

# Structures of Tetrasilylmethane Derivatives C(SiXMe<sub>2</sub>)<sub>4</sub> (X = H, F, Cl, Br) in the Gas Phase and their Dynamic Structures in Solution

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## Electronic Supplementary Information

**Table S1** Nozzle-to-film distances / mm, sample and nozzle temperatures / K, weighting functions / nm<sup>-1</sup>, scale factors, correlation parameters and electron wavelengths / pm used in the GED studies of C(SiXMe<sub>2</sub>)<sub>4</sub> (X = H, F, Cl, Br) (**1–4**).<sup>a</sup>

	<b>1</b>		<b>2</b>		<b>3</b>		<b>4</b>	
Nozzle-to-film distance	254.22	92.70	260.29	96.79	255.57	100.06	259.17	94.82
<i>T</i> <sub>sample</sub>	92	128	126	162	195	192	204	223
<i>T</i> <sub>nozzle</sub>	115	133	141	173	203	217	223	233
$\Delta s$	2.0	4.0	1.0	2.0	2.0	4.0	1.0	2.0
<i>s</i> <sub>min</sub>	30.0	80.0	20.0	100.0	20.0	80.0	20.0	90.0
<i>sw</i> <sub>1</sub>	50.0	100.0	40.0	120.0	40.0	100.0	40.0	100.0
<i>sw</i> <sub>2</sub>	128.0	292.0	129.0	275.2	128.0	276.0	103.2	276.0
<i>s</i> <sub>max</sub>	150.0	340.0	150.0	320.0	150.0	320.0	120.0	320.0
Scale factor <sup>b</sup>	7.74(11)	6.52(12)	6.31(6)	5.27(25)	1.43(2)	1.26(5)	1.70(3)	1.70(6)
Correlation parameter	0.496	0.380	0.498	0.329	0.479	0.212	0.496	0.267
Electron wavelength <sup>c</sup>	6.02	6.02	6.13	6.13	6.02	6.02	6.02	6.02

<sup>a</sup> From the *r*<sub>h1</sub> refinements. <sup>b</sup> Values in parentheses are the estimated standard deviations.

<sup>c</sup> Determined by reference to the scattering pattern of benzene.

**Table S2** Total free energies and relative energies of nine conformers of C(SiHMe<sub>2</sub>)<sub>4</sub> (**1**) calculated at the M06-2X/6-31G(d). Energies are relative to conformer 1, the lowest-energy conformer.

Conformer	Symmetry	Total free energy / kJ mol <sup>-1</sup>	Relative energy / kJ mol <sup>-1</sup>	Abundance / %
1	<i>C</i> <sub>2</sub>	-3983934.10	0.00	25.6
2	<i>C</i> <sub>1</sub>	-3983929.95	4.15	16.7
3	<i>C</i> <sub>1</sub>	-3983928.97	5.12	12.8
4	<i>C</i> <sub>1</sub>	-3983928.67	5.42	11.8
5	<i>D</i> <sub>2</sub>	-3983933.23	0.86	10.1
6	<i>C</i> <sub>1</sub>	-3983927.23	6.86	8.0
7	<i>C</i> <sub>1</sub>	-3983925.66	8.44	5.2
8	<i>C</i> <sub>2</sub>	-3983928.12	5.97	5.1
9	<i>C</i> <sub>2</sub>	-3983927.74	6.35	4.6

**Table S3** Total free energies and relative energies of nine conformers of C(SiFMe<sub>2</sub>)<sub>4</sub> (**2**) calculated at the M06-2X/6-31G(d). Energies are relative to conformer 1, the lowest-energy conformer. Those conformers marked with a star were not included in the refinement model.

Conformer	Symmetry	Total free energy / kJ mol <sup>-1</sup>	Relative energy / kJ mol <sup>-1</sup>	Abundance / %
1	<i>C</i> <sub>1</sub>	-5026839.49	0.00	32.0
2	<i>C</i> <sub>1</sub>	-5026838.74	0.75	26.2
3	<i>C</i> <sub>1</sub>	-5026835.58	3.91	11.1
4	<i>C</i> <sub>2</sub>	-5026837.89	1.60	10.4
5	<i>C</i> <sub>2</sub>	-5026836.66	2.83	7.5
6	<i>C</i> <sub>2</sub>	-5026835.95	3.54	6.2
7	<i>C</i> <sub>1</sub>	-5026832.72	6.77	5.1
8 *	<i>C</i> <sub>1</sub>	-5026827.25	12.24	1.2
9 *	<i>C</i> <sub>2</sub>	-5026825.27	14.22	0.3

**Table S4** Total free energies and relative energies of nine conformers of C(SiClMe<sub>2</sub>)<sub>4</sub> (**3**) calculated at the M06-2X/6-31G(d). Energies are relative to conformer 2 the lowest-energy conformer. Those conformers marked with a star were not included in the refinement model.

Conformer	Symmetry	Total free energy / kJ mol <sup>-1</sup>	Relative energy / kJ mol <sup>-1</sup>	Abundance / %
1	<i>C</i> <sub>1</sub>	-8811568.45	1.41	51.1
2	<i>C</i> <sub>2</sub>	-8811569.86	0.00	37.4
3 *	<i>C</i> <sub>1</sub>	-8811558.25	11.61	3.3
4 *	<i>C</i> <sub>1</sub>	-8811558.10	11.76	3.1
5 *	<i>C</i> <sub>1</sub>	-8811556.76	13.10	2.2
6 *	<i>C</i> <sub>2</sub>	-8811558.38	11.49	1.7
7 *	<i>D</i> <sub>2</sub>	-8811558.64	11.22	0.9
8 *	<i>C</i> <sub>1</sub>	-8811547.96	21.90	0.2
9 *	<i>C</i> <sub>2</sub>	-8811548.09	21.78	0.1

### GED model for C(SiXMe<sub>2</sub>)<sub>4</sub>

To describe the geometric structure of each of the C(SiXMe<sub>2</sub>)<sub>4</sub> (X = H, F, Cl, Br) species a set of twelve parameters was used comprising four distances, six angles and two dihedral angles. In addition to these twelve common parameters, additional parameters were used to define the dihedral angles that define the relative positions of SiXMe<sub>2</sub> substituents for the various conformers. The number of and symmetry of the conformers fitted dictates the number of additional dihedral angles required. For a C<sub>1</sub>-symmetric conformer four dihedral angles were required as the four substituents exist in distinct orientations. For C<sub>2</sub> symmetry, two dihedral angles are required, and for D<sub>2</sub> symmetry one dihedral angle was sufficient. The definitions of these dihedral angles, as well as the twelve common parameters, can be found in Tables S5–S8 for **1** to **4**, respectively. Non-geometric parameters were also used to control the amounts of each conformer present in the mixture, and are also listed in the Tables S5–S8.

The definitions of the common parameters for a given species are assumed to be the average values for the most dominant conformer. To account for small deviations from any average value within that conformer, or between the dominant conformer and any additional conformers, fixed (non-refinable) differences were included in the models. This was done to minimise the number of parameters used to define the structures.

The methyl groups in **1–4** were assumed in the models to have C<sub>3v</sub> symmetry, and so a single C–H distance (*p*<sub>4</sub>) and single Si–C–H angle (*p*<sub>5</sub>) can be used to define the groups. All four species are very close to tetrahedral in structure and parameter *p*<sub>10</sub>, as well as fixed differences from this average value are used to define the deviation from a perfect tetrahedral geometry.

Depending on the point-group symmetry of a particular conformer, there may be one (D<sub>2</sub>), two (C<sub>2</sub>) or four (C<sub>1</sub>) formally different SiXMe<sub>2</sub> groups, with many of the differences incorporated as fixed values applied to the parameters in Tables S5–S8. Generally, the two methyl groups and atom X are arranged around a given silicon atom in an approximately tetrahedral fashion. The deviations from a perfect tetrahedron are achieved using parameters *p*<sub>6–p</sub><sub>9</sub>. Parameters *p*<sub>11</sub> and *p*<sub>12</sub> are used to rotate the methyl groups around the C(12)–Si(2) and C(13)–Si(2) bonds, though both dihedral angles remain very close to 180°. The equivalent dihedral angles the other SiXMe<sub>2</sub> groups use the same parameters with fixed differences. Finally, parameters *p*<sub>1–p</sub><sub>3</sub> are different for each of the species and are described.

**(X = Cl)**

For the chlorine derivative, **3**, (see Table S7) the bonded distances  $r_{\text{SiCl}}$ ,  $r_{\text{CSi1}}$  [C(1)–Si(2/3/4/5)], and  $r_{\text{CSi2}}$  [Si(2/3/4/5)–C<sub>Me</sub>] are very similar in length and so lie under a single peak in the radial distribution curve. Such distances are hard to refine independently, and so the model defines these as a weighted average ( $p_1$ ) and two related difference parameters ( $p_2$  and  $p_3$ ). In doing this the average can often be refined without using a SARACEN restraint, while the differences are restrained. These parameters are defined as follows:

$$p_1 = (r_{\text{SiCl}})/4 + (r_{\text{CSi1}})/4 + (r_{\text{CSi2}})/2$$

$$p_2 = (r_{\text{SiCl}}) - [(r_{\text{CSi1}})/3 + 2 \times (r_{\text{CSi2}})/3]$$

$$p_3 = (r_{\text{CSi1}}) - (r_{\text{CSi2}})$$

**(X = H, F, Br)**

The bonded X–Si peak in species **1**, **2**, and **4** lies under a separate peak to the C–Si distances (unlike for the Cl derivative) and so should refine well. Only the two different types of C–Si distance, defined as above, are correlated and so these are described using the equations below:

$$p_1 = 2 \times (r_{\text{CSi2}})/3 + (r_{\text{CSi1}})/3$$

$$p_2 = (r_{\text{CSi2}}) - (r_{\text{CSi1}})$$



**Table S5** Refined ( $r_{h1}$ ) and calculated ( $r_e$ ) parameters for C(SiHMe<sub>2</sub>)<sub>4</sub> (**1**) from the GED study.<sup>a</sup>

	Parameter	GED ( $r_{h1}$ )	MP2/aug-cc-pVDZ ( $r_e$ )	Restraint
$p_1$	$r_{Si-C}$ average	189.21(9)	190.3	—
$p_2$	$r_{Si-C}$ difference	-0.2(4)	-1.3	—
$p_3$	$r_{Si-H}$	149.8(8)	150.3	0.9
$p_4$	$r_{C-H}$	109.6(2)	110.0	—
$p_5$	$\angle Si-C-H$	110.9(3)	111.0	0.3
$p_6$	$\angle C-Si-Me$	114.2(4)	113.1	—
$p_7$	$\angle Me-Si-Me$	106.7(6)	106.7	0.7
$p_8$	$\angle C-Si-H$	107.6(4)	107.7	0.5
$p_9$	$\angle Me-Si-H$	106.7(8)	108.0	1.2
$p_{10}$	$\angle Si-C-Si$	111.8(2)	109.5	—
$p_{11}$	$\phi_{H(37)C(12)Si(2)H(14)}$	186.6(45)	182.0	6.7
$p_{12}$	$\phi_{H(39)C(13)Si(2)H(14)}$	177.4(35)	175.9	3.3
$p_{13}$	$\phi_{Si(4)C(1)Si(2)H(14)}$	-74.9(40)	-74.6	3.3
$p_{14}$	$\phi_{Si(2)C(1)Si(4)H(15)}$	161.6(5)	161.6	0.6
$p_{15}$	$\phi_{Si(44)C(42)Si(43)H(55)}$	46.6(44)	47.5	2.8
$p_{16}$	$\phi_{Si(43)C(42)Si(44)H(57)}$	46.3(15)	46.6	1.6
$p_{17}$	$\phi_{Si(43)C(42)Si(45)H(56)}$	39.4(10)	39.4	1.1
$p_{18}$	$\phi_{Si(43)C(42)Si(46)H(58)}$	-79.8(11)	-79.7	1.2
$p_{19}$	$\phi_{Si(85)C(83)Si(84)H(96)}$	39.6(61)	40.3	3.2
$p_{20}$	$\phi_{Si(84)C(83)Si(85)H(98)}$	45.2(15)	45.3	1.4
$p_{21}$	$\phi_{Si(84)C(83)Si(86)H(97)}$	159.9(12)	160.0	1.1
$p_{22}$	$\phi_{Si(84)C(83)Si(87)H(99)}$	-75.9(8)	-75.9	0.8
$p_{23}$	$\phi_{Si(126)C(124)Si(125)H(137)}$	46.8(6)	46.9	0.7
$p_{24}$	$\phi_{Si(125)C(124)Si(126)H(139)}$	41.9(12)	41.9	1.1
$p_{25}$	$\phi_{Si(125)C(124)Si(127)H(138)}$	40.9(28)	41.0	1.9
$p_{26}$	$\phi_{Si(125)C(124)Si(128)H(140)}$	161.6(14)	161.7	1.4
$p_{27}$	$\phi_{Si(169)C(165)Si(167)H(180)}$	-76.8(17)	-76.3	1.7
$p_{28}$	$\phi_{Si(208)C(206)Si(207)H(219)}$	41.0(60)	42.0	3.5
$p_{29}$	$\phi_{Si(207)C(206)Si(208)H(221)}$	161.9(27)	162.2	2.5
$p_{30}$	$\phi_{Si(207)C(206)Si(209)H(220)}$	41.6(20)	41.7	1.8
$p_{31}$	$\phi_{Si(207)C(206)Si(210)H(222)}$	-81.5(23)	-81.3	1.7
$p_{32}$	$\phi_{Si(249)C(247)Si(248)H(260)}$	42.7(14)	42.8	1.2
$p_{33}$	$\phi_{Si(248)C(247)Si(249)H(262)}$	160.6(18)	160.6	1.3
$p_{34}$	$\phi_{Si(248)C(247)Si(250)H(261)}$	-77.1(7)	-77.1	0.7
$p_{35}$	$\phi_{Si(248)C(247)Si(251)H(263)}$	37.2(21)	37.3	1.6
$p_{36}$	$\phi_{Si(290)C(288)Si(289)H(301)}$	37.1(18)	37.3	2.0
$p_{37}$	$\phi_{Si(289)C(288)Si(290)H(303)}$	164.9(18)	165.0	1.7
$p_{38}$	$\phi_{Si(332)C(329)Si(330)H(342)}$	-76.9(9)	-76.9	0.8
$p_{39}$	$\phi_{Si(330)C(329)Si(332)H(343)}$	39.7(13)	39.8	1.3
$f_1$	Conformer 1	(fixed)	25.6	—
$f_2$	Conformer 2	(fixed)	16.7	—
$f_3$	Conformer 3	(fixed)	12.8	—

Parameter	GED ( $r_{h1}$ )	MP2/aug-cc-pVDZ ( $r_e$ )	Restraint
$f_4$ Conformer 4	(fixed)	11.8	—
$f_5$ Conformer 5	(fixed)	10.1	—
$f_6$ Conformer 6	(fixed)	8.0	—
$f_7$ Conformer 7	(fixed)	5.2	—
$f_8$ Conformer 8	(fixed)	5.1	—
$f_9$ Conformer 9	(fixed)	4.7	—

<sup>a</sup> Distances ( $r$ ) are in pm, angles ( $\angle$ ) and dihedral angles ( $\phi$ ) are in degrees. Atom numbering as described in Figure 1.

**Table S6** Refined ( $r_{h1}$ ) and calculated ( $r_e$ ) parameters for C(SiFMe<sub>2</sub>)<sub>4</sub> (**2**) from the GED study.<sup>a</sup>

	Parameter	GED ( $r_{h1}$ )	MP2/aug-cc-pVDZ ( $r_e$ )	Restraint
$p_1$	$r_{Si-C}$ average	188.5(2)	189.4	—
$p_2$	$r_{Si-C}$ difference	2.1(3)	2.2	—
$p_3$	$r_{Si-F}$	160.6(1)	167.6	—
$p_4$	$r_{C-H}$	109.3(3)	110.1	0.7
$p_5$	$\angle Si-C-H$	109.7(4)	110.6	0.5
$p_6$	$\angle C-Si-Me$	115.9(11)	114.5	1.8
$p_7$	$\angle Me-Si-Me$	113.1(13)	110.0	2.7
$p_8$	$\angle C-Si-F$	104.9(6)	104.7	1.1
$p_9$	$\angle Me-Si-F$	106.0(6)	106.2	—
$p_{10}$	$\angle Si-C-Si$	110.2(3)	109.5	—
$p_{11}$	$\phi_{H(37)C(12)Si(2)F(14)}$	185.5(149)	170.9	16.9
$p_{12}$	$\phi_{H(39)C(13)Si(2)F(14)}$	176.7(42)	175.5	4.3
$p_{13}$	$\phi_{Si(4)C(1)Si(2)F(14)}$	81.9(39)	83.2	4.0
$p_{14}$	$\phi_{Si(2)C(1)Si(4)F(15)}$	-167.2(10)	-167.2	1.0
$p_{15}$	$\phi_{Si(44)C(42)Si(43)F(55)}$	-153.2(20)	-152.4	2.1
$p_{16}$	$\phi_{Si(43)C(42)Si(44)F(57)}$	-39.1(29)	-39.4	3.0
$p_{17}$	$\phi_{Si(43)C(42)Si(45)F(56)}$	84.6(26)	85.8	2.7
$p_{18}$	$\phi_{Si(43)C(42)Si(46)F(58)}$	-40.8(33)	-40.2	3.5
$p_{19}$	$\phi_{Si(85)C(83)Si(84)F(96)}$	-166.1(46)	-166.1	4.9
$p_{20}$	$\phi_{Si(84)C(83)Si(85)F(98)}$	71.2(46)	71.9	5.0
$p_{21}$	$\phi_{Si(84)C(83)Si(86)F(97)}$	77.6(62)	79.8	6.7
$p_{22}$	$\phi_{Si(84)C(83)Si(87)F(99)}$	-163.9(46)	-163.8	4.8
$p_{23}$	$\phi_{Si(126)C(124)Si(125)F(137)}$	84.9(26)	85.7	2.7
$p_{24}$	$\phi_{Si(125)C(124)Si(126)F(139)}$	-41.9(17)	-41.3	1.7
$p_{25}$	$\phi_{Si(125)C(124)Si(127)F(138)}$	77.9(63)	77.3	6.5
$p_{26}$	$\phi_{Si(125)C(124)Si(128)F(140)}$	73.3(14)	73.4	1.5
$p_{27}$	$\phi_{Si(169)C(165)Si(167)F(180)}$	81.5(19)	81.7	2.0
$p_{28}$	$\phi_{Si(208)C(206)Si(207)F(219)}$	-170.6(23)	-170.7	2.3
$p_{29}$	$\phi_{Si(207)C(206)Si(208)F(221)}$	80.3(7)	80.3	0.8
$p_{30}$	$\phi_{Si(207)C(206)Si(209)F(220)}$	-36.7(23)	-36.8	2.4
$p_{31}$	$\phi_{Si(207)C(206)Si(210)F(222)}$	80.5(24)	80.6	2.5
$p_{32}$	$\phi_{Si(249)C(247)Si(248)F(260)}$	-161.8(20)	-161.7	2.1
$p_{33}$	$\phi_{Si(248)C(247)Si(249)F(262)}$	-157.6(25)	-157.5	2.6
$p_{34}$	$\phi_{Si(248)C(247)Si(250)F(261)}$	71.4(38)	71.4	3.9
$f_1$	Conformer 1	(fixed)	33.0	—
$f_2$	Conformer 2	(fixed)	26.2	—
$f_3$	Conformer 3	(fixed)	11.1	—
$f_4$	Conformer 4	(fixed)	10.4	—
$f_5$	Conformer 5	(fixed)	7.5	—
$f_6$	Conformer 6	(fixed)	6.2	—
$f_7$	Conformer 7	(fixed)	5.7	—

<sup>a</sup> Distances ( $r$ ) are in pm, angles ( $\angle$ ) and dihedral angles ( $\phi$ ) are in degrees. Atom numbering as described in Figure 1.

**Table S7** Refined ( $r_{h1}$ ) and calculated ( $r_e$ ) parameters for C(SiClMe<sub>2</sub>)<sub>4</sub> (**3**) from the GED study.<sup>a</sup>

Parameter	GED ( $r_{h1}$ )	MP2/aug-cc-pVDZ ( $r_e$ )	Restraint
$p_1$ $r(\text{SiCl/CSi1/CSi2})$ average	194.8(2)	195.5	—
$p_2$ $r\text{SiCl} - (r\text{CSi average})$	17.9(3)	23.9	—
$p_3$ $r\text{CSi1} - r\text{CSi2}^b$	2.5(5)	3.8	0.5
$p_4$ $r\text{C-H}$	110.8(6)	110.1	0.8
$p_5$ $\angle\text{Si-C-H}$	110.5(5)	110.4	0.5
$p_6$ $\angle\text{C-Si-Me}$	114.3(4)	115.3	0.4
$p_7$ $\angle\text{Me-Si-Me}$	109.7(19)	109.7	1.7
$p_8$ $\angle\text{C-Si-Cl}$	108.3(5)	107.1	—
$p_9$ $\angle\text{Me-Si-Cl}$	105.9(8)	104.0	—
$p_{10}$ $\angle\text{Si-C-Si}$	110.2(4)	109.5	—
$p_{11}$ $\phi\text{H(37)C(12)Si(2)Cl(14)}$	-176.7(24)	-177.0	2.1
$p_{12}$ $\phi\text{H(39)C(13)Si(2)Cl(14)}$	176.3(30)	176.1	2.7
$p_{13}$ $\phi\text{Si(3)C(1)Si(2)Cl(14)}$	39.9(4)	40.2	0.4
$p_{14}$ $\phi\text{Si(2)C(1)Si(3)Cl(16)}$	159.1(5)	159.4	0.4
$p_{15}$ $\phi\text{Si(2)C(1)Si(4)Cl(15)}$	-74.9(11)	-73.5	1.0
$p_{16}$ $\phi\text{Si(2)C(1)Si(5)Cl(17)}$	34.7(5)	35.1	0.5
$p_{17}$ $\phi\text{Si(45)C(42)Si(43)Cl(55)}$	-75.3(6)	-75.1	0.5
$p_{18}$ $\phi\text{Si(43)C(42)Si(45)Cl(56)}$	165.2(7)	165.6	0.7
$f_1$ Conformer 1	(fixed)	72.0	—
$f_2$ Conformer 2	(fixed)	28.0	—

<sup>a</sup> Distances ( $r$ ) are in pm, angles ( $\angle$ ) and dihedral angles ( $\phi$ ) are in degrees. Atom numbering as described in Figure 1. <sup>b</sup> For full explanation of parameter titles see model description above.

**Table S8** Refined ( $r_{\text{hl}}$ ) and calculated ( $r_{\text{e}}$ ) parameters for C(SiBrMe<sub>2</sub>)<sub>4</sub> (**4**) from the GED study.<sup>a</sup>

	Parameter	GED ( $r_{\text{hl}}$ )	MP2/aug-cc-pVDZ(-PP) ( $r_{\text{e}}$ )	Restraint
$p_1$	$r_{\text{Si-C}}$ average	187.5(2)	189.7	—
$p_2$	$r_{\text{Si-C}}$ difference	-5.2(7)	-4.0	—
$p_3$	$r_{\text{Si-Br}}$	226.6(2)	229.0	—
$p_4$	$r_{\text{C-H}}$	109.3(5)	110.1	0.7
$p_5$	$\angle \text{Si-C-H}$	110.5(4)	110.3	0.4
$p_6$	$\angle \text{C-Si-Me}$	117.0(5)	115.5	—
$p_7$	$\angle \text{Me-Si-Me}$	110.1(14)	110.1	1.4
$p_8$	$\angle \text{C-Si-Br}$	108.6(3)	108.2	—
$p_9$	$\angle \text{Me-Si-Br}$	102.3(3)	103.0	0.4
$p_{10}$	$\angle \text{Si-C-Si}$	110.1(2)	109.5	—
$p_{11}$	$\phi \text{H(37)C(12)Si(2)Br(14)}$	-177.2(12)	-177.5	1.2
$p_{12}$	$\phi \text{H(39)C(13)Si(2)Br(14)}$	177.8(33)	175.9	3.3
$p_{13}$	$\phi \text{Si(3)C(1)Si(2)Br(14)}$	39.6(8)	39.5	0.9
$p_{14}$	$\phi \text{Si(2)C(1)Si(3)Br(16)}$	158.7(6)	158.7	0.6
$p_{15}$	$\phi \text{Si(2)C(1)Si(4)Br(15)}$	-72.7(11)	-72.4	1.2
$p_{16}$	$\phi \text{Si(2)C(1)Si(5)Br(17)}$	35.0(14)	34.8	1.6
$p_{17}$	$\phi \text{Si(45)C(42)Si(43)Br(55)}$	-80.6(11)	-81.2	1.2
$p_{18}$	$\phi \text{Si(43)C(42)Si(45)Br(56)}$	166.4(8)	166.2	0.8
$f_1$	Conformer 1	0.73(16) <sup>i</sup>	0.75	—
$f_2$	Conformer 2	0.27(16) <sup>b</sup>	0.25	—

<sup>a</sup> Distances ( $r$ ) are in pm, angles ( $\angle$ ) and dihedral angles ( $\phi$ ) are in degrees. Atom numbering as described in Figure 1. <sup>b</sup> Uncertainties in conformer amounts obtained from Figure 2, and are approximately equal to  $2\sigma$ .

**Table S9** Refined and calculated [B3LYP/6-31G(d)] amplitudes of vibration ( $u_{h1}$ ), associated  $r_a$  distances and corresponding correction values ( $k_{h1}$ ) for the refinement of  $C(SiHMe_2)_4$  (**1**).<sup>a</sup>

	Atom pair	$r_a$	$u_{GED}$	Restraint	$k_{h1}$	$u_{calc.}$
<i>u32</i>	C(135)–H(159)	109.0(24)	10.5(tied to <i>u135</i> )	—	0.4	9.3
<i>u47</i>	C(135)–H(160)	109.0(24)	10.3(tied to <i>u135</i> )	—	0.4	9.1
<i>u158</i>	C(135)–H(161)	109.0(24)	10.2(tied to <i>u135</i> )	—	0.4	8.9
<i>u62</i>	C(134)–H(156)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.7
<i>u21</i>	C(134)–H(158)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.7
<i>u65</i>	C(92)–H(113)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.7
<i>u144</i>	C(134)–H(157)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.8
<i>u157</i>	C(92)–H(112)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.7
<i>u69</i>	C(47)–H(61)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u67</i>	C(256)–H(277)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u66</i>	C(215)–H(236)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u79</i>	C(88)–H(102)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u70</i>	C(91)–H(110)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u4</i>	C(92)–H(114)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u105</i>	C(252)–H(266)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u87</i>	C(293)–H(307)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u72</i>	C(136)–H(162)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u94</i>	C(132)–H(151)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u107</i>	C(259)–H(285)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u89</i>	C(9)–H(28)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u101</i>	C(50)–H(69)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u95</i>	C(218)–H(244)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u103</i>	C(133)–H(154)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u97</i>	C(129)–H(143)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u63</i>	C(53)–H(78)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u99</i>	C(211)–H(225)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u81</i>	C(217)–H(242)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u90</i>	C(95)–H(121)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u96</i>	C(254)–H(270)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u92</i>	C(212)–H(228)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u100</i>	C(213)–H(229)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u108</i>	C(334)–H(348)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u76</i>	C(335)–H(351)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u86</i>	C(253)–H(269)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u53</i>	C(216)–H(238)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u82</i>	C(257)–H(279)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u64</i>	C(337)–H(356)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u55</i>	C(171)–H(187)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u60</i>	C(52)–H(74)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u74</i>	C(258)–H(283)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u59</i>	C(49)–H(65)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7

<i>u68</i>	C(336)–H(352)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u61</i>	C(90)–H(106)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u83</i>	C(48)–H(64)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u85</i>	C(94)–H(119)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u78</i>	C(8)–H(24)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u88</i>	C(299)–H(324)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u80</i>	C(89)–H(105)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u73</i>	C(131)–H(147)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u84</i>	C(54)–H(80)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u91</i>	C(130)–H(146)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u75</i>	C(295)–H(311)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u13</i>	C(47)–H(59)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u71</i>	C(93)–H(115)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u93</i>	C(296)–H(315)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u156</i>	C(47)–H(60)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.7
<i>u159</i>	C(215)–H(235)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.7
<i>u161</i>	C(256)–H(276)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.7
<i>u56</i>	C(294)–H(309)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u58</i>	C(336)–H(354)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u46</i>	C(8)–H(26)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u54</i>	C(131)–H(149)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u40</i>	C(93)–H(117)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u28</i>	C(91)–H(111)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u50</i>	C(49)–H(67)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u51</i>	C(50)–H(70)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u48</i>	C(132)–H(152)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u30</i>	C(53)–H(77)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u52</i>	C(90)–H(108)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u5</i>	C(256)–H(278)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u2</i>	C(215)–H(237)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u49</i>	C(48)–H(63)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u33</i>	C(171)–H(186)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u24</i>	C(136)–H(163)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u37</i>	C(337)–H(357)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u45</i>	C(335)–H(350)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u31</i>	C(89)–H(104)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u135</i>	C(7)–H(21)	109.3(24)	8.8(5)	—	0.4	7.7
<i>u111</i>	C(91)–H(109)	109.3(24)	8.8(tied to <i>u135</i> )	—	0.4	7.7
<i>u34</i>	C(212)–H(227)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u19</i>	C(334)–H(346)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u26</i>	C(213)–H(231)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u1</i>	C(88)–H(100)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u9</i>	C(129)–H(141)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u18</i>	C(252)–H(264)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6



<i>u35</i>	C(94)–H(118)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u29</i>	C(130)–H(145)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u15</i>	C(217)–H(241)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u22</i>	C(216)–H(240)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u23</i>	C(254)–H(272)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u27</i>	C(293)–H(305)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u20</i>	C(52)–H(76)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u39</i>	C(54)–H(81)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u44</i>	C(257)–H(281)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u36</i>	C(258)–H(282)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u38</i>	C(9)–H(29)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u16</i>	C(295)–H(313)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u25</i>	C(211)–H(223)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u41</i>	C(95)–H(122)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u43</i>	C(253)–H(268)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u42</i>	C(170)–H(182)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u122</i>	C(95)–H(123)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u148</i>	C(218)–H(246)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u162</i>	C(296)–H(314)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u139</i>	C(88)–H(101)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u134</i>	C(339)–H(362)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u155</i>	C(6)–H(19)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u132</i>	C(334)–H(347)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u136</i>	C(49)–H(66)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u124</i>	C(136)–H(164)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u120</i>	C(89)–H(103)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u118</i>	C(53)–H(79)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u137</i>	C(51)–H(71)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u160</i>	C(216)–H(239)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u129</i>	C(293)–H(306)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u146</i>	C(211)–H(224)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u138</i>	C(52)–H(75)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u151</i>	C(254)–H(271)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u133</i>	C(337)–H(355)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u145</i>	C(171)–H(185)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u126</i>	C(217)–H(243)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u147</i>	C(214)–H(232)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u152</i>	C(255)–H(273)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u153</i>	C(257)–H(280)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u150</i>	C(253)–H(267)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u143</i>	C(133)–H(153)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u149</i>	C(252)–H(265)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u130</i>	C(295)–H(312)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u8</i>	C(259)–H(286)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6

<i>u11</i>	C(255)–H(275)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u6</i>	C(214)–H(234)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u14</i>	C(51)–H(73)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u10</i>	C(133)–H(155)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u12</i>	C(296)–H(316)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u7</i>	C(218)–H(245)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.6
<i>u131</i>	C(299)–H(325)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u154</i>	C(336)–H(353)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u117</i>	C(48)–H(62)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u114</i>	C(170)–H(183)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u142</i>	C(129)–H(142)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u125</i>	C(212)–H(226)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u116</i>	C(9)–H(27)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u141</i>	C(93)–H(116)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u109</i>	C(50)–H(68)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u110</i>	C(8)–H(25)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u140</i>	C(90)–H(107)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u128</i>	C(259)–H(287)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u119</i>	C(54)–H(82)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u127</i>	C(258)–H(284)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u115</i>	C(213)–H(230)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u113</i>	C(132)–H(150)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u123</i>	C(131)–H(148)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u121</i>	C(94)–H(120)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u112</i>	C(130)–H(144)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u102</i>	C(51)–H(72)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u106</i>	C(255)–H(274)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u104</i>	C(214)–H(233)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u98</i>	C(170)–H(184)	109.3(24)	8.7(tied to <i>u135</i> )	—	0.4	7.7
<i>u57</i>	C(7)–H(23)	143.3(638)	7.7(fixed)	—	0.4	7.7
<i>u77</i>	C(6)–H(20)	143.3(638)	7.7(fixed)	—	0.4	7.7
<i>u17</i>	C(7)–H(22)	143.3(638)	7.7(fixed)	—	0.4	7.7
<i>u3</i>	C(6)–H(18)	143.3(638)	7.6(fixed)	—	0.4	7.6
<i>u2140</i>	H(105)...H(117)	146.3(186)	59.4(fixed)	—	2.3	59.4
<i>u185</i>	Si(207)–H(219)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u186</i>	Si(248)–H(260)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u181</i>	Si(128)–H(140)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u178</i>	Si(45)–H(56)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u180</i>	Si(86)–H(97)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u179</i>	Si(332)–H(343)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u175</i>	Si(290)–H(303)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u166</i>	Si(251)–H(263)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u168</i>	Si(249)–H(262)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9
<i>u167</i>	Si(44)–H(57)	149.8(8)	8.2(tied to <i>u184</i> )	—	0.4	8.9

<i>u</i> 169	Si(250)–H(261)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 170	Si(43)–H(55)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 176	Si(85)–H(98)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 164	Si(84)–H(96)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 188	Si(127)–H(138)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 184	Si(4)–H(15)	149.8(8)	8.2(7)	0.9	0.4	8.9
<i>u</i> 189	Si(208)–H(221)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 187	Si(87)–H(99)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 183	Si(289)–H(301)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 182	Si(210)–H(222)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 172	Si(166)–H(178)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 174	Si(209)–H(220)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 177	Si(125)–H(137)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 173	Si(46)–H(58)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 171	Si(2)–H(14)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 163	Si(126)–H(139)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 165	Si(330)–H(342)	149.8(8)	8.2(tied to <i>u</i> 184)	—	0.4	8.9
<i>u</i> 251	H(21)...H(23)	152.3(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 288	H(18)...H(19)	152.4(39)	12.4(fixed)	—	–0.2	12.4
<i>u</i> 1890	H(141)...H(154)	153.6(176)	58.6(fixed)	—	2.8	58.6
<i>u</i> 3838	H(225)...H(236)	159.2(132)	61.6(fixed)	—	1.8	61.6
<i>u</i> 4931	H(268)...H(278)	160.5(88)	33.6(fixed)	—	4.7	33.6
<i>u</i> 5093	H(269)...H(278)	160.9(86)	40.9(fixed)	—	1.9	40.9
<i>u</i> 2170	H(113)...H(118)	162.5(251)	40.4(fixed)	—	–3.9	40.4
<i>u</i> 1925	H(228)...H(236)	171.2(113)	64.9(fixed)	—	–0.2	64.9
<i>u</i> 4093	H(61)...H(72)	173.6(123)	42.7(fixed)	—	5.3	42.7
<i>u</i> 255	H(160)...H(161)	174.4(39)	13.7(fixed)	—	–1.9	13.7
<i>u</i> 239	H(159)...H(161)	174.8(39)	14.0(fixed)	—	–1.4	14.0
<i>u</i> 216	H(159)...H(160)	175.0(39)	14.1(fixed)	—	–1.2	14.1
<i>u</i> 459	H(141)...H(155)	176.1(203)	45.3(fixed)	—	18.2	45.3
<i>u</i> 205	H(276)...H(277)	176.1(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 218	H(235)...H(236)	176.1(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 270	H(156)...H(157)	176.1(39)	12.6(fixed)	—	–0.3	12.6
<i>u</i> 209	H(112)...H(113)	176.1(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 246	H(157)...H(158)	176.1(39)	12.6(fixed)	—	–0.3	12.6
<i>u</i> 241	H(277)...H(278)	176.1(39)	12.4(fixed)	—	–0.3	12.4
<i>u</i> 215	H(156)...H(158)	176.1(39)	12.6(fixed)	—	–0.3	12.6
<i>u</i> 268	H(235)...H(237)	176.1(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 240	H(236)...H(237)	176.1(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 267	H(112)...H(114)	176.1(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 225	H(113)...H(114)	176.1(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 272	H(276)...H(278)	176.2(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 280	H(77)...H(79)	176.2(39)	12.5(fixed)	—	–0.3	12.5
<i>u</i> 245	H(77)...H(78)	176.2(39)	12.4(fixed)	—	–0.3	12.4

<i>u</i> 222	H(60)...H(61)	176.2(39)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 224	H(101)...H(102)	176.2(39)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 289	H(59)...H(60)	176.2(39)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 231	H(59)...H(61)	176.2(39)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 308	H(78)...H(79)	176.2(39)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 259	H(109)...H(110)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 285	H(110)...H(111)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 235	H(100)...H(102)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 274	H(100)...H(101)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 307	H(109)...H(111)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 282	H(185)...H(187)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 300	H(242)...H(243)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 201	H(285)...H(287)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 191	H(66)...H(67)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 250	H(305)...H(306)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 242	H(241)...H(242)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 311	H(285)...H(286)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 195	H(153)...H(154)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 198	H(306)...H(307)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 256	H(162)...H(164)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 248	H(185)...H(186)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 227	H(150)...H(151)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 244	H(239)...H(240)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 265	H(238)...H(239)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 269	H(65)...H(66)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 271	H(241)...H(243)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 249	H(75)...H(76)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 278	H(312)...H(313)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 252	H(286)...H(287)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 214	H(74)...H(76)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 217	H(186)...H(187)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 309	H(305)...H(307)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 212	H(238)...H(240)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 313	H(154)...H(155)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 298	H(65)...H(67)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 196	H(265)...H(266)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 190	H(107)...H(108)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 293	H(74)...H(75)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 310	H(163)...H(164)	176.2(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 197	H(282)...H(284)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 292	H(162)...H(163)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 260	H(153)...H(155)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 193	H(103)...H(104)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 247	H(311)...H(313)	176.2(39)	12.4(fixed)	—	-0.2	12.4

<i>u</i> 304	H(282)...H(283)	176.2(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 204	H(244)...H(246)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 192	H(71)...H(72)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 234	H(68)...H(69)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 254	H(103)...H(105)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 305	H(311)...H(312)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 258	H(283)...H(284)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 302	H(68)...H(70)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 295	H(150)...H(152)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 276	H(115)...H(116)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 279	H(71)...H(73)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 290	H(122)...H(123)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 257	H(264)...H(265)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 194	H(116)...H(117)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 203	H(144)...H(145)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 200	H(230)...H(231)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 261	H(232)...H(234)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 319	H(69)...H(70)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 324	H(151)...H(152)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 266	H(245)...H(246)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 312	H(106)...H(108)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 315	H(264)...H(266)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 306	H(104)...H(105)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 210	H(142)...H(143)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 277	H(270)...H(271)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 287	H(229)...H(230)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 296	H(144)...H(146)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 206	H(314)...H(315)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 208	H(273)...H(274)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 207	H(232)...H(233)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 273	H(279)...H(280)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 211	H(148)...H(149)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 284	H(267)...H(269)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 220	H(183)...H(184)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 236	H(121)...H(123)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 228	H(224)...H(225)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 223	H(80)...H(82)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 281	H(62)...H(64)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 303	H(182)...H(183)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 291	H(147)...H(148)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 283	H(226)...H(228)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 275	H(106)...H(107)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 286	H(308)...H(310)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 237	H(226)...H(227)	176.3(39)	12.4(fixed)	—	-0.2	12.4

<i>u</i> 253	H(314)...H(316)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 232	H(62)...H(63)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 229	H(271)...H(272)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 233	H(308)...H(309)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 202	H(25)...H(26)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 219	H(267)...H(268)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 226	H(118)...H(120)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 297	H(27)...H(29)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 299	H(81)...H(82)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 213	H(280)...H(281)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 264	H(223)...H(224)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 262	H(273)...H(275)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 263	H(141)...H(142)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 317	H(72)...H(73)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 316	H(229)...H(231)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 318	H(24)...H(26)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 320	H(145)...H(146)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 332	H(309)...H(310)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 314	H(115)...H(117)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 330	H(63)...H(64)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 326	H(182)...H(184)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 322	H(244)...H(245)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 321	H(233)...H(234)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 221	H(27)...H(28)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 301	H(24)...H(25)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 294	H(119)...H(120)	176.3(39)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 336	H(227)...H(228)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 329	H(147)...H(149)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 335	H(80)...H(81)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 334	H(28)...H(29)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 333	H(279)...H(281)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 323	H(141)...H(143)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 327	H(274)...H(275)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 331	H(268)...H(269)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 338	H(121)...H(122)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 325	H(223)...H(225)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 337	H(118)...H(119)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 339	H(270)...H(272)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 328	H(315)...H(316)	176.3(39)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 730	H(105)...H(115)	177.5(167)	56.4(fixed)	—	12.0	56.4
<i>u</i> 2984	H(63)...H(78)	179.6(115)	55.5(fixed)	—	7.2	55.5
<i>u</i> 2100	H(64)...H(72)	181.7(94)	48.8(fixed)	—	2.0	48.8
<i>u</i> 523	H(64)...H(73)	184.7(111)	43.7(fixed)	—	14.4	43.7
<i>u</i> 4110	H(102)...H(117)	186.7(79)	43.3(fixed)	—	6.2	43.3

<i>u</i> 2105	H(231)...H(240)	188.6(143)	49.4(fixed)	—	-3.1	49.4
<i>u</i> 384	Si(125)–C(135)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 382	Si(86)–C(93)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 389	Si(4)–C(11)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 385	Si(209)–C(216)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 393	Si(87)–C(89)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 376	Si(209)–C(215)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 386	Si(248)–C(258)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 373	Si(46)–C(47)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 387	Si(250)–C(256)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 375	Si(208)–C(213)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 374	Si(127)–C(134)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 377	Si(45)–C(51)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 372	Si(45)–C(52)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 388	Si(332)–C(338)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 366	Si(128)–C(130)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 383	Si(127)–C(133)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 378	Si(86)–C(92)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 369	Si(290)–C(296)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 363	Si(208)–C(214)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 391	Si(289)–C(300)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 379	Si(248)–C(259)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 370	Si(166)–C(176)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 380	Si(44)–C(49)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 392	Si(251)–C(252)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 371	Si(249)–C(255)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 381	Si(85)–C(90)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 390	Si(332)–C(339)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 368	Si(87)–C(88)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 362	Si(4)–C(10)	189.2(2)	5.7(1)	—	0.2	5.6
<i>u</i> 357	Si(126)–C(132)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 364	Si(210)–C(211)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 358	Si(251)–C(253)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 365	Si(128)–C(129)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 356	Si(290)–C(295)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 352	Si(44)–C(50)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 353	Si(46)–C(48)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 361	Si(250)–C(257)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 360	Si(2)–C(12)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 350	Si(330)–C(341)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 359	Si(207)–C(217)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 351	Si(43)–C(53)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 367	Si(207)–C(218)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 349	Si(249)–C(254)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6

<i>u</i> 355	Si(330)–C(340)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 348	Si(166)–C(177)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 345	Si(125)–C(136)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 347	Si(85)–C(91)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 343	Si(2)–C(13)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 354	Si(126)–C(131)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 342	Si(43)–C(54)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 344	Si(84)–C(95)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 341	Si(210)–C(212)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 340	Si(84)–C(94)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 346	Si(289)–C(299)	189.2(2)	5.7(tied to <i>u</i> 362)	—	0.2	5.6
<i>u</i> 2361	H(281)...H(282)	189.4(84)	48.5(fixed)	—	1.0	48.5
<i>u</i> 395	C(329)–Si(332)	189.4(4)	5.9(tied to <i>u</i> 362)	—	0.2	5.8
<i>u</i> 420	C(83)–Si(84)	189.4(4)	6.1(tied to <i>u</i> 362)	—	0.2	6.0
<i>u</i> 394	C(247)–Si(248)	189.4(4)	5.9(tied to <i>u</i> 362)	—	0.2	5.8
<i>u</i> 417	C(247)–Si(249)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 414	C(247)–Si(250)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 419	C(329)–Si(330)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 412	C(206)–Si(210)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 411	C(124)–Si(126)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 408	C(206)–Si(207)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 402	C(42)–Si(45)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 406	C(1)–Si(4)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 404	C(247)–Si(251)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 409	C(42)–Si(46)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 401	C(83)–Si(86)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 410	C(1)–Si(2)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 407	C(83)–Si(85)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 403	C(124)–Si(128)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 405	C(165)–Si(166)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 400	C(206)–Si(208)	189.4(4)	5.9(tied to <i>u</i> 362)	—	0.2	5.8
<i>u</i> 397	C(124)–Si(127)	189.4(4)	5.9(tied to <i>u</i> 362)	—	0.2	5.8
<i>u</i> 396	C(83)–Si(87)	189.4(4)	5.9(tied to <i>u</i> 362)	—	0.2	5.8
<i>u</i> 399	C(288)–Si(289)	189.4(4)	5.9(tied to <i>u</i> 362)	—	0.2	5.8
<i>u</i> 398	C(42)–Si(44)	189.4(4)	5.9(tied to <i>u</i> 362)	—	0.2	5.8
<i>u</i> 418	C(42)–Si(43)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 415	C(288)–Si(290)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 413	C(206)–Si(209)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 416	C(124)–Si(125)	189.4(4)	6.0(tied to <i>u</i> 362)	—	0.2	5.9
<i>u</i> 426	H(307)...H(326)	193.8(170)	42.5(fixed)	—	27.5	42.5
<i>u</i> 4901	C(253)...H(278)	198.2(60)	27.5(fixed)	—	1.3	27.5
<i>u</i> 5088	H(225)...H(238)	198.6(90)	36.4(fixed)	—	1.2	36.4
<i>u</i> 3513	H(143)...H(160)	201.3(78)	70.3(fixed)	—	20.6	70.3
<i>u</i> 1699	C(93)...H(105)	202.1(83)	49.3(fixed)	—	2.7	49.3



<i>u</i> 2067	H(100)...H(108)	202.6(92)	50.8(fixed)	—	0.7	50.8
<i>u</i> 2247	H(272)...H(277)	203.0(103)	39.6(fixed)	—	-5.8	39.6
<i>u</i> 1411	C(133)...H(141)	203.3(96)	38.8(fixed)	—	4.7	38.8
<i>u</i> 1964	H(59)...H(67)	203.7(103)	52.7(fixed)	—	2.8	52.7
<i>u</i> 3969	H(145)...H(149)	203.9(118)	36.2(fixed)	—	1.6	36.2
<i>u</i> 799	H(15)...H(22)	204.8(727)	52.9(fixed)	—	11.0	52.9
<i>u</i> 2946	H(227)...H(242)	205.8(111)	56.4(fixed)	—	7.3	56.4
<i>u</i> 5094	H(61)...H(74)	206.3(86)	38.5(fixed)	—	2.0	38.5
<i>u</i> 440	H(228)...H(237)	206.6(145)	45.6(fixed)	—	27.1	45.6
<i>u</i> 2200	H(151)...H(158)	206.6(114)	60.4(fixed)	—	-5.6	60.4
<i>u</i> 462	H(309)...H(316)	207.8(125)	41.9(fixed)	—	11.3	41.9
<i>u</i> 3296	H(104)...H(119)	208.5(341)	46.5(fixed)	—	6.1	46.5
<i>u</i> 5136	H(223)...H(238)	212.8(120)	38.9(fixed)	—	-0.5	38.9
<i>u</i> 5129	H(186)...H(199)	213.0(125)	38.2(fixed)	—	-0.7	38.2
<i>u</i> 4233	H(65)...H(76)	213.7(128)	37.0(fixed)	—	-2.0	37.0
<i>u</i> 804	H(14)...H(31)	214.7(758)	51.9(fixed)	—	7.6	51.9
<i>u</i> 4343	H(147)...H(158)	215.2(117)	44.1(fixed)	—	-7.7	44.1
<i>u</i> 2167	H(69)...H(76)	217.4(86)	50.7(fixed)	—	-2.0	50.7
<i>u</i> 4067	H(227)...H(244)	217.6(198)	40.0(fixed)	—	0.5	40.0
<i>u</i> 3128	H(261)...H(268)	218.7(77)	32.3(fixed)	—	1.5	32.3
<i>u</i> 1463	C(51)...H(64)	221.6(84)	38.5(fixed)	—	3.7	38.5
<i>u</i> 4888	C(256)...H(268)	221.6(94)	23.1(fixed)	—	-1.1	23.1
<i>u</i> 3968	H(73)...H(77)	224.8(80)	38.8(fixed)	—	4.7	38.8
<i>u</i> 431	H(18)...H(39)	226.5(285)	42.1(fixed)	—	22.8	42.1
<i>u</i> 5084	H(59)...H(74)	227.0(93)	42.0(fixed)	—	0.8	42.0
<i>u</i> 4285	H(237)...H(242)	227.3(63)	51.3(fixed)	—	2.1	51.3
<i>u</i> 527	H(310)...H(316)	228.2(76)	44.1(fixed)	—	13.2	44.1
<i>u</i> 4547	H(155)...H(160)	228.6(119)	82.1(fixed)	—	1.2	82.1
<i>u</i> 1371	C(215)...H(228)	229.6(108)	35.6(fixed)	—	4.9	35.6
<i>u</i> 3923	H(237)...H(241)	229.7(117)	40.7(fixed)	—	3.2	40.7
<i>u</i> 447	H(184)...H(201)	229.9(116)	44.3(fixed)	—	21.5	44.3
<i>u</i> 2568	C(89)...H(117)	230.6(130)	38.0(fixed)	—	-2.1	38.0
<i>u</i> 4024	H(155)...H(159)	230.6(95)	63.6(fixed)	—	21.7	63.6
<i>u</i> 2093	H(146)...H(162)	232.4(83)	39.9(fixed)	—	5.4	39.9
<i>u</i> 2442	C(129)...H(154)	233.7(112)	42.0(fixed)	—	-2.2	42.0
<i>u</i> 3666	H(140)...H(154)	235.4(98)	40.5(fixed)	—	-2.0	40.5
<i>u</i> 4215	H(104)...H(121)	235.5(257)	40.3(fixed)	—	-0.1	40.3
<i>u</i> 3369	H(59)...H(65)	236.2(78)	50.3(fixed)	—	-10.5	50.3
<i>u</i> 243	H(21)...H(22)	236.5(754)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 4040	H(272)...H(279)	236.5(147)	31.0(fixed)	—	0.2	31.0
<i>u</i> 674	H(192)...H(195)	236.5(183)	56.1(fixed)	—	14.6	56.1
<i>u</i> 238	H(19)...H(20)	236.5(754)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 3470	H(100)...H(106)	236.9(66)	47.6(fixed)	—	-10.0	47.6
<i>u</i> 199	H(22)...H(23)	238.0(1150)	12.5(fixed)	—	-0.3	12.5

<i>u</i> 230	H(18)...H(20)	238.0(1150)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 4657	H(140)...H(156)	238.8(104)	31.9(fixed)	—	-0.5	31.9
<i>u</i> 4169	H(64)...H(78)	239.3(167)	42.1(fixed)	—	0.9	42.1
<i>u</i> 4424	H(73)...H(78)	239.8(64)	50.8(fixed)	—	0.4	50.8
<i>u</i> 4172	C(211)...H(236)	240.6(104)	50.4(fixed)	—	-2.7	50.4
<i>u</i> 4159	H(228)...H(242)	242.2(269)	42.6(fixed)	—	0.7	42.6
<i>u</i> 458	H(274)...H(286)	243.4(97)	42.4(fixed)	—	14.9	42.4
<i>u</i> 4438	H(115)...H(119)	244.8(206)	36.6(fixed)	—	0.2	36.6
<i>u</i> 4166	H(63)...H(80)	244.9(182)	40.2(fixed)	—	0.0	40.2
<i>u</i> 4158	H(110)...H(114)	245.0(81)	43.9(fixed)	—	1.3	43.9
<i>u</i> 676	H(305)...H(324)	245.2(82)	57.7(fixed)	—	12.6	57.7
<i>u</i> 461	H(305)...H(318)	245.7(103)	44.6(fixed)	—	14.6	44.6
<i>u</i> 428	H(313)...H(322)	246.0(182)	38.8(fixed)	—	22.3	38.8
<i>u</i> 4306	C(47)...H(72)	246.4(86)	33.1(fixed)	—	-1.9	33.1
<i>u</i> 5038	C(211)...H(238)	247.0(87)	27.5(fixed)	—	-1.4	27.5
<i>u</i> 2916	H(65)...H(74)	247.4(122)	44.2(fixed)	—	8.8	44.2
<i>u</i> 4096	H(115)...H(118)	248.1(314)	32.2(fixed)	—	0.5	32.2
<i>u</i> 4316	C(88)...H(117)	248.4(66)	34.1(fixed)	—	-1.5	34.1
<i>u</i> 445	H(233)...H(245)	248.6(303)	41.2(fixed)	—	14.4	41.2
<i>u</i> 464	Si(249)...H(271)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 466	Si(210)...H(226)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 507	Si(166)...H(205)	249.2(16)	12.8(fixed)	—	-0.4	12.8
<i>u</i> 467	Si(84)...H(120)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 491	Si(128)...H(144)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 468	Si(250)...H(280)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 493	Si(166)...H(202)	249.2(16)	12.8(fixed)	—	-0.4	12.8
<i>u</i> 475	Si(330)...H(366)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 485	Si(289)...H(325)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 478	Si(126)...H(148)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 477	Si(2)...H(41)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 501	Si(85)...H(107)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 470	Si(290)...H(314)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 479	Si(209)...H(239)	249.2(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 471	Si(208)...H(232)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 476	Si(128)...H(142)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 472	Si(251)...H(267)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 481	Si(43)...H(82)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 474	Si(249)...H(273)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 482	Si(46)...H(62)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 502	Si(2)...H(38)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 469	Si(84)...H(123)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 480	Si(210)...H(224)	249.2(16)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 511	Si(332)...H(362)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 498	Si(45)...H(71)	249.2(16)	12.7(fixed)	—	-0.3	12.7

<i>u</i> 515	Si(248)...H(284)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 505	Si(127)...H(153)	249.2(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 473	Si(207)...H(246)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 496	Si(86)...H(116)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 504	Si(125)...H(164)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 508	Si(126)...H(150)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 506	Si(87)...H(103)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 520	Si(44)...H(68)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 500	Si(208)...H(230)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 509	Si(44)...H(66)	249.2(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 488	Si(45)...H(75)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 503	Si(290)...H(312)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 513	Si(251)...H(265)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 518	Si(332)...H(358)	249.2(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 486	Si(4)...H(30)	249.2(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 517	Si(289)...H(328)	249.2(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 497	Si(127)...H(157)	249.2(16)	13.0(fixed)	—	-0.3	13.0
<i>u</i> 576	Si(126)...H(149)	249.2(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 512	Si(207)...H(243)	249.3(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 516	Si(248)...H(287)	249.3(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 572	Si(330)...H(364)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 499	Si(330)...H(369)	249.3(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 489	Si(87)...H(101)	249.3(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 542	Si(128)...H(143)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 581	Si(289)...H(323)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 490	Si(4)...H(34)	249.3(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 573	Si(166)...H(203)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 563	Si(126)...H(152)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 561	Si(45)...H(72)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 540	Si(128)...H(146)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 590	Si(46)...H(63)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 601	Si(250)...H(281)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 612	Si(85)...H(108)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 596	Si(2)...H(40)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 555	Si(2)...H(39)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 495	Si(46)...H(60)	249.3(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 604	Si(84)...H(118)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 553	Si(210)...H(225)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 567	Si(127)...H(154)	249.3(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 623	Si(86)...H(117)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 618	Si(2)...H(36)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 538	Si(208)...H(229)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 539	Si(208)...H(233)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 543	Si(207)...H(244)	249.3(16)	12.6(fixed)	—	-0.3	12.6

<i>u559</i>	Si(249)...H(270)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u557</i>	Si(210)...H(228)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u562</i>	Si(84)...H(119)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u544</i>	Si(249)...H(274)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u546</i>	Si(290)...H(315)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u624</i>	Si(210)...H(223)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u603</i>	Si(126)...H(151)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u556</i>	Si(43)...H(80)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u585</i>	Si(289)...H(324)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u609</i>	Si(210)...H(227)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u597</i>	Si(251)...H(268)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u592</i>	Si(84)...H(122)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u514</i>	Si(85)...H(109)	249.3(16)	12.8(fixed)	—	-0.3	12.8
<i>u551</i>	Si(248)...H(283)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u631</i>	Si(128)...H(145)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u614</i>	Si(249)...H(272)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u552</i>	Si(125)...H(163)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u566</i>	Si(332)...H(361)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u617</i>	Si(44)...H(67)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u564</i>	Si(44)...H(70)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u579</i>	Si(44)...H(69)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u570</i>	Si(332)...H(359)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u607</i>	Si(330)...H(365)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u580</i>	Si(86)...H(115)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u574</i>	Si(251)...H(266)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u565</i>	Si(87)...H(105)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u577</i>	Si(166)...H(204)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u599</i>	Si(126)...H(147)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u545</i>	Si(2)...H(37)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u633</i>	Si(248)...H(282)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u600</i>	Si(250)...H(279)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u594</i>	Si(85)...H(106)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u643</i>	Si(208)...H(231)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u569</i>	Si(84)...H(121)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u588</i>	Si(46)...H(64)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u630</i>	Si(332)...H(363)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u593</i>	Si(43)...H(81)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u635</i>	Si(87)...H(104)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u595</i>	Si(289)...H(326)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u530</i>	Si(207)...H(242)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u611</i>	Si(289)...H(327)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u571</i>	Si(248)...H(285)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u642</i>	Si(208)...H(234)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u533</i>	Si(290)...H(311)	249.3(16)	12.6(fixed)	—	-0.3	12.6

<i>u</i> 632	Si(128)...H(141)	249.3(16)	12.3(fixed)	—	-0.3	12.3
<i>u</i> 629	Si(45)...H(73)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 636	Si(207)...H(245)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 589	Si(251)...H(269)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 626	Si(127)...H(155)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 641	Si(290)...H(316)	249.3(16)	12.3(fixed)	—	-0.3	12.3
<i>u</i> 560	Si(209)...H(238)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 640	Si(249)...H(275)	249.3(16)	12.3(fixed)	—	-0.3	12.3
<i>u</i> 620	Si(332)...H(360)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 625	Si(251)...H(264)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 492	Si(86)...H(112)	249.3(16)	12.9(fixed)	—	-0.2	12.9
<i>u</i> 634	Si(166)...H(200)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 549	Si(330)...H(368)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 550	Si(45)...H(74)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 510	Si(43)...H(79)	249.3(16)	12.8(fixed)	—	-0.3	12.8
<i>u</i> 554	Si(166)...H(201)	249.3(16)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 578	Si(44)...H(65)	249.3(16)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 646	Si(290)...H(313)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 638	Si(45)...H(76)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 483	Si(209)...H(235)	249.3(16)	12.9(fixed)	—	-0.2	12.9
<i>u</i> 644	Si(209)...H(240)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 619	Si(248)...H(286)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 548	Si(85)...H(111)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 602	Si(125)...H(162)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 616	Si(87)...H(100)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 613	Si(330)...H(367)	249.3(16)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 494	Si(250)...H(276)	249.3(16)	12.9(fixed)	—	-0.2	12.9
<i>u</i> 610	Si(46)...H(59)	249.3(16)	12.6(fixed)	—	-0.2	12.6
<i>u</i> 649	Si(207)...H(241)	249.3(16)	12.4(fixed)	—	-0.3	12.4
<i>u</i> 584	Si(87)...H(102)	249.3(16)	12.6(fixed)	—	-0.2	12.6
<i>u</i> 605	Si(85)...H(110)	249.4(16)	12.6(fixed)	—	-0.2	12.6
<i>u</i> 598	Si(46)...H(61)	249.4(16)	12.6(fixed)	—	-0.2	12.6
<i>u</i> 535	Si(43)...H(78)	249.4(16)	12.6(fixed)	—	-0.2	12.6
<i>u</i> 637	Si(43)...H(77)	249.4(16)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 583	Si(250)...H(277)	249.4(16)	12.7(fixed)	—	-0.2	12.7
<i>u</i> 541	Si(127)...H(156)	249.4(16)	12.7(fixed)	—	-0.2	12.7
<i>u</i> 587	Si(86)...H(113)	249.4(16)	12.7(fixed)	—	-0.2	12.7
<i>u</i> 621	Si(86)...H(114)	249.4(16)	12.6(fixed)	—	-0.2	12.6
<i>u</i> 586	Si(209)...H(236)	249.4(16)	12.7(fixed)	—	-0.2	12.7
<i>u</i> 645	Si(127)...H(158)	249.4(16)	12.7(fixed)	—	-0.1	12.7
<i>u</i> 622	Si(209)...H(237)	249.4(16)	12.6(fixed)	—	-0.1	12.6
<i>u</i> 627	Si(250)...H(278)	249.5(16)	12.5(fixed)	—	-0.1	12.5
<i>u</i> 484	Si(125)...H(161)	250.2(16)	14.4(fixed)	—	0.8	14.4
<i>u</i> 568	Si(125)...H(160)	250.9(16)	15.2(fixed)	—	1.6	15.2

<i>u</i> 2076	H(264)...H(285)	251.1(132)	44.9(fixed)	—	4.2	44.9
<i>u</i> 639	Si(125)...H(159)	251.4(16)	15.6(fixed)	—	2.2	15.6
<i>u</i> 4165	H(178)...H(196)	252.2(50)	27.7(fixed)	—	-3.5	27.7
<i>u</i> 2446	C(212)...H(236)	252.2(87)	45.9(fixed)	—	-5.0	45.9
<i>u</i> 4543	H(141)...H(160)	252.7(89)	56.3(fixed)	—	12.9	56.3
<i>u</i> 3651	C(215)...H(225)	253.0(100)	33.8(fixed)	—	0.7	33.8
<i>u</i> 785	H(310)...H(326)	254.4(125)	62.9(fixed)	—	9.9	62.9
<i>u</i> 2270	H(221)...H(223)	254.5(78)	42.0(fixed)	—	-2.0	42.0
<i>u</i> 3146	Si(250)...H(268)	254.6(74)	21.4(fixed)	—	-0.2	21.4
<i>u</i> 3057	C(48)...H(78)	254.8(125)	42.9(fixed)	—	5.9	42.9
<i>u</i> 667	H(187)...H(204)	254.9(82)	57.5(fixed)	—	15.7	57.5
<i>u</i> 4633	H(97)...H(102)	255.1(70)	28.6(fixed)	—	-0.9	28.6
<i>u</i> 3227	H(266)...H(275)	255.5(91)	39.5(fixed)	—	6.0	39.5
<i>u</i> 2119	H(262)...H(269)	255.9(71)	36.9(fixed)	—	-1.9	36.9
<i>u</i> 5348	H(268)...H(276)	256.3(126)	28.4(fixed)	—	-6.6	28.4
<i>u</i> 5002	C(47)...H(74)	257.8(66)	27.3(fixed)	—	-1.5	27.3
<i>u</i> 2465	C(94)...H(113)	257.9(179)	43.5(fixed)	—	-4.3	43.5
<i>u</i> 2551	C(48)...H(72)	258.2(95)	32.3(fixed)	—	-1.9	32.3
<i>u</i> 772	H(220)...H(241)	258.9(203)	46.7(fixed)	—	8.5	46.7
<i>u</i> 3791	C(51)...H(61)	259.0(86)	29.8(fixed)	—	3.8	29.8
<i>u</i> 450	H(275)...H(286)	259.2(84)	42.5(fixed)	—	16.0	42.5
<i>u</i> 793	C(294)...H(316)	259.3(65)	29.4(fixed)	—	9.6	29.4
<i>u</i> 4456	H(105)...H(119)	260.3(30)	40.2(fixed)	—	-2.5	40.2
<i>u</i> 2643	C(90)...H(100)	260.4(44)	47.9(fixed)	—	-4.9	47.9
<i>u</i> 2528	C(49)...H(59)	261.1(48)	49.1(fixed)	—	-4.1	49.1
<i>u</i> 2764	Si(87)...H(117)	261.5(69)	28.5(fixed)	—	-1.7	28.5
<i>u</i> 558	H(234)...H(245)	261.9(56)	47.3(fixed)	—	13.4	47.3
<i>u</i> 3072	H(147)...H(156)	262.8(90)	45.6(fixed)	—	10.3	45.6
<i>u</i> 532	H(14)...H(29)	262.9(102)	36.6(fixed)	—	13.0	36.6
<i>u</i> 4405	H(264)...H(275)	262.9(169)	33.6(fixed)	—	-0.9	33.6
<i>u</i> 5025	C(256)...H(269)	263.5(83)	25.0(fixed)	—	-1.9	25.0
<i>u</i> 939	H(261)...H(263)	264.2(80)	31.0(fixed)	—	1.8	31.0
<i>u</i> 441	H(139)...H(163)	264.2(37)	34.8(fixed)	—	18.8	34.8
<i>u</i> 4018	C(93)...H(102)	264.3(57)	30.0(fixed)	—	3.6	30.0
<i>u</i> 3813	H(262)...H(266)	265.3(68)	25.3(fixed)	—	-2.1	25.3
<i>u</i> 615	Si(4)...H(32)	265.9(341)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 575	Si(4)...H(31)	265.9(341)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 547	Si(4)...H(33)	265.9(341)	12.7(fixed)	—	-0.2	12.7
<i>u</i> 647	Si(4)...H(35)	265.9(341)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 436	H(23)...H(26)	266.1(379)	44.1(fixed)	—	24.9	44.1
<i>u</i> 443	H(96)...H(111)	266.3(47)	36.2(fixed)	—	20.6	36.2
<i>u</i> 1045	C(92)...H(118)	266.7(171)	31.4(fixed)	—	6.6	31.4
<i>u</i> 606	H(305)...H(319)	267.5(108)	47.4(fixed)	—	16.3	47.4
<i>u</i> 666	H(15)...H(24)	268.7(82)	42.2(fixed)	—	12.0	42.2

<i>u774</i>	H(56)...H(77)	268.8(146)	46.0(fixed)	—	10.1	46.0
<i>u1782</i>	H(20)...H(40)	269.1(925)	63.9(fixed)	—	3.4	63.9
<i>u3060</i>	C(212)...H(242)	269.4(189)	44.0(fixed)	—	5.5	44.0
<i>u780</i>	H(302)...H(323)	270.1(75)	39.9(fixed)	—	6.6	39.9
<i>u522</i>	H(57)...H(81)	270.5(93)	35.0(fixed)	—	12.2	35.0
<i>u451</i>	H(342)...H(357)	270.6(34)	36.0(fixed)	—	17.5	36.0
<i>u2705</i>	Si(128)...H(154)	270.7(60)	33.5(fixed)	—	-2.5	33.5
<i>u4256</i>	C(217)...H(237)	270.8(69)	24.0(fixed)	—	-1.2	24.0
<i>u2702</i>	Si(210)...H(236)	271.2(64)	38.8(fixed)	—	-3.6	38.8
<i>u4135</i>	H(143)...H(162)	271.2(108)	36.6(fixed)	—	2.7	36.6
<i>u455</i>	H(20)...H(26)	271.2(346)	45.8(fixed)	—	21.4	45.8
<i>u1169</i>	Si(4)...H(22)	271.5(277)	35.8(fixed)	—	11.4	35.8
<i>u4984</i>	C(216)...H(225)	271.5(87)	25.1(fixed)	—	-2.1	25.1
<i>u591</i>	H(55)...H(70)	271.8(59)	35.9(fixed)	—	13.0	35.9
<i>u740</i>	C(217)...H(219)	271.9(14)	13.5(fixed)	—	-0.1	13.5
<i>u707</i>	C(218)...H(219)	271.9(14)	13.5(fixed)	—	-0.1	13.5
<i>u731</i>	C(213)...H(221)	272.0(14)	13.6(fixed)	—	-0.1	13.6
<i>u692</i>	C(49)...H(57)	272.0(14)	13.6(fixed)	—	-0.1	13.6
<i>u689</i>	C(50)...H(57)	272.0(14)	13.6(fixed)	—	-0.1	13.6
<i>u684</i>	C(54)...H(55)	272.0(14)	13.5(fixed)	—	-0.1	13.5
<i>u732</i>	C(53)...H(55)	272.0(14)	13.6(fixed)	—	-0.1	13.6
<i>u717</i>	C(214)...H(221)	272.0(14)	13.5(fixed)	—	-0.1	13.5
<i>u710</i>	C(88)...H(99)	272.1(14)	13.6(fixed)	—	-0.1	13.6
<i>u712</i>	C(89)...H(99)	272.1(14)	13.6(fixed)	—	-0.1	13.6
<i>u716</i>	C(8)...H(16)	272.2(14)	13.6(fixed)	—	-0.1	13.6
<i>u706</i>	C(6)...H(17)	272.2(14)	13.6(fixed)	—	-0.1	13.6
<i>u708</i>	C(259)...H(260)	272.2(14)	13.6(fixed)	—	-0.1	13.6
<i>u683</i>	C(9)...H(16)	272.2(14)	13.5(fixed)	—	-0.1	13.5
<i>u738</i>	C(295)...H(303)	272.2(14)	13.5(fixed)	—	-0.1	13.5
<i>u711</i>	C(296)...H(303)	272.2(14)	13.5(fixed)	—	-0.1	13.5
<i>u722</i>	C(258)...H(260)	272.2(14)	13.5(fixed)	—	-0.1	13.5
<i>u724</i>	C(7)...H(17)	272.2(14)	13.5(fixed)	—	-0.1	13.5
<i>u719</i>	C(129)...H(140)	272.3(14)	13.6(fixed)	—	-0.1	13.6
<i>u705</i>	C(133)...H(138)	272.3(14)	13.6(fixed)	—	-0.1	13.6
<i>u728</i>	C(130)...H(140)	272.3(14)	13.6(fixed)	—	-0.1	13.6
<i>u726</i>	C(134)...H(138)	272.3(14)	13.6(fixed)	—	-0.1	13.6
<i>u695</i>	C(91)...H(98)	272.4(14)	13.6(fixed)	—	-0.1	13.6
<i>u697</i>	C(47)...H(58)	272.4(14)	13.6(fixed)	—	-0.1	13.6
<i>u685</i>	C(90)...H(98)	272.4(14)	13.6(fixed)	—	-0.1	13.6
<i>u680</i>	C(48)...H(58)	272.4(14)	13.5(fixed)	—	-0.1	13.5
<i>u734</i>	C(247)...H(261)	272.4(10)	13.2(fixed)	—	0.0	13.2
<i>u737</i>	C(247)...H(262)	272.4(10)	13.2(fixed)	—	0.0	13.2
<i>u681</i>	C(132)...H(139)	272.4(14)	13.7(fixed)	—	-0.1	13.7
<i>u704</i>	C(171)...H(181)	272.5(14)	13.6(fixed)	—	-0.1	13.6

<i>u678</i>	C(131)...H(139)	272.5(14)	13.6(fixed)	—	-0.1	13.6
<i>u3442</i>	C(53)...H(63)	272.5(76)	34.4(fixed)	—	1.5	34.4
<i>u714</i>	C(334)...H(345)	272.5(14)	13.5(fixed)	—	-0.1	13.5
<i>u687</i>	C(170)...H(181)	272.5(14)	13.6(fixed)	—	-0.1	13.6
<i>u720</i>	C(335)...H(345)	272.5(14)	13.5(fixed)	—	-0.1	13.5
<i>u648</i>	H(137)...H(152)	272.5(46)	37.8(fixed)	—	13.7	37.8
<i>u691</i>	C(212)...H(222)	272.5(14)	13.6(fixed)	—	-0.1	13.6
<i>u694</i>	C(293)...H(304)	272.5(14)	13.6(fixed)	—	-0.1	13.6
<i>u702</i>	C(211)...H(222)	272.5(14)	13.6(fixed)	—	-0.1	13.6
<i>u696</i>	C(136)...H(137)	272.6(14)	13.6(fixed)	—	-0.1	13.6
<i>u679</i>	C(294)...H(304)	272.6(14)	13.6(fixed)	—	-0.1	13.6
<i>u713</i>	C(92)...H(97)	272.6(14)	13.6(fixed)	—	-0.1	13.6
<i>u699</i>	C(135)...H(137)	272.6(14)	13.6(fixed)	—	-0.1	13.6
<i>u700</i>	C(93)...H(97)	272.6(14)	13.5(fixed)	—	-0.1	13.5
<i>u709</i>	C(51)...H(56)	272.6(14)	13.5(fixed)	—	-0.1	13.5
<i>u723</i>	C(52)...H(56)	272.6(14)	13.5(fixed)	—	-0.1	13.5
<i>u735</i>	C(247)...H(263)	272.6(10)	13.2(fixed)	—	0.0	13.2
<i>u651</i>	H(98)...H(122)	272.6(179)	38.4(fixed)	—	10.5	38.4
<i>u693</i>	C(94)...H(96)	272.6(14)	13.6(fixed)	—	-0.1	13.6
<i>u686</i>	C(95)...H(96)	272.6(14)	13.6(fixed)	—	-0.1	13.6
<i>u715</i>	C(215)...H(220)	272.7(14)	13.5(fixed)	—	-0.1	13.5
<i>u718</i>	C(216)...H(220)	272.7(14)	13.5(fixed)	—	-0.1	13.5
<i>u688</i>	C(337)...H(344)	272.7(14)	13.6(fixed)	—	-0.1	13.6
<i>u677</i>	C(336)...H(344)	272.8(14)	13.5(fixed)	—	-0.1	13.5
<i>u2345</i>	C(213)...H(240)	272.9(113)	49.7(fixed)	—	-2.9	49.7
<i>u690</i>	C(253)...H(263)	273.0(14)	13.6(fixed)	—	-0.1	13.6
<i>u725</i>	C(252)...H(263)	273.0(14)	13.6(fixed)	—	-0.1	13.6
<i>u703</i>	C(254)...H(262)	273.1(14)	13.6(fixed)	—	-0.1	13.6
<i>u729</i>	C(255)...H(262)	273.1(14)	13.6(fixed)	—	-0.1	13.6
<i>u747</i>	C(329)...H(342)	273.1(10)	13.2(fixed)	—	0.0	13.2
<i>u727</i>	C(256)...H(261)	273.1(14)	13.6(fixed)	—	-0.1	13.6
<i>u682</i>	C(257)...H(261)	273.1(14)	13.5(fixed)	—	-0.1	13.5
<i>u752</i>	C(206)...H(220)	273.3(10)	13.2(fixed)	—	0.0	13.2
<i>u757</i>	C(83)...H(96)	273.3(10)	13.2(fixed)	—	0.0	13.2
<i>u958</i>	H(15)...H(32)	273.4(142)	28.0(fixed)	—	0.8	28.0
<i>u739</i>	C(83)...H(97)	273.5(10)	13.2(fixed)	—	0.0	13.2
<i>u744</i>	C(206)...H(222)	273.5(10)	13.2(fixed)	—	0.0	13.2
<i>u754</i>	C(124)...H(137)	273.5(10)	13.3(fixed)	—	0.0	13.3
<i>u736</i>	C(288)...H(301)	273.5(10)	13.1(fixed)	—	0.0	13.1
<i>u745</i>	C(42)...H(56)	273.5(10)	13.2(fixed)	—	0.0	13.2
<i>u755</i>	C(165)...H(178)	273.6(10)	13.2(fixed)	—	0.0	13.2
<i>u742</i>	C(329)...H(343)	273.6(10)	13.1(fixed)	—	0.0	13.1
<i>u756</i>	C(124)...H(139)	273.6(10)	13.1(fixed)	—	0.0	13.1
<i>u1141</i>	C(293)...H(326)	273.7(127)	34.5(fixed)	—	10.9	34.5



<i>u</i> 751	C(83)...H(98)	273.8(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 753	C(42)...H(58)	273.8(10)	13.1(fixed)	—	0.0	13.1
<i>u</i> 746	C(124)...H(140)	274.0(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 743	C(124)...H(138)	274.0(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 3531	H(142)...H(154)	274.0(97)	45.5(fixed)	—	-6.5	45.5
<i>u</i> 762	C(288)...H(302)	274.1(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 741	C(247)...H(260)	274.2(10)	13.1(fixed)	—	0.0	13.1
<i>u</i> 759	C(1)...H(14)	274.2(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 760	C(1)...H(15)	274.2(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 3960	H(262)...H(277)	274.2(48)	31.3(fixed)	—	-7.2	31.3
<i>u</i> 4305	C(53)...H(73)	274.3(40)	23.6(fixed)	—	-1.3	23.6
<i>u</i> 748	C(83)...H(99)	274.3(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 3164	C(52)...H(65)	274.4(54)	33.0(fixed)	—	4.0	33.0
<i>u</i> 977	C(335)...H(365)	274.5(50)	37.2(fixed)	—	7.4	37.2
<i>u</i> 749	C(206)...H(221)	274.5(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 763	C(42)...H(55)	274.5(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 758	C(42)...H(57)	274.5(10)	13.1(fixed)	—	0.0	13.1
<i>u</i> 761	C(206)...H(219)	274.7(10)	13.2(fixed)	—	0.0	13.2
<i>u</i> 2771	Si(46)...H(72)	274.9(62)	26.5(fixed)	—	-2.0	26.5
<i>u</i> 733	H(303)...H(322)	275.3(102)	43.8(fixed)	—	7.6	43.8
<i>u</i> 3405	H(264)...H(286)	275.6(125)	44.7(fixed)	—	-7.1	44.7
<i>u</i> 4408	C(135)...H(155)	275.7(77)	24.7(fixed)	—	-1.7	24.7
<i>u</i> 3562	C(129)...H(160)	276.4(55)	55.9(fixed)	—	20.5	55.9
<i>u</i> 3776	H(221)...H(240)	276.4(88)	33.8(fixed)	—	-5.4	33.8
<i>u</i> 1675	Si(251)...H(261)	276.7(47)	20.2(fixed)	—	-0.3	20.2
<i>u</i> 3377	C(89)...H(119)	276.8(143)	40.2(fixed)	—	2.4	40.2
<i>u</i> 1016	Si(250)...Si(251)	277.1(33)	10.9(38)	—	-0.1	9.6
<i>u</i> 783	C(129)...H(155)	277.1(158)	31.2(fixed)	—	14.9	31.2
<i>u</i> 801	C(48)...H(73)	277.6(116)	30.3(fixed)	—	10.2	30.3
<i>u</i> 912	C(89)...H(115)	277.9(116)	35.7(fixed)	—	9.2	35.7
<i>u</i> 1520	H(19)...H(23)	279.0(527)	55.1(fixed)	—	-1.5	55.1
<i>u</i> 5016	C(52)...H(61)	279.4(84)	26.7(fixed)	—	-1.2	26.7
<i>u</i> 4759	C(253)...C(256)	279.7(61)	14.1(tied to <i>u</i> 1016)	—	-1.9	12.4
<i>u</i> 1787	H(22)...H(24)	279.8(922)	77.9(fixed)	—	2.9	77.9
<i>u</i> 2858	H(97)...H(106)	280.1(59)	31.7(fixed)	—	2.5	31.7
<i>u</i> 4217	H(111)...H(114)	280.7(146)	49.0(fixed)	—	3.8	49.0
<i>u</i> 3043	H(263)...H(283)	281.0(57)	36.5(fixed)	—	3.3	36.5
<i>u</i> 3668	H(103)...H(117)	281.4(89)	41.0(fixed)	—	-8.6	41.0
<i>u</i> 2633	C(258)...H(281)	282.0(62)	35.3(fixed)	—	-1.6	35.3
<i>u</i> 4019	H(178)...H(190)	282.1(75)	26.2(fixed)	—	-3.3	26.2
<i>u</i> 650	H(301)...H(311)	282.4(57)	38.4(fixed)	—	14.4	38.4
<i>u</i> 3393	H(146)...H(163)	282.6(81)	42.3(fixed)	—	-8.8	42.3
<i>u</i> 3332	C(134)...H(147)	282.6(51)	35.6(fixed)	—	0.9	35.6
<i>u</i> 782	H(343)...H(364)	282.8(50)	39.3(fixed)	—	6.6	39.3

<i>u</i> 806	H(138)...H(159)	283.1(87)	78.8(fixed)	—	29.0	78.8
<i>u</i> 1087	Si(127)...Si(128)	283.1(33)	11.1(tied to <i>u</i> 1016)	—	-0.1	9.8
<i>u</i> 3229	Si(209)...H(225)	283.3(66)	22.8(fixed)	—	-1.0	22.8
<i>u</i> 1357	Si(2)...H(31)	283.4(382)	35.4(fixed)	—	7.0	35.4
<i>u</i> 1153	C(296)...H(309)	283.6(108)	34.0(fixed)	—	4.8	34.0
<i>u</i> 2512	C(254)...H(277)	283.7(65)	41.0(fixed)	—	-6.1	41.0
<i>u</i> 830	C(170)...H(201)	284.7(58)	37.8(fixed)	—	15.5	37.8
<i>u</i> 1109	Si(86)...Si(87)	285.2(33)	11.1(tied to <i>u</i> 1016)	—	-0.1	9.8
<i>u</i> 5380	H(267)...H(278)	285.5(68)	27.0(fixed)	—	-3.6	27.0
<i>u</i> 3190	C(253)...H(261)	285.5(68)	23.7(fixed)	—	-1.0	23.7
<i>u</i> 1395	C(257)...H(282)	285.5(66)	42.8(fixed)	—	6.3	42.8
<i>u</i> 1042	Si(209)...Si(210)	285.7(33)	9.6(fixed)	—	-0.1	9.6
<i>u</i> 2895	H(222)...H(234)	286.1(80)	33.4(fixed)	—	2.4	33.4
<i>u</i> 1060	Si(45)...Si(46)	286.4(33)	11.2(tied to <i>u</i> 1016)	—	-0.1	9.9
<i>u</i> 1350	C(334)...H(359)	287.6(101)	35.4(fixed)	—	7.0	35.4
<i>u</i> 2595	Si(127)...H(140)	287.9(43)	13.4(fixed)	—	-1.6	13.4
<i>u</i> 2661	H(105)...H(116)	288.1(94)	54.3(fixed)	—	-2.6	54.3
<i>u</i> 4372	C(94)...H(115)	288.2(69)	21.1(fixed)	—	-1.5	21.1
<i>u</i> 807	H(301)...H(315)	288.2(81)	44.7(fixed)	—	6.2	44.7
<i>u</i> 4890	H(224)...H(236)	288.2(127)	54.2(fixed)	—	-7.4	54.2
<i>u</i> 956	H(343)...H(356)	288.2(65)	52.3(fixed)	—	5.5	52.3
<i>u</i> 4461	H(270)...H(279)	288.4(155)	36.4(fixed)	—	-0.8	36.4
<i>u</i> 2430	H(141)...H(153)	288.6(104)	43.8(fixed)	—	-2.2	43.8
<i>u</i> 3279	Si(45)...H(61)	288.6(54)	21.8(fixed)	—	0.4	21.8
<i>u</i> 1299	C(6)...H(23)	289.2(208)	32.7(fixed)	—	1.6	32.7
<i>u</i> 3863	C(135)...H(143)	289.6(62)	37.4(fixed)	—	0.6	37.4
<i>u</i> 2343	C(132)...H(158)	289.9(96)	64.3(fixed)	—	-4.4	64.3
<i>u</i> 3449	C(217)...H(227)	290.2(58)	36.8(fixed)	—	1.2	36.8
<i>u</i> 3250	C(130)...H(149)	290.4(65)	31.4(fixed)	—	2.6	31.4
<i>u</i> 4415	C(131)...H(145)	290.5(71)	24.6(fixed)	—	-2.1	24.6
<i>u</i> 1208	C(216)...H(231)	290.6(115)	34.7(fixed)	—	5.1	34.7
<i>u</i> 5034	H(101)...H(117)	290.6(100)	40.3(fixed)	—	-7.0	40.3
<i>u</i> 1903	C(89)...C(93)	291.0(75)	26.0(fixed)	—	1.1	26.0
<i>u</i> 1714	C(129)...C(133)	291.3(88)	23.5(tied to <i>u</i> 1082)	—	2.6	21.5
<i>u</i> 1000	H(99)...H(121)	291.3(47)	50.4(fixed)	—	5.3	50.4
<i>u</i> 3330	Si(86)...H(102)	291.5(51)	21.5(fixed)	—	0.5	21.5
<i>u</i> 794	C(336)...H(346)	291.8(49)	29.5(fixed)	—	10.4	29.5
<i>u</i> 1244	H(15)...H(28)	292.0(125)	53.4(fixed)	—	5.0	53.4
<i>u</i> 5045	H(60)...H(72)	292.1(103)	37.8(fixed)	—	-7.4	37.8
<i>u</i> 779	C(255)...H(286)	292.4(39)	29.4(fixed)	—	13.0	29.4
<i>u</i> 1349	C(336)...H(363)	292.5(93)	40.3(fixed)	—	5.8	40.3
<i>u</i> 884	C(334)...H(361)	292.5(55)	34.5(fixed)	—	10.3	34.5
<i>u</i> 914	H(221)...H(230)	293.7(31)	25.3(fixed)	—	0.1	25.3
<i>u</i> 4387	C(49)...H(76)	293.9(106)	31.5(fixed)	—	-5.0	31.5

<i>u</i> 918	H(14)...H(38)	294.0(31)	25.4(fixed)	—	0.1	25.4
<i>u</i> 919	H(140)...H(144)	294.1(31)	26.1(fixed)	—	0.1	26.1
<i>u</i> 890	H(219)...H(243)	294.3(31)	27.4(fixed)	—	1.2	27.4
<i>u</i> 879	H(99)...H(103)	294.3(31)	25.8(fixed)	—	0.6	25.8
<i>u</i> 858	H(57)...H(66)	294.5(31)	26.4(fixed)	—	1.0	26.4
<i>u</i> 880	H(55)...H(79)	294.6(31)	27.5(fixed)	—	1.4	27.5
<i>u</i> 895	H(302)...H(321)	294.6(31)	27.0(fixed)	—	1.0	27.0
<i>u</i> 954	H(58)...H(80)	294.6(57)	50.8(fixed)	—	5.6	50.8
<i>u</i> 1122	C(300)...H(310)	294.7(72)	41.8(fixed)	—	7.3	41.8
<i>u</i> 867	H(58)...H(62)	294.7(31)	24.5(fixed)	—	0.2	24.5
<i>u</i> 871	H(260)...H(284)	294.8(31)	25.9(fixed)	—	0.9	25.9
<i>u</i> 868	H(139)...H(148)	294.8(31)	24.9(fixed)	—	0.2	24.9
<i>u</i> 875	H(98)...H(107)	294.8(31)	25.9(fixed)	—	0.6	25.9
<i>u</i> 872	H(222)...H(226)	294.8(31)	25.0(fixed)	—	0.1	25.0
<i>u</i> 888	H(96)...H(120)	294.9(31)	25.1(fixed)	—	0.0	25.1
<i>u</i> 3808	C(94)...H(104)	295.0(263)	31.2(fixed)	—	2.7	31.2
<i>u</i> 885	H(97)...H(116)	295.0(31)	25.5(fixed)	—	0.4	25.5
<i>u</i> 866	H(301)...H(325)	295.0(31)	24.6(fixed)	—	0.2	24.6
<i>u</i> 878	H(343)...H(362)	295.1(31)	25.9(fixed)	—	0.7	25.9
<i>u</i> 777	H(140)...H(149)	295.3(111)	42.8(fixed)	—	7.2	42.8
<i>u</i> 4442	C(218)...H(227)	295.3(146)	27.3(fixed)	—	-3.0	27.3
<i>u</i> 869	H(342)...H(366)	295.3(31)	24.7(fixed)	—	0.2	24.7
<i>u</i> 873	H(56)...H(75)	295.5(31)	26.6(fixed)	—	1.1	26.6
<i>u</i> 845	H(178)...H(202)	295.5(31)	28.1(fixed)	—	1.5	28.1
<i>u</i> 4809	H(225)...H(235)	295.6(127)	39.3(fixed)	—	-10.8	39.3
<i>u</i> 1052	C(337)...H(363)	295.6(54)	31.1(fixed)	—	9.3	31.1
<i>u</i> 844	H(15)...H(34)	295.7(31)	28.5(fixed)	—	2.3	28.5
<i>u</i> 883	H(262)...H(271)	295.8(31)	25.1(fixed)	—	0.1	25.1
<i>u</i> 876	H(263)...H(267)	295.9(31)	24.6(fixed)	—	0.2	24.6
<i>u</i> 874	H(261)...H(280)	296.0(31)	24.7(fixed)	—	0.2	24.7
<i>u</i> 853	H(138)...H(157)	296.1(31)	29.6(fixed)	—	2.7	29.6
<i>u</i> 846	H(220)...H(239)	296.3(31)	27.6(fixed)	—	1.8	27.6
<i>u</i> 786	C(214)...H(245)	296.5(140)	29.6(fixed)	—	11.1	29.6
<i>u</i> 1186	C(6)...H(39)	296.5(55)	32.8(fixed)	—	6.7	32.8
<i>u</i> 4437	C(131)...H(158)	296.8(98)	41.8(fixed)	—	-7.8	41.8
<i>u</i> 2644	C(136)...H(146)	296.9(57)	34.0(fixed)	—	-2.9	34.0
<i>u</i> 4930	C(172)...H(200)	297.1(100)	26.1(fixed)	—	-0.1	26.1
<i>u</i> 848	H(219)...H(246)	297.2(29)	24.4(fixed)	—	0.7	24.4
<i>u</i> 812	H(260)...H(270)	297.4(44)	44.1(fixed)	—	7.8	44.1
<i>u</i> 837	H(221)...H(232)	297.4(29)	24.2(fixed)	—	0.7	24.2
<i>u</i> 817	H(55)...H(82)	297.5(29)	24.0(fixed)	—	0.8	24.0
<i>u</i> 825	H(57)...H(68)	297.6(29)	24.4(fixed)	—	0.9	24.4
<i>u</i> 765	C(212)...H(237)	297.6(160)	33.6(fixed)	—	22.0	33.6
<i>u</i> 769	H(219)...H(229)	297.7(74)	42.6(fixed)	—	10.0	42.6

<i>u</i> 841	H(302)...H(317)	297.8(29)	24.2(fixed)	—	0.7	24.2
<i>u</i> 838	H(140)...H(142)	297.8(29)	24.4(fixed)	—	0.6	24.4
<i>u</i> 864	H(260)...H(287)	297.8(29)	25.7(fixed)	—	1.0	25.7
<i>u</i> 863	H(99)...H(101)	297.8(29)	27.9(fixed)	—	1.6	27.9
<i>u</i> 2957	H(58)...H(67)	297.9(55)	32.3(fixed)	—	5.3	32.3
<i>u</i> 865	H(15)...H(30)	297.9(29)	27.0(fixed)	—	1.3	27.0
<i>u</i> 808	H(14)...H(41)	297.9(29)	23.9(fixed)	—	0.8	23.9
<i>u</i> 861	H(138)...H(153)	298.0(29)	26.0(fixed)	—	1.1	26.0
<i>u</i> 1080	H(219)...H(233)	298.0(166)	48.9(fixed)	—	5.4	48.9
<i>u</i> 795	C(296)...H(327)	298.1(59)	32.0(fixed)	—	12.9	32.0
<i>u</i> 855	H(222)...H(224)	298.2(29)	24.2(fixed)	—	0.5	24.2
<i>u</i> 850	H(343)...H(358)	298.4(29)	24.6(fixed)	—	0.9	24.6
<i>u</i> 821	H(139)...H(150)	298.4(29)	24.5(fixed)	—	0.9	24.5
<i>u</i> 854	H(137)...H(164)	298.5(29)	26.9(fixed)	—	1.2	26.9
<i>u</i> 843	H(98)...H(109)	298.6(29)	27.1(fixed)	—	1.7	27.1
<i>u</i> 819	H(178)...H(205)	298.6(29)	24.4(fixed)	—	1.1	24.4
<i>u</i> 836	H(56)...H(71)	298.6(29)	24.5(fixed)	—	0.9	24.5
<i>u</i> 818	H(96)...H(123)	298.6(29)	23.9(fixed)	—	0.7	23.9
<i>u</i> 2813	H(262)...H(278)	298.7(90)	31.2(fixed)	—	7.1	31.2
<i>u</i> 834	H(58)...H(60)	298.7(29)	27.3(fixed)	—	1.8	27.3
<i>u</i> 842	H(304)...H(306)	298.7(29)	26.2(fixed)	—	1.3	26.2
<i>u</i> 2418	C(50)...H(76)	298.8(67)	47.2(fixed)	—	-2.2	47.2
<i>u</i> 905	H(260)...H(274)	298.8(59)	44.8(fixed)	—	5.4	44.8
<i>u</i> 976	H(57)...H(70)	299.0(38)	25.3(fixed)	—	0.1	25.3
<i>u</i> 979	H(58)...H(59)	299.0(37)	29.3(fixed)	—	0.7	29.3
<i>u</i> 991	H(55)...H(81)	299.0(38)	24.6(fixed)	—	0.0	24.6
<i>u</i> 1013	H(14)...H(40)	299.0(37)	24.4(fixed)	—	-0.1	24.4
<i>u</i> 951	H(98)...H(111)	299.0(37)	29.0(fixed)	—	0.6	29.0
<i>u</i> 998	H(97)...H(114)	299.0(37)	31.1(fixed)	—	1.0	31.1
<i>u</i> 959	H(342)...H(368)	299.1(37)	28.9(fixed)	—	0.5	28.9
<i>u</i> 987	H(219)...H(245)	299.1(38)	24.9(fixed)	—	0.2	24.9
<i>u</i> 1017	H(221)...H(234)	299.1(38)	24.4(fixed)	—	0.1	24.4
<i>u</i> 1027	H(261)...H(278)	299.1(37)	31.6(fixed)	—	0.9	31.6
<i>u</i> 962	H(99)...H(100)	299.1(38)	29.5(fixed)	—	1.0	29.5
<i>u</i> 964	H(139)...H(152)	299.1(37)	25.7(fixed)	—	0.1	25.7
<i>u</i> 966	H(301)...H(327)	299.2(37)	27.4(fixed)	—	0.4	27.4
<i>u</i> 965	H(260)...H(286)	299.2(37)	26.6(fixed)	—	0.5	26.6
<i>u</i> 990	H(178)...H(204)	299.2(37)	25.0(fixed)	—	0.1	25.0
<i>u</i> 1014	H(140)...H(141)	299.2(37)	24.2(fixed)	—	0.0	24.2
<i>u</i> 1002	H(302)...H(319)	299.3(37)	24.4(fixed)	—	0.2	24.4
<i>u</i> 970	H(138)...H(155)	299.3(37)	26.6(fixed)	—	0.5	26.6
<i>u</i> 993	H(343)...H(360)	299.3(37)	25.4(fixed)	—	0.2	25.4
<i>u</i> 984	H(96)...H(122)	299.3(37)	24.4(fixed)	—	0.0	24.4
<i>u</i> 1005	H(56)...H(73)	299.4(37)	25.0(fixed)	—	0.2	25.0

<i>u</i> 859	H(220)...H(235)	299.4(29)	29.2(fixed)	—	2.3	29.2
<i>u</i> 938	H(137)...H(163)	299.4(37)	27.6(fixed)	—	0.6	27.6
<i>u</i> 852	H(262)...H(273)	299.4(29)	24.1(fixed)	—	0.6	24.1
<i>u</i> 851	H(263)...H(265)	299.4(29)	24.6(fixed)	—	0.9	24.6
<i>u</i> 967	H(222)...H(223)	299.4(37)	24.3(fixed)	—	0.1	24.3
<i>u</i> 824	H(342)...H(369)	299.4(29)	26.7(fixed)	—	1.8	26.7
<i>u</i> 971	H(220)...H(237)	299.4(37)	31.2(fixed)	—	1.4	31.2
<i>u</i> 839	H(97)...H(112)	299.5(29)	28.7(fixed)	—	2.5	28.7
<i>u</i> 822	H(137)...H(161)	299.5(31)	38.7(fixed)	—	7.7	38.7
<i>u</i> 997	H(263)...H(264)	299.6(37)	25.3(fixed)	—	0.2	25.3
<i>u</i> 1010	H(262)...H(275)	299.7(37)	24.0(fixed)	—	0.1	24.0
<i>u</i> 1036	C(256)...H(272)	299.8(70)	32.4(fixed)	—	4.9	32.4
<i>u</i> 3375	C(252)...H(275)	300.7(78)	30.9(fixed)	—	2.8	30.9
<i>u</i> 898	C(7)...H(35)	300.7(248)	32.6(fixed)	—	17.6	32.6
<i>u</i> 833	H(261)...H(276)	301.0(29)	28.5(fixed)	—	2.9	28.5
<i>u</i> 2981	H(99)...H(108)	301.1(54)	31.0(fixed)	—	3.6	31.0
<i>u</i> 1324	C(172)...H(195)	301.3(88)	35.8(fixed)	—	5.2	35.8
<i>u</i> 2935	H(261)...H(282)	301.7(84)	31.4(fixed)	—	4.5	31.4
<i>u</i> 1008	H(137)...H(159)	301.9(48)	47.5(fixed)	—	5.0	47.5
<i>u</i> 5042	H(102)...H(116)	301.9(93)	32.2(fixed)	—	-2.6	32.2
<i>u</i> 802	H(222)...H(244)	301.9(63)	49.0(fixed)	—	6.7	49.0
<i>u</i> 2924	Si(250)...C(253)	302.0(47)	12.2(tied to <i>u</i> 1082)	—	-1.0	11.2
<i>u</i> 944	H(57)...H(67)	302.2(48)	27.4(fixed)	—	0.7	27.4
<i>u</i> 999	H(220)...H(240)	302.3(47)	29.4(fixed)	—	0.8	29.4
<i>u</i> 963	H(260)...H(282)	302.4(47)	26.7(fixed)	—	0.6	26.7
<i>u</i> 994	H(55)...H(77)	302.4(48)	28.2(fixed)	—	1.0	28.2
<i>u</i> 1068	C(335)...H(367)	302.4(52)	32.9(fixed)	—	12.4	32.9
<i>u</i> 992	H(179)...H(199)	302.4(47)	28.3(fixed)	—	0.8	28.3
<i>u</i> 1007	H(219)...H(241)	302.4(48)	27.7(fixed)	—	1.0	27.7
<i>u</i> 941	H(99)...H(104)	302.5(47)	25.9(fixed)	—	0.6	25.9
<i>u</i> 901	H(58)...H(63)	302.6(47)	24.3(fixed)	—	0.3	24.3
<i>u</i> 969	H(56)...H(76)	302.6(47)	27.4(fixed)	—	0.8	27.4
<i>u</i> 947	H(343)...H(363)	302.6(47)	26.2(fixed)	—	0.6	26.2
<i>u</i> 892	H(139)...H(149)	302.6(47)	24.5(fixed)	—	0.4	24.5
<i>u</i> 900	H(304)...H(309)	302.6(47)	24.3(fixed)	—	0.3	24.3
<i>u</i> 906	H(98)...H(108)	302.6(47)	25.9(fixed)	—	0.6	25.9
<i>u</i> 995	H(303)...H(313)	302.6(47)	26.9(fixed)	—	0.9	26.9
<i>u</i> 1015	H(138)...H(158)	302.6(48)	31.0(fixed)	—	1.7	31.0
<i>u</i> 926	H(221)...H(231)	302.7(47)	24.6(fixed)	—	0.6	24.6
<i>u</i> 910	H(222)...H(227)	302.7(47)	23.9(fixed)	—	0.3	23.9
<i>u</i> 894	H(14)...H(36)	302.8(47)	24.9(fixed)	—	0.7	24.9
<i>u</i> 860	H(148)...H(150)	302.8(79)	35.4(fixed)	—	5.7	35.4
<i>u</i> 909	H(97)...H(117)	302.8(47)	25.2(fixed)	—	0.6	25.2
<i>u</i> 886	H(342)...H(364)	302.8(47)	24.4(fixed)	—	0.4	24.4

<i>u</i> 811	H(120)...H(123)	302.8(79)	33.3(fixed)	—	5.2	33.3
<i>u</i> 893	H(96)...H(118)	302.9(47)	24.1(fixed)	—	0.5	24.1
<i>u</i> 2654	Si(208)...H(240)	302.9(63)	38.0(fixed)	—	-1.9	38.0
<i>u</i> 902	H(263)...H(268)	302.9(47)	24.2(fixed)	—	0.3	24.2
<i>u</i> 903	H(140)...H(145)	302.9(47)	24.8(fixed)	—	0.8	24.8
<i>u</i> 1291	Si(291)...H(323)	302.9(58)	28.7(fixed)	—	3.9	28.7
<i>u</i> 896	H(261)...H(281)	302.9(47)	24.3(fixed)	—	0.4	24.3
<i>u</i> 826	H(25)...H(27)	303.0(79)	34.6(fixed)	—	5.7	34.6
<i>u</i> 911	H(262)...H(272)	303.0(47)	24.0(fixed)	—	0.4	24.0
<i>u</i> 4345	C(254)...H(279)	303.1(54)	20.5(fixed)	—	-2.0	20.5
<i>u</i> 790	H(271)...H(273)	303.2(79)	33.0(fixed)	—	5.5	33.0
<i>u</i> 815	H(265)...H(267)	303.2(79)	34.3(fixed)	—	5.8	34.3
<i>u</i> 3551	H(226)...H(236)	303.2(103)	49.2(fixed)	—	-9.6	49.2
<i>u</i> 791	H(224)...H(226)	303.2(79)	32.9(fixed)	—	5.5	32.9
<i>u</i> 973	C(131)...C(132)	303.4(23)	11.3(fixed)	—	-0.2	11.3
<i>u</i> 948	C(8)...C(9)	303.4(23)	11.2(fixed)	—	-0.2	11.2
<i>u</i> 932	C(133)...C(134)	303.4(23)	11.1(fixed)	—	-0.2	11.1
<i>u</i> 946	C(94)...C(95)	303.4(23)	11.1(fixed)	—	-0.2	11.1
<i>u</i> 968	C(49)...C(50)	303.4(23)	11.2(fixed)	—	-0.2	11.2
<i>u</i> 1171	C(88)...H(108)	303.4(82)	33.2(fixed)	—	8.7	33.2
<i>u</i> 960	C(293)...C(294)	303.4(23)	11.2(fixed)	—	-0.2	11.2
<i>u</i> 952	C(53)...C(54)	303.4(23)	11.2(fixed)	—	-0.2	11.2
<i>u</i> 957	C(170)...C(171)	303.4(23)	11.2(fixed)	—	-0.2	11.2
<i>u</i> 986	C(336)...C(337)	303.4(23)	11.2(fixed)	—	-0.2	11.2
<i>u</i> 972	C(135)...C(136)	303.4(23)	11.2(fixed)	—	-0.2	11.2
<i>u</i> 978	C(90)...C(91)	303.4(23)	11.1(fixed)	—	-0.2	11.1
<i>u</i> 961	C(47)...C(48)	303.4(23)	11.1(fixed)	—	-0.2	11.1
<i>u</i> 942	C(215)...C(216)	303.4(23)	11.1(fixed)	—	-0.2	11.1
<i>u</i> 950	C(256)...C(257)	303.4(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 945	C(92)...C(93)	303.4(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 929	C(211)...C(212)	303.4(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 934	C(258)...C(259)	303.4(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 921	C(217)...C(218)	303.4(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 916	C(129)...C(130)	303.4(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 931	C(51)...C(52)	303.4(23)	10.9(fixed)	—	-0.2	10.9
<i>u</i> 923	C(295)...C(296)	303.4(23)	10.9(fixed)	—	-0.2	10.9
<i>u</i> 935	C(6)...C(7)	303.4(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 907	C(213)...C(214)	303.4(23)	10.9(fixed)	—	-0.2	10.9
<i>u</i> 936	C(88)...C(89)	303.4(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 937	C(334)...C(335)	303.5(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 943	C(252)...C(253)	303.5(23)	11.0(fixed)	—	-0.2	11.0
<i>u</i> 915	C(254)...C(255)	303.5(23)	10.9(fixed)	—	-0.2	10.9
<i>u</i> 2658	C(259)...H(264)	303.5(50)	38.2(fixed)	—	-2.6	38.2
<i>u</i> 787	H(230)...H(232)	303.5(79)	34.0(fixed)	—	6.1	34.0

<i>u</i> 1741	C(48)...C(51)	303.8(78)	23.4(tied to <i>u</i> 1082)	—	1.9	21.5
<i>u</i> 823	H(306)...H(308)	303.8(79)	36.3(fixed)	—	6.9	36.3
<i>u</i> 4962	C(216)...H(223)	303.9(96)	24.0(fixed)	—	-1.5	24.0
<i>u</i> 4324	C(91)...H(114)	303.9(62)	24.7(fixed)	—	-1.1	24.7
<i>u</i> 887	H(66)...H(68)	303.9(79)	37.1(fixed)	—	7.2	37.1
<i>u</i> 789	H(142)...H(144)	304.0(79)	33.7(fixed)	—	6.5	33.7
<i>u</i> 4383	C(134)...H(140)	304.2(78)	15.2(fixed)	—	-2.4	15.2
<i>u</i> 881	H(79)...H(82)	304.4(79)	37.6(fixed)	—	7.8	37.6
<i>u</i> 897	H(189)...H(191)	304.4(79)	39.8(fixed)	—	8.4	39.8
<i>u</i> 835	H(60)...H(62)	304.4(79)	38.2(fixed)	—	8.0	38.2
<i>u</i> 828	H(71)...H(75)	304.5(79)	37.1(fixed)	—	7.8	37.1
<i>u</i> 4582	H(97)...H(100)	304.6(87)	28.3(fixed)	—	-0.2	28.3
<i>u</i> 813	H(312)...H(314)	304.7(79)	36.5(fixed)	—	7.8	36.5
<i>u</i> 3355	C(212)...H(244)	304.7(168)	35.2(fixed)	—	1.5	35.2
<i>u</i> 829	H(276)...H(280)	304.7(79)	42.2(fixed)	—	9.4	42.2
<i>u</i> 1095	C(47)...H(67)	304.8(88)	33.6(fixed)	—	11.3	33.6
<i>u</i> 3207	C(51)...H(77)	304.8(57)	33.2(fixed)	—	7.6	33.2
<i>u</i> 4036	H(260)...H(281)	304.8(72)	26.7(fixed)	—	-3.6	26.7
<i>u</i> 1281	Si(86)...H(118)	305.2(15)	29.3(fixed)	—	4.6	29.3
<i>u</i> 810	H(243)...H(246)	305.2(79)	37.0(fixed)	—	8.5	37.0
<i>u</i> 814	H(284)...H(287)	305.3(79)	36.6(fixed)	—	8.4	36.6
<i>u</i> 2927	H(220)...H(231)	305.5(69)	29.5(fixed)	—	3.0	29.5
<i>u</i> 3162	Si(207)...H(227)	305.6(40)	23.8(fixed)	—	-0.7	23.8
<i>u</i> 857	H(107)...H(109)	305.6(79)	38.2(fixed)	—	9.2	38.2
<i>u</i> 3321	C(133)...H(140)	305.9(80)	20.6(fixed)	—	-1.6	20.6
<i>u</i> 1345	Si(330)...H(350)	305.9(54)	29.7(fixed)	—	5.8	29.7
<i>u</i> 3253	H(139)...H(145)	305.9(97)	35.1(fixed)	—	1.9	35.1
<i>u</i> 1063	Si(4)...Si(5)	306.0(8)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1229	Si(289)...Si(292)	306.0(8)	10.4(tied to <i>u</i> 1082)	—	-0.1	9.6
<i>u</i> 1058	Si(251)...H(262)	306.1(20)	21.4(fixed)	—	0.6	21.4
<i>u</i> 816	H(112)...H(116)	306.2(79)	40.9(fixed)	—	10.5	40.9
<i>u</i> 3159	Si(43)...H(63)	306.2(53)	22.9(fixed)	—	-0.5	22.9
<i>u</i> 1082	Si(2)...Si(5)	306.3(8)	10.4(3)	—	-0.1	9.5
<i>u</i> 1151	C(334)...H(354)	306.4(84)	34.3(fixed)	—	4.8	34.3
<i>u</i> 1061	Si(166)...Si(168)	306.6(8)	10.7(tied to <i>u</i> 1082)	—	-0.1	9.9
<i>u</i> 1032	Si(2)...Si(3)	306.6(8)	10.7(tied to <i>u</i> 1082)	—	-0.1	9.8
<i>u</i> 1144	Si(166)...Si(169)	306.6(8)	10.1(tied to <i>u</i> 1082)	—	-0.1	9.3
<i>u</i> 927	Si(330)...Si(331)	306.6(8)	10.5(tied to <i>u</i> 1082)	—	-0.1	9.6
<i>u</i> 1099	Si(330)...Si(333)	306.7(8)	10.4(tied to <i>u</i> 1082)	—	-0.1	9.5
<i>u</i> 800	H(101)...H(103)	306.7(79)	38.2(fixed)	—	10.3	38.2
<i>u</i> 975	Si(84)...Si(85)	306.8(6)	10.6(tied to <i>u</i> 1082)	—	-0.1	9.7
<i>u</i> 1167	Si(332)...Si(333)	306.8(8)	9.9(tied to <i>u</i> 1082)	—	-0.1	9.1
<i>u</i> 3868	H(96)...H(113)	307.0(117)	33.5(fixed)	—	-7.5	33.5
<i>u</i> 831	H(153)...H(157)	307.0(79)	44.5(fixed)	—	12.3	44.5

<i>u</i> 2663	Si(126)...H(158)	307.1(70)	48.6(fixed)	—	-2.8	48.6
<i>u</i> 1021	Si(249)...Si(251)	307.3(6)	10.5(tied to <i>u</i> 1082)	—	-0.1	9.6
<i>u</i> 4377	C(88)...H(97)	307.4(51)	15.3(fixed)	—	-2.2	15.3
<i>u</i> 3184	C(215)...H(241)	307.7(9)	34.0(fixed)	—	6.9	34.0
<i>u</i> 1084	Si(289)...Si(291)	307.7(8)	10.7(tied to <i>u</i> 1082)	—	-0.1	9.9
<i>u</i> 832	H(19)...H(21)	307.8(79)	41.7(fixed)	—	12.3	41.7
<i>u</i> 2762	Si(249)...H(277)	307.9(43)	36.0(fixed)	—	-4.4	36.0
<i>u</i> 974	Si(125)...Si(126)	308.0(6)	10.6(tied to <i>u</i> 1082)	—	-0.1	9.7
<i>u</i> 2402	H(64)...H(71)	308.0(96)	45.2(fixed)	—	-0.8	45.2
<i>u</i> 2695	Si(44)...H(76)	308.6(59)	35.1(fixed)	—	-1.9	35.1
<i>u</i> 3649	H(62)...H(72)	308.8(133)	34.9(fixed)	—	-6.4	34.9
<i>u</i> 840	H(235)...H(239)	308.8(79)	43.4(fixed)	—	13.8	43.4
<i>u</i> 4878	H(61)...H(71)	309.4(95)	33.5(fixed)	—	-2.1	33.5
<i>u</i> 1030	Si(43)...Si(45)	309.5(6)	10.4(tied to <i>u</i> 1082)	—	-0.1	9.5
<i>u</i> 608	H(104)...H(115)	309.6(81)	48.0(fixed)	—	13.2	48.0
<i>u</i> 985	Si(249)...Si(250)	309.6(6)	10.3(tied to <i>u</i> 1082)	—	-0.1	9.5
<i>u</i> 1006	Si(290)...Si(291)	309.7(8)	10.2(tied to <i>u</i> 1082)	—	-0.1	9.3
<i>u</i> 1023	Si(84)...Si(86)	309.9(6)	10.6(tied to <i>u</i> 1082)	—	-0.1	9.8
<i>u</i> 1508	C(1)...H(22)	309.9(135)	26.5(fixed)	—	2.8	26.5
<i>u</i> 1644	C(212)...C(215)	310.1(101)	20.8(tied to <i>u</i> 1082)	—	2.9	19.1
<i>u</i> 1031	Si(43)...Si(46)	310.1(6)	10.4(tied to <i>u</i> 1082)	—	-0.1	9.5
<i>u</i> 2289	H(228)...H(235)	310.2(125)	45.5(fixed)	—	-5.0	45.5
<i>u</i> 1136	Si(209)...H(241)	310.4(94)	32.3(fixed)	—	8.3	32.3
<i>u</i> 537	H(63)...H(73)	310.5(158)	43.9(fixed)	—	11.1	43.9
<i>u</i> 2290	Si(87)...C(93)	310.6(51)	18.4(tied to <i>u</i> 1082)	—	-0.4	16.9
<i>u</i> 1037	Si(207)...Si(210)	310.6(6)	10.4(tied to <i>u</i> 1082)	—	-0.1	9.5
<i>u</i> 1035	Si(207)...Si(209)	310.6(6)	10.5(tied to <i>u</i> 1082)	—	-0.1	9.7
<i>u</i> 1128	H(24)...H(28)	310.7(92)	38.0(fixed)	—	4.1	38.0
<i>u</i> 1025	Si(289)...Si(290)	310.8(6)	10.2(tied to <i>u</i> 1082)	—	-0.1	9.4
<i>u</i> 1043	H(229)...H(233)	311.1(92)	37.3(fixed)	—	4.3	37.3
<i>u</i> 1074	H(143)...H(146)	311.1(92)	37.6(fixed)	—	4.4	37.6
<i>u</i> 1198	H(147)...H(151)	311.1(92)	37.6(fixed)	—	4.5	37.6
<i>u</i> 1135	H(119)...H(121)	311.2(91)	35.4(fixed)	—	4.1	35.4
<i>u</i> 1096	H(225)...H(228)	311.3(91)	35.3(fixed)	—	4.1	35.3
<i>u</i> 5139	H(269)...H(277)	311.3(112)	39.3(fixed)	—	1.2	39.3
<i>u</i> 1102	H(266)...H(269)	311.3(92)	37.0(fixed)	—	4.5	37.0
<i>u</i> 1047	H(270)...H(274)	311.4(91)	35.4(fixed)	—	4.2	35.4
<i>u</i> 1547	C(173)...H(195)	311.5(129)	47.3(fixed)	—	5.9	47.3
<i>u</i> 1168	H(307)...H(310)	311.5(92)	39.7(fixed)	—	5.4	39.7
<i>u</i> 1585	C(1)...H(20)	311.8(202)	25.4(fixed)	—	1.1	25.4
<i>u</i> 4723	H(141)...H(159)	311.8(155)	78.6(fixed)	—	2.2	78.6
<i>u</i> 917	H(97)...H(110)	311.9(59)	52.6(fixed)	—	6.5	52.6
<i>u</i> 1079	H(65)...H(69)	312.0(92)	40.5(fixed)	—	6.1	40.5
<i>u</i> 983	H(311)...H(315)	312.1(92)	40.4(fixed)	—	6.1	40.4



<i>u2737</i>	Si(84)...H(113)	312.1(45)	37.2(fixed)	—	-4.0	37.2
<i>u1085</i>	Si(84)...Si(87)	312.1(6)	10.5(tied to <i>u1082</i> )	—	-0.1	9.6
<i>u1062</i>	H(283)...H(285)	312.1(92)	41.5(fixed)	—	6.5	41.5
<i>u1004</i>	H(78)...H(80)	312.2(92)	41.9(fixed)	—	6.6	41.9
<i>u1020</i>	H(72)...H(74)	312.2(92)	40.9(fixed)	—	6.4	40.9
<i>u1159</i>	H(61)...H(64)	312.2(92)	41.6(fixed)	—	6.6	41.6
<i>u1498</i>	Si(292)...H(326)	312.3(46)	36.1(fixed)	—	5.3	36.1
<i>u980</i>	H(242)...H(244)	312.3(92)	41.7(fixed)	—	6.7	41.7
<i>u1041</i>	Si(43)...Si(44)	312.3(6)	10.6(tied to <i>u1082</i> )	—	-0.1	9.7
<i>u1238</i>	H(106)...H(110)	312.4(92)	43.2(fixed)	—	7.1	43.2
<i>u4507</i>	C(95)...H(104)	312.4(164)	24.9(fixed)	—	-2.6	24.9
<i>u1111</i>	H(102)...H(105)	312.4(92)	44.6(fixed)	—	7.6	44.6
<i>u953</i>	C(295)...H(322)	312.4(121)	29.9(fixed)	—	11.1	29.9
<i>u1066</i>	Si(125)...Si(127)	312.5(6)	11.0(tied to <i>u1082</i> )	—	-0.1	10.1
<i>u2060</i>	H(22)...H(26)	312.8(268)	53.7(fixed)	—	-2.6	53.7
<i>u1199</i>	C(7)...H(26)	313.0(122)	34.1(fixed)	—	6.6	34.1
<i>u1116</i>	Si(208)...Si(210)	313.0(6)	10.7(tied to <i>u1082</i> )	—	-0.1	9.8
<i>u1059</i>	Si(330)...Si(332)	313.0(6)	10.7(tied to <i>u1082</i> )	—	-0.1	9.9
<i>u1075</i>	Si(208)...Si(209)	313.1(6)	10.2(tied to <i>u1082</i> )	—	-0.1	9.4
<i>u889</i>	H(161)...H(164)	313.2(80)	57.1(fixed)	—	22.8	57.1
<i>u1018</i>	Si(166)...Si(167)	313.2(6)	10.8(tied to <i>u1082</i> )	—	-0.1	9.9
<i>u1175</i>	Si(45)...H(77)	313.3(84)	31.6(fixed)	—	9.0	31.6
<i>u2565</i>	H(55)...H(56)	313.5(88)	25.8(fixed)	—	-1.4	25.8
<i>u1110</i>	H(113)...H(115)	313.5(92)	44.7(fixed)	—	8.8	44.7
<i>u775</i>	C(9)...H(32)	313.6(512)	32.6(fixed)	—	17.8	32.6
<i>u1067</i>	Si(125)...Si(128)	313.6(6)	10.3(tied to <i>u1082</i> )	—	-0.1	9.5
<i>u3587</i>	H(113)...H(120)	313.7(68)	46.4(fixed)	—	-9.1	46.4
<i>u1094</i>	H(277)...H(279)	313.8(92)	43.5(fixed)	—	8.7	43.5
<i>u1077</i>	Si(2)...Si(4)	313.8(6)	10.2(tied to <i>u1082</i> )	—	-0.1	9.4
<i>u2153</i>	Si(128)...C(133)	313.9(59)	16.8(tied to <i>u1082</i> )	—	-0.1	15.4
<i>u3262</i>	Si(84)...H(104)	313.9(49)	21.0(fixed)	—	0.1	21.0
<i>u1011</i>	H(201)...H(203)	313.9(92)	40.5(fixed)	—	8.0	40.5
<i>u1093</i>	Si(85)...H(96)	314.1(60)	23.7(fixed)	—	0.9	23.7
<i>u2126</i>	H(20)...H(39)	314.7(461)	45.9(fixed)	—	-2.1	45.9
<i>u2219</i>	Si(46)...C(51)	314.7(48)	16.5(tied to <i>u1082</i> )	—	-0.2	15.1
<i>u1401</i>	C(134)...H(151)	314.7(78)	39.2(fixed)	—	5.2	39.2
<i>u4482</i>	C(54)...H(63)	314.8(136)	26.8(fixed)	—	-3.0	26.8
<i>u1302</i>	C(6)...H(26)	315.0(123)	36.5(fixed)	—	7.6	36.5
<i>u988</i>	H(342)...H(344)	315.1(38)	38.7(fixed)	—	0.5	38.7
<i>u1462</i>	C(296)...H(310)	315.1(82)	38.9(fixed)	—	3.6	38.9
<i>u1289</i>	H(96)...H(98)	315.1(114)	41.9(fixed)	—	0.3	41.9
<i>u1476</i>	Si(332)...H(348)	315.2(43)	31.3(fixed)	—	3.8	31.3
<i>u3242</i>	Si(166)...H(190)	315.3(58)	21.8(fixed)	—	0.5	21.8
<i>u5217</i>	H(268)...H(277)	315.3(89)	34.1(fixed)	—	-3.0	34.1

<i>u</i> 582	H(18)...H(40)	315.4(742)	52.0(fixed)	—	18.8	52.0
<i>u</i> 1038	H(236)...H(238)	315.6(92)	48.3(fixed)	—	11.8	48.3
<i>u</i> 1046	H(342)...H(343)	315.6(27)	32.5(fixed)	—	1.7	32.5
<i>u</i> 1118	Si(44)...Si(46)	315.6(6)	10.6(tied to <i>u</i> 1082)	—	-0.1	9.8
<i>u</i> 1009	H(154)...H(156)	315.6(92)	45.0(fixed)	—	10.9	45.0
<i>u</i> 1103	Si(248)...Si(249)	315.8(6)	10.5(tied to <i>u</i> 1082)	—	-0.1	9.7
<i>u</i> 2979	C(256)...H(262)	315.8(43)	22.2(fixed)	—	-1.4	22.2
<i>u</i> 1157	Si(44)...Si(45)	316.0(6)	10.0(tied to <i>u</i> 1082)	—	-0.1	9.2
<i>u</i> 1012	Si(330)...H(344)	316.0(16)	22.1(fixed)	—	0.6	22.1
<i>u</i> 1719	Si(166)...H(179)	316.0(20)	21.8(fixed)	—	-0.2	21.8
<i>u</i> 1053	Si(126)...Si(128)	316.0(6)	10.9(tied to <i>u</i> 1082)	—	-0.1	10.0
<i>u</i> 1121	Si(207)...Si(208)	316.2(6)	10.6(tied to <i>u</i> 1082)	—	-0.1	9.7
<i>u</i> 3144	C(257)...H(272)	316.3(109)	29.5(fixed)	—	2.8	29.5
<i>u</i> 2610	H(178)...H(179)	316.3(65)	27.6(fixed)	—	-1.7	27.6
<i>u</i> 1092	Si(290)...H(322)	316.3(49)	30.7(fixed)	—	7.2	30.7
<i>u</i> 989	H(343)...H(357)	316.4(84)	56.7(fixed)	—	5.0	56.7
<i>u</i> 3064	H(263)...H(285)	316.4(83)	34.7(fixed)	—	2.9	34.7
<i>u</i> 2137	Si(210)...C(215)	316.4(53)	15.6(tied to <i>u</i> 1082)	—	-0.1	14.4
<i>u</i> 1129	Si(248)...Si(250)	316.5(6)	10.6(tied to <i>u</i> 1082)	—	-0.1	9.8
<i>u</i> 1170	Si(126)...Si(127)	316.7(6)	10.0(tied to <i>u</i> 1082)	—	-0.1	9.2
<i>u</i> 454	H(143)...H(155)	316.7(110)	43.7(fixed)	—	17.2	43.7
<i>u</i> 1328	Si(2)...H(17)	316.8(14)	21.5(fixed)	—	0.4	21.5
<i>u</i> 421	H(22)...H(35)	316.9(1182)	43.4(fixed)	—	34.6	43.4
<i>u</i> 1424	C(335)...H(359)	317.0(76)	40.3(fixed)	—	3.9	40.3
<i>u</i> 1308	Si(332)...H(364)	317.1(55)	29.3(fixed)	—	3.9	29.3
<i>u</i> 2827	H(221)...H(238)	317.1(90)	31.8(fixed)	—	5.5	31.8
<i>u</i> 1717	Si(43)...H(56)	317.2(14)	20.3(fixed)	—	-0.3	20.3
<i>u</i> 1204	C(165)...C(170)	317.2(7)	11.2(tied to <i>u</i> 1082)	—	-0.1	10.3
<i>u</i> 1222	C(124)...C(130)	317.3(7)	11.5(tied to <i>u</i> 1082)	—	-0.1	10.5
<i>u</i> 1215	C(124)...C(133)	317.3(7)	11.3(tied to <i>u</i> 1082)	—	-0.1	10.4
<i>u</i> 1249	C(124)...C(129)	317.3(7)	11.2(tied to <i>u</i> 1082)	—	-0.1	10.3
<i>u</i> 1258	C(124)...C(131)	317.3(7)	11.3(tied to <i>u</i> 1082)	—	-0.1	10.4
<i>u</i> 1242	C(206)...C(215)	317.3(7)	11.3(tied to <i>u</i> 1082)	—	-0.1	10.4
<i>u</i> 1264	C(124)...C(135)	317.3(7)	11.3(tied to <i>u</i> 1082)	—	-0.1	10.4
<i>u</i> 1196	C(124)...C(132)	317.3(7)	11.2(tied to <i>u</i> 1082)	—	-0.1	10.3
<i>u</i> 1203	C(206)...C(213)	317.3(7)	11.2(tied to <i>u</i> 1082)	—	-0.1	10.3
<i>u</i> 1212	C(1)...C(8)	317.3(7)	11.2(tied to <i>u</i> 1082)	—	-0.1	10.3
<i>u</i> 1260	C(206)...C(214)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1220	C(42)...C(49)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1236	C(165)...C(171)	317.3(7)	11.2(tied to <i>u</i> 1082)	—	-0.1	10.3
<i>u</i> 1176	C(42)...C(50)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1246	C(206)...C(218)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1239	C(247)...C(256)	317.3(7)	11.2(tied to <i>u</i> 1082)	—	-0.1	10.3
<i>u</i> 1237	C(206)...C(211)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2

<i>u</i> 1216	C(329)...C(335)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1262	C(247)...C(255)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1206	C(247)...C(258)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1224	C(124)...C(134)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1241	C(42)...C(51)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1251	C(83)...C(90)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1200	C(288)...C(293)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1207	C(42)...C(47)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1243	C(83)...C(93)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1276	C(329)...C(336)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1240	C(1)...C(7)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1263	C(288)...C(296)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1223	C(247)...C(252)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1232	C(42)...C(54)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1248	C(206)...C(216)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 4904	C(52)...H(59)	317.3(96)	26.5(fixed)	—	-0.1	26.5
<i>u</i> 1181	C(206)...C(217)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1256	C(288)...C(294)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1201	C(247)...C(259)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1266	C(83)...C(94)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1230	C(83)...C(92)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1277	C(206)...C(212)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1217	C(83)...C(89)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1259	C(247)...C(253)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1257	C(42)...C(48)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1205	C(329)...C(334)	317.3(7)	10.9(tied to <i>u</i> 1082)	—	-0.1	10.0
<i>u</i> 1193	C(124)...C(136)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1190	C(329)...C(337)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1192	C(42)...C(53)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1185	C(288)...C(295)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1235	C(1)...C(9)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1247	C(83)...C(95)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1219	C(1)...C(6)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1270	C(247)...C(257)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1225	C(42)...C(52)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1179	C(83)...C(91)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1272	C(247)...C(254)	317.3(7)	11.1(tied to <i>u</i> 1082)	—	-0.1	10.2
<i>u</i> 1218	C(83)...C(88)	317.3(7)	11.0(tied to <i>u</i> 1082)	—	-0.1	10.1
<i>u</i> 1130	Si(85)...Si(87)	317.4(6)	10.6(tied to <i>u</i> 1082)	—	-0.1	9.8
<i>u</i> 1253	C(8)...H(20)	317.5(98)	37.6(fixed)	—	12.0	37.6
<i>u</i> 1284	Si(128)...H(149)	317.5(54)	29.5(fixed)	—	4.5	29.5
<i>u</i> 1123	Si(250)...H(272)	317.7(34)	27.5(fixed)	—	4.0	27.5
<i>u</i> 4504	C(53)...H(64)	317.7(140)	24.9(fixed)	—	-3.7	24.9
<i>u</i> 1373	C(52)...H(69)	317.8(68)	37.9(fixed)	—	5.1	37.9

<i>u</i> 1078	Si(290)...H(301)	317.8(19)	21.4(fixed)	—	0.6	21.4
<i>u</i> 2797	Si(248)...H(281)	318.0(50)	26.0(fixed)	—	-1.5	26.0
<i>u</i> 3498	C(89)...H(121)	318.0(196)	35.8(fixed)	—	1.7	35.8
<i>u</i> 2287	H(104)...H(117)	318.1(174)	47.3(fixed)	—	-0.5	47.3
<i>u</i> 1292	C(259)...H(274)	318.1(73)	34.9(fixed)	—	4.2	34.9
<i>u</i> 3068	H(138)...H(151)	318.2(101)	33.2(fixed)	—	2.3	33.2
<i>u</i> 1076	Si(125)...H(139)	318.2(17)	23.0(fixed)	—	0.8	23.0
<i>u</i> 2645	H(137)...H(138)	318.3(28)	26.7(fixed)	—	-1.6	26.7
<i>u</i> 1297	C(172)...H(191)	318.3(39)	26.1(fixed)	—	0.3	26.1
<i>u</i> 1252	C(293)...H(318)	318.3(71)	35.7(fixed)	—	4.3	35.7
<i>u</i> 1296	C(8)...H(27)	318.4(39)	24.6(fixed)	—	0.1	24.6
<i>u</i> 1287	C(53)...H(82)	318.5(39)	24.6(fixed)	—	0.2	24.6
<i>u</i> 1233	C(94)...H(123)	318.6(39)	24.2(fixed)	—	0.2	24.2
<i>u</i> 1189	C(52)...H(71)	318.6(39)	25.4(fixed)	—	0.5	25.4
<i>u</i> 1160	C(295)...H(314)	318.6(39)	24.8(fixed)	—	0.4	24.8
<i>u</i> 1098	Si(85)...Si(86)	318.6(6)	10.4(tied to <i>u</i> 1082)	—	-0.1	9.5
<i>u</i> 1290	C(131)...H(150)	318.6(39)	25.5(fixed)	—	0.5	25.5
<i>u</i> 1295	C(49)...H(68)	318.7(39)	25.1(fixed)	—	0.5	25.1
<i>u</i> 1133	C(213)...H(232)	318.7(39)	24.3(fixed)	—	0.4	24.3
<i>u</i> 1531	Si(166)...H(184)	318.8(41)	33.0(fixed)	—	3.6	33.0
<i>u</i> 1255	C(257)...H(276)	318.8(39)	32.5(fixed)	—	1.9	32.5
<i>u</i> 1155	C(130)...H(142)	318.8(39)	23.8(fixed)	—	0.4	23.8
<i>u</i> 1140	C(217)...H(246)	318.8(39)	24.6(fixed)	—	0.5	24.6
<i>u</i> 1180	C(335)...H(347)	318.8(39)	25.2(fixed)	—	0.6	25.2
<i>u</i> 1126	C(254)...H(273)	318.8(39)	23.8(fixed)	—	0.4	23.8
<i>u</i> 1187	C(253)...H(265)	318.9(39)	24.8(fixed)	—	0.7	24.8
<i>u</i> 1113	C(212)...H(224)	319.0(39)	23.6(fixed)	—	0.5	23.6
<i>u</i> 3427	Si(251)...H(278)	319.0(41)	23.1(fixed)	—	-0.4	23.1
<i>u</i> 3237	C(93)...H(118)	319.0(215)	31.4(fixed)	—	3.1	31.4
<i>u</i> 2249	H(140)...H(147)	319.1(77)	41.0(fixed)	—	-2.2	41.0
<i>u</i> 1301	C(336)...H(355)	319.1(39)	28.1(fixed)	—	1.4	28.1
<i>u</i> 1137	C(134)...H(153)	319.1(39)	26.6(fixed)	—	1.1	26.6
<i>u</i> 1209	C(299)...H(328)	319.2(39)	26.5(fixed)	—	1.2	26.5
<i>u</i> 1323	Si(2)...H(16)	319.2(44)	22.9(fixed)	—	0.5	22.9
<i>u</i> 1231	C(48)...H(60)	319.2(39)	28.5(fixed)	—	1.6	28.5
<i>u</i> 1202	C(93)...H(112)	319.2(39)	31.1(fixed)	—	2.1	31.1
<i>u</i> 1138	C(258)...H(287)	319.2(39)	25.9(fixed)	—	1.2	25.9
<i>u</i> 4655	C(135)...H(141)	319.2(83)	25.8(fixed)	—	-3.3	25.8
<i>u</i> 1234	C(135)...H(164)	319.3(39)	26.6(fixed)	—	1.4	26.6
<i>u</i> 1280	C(90)...H(109)	319.4(39)	27.8(fixed)	—	1.6	27.8
<i>u</i> 1148	C(216)...H(235)	319.4(39)	31.8(fixed)	—	2.4	31.8
<i>u</i> 1125	C(7)...H(19)	319.4(39)	27.4(fixed)	—	1.6	27.4
<i>u</i> 3276	Si(249)...H(266)	319.7(39)	20.9(fixed)	—	-0.4	20.9
<i>u</i> 1124	C(89)...H(101)	319.8(39)	28.3(fixed)	—	2.1	28.3

<i>u</i> 1172	Si(84)...H(98)	319.8(18)	22.0(fixed)	—	0.4	22.0
<i>u</i> 1516	Si(4)...H(28)	320.1(69)	34.6(fixed)	—	3.5	34.6
<i>u</i> 1197	Si(248)...Si(251)	320.1(6)	10.1(tied to <i>u</i> 1082)	—	-0.1	9.3
<i>u</i> 1362	Si(250)...H(282)	320.2(61)	30.4(fixed)	—	6.3	30.4
<i>u</i> 4204	C(133)...H(160)	320.4(130)	79.1(fixed)	—	-5.3	79.1
<i>u</i> 1415	Si(333)...H(367)	320.5(38)	36.7(fixed)	—	6.2	36.7
<i>u</i> 3986	C(215)...H(242)	320.5(8)	46.6(fixed)	—	-1.6	46.6
<i>u</i> 1690	Si(207)...H(220)	320.6(20)	20.0(fixed)	—	-0.2	20.0
<i>u</i> 3224	Si(126)...H(145)	321.3(44)	22.7(fixed)	—	-0.2	22.7
<i>u</i> 1966	Si(127)...H(141)	321.4(61)	32.8(fixed)	—	0.3	32.8
<i>u</i> 1072	H(160)...H(162)	321.4(94)	61.9(fixed)	—	22.5	61.9
<i>u</i> 1410	Si(4)...H(36)	321.5(25)	28.7(fixed)	—	5.1	28.7
<i>u</i> 1360	Si(210)...H(221)	321.5(24)	22.1(fixed)	—	0.4	22.1
<i>u</i> 3095	H(56)...H(69)	321.6(62)	33.4(fixed)	—	1.7	33.4
<i>u</i> 3395	H(230)...H(240)	321.7(146)	53.6(fixed)	—	-8.2	53.6
<i>u</i> 1285	C(136)...H(161)	322.0(50)	48.0(fixed)	—	5.6	48.0
<i>u</i> 1162	C(133)...H(157)	322.2(49)	34.1(fixed)	—	2.3	34.1
<i>u</i> 1355	Si(209)...H(231)	322.3(61)	28.0(fixed)	—	4.6	28.0
<i>u</i> 1423	C(9)...H(24)	322.4(54)	26.0(fixed)	—	-0.3	26.0
<i>u</i> 1389	C(129)...H(146)	322.5(54)	26.2(fixed)	—	-0.1	26.2
<i>u</i> 1117	C(293)...H(308)	322.5(49)	23.4(fixed)	—	0.7	23.4
<i>u</i> 1119	C(47)...H(62)	322.5(49)	23.3(fixed)	—	0.7	23.3
<i>u</i> 1311	C(218)...H(242)	322.6(54)	30.5(fixed)	—	0.7	30.5
<i>u</i> 1320	C(296)...H(311)	322.6(54)	29.4(fixed)	—	0.5	29.4
<i>u</i> 1368	C(214)...H(229)	322.6(54)	25.6(fixed)	—	-0.2	25.6
<i>u</i> 1055	C(211)...H(226)	322.6(49)	23.1(fixed)	—	0.7	23.1
<i>u</i> 1174	Si(126)...H(137)	322.6(13)	22.2(fixed)	—	0.4	22.2
<i>u</i> 1146	C(337)...H(353)	322.6(49)	23.5(fixed)	—	0.8	23.5
<i>u</i> 1177	C(6)...H(21)	322.6(49)	30.6(fixed)	—	2.0	30.6
<i>u</i> 1337	C(51)...H(74)	322.6(54)	29.4(fixed)	—	0.5	29.4
<i>u</i> 1131	C(132)...H(148)	322.6(49)	23.4(fixed)	—	0.8	23.4
<i>u</i> 1211	C(170)...H(185)	322.6(49)	28.7(fixed)	—	1.6	28.7
<i>u</i> 2378	H(99)...H(122)	322.6(83)	41.8(fixed)	—	-2.2	41.8
<i>u</i> 1081	C(256)...H(280)	322.6(49)	23.2(fixed)	—	0.8	23.2
<i>u</i> 1339	C(54)...H(78)	322.6(54)	30.6(fixed)	—	0.8	30.6
<i>u</i> 1083	C(252)...H(267)	322.7(49)	23.0(fixed)	—	0.7	23.0
<i>u</i> 1392	C(92)...H(115)	322.7(54)	26.2(fixed)	—	0.1	26.2
<i>u</i> 1352	C(334)...H(351)	322.7(54)	27.5(fixed)	—	0.3	27.5
<i>u</i> 1416	C(91)...H(106)	322.7(54)	26.7(fixed)	—	0.2	26.7
<i>u</i> 1033	C(255)...H(271)	322.7(49)	22.8(fixed)	—	0.8	22.8
<i>u</i> 1359	C(88)...H(105)	322.7(54)	27.0(fixed)	—	0.2	27.0
<i>u</i> 2966	Si(209)...C(211)	322.7(46)	12.0(tied to <i>u</i> 1082)	—	-1.3	11.0
<i>u</i> 1336	C(259)...H(283)	322.7(54)	28.0(fixed)	—	0.4	28.0
<i>u</i> 1173	C(215)...H(239)	322.8(49)	28.7(fixed)	—	1.8	28.7

<i>u</i> 1374	C(50)...H(65)	322.8(54)	28.5(fixed)	—	0.5	28.5
<i>u</i> 1406	C(95)...H(119)	322.8(54)	24.3(fixed)	—	-0.2	24.3
<i>u</i> 1182	C(50)...H(66)	322.8(49)	26.2(fixed)	—	1.4	26.2
<i>u</i> 1049	C(95)...H(120)	322.8(49)	22.8(fixed)	—	0.9	22.8
<i>u</i> 1316	Si(289)...H(302)	322.8(23)	21.3(fixed)	—	0.3	21.3
<i>u</i> 1114	C(259)...H(284)	322.8(49)	25.5(fixed)	—	1.3	25.5
<i>u</i> 1419	C(132)...H(147)	322.8(54)	24.6(fixed)	—	-0.1	24.6
<i>u</i> 1267	H(301)...H(302)	322.8(43)	32.4(fixed)	—	1.6	32.4
<i>u</i> 1312	C(215)...H(238)	322.9(54)	31.5(fixed)	—	1.2	31.5
<i>u</i> 3232	C(133)...H(159)	322.9(66)	54.5(fixed)	—	29.2	54.5
<i>u</i> 1090	C(88)...H(103)	322.9(49)	24.5(fixed)	—	1.2	24.5
<i>u</i> 1396	C(256)...H(279)	322.9(54)	24.3(fixed)	—	0.0	24.3
<i>u</i> 1152	C(91)...H(107)	322.9(49)	24.5(fixed)	—	1.2	24.5
<i>u</i> 1399	C(293)...H(310)	322.9(54)	24.3(fixed)	—	0.0	24.3
<i>u</i> 1662	C(294)...H(326)	322.9(91)	54.1(fixed)	—	4.4	54.1
<i>u</i> 1430	C(337)...H(352)	322.9(54)	24.1(fixed)	—	0.0	24.1
<i>u</i> 1379	C(252)...H(269)	322.9(54)	24.3(fixed)	—	0.0	24.3
<i>u</i> 1327	C(136)...H(160)	322.9(55)	51.8(fixed)	—	6.4	51.8
<i>u</i> 1100	C(334)...H(349)	322.9(49)	24.9(fixed)	—	1.3	24.9
<i>u</i> 1073	C(92)...H(116)	322.9(49)	24.1(fixed)	—	1.2	24.1
<i>u</i> 1354	C(255)...H(270)	322.9(54)	24.1(fixed)	—	0.0	24.1
<i>u</i> 1400	C(47)...H(64)	323.0(54)	24.2(fixed)	—	0.0	24.2
<i>u</i> 2904	H(221)...H(222)	323.0(65)	22.6(fixed)	—	-2.3	22.6
<i>u</i> 1367	C(211)...H(228)	323.0(54)	23.9(fixed)	—	0.0	23.9
<i>u</i> 1158	C(54)...H(79)	323.0(49)	27.5(fixed)	—	1.8	27.5
<i>u</i> 1101	C(51)...H(75)	323.0(49)	26.2(fixed)	—	1.6	26.2
<i>u</i> 1001	C(214)...H(230)	323.1(49)	23.1(fixed)	—	1.2	23.1
<i>u</i> 5371	H(225)...H(239)	323.1(134)	26.9(fixed)	—	-7.2	26.9
<i>u</i> 1089	C(218)...H(243)	323.1(49)	27.2(fixed)	—	1.9	27.2
<i>u</i> 1071	C(296)...H(312)	323.1(49)	26.2(fixed)	—	1.7	26.2
<i>u</i> 1039	C(9)...H(25)	323.2(49)	23.1(fixed)	—	1.3	23.1
<i>u</i> 1003	C(129)...H(144)	323.2(49)	23.5(fixed)	—	1.4	23.5
<i>u</i> 1513	H(14)...H(16)	323.2(159)	41.4(fixed)	—	-0.1	41.4
<i>u</i> 1334	C(177)...H(201)	323.3(54)	29.7(fixed)	—	1.2	29.7
<i>u</i> 1226	Si(330)...H(343)	323.3(16)	21.2(fixed)	—	0.4	21.2
<i>u</i> 1390	Si(46)...H(67)	323.3(54)	31.2(fixed)	—	7.4	31.2
<i>u</i> 1300	C(133)...H(156)	323.4(54)	33.4(fixed)	—	2.0	33.4
<i>u</i> 1776	Si(125)...H(138)	323.4(26)	20.8(fixed)	—	-0.3	20.8
<i>u</i> 3625	H(261)...H(283)	323.5(65)	39.0(fixed)	—	-1.9	39.0
<i>u</i> 1273	C(218)...H(233)	323.9(213)	34.5(fixed)	—	5.5	34.5
<i>u</i> 1405	Si(87)...H(108)	323.9(58)	29.6(fixed)	—	5.4	29.6
<i>u</i> 4772	C(211)...C(216)	324.0(73)	13.5(tied to <i>u</i> 1082)	—	-2.2	12.4
<i>u</i> 1070	C(91)...H(96)	324.3(49)	24.9(fixed)	—	4.3	24.9
<i>u</i> 2844	H(57)...H(58)	324.5(40)	26.9(fixed)	—	-1.4	26.9

<i>u</i> 1051	C(136)...H(139)	324.5(25)	24.5(fixed)	—	4.2	24.5
<i>u</i> 1164	H(302)...H(311)	324.6(84)	55.0(fixed)	—	2.3	55.0
<i>u</i> 1268	H(137)...H(139)	324.6(30)	41.9(fixed)	—	0.2	41.9
<i>u</i> 1394	C(253)...H(262)	324.7(47)	29.5(fixed)	—	1.0	29.5
<i>u</i> 4592	H(64)...H(77)	324.7(144)	46.9(fixed)	—	-2.2	46.9
<i>u</i> 1684	H(112)...H(118)	324.9(186)	57.5(fixed)	—	3.7	57.5
<i>u</i> 3315	Si(125)...H(143)	325.0(45)	23.4(fixed)	—	-1.3	23.4
<i>u</i> 4511	C(217)...H(228)	325.2(226)	25.0(fixed)	—	-4.0	25.0
<i>u</i> 3422	C(170)...H(180)	325.4(39)	24.1(fixed)	—	-1.5	24.1
<i>u</i> 3730	C(211)...C(215)	325.8(84)	23.0(tied to <i>u</i> 1082)	—	-1.4	21.2
<i>u</i> 1340	C(89)...H(102)	326.0(47)	32.4(fixed)	—	0.9	32.4
<i>u</i> 3840	C(255)...H(266)	326.1(57)	28.2(fixed)	—	1.7	28.2
<i>u</i> 3035	C(216)...H(221)	326.2(54)	22.7(fixed)	—	-1.5	22.7
<i>u</i> 3476	C(48)...H(80)	326.3(160)	35.6(fixed)	—	1.4	35.6
<i>u</i> 1335	C(216)...H(236)	326.4(47)	33.9(fixed)	—	1.6	33.9
<i>u</i> 1325	C(258)...H(285)	326.4(47)	28.1(fixed)	—	0.5	28.1
<i>u</i> 1348	C(294)...H(307)	326.4(47)	28.9(fixed)	—	0.7	28.9
<i>u</i> 1372	C(90)...H(110)	326.5(47)	30.6(fixed)	—	1.1	30.6
<i>u</i> 1341	C(48)...H(61)	326.5(47)	31.2(fixed)	—	1.2	31.2
<i>u</i> 1318	C(134)...H(154)	326.5(47)	28.1(fixed)	—	0.6	28.1
<i>u</i> 1319	C(212)...H(225)	326.5(47)	25.0(fixed)	—	0.2	25.0
<i>u</i> 1376	C(135)...H(162)	326.6(47)	28.7(fixed)	—	0.8	28.7
<i>u</i> 1313	C(93)...H(113)	326.6(47)	33.7(fixed)	—	1.8	33.7
<i>u</i> 1385	Si(289)...H(315)	326.6(48)	31.9(fixed)	—	3.4	31.9
<i>u</i> 1315	C(253)...H(266)	326.6(47)	26.0(fixed)	—	0.4	26.0
<i>u</i> 1274	C(217)...H(244)	326.7(47)	25.6(fixed)	—	0.4	25.6
<i>u</i> 1346	C(131)...H(151)	326.7(47)	26.1(fixed)	—	0.5	26.1
<i>u</i> 1375	C(336)...H(356)	326.7(47)	29.8(fixed)	—	1.1	29.8
<i>u</i> 1310	C(335)...H(348)	326.7(47)	26.2(fixed)	—	0.5	26.2
<i>u</i> 2603	H(219)...H(220)	326.7(115)	25.3(fixed)	—	-1.4	25.3
<i>u</i> 1275	C(254)...H(274)	326.7(47)	24.6(fixed)	—	0.3	24.6
<i>u</i> 1330	C(49)...H(69)	326.8(47)	25.7(fixed)	—	0.5	25.7
<i>u</i> 1245	C(130)...H(143)	326.8(47)	24.8(fixed)	—	0.4	24.8
<i>u</i> 1213	C(213)...H(233)	326.8(47)	25.0(fixed)	—	0.4	25.0
<i>u</i> 1305	C(94)...H(121)	326.8(47)	24.4(fixed)	—	0.4	24.4
<i>u</i> 1250	C(295)...H(315)	326.8(47)	24.8(fixed)	—	0.4	24.8
<i>u</i> 1283	C(52)...H(72)	326.8(47)	25.4(fixed)	—	0.5	25.4
<i>u</i> 1286	C(53)...H(80)	326.9(47)	24.9(fixed)	—	0.5	24.9
<i>u</i> 1306	C(257)...H(277)	326.9(47)	33.7(fixed)	—	2.1	33.7
<i>u</i> 2980	Si(45)...C(47)	326.9(40)	11.6(tied to <i>u</i> 1082)	—	-1.1	10.6
<i>u</i> 1265	C(8)...H(28)	326.9(47)	24.7(fixed)	—	0.5	24.7
<i>u</i> 1161	C(130)...H(162)	327.0(68)	35.1(fixed)	—	11.6	35.1
<i>u</i> 1309	C(171)...H(184)	327.0(47)	25.0(fixed)	—	0.6	25.0
<i>u</i> 3845	C(47)...C(51)	327.1(74)	20.3(tied to <i>u</i> 1082)	—	-1.2	18.6

<i>u</i> 2072	Si(86)...H(105)	327.3(53)	36.3(fixed)	—	-0.4	36.3
<i>u</i> 2588	Si(208)...H(222)	327.4(28)	13.7(fixed)	—	-1.6	13.7
<i>u</i> 2252	H(143)...H(154)	327.4(150)	43.9(fixed)	—	-2.5	43.9
<i>u</i> 2372	C(9)...H(31)	327.6(711)	46.0(fixed)	—	-2.0	46.0
<i>u</i> 1303	C(9)...H(14)	328.1(65)	27.5(fixed)	—	3.9	27.5
<i>u</i> 1768	C(340)...H(351)	328.2(86)	51.8(fixed)	—	2.4	51.8
<i>u</i> 1418	C(8)...H(15)	328.2(90)	31.2(fixed)	—	2.6	31.2
<i>u</i> 1646	C(299)...H(305)	328.2(87)	50.5(fixed)	—	5.0	50.5
<i>u</i> 1459	C(171)...H(204)	328.3(91)	48.4(fixed)	—	3.8	48.4
<i>u</i> 1537	C(335)...H(360)	328.3(87)	44.7(fixed)	—	3.1	44.7
<i>u</i> 1763	Si(85)...H(97)	328.6(16)	20.5(fixed)	—	-0.3	20.5
<i>u</i> 1586	H(160)...H(164)	328.6(58)	79.9(fixed)	—	-1.8	79.9
<i>u</i> 1434	C(7)...H(15)	328.7(17)	33.3(fixed)	—	1.5	33.3
<i>u</i> 2273	H(222)...H(245)	328.8(218)	45.8(fixed)	—	-2.9	45.8
<i>u</i> 1091	C(337)...H(342)	328.9(28)	25.0(fixed)	—	2.8	25.0
<i>u</i> 3177	C(49)...H(74)	329.0(76)	33.1(fixed)	—	4.1	33.1
<i>u</i> 4041	C(88)...C(93)	329.2(59)	21.3(tied to <i>u</i> 1082)	—	-1.4	19.6
<i>u</i> 1378	Si(210)...H(244)	329.2(49)	32.6(fixed)	—	3.9	32.6
<i>u</i> 2617	Si(248)...H(263)	329.3(19)	13.2(fixed)	—	-1.2	13.2
<i>u</i> 1278	C(295)...H(302)	329.4(29)	28.6(fixed)	—	1.5	28.6
<i>u</i> 1054	Si(250)...H(263)	329.5(52)	21.0(fixed)	—	0.5	21.0
<i>u</i> 1331	Si(43)...H(57)	329.5(18)	21.6(fixed)	—	0.5	21.6
<i>u</i> 1447	Si(87)...H(121)	329.5(90)	33.8(fixed)	—	3.6	33.8
<i>u</i> 1361	Si(44)...H(55)	329.7(41)	22.0(fixed)	—	0.4	22.0
<i>u</i> 3024	Si(86)...C(88)	330.0(38)	11.2(tied to <i>u</i> 1082)	—	-1.1	10.3
<i>u</i> 1332	C(217)...H(220)	330.0(142)	29.5(fixed)	—	1.6	29.5
<i>u</i> 1661	C(211)...H(221)	330.0(54)	36.3(fixed)	—	0.5	36.3
<i>u</i> 1384	Si(208)...H(219)	330.1(50)	21.6(fixed)	—	0.3	21.6
<i>u</i> 3623	H(271)...H(277)	330.2(52)	43.7(fixed)	—	-11.1	43.7
<i>u</i> 448	H(227)...H(237)	330.5(233)	45.2(fixed)	—	21.9	45.2
<i>u</i> 1343	Si(249)...H(260)	330.5(16)	21.3(fixed)	—	0.3	21.3
<i>u</i> 1429	Si(248)...H(274)	330.7(50)	32.5(fixed)	—	3.0	32.5
<i>u</i> 3183	C(252)...H(262)	330.8(50)	21.5(fixed)	—	-0.9	21.5
<i>u</i> 2901	H(98)...H(99)	330.8(39)	25.1(fixed)	—	-1.4	25.1
<i>u</i> 2579	Si(44)...H(58)	331.3(18)	13.9(fixed)	—	-1.4	13.9
<i>u</i> 4810	H(59)...H(72)	331.4(99)	43.6(fixed)	—	-4.5	43.6
<i>u</i> 3563	C(48)...C(53)	331.4(88)	25.2(tied to <i>u</i> 1082)	—	-1.0	23.2
<i>u</i> 4775	H(223)...H(236)	331.5(103)	49.8(fixed)	—	-2.9	49.8
<i>u</i> 2000	H(113)...H(119)	331.6(306)	63.8(fixed)	—	0.4	63.8
<i>u</i> 4098	C(51)...H(78)	331.8(54)	47.5(fixed)	—	-2.3	47.5
<i>u</i> 2310	C(8)...H(22)	332.1(603)	56.2(fixed)	—	-2.7	56.2
<i>u</i> 5415	H(269)...H(276)	332.1(100)	25.9(fixed)	—	-10.0	25.9
<i>u</i> 1427	C(6)...H(40)	332.1(75)	42.4(fixed)	—	4.6	42.4
<i>u</i> 4031	C(93)...H(119)	332.3(153)	31.8(fixed)	—	-0.8	31.8



<i>u</i> 3815	H(178)...H(188)	332.5(76)	25.6(fixed)	—	-1.8	25.6
<i>u</i> 1468	Si(207)...H(233)	332.6(50)	33.5(fixed)	—	3.4	33.5
<i>u</i> 5389	H(61)...H(75)	333.1(120)	26.7(fixed)	—	-5.3	26.7
<i>u</i> 1402	C(337)...H(343)	333.3(31)	30.8(fixed)	—	1.4	30.8
<i>u</i> 4758	C(47)...C(52)	333.5(59)	13.6(tied to <i>u</i> 1082)	—	-2.1	12.5
<i>u</i> 1439	Si(46)...H(80)	334.3(65)	33.3(fixed)	—	3.6	33.3
<i>u</i> 3757	H(143)...H(159)	334.3(94)	101.4(fixed)	—	8.9	101.4
<i>u</i> 3425	C(92)...H(110)	334.3(59)	38.4(fixed)	—	5.2	38.4
<i>u</i> 1930	H(305)...H(326)	334.3(159)	50.2(fixed)	—	4.2	50.2
<i>u</i> 2085	H(306)...H(326)	334.6(126)	43.8(fixed)	—	6.3	43.8
<i>u</i> 1574	C(329)...H(354)	334.9(38)	21.4(fixed)	—	0.5	21.4
<i>u</i> 1565	C(124)...H(149)	335.0(38)	21.3(fixed)	—	0.5	21.3
<i>u</i> 1606	C(1)...H(26)	335.0(38)	21.4(fixed)	—	0.5	21.4
<i>u</i> 1554	C(288)...H(309)	335.0(38)	20.9(fixed)	—	0.5	20.9
<i>u</i> 1601	C(83)...H(118)	335.0(38)	20.6(fixed)	—	0.4	20.6
<i>u</i> 1597	C(206)...H(231)	335.0(38)	21.2(fixed)	—	0.5	21.2
<i>u</i> 1578	C(247)...H(281)	335.0(38)	20.7(fixed)	—	0.5	20.7
<i>u</i> 1555	C(42)...H(63)	335.0(38)	20.8(fixed)	—	0.5	20.8
<i>u</i> 1614	C(124)...H(145)	335.1(38)	21.6(fixed)	—	0.6	21.6
<i>u</i> 1588	C(206)...H(227)	335.1(38)	20.5(fixed)	—	0.5	20.5
<i>u</i> 1397	C(53)...H(56)	335.1(101)	30.5(fixed)	—	1.7	30.5
<i>u</i> 1568	C(247)...H(268)	335.1(38)	20.5(fixed)	—	0.5	20.5
<i>u</i> 1596	C(247)...H(272)	335.1(38)	20.2(fixed)	—	0.5	20.2
<i>u</i> 2763	H(96)...H(114)	335.1(171)	33.7(fixed)	—	6.8	33.7
<i>u</i> 1576	C(83)...H(117)	335.2(38)	21.9(fixed)	—	0.8	21.9
<i>u</i> 1317	C(132)...H(137)	335.2(31)	27.3(fixed)	—	3.1	27.3
<i>u</i> 1567	C(83)...H(108)	335.3(38)	22.4(fixed)	—	0.9	22.4
<i>u</i> 1227	Si(127)...H(159)	335.3(53)	54.3(fixed)	—	32.0	54.3
<i>u</i> 1551	C(83)...H(104)	335.4(38)	22.1(fixed)	—	1.0	22.1
<i>u</i> 1546	C(329)...H(350)	335.4(38)	22.6(fixed)	—	1.1	22.6
<i>u</i> 2716	C(47)...H(65)	335.4(90)	37.6(fixed)	—	-4.5	37.6
<i>u</i> 1532	C(247)...H(282)	335.5(38)	23.0(fixed)	—	1.2	23.0
<i>u</i> 1269	C(54)...H(57)	335.5(86)	26.4(fixed)	—	3.2	26.4
<i>u</i> 1527	C(42)...H(67)	335.5(38)	23.8(fixed)	—	1.4	23.8
<i>u</i> 3778	H(281)...H(284)	335.5(97)	38.3(fixed)	—	-8.7	38.3
<i>u</i> 2706	C(88)...H(106)	335.6(76)	35.7(fixed)	—	-3.5	35.7
<i>u</i> 1534	C(288)...H(322)	335.7(38)	23.6(fixed)	—	1.5	23.6
<i>u</i> 1539	C(42)...H(76)	335.7(38)	23.3(fixed)	—	1.5	23.3
<i>u</i> 1729	C(294)...C(296)	335.8(47)	20.2(tied to <i>u</i> 1859)	—	1.9	21.0
<i>u</i> 1530	C(206)...H(241)	335.8(38)	24.5(fixed)	—	1.7	24.5
<i>u</i> 1509	C(42)...H(77)	335.9(38)	24.8(fixed)	—	1.9	24.8
<i>u</i> 1329	C(50)...H(55)	336.0(39)	26.9(fixed)	—	3.1	26.9
<i>u</i> 1761	C(95)...H(99)	336.0(41)	37.6(fixed)	—	0.3	37.6
<i>u</i> 1505	C(165)...H(186)	336.1(38)	25.1(fixed)	—	2.1	25.1

<i>u4710</i>	H(63)...H(79)	336.2(82)	37.4(fixed)	—	-7.7	37.4
<i>u2601</i>	Si(85)...H(99)	336.2(16)	13.6(fixed)	—	-1.3	13.6
<i>u1507</i>	C(124)...H(158)	336.3(38)	29.7(fixed)	—	3.1	29.7
<i>u1514</i>	C(206)...H(240)	336.3(38)	24.9(fixed)	—	2.4	24.9
<i>u5417</i>	H(224)...H(238)	336.5(93)	26.9(fixed)	—	-6.1	26.9
<i>u1344</i>	C(6)...H(16)	336.6(83)	36.0(fixed)	—	2.0	36.0
<i>u1627</i>	H(21)...H(35)	336.6(209)	56.4(fixed)	—	14.4	56.4
<i>u3286</i>	C(171)...H(179)	336.6(28)	21.8(fixed)	—	-1.6	21.8
<i>u1500</i>	C(131)...H(140)	336.7(33)	33.1(fixed)	—	1.1	33.1
<i>u1836</i>	H(309)...H(314)	336.8(130)	44.3(fixed)	—	4.3	44.3
<i>u1293</i>	C(295)...H(301)	336.9(45)	27.3(fixed)	—	2.2	27.3
<i>u1953</i>	Si(45)...H(64)	337.0(55)	31.4(fixed)	—	0.1	31.4
<i>u1314</i>	C(95)...H(98)	337.1(129)	28.7(fixed)	—	3.0	28.7
<i>u3511</i>	Si(250)...H(269)	337.1(64)	19.9(fixed)	—	-1.9	19.9
<i>u1559</i>	H(235)...H(238)	337.1(56)	58.2(fixed)	—	-1.9	58.2
<i>u4993</i>	H(143)...H(161)	337.4(87)	41.7(fixed)	—	-27.0	41.7
<i>u1387</i>	C(259)...H(275)	337.5(52)	36.6(fixed)	—	3.9	36.6
<i>u1543</i>	C(294)...H(303)	337.7(60)	30.6(fixed)	—	0.8	30.6
<i>u4838</i>	H(100)...H(117)	337.8(66)	43.0(fixed)	—	-4.3	43.0
<i>u3325</i>	H(63)...H(77)	338.1(106)	55.7(fixed)	—	5.1	55.7
<i>u1511</i>	C(206)...H(223)	338.1(30)	21.6(fixed)	—	0.7	21.6
<i>u1449</i>	C(124)...H(152)	338.2(30)	23.7(fixed)	—	1.0	23.7
<i>u1526</i>	C(288)...H(316)	338.2(30)	22.3(fixed)	—	0.8	22.3
<i>u1445</i>	C(165)...H(182)	338.2(30)	23.8(fixed)	—	1.0	23.8
<i>u1528</i>	C(206)...H(245)	338.2(30)	22.3(fixed)	—	0.8	22.3
<i>u1519</i>	C(247)...H(275)	338.2(30)	21.5(fixed)	—	0.7	21.5
<i>u1522</i>	C(206)...H(234)	338.2(30)	22.0(fixed)	—	0.8	22.0
<i>u1471</i>	C(83)...H(122)	338.2(30)	21.7(fixed)	—	0.8	21.7
<i>u1442</i>	C(42)...H(70)	338.2(30)	23.0(fixed)	—	0.9	23.0
<i>u1466</i>	C(42)...H(81)	338.2(30)	22.1(fixed)	—	0.8	22.1
<i>u1896</i>	Si(46)...H(73)	338.2(79)	26.6(fixed)	—	4.2	26.6
<i>u1502</i>	C(124)...H(141)	338.3(30)	21.4(fixed)	—	0.8	21.4
<i>u1489</i>	C(42)...H(73)	338.3(30)	22.9(fixed)	—	1.0	22.9
<i>u1484</i>	C(329)...H(346)	338.3(30)	22.8(fixed)	—	1.0	22.8
<i>u1458</i>	C(1)...H(29)	338.3(30)	21.9(fixed)	—	0.9	21.9
<i>u1486</i>	C(247)...H(264)	338.4(30)	22.5(fixed)	—	1.0	22.5
<i>u1506</i>	C(124)...H(155)	338.4(30)	24.0(fixed)	—	1.2	24.0
<i>u1501</i>	C(247)...H(286)	338.5(30)	23.4(fixed)	—	1.2	23.4
<i>u2394</i>	H(58)...H(81)	338.5(152)	44.8(fixed)	—	-2.9	44.8
<i>u1545</i>	H(153)...H(156)	338.6(56)	54.4(fixed)	—	-1.7	54.4
<i>u1464</i>	C(124)...H(163)	338.7(30)	24.0(fixed)	—	1.6	24.0
<i>u1473</i>	C(288)...H(305)	338.7(30)	23.9(fixed)	—	1.6	23.9
<i>u4490</i>	C(136)...H(143)	338.8(81)	23.1(fixed)	—	-3.5	23.1
<i>u1521</i>	C(83)...H(100)	339.0(30)	25.6(fixed)	—	2.1	25.6

<i>u</i> 1451	C(83)...H(111)	339.0(30)	25.1(fixed)	—	2.1	25.1
<i>u</i> 1441	C(329)...H(357)	339.1(30)	25.4(fixed)	—	2.1	25.4
<i>u</i> 1686	H(161)...H(162)	339.1(61)	75.8(fixed)	—	-3.5	75.8
<i>u</i> 1472	C(42)...H(59)	339.2(30)	25.5(fixed)	—	2.3	25.5
<i>u</i> 1512	C(206)...H(237)	339.3(30)	28.5(fixed)	—	2.8	28.5
<i>u</i> 1480	Si(127)...H(151)	339.4(44)	31.8(fixed)	—	4.5	31.8
<i>u</i> 1482	C(83)...H(114)	339.7(30)	27.3(fixed)	—	3.1	27.3
<i>u</i> 1651	H(182)...H(200)	339.8(140)	72.1(fixed)	—	3.9	72.1
<i>u</i> 1709	H(112)...H(115)	339.9(56)	48.4(fixed)	—	-2.2	48.4
<i>u</i> 1470	C(247)...H(278)	339.9(30)	28.1(fixed)	—	3.4	28.1
<i>u</i> 1736	H(276)...H(279)	340.1(56)	47.5(fixed)	—	-2.2	47.5
<i>u</i> 1670	H(183)...H(187)	340.2(56)	47.3(fixed)	—	-2.1	47.3
<i>u</i> 3911	C(129)...C(135)	340.4(39)	26.4(tied to <i>u</i> 1082)	—	-1.5	24.2
<i>u</i> 1612	H(242)...H(246)	340.5(56)	46.2(fixed)	—	-2.1	46.2
<i>u</i> 5294	C(253)...H(276)	340.5(97)	17.0(fixed)	—	-7.9	17.0
<i>u</i> 1691	H(78)...H(82)	340.7(56)	45.2(fixed)	—	-2.2	45.2
<i>u</i> 1658	H(71)...H(74)	340.7(56)	45.2(fixed)	—	-2.2	45.2
<i>u</i> 1645	H(311)...H(314)	340.8(56)	44.7(fixed)	—	-2.3	44.7
<i>u</i> 1626	H(101)...H(105)	341.0(56)	47.1(fixed)	—	-1.4	47.1
<i>u</i> 1499	C(124)...H(159)	341.0(39)	41.1(fixed)	—	10.2	41.1
<i>u</i> 1911	Si(209)...H(228)	341.1(50)	29.8(fixed)	—	0.5	29.8
<i>u</i> 2592	Si(87)...H(97)	341.2(34)	13.4(fixed)	—	-1.2	13.4
<i>u</i> 1732	H(106)...H(109)	341.3(56)	45.1(fixed)	—	-1.7	45.1
<i>u</i> 3299	C(258)...H(261)	341.3(19)	17.5(fixed)	—	-1.3	17.5
<i>u</i> 1602	H(283)...H(287)	341.4(56)	45.2(fixed)	—	-1.6	45.2
<i>u</i> 4665	C(94)...H(105)	341.4(29)	26.5(fixed)	—	-4.1	26.5
<i>u</i> 1703	H(65)...H(68)	341.5(56)	43.5(fixed)	—	-1.9	43.5
<i>u</i> 3044	C(90)...H(97)	341.5(35)	22.8(fixed)	—	-1.4	22.8
<i>u</i> 1632	C(124)...H(143)	341.5(30)	22.7(fixed)	—	0.0	22.7
<i>u</i> 1663	C(1)...H(28)	341.5(30)	22.0(fixed)	—	0.0	22.0
<i>u</i> 1643	C(165)...H(184)	341.6(30)	22.5(fixed)	—	0.1	22.5
<i>u</i> 1655	C(83)...H(121)	341.6(30)	21.8(fixed)	—	0.0	21.8
<i>u</i> 4230	H(67)...H(74)	341.7(69)	38.0(fixed)	—	-1.9	38.0
<i>u</i> 1629	C(247)...H(274)	341.7(30)	22.0(fixed)	—	0.1	22.0
<i>u</i> 1647	C(42)...H(80)	341.7(30)	22.0(fixed)	—	0.1	22.0
<i>u</i> 1635	C(206)...H(233)	341.7(30)	22.2(fixed)	—	0.1	22.2
<i>u</i> 1503	Si(45)...H(69)	341.7(48)	32.1(fixed)	—	3.9	32.1
<i>u</i> 1615	C(42)...H(69)	341.7(30)	22.6(fixed)	—	0.2	22.6
<i>u</i> 1604	C(206)...H(225)	341.7(30)	22.0(fixed)	—	0.1	22.0
<i>u</i> 1637	C(42)...H(72)	341.7(30)	22.6(fixed)	—	0.2	22.6
<i>u</i> 2204	H(227)...H(236)	341.8(106)	42.8(fixed)	—	-5.3	42.8
<i>u</i> 1630	C(288)...H(315)	341.8(30)	22.0(fixed)	—	0.2	22.0
<i>u</i> 1623	C(247)...H(266)	341.8(30)	22.7(fixed)	—	0.3	22.7
<i>u</i> 1633	C(124)...H(151)	341.8(30)	22.6(fixed)	—	0.3	22.6

<i>u</i> 1616	C(288)...H(326)	341.8(30)	24.8(fixed)	—	0.6	24.8
<i>u</i> 1610	C(206)...H(244)	341.8(30)	22.3(fixed)	—	0.3	22.3
<i>u</i> 1634	C(329)...H(356)	341.9(30)	25.7(fixed)	—	0.8	25.7
<i>u</i> 1593	C(124)...H(162)	341.9(30)	25.6(fixed)	—	0.8	25.6
<i>u</i> 1591	C(124)...H(154)	341.9(30)	24.6(fixed)	—	0.7	24.6
<i>u</i> 1609	C(329)...H(348)	341.9(30)	22.5(fixed)	—	0.4	22.5
<i>u</i> 1599	C(83)...H(110)	341.9(30)	26.2(fixed)	—	0.9	26.2
<i>u</i> 1656	C(247)...H(277)	341.9(30)	28.3(fixed)	—	1.3	28.3
<i>u</i> 1625	C(42)...H(61)	341.9(30)	26.3(fixed)	—	1.0	26.3
<i>u</i> 1579	C(247)...H(285)	342.0(30)	24.0(fixed)	—	0.7	24.0
<i>u</i> 1704	H(60)...H(64)	342.0(56)	42.8(fixed)	—	-1.5	42.8
<i>u</i> 1636	C(83)...H(113)	342.0(30)	28.2(fixed)	—	1.4	28.2
<i>u</i> 1865	H(24)...H(27)	342.1(55)	38.3(fixed)	—	-2.5	38.3
<i>u</i> 1563	H(55)...H(57)	342.1(92)	37.6(fixed)	—	0.0	37.6
<i>u</i> 1730	H(142)...H(146)	342.2(55)	39.1(fixed)	—	-2.1	39.1
<i>u</i> 1693	H(229)...H(232)	342.3(55)	39.0(fixed)	—	-2.1	39.0
<i>u</i> 1590	C(83)...H(102)	342.3(30)	26.4(fixed)	—	1.4	26.4
<i>u</i> 1322	C(252)...H(285)	342.4(96)	36.2(fixed)	—	9.0	36.2
<i>u</i> 1611	C(206)...H(236)	342.4(30)	28.1(fixed)	—	1.8	28.1
<i>u</i> 1382	Si(128)...H(162)	342.5(41)	36.0(fixed)	—	6.5	36.0
<i>u</i> 1765	H(119)...H(123)	342.6(55)	37.9(fixed)	—	-2.0	37.9
<i>u</i> 3367	C(258)...H(263)	342.6(31)	21.2(fixed)	—	-1.3	21.2
<i>u</i> 1695	H(324)...H(328)	342.7(56)	40.3(fixed)	—	-1.4	40.3
<i>u</i> 1766	H(147)...H(150)	342.7(55)	38.8(fixed)	—	-1.7	38.8
<i>u</i> 2090	H(280)...H(282)	343.0(112)	48.1(fixed)	—	5.9	48.1
<i>u</i> 1681	H(265)...H(269)	343.0(55)	38.5(fixed)	—	-1.5	38.5
<i>u</i> 1659	H(270)...H(273)	343.0(55)	37.8(fixed)	—	-1.7	37.8
<i>u</i> 1875	Si(128)...H(155)	343.1(111)	27.3(fixed)	—	5.9	27.3
<i>u</i> 1448	C(218)...H(234)	343.2(49)	41.6(fixed)	—	4.2	41.6
<i>u</i> 1640	H(224)...H(228)	343.3(55)	37.7(fixed)	—	-1.4	37.7
<i>u</i> 2038	H(231)...H(239)	343.4(144)	47.9(fixed)	—	1.0	47.9
<i>u</i> 4987	H(223)...H(240)	343.7(120)	35.8(fixed)	—	3.1	35.8
<i>u</i> 1558	C(218)...H(222)	343.8(85)	38.2(fixed)	—	0.3	38.2
<i>u</i> 1692	C(54)...H(58)	343.9(55)	39.2(fixed)	—	0.0	39.2
<i>u</i> 2006	C(293)...C(300)	344.0(101)	24.1(tied to <i>u</i> 1859)	—	0.7	24.3
<i>u</i> 3398	H(138)...H(152)	344.0(71)	39.0(fixed)	—	-1.0	39.0
<i>u</i> 1481	C(135)...H(138)	344.2(62)	32.2(fixed)	—	1.8	32.2
<i>u</i> 3581	C(212)...C(217)	344.2(131)	24.6(tied to <i>u</i> 1859)	—	-1.4	24.8
<i>u</i> 1677	Si(290)...C(294)	344.3(20)	16.5(tied to <i>u</i> 1859)	—	0.5	16.6
<i>u</i> 4618	H(228)...H(241)	344.3(213)	45.8(fixed)	—	-2.5	45.8
<i>u</i> 1842	Si(289)...C(293)	344.6(24)	17.4(tied to <i>u</i> 1859)	—	0.3	17.5
<i>u</i> 1581	C(206)...H(228)	344.9(37)	23.5(fixed)	—	0.2	23.5
<i>u</i> 1613	C(165)...H(188)	344.9(37)	28.0(fixed)	—	0.9	28.0
<i>u</i> 1569	C(247)...H(270)	344.9(37)	23.5(fixed)	—	0.3	23.5

<i>u1573</i>	C(124)...H(147)	344.9(37)	23.5(fixed)	—	0.3	23.5
<i>u1583</i>	C(288)...H(310)	345.0(37)	22.7(fixed)	—	0.2	22.7
<i>u1544</i>	C(83)...H(119)	345.0(37)	23.5(fixed)	—	0.4	23.5
<i>u1577</i>	C(247)...H(269)	345.0(37)	22.8(fixed)	—	0.3	22.8
<i>u1580</i>	C(42)...H(64)	345.0(37)	22.6(fixed)	—	0.3	22.6
<i>u1487</i>	C(124)...H(146)	345.0(37)	25.2(fixed)	—	0.6	25.2
<i>u1589</i>	C(247)...H(279)	345.0(37)	22.7(fixed)	—	0.3	22.7
<i>u1587</i>	C(329)...H(352)	345.1(37)	22.7(fixed)	—	0.4	22.7
<i>u1485</i>	C(206)...H(229)	345.1(37)	23.9(fixed)	—	0.6	23.9
<i>u1571</i>	C(83)...H(106)	345.1(37)	24.2(fixed)	—	0.6	24.2
<i>u1556</i>	C(329)...H(351)	345.2(37)	24.4(fixed)	—	0.7	24.4
<i>u1550</i>	C(83)...H(105)	345.2(37)	24.1(fixed)	—	0.6	24.1
<i>u1549</i>	C(83)...H(115)	345.2(37)	23.8(fixed)	—	0.6	23.8
<i>u1621</i>	C(206)...H(238)	345.2(37)	26.8(fixed)	—	1.0	26.8
<i>u1566</i>	C(247)...H(283)	345.2(37)	24.4(fixed)	—	0.7	24.4
<i>u1504</i>	C(288)...H(311)	345.2(37)	26.3(fixed)	—	1.0	26.3
<i>u1538</i>	C(42)...H(78)	345.2(37)	26.9(fixed)	—	1.1	26.9
<i>u1584</i>	C(42)...H(65)	345.2(37)	25.0(fixed)	—	0.8	25.0
<i>u1477</i>	C(1)...H(24)	345.2(37)	23.9(fixed)	—	0.7	23.9
<i>u5205</i>	H(155)...H(161)	345.2(83)	36.6(fixed)	—	-27.1	36.6
<i>u1510</i>	C(206)...H(242)	345.2(37)	26.8(fixed)	—	1.1	26.8
<i>u1570</i>	C(42)...H(74)	345.2(37)	25.5(fixed)	—	0.9	25.5
<i>u1603</i>	C(124)...H(156)	345.3(37)	29.8(fixed)	—	1.6	29.8
<i>u1491</i>	C(300)...H(316)	345.3(77)	41.5(fixed)	—	3.0	41.5
<i>u1650</i>	Si(86)...C(94)	345.4(48)	16.9(tied to <i>u1859</i> )	—	1.1	17.0
<i>u3112</i>	H(225)...H(237)	345.5(104)	53.9(fixed)	—	11.6	53.9
<i>u1674</i>	Si(4)...C(7)	345.5(14)	17.5(tied to <i>u1859</i> )	—	0.4	17.6
<i>u2292</i>	H(63)...H(72)	345.7(92)	39.8(fixed)	—	-1.1	39.8
<i>u2001</i>	Si(87)...H(115)	345.7(96)	29.7(fixed)	—	3.6	29.7
<i>u5412</i>	H(60)...H(74)	345.8(73)	27.3(fixed)	—	-8.3	27.3
<i>u1409</i>	Si(86)...H(110)	345.8(42)	36.8(fixed)	—	6.8	36.8
<i>u3185</i>	H(61)...H(73)	345.9(105)	44.1(fixed)	—	9.1	44.1
<i>u5365</i>	H(185)...H(199)	345.9(133)	26.7(fixed)	—	-6.2	26.7
<i>u1652</i>	C(124)...H(160)	346.2(37)	41.5(fixed)	—	4.9	41.5
<i>u5154</i>	H(145)...H(148)	346.2(68)	29.4(fixed)	—	-5.8	29.4
<i>u1753</i>	Si(330)...C(335)	346.4(17)	15.7(tied to <i>u1859</i> )	—	0.3	15.8
<i>u3261</i>	C(131)...H(156)	346.4(59)	35.1(fixed)	—	8.3	35.1
<i>u1919</i>	C(335)...C(340)	346.7(35)	27.0(tied to <i>u1859</i> )	—	1.0	27.2
<i>u3621</i>	H(144)...H(149)	347.0(76)	37.4(fixed)	—	3.6	37.4
<i>u3559</i>	Si(128)...H(156)	347.0(79)	24.2(fixed)	—	-2.0	24.2
<i>u1631</i>	Si(209)...C(217)	347.1(54)	16.6(tied to <i>u1859</i> )	—	0.4	16.7
<i>u1523</i>	C(336)...H(345)	347.2(35)	29.9(fixed)	—	0.8	29.9
<i>u1620</i>	H(236)...H(239)	347.4(60)	57.0(fixed)	—	-2.2	57.0
<i>u3589</i>	H(62)...H(78)	347.5(121)	47.4(fixed)	—	6.7	47.4

<i>u1479</i>	Si(251)...H(285)	347.6(39)	33.7(fixed)	—	5.1	33.7
<i>u3522</i>	C(49)...C(52)	347.6(44)	21.7(tied to <i>u1859</i> )	—	-1.5	21.9
<i>u1605</i>	H(154)...H(157)	347.8(60)	56.1(fixed)	—	-2.2	56.1
<i>u1557</i>	C(296)...H(301)	347.9(59)	34.4(fixed)	—	0.3	34.4
<i>u1848</i>	Si(332)...C(334)	348.3(21)	16.7(tied to <i>u1859</i> )	—	0.1	16.8
<i>u1853</i>	Si(210)...H(237)	348.3(90)	29.8(fixed)	—	10.6	29.8
<i>u2048</i>	H(310)...H(315)	348.3(115)	48.3(fixed)	—	2.5	48.3
<i>u2138</i>	Si(249)...C(256)	348.5(15)	14.2(tied to <i>u1859</i> )	—	-0.2	14.3
<i>u1660</i>	C(92)...C(94)	348.7(140)	19.3(tied to <i>u1859</i> )	—	3.2	19.4
<i>u2941</i>	Si(207)...C(212)	348.9(21)	11.9(tied to <i>u1859</i> )	—	-1.5	11.9
<i>u3383</i>	C(129)...H(162)	349.1(82)	38.0(fixed)	—	4.4	38.0
<i>u1702</i>	C(6)...C(13)	349.1(32)	21.7(tied to <i>u1859</i> )	—	3.1	21.8
<i>u1876</i>	C(7)...C(11)	349.2(46)	19.2(tied to <i>u1859</i> )	—	1.1	19.4
<i>u2951</i>	C(92)...H(96)	349.4(131)	25.6(fixed)	—	-1.6	25.6
<i>u1950</i>	H(19)...H(39)	349.6(27)	48.7(fixed)	—	3.2	48.7
<i>u2237</i>	Si(208)...C(216)	349.9(20)	15.4(tied to <i>u1859</i> )	—	-0.3	15.5
<i>u2940</i>	Si(43)...C(48)	349.9(13)	11.8(tied to <i>u1859</i> )	—	-1.3	11.8
<i>u4125</i>	H(139)...H(146)	349.9(92)	28.2(fixed)	—	-4.1	28.2
<i>u3647</i>	C(215)...C(217)	350.1(47)	17.6(tied to <i>u1859</i> )	—	-0.9	17.7
<i>u3366</i>	H(150)...H(158)	350.3(79)	69.9(fixed)	—	-10.5	69.9
<i>u4708</i>	H(227)...H(243)	350.3(111)	40.1(fixed)	—	-7.7	40.1
<i>u1548</i>	H(102)...H(103)	350.3(59)	49.7(fixed)	—	-1.5	49.7
<i>u3483</i>	Si(209)...H(223)	350.4(59)	19.7(fixed)	—	-1.6	19.7
<i>u1669</i>	Si(45)...C(53)	350.4(45)	17.1(tied to <i>u1859</i> )	—	0.4	17.2
<i>u1665</i>	Si(250)...H(262)	350.4(24)	20.9(fixed)	—	-0.2	20.9
<i>u1467</i>	H(113)...H(116)	350.5(59)	51.7(fixed)	—	-0.8	51.7
<i>u1779</i>	C(170)...C(176)	350.6(41)	25.2(tied to <i>u1859</i> )	—	1.9	25.4
<i>u2971</i>	H(260)...H(279)	350.9(97)	33.3(fixed)	—	0.9	33.3
<i>u4646</i>	C(255)...H(264)	350.9(133)	24.0(fixed)	—	-2.9	24.0
<i>u1494</i>	C(334)...H(352)	350.9(79)	39.4(fixed)	—	3.2	39.4
<i>u2008</i>	H(308)...H(316)	350.9(68)	31.8(fixed)	—	6.1	31.8
<i>u1461</i>	H(277)...H(280)	350.9(59)	50.4(fixed)	—	-0.7	50.4
<i>u3269</i>	H(100)...H(107)	350.9(48)	60.7(fixed)	—	-7.8	60.7
<i>u3284</i>	C(214)...H(222)	351.3(62)	21.8(fixed)	—	-1.5	21.8
<i>u3073</i>	H(59)...H(66)	351.4(53)	63.0(fixed)	—	-6.8	63.0
<i>u1572</i>	H(107)...H(110)	351.6(59)	47.3(fixed)	—	-0.9	47.3
<i>u1533</i>	H(61)...H(62)	351.8(59)	46.1(fixed)	—	-1.0	46.1
<i>u1564</i>	H(284)...H(285)	351.8(59)	45.2(fixed)	—	-1.2	45.2
<i>u3550</i>	Si(210)...H(238)	351.9(61)	21.9(fixed)	—	-1.9	21.9
<i>u1561</i>	H(184)...H(185)	351.9(59)	46.3(fixed)	—	-0.8	46.3
<i>u1892</i>	C(9)...H(15)	351.9(87)	39.8(fixed)	—	-0.2	39.8
<i>u1022</i>	H(15)...H(35)	352.2(581)	30.3(fixed)	—	1.0	30.3
<i>u438</i>	H(114)...H(118)	352.2(208)	43.3(fixed)	—	22.3	43.3
<i>u1478</i>	H(243)...H(244)	352.4(59)	45.0(fixed)	—	-0.6	45.0

<i>u</i> 1541	H(307)...H(308)	352.6(59)	43.0(fixed)	—	-0.9	43.0
<i>u</i> 827	C(8)...H(23)	352.8(453)	37.4(fixed)	—	18.6	37.4
<i>u</i> 1347	C(93)...H(104)	352.8(111)	40.3(fixed)	—	5.5	40.3
<i>u</i> 1483	H(72)...H(75)	352.9(59)	43.3(fixed)	—	-0.6	43.3
<i>u</i> 1560	H(66)...H(69)	352.9(59)	42.9(fixed)	—	-0.7	42.9
<i>u</i> 1492	H(79)...H(80)	353.0(59)	44.0(fixed)	—	-0.4	44.0
<i>u</i> 1859	Si(166)...C(170)	353.0(26)	19.2(11)	—	0.1	19.3
<i>u</i> 4080	H(261)...H(267)	353.0(101)	30.6(fixed)	—	-3.1	30.6
<i>u</i> 3854	C(89)...C(94)	353.1(149)	23.2(tied to <i>u</i> 1859)	—	-1.0	23.4
<i>u</i> 1455	H(312)...H(315)	353.1(59)	43.2(fixed)	—	-0.4	43.2
<i>u</i> 1687	Si(332)...C(337)	353.2(19)	17.9(tied to <i>u</i> 1859)	—	0.3	18.0
<i>u</i> 5168	H(227)...H(246)	353.4(88)	31.7(fixed)	—	-7.1	31.7
<i>u</i> 3437	H(220)...H(229)	353.5(103)	35.5(fixed)	—	-0.9	35.5
<i>u</i> 1493	H(225)...H(226)	353.6(59)	39.1(fixed)	—	-0.9	39.1
<i>u</i> 3688	C(51)...C(53)	353.6(29)	17.9(tied to <i>u</i> 1859)	—	-0.9	18.0
<i>u</i> 1488	H(266)...H(267)	353.6(59)	39.7(fixed)	—	-0.7	39.7
<i>u</i> 2143	Si(84)...C(92)	353.7(18)	14.2(tied to <i>u</i> 1859)	—	-0.1	14.3
<i>u</i> 1518	H(148)...H(151)	353.8(59)	39.5(fixed)	—	-0.5	39.5
<i>u</i> 2020	C(88)...C(90)	353.9(31)	24.0(tied to <i>u</i> 1859)	—	0.5	24.2
<i>u</i> 1438	H(271)...H(274)	354.0(59)	38.7(fixed)	—	-0.6	38.7
<i>u</i> 5058	C(253)...H(277)	354.0(74)	27.6(fixed)	—	-1.0	27.6
<i>u</i> 2272	Si(44)...C(52)	354.1(13)	16.4(tied to <i>u</i> 1859)	—	-0.3	16.5
<i>u</i> 1975	C(47)...C(49)	354.2(36)	23.4(tied to <i>u</i> 1859)	—	0.7	23.5
<i>u</i> 1895	Si(289)...H(319)	354.2(47)	26.4(fixed)	—	3.8	26.4
<i>u</i> 675	H(23)...H(24)	354.2(497)	57.8(fixed)	—	18.8	57.8
<i>u</i> 1799	H(137)...H(160)	354.2(25)	18.3(fixed)	—	-11.2	18.3
<i>u</i> 1388	H(143)...H(144)	354.3(59)	40.0(fixed)	—	0.0	40.0
<i>u</i> 1391	H(230)...H(233)	354.3(59)	39.4(fixed)	—	-0.1	39.4
<i>u</i> 1433	H(120)...H(121)	354.3(59)	38.7(fixed)	—	-0.2	38.7
<i>u</i> 3490	H(56)...H(70)	354.5(77)	37.5(fixed)	—	-1.4	37.5
<i>u</i> 1553	C(213)...H(219)	354.8(58)	31.6(fixed)	—	1.9	31.6
<i>u</i> 3412	Si(166)...H(196)	355.0(37)	21.2(fixed)	—	-1.5	21.2
<i>u</i> 1377	H(25)...H(28)	355.0(59)	38.4(fixed)	—	0.5	38.4
<i>u</i> 1829	Si(4)...C(9)	355.1(44)	20.8(tied to <i>u</i> 1859)	—	0.4	20.9
<i>u</i> 1721	Si(127)...C(135)	355.2(11)	17.2(tied to <i>u</i> 1859)	—	0.6	17.3
<i>u</i> 1967	H(142)...H(155)	355.3(198)	33.7(fixed)	—	11.8	33.7
<i>u</i> 1598	Si(290)...C(298)	355.4(23)	15.9(tied to <i>u</i> 1859)	—	0.3	16.0
<i>u</i> 2967	Si(249)...C(252)	355.6(33)	10.5(tied to <i>u</i> 1859)	—	-1.0	10.5
<i>u</i> 2962	Si(251)...C(256)	355.7(36)	10.4(tied to <i>u</i> 1859)	—	-1.0	10.4
<i>u</i> 3275	C(130)...H(139)	355.8(33)	25.8(fixed)	—	-1.4	25.8
<i>u</i> 1638	C(254)...H(260)	356.0(49)	32.6(fixed)	—	1.5	32.6
<i>u</i> 3447	Si(45)...H(59)	356.0(68)	21.9(fixed)	—	-1.2	21.9
<i>u</i> 1594	Si(2)...H(29)	356.1(90)	30.0(fixed)	—	4.3	30.0
<i>u</i> 3137	C(257)...H(260)	356.1(31)	24.0(fixed)	—	-1.6	24.0

<i>u3761</i>	C(133)...C(135)	356.4(62)	18.1(tied to <i>u1859</i> )	—	-0.9	18.2
<i>u3223</i>	C(213)...H(220)	356.5(44)	17.1(fixed)	—	-0.8	17.1
<i>u5177</i>	H(225)...H(240)	356.6(87)	33.9(fixed)	—	-2.1	33.9
<i>u1676</i>	Si(128)...C(131)	356.9(13)	17.3(tied to <i>u1859</i> )	—	0.7	17.4
<i>u3004</i>	Si(84)...C(89)	357.0(12)	10.9(tied to <i>u1859</i> )	—	-1.0	11.0
<i>u4816</i>	H(105)...H(118)	357.0(228)	36.4(fixed)	—	-3.9	36.4
<i>u1666</i>	Si(290)...H(302)	357.0(24)	19.7(fixed)	—	-0.2	19.7
<i>u1524</i>	Si(126)...H(163)	357.3(30)	27.1(fixed)	—	7.6	27.1
<i>u1026</i>	H(20)...H(23)	357.3(832)	46.2(fixed)	—	10.7	46.2
<i>u3604</i>	C(131)...C(134)	357.4(47)	23.0(tied to <i>u1859</i> )	—	-1.9	23.2
<i>u2964</i>	Si(166)...C(172)	357.4(18)	11.1(tied to <i>u1859</i> )	—	-1.3	11.2
<i>u1771</i>	Si(250)...C(258)	357.6(17)	15.7(tied to <i>u1859</i> )	—	0.3	15.8
<i>u2263</i>	Si(126)...C(134)	357.6(28)	17.1(tied to <i>u1859</i> )	—	-0.3	17.2
<i>u1536</i>	C(7)...H(24)	357.7(148)	48.9(fixed)	—	3.8	48.9
<i>u1775</i>	H(229)...H(240)	357.7(121)	69.6(fixed)	—	2.4	69.6
<i>u3481</i>	H(68)...H(76)	357.7(69)	51.1(fixed)	—	-7.8	51.1
<i>u2111</i>	C(334)...C(338)	357.7(79)	25.9(tied to <i>u1859</i> )	—	0.0	26.0
<i>u2280</i>	H(281)...H(283)	357.8(93)	57.8(fixed)	—	2.7	57.8
<i>u3499</i>	H(102)...H(115)	357.8(77)	46.2(fixed)	—	7.9	46.2
<i>u3536</i>	Si(46)...H(74)	357.9(45)	21.7(fixed)	—	-1.9	21.7
<i>u1762</i>	Si(4)...H(17)	358.1(13)	21.4(fixed)	—	-0.3	21.4
<i>u1608</i>	H(272)...H(276)	358.2(100)	60.4(fixed)	—	2.6	60.4
<i>u1921</i>	Si(208)...H(223)	358.2(59)	31.2(fixed)	—	0.5	31.2
<i>u1759</i>	Si(209)...H(221)	358.2(34)	21.5(fixed)	—	-0.3	21.5
<i>u1988</i>	Si(85)...H(100)	358.3(33)	46.4(fixed)	—	0.0	46.4
<i>u4817</i>	H(154)...H(160)	358.3(201)	71.6(fixed)	—	-10.5	71.6
<i>u4103</i>	C(129)...H(159)	358.3(107)	88.1(fixed)	—	0.8	88.1
<i>u1683</i>	Si(332)...C(340)	358.4(13)	16.6(tied to <i>u1859</i> )	—	0.4	16.7
<i>u1713</i>	H(312)...H(322)	358.4(118)	46.5(fixed)	—	8.9	46.5
<i>u4937</i>	H(59)...H(76)	358.5(140)	35.2(fixed)	—	4.5	35.2
<i>u1749</i>	Si(330)...H(345)	358.7(21)	20.4(fixed)	—	-0.3	20.4
<i>u1889</i>	C(334)...C(339)	358.8(43)	24.2(tied to <i>u1859</i> )	—	0.8	24.3
<i>u3304</i>	C(132)...H(138)	358.9(58)	19.1(fixed)	—	-1.5	19.1
<i>u5163</i>	H(237)...H(243)	358.9(79)	25.8(fixed)	—	-10.0	25.8
<i>u1976</i>	Si(289)...H(305)	359.0(67)	39.3(fixed)	—	0.7	39.3
<i>u2819</i>	C(133)...H(142)	359.1(120)	24.4(fixed)	—	-1.2	24.4
<i>u1869</i>	C(214)...H(219)	359.1(144)	36.9(fixed)	—	-0.1	36.9
<i>u2159</i>	H(103)...H(115)	359.2(160)	38.4(fixed)	—	3.8	38.4
<i>u1823</i>	H(138)...H(156)	359.4(25)	15.8(fixed)	—	-6.1	15.8
<i>u1866</i>	Si(44)...H(59)	359.4(35)	46.2(fixed)	—	1.0	46.2
<i>u1529</i>	Si(84)...H(111)	359.5(32)	28.1(fixed)	—	8.5	28.1
<i>u2014</i>	H(101)...H(108)	359.6(108)	46.1(fixed)	—	3.8	46.1
<i>u1706</i>	C(255)...H(260)	359.7(39)	33.5(fixed)	—	0.3	33.5
<i>u1582</i>	Si(250)...C(254)	359.7(22)	15.4(tied to <i>u1859</i> )	—	0.7	15.5



<i>u</i> 2647	C(130)...H(163)	359.7(99)	44.2(fixed)	—	-4.2	44.2
<i>u</i> 3009	Si(125)...C(129)	359.7(19)	10.7(tied to <i>u</i> 1859)	—	-1.5	10.7
<i>u</i> 5032	H(66)...H(76)	360.0(54)	39.3(fixed)	—	-8.6	39.3
<i>u</i> 1575	Si(44)...H(81)	360.0(68)	28.7(fixed)	—	4.4	28.7
<i>u</i> 1850	H(220)...H(236)	360.0(25)	15.9(fixed)	—	-5.8	15.9
<i>u</i> 3345	C(49)...H(58)	360.1(40)	18.3(fixed)	—	-1.5	18.3
<i>u</i> 1718	Si(289)...C(296)	360.1(24)	18.1(tied to <i>u</i> 1859)	—	0.1	18.2
<i>u</i> 1834	H(97)...H(113)	360.1(25)	15.7(fixed)	—	-5.7	15.7
<i>u</i> 4112	H(261)...H(269)	360.1(74)	26.4(fixed)	—	-3.4	26.4
<i>u</i> 1758	Si(127)...C(129)	360.2(49)	20.4(tied to <i>u</i> 1859)	—	0.4	20.5
<i>u</i> 3669	H(226)...H(244)	360.3(236)	41.8(fixed)	—	1.9	41.8
<i>u</i> 1844	H(261)...H(277)	360.3(25)	16.2(fixed)	—	-5.9	16.2
<i>u</i> 2046	H(60)...H(67)	360.4(109)	44.3(fixed)	—	6.4	44.3
<i>u</i> 1849	H(99)...H(102)	360.5(25)	15.5(fixed)	—	-5.0	15.5
<i>u</i> 2031	H(62)...H(73)	360.5(112)	32.9(fixed)	—	6.6	32.9
<i>u</i> 1855	H(219)...H(242)	360.6(25)	15.2(fixed)	—	-4.5	15.2
<i>u</i> 1809	H(178)...H(201)	360.7(25)	15.6(fixed)	—	-4.9	15.6
<i>u</i> 1838	H(55)...H(78)	360.7(25)	15.2(fixed)	—	-4.5	15.2
<i>u</i> 1821	H(220)...H(238)	360.8(25)	15.6(fixed)	—	-5.0	15.6
<i>u</i> 1592	Si(43)...H(70)	360.8(41)	29.1(fixed)	—	4.8	29.1
<i>u</i> 1841	Si(46)...C(49)	360.8(18)	16.7(tied to <i>u</i> 1859)	—	0.4	16.8
<i>u</i> 1816	H(58)...H(61)	360.9(25)	15.4(fixed)	—	-4.8	15.4
<i>u</i> 1711	Si(2)...C(10)	360.9(16)	19.2(tied to <i>u</i> 1859)	—	0.2	19.3
<i>u</i> 2028	H(20)...H(25)	361.0(72)	46.6(fixed)	—	10.4	46.6
<i>u</i> 1282	C(133)...H(143)	361.0(97)	34.8(fixed)	—	5.3	34.8
<i>u</i> 1825	H(98)...H(110)	361.0(25)	15.2(fixed)	—	-4.7	15.2
<i>u</i> 3674	C(93)...C(94)	361.2(51)	17.5(tied to <i>u</i> 1859)	—	-0.5	17.6
<i>u</i> 1856	H(302)...H(320)	361.2(25)	15.1(fixed)	—	-4.2	15.1
<i>u</i> 1806	H(57)...H(65)	361.3(25)	15.0(fixed)	—	-4.0	15.0
<i>u</i> 2081	H(184)...H(200)	361.3(98)	53.0(fixed)	—	-2.7	53.0
<i>u</i> 3573	H(71)...H(77)	361.4(94)	38.5(fixed)	—	9.6	38.5
<i>u</i> 1818	H(342)...H(367)	361.5(25)	15.3(fixed)	—	-4.5	15.3
<i>u</i> 1678	Si(4)...H(14)	361.5(47)	23.0(fixed)	—	-0.1	23.0
<i>u</i> 1326	Si(84)...H(99)	361.6(14)	21.6(fixed)	—	0.4	21.6
<i>u</i> 1839	H(56)...H(74)	361.6(25)	15.1(fixed)	—	-4.1	15.1
<i>u</i> 1830	H(137)...H(162)	361.6(25)	15.1(fixed)	—	-4.3	15.1
<i>u</i> 4715	H(236)...H(242)	361.6(129)	44.6(fixed)	—	-6.3	44.6
<i>u</i> 1835	H(260)...H(283)	361.6(25)	15.0(fixed)	—	-3.8	15.0
<i>u</i> 1826	H(138)...H(154)	361.8(25)	15.1(fixed)	—	-3.9	15.1
<i>u</i> 1757	Si(4)...C(12)	361.8(38)	16.4(tied to <i>u</i> 1859)	—	0.8	16.5
<i>u</i> 1833	H(260)...H(285)	361.8(25)	15.0(fixed)	—	-3.8	15.0
<i>u</i> 1813	H(301)...H(326)	361.8(25)	15.2(fixed)	—	-4.0	15.2
<i>u</i> 1837	H(99)...H(105)	361.9(25)	14.9(fixed)	—	-3.5	14.9
<i>u</i> 1723	Si(332)...H(342)	362.0(16)	20.9(fixed)	—	-0.2	20.9

<i>u</i> 1649	Si(46)...H(78)	362.0(97)	32.2(fixed)	—	7.5	32.2
<i>u</i> 1843	H(343)...H(361)	362.0(25)	14.9(fixed)	—	-3.6	14.9
<i>u</i> 3472	Si(207)...H(237)	362.1(41)	22.8(fixed)	—	-0.8	22.8
<i>u</i> 1948	Si(249)...H(269)	362.1(60)	31.4(fixed)	—	-0.2	31.4
<i>u</i> 1810	H(98)...H(106)	362.1(25)	14.9(fixed)	—	-3.5	14.9
<i>u</i> 1846	H(140)...H(146)	362.2(25)	14.8(fixed)	—	-3.3	14.8
<i>u</i> 3402	H(227)...H(241)	362.2(27)	56.7(fixed)	—	4.2	56.7
<i>u</i> 1854	H(221)...H(229)	362.2(25)	14.7(fixed)	—	-3.1	14.7
<i>u</i> 1820	H(14)...H(37)	362.3(25)	14.8(fixed)	—	-3.1	14.8
<i>u</i> 1733	Si(210)...C(218)	362.3(74)	19.5(tied to <i>u</i> 1859)	—	0.1	19.6
<i>u</i> 1796	H(57)...H(69)	362.3(25)	14.8(fixed)	—	-3.1	14.8
<i>u</i> 1807	H(219)...H(244)	362.3(25)	14.8(fixed)	—	-3.0	14.8
<i>u</i> 3517	Si(86)...H(100)	362.4(64)	21.6(fixed)	—	-1.1	21.6
<i>u</i> 5180	H(73)...H(79)	362.5(41)	25.4(fixed)	—	-9.7	25.4
<i>u</i> 1828	H(97)...H(115)	362.5(25)	14.8(fixed)	—	-3.3	14.8
<i>u</i> 2375	Si(248)...C(257)	362.5(11)	17.1(tied to <i>u</i> 1859)	—	-0.4	17.2
<i>u</i> 2016	C(293)...C(299)	362.5(52)	30.9(tied to <i>u</i> 1859)	—	1.1	31.1
<i>u</i> 1804	H(221)...H(233)	362.5(25)	14.9(fixed)	—	-2.9	14.9
<i>u</i> 1788	H(55)...H(80)	362.6(25)	14.8(fixed)	—	-2.9	14.8
<i>u</i> 1789	Si(87)...C(90)	362.6(17)	16.0(tied to <i>u</i> 1859)	—	0.4	16.1
<i>u</i> 3881	C(92)...H(111)	362.6(103)	46.4(fixed)	—	-0.3	46.4
<i>u</i> 1824	H(343)...H(359)	362.6(25)	14.9(fixed)	—	-3.2	14.9
<i>u</i> 1797	H(139)...H(151)	362.6(25)	14.9(fixed)	—	-3.2	14.9
<i>u</i> 1805	H(302)...H(318)	362.7(25)	14.9(fixed)	—	-2.9	14.9
<i>u</i> 4933	H(104)...H(120)	362.7(158)	33.5(fixed)	—	-2.0	33.5
<i>u</i> 2264	H(318)...H(323)	362.7(102)	38.6(fixed)	—	-0.6	38.6
<i>u</i> 1792	H(178)...H(203)	362.7(25)	15.0(fixed)	—	-3.1	15.0
<i>u</i> 1755	Si(86)...C(89)	362.7(42)	15.5(tied to <i>u</i> 1859)	—	0.4	15.6
<i>u</i> 5194	H(61)...H(76)	362.7(82)	35.4(fixed)	—	-2.3	35.4
<i>u</i> 1811	H(56)...H(72)	362.7(25)	14.9(fixed)	—	-3.1	14.9
<i>u</i> 1786	H(14)...H(39)	362.8(25)	14.9(fixed)	—	-2.8	14.9
<i>u</i> 4905	H(67)...H(76)	362.8(161)	36.0(fixed)	—	-7.2	36.0
<i>u</i> 1653	Si(125)...H(152)	362.8(35)	30.3(fixed)	—	4.9	30.3
<i>u</i> 1795	H(139)...H(147)	362.8(25)	14.7(fixed)	—	-2.9	14.7
<i>u</i> 1808	H(140)...H(143)	362.8(25)	14.9(fixed)	—	-2.9	14.9
<i>u</i> 1800	H(58)...H(64)	362.8(25)	14.7(fixed)	—	-2.8	14.7
<i>u</i> 1642	Si(45)...H(55)	362.9(57)	21.1(fixed)	—	-0.1	21.1
<i>u</i> 1803	H(96)...H(119)	363.0(25)	14.7(fixed)	—	-2.9	14.7
<i>u</i> 1802	H(222)...H(228)	363.0(25)	14.7(fixed)	—	-2.8	14.7
<i>u</i> 1798	H(301)...H(324)	363.0(25)	14.7(fixed)	—	-2.8	14.7
<i>u</i> 1705	C(255)...C(259)	363.0(33)	20.2(tied to <i>u</i> 1859)	—	1.9	20.4
<i>u</i> 5018	H(148)...H(158)	363.1(51)	50.9(fixed)	—	-11.0	50.9
<i>u</i> 1793	H(342)...H(365)	363.1(25)	14.7(fixed)	—	-2.8	14.7
<i>u</i> 1845	H(263)...H(266)	363.1(25)	14.9(fixed)	—	-3.2	14.9

<i>u</i> 1814	H(222)...H(225)	363.1(25)	14.8(fixed)	—	-2.8	14.8
<i>u</i> 1751	Si(248)...C(255)	363.1(20)	18.0(tied to <i>u</i> 1859)	—	0.3	18.2
<i>u</i> 1791	H(96)...H(121)	363.2(25)	14.8(fixed)	—	-2.8	14.8
<i>u</i> 1694	Si(209)...C(213)	363.2(32)	15.0(tied to <i>u</i> 1859)	—	0.7	15.1
<i>u</i> 1744	C(334)...C(336)	363.2(36)	20.8(tied to <i>u</i> 1859)	—	1.7	21.0
<i>u</i> 1271	Si(166)...H(180)	363.3(24)	22.3(fixed)	—	0.5	22.3
<i>u</i> 1870	H(275)...H(285)	363.3(54)	54.8(fixed)	—	2.3	54.8
<i>u</i> 4351	H(149)...H(156)	363.3(74)	34.8(fixed)	—	3.1	34.8
<i>u</i> 1817	H(263)...H(269)	363.4(25)	14.6(fixed)	—	-2.8	14.6
<i>u</i> 1827	H(262)...H(270)	363.4(25)	14.7(fixed)	—	-2.8	14.7
<i>u</i> 1754	Si(87)...C(95)	363.4(63)	19.6(tied to <i>u</i> 1859)	—	0.7	19.7
<i>u</i> 1812	H(261)...H(279)	363.4(25)	14.7(fixed)	—	-2.8	14.7
<i>u</i> 1097	Si(43)...H(58)	363.6(17)	22.0(fixed)	—	0.6	22.0
<i>u</i> 1832	H(262)...H(274)	363.6(25)	14.8(fixed)	—	-2.8	14.8
<i>u</i> 1562	Si(330)...H(357)	363.6(26)	28.3(fixed)	—	8.1	28.3
<i>u</i> 2958	Si(126)...C(130)	363.7(17)	11.4(tied to <i>u</i> 1859)	—	-1.4	11.5
<i>u</i> 3615	H(226)...H(242)	363.8(185)	49.9(fixed)	—	5.8	49.9
<i>u</i> 3549	H(235)...H(241)	363.9(38)	39.5(fixed)	—	10.5	39.5
<i>u</i> 2703	C(252)...H(286)	364.1(80)	41.7(fixed)	—	-3.6	41.7
<i>u</i> 1664	Si(85)...H(122)	364.1(130)	31.0(fixed)	—	3.7	31.0
<i>u</i> 3951	H(104)...H(118)	364.2(391)	40.0(fixed)	—	4.5	40.0
<i>u</i> 1195	Si(126)...H(140)	364.2(19)	22.5(fixed)	—	0.6	22.5
<i>u</i> 3459	Si(43)...H(73)	364.4(29)	20.2(fixed)	—	-1.3	20.2
<i>u</i> 1746	Si(4)...H(24)	364.4(49)	33.7(fixed)	—	4.3	33.7
<i>u</i> 2145	H(189)...H(195)	364.4(111)	46.2(fixed)	—	0.5	46.2
<i>u</i> 1710	Si(127)...H(137)	364.5(15)	22.7(fixed)	—	-0.3	22.7
<i>u</i> 1965	C(257)...C(258)	364.6(49)	26.7(tied to <i>u</i> 1859)	—	0.9	26.9
<i>u</i> 1794	Si(290)...H(304)	364.7(27)	20.8(fixed)	—	-0.3	20.8
<i>u</i> 4734	H(145)...H(147)	364.7(136)	35.0(fixed)	—	-4.2	35.0
<i>u</i> 1801	Si(207)...C(214)	364.7(32)	19.7(tied to <i>u</i> 1859)	—	0.2	19.8
<i>u</i> 1945	C(335)...C(341)	364.8(40)	22.1(tied to <i>u</i> 1859)	—	0.6	22.3
<i>u</i> 1747	C(213)...C(216)	364.9(86)	22.4(tied to <i>u</i> 1859)	—	1.7	22.6
<i>u</i> 3350	C(50)...H(56)	365.0(34)	19.6(fixed)	—	-1.7	19.6
<i>u</i> 3331	C(90)...H(99)	365.1(36)	17.8(fixed)	—	-1.4	17.8
<i>u</i> 3501	Si(125)...H(155)	365.1(43)	21.0(fixed)	—	-1.7	21.0
<i>u</i> 2583	Si(248)...H(261)	365.1(13)	13.5(fixed)	—	-1.2	13.5
<i>u</i> 4566	H(140)...H(158)	365.2(77)	31.3(fixed)	—	0.6	31.3
<i>u</i> 2199	H(151)...H(157)	365.2(112)	54.1(fixed)	—	-1.3	54.1
<i>u</i> 2955	C(93)...H(103)	365.3(99)	28.7(fixed)	—	-4.8	28.7
<i>u</i> 2147	Si(127)...H(160)	365.3(73)	75.5(fixed)	—	-5.5	75.5
<i>u</i> 2012	Si(332)...H(346)	365.4(64)	35.2(fixed)	—	0.1	35.2
<i>u</i> 1086	Si(207)...H(222)	366.0(28)	22.0(fixed)	—	0.8	22.0
<i>u</i> 1178	C(51)...H(63)	366.2(104)	35.3(fixed)	—	4.7	35.3
<i>u</i> 1764	C(293)...C(297)	366.6(43)	22.0(tied to <i>u</i> 1859)	—	1.3	22.1

<i>u</i> 1672	H(152)...H(158)	366.7(118)	85.5(fixed)	—	2.6	85.5
<i>u</i> 1978	Si(209)...H(242)	367.1(34)	43.5(fixed)	—	-1.1	43.5
<i>u</i> 3842	H(65)...H(75)	367.3(57)	42.1(fixed)	—	3.2	42.1
<i>u</i> 1715	Si(46)...H(57)	367.8(23)	22.2(fixed)	—	-0.2	22.2
<i>u</i> 1941	Si(86)...H(119)	367.9(177)	30.9(fixed)	—	0.5	30.9
<i>u</i> 1769	Si(46)...C(54)	367.9(62)	20.3(tied to <i>u</i> 1859)	—	0.1	20.4
<i>u</i> 1819	H(15)...H(33)	368.0(234)	15.8(fixed)	—	-5.5	15.8
<i>u</i> 2094	H(15)...H(26)	368.0(192)	42.9(fixed)	—	-0.9	42.9
<i>u</i> 2050	Si(332)...H(352)	368.1(42)	30.1(fixed)	—	2.8	30.1
<i>u</i> 2102	H(305)...H(323)	368.1(145)	55.3(fixed)	—	5.5	55.3
<i>u</i> 3707	C(130)...C(131)	368.1(54)	17.9(tied to <i>u</i> 1859)	—	-1.3	18.0
<i>u</i> 3667	C(48)...H(77)	368.2(101)	47.8(fixed)	—	-0.3	47.8
<i>u</i> 1742	C(214)...C(218)	368.4(120)	21.6(tied to <i>u</i> 1859)	—	2.3	21.7
<i>u</i> 4042	H(103)...H(119)	368.7(197)	48.9(fixed)	—	1.9	48.9
<i>u</i> 1893	H(139)...H(162)	369.1(61)	45.8(fixed)	—	-1.4	45.8
<i>u</i> 4957	H(149)...H(158)	369.1(144)	39.8(fixed)	—	-8.5	39.8
<i>u</i> 4701	H(117)...H(119)	369.3(61)	32.4(fixed)	—	-3.5	32.4
<i>u</i> 4004	C(257)...H(270)	369.4(105)	31.2(fixed)	—	-1.3	31.2
<i>u</i> 1654	Si(45)...C(48)	369.5(43)	15.9(tied to <i>u</i> 1859)	—	0.6	16.0
<i>u</i> 2077	H(270)...H(277)	369.5(113)	61.0(fixed)	—	-1.9	61.0
<i>u</i> 1774	C(7)...C(8)	369.5(33)	24.5(tied to <i>u</i> 1859)	—	2.4	24.6
<i>u</i> 2429	H(191)...H(195)	369.6(117)	55.7(fixed)	—	3.1	55.7
<i>u</i> 1979	Si(290)...H(310)	369.6(71)	32.0(fixed)	—	0.0	32.0
<i>u</i> 4101	H(146)...H(149)	369.7(123)	32.6(fixed)	—	-0.3	32.6
<i>u</i> 5199	H(63)...H(82)	369.7(107)	30.4(fixed)	—	-7.0	30.4
<i>u</i> 1671	Si(86)...H(96)	370.2(71)	23.4(fixed)	—	-0.2	23.4
<i>u</i> 655	H(279)...H(282)	370.2(86)	50.4(fixed)	—	12.2	50.4
<i>u</i> 1752	Si(87)...H(98)	370.5(23)	21.3(fixed)	—	-0.3	21.3
<i>u</i> 1904	Si(87)...H(119)	370.6(67)	37.1(fixed)	—	2.9	37.1
<i>u</i> 1708	Si(209)...H(219)	370.9(74)	20.7(fixed)	—	-0.2	20.7
<i>u</i> 1783	Si(127)...C(132)	371.0(22)	17.6(tied to <i>u</i> 1859)	—	0.5	17.8
<i>u</i> 1697	Si(210)...H(242)	371.2(134)	32.6(fixed)	—	7.0	32.6
<i>u</i> 1648	C(254)...C(256)	371.2(45)	19.0(tied to <i>u</i> 1859)	—	2.1	19.2
<i>u</i> 1932	Si(167)...H(197)	371.4(50)	33.0(fixed)	—	7.0	33.0
<i>u</i> 5245	H(104)...H(123)	371.6(169)	27.8(fixed)	—	-6.4	27.8
<i>u</i> 1428	C(91)...H(97)	371.7(41)	31.4(fixed)	—	1.3	31.4
<i>u</i> 4756	H(72)...H(78)	371.7(109)	44.3(fixed)	—	-5.5	44.3
<i>u</i> 1908	H(96)...H(110)	371.8(71)	46.9(fixed)	—	-1.8	46.9
<i>u</i> 4769	C(171)...C(175)	371.8(77)	12.7(tied to <i>u</i> 1859)	—	-2.2	12.7
<i>u</i> 1877	H(306)...H(318)	372.0(43)	50.4(fixed)	—	2.8	50.4
<i>u</i> 2586	Si(208)...H(220)	372.3(29)	13.3(fixed)	—	-1.1	13.3
<i>u</i> 1619	Si(209)...C(212)	372.3(54)	15.9(tied to <i>u</i> 1859)	—	1.0	16.0
<i>u</i> 1924	Si(45)...H(65)	372.3(44)	29.7(fixed)	—	5.6	29.7
<i>u</i> 4738	H(227)...H(245)	372.4(199)	35.9(fixed)	—	-4.7	35.9

<i>u</i> 2116	H(102)...H(106)	372.5(121)	42.3(fixed)	—	7.7	42.3
<i>u</i> 3851	H(103)...H(121)	372.6(117)	41.9(fixed)	—	3.3	41.9
<i>u</i> 1873	Si(332)...H(357)	372.6(67)	44.5(fixed)	—	0.6	44.5
<i>u</i> 4132	H(147)...H(157)	372.7(57)	49.7(fixed)	—	-2.4	49.7
<i>u</i> 1871	Si(249)...H(286)	372.8(27)	26.5(fixed)	—	5.6	26.5
<i>u</i> 3378	C(259)...H(263)	372.9(67)	19.2(fixed)	—	-1.6	19.2
<i>u</i> 3903	C(252)...C(255)	372.9(58)	18.0(tied to <i>u</i> 1859)	—	-0.9	18.2
<i>u</i> 1065	C(215)...H(227)	372.9(156)	32.2(fixed)	—	5.5	32.2
<i>u</i> 1720	Si(128)...C(136)	373.0(21)	20.7(tied to <i>u</i> 1859)	—	0.1	20.8
<i>u</i> 1899	H(234)...H(244)	373.2(190)	52.8(fixed)	—	4.0	52.8
<i>u</i> 1888	Si(330)...H(360)	373.2(35)	26.2(fixed)	—	4.4	26.2
<i>u</i> 1831	Si(249)...H(278)	373.2(59)	28.7(fixed)	—	10.8	28.7
<i>u</i> 2629	Si(126)...H(138)	373.3(37)	13.3(fixed)	—	-1.4	13.3
<i>u</i> 3777	C(212)...C(218)	373.4(123)	20.2(tied to <i>u</i> 1859)	—	-2.3	20.3
<i>u</i> 1840	H(15)...H(31)	373.5(234)	15.2(fixed)	—	-4.5	15.2
<i>u</i> 1726	Si(128)...H(139)	373.5(19)	22.4(fixed)	—	-0.3	22.4
<i>u</i> 1863	Si(45)...C(50)	373.7(27)	18.7(tied to <i>u</i> 1859)	—	0.2	18.8
<i>u</i> 2002	Si(166)...H(182)	373.8(74)	37.1(fixed)	—	0.0	37.1
<i>u</i> 2092	Si(330)...H(351)	374.0(71)	37.0(fixed)	—	-0.7	37.0
<i>u</i> 2141	H(69)...H(75)	374.2(101)	47.4(fixed)	—	1.9	47.4
<i>u</i> 2115	H(61)...H(65)	374.2(132)	43.2(fixed)	—	6.3	43.2
<i>u</i> 1937	H(274)...H(287)	374.5(32)	48.0(fixed)	—	2.3	48.0
<i>u</i> 1777	Si(250)...H(260)	374.6(22)	21.1(fixed)	—	-0.3	21.1
<i>u</i> 1689	Si(289)...H(311)	374.6(43)	31.8(fixed)	—	6.1	31.8
<i>u</i> 1878	Si(208)...H(245)	374.7(79)	26.5(fixed)	—	4.1	26.5
<i>u</i> 2070	Si(45)...H(78)	374.7(47)	44.4(fixed)	—	-1.6	44.4
<i>u</i> 2938	H(140)...H(155)	375.1(119)	33.9(fixed)	—	4.1	33.9
<i>u</i> 4914	H(266)...H(273)	375.2(50)	31.0(fixed)	—	-2.9	31.0
<i>u</i> 2095	H(145)...H(163)	375.3(179)	47.8(fixed)	—	1.5	47.8
<i>u</i> 1728	Si(86)...C(91)	375.3(27)	18.5(tied to <i>u</i> 1859)	—	0.2	18.6
<i>u</i> 1992	C(130)...C(136)	375.3(55)	24.8(tied to <i>u</i> 1859)	—	0.8	25.0
<i>u</i> 3504	Si(84)...H(115)	375.5(32)	20.5(fixed)	—	-1.7	20.5
<i>u</i> 2619	Si(44)...H(56)	375.6(19)	13.1(fixed)	—	-1.2	13.1
<i>u</i> 2996	Si(128)...C(134)	375.7(49)	11.1(tied to <i>u</i> 1859)	—	-1.1	11.2
<i>u</i> 5304	C(256)...H(267)	375.7(77)	15.5(fixed)	—	-5.0	15.5
<i>u</i> 2054	H(19)...H(26)	375.7(149)	48.2(fixed)	—	4.1	48.2
<i>u</i> 3628	C(254)...C(257)	375.8(40)	16.4(tied to <i>u</i> 1859)	—	-0.8	16.5
<i>u</i> 2057	H(316)...H(326)	376.0(65)	58.4(fixed)	—	0.8	58.4
<i>u</i> 2043	Si(127)...H(147)	376.1(37)	32.7(fixed)	—	2.9	32.7
<i>u</i> 1883	C(295)...C(298)	376.3(94)	19.9(tied to <i>u</i> 1859)	—	0.6	20.0
<i>u</i> 3524	Si(207)...H(228)	376.4(104)	20.2(fixed)	—	-2.4	20.2
<i>u</i> 2066	H(188)...H(194)	376.4(62)	39.4(fixed)	—	11.5	39.4
<i>u</i> 1879	Si(290)...H(327)	376.5(42)	27.3(fixed)	—	6.1	27.3
<i>u</i> 2062	H(21)...H(26)	376.8(42)	48.0(fixed)	—	1.4	48.0

<i>u</i> 4219	H(142)...H(160)	377.2(55)	55.1(fixed)	—	24.4	55.1
<i>u</i> 1928	Si(125)...H(146)	377.3(32)	36.1(fixed)	—	0.4	36.1
<i>u</i> 1862	H(70)...H(76)	377.5(77)	66.3(fixed)	—	3.1	66.3
<i>u</i> 1951	H(301)...H(313)	377.8(102)	44.6(fixed)	—	-2.0	44.6
<i>u</i> 1874	Si(251)...C(259)	377.8(26)	17.9(tied to <i>u</i> 1859)	—	0.1	18.0
<i>u</i> 2653	Si(2)...H(35)	377.8(484)	42.2(fixed)	—	-2.2	42.2
<i>u</i> 2685	Si(2)...H(20)	377.8(571)	36.2(fixed)	—	-2.7	36.2
<i>u</i> 1962	Si(86)...H(106)	378.0(50)	29.4(fixed)	—	4.2	29.4
<i>u</i> 1977	Si(332)...H(351)	378.0(40)	29.8(fixed)	—	4.4	29.8
<i>u</i> 1998	H(342)...H(356)	378.1(75)	43.6(fixed)	—	-3.3	43.6
<i>u</i> 2268	C(173)...C(174)	378.1(100)	35.2(tied to <i>u</i> 1859)	—	-0.4	35.4
<i>u</i> 2007	Si(4)...H(29)	378.4(62)	34.2(fixed)	—	0.2	34.2
<i>u</i> 1897	Si(210)...H(234)	378.5(55)	26.6(fixed)	—	3.9	26.6
<i>u</i> 2017	H(14)...H(28)	378.6(107)	37.5(fixed)	—	0.6	37.5
<i>u</i> 3528	Si(43)...H(64)	378.9(69)	19.8(fixed)	—	-2.1	19.8
<i>u</i> 3888	H(97)...H(108)	378.9(76)	29.0(fixed)	—	-4.0	29.0
<i>u</i> 3497	Si(125)...H(141)	379.0(56)	19.6(fixed)	—	-1.6	19.6
<i>u</i> 2118	Si(250)...H(283)	379.5(59)	37.6(fixed)	—	-0.8	37.6
<i>u</i> 3446	Si(249)...H(264)	379.6(86)	19.9(fixed)	—	-1.1	19.9
<i>u</i> 2830	C(51)...H(62)	379.6(98)	24.4(fixed)	—	-2.1	24.4
<i>u</i> 2960	Si(210)...C(216)	379.8(40)	12.7(tied to <i>u</i> 2037)	—	-0.9	10.9
<i>u</i> 1997	H(55)...H(69)	379.9(73)	40.4(fixed)	—	-0.4	40.4
<i>u</i> 1954	H(57)...H(80)	379.9(165)	38.5(fixed)	—	0.1	38.5
<i>u</i> 2114	Si(289)...H(310)	379.9(48)	32.2(fixed)	—	2.5	32.2
<i>u</i> 1983	Si(251)...H(283)	380.0(51)	29.8(fixed)	—	4.8	29.8
<i>u</i> 3480	Si(85)...H(114)	380.0(39)	22.8(fixed)	—	-0.4	22.8
<i>u</i> 3603	H(263)...H(282)	380.0(63)	39.8(fixed)	—	-0.8	39.8
<i>u</i> 1993	Si(128)...H(147)	380.1(77)	33.9(fixed)	—	0.0	33.9
<i>u</i> 1958	Si(248)...H(275)	380.2(45)	31.1(fixed)	—	0.3	31.1
<i>u</i> 4574	H(140)...H(153)	380.4(81)	24.5(fixed)	—	-7.5	24.5
<i>u</i> 1952	Si(208)...H(238)	380.5(61)	30.6(fixed)	—	7.1	30.6
<i>u</i> 5212	H(115)...H(120)	380.5(77)	22.4(fixed)	—	-6.1	22.4
<i>u</i> 1940	Si(128)...H(160)	380.8(39)	43.1(fixed)	—	23.7	43.1
<i>u</i> 3827	H(62)...H(80)	381.0(216)	41.9(fixed)	—	2.2	41.9
<i>u</i> 1991	Si(289)...H(316)	381.0(55)	33.3(fixed)	—	-0.2	33.3
<i>u</i> 1338	C(7)...H(20)	381.2(694)	30.1(fixed)	—	0.8	30.1
<i>u</i> 1981	Si(248)...H(264)	381.3(32)	34.0(fixed)	—	0.4	34.0
<i>u</i> 3747	C(91)...C(92)	381.4(42)	22.5(tied to <i>u</i> 2037)	—	-1.2	19.3
<i>u</i> 1905	Si(251)...H(275)	381.4(50)	26.2(fixed)	—	3.2	26.2
<i>u</i> 3597	H(116)...H(118)	381.9(110)	37.3(fixed)	—	4.6	37.3
<i>u</i> 1914	H(226)...H(237)	382.0(139)	35.7(fixed)	—	19.4	35.7
<i>u</i> 1955	H(233)...H(246)	382.0(128)	44.1(fixed)	—	4.3	44.1
<i>u</i> 5101	H(140)...H(157)	382.1(111)	18.4(fixed)	—	-9.4	18.4
<i>u</i> 2023	Si(207)...H(234)	382.2(72)	34.3(fixed)	—	0.1	34.3

<i>u</i> 1852	Si(84)...H(114)	382.2(55)	28.3(fixed)	—	10.3	28.3
<i>u</i> 2052	C(6)...C(8)	382.3(87)	31.2(tied to <i>u</i> 2037)	—	0.6	26.7
<i>u</i> 673	H(262)...H(268)	382.3(73)	37.5(fixed)	—	6.7	37.5
<i>u</i> 444	H(231)...H(238)	382.7(125)	43.6(fixed)	—	20.0	43.6
<i>u</i> 1963	Si(44)...H(74)	382.8(66)	30.2(fixed)	—	5.6	30.2
<i>u</i> 2393	H(308)...H(326)	383.5(115)	59.4(fixed)	—	4.3	59.4
<i>u</i> 1882	Si(207)...H(229)	383.7(60)	33.8(fixed)	—	3.5	33.8
<i>u</i> 1790	C(132)...C(134)	383.7(65)	31.1(tied to <i>u</i> 2037)	—	1.9	26.7
<i>u</i> 3505	Si(249)...H(279)	383.9(35)	19.7(fixed)	—	-1.8	19.7
<i>u</i> 5029	H(186)...H(197)	384.0(109)	39.2(fixed)	—	4.7	39.2
<i>u</i> 2089	H(137)...H(151)	384.2(64)	40.0(fixed)	—	-1.3	40.0
<i>u</i> 4174	H(228)...H(244)	384.3(125)	35.0(fixed)	—	-1.0	35.0
<i>u</i> 1968	Si(248)...H(270)	384.3(27)	34.7(fixed)	—	2.6	34.7
<i>u</i> 2961	Si(46)...C(52)	384.3(32)	12.9(tied to <i>u</i> 2037)	—	-1.0	11.0
<i>u</i> 1872	C(50)...C(52)	384.6(49)	29.8(tied to <i>u</i> 2037)	—	1.4	25.5
<i>u</i> 2022	Si(210)...H(245)	384.7(165)	35.6(fixed)	—	-0.4	35.6
<i>u</i> 1959	Si(291)...H(311)	384.8(81)	41.1(fixed)	—	-1.0	41.1
<i>u</i> 5397	H(223)...H(239)	384.8(121)	25.5(fixed)	—	-8.1	25.5
<i>u</i> 3502	H(178)...H(195)	384.8(91)	33.3(fixed)	—	0.8	33.3
<i>u</i> 2385	H(306)...H(324)	384.9(75)	45.4(fixed)	—	0.4	45.4
<i>u</i> 2098	C(252)...C(259)	384.9(41)	30.7(tied to <i>u</i> 2037)	—	0.1	26.3
<i>u</i> 1933	Si(87)...H(122)	385.4(72)	31.5(fixed)	—	0.6	31.5
<i>u</i> 1261	H(220)...H(242)	385.5(119)	58.0(fixed)	—	2.5	58.0
<i>u</i> 2013	Si(46)...C(53)	385.5(54)	20.4(tied to <i>u</i> 2037)	—	-0.1	17.5
<i>u</i> 457	H(272)...H(278)	385.7(70)	45.5(fixed)	—	19.4	45.5
<i>u</i> 3464	H(272)...H(280)	385.7(43)	35.3(fixed)	—	3.9	35.3
<i>u</i> 2581	C(129)...H(153)	386.1(100)	33.5(fixed)	—	-2.5	33.5
<i>u</i> 3612	H(153)...H(159)	386.1(81)	58.9(fixed)	—	34.9	58.9
<i>u</i> 2757	C(215)...H(226)	386.2(90)	21.9(fixed)	—	-0.5	21.9
<i>u</i> 3806	C(89)...C(95)	386.2(139)	22.7(tied to <i>u</i> 2037)	—	-1.1	19.4
<i>u</i> 2188	Si(46)...H(65)	386.4(72)	39.9(fixed)	—	-1.1	39.9
<i>u</i> 2718	C(89)...H(116)	386.4(91)	35.1(fixed)	—	-2.7	35.1
<i>u</i> 1552	H(138)...H(160)	386.6(68)	98.9(fixed)	—	0.7	98.9
<i>u</i> 2376	H(184)...H(204)	386.7(159)	51.6(fixed)	—	1.4	51.6
<i>u</i> 1969	Si(126)...C(136)	386.8(13)	17.9(tied to <i>u</i> 2037)	—	0.2	15.4
<i>u</i> 1961	H(273)...H(286)	386.8(41)	31.7(fixed)	—	9.9	31.7
<i>u</i> 2207	Si(289)...C(297)	386.9(27)	17.4(tied to <i>u</i> 2037)	—	-0.2	14.9
<i>u</i> 3363	H(146)...H(164)	387.0(59)	46.2(fixed)	—	-6.5	46.2
<i>u</i> 2243	C(136)...H(159)	387.1(24)	16.2(fixed)	—	-13.0	16.2
<i>u</i> 1980	Si(84)...C(91)	387.4(22)	18.1(tied to <i>u</i> 2037)	—	0.0	15.5
<i>u</i> 3529	Si(166)...H(188)	387.6(59)	22.5(fixed)	—	-2.1	22.5
<i>u</i> 1517	C(1)...H(18)	387.7(635)	24.8(fixed)	—	1.7	24.8
<i>u</i> 4349	C(52)...H(67)	387.8(101)	32.8(fixed)	—	-5.0	32.8
<i>u</i> 4925	C(211)...H(240)	387.8(85)	25.3(fixed)	—	0.1	25.3

<i>u</i> 2262	C(170)...H(200)	387.9(84)	52.7(fixed)	—	-2.0	52.7
<i>u</i> 1999	Si(332)...H(365)	387.9(61)	32.0(fixed)	—	-0.1	32.0
<i>u</i> 2120	Si(87)...H(106)	388.0(62)	36.7(fixed)	—	-0.5	36.7
<i>u</i> 2037	Si(2)...C(9)	388.1(57)	20.7(12)	—	0.1	17.8
<i>u</i> 3541	Si(84)...H(105)	388.5(69)	20.8(fixed)	—	-1.7	20.8
<i>u</i> 4687	H(111)...H(113)	388.5(58)	44.9(fixed)	—	-5.2	44.9
<i>u</i> 3745	C(212)...H(241)	388.8(108)	47.3(fixed)	—	-0.9	47.3
<i>u</i> 2261	H(274)...H(285)	388.9(120)	42.6(fixed)	—	-2.6	42.6
<i>u</i> 3760	H(272)...H(281)	389.0(180)	34.3(fixed)	—	1.6	34.3
<i>u</i> 3829	C(48)...C(54)	389.2(113)	24.0(tied to <i>u</i> 2037)	—	-2.0	20.6
<i>u</i> 4023	H(72)...H(77)	389.2(66)	33.0(fixed)	—	5.7	33.0
<i>u</i> 2125	Si(4)...C(8)	389.6(60)	23.4(tied to <i>u</i> 2037)	—	-0.2	20.0
<i>u</i> 2192	Si(128)...C(135)	389.6(17)	19.7(tied to <i>u</i> 2037)	—	-0.2	16.9
<i>u</i> 4818	C(211)...H(235)	389.6(109)	30.0(fixed)	—	-11.2	30.0
<i>u</i> 4692	H(104)...H(122)	389.9(192)	32.4(fixed)	—	-3.7	32.4
<i>u</i> 2995	Si(166)...C(174)	389.9(27)	12.4(tied to <i>u</i> 2037)	—	-1.4	10.7
<i>u</i> 862	H(221)...H(225)	389.9(67)	47.8(fixed)	—	5.9	47.8
<i>u</i> 5006	C(88)...H(116)	390.2(87)	23.1(fixed)	—	-6.2	23.1
<i>u</i> 2139	Si(2)...C(6)	390.8(16)	17.7(tied to <i>u</i> 2037)	—	-0.1	15.2
<i>u</i> 1985	H(232)...H(245)	390.8(163)	32.0(fixed)	—	7.4	32.0
<i>u</i> 1990	Si(330)...C(337)	390.8(17)	18.3(tied to <i>u</i> 2037)	—	-0.1	15.7
<i>u</i> 3738	H(262)...H(264)	390.8(85)	25.2(fixed)	—	-1.4	25.2
<i>u</i> 1929	Si(127)...H(152)	391.2(58)	37.5(fixed)	—	0.4	37.5
<i>u</i> 2069	H(311)...H(322)	391.8(162)	37.8(fixed)	—	3.7	37.8
<i>u</i> 2091	H(98)...H(121)	391.8(138)	36.6(fixed)	—	-0.2	36.6
<i>u</i> 2282	H(307)...H(318)	391.8(114)	42.7(fixed)	—	-3.1	42.7
<i>u</i> 2015	Si(5)...H(24)	391.9(132)	35.6(fixed)	—	0.1	35.6
<i>u</i> 2011	Si(44)...C(54)	391.9(58)	19.9(tied to <i>u</i> 2037)	—	0.0	17.0
<i>u</i> 1972	Si(126)...H(156)	392.1(52)	33.7(fixed)	—	9.7	33.7
<i>u</i> 2019	H(305)...H(317)	392.2(61)	34.5(fixed)	—	9.0	34.5
<i>u</i> 1622	Si(249)...C(253)	392.2(29)	18.2(tied to <i>u</i> 2037)	—	0.4	15.6
<i>u</i> 2035	Si(43)...C(50)	392.2(23)	20.2(tied to <i>u</i> 2037)	—	-0.1	17.3
<i>u</i> 2499	C(294)...H(315)	392.5(67)	31.4(fixed)	—	-1.4	31.4
<i>u</i> 2056	Si(125)...C(132)	392.8(19)	20.6(tied to <i>u</i> 2037)	—	-0.1	17.6
<i>u</i> 4731	C(93)...H(101)	392.9(94)	27.6(fixed)	—	-4.6	27.6
<i>u</i> 2196	C(133)...H(158)	393.0(24)	14.1(fixed)	—	-7.3	14.1
<i>u</i> 4666	C(51)...H(60)	393.1(90)	26.2(fixed)	—	-4.5	26.2
<i>u</i> 2235	Si(166)...C(171)	393.3(24)	19.5(tied to <i>u</i> 2037)	—	-0.2	16.7
<i>u</i> 2071	Si(210)...C(217)	393.3(76)	20.6(tied to <i>u</i> 2037)	—	-0.2	17.7
<i>u</i> 2340	Si(332)...C(336)	393.3(18)	20.0(tied to <i>u</i> 2037)	—	-0.4	17.2
<i>u</i> 2209	C(257)...H(278)	393.4(24)	14.1(fixed)	—	-6.7	14.1
<i>u</i> 4003	H(236)...H(241)	393.4(101)	34.0(fixed)	—	4.5	34.0
<i>u</i> 2195	C(216)...H(237)	393.5(24)	14.2(fixed)	—	-6.6	14.2
<i>u</i> 5231	H(143)...H(164)	393.7(99)	26.3(fixed)	—	-9.7	26.3



<i>u</i> 2201	C(93)...H(114)	393.7(24)	13.7(fixed)	—	-6.5	13.7
<i>u</i> 5333	H(141)...H(161)	393.8(80)	30.7(fixed)	—	-25.5	30.7
<i>u</i> 4586	C(215)...H(224)	394.0(108)	26.8(fixed)	—	-3.7	26.8
<i>u</i> 5197	H(271)...H(279)	394.0(58)	22.0(fixed)	—	-6.5	22.0
<i>u</i> 5203	H(109)...H(114)	394.1(51)	26.0(fixed)	—	-9.7	26.0
<i>u</i> 1716	Si(208)...C(211)	394.2(34)	21.9(tied to <i>u</i> 2037)	—	0.5	18.7
<i>u</i> 2436	H(310)...H(314)	394.3(81)	44.7(fixed)	—	-0.7	44.7
<i>u</i> 1413	H(56)...H(78)	394.4(97)	60.4(fixed)	—	1.9	60.4
<i>u</i> 1939	H(18)...H(41)	394.5(359)	34.8(fixed)	—	14.5	34.8
<i>u</i> 1912	Si(250)...H(270)	394.5(94)	30.1(fixed)	—	0.1	30.1
<i>u</i> 2181	C(89)...H(100)	394.6(24)	13.6(fixed)	—	-5.6	13.6
<i>u</i> 2064	Si(85)...C(95)	394.6(83)	21.6(tied to <i>u</i> 2037)	—	0.0	18.5
<i>u</i> 2026	Si(46)...H(81)	394.7(120)	34.9(fixed)	—	-0.4	34.9
<i>u</i> 2211	C(215)...H(240)	394.7(24)	13.7(fixed)	—	-5.6	13.7
<i>u</i> 1926	Si(86)...H(111)	394.8(71)	44.8(fixed)	—	0.0	44.8
<i>u</i> 2570	C(300)...H(305)	394.8(130)	44.1(fixed)	—	-3.2	44.1
<i>u</i> 4845	H(264)...H(274)	394.8(87)	36.5(fixed)	—	-3.1	36.5
<i>u</i> 2221	C(48)...H(59)	394.8(24)	13.3(fixed)	—	-5.4	13.3
<i>u</i> 2080	Si(248)...H(279)	395.0(70)	30.0(fixed)	—	2.6	30.0
<i>u</i> 2596	C(335)...H(364)	395.0(82)	35.4(fixed)	—	-1.7	35.4
<i>u</i> 2231	C(170)...H(186)	395.0(24)	13.6(fixed)	—	-5.3	13.6
<i>u</i> 2230	C(90)...H(111)	395.0(24)	13.2(fixed)	—	-5.2	13.2
<i>u</i> 3458	Si(126)...H(146)	395.0(82)	21.7(fixed)	—	-2.2	21.7
<i>u</i> 434	H(102)...H(108)	395.2(75)	43.5(fixed)	—	26.0	43.5
<i>u</i> 2239	C(336)...H(357)	395.2(24)	13.3(fixed)	—	-5.0	13.3
<i>u</i> 2218	C(54)...H(77)	395.3(24)	13.3(fixed)	—	-5.0	13.3
<i>u</i> 2175	C(218)...H(241)	395.3(24)	13.4(fixed)	—	-5.0	13.4
<i>u</i> 2240	Si(45)...C(49)	395.6(23)	19.0(tied to <i>u</i> 2037)	—	-0.2	16.3
<i>u</i> 2222	C(135)...H(163)	395.7(24)	13.1(fixed)	—	-4.5	13.1
<i>u</i> 2171	C(296)...H(313)	395.7(24)	13.3(fixed)	—	-4.6	13.3
<i>u</i> 1956	Si(209)...H(229)	395.8(73)	33.4(fixed)	—	0.2	33.4
<i>u</i> 2185	C(51)...H(76)	395.8(24)	13.2(fixed)	—	-4.6	13.2
<i>u</i> 2216	C(294)...H(305)	395.8(24)	13.1(fixed)	—	-4.4	13.1
<i>u</i> 3311	C(47)...H(73)	395.8(95)	32.8(fixed)	—	3.4	32.8
<i>u</i> 2232	C(50)...H(67)	395.9(24)	13.2(fixed)	—	-4.4	13.2
<i>u</i> 2180	C(134)...H(155)	396.0(24)	13.1(fixed)	—	-4.2	13.1
<i>u</i> 2224	H(233)...H(244)	396.1(313)	41.1(fixed)	—	-0.4	41.1
<i>u</i> 2178	C(258)...H(286)	396.1(24)	12.9(fixed)	—	-4.1	12.9
<i>u</i> 2982	Si(207)...C(215)	396.1(29)	12.2(tied to <i>u</i> 2037)	—	-1.0	10.5
<i>u</i> 2665	H(138)...H(161)	396.2(99)	42.9(fixed)	—	-24.0	42.9
<i>u</i> 2248	H(219)...H(231)	396.2(84)	41.0(fixed)	—	-1.1	41.0
<i>u</i> 2191	C(259)...H(282)	396.2(24)	13.1(fixed)	—	-4.2	13.1
<i>u</i> 4210	C(89)...H(118)	396.2(296)	32.1(fixed)	—	-1.1	32.1
<i>u</i> 2238	Si(87)...C(94)	396.3(86)	25.5(tied to <i>u</i> 2037)	—	-0.4	21.9

<i>u</i> 4678	H(270)...H(281)	396.3(53)	31.8(fixed)	—	-3.6	31.8
<i>u</i> 1617	C(1)...H(23)	396.4(585)	28.2(fixed)	—	1.2	28.2
<i>u</i> 2187	C(334)...H(350)	396.4(24)	13.0(fixed)	—	-3.9	13.0
<i>u</i> 4730	H(63)...H(81)	396.6(163)	34.8(fixed)	—	-4.4	34.8
<i>u</i> 2189	C(88)...H(104)	396.6(24)	12.9(fixed)	—	-3.8	12.9
<i>u</i> 2228	C(131)...H(152)	396.6(24)	12.7(fixed)	—	-3.6	12.7
<i>u</i> 2236	C(91)...H(108)	396.6(24)	13.1(fixed)	—	-3.8	13.1
<i>u</i> 439	H(145)...H(162)	396.7(102)	42.7(fixed)	—	21.8	42.7
<i>u</i> 2193	C(335)...H(346)	396.7(24)	12.7(fixed)	—	-3.6	12.7
<i>u</i> 2214	C(171)...H(182)	396.7(24)	12.8(fixed)	—	-3.5	12.8
<i>u</i> 2065	Si(289)...C(295)	396.7(29)	19.9(tied to <i>u</i> 2037)	—	-0.3	17.0
<i>u</i> 2183	C(52)...H(73)	396.8(24)	12.7(fixed)	—	-3.5	12.7
<i>u</i> 2198	C(253)...H(264)	396.8(24)	12.7(fixed)	—	-3.5	12.7
<i>u</i> 1970	Si(128)...H(163)	396.8(57)	44.5(fixed)	—	-0.5	44.5
<i>u</i> 2220	C(49)...H(70)	396.8(24)	12.7(fixed)	—	-3.4	12.7
<i>u</i> 2190	C(92)...H(117)	396.9(24)	13.0(fixed)	—	-3.5	13.0
<i>u</i> 2021	Si(45)...H(70)	396.9(61)	36.9(fixed)	—	-0.1	36.9
<i>u</i> 2168	C(217)...H(245)	396.9(24)	12.6(fixed)	—	-3.3	12.6
<i>u</i> 2149	C(129)...H(145)	396.9(24)	13.0(fixed)	—	-3.4	13.0
<i>u</i> 2169	C(295)...H(316)	397.0(24)	12.6(fixed)	—	-3.2	12.6
<i>u</i> 2157	C(213)...H(234)	397.1(24)	12.6(fixed)	—	-3.2	12.6
<i>u</i> 2173	C(9)...H(26)	397.1(24)	13.1(fixed)	—	-3.3	13.1
<i>u</i> 4906	C(47)...H(76)	397.1(85)	24.5(fixed)	—	-0.3	24.5
<i>u</i> 2205	C(53)...H(81)	397.1(24)	12.6(fixed)	—	-3.2	12.6
<i>u</i> 2197	C(8)...H(29)	397.1(24)	12.7(fixed)	—	-3.1	12.7
<i>u</i> 2253	H(303)...H(310)	397.1(98)	38.3(fixed)	—	-2.0	38.3
<i>u</i> 2148	C(214)...H(231)	397.2(24)	12.8(fixed)	—	-3.2	12.8
<i>u</i> 2165	C(130)...H(141)	397.2(24)	12.6(fixed)	—	-3.1	12.6
<i>u</i> 2174	C(212)...H(223)	397.2(24)	12.6(fixed)	—	-3.1	12.6
<i>u</i> 2194	C(94)...H(122)	397.2(24)	12.6(fixed)	—	-3.1	12.6
<i>u</i> 2163	C(254)...H(275)	397.2(24)	12.5(fixed)	—	-3.1	12.5
<i>u</i> 2217	C(132)...H(149)	397.3(24)	12.9(fixed)	—	-3.0	12.9
<i>u</i> 4589	C(215)...H(223)	397.4(86)	24.0(fixed)	—	-3.2	24.0
<i>u</i> 2233	C(337)...H(354)	397.4(24)	12.9(fixed)	—	-3.0	12.9
<i>u</i> 2350	C(124)...H(161)	397.4(21)	16.3(fixed)	—	-13.1	16.3
<i>u</i> 4611	C(51)...H(59)	397.4(89)	28.7(fixed)	—	-4.6	28.7
<i>u</i> 2172	C(95)...H(118)	397.4(24)	12.8(fixed)	—	-2.9	12.8
<i>u</i> 2203	C(293)...H(309)	397.5(24)	12.8(fixed)	—	-2.9	12.8
<i>u</i> 2184	C(256)...H(281)	397.5(24)	12.7(fixed)	—	-2.9	12.7
<i>u</i> 2208	C(47)...H(63)	397.5(24)	12.7(fixed)	—	-2.9	12.7
<i>u</i> 1756	Si(85)...C(88)	397.5(16)	22.2(tied to <i>u</i> 2037)	—	0.2	19.1
<i>u</i> 2177	C(252)...H(268)	397.5(24)	12.7(fixed)	—	-2.9	12.7
<i>u</i> 2152	C(255)...H(272)	397.5(24)	12.7(fixed)	—	-2.9	12.7
<i>u</i> 2162	C(211)...H(227)	397.5(24)	12.7(fixed)	—	-2.8	12.7

<i>u</i> 1679	Si(44)...C(47)	397.6(19)	21.9(tied to <i>u</i> 2037)	—	0.4	18.8
<i>u</i> 2975	Si(43)...C(51)	397.6(17)	12.4(tied to <i>u</i> 2037)	—	-1.0	10.6
<i>u</i> 2130	H(266)...H(286)	397.7(62)	47.0(fixed)	—	1.5	47.0
<i>u</i> 4126	H(265)...H(275)	397.8(73)	36.5(fixed)	—	1.5	36.5
<i>u</i> 3372	H(264)...H(287)	397.9(56)	47.7(fixed)	—	-6.0	47.7
<i>u</i> 429	H(61)...H(67)	398.1(82)	43.4(fixed)	—	28.7	43.4
<i>u</i> 5310	C(211)...H(239)	398.1(114)	16.3(fixed)	—	-7.2	16.3
<i>u</i> 2088	Si(251)...H(286)	398.3(72)	38.7(fixed)	—	-0.2	38.7
<i>u</i> 4855	C(47)...H(71)	398.4(87)	24.1(fixed)	—	-5.8	24.1
<i>u</i> 2312	H(260)...H(272)	398.8(120)	38.7(fixed)	—	-0.9	38.7
<i>u</i> 2999	Si(125)...C(133)	398.9(37)	12.9(tied to <i>u</i> 2037)	—	-1.2	11.1
<i>u</i> 3779	Si(250)...H(267)	399.0(67)	16.7(fixed)	—	-3.2	16.7
<i>u</i> 5383	H(59)...H(75)	399.1(92)	26.7(fixed)	—	-6.4	26.7
<i>u</i> 3970	H(117)...H(118)	399.7(302)	36.3(fixed)	—	1.7	36.3
<i>u</i> 2277	Si(332)...C(335)	399.9(22)	19.0(tied to <i>u</i> 2037)	—	-0.3	16.2
<i>u</i> 2003	H(144)...H(162)	400.3(78)	46.4(fixed)	—	9.9	46.4
<i>u</i> 4516	H(235)...H(242)	400.4(86)	53.3(fixed)	—	-2.5	53.3
<i>u</i> 2108	H(96)...H(109)	400.6(50)	37.9(fixed)	—	-2.1	37.9
<i>u</i> 2346	Si(127)...C(131)	400.7(22)	22.4(tied to <i>u</i> 2037)	—	-0.4	19.2
<i>u</i> 4225	H(105)...H(121)	400.9(258)	35.4(fixed)	—	-0.7	35.4
<i>u</i> 2563	H(309)...H(326)	401.0(101)	57.8(fixed)	—	-1.0	57.8
<i>u</i> 3769	H(110)...H(112)	401.1(38)	44.1(fixed)	—	8.3	44.1
<i>u</i> 2156	Si(249)...C(259)	401.2(20)	17.2(tied to <i>u</i> 2037)	—	-0.1	14.7
<i>u</i> 4494	C(134)...H(149)	401.3(100)	26.1(fixed)	—	-4.3	26.1
<i>u</i> 2265	Si(86)...C(90)	401.3(22)	19.0(tied to <i>u</i> 2037)	—	-0.3	16.3
<i>u</i> 2511	C(48)...H(71)	401.5(91)	34.1(fixed)	—	-1.2	34.1
<i>u</i> 2186	Si(330)...C(338)	401.8(20)	17.4(tied to <i>u</i> 2037)	—	-0.2	14.9
<i>u</i> 1851	Si(2)...H(18)	401.8(551)	27.8(fixed)	—	7.4	27.8
<i>u</i> 2461	C(212)...H(235)	401.9(111)	42.2(fixed)	—	-4.4	42.2
<i>u</i> 2944	Si(84)...C(93)	402.0(23)	13.1(tied to <i>u</i> 2037)	—	-1.0	11.2
<i>u</i> 3225	C(211)...H(237)	402.3(95)	41.1(fixed)	—	9.4	41.1
<i>u</i> 2182	C(7)...H(18)	402.4(168)	13.4(fixed)	—	-5.0	13.4
<i>u</i> 4700	C(93)...H(100)	402.4(64)	28.4(fixed)	—	-4.8	28.4
<i>u</i> 2410	Si(289)...C(294)	402.4(28)	21.8(tied to <i>u</i> 2037)	—	-0.5	18.7
<i>u</i> 2166	Si(290)...C(300)	402.5(26)	18.0(tied to <i>u</i> 2037)	—	-0.2	15.4
<i>u</i> 4693	H(153)...H(160)	402.5(109)	88.0(fixed)	—	-8.1	88.0
<i>u</i> 2279	Si(251)...C(258)	402.6(20)	19.2(tied to <i>u</i> 2037)	—	-0.3	16.5
<i>u</i> 2258	H(301)...H(316)	403.3(73)	41.1(fixed)	—	-2.4	41.1
<i>u</i> 2424	H(18)...H(21)	403.5(110)	29.5(fixed)	—	-4.0	29.5
<i>u</i> 2150	H(265)...H(285)	403.5(43)	44.0(fixed)	—	6.1	44.0
<i>u</i> 2448	H(159)...H(164)	403.5(54)	32.2(fixed)	—	-16.1	32.2
<i>u</i> 4001	H(99)...H(117)	403.5(76)	28.7(fixed)	—	-4.0	28.7
<i>u</i> 2533	H(220)...H(243)	403.6(162)	32.4(fixed)	—	-6.4	32.4
<i>u</i> 2103	H(139)...H(164)	403.7(44)	35.4(fixed)	—	-1.7	35.4

<i>u</i> 2161	Si(208)...C(218)	403.8(75)	17.6(tied to <i>u</i> 2037)	—	-0.1	15.1
<i>u</i> 2317	C(124)...H(157)	404.0(21)	13.8(fixed)	—	-6.7	13.8
<i>u</i> 2242	Si(2)...C(11)	404.6(16)	18.9(tied to <i>u</i> 2037)	—	-0.3	16.2
<i>u</i> 2326	C(247)...H(276)	404.7(21)	14.2(fixed)	—	-6.2	14.2
<i>u</i> 5264	H(64)...H(79)	404.7(161)	26.8(fixed)	—	-11.5	26.8
<i>u</i> 2341	C(206)...H(235)	404.8(21)	13.9(fixed)	—	-6.1	13.9
<i>u</i> 2333	C(1)...H(21)	405.0(21)	13.7(fixed)	—	-5.7	13.7
<i>u</i> 2318	C(83)...H(112)	405.0(21)	13.6(fixed)	—	-5.9	13.6
<i>u</i> 2206	C(6)...H(22)	405.1(260)	13.9(fixed)	—	-6.2	13.9
<i>u</i> 1437	H(15)...H(23)	405.4(919)	66.2(fixed)	—	2.1	66.2
<i>u</i> 2573	H(56)...H(79)	405.4(122)	33.0(fixed)	—	-6.5	33.0
<i>u</i> 1688	Si(125)...C(130)	405.6(25)	18.6(tied to <i>u</i> 2037)	—	1.0	15.9
<i>u</i> 2059	H(342)...H(355)	405.6(46)	39.0(fixed)	—	-2.7	39.0
<i>u</i> 2342	C(206)...H(239)	405.6(21)	13.5(fixed)	—	-5.1	13.5
<i>u</i> 2334	C(165)...H(185)	405.7(21)	13.4(fixed)	—	-5.0	13.4
<i>u</i> 487	H(69)...H(74)	405.7(73)	45.5(fixed)	—	18.2	45.5
<i>u</i> 2315	C(83)...H(101)	405.9(21)	13.3(fixed)	—	-5.1	13.3
<i>u</i> 2609	Si(128)...H(159)	405.9(73)	72.4(fixed)	—	-3.6	72.4
<i>u</i> 2135	H(20)...H(24)	406.0(132)	43.2(fixed)	—	6.1	43.2
<i>u</i> 2316	C(42)...H(79)	406.1(21)	12.9(fixed)	—	-4.7	12.9
<i>u</i> 2300	C(206)...H(243)	406.1(21)	13.0(fixed)	—	-4.6	13.0
<i>u</i> 2307	C(42)...H(60)	406.1(21)	13.2(fixed)	—	-4.9	13.2
<i>u</i> 4320	H(178)...H(194)	406.3(47)	29.8(fixed)	—	-4.2	29.8
<i>u</i> 2223	Si(207)...C(213)	406.3(36)	23.2(tied to <i>u</i> 2037)	—	-0.4	19.9
<i>u</i> 2293	C(83)...H(109)	406.3(21)	13.0(fixed)	—	-4.7	13.0
<i>u</i> 2225	Si(210)...C(214)	406.3(36)	17.5(tied to <i>u</i> 2037)	—	0.0	15.0
<i>u</i> 2295	C(329)...H(355)	406.3(21)	13.3(fixed)	—	-4.6	13.3
<i>u</i> 2305	C(288)...H(312)	406.4(21)	12.9(fixed)	—	-4.3	12.9
<i>u</i> 2325	C(1)...H(19)	406.5(21)	13.1(fixed)	—	-4.5	13.1
<i>u</i> 2329	C(42)...H(75)	406.6(21)	12.8(fixed)	—	-4.2	12.8
<i>u</i> 2327	C(42)...H(66)	406.7(21)	12.8(fixed)	—	-4.1	12.8
<i>u</i> 2308	C(124)...H(164)	406.7(21)	13.0(fixed)	—	-4.3	13.0
<i>u</i> 3740	C(129)...C(136)	406.8(61)	25.4(tied to <i>u</i> 2037)	—	-1.9	21.8
<i>u</i> 2301	C(288)...H(306)	406.9(21)	12.9(fixed)	—	-4.1	12.9
<i>u</i> 2309	C(247)...H(284)	407.0(21)	12.7(fixed)	—	-3.8	12.7
<i>u</i> 1112	H(14)...H(32)	407.0(1086)	61.5(fixed)	—	4.2	61.5
<i>u</i> 3571	C(88)...H(115)	407.0(96)	35.5(fixed)	—	2.5	35.5
<i>u</i> 2314	C(124)...H(153)	407.1(21)	12.8(fixed)	—	-3.9	12.8
<i>u</i> 2319	C(329)...H(349)	407.1(21)	12.7(fixed)	—	-3.6	12.7
<i>u</i> 2215	Si(251)...C(255)	407.1(27)	17.6(tied to <i>u</i> 2037)	—	-0.2	15.1
<i>u</i> 2351	C(83)...H(107)	407.2(21)	12.7(fixed)	—	-3.5	12.7
<i>u</i> 2302	C(247)...H(287)	407.3(21)	12.6(fixed)	—	-3.7	12.6
<i>u</i> 5102	H(97)...H(101)	407.3(63)	18.0(fixed)	—	-7.2	18.0
<i>u</i> 2320	C(83)...H(103)	407.3(21)	12.6(fixed)	—	-3.5	12.6

<i>u</i> 4037	H(154)...H(159)	407.4(81)	48.2(fixed)	—	26.9	48.2
<i>u</i> 2321	C(124)...H(144)	407.4(21)	12.8(fixed)	—	-3.3	12.8
<i>u</i> 2274	Si(248)...C(254)	407.4(31)	23.4(tied to <i>u</i> 2037)	—	-0.5	20.1
<i>u</i> 2344	C(83)...H(116)	407.5(21)	12.6(fixed)	—	-3.3	12.6
<i>u</i> 3178	Si(87)...H(116)	407.6(66)	22.2(fixed)	—	-4.1	22.2
<i>u</i> 2322	C(1)...H(25)	407.6(21)	12.6(fixed)	—	-3.1	12.6
<i>u</i> 2306	C(206)...H(230)	407.7(21)	12.5(fixed)	—	-3.1	12.5
<i>u</i> 2299	C(165)...H(183)	407.7(21)	12.8(fixed)	—	-3.3	12.8
<i>u</i> 2296	C(124)...H(150)	407.7(21)	12.7(fixed)	—	-3.3	12.7
<i>u</i> 2303	C(329)...H(347)	407.8(21)	12.6(fixed)	—	-3.2	12.6
<i>u</i> 2331	C(42)...H(71)	407.8(21)	12.7(fixed)	—	-3.2	12.7
<i>u</i> 2324	C(247)...H(265)	407.8(21)	12.6(fixed)	—	-3.2	12.6
<i>u</i> 2291	C(42)...H(68)	407.9(21)	12.6(fixed)	—	-3.1	12.6
<i>u</i> 2355	C(124)...H(148)	407.9(21)	12.5(fixed)	—	-2.9	12.5
<i>u</i> 2363	C(329)...H(353)	407.9(21)	12.5(fixed)	—	-2.8	12.5
<i>u</i> 2359	C(83)...H(120)	407.9(21)	12.5(fixed)	—	-2.8	12.5
<i>u</i> 2339	C(206)...H(246)	408.0(21)	12.5(fixed)	—	-3.0	12.5
<i>u</i> 2357	C(247)...H(271)	408.0(21)	12.5(fixed)	—	-2.8	12.5
<i>u</i> 2360	C(247)...H(280)	408.0(21)	12.4(fixed)	—	-2.8	12.4
<i>u</i> 2358	C(206)...H(226)	408.0(21)	12.4(fixed)	—	-2.8	12.4
<i>u</i> 2349	C(288)...H(314)	408.0(21)	12.6(fixed)	—	-3.0	12.6
<i>u</i> 3654	H(222)...H(233)	408.0(90)	35.3(fixed)	—	-1.7	35.3
<i>u</i> 2347	C(288)...H(308)	408.0(21)	12.4(fixed)	—	-2.7	12.4
<i>u</i> 2353	C(42)...H(62)	408.0(21)	12.4(fixed)	—	-2.7	12.4
<i>u</i> 2348	C(247)...H(267)	408.0(21)	12.4(fixed)	—	-2.7	12.4
<i>u</i> 2328	C(42)...H(82)	408.1(21)	12.6(fixed)	—	-2.9	12.6
<i>u</i> 2458	C(334)...H(363)	408.1(93)	40.9(fixed)	—	-2.3	40.9
<i>u</i> 2338	C(206)...H(232)	408.1(21)	12.5(fixed)	—	-2.9	12.5
<i>u</i> 2335	C(124)...H(142)	408.2(21)	12.5(fixed)	—	-2.8	12.5
<i>u</i> 2311	C(1)...H(27)	408.2(21)	12.6(fixed)	—	-2.8	12.6
<i>u</i> 2352	C(247)...H(273)	408.2(21)	12.5(fixed)	—	-2.8	12.5
<i>u</i> 2337	C(206)...H(224)	408.3(21)	12.5(fixed)	—	-2.7	12.5
<i>u</i> 2336	C(83)...H(123)	408.3(21)	12.5(fixed)	—	-2.7	12.5
<i>u</i> 2917	Si(249)...C(257)	408.3(21)	13.1(tied to <i>u</i> 2037)	—	-1.0	11.2
<i>u</i> 4164	H(110)...H(113)	408.4(106)	37.6(fixed)	—	3.4	37.6
<i>u</i> 5316	C(47)...H(75)	408.4(85)	15.7(fixed)	—	-6.4	15.7
<i>u</i> 2477	H(18)...H(23)	408.6(48)	31.2(fixed)	—	-5.0	31.2
<i>u</i> 1363	Si(86)...H(104)	408.7(76)	29.1(fixed)	—	5.5	29.1
<i>u</i> 2541	C(294)...H(314)	408.7(69)	32.4(fixed)	—	-1.1	32.4
<i>u</i> 4237	H(64)...H(80)	408.7(124)	35.0(fixed)	—	-0.9	35.0
<i>u</i> 4971	C(129)...H(161)	409.2(53)	30.7(fixed)	—	-25.5	30.7
<i>u</i> 2604	C(7)...H(34)	409.2(74)	43.9(fixed)	—	-5.3	43.9
<i>u</i> 2255	H(343)...H(365)	409.6(64)	37.6(fixed)	—	-2.1	37.6
<i>u</i> 2246	H(14)...H(27)	409.7(61)	35.7(fixed)	—	0.7	35.7

<i>u</i> 5265	H(228)...H(243)	409.9(255)	27.4(fixed)	—	-11.7	27.4
<i>u</i> 2529	H(159)...H(162)	410.0(54)	34.1(fixed)	—	-16.3	34.1
<i>u</i> 2451	H(219)...H(234)	410.1(194)	43.6(fixed)	—	-2.6	43.6
<i>u</i> 536	H(151)...H(156)	410.3(77)	50.1(fixed)	—	25.5	50.1
<i>u</i> 2304	H(260)...H(275)	410.5(58)	39.3(fixed)	—	-2.0	39.3
<i>u</i> 2455	H(15)...H(29)	410.5(97)	45.1(fixed)	—	-2.9	45.1
<i>u</i> 2370	H(262)...H(267)	410.6(77)	35.3(fixed)	—	-1.6	35.3
<i>u</i> 1426	C(92)...H(119)	410.7(277)	37.9(fixed)	—	4.8	37.9
<i>u</i> 3019	Si(85)...C(92)	410.8(20)	12.0(tied to <i>u</i> 2037)	—	-1.0	10.3
<i>u</i> 2621	H(305)...H(325)	411.5(69)	55.7(fixed)	—	0.6	55.7
<i>u</i> 4142	H(266)...H(274)	411.7(93)	39.9(fixed)	—	2.3	39.9
<i>u</i> 2641	H(221)...H(224)	411.8(70)	41.2(fixed)	—	-2.5	41.2
<i>u</i> 2432	C(255)...H(285)	412.0(80)	39.3(fixed)	—	-2.3	39.3
<i>u</i> 2467	H(19)...H(40)	412.2(99)	48.2(fixed)	—	-3.9	48.2
<i>u</i> 2420	H(153)...H(158)	412.2(54)	28.8(fixed)	—	-7.9	28.8
<i>u</i> 3026	Si(210)...H(235)	412.4(63)	27.8(fixed)	—	-7.3	27.8
<i>u</i> 4595	H(71)...H(78)	412.9(76)	55.0(fixed)	—	-3.7	55.0
<i>u</i> 3058	Si(128)...H(153)	413.0(63)	22.2(fixed)	—	-4.6	22.2
<i>u</i> 2479	Si(46)...H(77)	413.2(50)	40.2(fixed)	—	-2.0	40.2
<i>u</i> 1822	Si(248)...C(252)	413.2(27)	19.4(tied to <i>u</i> 2037)	—	0.1	16.6
<i>u</i> 3795	H(262)...H(265)	413.3(57)	27.2(fixed)	—	-1.6	27.2
<i>u</i> 3298	Si(251)...H(277)	413.5(54)	22.0(fixed)	—	1.1	22.0
<i>u</i> 2692	C(334)...H(360)	413.5(106)	38.6(fixed)	—	-2.9	38.6
<i>u</i> 2397	H(278)...H(280)	413.7(60)	26.4(fixed)	—	-7.8	26.4
<i>u</i> 4739	C(48)...H(79)	413.8(109)	27.2(fixed)	—	-9.1	27.2
<i>u</i> 1321	Si(128)...H(138)	413.8(32)	22.1(fixed)	—	0.4	22.1
<i>u</i> 4432	C(217)...H(236)	413.8(118)	20.9(fixed)	—	-2.6	20.9
<i>u</i> 2453	H(183)...H(186)	414.3(54)	27.5(fixed)	—	-6.1	27.5
<i>u</i> 2389	H(114)...H(116)	414.4(60)	26.3(fixed)	—	-7.1	26.3
<i>u</i> 2569	H(182)...H(202)	414.5(81)	51.2(fixed)	—	-5.0	51.2
<i>u</i> 2427	H(237)...H(239)	414.5(60)	29.6(fixed)	—	-6.5	29.6
<i>u</i> 2508	H(302)...H(325)	414.5(72)	36.1(fixed)	—	-2.0	36.1
<i>u</i> 1210	Si(46)...H(56)	414.7(30)	21.2(fixed)	—	0.4	21.2
<i>u</i> 3944	H(222)...H(236)	414.7(70)	34.6(fixed)	—	-7.1	34.6
<i>u</i> 2447	H(77)...H(82)	414.9(54)	26.6(fixed)	—	-5.6	26.6
<i>u</i> 1188	Si(210)...H(220)	415.0(30)	21.1(fixed)	—	0.4	21.1
<i>u</i> 2426	H(235)...H(240)	415.1(54)	30.7(fixed)	—	-4.8	30.7
<i>u</i> 2403	H(241)...H(246)	415.1(54)	26.3(fixed)	—	-5.4	26.3
<i>u</i> 4703	H(143)...H(163)	415.2(84)	43.3(fixed)	—	-5.4	43.3
<i>u</i> 1221	Si(45)...H(63)	415.3(75)	28.2(fixed)	—	4.1	28.2
<i>u</i> 2406	H(313)...H(314)	415.5(54)	26.3(fixed)	—	-5.0	26.3
<i>u</i> 1435	Si(127)...H(143)	415.6(64)	35.3(fixed)	—	3.3	35.3
<i>u</i> 2428	H(71)...H(76)	415.6(54)	26.7(fixed)	—	-4.9	26.7
<i>u</i> 2409	H(59)...H(62)	415.6(60)	25.4(fixed)	—	-6.0	25.4

<i>u2384</i>	H(100)...H(103)	415.7(60)	26.4(fixed)	—	-5.7	26.4
<i>u2449</i>	H(67)...H(68)	415.8(54)	26.4(fixed)	—	-4.7	26.4
<i>u2227</i>	H(137)...H(150)	415.8(48)	37.1(fixed)	—	-0.8	37.1
<i>u3046</i>	Si(46)...H(71)	415.9(61)	22.8(fixed)	—	-3.6	22.8
<i>u2354</i>	H(138)...H(141)	415.9(99)	43.8(fixed)	—	-2.3	43.8
<i>u3700</i>	H(142)...H(162)	416.2(94)	44.3(fixed)	—	5.8	44.3
<i>u2413</i>	H(15)...H(25)	416.2(46)	38.2(fixed)	—	-1.3	38.2
<i>u4480</i>	C(135)...H(154)	416.2(120)	21.6(fixed)	—	-2.4	21.6
<i>u2422</i>	H(107)...H(111)	416.3(60)	25.7(fixed)	—	-5.2	25.7
<i>u4457</i>	C(53)...H(72)	416.4(73)	21.4(fixed)	—	-2.3	21.4
<i>u3596</i>	H(60)...H(65)	416.6(88)	48.9(fixed)	—	-10.2	48.9
<i>u2400</i>	H(282)...H(287)	416.7(54)	26.4(fixed)	—	-3.8	26.4
<i>u1781</i>	Si(209)...H(222)	416.7(29)	21.9(fixed)	—	-0.3	21.9
<i>u2401</i>	H(305)...H(308)	416.9(60)	24.8(fixed)	—	-4.8	24.8
<i>u3684</i>	H(262)...H(276)	417.1(49)	38.4(fixed)	—	-5.1	38.4
<i>u2414</i>	H(26)...H(27)	417.3(54)	25.9(fixed)	—	-3.2	25.9
<i>u2371</i>	H(142)...H(145)	417.3(54)	25.3(fixed)	—	-3.2	25.3
<i>u3506</i>	H(101)...H(106)	417.4(76)	49.3(fixed)	—	-8.7	49.3
<i>u2226</i>	H(98)...H(123)	417.5(131)	35.9(fixed)	—	0.5	35.9
<i>u2367</i>	H(231)...H(232)	417.5(54)	25.4(fixed)	—	-3.0	25.4
<i>u4034</i>	H(58)...H(72)	417.6(68)	27.6(fixed)	—	-4.2	27.6
<i>u2437</i>	H(108)...H(109)	417.8(54)	27.6(fixed)	—	-2.6	27.6
<i>u2399</i>	H(118)...H(123)	417.8(54)	24.7(fixed)	—	-2.9	24.7
<i>u2487</i>	H(237)...H(238)	417.8(55)	31.1(fixed)	—	-7.5	31.1
<i>u2434</i>	H(149)...H(150)	417.8(54)	25.9(fixed)	—	-2.7	25.9
<i>u2419</i>	H(155)...H(157)	417.8(60)	31.7(fixed)	—	-2.9	31.7
<i>u2396</i>	H(284)...H(286)	417.8(60)	25.9(fixed)	—	-3.7	25.9
<i>u2538</i>	H(278)...H(279)	417.8(55)	27.5(fixed)	—	-8.0	27.5
<i>u2374</i>	H(272)...H(273)	418.0(54)	24.5(fixed)	—	-2.7	24.5
<i>u4537</i>	H(116)...H(119)	418.0(238)	37.3(fixed)	—	-1.6	37.3
<i>u2377</i>	H(224)...H(227)	418.0(54)	24.2(fixed)	—	-2.7	24.2
<i>u2387</i>	H(101)...H(104)	418.0(54)	27.6(fixed)	—	-2.3	27.6
<i>u2539</i>	H(114)...H(115)	418.1(55)	28.0(fixed)	—	-7.7	28.0
<i>u2417</i>	H(148)...H(152)	418.1(60)	24.1(fixed)	—	-3.7	24.1
<i>u2404</i>	H(265)...H(268)	418.1(54)	25.2(fixed)	—	-2.5	25.2
<i>u2390</i>	H(264)...H(267)	418.2(60)	23.8(fixed)	—	-3.5	23.8
<i>u1780</i>	Si(45)...H(58)	418.3(27)	21.4(fixed)	—	-0.3	21.4
<i>u2407</i>	H(112)...H(117)	418.4(54)	29.6(fixed)	—	-1.7	29.6
<i>u2444</i>	H(182)...H(185)	418.4(60)	27.5(fixed)	—	-2.9	27.5
<i>u2415</i>	H(306)...H(309)	418.5(54)	26.3(fixed)	—	-2.0	26.3
<i>u1773</i>	Si(86)...H(99)	418.5(28)	21.2(fixed)	—	-0.3	21.2
<i>u2489</i>	H(154)...H(158)	418.5(54)	29.0(fixed)	—	-8.6	29.0
<i>u4362</i>	C(94)...H(117)	418.6(150)	23.8(fixed)	—	-1.6	23.8
<i>u3732</i>	H(263)...H(278)	418.6(55)	25.1(fixed)	—	-1.5	25.1

<i>u</i> 2438	H(66)...H(70)	418.7(60)	25.8(fixed)	—	-2.9	25.8
<i>u</i> 2368	H(223)...H(226)	418.7(60)	23.5(fixed)	—	-3.1	23.5
<i>u</i> 2516	C(336)...H(348)	418.7(67)	33.5(fixed)	—	-2.0	33.5
<i>u</i> 2379	H(120)...H(122)	418.7(60)	23.2(fixed)	—	-3.1	23.2
<i>u</i> 2425	H(60)...H(63)	418.8(54)	27.6(fixed)	—	-1.5	27.6
<i>u</i> 2405	H(73)...H(75)	418.8(60)	26.0(fixed)	—	-2.7	26.0
<i>u</i> 2356	H(271)...H(275)	418.8(60)	23.4(fixed)	—	-3.0	23.4
<i>u</i> 2650	C(293)...H(323)	418.8(98)	38.6(fixed)	—	-1.4	38.6
<i>u</i> 2445	H(161)...H(163)	418.8(60)	40.9(fixed)	—	-0.3	40.9
<i>u</i> 1641	H(20)...H(21)	418.9(777)	54.3(fixed)	—	-2.2	54.3
<i>u</i> 2423	H(276)...H(281)	418.9(54)	30.4(fixed)	—	-1.0	30.4
<i>u</i> 2323	H(230)...H(234)	418.9(60)	23.7(fixed)	—	-2.9	23.7
<i>u</i> 2876	C(293)...H(328)	419.0(101)	32.8(fixed)	—	-4.6	32.8
<i>u</i> 2382	H(25)...H(29)	419.0(60)	23.5(fixed)	—	-2.8	23.5
<i>u</i> 2525	H(100)...H(105)	419.0(55)	27.8(fixed)	—	-6.7	27.8
<i>u</i> 1149	C(90)...H(102)	419.1(67)	35.8(fixed)	—	14.2	35.8
<i>u</i> 2332	H(141)...H(144)	419.2(60)	23.8(fixed)	—	-2.6	23.8
<i>u</i> 1184	Si(209)...H(227)	419.2(107)	28.5(fixed)	—	4.3	28.5
<i>u</i> 2392	H(312)...H(316)	419.2(60)	25.8(fixed)	—	-2.3	25.8
<i>u</i> 2395	H(243)...H(245)	419.2(60)	26.4(fixed)	—	-2.2	26.4
<i>u</i> 2435	H(79)...H(81)	419.2(60)	26.6(fixed)	—	-2.2	26.6
<i>u</i> 2398	H(275)...H(287)	419.4(79)	41.5(fixed)	—	-2.3	41.5
<i>u</i> 2457	C(94)...H(112)	419.6(173)	42.8(fixed)	—	-3.5	42.8
<i>u</i> 2545	H(59)...H(64)	419.6(55)	25.9(fixed)	—	-6.4	25.9
<i>u</i> 2518	C(296)...H(326)	419.6(76)	39.5(fixed)	—	-3.6	39.5
<i>u</i> 2286	H(55)...H(68)	419.7(68)	35.1(fixed)	—	-1.0	35.1
<i>u</i> 2557	H(106)...H(111)	419.8(55)	27.3(fixed)	—	-6.1	27.3
<i>u</i> 2254	H(57)...H(82)	419.9(64)	33.9(fixed)	—	-0.3	33.9
<i>u</i> 2441	C(214)...H(244)	420.0(235)	35.4(fixed)	—	-0.8	35.4
<i>u</i> 3928	H(66)...H(74)	420.0(111)	41.1(fixed)	—	3.2	41.1
<i>u</i> 3685	H(58)...H(65)	420.1(81)	41.2(fixed)	—	-2.6	41.2
<i>u</i> 1166	C(136)...H(145)	420.1(123)	34.5(fixed)	—	8.4	34.5
<i>u</i> 2769	C(92)...H(120)	420.5(46)	22.1(fixed)	—	-0.3	22.1
<i>u</i> 1088	C(49)...H(61)	420.6(70)	34.9(fixed)	—	13.8	34.9
<i>u</i> 2549	H(305)...H(310)	420.8(55)	25.3(fixed)	—	-5.3	25.3
<i>u</i> 2521	C(335)...H(368)	420.9(73)	46.3(fixed)	—	-3.9	46.3
<i>u</i> 2500	H(236)...H(240)	421.0(54)	32.6(fixed)	—	-5.6	32.6
<i>u</i> 2504	H(283)...H(286)	421.1(55)	27.6(fixed)	—	-4.7	27.6
<i>u</i> 2483	H(184)...H(186)	421.5(54)	26.0(fixed)	—	-6.0	26.0
<i>u</i> 2468	H(241)...H(244)	421.5(54)	26.5(fixed)	—	-5.9	26.5
<i>u</i> 2615	C(9)...H(30)	421.6(47)	35.3(fixed)	—	-3.4	35.3
<i>u</i> 2278	H(301)...H(312)	421.6(49)	36.9(fixed)	—	-3.4	36.9
<i>u</i> 2475	H(77)...H(80)	421.6(54)	26.0(fixed)	—	-5.9	26.0
<i>u</i> 2476	H(155)...H(156)	421.7(55)	31.2(fixed)	—	-3.6	31.2



<i>u</i> 2494	H(160)...H(163)	421.7(55)	45.1(fixed)	—	-1.1	45.1
<i>u</i> 4136	H(141)...H(162)	421.8(90)	42.6(fixed)	—	2.0	42.6
<i>u</i> 2559	H(147)...H(152)	421.9(55)	24.8(fixed)	—	-4.2	24.8
<i>u</i> 2484	H(343)...H(366)	421.9(66)	36.0(fixed)	—	-2.1	36.0
<i>u</i> 2537	H(264)...H(269)	422.1(55)	24.7(fixed)	—	-4.1	24.7
<i>u</i> 2493	H(73)...H(74)	422.1(55)	28.3(fixed)	—	-3.6	28.3
<i>u</i> 2464	H(313)...H(315)	422.1(54)	25.7(fixed)	—	-5.4	25.7
<i>u</i> 2471	H(72)...H(76)	422.2(54)	26.1(fixed)	—	-5.2	26.1
<i>u</i> 2519	H(65)...H(70)	422.3(55)	27.5(fixed)	—	-3.5	27.5
<i>u</i> 2473	H(242)...H(245)	422.3(55)	29.0(fixed)	—	-3.3	29.0
<i>u</i> 2514	H(229)...H(234)	422.3(55)	25.6(fixed)	—	-3.7	25.6
<i>u</i> 2548	H(24)...H(29)	422.3(55)	26.0(fixed)	—	-3.7	26.0
<i>u</i> 2481	H(311)...H(316)	422.4(55)	28.2(fixed)	—	-3.3	28.2
<i>u</i> 2536	H(141)...H(146)	422.4(55)	26.0(fixed)	—	-3.6	26.0
<i>u</i> 2509	H(67)...H(69)	422.4(54)	26.0(fixed)	—	-5.1	26.0
<i>u</i> 2503	H(282)...H(285)	422.6(54)	27.8(fixed)	—	-4.7	27.8
<i>u</i> 2530	H(223)...H(228)	422.6(55)	23.9(fixed)	—	-3.7	23.9
<i>u</i> 2546	H(119)...H(122)	422.6(55)	24.2(fixed)	—	-3.6	24.2
<i>u</i> 2515	H(270)...H(275)	422.6(55)	24.3(fixed)	—	-3.6	24.3
<i>u</i> 3861	Si(209)...H(224)	422.6(64)	15.4(fixed)	—	-3.8	15.4
<i>u</i> 2486	H(182)...H(187)	422.7(55)	28.1(fixed)	—	-3.1	28.1
<i>u</i> 2485	H(78)...H(81)	422.7(55)	29.0(fixed)	—	-2.9	29.0
<i>u</i> 5421	H(267)...H(276)	422.8(125)	20.8(fixed)	—	-9.9	20.8
<i>u</i> 2520	H(102)...H(104)	422.8(54)	30.7(fixed)	—	-4.1	30.7
<i>u</i> 2547	H(108)...H(110)	423.1(54)	29.2(fixed)	—	-4.0	29.2
<i>u</i> 5315	C(216)...H(224)	423.3(86)	15.5(fixed)	—	-5.5	15.5
<i>u</i> 2469	H(143)...H(145)	423.5(54)	24.7(fixed)	—	-4.2	24.7
<i>u</i> 2502	H(113)...H(117)	423.5(54)	31.6(fixed)	—	-3.2	31.6
<i>u</i> 2662	Si(45)...H(67)	423.6(71)	35.6(fixed)	—	-1.7	35.6
<i>u</i> 4744	C(212)...H(243)	423.6(165)	29.3(fixed)	—	-9.3	29.3
<i>u</i> 2626	H(15)...H(21)	423.7(34)	36.9(fixed)	—	-9.0	36.9
<i>u</i> 2480	H(26)...H(28)	423.8(54)	24.6(fixed)	—	-3.9	24.6
<i>u</i> 2462	H(231)...H(233)	423.8(54)	24.9(fixed)	—	-3.8	24.9
<i>u</i> 3590	H(97)...H(105)	423.8(51)	38.0(fixed)	—	-1.6	38.0
<i>u</i> 768	C(94)...H(114)	423.9(126)	32.6(fixed)	—	21.5	32.6
<i>u</i> 2672	Si(5)...H(36)	424.1(132)	30.7(fixed)	—	-1.9	30.7
<i>u</i> 2531	H(149)...H(151)	424.2(54)	25.5(fixed)	—	-3.4	25.5
<i>u</i> 2558	Si(210)...H(241)	424.2(26)	38.0(fixed)	—	-2.2	38.0
<i>u</i> 2527	H(307)...H(309)	424.2(54)	27.5(fixed)	—	-3.1	27.5
<i>u</i> 2495	H(118)...H(121)	424.2(54)	24.1(fixed)	—	-3.5	24.1
<i>u</i> 2507	H(225)...H(227)	424.2(54)	24.4(fixed)	—	-3.4	24.4
<i>u</i> 2522	H(61)...H(63)	424.3(54)	29.3(fixed)	—	-2.7	29.3
<i>u</i> 2474	H(272)...H(274)	424.3(54)	24.3(fixed)	—	-3.4	24.3
<i>u</i> 4275	C(217)...H(235)	424.3(75)	24.9(fixed)	—	-1.0	24.9

<i>u</i> 2497	H(266)...H(268)	424.3(54)	25.4(fixed)	—	-3.2	25.4
<i>u</i> 1864	C(257)...H(283)	424.6(80)	51.7(fixed)	—	2.3	51.7
<i>u</i> 2492	H(277)...H(281)	424.6(54)	31.4(fixed)	—	-2.1	31.4
<i>u</i> 3620	H(99)...H(106)	424.7(66)	38.6(fixed)	—	-1.8	38.6
<i>u</i> 3914	Si(45)...H(60)	425.2(56)	15.5(fixed)	—	-4.5	15.5
<i>u</i> 2452	H(306)...H(319)	425.3(105)	47.3(fixed)	—	-3.4	47.3
<i>u</i> 3244	Si(128)...H(158)	425.5(51)	22.9(fixed)	—	1.9	22.9
<i>u</i> 3410	H(20)...H(41)	426.4(753)	49.6(fixed)	—	-6.5	49.6
<i>u</i> 2459	H(234)...H(246)	426.4(63)	46.1(fixed)	—	-0.8	46.1
<i>u</i> 2482	H(302)...H(312)	426.6(49)	31.1(fixed)	—	-5.6	31.1
<i>u</i> 452	H(266)...H(285)	426.6(166)	43.1(fixed)	—	19.9	43.1
<i>u</i> 4027	H(221)...H(239)	427.0(62)	33.1(fixed)	—	-6.0	33.1
<i>u</i> 3987	Si(86)...H(101)	427.0(55)	15.4(fixed)	—	-4.5	15.4
<i>u</i> 4290	C(257)...H(268)	427.0(81)	23.2(fixed)	—	-1.9	23.2
<i>u</i> 2630	Si(166)...H(186)	427.1(58)	39.0(fixed)	—	-1.7	39.0
<i>u</i> 3880	H(220)...H(225)	427.2(71)	25.4(fixed)	—	-2.7	25.4
<i>u</i> 4265	C(254)...H(281)	427.2(98)	23.3(fixed)	—	-1.8	23.3
<i>u</i> 1145	H(97)...H(111)	427.4(73)	57.9(fixed)	—	4.1	57.9
<i>u</i> 2552	Si(126)...H(162)	427.8(49)	36.6(fixed)	—	-2.8	36.6
<i>u</i> 2865	C(49)...H(60)	428.0(56)	33.8(fixed)	—	-6.0	33.8
<i>u</i> 4314	C(53)...H(71)	428.2(66)	25.2(fixed)	—	-1.6	25.2
<i>u</i> 2739	C(335)...H(366)	428.4(58)	35.3(fixed)	—	-2.1	35.3
<i>u</i> 2854	C(90)...H(101)	428.5(57)	36.6(fixed)	—	-6.0	36.6
<i>u</i> 3592	H(263)...H(286)	428.5(108)	39.2(fixed)	—	-1.3	39.2
<i>u</i> 3210	Si(210)...H(240)	428.8(56)	20.8(fixed)	—	1.4	20.8
<i>u</i> 4087	C(130)...H(147)	428.9(114)	34.9(fixed)	—	-1.8	34.9
<i>u</i> 2532	H(301)...H(314)	429.0(71)	40.0(fixed)	—	-2.9	40.0
<i>u</i> 2624	Si(289)...H(304)	429.0(14)	13.4(fixed)	—	-1.4	13.4
<i>u</i> 2577	Si(84)...H(110)	429.0(61)	37.6(fixed)	—	-3.3	37.6
<i>u</i> 2567	Si(289)...H(313)	429.3(77)	34.9(fixed)	—	-2.0	34.9
<i>u</i> 2838	C(216)...H(230)	429.4(112)	25.2(fixed)	—	-2.8	25.2
<i>u</i> 2781	Si(332)...H(354)	429.6(59)	26.1(fixed)	—	-1.6	26.1
<i>u</i> 2726	C(337)...H(362)	429.9(83)	35.6(fixed)	—	-3.3	35.6
<i>u</i> 2725	Si(87)...H(118)	430.0(176)	27.8(fixed)	—	-1.7	27.8
<i>u</i> 2678	C(337)...H(361)	430.0(62)	34.4(fixed)	—	-3.6	34.4
<i>u</i> 2136	H(56)...H(64)	430.2(68)	37.2(fixed)	—	-1.8	37.2
<i>u</i> 5290	H(264)...H(273)	430.3(168)	25.4(fixed)	—	-6.9	25.4
<i>u</i> 4310	C(53)...H(62)	430.5(91)	31.0(fixed)	—	-2.9	31.0
<i>u</i> 2723	Si(86)...H(108)	430.5(61)	29.8(fixed)	—	-1.7	29.8
<i>u</i> 2699	Si(251)...H(282)	430.6(57)	33.2(fixed)	—	-1.6	33.2
<i>u</i> 2032	H(22)...H(33)	430.7(759)	42.8(fixed)	—	6.7	42.8
<i>u</i> 2731	C(170)...H(202)	430.8(56)	33.2(fixed)	—	-5.4	33.2
<i>u</i> 4540	H(222)...H(232)	430.9(62)	24.4(fixed)	—	-5.7	24.4
<i>u</i> 2745	Si(289)...H(318)	431.0(49)	25.9(fixed)	—	-1.8	25.9

<i>u2622</i>	Si(332)...H(345)	431.0(13)	13.1(fixed)	—	-1.1	13.1
<i>u5308</i>	C(52)...H(60)	431.5(71)	15.9(fixed)	—	-6.8	15.9
<i>u1024</i>	Si(249)...H(261)	431.5(12)	20.9(fixed)	—	0.5	20.9
<i>u2786</i>	H(15)...H(27)	431.6(99)	44.0(fixed)	—	-3.4	44.0
<i>u1147</i>	Si(249)...H(268)	431.6(54)	27.1(fixed)	—	3.8	27.1
<i>u3938</i>	H(56)...H(61)	431.7(58)	25.0(fixed)	—	-2.5	25.0
<i>u4631</i>	H(263)...H(284)	431.9(52)	23.4(fixed)	—	-7.1	23.4
<i>u2606</i>	H(343)...H(355)	431.9(41)	33.9(fixed)	—	-6.9	33.9
<i>u2580</i>	Si(332)...H(344)	432.0(12)	13.6(fixed)	—	-1.3	13.6
<i>u2761</i>	Si(127)...H(149)	432.0(75)	28.4(fixed)	—	-1.7	28.4
<i>u3386</i>	H(22)...H(25)	432.1(638)	60.1(fixed)	—	-8.5	60.1
<i>u2625</i>	Si(166)...H(181)	432.1(12)	13.4(fixed)	—	-1.5	13.4
<i>u5324</i>	H(105)...H(120)	432.1(43)	27.6(fixed)	—	-8.2	27.6
<i>u4463</i>	C(52)...H(66)	432.4(53)	29.6(fixed)	—	-4.9	29.6
<i>u2605</i>	Si(4)...H(16)	432.6(17)	13.3(fixed)	—	-1.7	13.3
<i>u2682</i>	C(213)...H(239)	432.7(113)	33.2(fixed)	—	-5.4	33.2
<i>u3992</i>	H(97)...H(107)	432.7(60)	30.1(fixed)	—	-4.2	30.1
<i>u4580</i>	H(58)...H(66)	432.8(61)	23.1(fixed)	—	-7.8	23.1
<i>u4821</i>	H(266)...H(278)	433.1(123)	46.7(fixed)	—	-4.5	46.7
<i>u1680</i>	Si(249)...H(263)	433.1(11)	20.4(fixed)	—	-0.3	20.4
<i>u2753</i>	Si(127)...H(161)	433.1(34)	39.5(fixed)	—	-20.0	39.5
<i>u2659</i>	Si(2)...H(28)	433.2(60)	27.4(fixed)	—	-1.9	27.4
<i>u2058</i>	H(23)...H(25)	433.2(370)	38.8(fixed)	—	14.9	38.8
<i>u2943</i>	C(334)...H(358)	433.3(82)	33.5(fixed)	—	-3.9	33.5
<i>u4419</i>	C(135)...H(153)	433.4(52)	24.9(fixed)	—	-1.2	24.9
<i>u3200</i>	Si(46)...H(76)	433.4(59)	20.9(fixed)	—	0.8	20.9
<i>u2780</i>	C(258)...H(280)	433.6(84)	34.6(fixed)	—	-2.1	34.6
<i>u4823</i>	C(133)...H(161)	433.8(65)	40.9(fixed)	—	-23.9	40.9
<i>u3031</i>	C(257)...H(284)	433.9(77)	30.1(fixed)	—	-5.7	30.1
<i>u4505</i>	C(91)...H(113)	433.9(56)	22.3(fixed)	—	-2.9	22.3
<i>u2638</i>	Si(331)...H(367)	433.9(56)	35.1(fixed)	—	-3.5	35.1
<i>u2627</i>	Si(43)...H(69)	434.0(51)	30.4(fixed)	—	-2.1	30.4
<i>u2608</i>	Si(44)...H(80)	434.1(106)	28.6(fixed)	—	-1.8	28.6
<i>u1957</i>	Si(2)...H(33)	434.1(521)	31.7(fixed)	—	8.5	31.7
<i>u1107</i>	Si(84)...H(97)	434.2(12)	21.5(fixed)	—	0.4	21.5
<i>u2823</i>	C(297)...H(325)	434.2(60)	23.8(fixed)	—	-2.0	23.8
<i>u2760</i>	C(256)...H(271)	434.5(45)	22.0(fixed)	—	-1.6	22.0
<i>u2491</i>	H(70)...H(81)	435.5(195)	55.0(fixed)	—	4.2	55.0
<i>u2829</i>	C(335)...H(369)	435.6(53)	32.1(fixed)	—	-5.6	32.1
<i>u2875</i>	H(138)...H(140)	435.9(43)	22.6(fixed)	—	-2.3	22.6
<i>u2591</i>	Si(87)...H(96)	435.9(21)	13.6(fixed)	—	-1.8	13.6
<i>u2575</i>	Si(289)...H(303)	436.0(12)	13.0(fixed)	—	-1.2	13.0
<i>u2555</i>	H(14)...H(30)	436.0(81)	38.4(fixed)	—	-6.1	38.4
<i>u4117</i>	C(212)...H(245)	436.1(203)	36.0(fixed)	—	-2.7	36.0

<i>u</i> 1457	C(216)...H(229)	436.1(101)	44.1(fixed)	—	3.5	44.1
<i>u</i> 2561	H(302)...H(303)	436.3(55)	24.5(fixed)	—	-1.3	24.5
<i>u</i> 2585	Si(210)...H(219)	436.6(14)	13.2(fixed)	—	-1.4	13.2
<i>u</i> 4403	C(131)...H(146)	436.6(111)	22.3(fixed)	—	-2.5	22.3
<i>u</i> 2127	H(220)...H(228)	436.7(63)	36.3(fixed)	—	-1.6	36.3
<i>u</i> 2589	Si(248)...H(262)	436.7(13)	13.3(fixed)	—	-1.4	13.3
<i>u</i> 1745	Si(125)...H(140)	436.8(12)	23.1(fixed)	—	-0.4	23.1
<i>u</i> 2593	Si(2)...H(15)	436.8(11)	13.6(fixed)	—	-1.4	13.6
<i>u</i> 2587	Si(46)...H(55)	436.9(10)	13.2(fixed)	—	-1.5	13.2
<i>u</i> 2542	C(336)...H(347)	437.0(58)	33.3(fixed)	—	-1.7	33.3
<i>u</i> 2733	Si(4)...H(21)	437.1(37)	25.7(fixed)	—	-8.1	25.7
<i>u</i> 2713	Si(332)...H(350)	437.2(64)	31.2(fixed)	—	-1.6	31.2
<i>u</i> 1044	C(258)...H(279)	437.3(78)	36.9(fixed)	—	7.2	36.9
<i>u</i> 4359	C(252)...H(274)	437.5(52)	30.5(fixed)	—	-1.7	30.5
<i>u</i> 2738	C(334)...H(362)	437.5(54)	33.4(fixed)	—	-3.9	33.4
<i>u</i> 5311	C(171)...H(198)	437.8(106)	16.3(fixed)	—	-7.5	16.3
<i>u</i> 2683	Si(125)...H(151)	437.8(48)	29.7(fixed)	—	-2.4	29.7
<i>u</i> 4344	C(131)...H(144)	437.8(58)	25.0(fixed)	—	-2.3	25.0
<i>u</i> 3346	Si(166)...H(195)	438.1(63)	21.6(fixed)	—	-1.0	21.6
<i>u</i> 4899	C(89)...H(120)	438.2(71)	26.8(fixed)	—	-5.0	26.8
<i>u</i> 2578	C(255)...H(287)	438.4(39)	32.6(fixed)	—	-2.8	32.6
<i>u</i> 2785	C(170)...H(204)	438.6(131)	43.0(fixed)	—	-3.4	43.0
<i>u</i> 2590	Si(128)...H(137)	438.7(11)	13.5(fixed)	—	-1.5	13.5
<i>u</i> 2614	Si(207)...H(221)	438.7(13)	13.3(fixed)	—	-1.5	13.3
<i>u</i> 3853	Si(251)...H(276)	438.7(57)	15.9(fixed)	—	-5.3	15.9
<i>u</i> 2642	C(295)...H(321)	439.2(97)	36.1(fixed)	—	-3.8	36.1
<i>u</i> 2560	C(296)...H(328)	439.2(56)	36.0(fixed)	—	-3.3	36.0
<i>u</i> 3996	H(148)...H(156)	439.4(87)	42.7(fixed)	—	8.9	42.7
<i>u</i> 4826	C(130)...H(148)	439.5(55)	21.4(fixed)	—	-5.6	21.4
<i>u</i> 2616	Si(127)...H(139)	439.6(11)	13.5(fixed)	—	-1.6	13.5
<i>u</i> 2707	H(99)...H(123)	439.7(48)	42.5(fixed)	—	-2.6	42.5
<i>u</i> 2721	Si(207)...H(231)	439.7(69)	29.4(fixed)	—	-1.8	29.4
<i>u</i> 2767	H(18)...H(37)	439.9(137)	54.2(fixed)	—	6.3	54.2
<i>u</i> 4469	C(218)...H(228)	439.9(62)	22.8(fixed)	—	-3.3	22.8
<i>u</i> 4593	H(99)...H(107)	440.0(64)	21.1(fixed)	—	-6.7	21.1
<i>u</i> 2466	H(140)...H(148)	440.2(47)	38.5(fixed)	—	-1.7	38.5
<i>u</i> 809	C(213)...H(238)	440.3(95)	34.7(fixed)	—	15.7	34.7
<i>u</i> 4016	H(178)...H(189)	440.4(37)	28.1(fixed)	—	-2.5	28.1
<i>u</i> 2632	Si(45)...H(57)	440.7(11)	13.2(fixed)	—	-1.4	13.2
<i>u</i> 2843	C(293)...H(325)	440.7(61)	37.9(fixed)	—	-1.9	37.9
<i>u</i> 2562	H(29)...H(40)	440.8(249)	58.7(fixed)	—	2.8	58.7
<i>u</i> 1398	Si(208)...H(225)	440.8(47)	32.9(fixed)	—	3.4	32.9
<i>u</i> 3194	Si(84)...H(117)	441.0(73)	21.4(fixed)	—	0.2	21.4
<i>u</i> 5020	C(171)...H(197)	441.2(88)	29.3(fixed)	—	-1.3	29.3

<i>u</i> 4671	C(135)...H(142)	441.3(46)	29.3(fixed)	—	-4.1	29.3
<i>u</i> 3636	H(142)...H(153)	441.7(131)	38.5(fixed)	—	-6.5	38.5
<i>u</i> 2597	Si(86)...H(98)	441.7(11)	13.5(fixed)	—	-1.3	13.5
<i>u</i> 2687	Si(85)...H(121)	441.9(73)	26.2(fixed)	—	-1.8	26.2
<i>u</i> 2801	Si(330)...H(349)	441.9(38)	20.0(fixed)	—	-4.8	20.0
<i>u</i> 2612	H(21)...H(24)	442.0(202)	51.7(fixed)	—	-6.6	51.7
<i>u</i> 2803	Si(289)...H(309)	442.1(64)	27.0(fixed)	—	-1.6	27.0
<i>u</i> 4301	C(94)...H(116)	442.1(61)	24.7(fixed)	—	-1.0	24.7
<i>u</i> 4564	H(261)...H(284)	442.1(31)	21.9(fixed)	—	-7.1	21.9
<i>u</i> 2416	H(19)...H(22)	442.2(394)	28.2(fixed)	—	-6.4	28.2
<i>u</i> 2750	Si(248)...H(272)	442.2(89)	26.9(fixed)	—	-1.5	26.9
<i>u</i> 2623	C(295)...H(320)	442.4(134)	35.7(fixed)	—	-4.4	35.7
<i>u</i> 5114	H(268)...H(280)	442.6(86)	28.4(fixed)	—	-5.3	28.4
<i>u</i> 2765	Si(290)...H(308)	442.7(38)	19.2(fixed)	—	-3.1	19.2
<i>u</i> 2513	H(219)...H(230)	442.8(45)	38.8(fixed)	—	-1.8	38.8
<i>u</i> 2720	Si(209)...H(243)	442.8(62)	21.8(fixed)	—	-6.3	21.8
<i>u</i> 2700	Si(249)...H(285)	442.9(61)	31.9(fixed)	—	-2.2	31.9
<i>u</i> 2755	H(219)...H(232)	443.0(108)	41.6(fixed)	—	-3.4	41.6
<i>u</i> 2634	Si(251)...H(260)	443.0(10)	13.2(fixed)	—	-1.2	13.2
<i>u</i> 4492	C(134)...H(148)	443.0(45)	30.2(fixed)	—	-4.2	30.2
<i>u</i> 2983	C(336)...H(362)	443.3(47)	29.8(fixed)	—	-5.1	29.8
<i>u</i> 770	C(254)...H(278)	443.4(47)	33.5(fixed)	—	20.4	33.5
<i>u</i> 2892	Si(289)...H(306)	443.8(33)	20.6(fixed)	—	-5.8	20.6
<i>u</i> 4872	C(252)...H(273)	443.9(88)	22.9(fixed)	—	-4.7	22.9
<i>u</i> 2681	H(260)...H(273)	444.0(54)	38.9(fixed)	—	-2.9	38.9
<i>u</i> 4373	C(217)...H(226)	444.0(131)	33.6(fixed)	—	-3.7	33.6
<i>u</i> 2421	C(254)...H(276)	444.3(78)	45.9(fixed)	—	-4.3	45.9
<i>u</i> 4414	C(218)...H(226)	444.4(189)	27.9(fixed)	—	-3.8	27.9
<i>u</i> 2730	Si(45)...H(79)	444.5(56)	22.4(fixed)	—	-6.2	22.4
<i>u</i> 2668	H(15)...H(17)	444.6(22)	26.4(fixed)	—	-1.6	26.4
<i>u</i> 1333	C(259)...H(266)	444.7(102)	35.7(fixed)	—	7.0	35.7
<i>u</i> 2576	H(260)...H(271)	444.7(30)	38.8(fixed)	—	-1.6	38.8
<i>u</i> 1425	C(134)...H(152)	444.9(98)	49.6(fixed)	—	4.4	49.6
<i>u</i> 1414	H(178)...H(180)	445.0(52)	38.8(fixed)	—	0.2	38.8
<i>u</i> 2742	Si(86)...H(120)	445.0(22)	19.6(fixed)	—	-2.3	19.6
<i>u</i> 3300	Si(207)...H(236)	445.0(63)	21.9(fixed)	—	1.1	21.9
<i>u</i> 2618	C(214)...H(246)	445.0(61)	31.3(fixed)	—	-1.3	31.3
<i>u</i> 4610	C(252)...H(278)	445.1(74)	30.5(fixed)	—	-4.5	30.5
<i>u</i> 2669	H(152)...H(163)	445.2(69)	56.2(fixed)	—	5.1	56.2
<i>u</i> 3180	C(256)...H(263)	445.2(54)	21.2(fixed)	—	-1.0	21.2
<i>u</i> 4418	C(130)...H(154)	445.3(69)	33.7(fixed)	—	-6.3	33.7
<i>u</i> 1364	Si(125)...H(145)	445.4(79)	29.2(fixed)	—	5.4	29.2
<i>u</i> 2840	Si(127)...H(142)	445.6(67)	22.2(fixed)	—	-3.4	22.2
<i>u</i> 1408	Si(85)...H(102)	445.9(53)	38.1(fixed)	—	7.7	38.1

<i>u</i> 3153	Si(208)...H(239)	446.0(38)	22.1(fixed)	—	-6.8	22.1
<i>u</i> 1407	Si(44)...H(61)	446.0(55)	39.0(fixed)	—	6.8	39.0
<i>u</i> 1417	C(256)...H(270)	446.1(108)	36.5(fixed)	—	3.7	36.5
<i>u</i> 4866	C(212)...H(246)	446.2(65)	23.4(fixed)	—	-7.1	23.4
<i>u</i> 3281	Si(43)...H(72)	446.2(52)	21.5(fixed)	—	-0.5	21.5
<i>u</i> 4796	C(215)...H(243)	446.2(56)	22.5(fixed)	—	-8.4	22.5
<i>u</i> 3272	Si(125)...H(154)	446.2(80)	22.2(fixed)	—	-0.4	22.2
<i>u</i> 2959	Si(249)...H(276)	446.3(28)	30.2(fixed)	—	-6.8	30.2
<i>u</i> 2751	Si(330)...H(359)	446.3(51)	27.5(fixed)	—	-2.1	27.5
<i>u</i> 2637	H(58)...H(82)	446.6(47)	43.8(fixed)	—	-3.0	43.8
<i>u</i> 2704	Si(208)...H(244)	447.0(141)	28.1(fixed)	—	-1.8	28.1
<i>u</i> 4441	C(49)...H(75)	447.2(54)	30.8(fixed)	—	-4.8	30.8
<i>u</i> 4313	H(141)...H(156)	447.2(86)	37.8(fixed)	—	2.2	37.8
<i>u</i> 2758	Si(290)...H(326)	447.3(53)	32.1(fixed)	—	-2.9	32.1
<i>u</i> 2146	H(18)...H(26)	447.4(661)	49.0(fixed)	—	0.4	49.0
<i>u</i> 2517	H(222)...H(246)	447.6(72)	42.8(fixed)	—	-2.8	42.8
<i>u</i> 3803	Si(207)...H(226)	447.7(26)	17.7(fixed)	—	-4.0	17.7
<i>u</i> 2498	H(20)...H(22)	447.9(493)	30.3(fixed)	—	-7.0	30.3
<i>u</i> 1542	C(52)...H(70)	448.0(73)	48.0(fixed)	—	3.2	48.0
<i>u</i> 2811	C(6)...H(41)	448.3(46)	24.4(fixed)	—	-1.0	24.4
<i>u</i> 2636	H(97)...H(109)	448.3(50)	34.4(fixed)	—	-7.2	34.4
<i>u</i> 3807	Si(43)...H(62)	448.4(34)	17.1(fixed)	—	-3.5	17.1
<i>u</i> 2711	C(8)...H(21)	448.5(72)	34.6(fixed)	—	-6.1	34.6
<i>u</i> 2884	Si(332)...H(347)	448.5(32)	19.1(fixed)	—	-4.5	19.1
<i>u</i> 2086	Si(4)...H(23)	448.6(818)	48.2(fixed)	—	-1.9	48.2
<i>u</i> 2701	Si(290)...H(321)	448.7(39)	20.7(fixed)	—	-5.7	20.7
<i>u</i> 3143	Si(249)...H(281)	448.8(64)	21.6(fixed)	—	-0.2	21.6
<i>u</i> 4804	C(51)...H(79)	448.9(39)	23.0(fixed)	—	-8.4	23.0
<i>u</i> 3972	C(89)...H(122)	449.0(151)	31.7(fixed)	—	-0.7	31.7
<i>u</i> 2728	C(132)...H(157)	449.2(96)	35.6(fixed)	—	-8.3	35.6
<i>u</i> 3832	H(103)...H(116)	449.2(112)	39.6(fixed)	—	-8.6	39.6
<i>u</i> 2868	C(171)...H(205)	449.4(50)	28.1(fixed)	—	-3.1	28.1
<i>u</i> 2696	C(6)...H(24)	449.5(171)	36.5(fixed)	—	-3.0	36.5
<i>u</i> 2855	C(6)...H(25)	449.5(42)	35.6(fixed)	—	-2.7	35.6
<i>u</i> 5343	H(101)...H(116)	449.6(105)	31.9(fixed)	—	-8.9	31.9
<i>u</i> 2804	Si(332)...H(355)	449.7(30)	20.7(fixed)	—	-6.8	20.7
<i>u</i> 3001	Si(84)...H(112)	450.6(30)	28.4(fixed)	—	-6.8	28.4
<i>u</i> 3192	Si(126)...H(157)	450.6(43)	23.7(fixed)	—	-9.2	23.7
<i>u</i> 2717	C(47)...H(66)	450.7(50)	38.6(fixed)	—	-3.5	38.6
<i>u</i> 2863	H(301)...H(319)	450.8(62)	31.2(fixed)	—	1.8	31.2
<i>u</i> 3557	H(265)...H(286)	451.1(115)	50.2(fixed)	—	-6.8	50.2
<i>u</i> 1228	H(98)...H(100)	451.2(37)	60.5(fixed)	—	4.5	60.5
<i>u</i> 3680	H(96)...H(112)	451.4(130)	41.2(fixed)	—	-5.5	41.2
<i>u</i> 2792	C(88)...H(107)	451.5(46)	36.0(fixed)	—	-3.3	36.0

<i>u4465</i>	H(111)...H(112)	451.6(131)	54.3(fixed)	—	-1.1	54.3
<i>u3206</i>	C(6)...H(35)	451.6(379)	37.1(fixed)	—	10.0	37.1
<i>u3097</i>	C(173)...H(194)	451.7(92)	42.6(fixed)	—	-4.3	42.6
<i>u2913</i>	H(220)...H(221)	451.8(52)	25.0(fixed)	—	-1.3	25.0
<i>u3179</i>	Si(44)...H(75)	451.8(34)	21.6(fixed)	—	-5.5	21.6
<i>u4623</i>	C(94)...H(103)	451.9(179)	32.7(fixed)	—	-3.3	32.7
<i>u2899</i>	Si(166)...H(183)	452.1(32)	20.8(fixed)	—	-4.4	20.8
<i>u4099</i>	H(60)...H(73)	452.2(90)	39.1(fixed)	—	1.7	39.1
<i>u4643</i>	H(263)...H(287)	452.4(48)	21.5(fixed)	—	-7.4	21.5
<i>u2747</i>	Si(210)...H(233)	452.4(59)	25.9(fixed)	—	-1.7	25.9
<i>u5281</i>	H(223)...H(235)	452.8(102)	29.0(fixed)	—	-12.9	29.0
<i>u2176</i>	Si(250)...C(252)	452.8(26)	14.8(fixed)	—	-0.2	14.8
<i>u778</i>	H(97)...H(118)	453.0(21)	42.7(fixed)	—	6.7	42.7
<i>u4530</i>	H(55)...H(63)	453.0(49)	25.9(fixed)	—	-1.6	25.9
<i>u4249</i>	H(222)...H(238)	453.0(95)	30.2(fixed)	—	-5.0	30.2
<i>u924</i>	H(57)...H(59)	453.1(45)	59.8(fixed)	—	6.2	59.8
<i>u3384</i>	H(144)...H(163)	453.3(82)	57.3(fixed)	—	-7.2	57.3
<i>u4554</i>	H(219)...H(227)	453.3(38)	26.1(fixed)	—	-1.8	26.1
<i>u2919</i>	H(342)...H(350)	453.4(54)	31.0(fixed)	—	4.0	31.0
<i>u2809</i>	Si(86)...H(103)	453.4(61)	19.4(fixed)	—	-4.5	19.4
<i>u5259</i>	H(224)...H(235)	453.5(151)	38.2(fixed)	—	-13.2	38.2
<i>u4556</i>	C(131)...H(157)	453.6(57)	36.3(fixed)	—	-8.1	36.3
<i>u2034</i>	H(104)...H(116)	453.8(116)	48.1(fixed)	—	4.4	48.1
<i>u5398</i>	H(267)...H(277)	453.9(90)	26.7(fixed)	—	-3.8	26.7
<i>u1624</i>	Si(251)...C(257)	453.9(29)	15.6(fixed)	—	0.4	15.6
<i>u4961</i>	H(182)...H(193)	454.0(136)	38.9(fixed)	—	-0.6	38.9
<i>u3922</i>	Si(84)...H(103)	454.2(34)	16.1(fixed)	—	-3.6	16.1
<i>u3826</i>	Si(166)...H(189)	454.3(38)	17.1(fixed)	—	-4.5	17.1
<i>u2883</i>	Si(4)...H(27)	454.4(54)	22.1(fixed)	—	-3.4	22.1
<i>u2816</i>	Si(250)...H(284)	454.5(37)	20.6(fixed)	—	-5.1	20.6
<i>u4022</i>	C(134)...H(141)	454.5(67)	32.9(fixed)	—	-1.2	32.9
<i>u949</i>	H(262)...H(263)	454.6(22)	31.3(fixed)	—	2.1	31.3
<i>u2698</i>	Si(250)...H(271)	454.6(27)	18.6(fixed)	—	-2.7	18.6
<i>u3274</i>	C(89)...H(97)	454.8(43)	17.4(fixed)	—	-1.2	17.4
<i>u1974</i>	Si(2)...H(32)	455.0(910)	44.7(fixed)	—	-0.4	44.7
<i>u2768</i>	Si(332)...H(366)	455.0(36)	19.5(fixed)	—	-3.3	19.5
<i>u4820</i>	H(142)...H(159)	455.2(114)	95.4(fixed)	—	-7.4	95.4
<i>u2759</i>	Si(128)...H(148)	455.7(32)	19.8(fixed)	—	-3.1	19.8
<i>u2837</i>	Si(46)...H(66)	455.8(36)	21.8(fixed)	—	-5.4	21.8
<i>u2749</i>	C(50)...H(75)	455.9(82)	33.8(fixed)	—	-4.5	33.8
<i>u5344</i>	H(100)...H(116)	456.1(106)	28.3(fixed)	—	-9.5	28.3
<i>u3856</i>	Si(249)...H(265)	456.1(28)	15.2(fixed)	—	-3.4	15.2
<i>u521</i>	H(58)...H(78)	456.2(121)	39.4(fixed)	—	17.7	39.4
<i>u4453</i>	C(95)...H(103)	456.4(78)	26.6(fixed)	—	-1.6	26.6

<i>u</i> 4102	C(48)...H(81)	456.7(159)	35.0(fixed)	—	-2.2	35.0
<i>u</i> 4548	H(220)...H(230)	457.0(44)	19.4(fixed)	—	-5.4	19.4
<i>u</i> 4411	C(95)...H(105)	457.0(203)	22.2(fixed)	—	-1.7	22.2
<i>u</i> 2774	Si(251)...H(274)	457.1(35)	24.0(fixed)	—	-1.8	24.0
<i>u</i> 2679	H(111)...H(122)	457.1(158)	55.3(fixed)	—	5.2	55.3
<i>u</i> 870	C(50)...H(74)	457.4(69)	35.9(fixed)	—	12.9	35.9
<i>u</i> 1040	H(139)...H(140)	457.4(30)	35.1(fixed)	—	2.3	35.1
<i>u</i> 2825	Si(4)...H(38)	457.4(25)	18.6(fixed)	—	-3.5	18.6
<i>u</i> 4474	C(54)...H(64)	457.6(69)	22.6(fixed)	—	-2.8	22.6
<i>u</i> 904	H(261)...H(262)	457.7(26)	32.1(fixed)	—	1.8	32.1
<i>u</i> 3077	H(304)...H(326)	457.8(51)	36.6(fixed)	—	3.0	36.6
<i>u</i> 4181	H(137)...H(155)	457.9(72)	30.0(fixed)	—	-4.1	30.0
<i>u</i> 2856	C(8)...H(19)	457.9(120)	37.8(fixed)	—	-4.6	37.8
<i>u</i> 4197	H(139)...H(144)	458.0(41)	33.6(fixed)	—	-4.1	33.6
<i>u</i> 2915	C(52)...H(68)	458.1(59)	28.2(fixed)	—	-3.7	28.2
<i>u</i> 3111	C(93)...H(99)	458.1(53)	24.2(fixed)	—	-1.6	24.2
<i>u</i> 3354	Si(85)...H(113)	458.2(43)	22.2(fixed)	—	0.9	22.2
<i>u</i> 2788	Si(209)...H(230)	458.2(42)	17.8(fixed)	—	-3.4	17.8
<i>u</i> 2213	Si(127)...C(130)	458.2(27)	21.2(fixed)	—	-0.5	21.2
<i>u</i> 3670	H(57)...H(76)	458.2(60)	42.4(fixed)	—	-1.3	42.4
<i>u</i> 2885	H(260)...H(261)	458.2(27)	24.6(fixed)	—	-1.3	24.6
<i>u</i> 3567	H(139)...H(158)	458.3(71)	58.5(fixed)	—	-1.1	58.5
<i>u</i> 2939	C(335)...H(358)	458.3(49)	27.2(fixed)	—	-4.4	27.2
<i>u</i> 1927	H(143)...H(153)	458.5(111)	48.4(fixed)	—	3.2	48.4
<i>u</i> 1734	Si(87)...C(92)	458.5(27)	18.3(fixed)	—	0.1	18.3
<i>u</i> 2796	Si(2)...H(30)	458.7(27)	22.1(fixed)	—	-6.5	22.1
<i>u</i> 2928	H(343)...H(352)	459.0(42)	32.5(fixed)	—	1.1	32.5
<i>u</i> 2882	C(134)...H(150)	459.0(58)	29.6(fixed)	—	-3.4	29.6
<i>u</i> 2849	Si(87)...H(107)	459.0(37)	19.7(fixed)	—	-4.5	19.7
<i>u</i> 4075	H(260)...H(280)	459.6(33)	30.4(fixed)	—	-3.8	30.4
<i>u</i> 3709	H(14)...H(20)	459.6(799)	43.2(fixed)	—	-2.3	43.2
<i>u</i> 2798	Si(289)...H(314)	459.6(34)	20.6(fixed)	—	-4.0	20.6
<i>u</i> 2656	C(92)...H(105)	459.7(79)	34.8(fixed)	—	-3.4	34.8
<i>u</i> 776	H(99)...H(119)	459.9(152)	47.2(fixed)	—	8.8	47.2
<i>u</i> 3219	Si(248)...H(280)	459.9(32)	21.5(fixed)	—	-3.5	21.5
<i>u</i> 4915	C(48)...H(82)	460.0(85)	23.0(fixed)	—	-6.5	23.0
<i>u</i> 3309	H(305)...H(328)	460.1(121)	51.4(fixed)	—	-7.1	51.4
<i>u</i> 4139	H(55)...H(73)	460.1(86)	27.0(fixed)	—	-3.0	27.0
<i>u</i> 3094	C(294)...H(328)	460.4(58)	34.6(fixed)	—	-6.2	34.6
<i>u</i> 4201	C(254)...H(280)	460.6(59)	23.7(fixed)	—	-1.4	23.7
<i>u</i> 2746	Si(45)...H(62)	460.6(61)	18.9(fixed)	—	-3.0	18.9
<i>u</i> 3869	Si(126)...H(144)	460.6(30)	16.9(fixed)	—	-4.2	16.9
<i>u</i> 5287	H(59)...H(71)	460.6(84)	29.1(fixed)	—	-9.3	29.1
<i>u</i> 4472	C(54)...H(62)	460.7(165)	27.9(fixed)	—	-3.1	27.9



<i>u</i> 5278	H(60)...H(71)	460.9(129)	32.8(fixed)	—	-8.2	32.8
<i>u</i> 4497	H(270)...H(280)	461.0(152)	36.3(fixed)	—	-2.2	36.3
<i>u</i> 1495	Si(248)...H(266)	461.0(69)	32.2(fixed)	—	3.5	32.2
<i>u</i> 4616	H(138)...H(150)	461.1(66)	20.3(fixed)	—	-6.7	20.3
<i>u</i> 2872	H(14)...H(17)	461.1(19)	22.0(fixed)	—	-2.4	22.0
<i>u</i> 2800	Si(210)...H(246)	461.2(42)	21.5(fixed)	—	-4.0	21.5
<i>u</i> 4923	C(89)...H(123)	461.3(149)	21.5(fixed)	—	-5.2	21.5
<i>u</i> 4590	H(96)...H(104)	461.4(59)	25.7(fixed)	—	-1.4	25.7
<i>u</i> 3941	Si(125)...H(142)	461.5(30)	15.1(fixed)	—	-4.0	15.1
<i>u</i> 4811	C(93)...H(120)	461.7(62)	21.2(fixed)	—	-4.4	21.2
<i>u</i> 4705	H(269)...H(272)	461.9(143)	32.8(fixed)	—	-3.9	32.8
<i>u</i> 2835	C(334)...H(353)	462.0(47)	23.8(fixed)	—	-2.4	23.8
<i>u</i> 3062	H(343)...H(348)	462.2(45)	32.6(fixed)	—	1.9	32.6
<i>u</i> 4194	H(58)...H(74)	462.2(55)	29.3(fixed)	—	-4.5	29.3
<i>u</i> 3218	H(305)...H(327)	462.4(149)	52.3(fixed)	—	-8.3	52.3
<i>u</i> 3065	C(51)...H(58)	462.5(50)	23.9(fixed)	—	-1.5	23.9
<i>u</i> 4212	H(219)...H(237)	462.6(116)	31.1(fixed)	—	-4.6	31.1
<i>u</i> 3337	C(9)...H(20)	462.6(485)	37.8(fixed)	—	4.7	37.8
<i>u</i> 4258	H(101)...H(115)	462.7(145)	41.9(fixed)	—	1.5	41.9
<i>u</i> 2905	H(97)...H(99)	462.7(32)	24.5(fixed)	—	-1.3	24.5
<i>u</i> 2727	Si(209)...H(226)	462.8(53)	18.9(fixed)	—	-2.3	18.9
<i>u</i> 3936	H(224)...H(237)	462.9(105)	43.5(fixed)	—	9.6	43.5
<i>u</i> 2817	C(136)...H(144)	463.1(47)	36.1(fixed)	—	-2.6	36.1
<i>u</i> 2770	H(301)...H(303)	463.2(21)	22.1(fixed)	—	-1.4	22.1
<i>u</i> 3901	Si(128)...H(157)	463.2(73)	16.9(fixed)	—	-5.2	16.9
<i>u</i> 4985	H(144)...H(154)	463.3(81)	40.2(fixed)	—	-9.5	40.2
<i>u</i> 2807	H(342)...H(360)	463.3(41)	31.6(fixed)	—	2.3	31.6
<i>u</i> 2846	Si(87)...H(123)	463.4(67)	21.3(fixed)	—	-2.8	21.3
<i>u</i> 4413	C(91)...H(112)	463.6(64)	26.4(fixed)	—	-1.7	26.4
<i>u</i> 2041	H(105)...H(113)	463.7(90)	41.3(fixed)	—	9.7	41.3
<i>u</i> 2815	C(259)...H(273)	463.9(45)	23.3(fixed)	—	-1.9	23.3
<i>u</i> 4385	H(228)...H(238)	464.0(107)	37.0(fixed)	—	0.6	37.0
<i>u</i> 3038	C(215)...H(222)	464.2(55)	23.5(fixed)	—	-1.6	23.5
<i>u</i> 2839	Si(248)...H(273)	464.3(33)	20.3(fixed)	—	-3.4	20.3
<i>u</i> 4462	H(64)...H(74)	464.5(79)	37.2(fixed)	—	-0.2	37.2
<i>u</i> 2954	C(259)...H(265)	464.6(47)	33.8(fixed)	—	-3.8	33.8
<i>u</i> 3016	C(252)...H(261)	464.9(47)	22.4(fixed)	—	-1.3	22.4
<i>u</i> 2708	C(50)...H(81)	465.0(151)	41.5(fixed)	—	2.0	41.5
<i>u</i> 3263	H(21)...H(34)	465.2(131)	57.5(fixed)	—	-13.7	57.5
<i>u</i> 4428	C(129)...H(156)	465.3(79)	22.9(fixed)	—	-1.9	22.9
<i>u</i> 847	C(132)...H(156)	465.4(65)	39.4(fixed)	—	20.5	39.4
<i>u</i> 4070	H(22)...H(28)	465.4(836)	65.5(fixed)	—	3.3	65.5
<i>u</i> 2712	C(54)...H(70)	465.4(124)	41.9(fixed)	—	2.4	41.9
<i>u</i> 2873	Si(207)...H(232)	465.5(34)	21.4(fixed)	—	-3.7	21.4

<i>u</i> 2842	Si(46)...H(82)	465.6(44)	21.9(fixed)	—	-3.8	21.9
<i>u</i> 4338	C(136)...H(141)	465.8(76)	26.8(fixed)	—	-1.9	26.8
<i>u</i> 1778	H(63)...H(71)	465.9(122)	46.6(fixed)	—	4.3	46.6
<i>u</i> 3117	H(179)...H(192)	466.0(42)	34.3(fixed)	—	1.2	34.3
<i>u</i> 4114	H(262)...H(279)	466.1(46)	26.7(fixed)	—	-3.3	26.7
<i>u</i> 2735	C(9)...H(40)	466.4(201)	45.5(fixed)	—	1.4	45.5
<i>u</i> 3052	H(56)...H(65)	466.7(49)	36.4(fixed)	—	3.8	36.4
<i>u</i> 2857	C(293)...H(317)	466.7(51)	24.9(fixed)	—	-3.2	24.9
<i>u</i> 4642	H(56)...H(68)	467.3(37)	20.8(fixed)	—	-6.5	20.8
<i>u</i> 2864	C(7)...H(25)	467.5(44)	26.8(fixed)	—	-2.5	26.8
<i>u</i> 1748	H(227)...H(235)	467.7(176)	57.7(fixed)	—	2.2	57.7
<i>u</i> 4561	H(62)...H(77)	468.1(116)	54.8(fixed)	—	-4.2	54.8
<i>u</i> 3824	Si(210)...H(239)	468.2(64)	17.0(fixed)	—	-4.2	17.0
<i>u</i> 2806	Si(128)...H(164)	468.4(28)	22.8(fixed)	—	-6.2	22.8
<i>u</i> 3558	H(62)...H(71)	468.4(122)	38.9(fixed)	—	-4.9	38.9
<i>u</i> 1712	C(129)...H(138)	468.4(69)	39.1(fixed)	—	0.2	39.1
<i>u</i> 670	H(261)...H(272)	468.9(33)	38.1(fixed)	—	6.7	38.1
<i>u</i> 3500	H(226)...H(235)	468.9(109)	47.9(fixed)	—	-7.6	47.9
<i>u</i> 4495	C(92)...H(102)	469.0(55)	21.9(fixed)	—	-3.1	21.9
<i>u</i> 2841	C(218)...H(232)	469.1(139)	24.5(fixed)	—	-1.9	24.5
<i>u</i> 2381	H(112)...H(119)	469.3(336)	47.7(fixed)	—	-4.5	47.7
<i>u</i> 3134	H(138)...H(147)	469.5(59)	38.3(fixed)	—	1.6	38.3
<i>u</i> 2986	H(15)...H(36)	469.6(26)	30.2(fixed)	—	3.3	30.2
<i>u</i> 2871	Si(127)...H(150)	469.8(29)	19.2(fixed)	—	-4.2	19.2
<i>u</i> 2930	Si(251)...C(254)	469.9(14)	12.3(tied to <i>u</i> 2976)	—	-1.2	11.3
<i>u</i> 2790	C(132)...H(163)	470.0(46)	39.9(fixed)	—	4.2	39.9
<i>u</i> 3139	Si(128)...H(161)	470.2(33)	30.7(fixed)	—	-18.6	30.7
<i>u</i> 4522	H(106)...H(114)	470.5(54)	40.5(fixed)	—	-3.1	40.5
<i>u</i> 3962	C(129)...H(163)	470.9(73)	47.4(fixed)	—	-1.9	47.4
<i>u</i> 4648	H(137)...H(143)	471.2(46)	28.7(fixed)	—	-3.2	28.7
<i>u</i> 2821	Si(86)...H(109)	471.2(27)	21.5(fixed)	—	-7.0	21.5
<i>u</i> 2852	C(136)...H(152)	471.5(50)	41.6(fixed)	—	1.7	41.6
<i>u</i> 3251	C(211)...H(220)	471.7(47)	21.2(fixed)	—	-1.7	21.2
<i>u</i> 2878	H(342)...H(345)	471.7(24)	25.2(fixed)	—	-1.4	25.2
<i>u</i> 2898	Si(45)...H(68)	471.8(32)	20.2(fixed)	—	-4.2	20.2
<i>u</i> 2914	H(97)...H(98)	472.4(20)	24.7(fixed)	—	-1.5	24.7
<i>u</i> 3843	Si(46)...H(75)	472.5(56)	16.7(fixed)	—	-3.8	16.7
<i>u</i> 2832	H(187)...H(201)	472.8(105)	47.2(fixed)	—	13.0	47.2
<i>u</i> 3766	H(260)...H(263)	472.9(20)	17.4(fixed)	—	-2.2	17.4
<i>u</i> 653	H(222)...H(242)	473.0(141)	39.9(fixed)	—	16.9	39.9
<i>u</i> 4847	H(145)...H(156)	473.1(130)	42.6(fixed)	—	-7.3	42.6
<i>u</i> 2881	H(14)...H(15)	473.2(35)	26.9(fixed)	—	-1.3	26.9
<i>u</i> 2810	C(130)...H(164)	473.4(55)	34.2(fixed)	—	-4.0	34.2
<i>u</i> 1443	C(48)...H(56)	473.5(49)	29.0(fixed)	—	1.1	29.0

<i>u</i> 2933	Si(85)...C(94)	473.5(27)	12.8(tied to <i>u</i> 2976)	—	-1.8	11.8
<i>u</i> 4048	C(52)...H(64)	473.6(62)	32.4(fixed)	—	-1.2	32.4
<i>u</i> 2891	H(260)...H(262)	473.7(19)	21.9(fixed)	—	-1.9	21.9
<i>u</i> 2866	Si(84)...H(109)	473.9(33)	24.9(fixed)	—	-5.5	24.9
<i>u</i> 2918	H(219)...H(221)	473.9(44)	22.1(fixed)	—	-2.1	22.1
<i>u</i> 3123	H(301)...H(310)	474.0(44)	37.8(fixed)	—	1.3	37.8
<i>u</i> 1139	C(53)...H(58)	474.0(73)	27.5(fixed)	—	2.9	27.5
<i>u</i> 4774	C(257)...H(271)	474.1(51)	20.8(fixed)	—	-4.7	20.8
<i>u</i> 3109	H(159)...H(163)	474.1(38)	18.5(fixed)	—	-13.8	18.5
<i>u</i> 4695	H(223)...H(231)	474.3(88)	32.5(fixed)	—	-3.5	32.5
<i>u</i> 4319	H(59)...H(73)	474.3(111)	38.6(fixed)	—	-2.5	38.6
<i>u</i> 2869	Si(126)...H(164)	474.5(32)	23.2(fixed)	—	-4.9	23.2
<i>u</i> 2974	Si(86)...C(95)	474.7(28)	11.7(tied to <i>u</i> 2976)	—	-1.6	10.8
<i>u</i> 3002	Si(2)...C(7)	474.9(7)	11.9(tied to <i>u</i> 2976)	—	-1.1	10.9
<i>u</i> 2908	Si(330)...C(336)	475.0(8)	12.7(tied to <i>u</i> 2976)	—	-1.2	11.7
<i>u</i> 3000	Si(290)...C(293)	475.1(10)	11.7(tied to <i>u</i> 2976)	—	-1.1	10.7
<i>u</i> 4680	C(255)...H(265)	475.1(54)	24.6(fixed)	—	-3.4	24.6
<i>u</i> 3988	C(216)...H(228)	475.1(76)	30.9(fixed)	—	-0.9	30.9
<i>u</i> 2992	Si(4)...C(6)	475.4(6)	11.6(tied to <i>u</i> 2976)	—	-1.2	10.7
<i>u</i> 4871	C(170)...H(193)	475.4(94)	26.7(fixed)	—	-1.9	26.7
<i>u</i> 2766	Si(250)...H(266)	475.4(31)	26.8(fixed)	—	-2.2	26.8
<i>u</i> 2900	Si(251)...H(287)	475.5(26)	20.8(fixed)	—	-5.4	20.8
<i>u</i> 2925	Si(125)...C(131)	475.5(7)	13.2(tied to <i>u</i> 2976)	—	-1.5	12.1
<i>u</i> 2976	Si(2)...C(8)	475.5(15)	12.0(4)	—	-1.5	11.0
<i>u</i> 2936	Si(290)...C(299)	475.8(10)	12.8(tied to <i>u</i> 2976)	—	-1.2	11.8
<i>u</i> 3256	C(47)...H(56)	475.9(41)	21.3(fixed)	—	-1.3	21.3
<i>u</i> 2877	H(96)...H(99)	475.9(67)	22.2(fixed)	—	-2.5	22.2
<i>u</i> 3022	Si(330)...C(334)	476.0(7)	11.3(tied to <i>u</i> 2976)	—	-1.0	10.4
<i>u</i> 1685	Si(166)...C(175)	476.3(9)	19.6(tied to <i>u</i> 2976)	—	0.5	18.0
<i>u</i> 2948	Si(84)...C(90)	476.3(6)	12.1(tied to <i>u</i> 2976)	—	-1.1	11.1
<i>u</i> 2985	Si(209)...C(218)	476.4(28)	11.7(tied to <i>u</i> 2976)	—	-1.2	10.7
<i>u</i> 2911	H(262)...H(286)	476.4(32)	33.4(fixed)	—	4.0	33.4
<i>u</i> 3059	Si(289)...H(317)	476.5(43)	21.8(fixed)	—	-3.4	21.8
<i>u</i> 4882	C(129)...H(164)	476.5(72)	23.3(fixed)	—	-9.0	23.3
<i>u</i> 3042	Si(2)...H(19)	476.6(36)	23.1(fixed)	—	-5.4	23.1
<i>u</i> 2853	Si(330)...H(355)	476.8(34)	26.1(fixed)	—	-5.2	26.1
<i>u</i> 2879	H(58)...H(73)	476.8(83)	31.4(fixed)	—	1.8	31.4
<i>u</i> 2947	C(6)...H(37)	476.9(113)	42.1(fixed)	—	1.8	42.1
<i>u</i> 3013	Si(210)...C(213)	477.1(15)	11.9(tied to <i>u</i> 2976)	—	-1.2	10.9
<i>u</i> 1618	Si(43)...C(52)	477.2(7)	17.9(tied to <i>u</i> 2976)	—	0.4	16.4
<i>u</i> 2888	Si(2)...H(27)	477.3(63)	24.0(fixed)	—	-2.8	24.0
<i>u</i> 2949	Si(126)...C(135)	477.4(5)	12.1(tied to <i>u</i> 2976)	—	-1.3	11.1
<i>u</i> 2977	Si(289)...C(298)	477.5(9)	11.7(tied to <i>u</i> 2976)	—	-1.0	10.8
<i>u</i> 2988	Si(45)...C(54)	477.6(17)	11.5(tied to <i>u</i> 2976)	—	-1.3	10.5

<i>u</i> 3110	H(237)...H(240)	477.9(38)	16.9(fixed)	—	-10.2	16.9
<i>u</i> 3069	H(343)...H(351)	478.0(45)	36.1(fixed)	—	2.9	36.1
<i>u</i> 2635	C(7)...H(33)	478.1(753)	40.8(fixed)	—	-6.7	40.8
<i>u</i> 3056	C(296)...H(304)	478.2(46)	23.5(fixed)	—	-1.4	23.5
<i>u</i> 2793	C(95)...H(111)	478.2(112)	41.0(fixed)	—	4.9	41.0
<i>u</i> 3102	H(155)...H(158)	478.5(38)	16.4(fixed)	—	-9.7	16.4
<i>u</i> 2245	Si(207)...C(211)	478.5(9)	17.7(tied to <i>u</i> 2976)	—	-0.2	16.3
<i>u</i> 940	H(96)...H(97)	478.5(51)	36.3(fixed)	—	2.1	36.3
<i>u</i> 1725	Si(208)...C(215)	478.5(12)	20.4(tied to <i>u</i> 2976)	—	0.1	18.7
<i>u</i> 1657	Si(207)...C(216)	478.8(9)	18.2(tied to <i>u</i> 2976)	—	0.3	16.7
<i>u</i> 1431	C(212)...H(220)	478.8(68)	30.7(fixed)	—	1.3	30.7
<i>u</i> 2155	Si(43)...C(47)	478.8(6)	16.9(tied to <i>u</i> 2976)	—	-0.2	15.5
<i>u</i> 3939	Si(166)...H(194)	478.8(37)	15.3(fixed)	—	-4.0	15.3
<i>u</i> 2968	Si(330)...C(339)	478.9(7)	12.0(tied to <i>u</i> 2976)	—	-0.9	11.1
<i>u</i> 4895	C(92)...H(109)	478.9(40)	21.8(fixed)	—	-9.0	21.8
<i>u</i> 2969	Si(46)...H(79)	479.0(69)	23.0(fixed)	—	-6.2	23.0
<i>u</i> 2862	C(91)...H(122)	479.1(163)	42.0(fixed)	—	0.9	42.0
<i>u</i> 4131	H(96)...H(115)	479.3(99)	27.9(fixed)	—	-3.5	27.9
<i>u</i> 4670	C(130)...H(156)	479.3(97)	31.5(fixed)	—	-7.4	31.5
<i>u</i> 3092	H(114)...H(117)	479.5(38)	16.4(fixed)	—	-8.7	16.4
<i>u</i> 2970	Si(290)...C(297)	479.5(7)	11.4(tied to <i>u</i> 2976)	—	-1.0	10.5
<i>u</i> 3090	H(278)...H(281)	479.7(38)	16.4(fixed)	—	-8.5	16.4
<i>u</i> 2972	H(221)...H(245)	479.8(36)	31.9(fixed)	—	2.4	31.9
<i>u</i> 1668	Si(125)...C(134)	479.8(12)	19.9(tied to <i>u</i> 2976)	—	0.4	18.3
<i>u</i> 2997	Si(127)...C(136)	479.8(5)	11.4(tied to <i>u</i> 2976)	—	-1.3	10.5
<i>u</i> 3091	H(100)...H(104)	480.0(38)	16.4(fixed)	—	-8.1	16.4
<i>u</i> 5043	H(237)...H(244)	480.0(241)	37.0(fixed)	—	3.3	37.0
<i>u</i> 2950	Si(250)...C(255)	480.1(4)	11.7(tied to <i>u</i> 2976)	—	-1.1	10.7
<i>u</i> 2729	Si(127)...H(145)	480.1(29)	29.9(fixed)	—	-2.0	29.9
<i>u</i> 3089	H(108)...H(111)	480.4(38)	16.3(fixed)	—	-7.7	16.3
<i>u</i> 2990	Si(43)...C(49)	480.5(6)	11.9(tied to <i>u</i> 2976)	—	-1.2	10.9
<i>u</i> 2978	Si(44)...C(53)	480.5(13)	11.6(tied to <i>u</i> 2976)	—	-1.3	10.6
<i>u</i> 3103	C(340)...H(345)	480.5(28)	23.0(fixed)	—	-1.5	23.0
<i>u</i> 1163	Si(251)...H(281)	480.6(35)	27.5(fixed)	—	3.8	27.5
<i>u</i> 1847	Si(44)...C(51)	480.6(7)	19.4(tied to <i>u</i> 2976)	—	0.1	17.8
<i>u</i> 3122	H(178)...H(187)	480.6(44)	39.7(fixed)	—	4.7	39.7
<i>u</i> 2989	Si(128)...C(132)	480.6(6)	11.6(tied to <i>u</i> 2976)	—	-1.4	10.7
<i>u</i> 2364	Si(208)...C(212)	480.6(8)	23.4(tied to <i>u</i> 2976)	—	-0.6	21.5
<i>u</i> 3104	H(182)...H(186)	480.6(38)	15.9(fixed)	—	-7.5	15.9
<i>u</i> 1540	C(94)...H(99)	480.7(107)	34.9(fixed)	—	2.0	34.9
<i>u</i> 2902	Si(125)...H(150)	480.8(35)	24.5(fixed)	—	-3.6	24.5
<i>u</i> 3991	H(18)...H(35)	480.8(646)	43.7(fixed)	—	6.0	43.7
<i>u</i> 3088	H(59)...H(63)	480.9(38)	16.0(fixed)	—	-7.3	16.0
<i>u</i> 3100	H(241)...H(245)	480.9(38)	15.7(fixed)	—	-7.2	15.7

<i>u</i> 3093	H(282)...H(286)	481.0(38)	15.8(fixed)	—	-7.2	15.8
<i>u</i> 3173	Si(251)...H(272)	481.0(24)	22.0(fixed)	—	-0.4	22.0
<i>u</i> 3105	H(77)...H(81)	481.0(38)	15.6(fixed)	—	-7.2	15.6
<i>u</i> 2867	C(337)...H(368)	481.0(57)	36.2(fixed)	—	4.7	36.2
<i>u</i> 2744	H(280)...H(283)	481.1(76)	56.5(fixed)	—	-2.1	56.5
<i>u</i> 3098	H(73)...H(76)	481.1(38)	15.7(fixed)	—	-7.0	15.7
<i>u</i> 3011	H(270)...H(286)	481.2(56)	46.2(fixed)	—	4.8	46.2
<i>u</i> 2777	H(219)...H(222)	481.2(71)	22.6(fixed)	—	-1.5	22.6
<i>u</i> 2987	Si(332)...C(341)	481.2(5)	11.4(tied to <i>u</i> 2976)	—	-1.1	10.5
<i>u</i> 3096	H(67)...H(70)	481.3(38)	15.7(fixed)	—	-6.9	15.7
<i>u</i> 3099	H(313)...H(316)	481.3(38)	15.6(fixed)	—	-6.9	15.6
<i>u</i> 3033	Si(250)...C(259)	481.3(8)	11.3(tied to <i>u</i> 2976)	—	-1.1	10.4
<i>u</i> 4334	C(212)...H(238)	481.3(67)	20.9(fixed)	—	-1.9	20.9
<i>u</i> 3010	Si(208)...C(217)	481.4(24)	11.7(tied to <i>u</i> 2976)	—	-1.1	10.7
<i>u</i> 4289	H(223)...H(237)	481.5(102)	42.0(fixed)	—	4.7	42.0
<i>u</i> 2144	Si(84)...C(88)	481.6(4)	15.9(tied to <i>u</i> 2976)	—	-0.1	14.6
<i>u</i> 3087	H(305)...H(309)	481.7(38)	15.8(fixed)	—	-6.5	15.8
<i>u</i> 3020	Si(4)...C(13)	481.7(10)	11.4(tied to <i>u</i> 2976)	—	-1.6	10.4
<i>u</i> 2040	Si(166)...C(173)	481.9(6)	18.9(tied to <i>u</i> 2976)	—	-0.1	17.4
<i>u</i> 2880	H(229)...H(245)	481.9(212)	48.4(fixed)	—	4.0	48.4
<i>u</i> 3008	Si(249)...C(258)	481.9(7)	11.9(tied to <i>u</i> 2976)	—	-1.0	10.9
<i>u</i> 3222	H(307)...H(316)	482.1(92)	42.3(fixed)	—	7.1	42.3
<i>u</i> 3015	Si(209)...C(214)	482.1(7)	11.6(tied to <i>u</i> 2976)	—	-1.3	10.6
<i>u</i> 2907	Si(43)...H(68)	482.2(37)	23.3(fixed)	—	-3.6	23.3
<i>u</i> 3030	Si(46)...C(50)	482.3(7)	11.4(tied to <i>u</i> 2976)	—	-1.3	10.5
<i>u</i> 3083	H(149)...H(152)	482.3(38)	15.6(fixed)	—	-5.8	15.6
<i>u</i> 1861	Si(126)...C(133)	482.3(13)	20.8(tied to <i>u</i> 2976)	—	0.2	19.1
<i>u</i> 2894	Si(44)...H(82)	482.4(49)	22.9(fixed)	—	-3.1	22.9
<i>u</i> 3084	H(26)...H(29)	482.4(38)	15.5(fixed)	—	-5.7	15.5
<i>u</i> 3079	H(141)...H(145)	482.5(38)	15.4(fixed)	—	-5.7	15.4
<i>u</i> 3082	H(231)...H(234)	482.5(38)	15.3(fixed)	—	-5.7	15.3
<i>u</i> 2890	H(305)...H(320)	482.6(80)	44.7(fixed)	—	7.3	44.7
<i>u</i> 3086	H(264)...H(268)	482.6(38)	15.4(fixed)	—	-5.6	15.4
<i>u</i> 2903	Si(85)...H(123)	482.6(84)	24.4(fixed)	—	-2.7	24.4
<i>u</i> 1740	Si(85)...C(93)	482.7(8)	17.0(tied to <i>u</i> 2976)	—	0.3	15.6
<i>u</i> 2391	Si(44)...C(48)	482.7(6)	19.9(tied to <i>u</i> 2976)	—	-0.5	18.3
<i>u</i> 2380	Si(248)...C(253)	482.7(11)	19.2(tied to <i>u</i> 2976)	—	-0.4	17.6
<i>u</i> 4052	C(254)...H(269)	482.7(95)	32.6(fixed)	—	-1.9	32.6
<i>u</i> 3080	H(272)...H(275)	483.0(38)	15.1(fixed)	—	-5.2	15.1
<i>u</i> 3076	H(118)...H(122)	483.1(38)	15.2(fixed)	—	-5.1	15.2
<i>u</i> 3078	H(223)...H(227)	483.1(38)	15.2(fixed)	—	-5.1	15.2
<i>u</i> 2956	H(111)...H(118)	483.2(172)	53.2(fixed)	—	8.2	53.2
<i>u</i> 3021	Si(4)...H(25)	483.4(33)	24.8(fixed)	—	-3.8	24.8
<i>u</i> 3025	Si(87)...C(91)	483.4(7)	11.2(tied to <i>u</i> 2976)	—	-1.2	10.3

<i>u</i> 2910	H(99)...H(115)	483.4(98)	33.0(fixed)	—	1.7	33.0
<i>u</i> 3167	Si(166)...H(185)	483.5(43)	22.0(fixed)	—	-6.6	22.0
<i>u</i> 1380	C(257)...H(263)	483.6(57)	28.7(fixed)	—	0.9	28.7
<i>u</i> 1356	C(47)...H(57)	483.6(33)	34.3(fixed)	—	1.8	34.3
<i>u</i> 2952	H(302)...H(305)	483.7(43)	32.7(fixed)	—	5.1	32.7
<i>u</i> 3882	Si(207)...H(235)	483.8(37)	16.0(fixed)	—	-5.1	16.0
<i>u</i> 2799	Si(44)...H(60)	484.0(34)	21.6(fixed)	—	-7.3	21.6
<i>u</i> 1727	Si(248)...C(256)	484.2(4)	20.0(tied to <i>u</i> 2976)	—	0.1	18.3
<i>u</i> 449	H(223)...H(234)	484.2(102)	41.3(fixed)	—	14.5	41.3
<i>u</i> 5283	H(265)...H(278)	484.2(53)	30.1(fixed)	—	-9.3	30.1
<i>u</i> 1432	C(88)...H(98)	484.4(29)	33.3(fixed)	—	1.5	33.3
<i>u</i> 2834	Si(85)...H(101)	484.5(33)	22.9(fixed)	—	-7.6	22.9
<i>u</i> 2814	Si(208)...H(224)	484.5(46)	20.8(fixed)	—	-3.1	20.8
<i>u</i> 2229	Si(126)...C(129)	484.5(5)	16.9(tied to <i>u</i> 2976)	—	-0.1	15.5
<i>u</i> 2775	H(55)...H(58)	484.5(41)	22.3(fixed)	—	-1.8	22.3
<i>u</i> 3189	C(257)...H(262)	484.6(37)	24.3(fixed)	—	-0.9	24.3
<i>u</i> 2283	Si(85)...C(89)	484.6(5)	18.4(tied to <i>u</i> 2976)	—	-0.4	16.8
<i>u</i> 1923	H(114)...H(120)	484.7(11)	34.8(fixed)	—	18.7	34.8
<i>u</i> 2870	H(263)...H(275)	484.7(76)	30.2(fixed)	—	1.2	30.2
<i>u</i> 3006	C(334)...H(344)	484.7(29)	23.8(fixed)	—	-1.3	23.8
<i>u</i> 4395	C(48)...H(74)	484.8(57)	21.1(fixed)	—	-2.2	21.1
<i>u</i> 4696	H(268)...H(279)	485.2(100)	32.7(fixed)	—	-3.7	32.7
<i>u</i> 5125	H(115)...H(121)	485.2(234)	35.9(fixed)	—	-0.8	35.9
<i>u</i> 657	H(146)...H(160)	485.3(97)	66.3(fixed)	—	43.9	66.3
<i>u</i> 3007	Si(210)...H(243)	485.5(92)	24.0(fixed)	—	-6.1	24.0
<i>u</i> 1421	C(135)...H(146)	485.5(65)	51.1(fixed)	—	4.6	51.1
<i>u</i> 2909	C(252)...H(287)	485.6(54)	35.2(fixed)	—	-4.5	35.2
<i>u</i> 2953	C(7)...H(16)	485.6(66)	25.0(fixed)	—	-1.6	25.0
<i>u</i> 3579	H(19)...H(35)	485.8(394)	42.2(fixed)	—	13.2	42.2
<i>u</i> 2998	C(8)...H(32)	485.8(268)	38.8(fixed)	—	4.5	38.8
<i>u</i> 5247	H(102)...H(112)	486.0(64)	26.4(fixed)	—	-11.9	26.4
<i>u</i> 3360	C(133)...H(137)	486.0(48)	25.4(fixed)	—	-1.5	25.4
<i>u</i> 3780	H(138)...H(139)	486.0(37)	17.4(fixed)	—	-2.9	17.4
<i>u</i> 3257	C(298)...H(323)	486.1(58)	30.2(fixed)	—	2.4	30.2
<i>u</i> 1436	Si(87)...H(113)	486.1(36)	42.1(fixed)	—	7.8	42.1
<i>u</i> 2719	Si(249)...H(267)	486.1(48)	18.5(fixed)	—	-3.1	18.5
<i>u</i> 3871	Si(43)...H(71)	486.2(32)	15.3(fixed)	—	-3.6	15.3
<i>u</i> 1298	C(217)...H(222)	486.2(78)	28.1(fixed)	—	2.9	28.1
<i>u</i> 4549	H(100)...H(115)	486.2(84)	39.5(fixed)	—	-3.5	39.5
<i>u</i> 3303	C(51)...H(55)	486.3(76)	23.5(fixed)	—	-1.0	23.5
<i>u</i> 3283	Si(4)...H(20)	486.4(44)	21.5(fixed)	—	0.1	21.5
<i>u</i> 3811	C(129)...C(134)	486.8(58)	22.2(tied to <i>u</i> 2976)	—	-1.6	20.4
<i>u</i> 3252	Si(2)...H(22)	486.9(12)	21.5(fixed)	—	1.5	21.5
<i>u</i> 3191	Si(332)...H(353)	486.9(39)	21.8(fixed)	—	-3.5	21.8

<i>u</i> 658	H(264)...H(283)	487.0(94)	49.4(fixed)	—	14.0	49.4
<i>u</i> 4577	H(144)...H(147)	487.2(83)	40.6(fixed)	—	-2.9	40.6
<i>u</i> 2828	H(222)...H(237)	487.3(100)	32.1(fixed)	—	7.3	32.1
<i>u</i> 671	H(263)...H(281)	487.5(64)	37.0(fixed)	—	6.8	37.0
<i>u</i> 4396	C(136)...H(142)	487.6(70)	30.3(fixed)	—	-3.0	30.3
<i>u</i> 3291	H(183)...H(200)	487.6(92)	57.2(fixed)	—	-7.5	57.2
<i>u</i> 3929	Si(125)...H(153)	488.2(35)	15.7(fixed)	—	-3.9	15.7
<i>u</i> 4992	H(67)...H(75)	488.5(101)	41.2(fixed)	—	-8.5	41.2
<i>u</i> 3477	H(112)...H(120)	488.5(95)	48.9(fixed)	—	-6.8	48.9
<i>u</i> 3032	Si(291)...H(306)	488.5(38)	23.7(fixed)	—	-4.6	23.7
<i>u</i> 2994	Si(289)...H(312)	488.7(34)	23.8(fixed)	—	-5.6	23.8
<i>u</i> 3646	C(253)...C(257)	488.8(49)	18.1(tied to <i>u</i> 2976)	—	-1.1	16.6
<i>u</i> 4138	C(214)...H(240)	488.9(65)	48.5(fixed)	—	-1.0	48.5
<i>u</i> 3802	H(268)...H(272)	489.1(58)	33.5(fixed)	—	1.5	33.5
<i>u</i> 5357	H(224)...H(240)	489.3(97)	26.1(fixed)	—	-3.1	26.1
<i>u</i> 3964	C(213)...H(223)	489.4(78)	31.5(fixed)	—	-1.0	31.5
<i>u</i> 4636	H(226)...H(241)	489.6(133)	54.4(fixed)	—	-4.9	54.4
<i>u</i> 5425	H(224)...H(239)	489.7(138)	20.4(fixed)	—	-9.5	20.4
<i>u</i> 3066	Si(249)...H(287)	489.7(30)	21.9(fixed)	—	-4.5	21.9
<i>u</i> 3045	Si(330)...H(358)	489.8(34)	22.3(fixed)	—	-3.7	22.3
<i>u</i> 3216	Si(85)...H(118)	489.9(50)	23.8(fixed)	—	-1.2	23.8
<i>u</i> 3158	Si(45)...H(66)	490.1(35)	20.9(fixed)	—	-5.3	20.9
<i>u</i> 3942	H(306)...H(328)	490.2(123)	41.7(fixed)	—	-11.1	41.7
<i>u</i> 3373	C(49)...H(56)	490.3(31)	20.8(fixed)	—	-1.2	20.8
<i>u</i> 3145	Si(290)...H(323)	490.3(29)	23.1(fixed)	—	-0.5	23.1
<i>u</i> 877	H(140)...H(162)	490.3(42)	53.9(fixed)	—	7.1	53.9
<i>u</i> 3955	H(186)...H(193)	490.6(62)	41.4(fixed)	—	4.5	41.4
<i>u</i> 3348	C(293)...H(316)	490.7(61)	31.8(fixed)	—	2.9	31.8
<i>u</i> 3187	Si(332)...H(349)	490.8(37)	21.4(fixed)	—	-4.7	21.4
<i>u</i> 3305	Si(210)...H(231)	490.9(39)	21.2(fixed)	—	-0.4	21.2
<i>u</i> 2923	H(149)...H(163)	490.9(54)	51.8(fixed)	—	7.6	51.8
<i>u</i> 3115	Si(87)...H(120)	491.3(40)	26.0(fixed)	—	-3.5	26.0
<i>u</i> 3344	C(293)...H(301)	491.6(27)	18.8(fixed)	—	-1.6	18.8
<i>u</i> 3696	H(140)...H(159)	491.8(69)	58.3(fixed)	—	-11.7	58.3
<i>u</i> 3785	H(56)...H(57)	491.8(26)	17.3(fixed)	—	-2.4	17.3
<i>u</i> 3317	Si(86)...H(121)	491.8(81)	22.8(fixed)	—	-1.5	22.8
<i>u</i> 1386	C(214)...H(223)	491.9(83)	36.2(fixed)	—	5.1	36.2
<i>u</i> 3119	C(171)...H(201)	492.1(83)	36.0(fixed)	—	5.9	36.0
<i>u</i> 3492	C(131)...H(138)	492.4(41)	24.2(fixed)	—	-1.6	24.2
<i>u</i> 3403	C(215)...H(219)	492.4(101)	22.5(fixed)	—	-1.1	22.5
<i>u</i> 3041	Si(251)...H(273)	492.4(41)	21.9(fixed)	—	-3.0	21.9
<i>u</i> 3014	C(94)...H(111)	492.7(86)	38.4(fixed)	—	6.5	38.4
<i>u</i> 5082	H(73)...H(80)	492.7(170)	35.1(fixed)	—	-0.1	35.1
<i>u</i> 3619	H(308)...H(315)	492.8(81)	34.2(fixed)	—	-5.8	34.2

<i>u</i> 4348	C(255)...H(277)	492.9(44)	47.4(fixed)	—	-3.8	47.4
<i>u</i> 3061	Si(208)...H(246)	493.0(48)	20.9(fixed)	—	-3.5	20.9
<i>u</i> 1475	C(94)...H(97)	493.0(49)	32.1(fixed)	—	1.1	32.1
<i>u</i> 3787	H(268)...H(281)	493.1(69)	33.5(fixed)	—	1.5	33.5
<i>u</i> 3349	C(216)...H(222)	493.1(51)	23.7(fixed)	—	-0.9	23.7
<i>u</i> 3181	Si(125)...H(149)	493.2(20)	23.5(fixed)	—	-1.0	23.5
<i>u</i> 3163	Si(330)...H(354)	493.3(25)	22.7(fixed)	—	-0.6	22.7
<i>u</i> 2754	H(14)...H(33)	493.4(345)	34.6(fixed)	—	6.9	34.6
<i>u</i> 3268	C(335)...H(342)	493.5(17)	17.6(fixed)	—	-1.4	17.6
<i>u</i> 2929	H(309)...H(320)	493.8(93)	53.5(fixed)	—	6.8	53.5
<i>u</i> 3683	H(14)...H(35)	493.8(305)	37.1(fixed)	—	-6.4	37.1
<i>u</i> 2783	Si(248)...H(268)	493.8(36)	26.5(fixed)	—	-1.4	26.5
<i>u</i> 3886	H(220)...H(223)	493.9(62)	25.7(fixed)	—	-2.1	25.7
<i>u</i> 4292	C(171)...H(193)	493.9(45)	25.8(fixed)	—	-1.6	25.8
<i>u</i> 3071	Si(210)...H(232)	493.9(42)	21.5(fixed)	—	-3.1	21.5
<i>u</i> 3270	Si(289)...H(308)	493.9(41)	22.4(fixed)	—	-3.6	22.4
<i>u</i> 3156	Si(2)...H(34)	493.9(32)	22.7(fixed)	—	-7.7	22.7
<i>u</i> 4222	C(9)...H(22)	494.0(714)	52.6(fixed)	—	-1.4	52.6
<i>u</i> 3755	H(230)...H(239)	494.2(159)	37.8(fixed)	—	-10.2	37.8
<i>u</i> 4573	H(98)...H(114)	494.3(56)	29.6(fixed)	—	0.6	29.6
<i>u</i> 2030	H(230)...H(238)	494.3(100)	36.5(fixed)	—	12.3	36.5
<i>u</i> 2534	H(229)...H(239)	494.3(111)	47.2(fixed)	—	-5.3	47.2
<i>u</i> 3455	H(105)...H(112)	494.5(102)	48.1(fixed)	—	-9.9	48.1
<i>u</i> 3282	Si(209)...H(244)	494.7(54)	21.5(fixed)	—	-0.8	21.5
<i>u</i> 4955	C(218)...H(237)	494.7(143)	29.2(fixed)	—	0.0	29.2
<i>u</i> 3469	H(260)...H(264)	494.8(43)	35.1(fixed)	—	-0.8	35.1
<i>u</i> 3310	Si(2)...H(26)	495.1(29)	21.6(fixed)	—	-0.9	21.6
<i>u</i> 4357	C(48)...H(55)	495.1(19)	15.1(fixed)	—	-2.5	15.1
<i>u</i> 3214	Si(330)...H(363)	495.3(23)	21.2(fixed)	—	0.5	21.2
<i>u</i> 3817	Si(84)...H(116)	495.3(30)	16.6(fixed)	—	-3.5	16.6
<i>u</i> 3295	Si(290)...H(307)	495.4(29)	21.9(fixed)	—	-0.1	21.9
<i>u</i> 4720	H(100)...H(110)	495.4(94)	46.4(fixed)	—	-5.2	46.4
<i>u</i> 3186	H(26)...H(40)	495.6(97)	44.0(fixed)	—	5.0	44.0
<i>u</i> 3342	C(334)...H(343)	495.7(22)	18.2(fixed)	—	-1.5	18.2
<i>u</i> 2756	Si(43)...H(61)	495.7(22)	35.6(fixed)	—	-3.6	35.6
<i>u</i> 1938	H(271)...H(278)	495.7(80)	36.0(fixed)	—	17.2	36.0
<i>u</i> 4346	C(95)...H(113)	495.8(60)	49.1(fixed)	—	-3.7	49.1
<i>u</i> 701	H(56)...H(63)	495.9(94)	37.9(fixed)	—	7.0	37.9
<i>u</i> 4382	C(212)...H(219)	495.9(26)	15.1(fixed)	—	-2.7	15.1
<i>u</i> 2991	C(131)...H(163)	496.3(46)	36.6(fixed)	—	5.9	36.6
<i>u</i> 3213	Si(127)...H(148)	496.4(32)	22.7(fixed)	—	-3.6	22.7
<i>u</i> 5409	H(185)...H(197)	496.5(94)	29.0(fixed)	—	-8.3	29.0
<i>u</i> 3148	Si(86)...H(107)	496.5(39)	21.8(fixed)	—	-4.3	21.8
<i>u</i> 3241	Si(84)...H(108)	496.7(26)	21.3(fixed)	—	-0.1	21.3



<i>u2795</i>	H(140)...H(160)	496.7(62)	38.8(fixed)	—	22.3	38.8
<i>u2285</i>	H(279)...H(284)	496.8(65)	39.8(fixed)	—	0.9	39.8
<i>u4347</i>	C(256)...H(266)	497.0(71)	33.8(fixed)	—	-2.0	33.8
<i>u3235</i>	H(311)...H(321)	497.0(119)	52.0(fixed)	—	-8.2	52.0
<i>u4885</i>	H(103)...H(118)	497.2(307)	40.0(fixed)	—	-5.0	40.0
<i>u4669</i>	C(90)...H(114)	497.2(39)	30.1(fixed)	—	-4.5	30.1
<i>u3661</i>	H(20)...H(27)	497.4(501)	43.8(fixed)	—	6.1	43.8
<i>u2773</i>	Si(207)...H(225)	497.4(35)	25.1(fixed)	—	-1.7	25.1
<i>u3199</i>	Si(251)...H(284)	497.6(39)	21.2(fixed)	—	-4.9	21.2
<i>u5055</i>	H(155)...H(162)	497.6(66)	37.8(fixed)	—	1.3	37.8
<i>u4619</i>	H(59)...H(69)	497.7(81)	46.2(fixed)	—	-3.5	46.2
<i>u5355</i>	H(60)...H(76)	497.7(96)	26.9(fixed)	—	-4.8	26.9
<i>u4607</i>	H(226)...H(245)	497.8(294)	42.7(fixed)	—	-4.6	42.7
<i>u3055</i>	C(9)...C(13)	497.9(152)	32.4(fixed)	—	-1.7	32.4
<i>u2787</i>	Si(125)...H(144)	498.1(28)	18.4(fixed)	—	-3.5	18.4
<i>u3580</i>	H(308)...H(314)	498.1(95)	36.9(fixed)	—	-4.9	36.9
<i>u5216</i>	H(146)...H(148)	498.2(81)	23.3(fixed)	—	-7.5	23.3
<i>u3169</i>	C(8)...H(40)	498.2(35)	33.4(fixed)	—	2.7	33.4
<i>u3287</i>	Si(208)...H(241)	498.3(77)	21.1(fixed)	—	0.7	21.1
<i>u2791</i>	Si(208)...H(227)	498.4(14)	26.9(fixed)	—	-1.7	26.9
<i>u3040</i>	C(50)...C(54)	498.4(101)	29.5(fixed)	—	-1.5	29.5
<i>u3983</i>	Si(85)...H(112)	498.5(33)	15.4(fixed)	—	-5.2	15.4
<i>u3368</i>	H(312)...H(321)	498.6(137)	47.8(fixed)	—	-9.3	47.8
<i>u3353</i>	Si(330)...H(348)	498.8(24)	20.8(fixed)	—	-0.4	20.8
<i>u3341</i>	C(170)...H(178)	498.9(23)	19.9(fixed)	—	-2.0	19.9
<i>u3400</i>	H(137)...H(146)	498.9(42)	39.3(fixed)	—	-0.9	39.3
<i>u1104</i>	Si(43)...H(76)	499.0(23)	30.7(fixed)	—	7.4	30.7
<i>u5427</i>	H(60)...H(75)	499.0(111)	20.1(fixed)	—	-10.0	20.1
<i>u3448</i>	C(130)...C(133)	499.1(62)	27.6(fixed)	—	-2.1	27.6
<i>u1365</i>	Si(85)...H(117)	499.1(23)	29.0(fixed)	—	4.7	29.0
<i>u3240</i>	Si(289)...H(322)	499.3(24)	20.9(fixed)	—	0.8	20.9
<i>u628</i>	H(269)...H(275)	499.4(66)	44.9(fixed)	—	11.4	44.9
<i>u5166</i>	H(154)...H(161)	499.4(133)	46.6(fixed)	—	-22.1	46.6
<i>u3327</i>	Si(128)...H(151)	499.4(26)	21.7(fixed)	—	-0.8	21.7
<i>u2812</i>	Si(44)...H(63)	499.4(22)	26.4(fixed)	—	-1.6	26.4
<i>u3359</i>	Si(45)...H(80)	499.4(44)	21.3(fixed)	—	-1.2	21.3
<i>u3259</i>	Si(249)...H(282)	499.5(29)	21.2(fixed)	—	0.3	21.2
<i>u2506</i>	H(152)...H(157)	499.6(139)	50.8(fixed)	—	-7.9	50.8
<i>u3554</i>	C(92)...H(106)	499.8(44)	35.3(fixed)	—	3.3	35.3
<i>u922</i>	H(221)...H(236)	499.8(57)	57.4(fixed)	—	7.8	57.4
<i>u3314</i>	C(52)...H(58)	499.8(31)	23.4(fixed)	—	-1.0	23.4
<i>u925</i>	C(216)...H(241)	499.9(113)	30.8(fixed)	—	13.1	30.8
<i>u5113</i>	H(149)...H(157)	499.9(102)	37.1(fixed)	—	-10.4	37.1
<i>u3012</i>	C(293)...H(320)	500.1(64)	33.8(fixed)	—	4.3	33.8

<i>u</i> 4064	H(61)...H(78)	500.1(67)	38.7(fixed)	—	-2.6	38.7
<i>u</i> 3101	Si(207)...H(230)	500.2(44)	24.7(fixed)	—	-3.9	24.7
<i>u</i> 1496	Si(44)...H(72)	500.3(24)	32.5(fixed)	—	3.5	32.5
<i>u</i> 3463	C(52)...H(57)	500.3(14)	22.0(fixed)	—	-1.6	22.0
<i>u</i> 3129	C(132)...C(136)	500.3(35)	27.6(fixed)	—	-1.7	27.6
<i>u</i> 4084	H(20)...H(29)	500.4(618)	43.0(fixed)	—	1.8	43.0
<i>u</i> 3973	H(280)...H(284)	500.4(133)	39.6(fixed)	—	-8.8	39.6
<i>u</i> 3343	Si(250)...H(285)	500.4(23)	21.3(fixed)	—	-0.2	21.3
<i>u</i> 3850	H(56)...H(59)	500.4(68)	25.8(fixed)	—	-2.0	25.8
<i>u</i> 5165	H(153)...H(161)	500.4(66)	50.8(fixed)	—	-25.6	50.8
<i>u</i> 3230	C(93)...H(96)	500.5(96)	25.1(fixed)	—	-0.8	25.1
<i>u</i> 3742	Si(249)...H(280)	500.5(31)	16.7(fixed)	—	-3.2	16.7
<i>u</i> 2154	H(67)...H(72)	500.5(112)	50.7(fixed)	—	-3.0	50.7
<i>u</i> 2690	Si(84)...H(102)	500.6(21)	38.1(fixed)	—	-3.0	38.1
<i>u</i> 4154	H(225)...H(242)	500.6(127)	34.4(fixed)	—	0.3	34.4
<i>u</i> 3265	Si(43)...H(67)	500.6(24)	21.3(fixed)	—	-0.1	21.3
<i>u</i> 3205	C(90)...H(96)	501.0(54)	23.1(fixed)	—	-1.2	23.1
<i>u</i> 3150	C(296)...H(322)	501.0(50)	32.4(fixed)	—	6.0	32.4
<i>u</i> 3174	C(254)...H(286)	501.1(38)	33.6(fixed)	—	3.3	33.6
<i>u</i> 4567	H(141)...H(157)	501.1(95)	41.0(fixed)	—	-1.7	41.0
<i>u</i> 3292	Si(44)...H(77)	501.1(53)	20.9(fixed)	—	0.1	20.9
<i>u</i> 2740	Si(85)...H(104)	501.1(21)	30.4(fixed)	—	-1.7	30.4
<i>u</i> 2889	Si(248)...H(265)	501.1(30)	19.0(fixed)	—	-4.4	19.0
<i>u</i> 3149	Si(248)...H(271)	501.4(24)	24.1(fixed)	—	-3.6	24.1
<i>u</i> 4304	C(253)...H(272)	501.4(66)	23.3(fixed)	—	-2.0	23.3
<i>u</i> 1910	Si(87)...H(114)	501.4(33)	48.5(fixed)	—	0.8	48.5
<i>u</i> 3124	H(108)...H(122)	501.7(80)	41.7(fixed)	—	6.4	41.7
<i>u</i> 2965	C(336)...H(368)	501.7(45)	36.4(fixed)	—	7.6	36.4
<i>u</i> 5040	C(254)...H(266)	501.8(42)	24.1(fixed)	—	-2.1	24.1
<i>u</i> 3982	H(140)...H(151)	501.9(36)	26.0(fixed)	—	-2.7	26.0
<i>u</i> 3127	C(295)...H(327)	501.9(62)	33.0(fixed)	—	3.4	33.0
<i>u</i> 1183	Si(166)...H(199)	501.9(29)	34.0(fixed)	—	9.3	34.0
<i>u</i> 3005	C(135)...H(140)	502.1(22)	23.6(fixed)	—	-1.9	23.6
<i>u</i> 3329	Si(127)...H(162)	502.1(22)	21.6(fixed)	—	-0.4	21.6
<i>u</i> 3106	C(213)...H(245)	502.1(168)	35.6(fixed)	—	1.9	35.6
<i>u</i> 3264	C(335)...H(354)	502.2(54)	30.8(fixed)	—	2.6	30.8
<i>u</i> 1497	C(255)...H(269)	502.3(53)	39.9(fixed)	—	3.1	39.9
<i>u</i> 1947	Si(251)...H(279)	502.3(37)	31.3(fixed)	—	-0.2	31.3
<i>u</i> 1019	C(52)...H(77)	502.4(93)	32.7(fixed)	—	12.9	32.7
<i>u</i> 2657	Si(166)...H(192)	502.4(23)	28.5(fixed)	—	-2.1	28.5
<i>u</i> 4384	C(89)...H(96)	502.5(19)	15.1(fixed)	—	-2.6	15.1
<i>u</i> 4632	H(261)...H(285)	502.5(40)	27.1(fixed)	—	-1.6	27.1
<i>u</i> 4404	C(129)...H(137)	502.6(18)	15.4(fixed)	—	-3.2	15.4
<i>u</i> 920	H(138)...H(143)	502.7(74)	52.3(fixed)	—	5.5	52.3

<i>u</i> 3648	C(212)...C(216)	502.7(57)	16.8(fixed)	—	-0.6	16.8
<i>u</i> 3141	C(336)...H(342)	502.8(14)	22.4(fixed)	—	-1.6	22.4
<i>u</i> 5258	H(228)...H(246)	502.8(60)	23.7(fixed)	—	-8.6	23.7
<i>u</i> 698	H(220)...H(227)	503.0(139)	40.6(fixed)	—	6.9	40.6
<i>u</i> 3246	H(342)...H(363)	503.0(36)	30.7(fixed)	—	2.6	30.7
<i>u</i> 5423	H(185)...H(198)	503.0(157)	21.0(fixed)	—	-11.0	21.0
<i>u</i> 1891	Si(250)...H(264)	503.1(33)	25.9(fixed)	—	4.1	25.9
<i>u</i> 4417	H(268)...H(283)	503.2(67)	32.3(fixed)	—	-0.5	32.3
<i>u</i> 1393	Si(208)...H(236)	503.2(31)	39.8(fixed)	—	9.0	39.8
<i>u</i> 5005	H(268)...H(282)	503.3(117)	31.2(fixed)	—	-5.3	31.2
<i>u</i> 5337	H(142)...H(161)	503.3(74)	38.6(fixed)	—	-28.5	38.6
<i>u</i> 3718	C(170)...H(199)	503.4(59)	31.3(fixed)	—	3.1	31.3
<i>u</i> 3632	H(183)...H(204)	503.4(116)	52.7(fixed)	—	-6.8	52.7
<i>u</i> 3364	C(134)...H(139)	503.6(26)	24.2(fixed)	—	-1.7	24.2
<i>u</i> 3675	C(48)...C(52)	503.6(49)	16.8(fixed)	—	-0.8	16.8
<i>u</i> 3208	C(259)...H(270)	503.6(44)	38.6(fixed)	—	1.0	38.6
<i>u</i> 3462	C(294)...H(301)	503.7(17)	23.7(fixed)	—	-1.6	23.7
<i>u</i> 1115	Si(207)...H(240)	503.7(32)	33.0(fixed)	—	9.6	33.0
<i>u</i> 4953	C(54)...H(73)	504.0(99)	25.3(fixed)	—	-1.6	25.3
<i>u</i> 3409	Si(46)...H(69)	504.2(28)	21.2(fixed)	—	-1.1	21.2
<i>u</i> 456	H(114)...H(119)	504.2(232)	46.8(fixed)	—	25.7	46.8
<i>u</i> 3193	C(135)...H(139)	504.3(15)	22.5(fixed)	—	-1.7	22.5
<i>u</i> 4389	C(259)...H(281)	504.4(49)	31.7(fixed)	—	-1.6	31.7
<i>u</i> 3466	C(54)...H(56)	504.4(14)	23.3(fixed)	—	-1.5	23.3
<i>u</i> 3063	C(218)...H(229)	504.4(149)	39.7(fixed)	—	1.6	39.7
<i>u</i> 3290	Si(290)...H(318)	504.5(28)	21.1(fixed)	—	-0.6	21.1
<i>u</i> 3574	C(7)...H(39)	504.5(74)	36.2(fixed)	—	1.3	36.2
<i>u</i> 5153	H(62)...H(79)	504.6(113)	36.7(fixed)	—	-11.0	36.7
<i>u</i> 5013	C(95)...H(115)	504.7(154)	25.8(fixed)	—	-2.2	25.8
<i>u</i> 3228	Si(126)...H(159)	504.8(19)	24.7(fixed)	—	6.2	24.7
<i>u</i> 4228	H(146)...H(154)	504.9(76)	42.9(fixed)	—	-4.8	42.9
<i>u</i> 3865	C(252)...C(256)	505.0(45)	17.7(fixed)	—	-1.0	17.7
<i>u</i> 3503	H(301)...H(305)	505.0(62)	39.6(fixed)	—	-0.7	39.6
<i>u</i> 1469	C(258)...H(264)	505.0(67)	42.5(fixed)	—	3.6	42.5
<i>u</i> 3382	Si(87)...H(110)	505.0(23)	21.6(fixed)	—	-0.1	21.6
<i>u</i> 3288	C(6)...C(12)	505.1(77)	27.9(fixed)	—	-1.8	27.9
<i>u</i> 1143	C(129)...H(149)	505.1(54)	35.6(fixed)	—	5.8	35.6
<i>u</i> 3333	Si(332)...H(367)	505.2(19)	21.3(fixed)	—	0.1	21.3
<i>u</i> 3371	H(271)...H(276)	505.2(58)	52.1(fixed)	—	-7.6	52.1
<i>u</i> 4374	H(227)...H(234)	505.2(72)	33.7(fixed)	—	-2.1	33.7
<i>u</i> 3320	C(8)...H(14)	505.4(34)	21.8(fixed)	—	-2.0	21.8
<i>u</i> 2234	H(108)...H(117)	505.4(78)	45.2(fixed)	—	-1.2	45.2
<i>u</i> 4849	H(61)...H(77)	505.4(74)	40.5(fixed)	—	-9.5	40.5
<i>u</i> 4757	C(170)...C(173)	505.5(70)	12.9(fixed)	—	-2.8	12.9

<i>u</i> 3415	Si(4)...H(39)	505.5(47)	22.3(fixed)	—	-1.7	22.3
<i>u</i> 3243	C(94)...H(98)	505.5(17)	21.9(fixed)	—	-2.6	21.9
<i>u</i> 3433	C(334)...H(367)	505.6(39)	38.2(fixed)	—	4.8	38.2
<i>u</i> 1440	C(215)...H(221)	505.6(38)	34.2(fixed)	—	1.2	34.2
<i>u</i> 1404	C(171)...H(180)	505.7(18)	34.3(fixed)	—	1.9	34.3
<i>u</i> 3416	C(335)...H(343)	505.7(16)	20.7(fixed)	—	-1.3	20.7
<i>u</i> 1465	Si(126)...H(154)	505.7(30)	34.5(fixed)	—	5.7	34.5
<i>u</i> 3132	C(91)...C(95)	505.7(103)	28.6(fixed)	—	-1.8	28.6
<i>u</i> 5244	H(142)...H(156)	505.9(88)	24.0(fixed)	—	-7.0	24.0
<i>u</i> 3226	C(7)...H(37)	506.0(26)	38.0(fixed)	—	3.2	38.0
<i>u</i> 3152	C(90)...H(122)	506.1(119)	33.1(fixed)	—	3.2	33.1
<i>u</i> 3959	C(91)...H(100)	506.2(59)	48.5(fixed)	—	-0.4	48.5
<i>u</i> 3411	C(171)...H(178)	506.2(17)	22.1(fixed)	—	-1.5	22.1
<i>u</i> 721	H(55)...H(76)	506.3(39)	44.3(fixed)	—	7.8	44.3
<i>u</i> 3151	C(337)...C(341)	506.4(42)	23.2(fixed)	—	-1.4	23.2
<i>u</i> 788	C(211)...H(234)	506.4(86)	29.7(fixed)	—	10.7	29.7
<i>u</i> 1165	Si(125)...H(158)	506.4(42)	39.1(fixed)	—	12.9	39.1
<i>u</i> 3053	C(294)...H(320)	506.5(53)	41.9(fixed)	—	4.9	41.9
<i>u</i> 4947	C(136)...H(155)	506.6(38)	26.4(fixed)	—	-1.8	26.4
<i>u</i> 3387	C(6)...H(14)	506.6(45)	20.6(fixed)	—	-1.8	20.6
<i>u</i> 5172	H(144)...H(148)	506.6(106)	29.4(fixed)	—	-6.9	29.4
<i>u</i> 2772	Si(126)...H(143)	506.7(25)	24.9(fixed)	—	-1.8	24.9
<i>u</i> 4998	H(145)...H(154)	506.7(70)	34.7(fixed)	—	-7.6	34.7
<i>u</i> 1358	C(254)...H(261)	506.8(21)	29.3(fixed)	—	1.1	29.3
<i>u</i> 4936	C(132)...H(145)	506.9(43)	25.2(fixed)	—	-1.7	25.2
<i>u</i> 3248	Si(250)...H(274)	507.2(29)	22.0(fixed)	—	-0.9	22.0
<i>u</i> 3694	C(50)...H(59)	507.5(52)	48.5(fixed)	—	0.5	48.5
<i>u</i> 3370	C(218)...H(220)	507.6(22)	23.0(fixed)	—	-1.3	23.0
<i>u</i> 3319	Si(209)...H(233)	507.8(30)	22.4(fixed)	—	-1.0	22.4
<i>u</i> 3271	C(8)...H(17)	507.8(34)	18.1(fixed)	—	-1.0	18.1
<i>u</i> 3140	C(135)...H(152)	508.0(45)	35.5(fixed)	—	3.9	35.5
<i>u</i> 3155	C(49)...H(81)	508.0(46)	32.1(fixed)	—	3.0	32.1
<i>u</i> 3247	C(131)...H(137)	508.3(12)	22.2(fixed)	—	-2.3	22.2
<i>u</i> 3426	H(310)...H(324)	508.4(117)	43.3(fixed)	—	2.4	43.3
<i>u</i> 2689	C(8)...H(18)	508.4(773)	45.0(fixed)	—	-4.5	45.0
<i>u</i> 3201	H(67)...H(81)	508.7(51)	43.9(fixed)	—	5.5	43.9
<i>u</i> 3197	C(53)...H(70)	508.8(92)	33.0(fixed)	—	3.1	33.0
<i>u</i> 3774	H(261)...H(265)	508.8(64)	31.3(fixed)	—	-3.5	31.3
<i>u</i> 3289	C(259)...H(262)	508.8(30)	20.0(fixed)	—	-1.3	20.0
<i>u</i> 3273	C(335)...H(344)	508.9(24)	22.9(fixed)	—	-1.0	22.9
<i>u</i> 882	C(252)...H(283)	509.0(70)	34.7(fixed)	—	11.0	34.7
<i>u</i> 3509	H(343)...H(346)	509.1(61)	36.3(fixed)	—	-1.0	36.3
<i>u</i> 3418	H(309)...H(322)	509.3(111)	52.8(fixed)	—	3.8	52.8
<i>u</i> 1880	Si(127)...H(146)	509.4(36)	36.3(fixed)	—	3.9	36.3

<i>u1412</i>	C(48)...H(67)	509.5(54)	44.4(fixed)	—	8.0	44.4
<i>u2602</i>	H(70)...H(75)	509.5(120)	51.5(fixed)	—	-4.3	51.5
<i>u3334</i>	C(293)...H(303)	509.6(20)	21.2(fixed)	—	-1.4	21.2
<i>u1944</i>	C(89)...C(92)	509.6(53)	21.5(fixed)	—	0.6	21.5
<i>u4531</i>	H(103)...H(122)	509.7(96)	38.0(fixed)	—	-1.7	38.0
<i>u3556</i>	H(182)...H(204)	509.7(151)	43.8(fixed)	—	-7.0	43.8
<i>u3255</i>	C(337)...H(345)	509.7(15)	21.3(fixed)	—	-1.3	21.3
<i>u4234</i>	H(102)...H(119)	509.9(49)	44.8(fixed)	—	-6.5	44.8
<i>u1731</i>	C(212)...H(221)	509.9(22)	35.3(fixed)	—	1.6	35.3
<i>u3278</i>	H(70)...H(77)	509.9(128)	45.4(fixed)	—	6.2	45.4
<i>u2906</i>	C(47)...H(78)	510.3(85)	36.7(fixed)	—	5.6	36.7
<i>u4596</i>	H(137)...H(141)	510.3(57)	25.5(fixed)	—	-2.3	25.5
<i>u3482</i>	C(136)...H(138)	510.4(24)	23.0(fixed)	—	-1.4	23.0
<i>u460</i>	H(65)...H(72)	510.6(62)	45.4(fixed)	—	16.9	45.4
<i>u3414</i>	C(6)...H(15)	510.7(14)	23.6(fixed)	—	-1.4	23.6
<i>u3782</i>	H(263)...H(276)	510.7(70)	27.2(fixed)	—	-1.7	27.2
<i>u1342</i>	C(89)...H(108)	510.7(59)	38.8(fixed)	—	5.8	38.8
<i>u3249</i>	C(132)...H(140)	510.8(24)	22.5(fixed)	—	-1.5	22.5
<i>u4353</i>	C(259)...H(261)	511.1(25)	15.3(fixed)	—	-2.2	15.3
<i>u1214</i>	C(52)...H(55)	511.1(43)	31.1(fixed)	—	1.8	31.1
<i>u1028</i>	C(256)...H(282)	511.1(61)	30.8(fixed)	—	10.3	30.8
<i>u2276</i>	H(270)...H(276)	511.2(154)	49.5(fixed)	—	-5.3	49.5
<i>u4478</i>	H(146)...H(147)	511.3(159)	39.8(fixed)	—	-0.9	39.8
<i>u2202</i>	H(97)...H(119)	511.4(157)	37.8(fixed)	—	-1.9	37.8
<i>u3362</i>	C(294)...H(318)	511.4(51)	34.0(fixed)	—	1.7	34.0
<i>u3107</i>	H(18)...H(22)	511.4(687)	16.5(fixed)	—	-9.4	16.5
<i>u3617</i>	C(334)...H(365)	511.5(59)	34.8(fixed)	—	2.1	34.8
<i>u1456</i>	Si(248)...H(277)	511.5(22)	43.0(fixed)	—	7.5	43.0
<i>u797</i>	H(279)...H(283)	511.7(121)	59.2(fixed)	—	9.6	59.2
<i>u3254</i>	C(335)...H(361)	512.0(68)	31.5(fixed)	—	3.0	31.5
<i>u5138</i>	H(235)...H(243)	512.1(84)	30.5(fixed)	—	-8.8	30.5
<i>u4924</i>	H(225)...H(241)	512.2(51)	34.6(fixed)	—	-7.1	34.6
<i>u1069</i>	C(215)...H(231)	512.2(65)	30.9(fixed)	—	7.5	30.9
<i>u784</i>	H(137)...H(158)	512.3(65)	55.5(fixed)	—	12.0	55.5
<i>u3439</i>	H(178)...H(182)	512.4(64)	38.6(fixed)	—	-1.5	38.6
<i>u3657</i>	H(19)...H(41)	512.5(57)	40.0(fixed)	—	-7.7	40.0
<i>u3441</i>	H(15)...H(20)	512.8(137)	32.2(fixed)	—	2.6	32.2
<i>u5175</i>	H(236)...H(243)	512.8(133)	27.2(fixed)	—	-8.9	27.2
<i>u3515</i>	H(273)...H(285)	512.9(88)	42.7(fixed)	—	-6.6	42.7
<i>u3037</i>	C(211)...H(242)	513.1(140)	36.3(fixed)	—	4.8	36.3
<i>u3358</i>	C(218)...H(221)	513.3(55)	20.1(fixed)	—	-1.5	20.1
<i>u3445</i>	C(171)...C(176)	513.3(59)	23.1(fixed)	—	-1.5	23.1
<i>u1383</i>	C(134)...H(137)	513.6(39)	34.8(fixed)	—	1.5	34.8
<i>u4679</i>	H(55)...H(64)	513.7(102)	26.2(fixed)	—	-2.4	26.2

<i>u5224</i>	H(117)...H(121)	513.8(68)	30.1(fixed)	—	-3.2	30.1
<i>u463</i>	H(106)...H(117)	513.8(107)	44.4(fixed)	—	13.8	44.4
<i>u4367</i>	C(213)...H(222)	513.9(26)	15.3(fixed)	—	-2.6	15.3
<i>u3994</i>	H(57)...H(63)	513.9(34)	27.2(fixed)	—	-3.9	27.2
<i>u664</i>	H(147)...H(154)	514.0(71)	58.9(fixed)	—	13.3	58.9
<i>u1698</i>	C(130)...C(135)	514.0(48)	26.1(fixed)	—	2.5	26.1
<i>u3356</i>	H(229)...H(241)	514.1(58)	47.3(fixed)	—	6.9	47.3
<i>u1973</i>	Si(208)...H(237)	514.3(25)	50.8(fixed)	—	-0.2	50.8
<i>u3965</i>	H(261)...H(266)	514.4(46)	26.5(fixed)	—	-4.2	26.5
<i>u5321</i>	H(144)...H(156)	514.4(79)	32.6(fixed)	—	-12.1	32.6
<i>u5145</i>	H(71)...H(79)	514.4(84)	30.8(fixed)	—	-9.6	30.8
<i>u3454</i>	Si(250)...H(275)	514.5(25)	19.3(fixed)	—	-1.3	19.3
<i>u3487</i>	Si(330)...H(346)	514.8(23)	20.4(fixed)	—	-1.1	20.4
<i>u3316</i>	C(53)...H(57)	514.8(17)	20.8(fixed)	—	-1.7	20.8
<i>u5191</i>	H(226)...H(246)	514.8(137)	32.3(fixed)	—	-9.0	32.3
<i>u3165</i>	H(152)...H(159)	514.8(45)	61.5(fixed)	—	18.5	61.5
<i>u3650</i>	H(60)...H(66)	515.1(83)	47.0(fixed)	—	-11.6	47.0
<i>u3374</i>	C(49)...H(55)	515.1(36)	21.2(fixed)	—	-1.6	21.2
<i>u4512</i>	H(228)...H(245)	515.1(124)	40.0(fixed)	—	-1.7	40.0
<i>u3385</i>	C(293)...H(302)	515.2(28)	19.9(fixed)	—	-1.3	19.9
<i>u3474</i>	Si(290)...H(305)	515.2(24)	21.2(fixed)	—	-1.2	21.2
<i>u3605</i>	H(342)...H(351)	515.3(72)	38.9(fixed)	—	-2.0	38.9
<i>u2033</i>	H(178)...H(192)	515.4(35)	38.0(fixed)	—	-0.5	38.0
<i>u3471</i>	Si(290)...H(319)	515.5(24)	19.7(fixed)	—	-1.2	19.7
<i>u3417</i>	Si(86)...H(122)	515.5(20)	20.0(fixed)	—	-1.7	20.0
<i>u5176</i>	H(72)...H(79)	515.6(86)	28.0(fixed)	—	-8.6	28.0
<i>u3118</i>	H(27)...H(40)	515.7(229)	53.2(fixed)	—	1.8	53.2
<i>u3406</i>	Si(45)...H(81)	515.7(22)	20.0(fixed)	—	-1.5	20.0
<i>u3361</i>	C(296)...H(302)	515.7(13)	22.3(fixed)	—	-1.1	22.3
<i>u1050</i>	C(89)...H(113)	515.8(63)	34.8(fixed)	—	16.5	34.8
<i>u5167</i>	H(226)...H(243)	516.0(166)	39.7(fixed)	—	-11.6	39.7
<i>u4121</i>	H(225)...H(231)	516.0(107)	39.4(fixed)	—	0.2	39.4
<i>u3516</i>	Si(209)...H(234)	516.2(24)	20.0(fixed)	—	-1.5	20.0
<i>u2388</i>	H(149)...H(154)	516.2(161)	56.0(fixed)	—	0.3	56.0
<i>u3489</i>	Si(209)...H(245)	516.2(28)	19.8(fixed)	—	-1.5	19.8
<i>u4672</i>	H(219)...H(228)	516.2(138)	27.2(fixed)	—	-2.6	27.2
<i>u3113</i>	H(68)...H(81)	516.3(159)	48.3(fixed)	—	2.4	48.3
<i>u2851</i>	H(261)...H(264)	516.3(59)	30.1(fixed)	—	2.0	30.1
<i>u3788</i>	H(306)...H(323)	516.4(109)	42.3(fixed)	—	-8.9	42.3
<i>u2099</i>	Si(166)...H(197)	516.6(31)	45.1(fixed)	—	-1.5	45.1
<i>u3457</i>	C(258)...H(274)	516.6(51)	34.2(fixed)	—	1.4	34.2
<i>u3453</i>	H(19)...H(24)	516.8(222)	49.9(fixed)	—	-7.2	49.9
<i>u4857</i>	H(232)...H(240)	516.8(62)	53.2(fixed)	—	-5.7	53.2
<i>u3432</i>	Si(4)...H(40)	516.8(27)	20.4(fixed)	—	-1.7	20.4

<i>u</i> 4335	C(50)...H(58)	516.8(17)	15.7(fixed)	—	-2.8	15.7
<i>u</i> 773	H(219)...H(240)	516.9(49)	48.2(fixed)	—	9.8	48.2
<i>u</i> 3116	H(70)...H(82)	516.9(119)	49.1(fixed)	—	2.8	49.1
<i>u</i> 3428	Si(127)...H(163)	517.0(23)	20.6(fixed)	—	-1.4	20.6
<i>u</i> 3607	H(178)...H(186)	517.1(73)	46.4(fixed)	—	-0.7	46.4
<i>u</i> 4410	C(257)...H(269)	517.1(64)	20.7(fixed)	—	-2.3	20.7
<i>u</i> 3695	H(101)...H(107)	517.2(83)	46.1(fixed)	—	-11.1	46.1
<i>u</i> 1881	Si(248)...H(278)	517.3(23)	50.3(fixed)	—	1.4	50.3
<i>u</i> 3277	C(212)...H(234)	517.3(56)	35.2(fixed)	—	1.2	35.2
<i>u</i> 3396	Si(332)...H(368)	517.4(22)	21.7(fixed)	—	-1.0	21.7
<i>u</i> 3324	C(253)...H(283)	517.4(46)	32.0(fixed)	—	3.3	32.0
<i>u</i> 3900	H(98)...H(104)	517.4(29)	29.9(fixed)	—	-4.2	29.9
<i>u</i> 798	C(130)...H(160)	517.6(57)	51.4(fixed)	—	44.9	51.4
<i>u</i> 3392	C(337)...H(346)	517.6(52)	31.3(fixed)	—	3.5	31.3
<i>u</i> 2063	Si(125)...H(156)	517.6(32)	52.8(fixed)	—	-2.1	52.8
<i>u</i> 2079	Si(126)...H(155)	517.6(25)	41.1(fixed)	—	-0.2	41.1
<i>u</i> 3443	H(311)...H(320)	517.7(168)	39.5(fixed)	—	-10.4	39.5
<i>u</i> 1304	C(211)...H(244)	517.8(55)	37.1(fixed)	—	5.5	37.1
<i>u</i> 805	C(253)...H(275)	517.9(48)	30.2(fixed)	—	7.8	30.2
<i>u</i> 3136	C(130)...H(155)	517.9(120)	38.1(fixed)	—	2.8	38.1
<i>u</i> 3381	H(270)...H(282)	517.9(60)	45.9(fixed)	—	5.6	45.9
<i>u</i> 3639	H(309)...H(312)	518.1(55)	36.0(fixed)	—	4.1	36.0
<i>u</i> 3029	C(255)...H(263)	518.2(40)	22.6(fixed)	—	-1.4	22.6
<i>u</i> 3767	C(88)...C(92)	518.2(38)	19.2(fixed)	—	-1.3	19.2
<i>u</i> 4143	H(266)...H(277)	518.2(64)	43.7(fixed)	—	6.8	43.7
<i>u</i> 3419	Si(46)...H(70)	518.2(23)	20.9(fixed)	—	-1.5	20.9
<i>u</i> 3544	C(217)...H(233)	518.2(49)	35.0(fixed)	—	1.3	35.0
<i>u</i> 3407	Si(128)...H(152)	518.3(24)	21.1(fixed)	—	-1.7	21.1
<i>u</i> 1422	C(136)...H(140)	518.4(20)	38.2(fixed)	—	1.5	38.2
<i>u</i> 2004	Si(44)...H(73)	518.4(25)	35.2(fixed)	—	0.2	35.2
<i>u</i> 3389	C(295)...H(304)	518.5(32)	22.5(fixed)	—	-1.0	22.5
<i>u</i> 3423	H(302)...H(315)	518.6(33)	31.1(fixed)	—	0.9	31.1
<i>u</i> 3687	H(304)...H(323)	518.6(73)	34.7(fixed)	—	-1.6	34.7
<i>u</i> 3380	H(301)...H(322)	518.6(45)	30.3(fixed)	—	3.3	30.3
<i>u</i> 2078	Si(207)...H(238)	518.6(31)	44.1(fixed)	—	-1.7	44.1
<i>u</i> 3496	Si(251)...H(270)	518.8(37)	20.2(fixed)	—	-2.0	20.2
<i>u</i> 4481	C(211)...H(231)	518.9(78)	24.9(fixed)	—	-2.5	24.9
<i>u</i> 3643	H(343)...H(350)	518.9(74)	37.4(fixed)	—	-1.0	37.4
<i>u</i> 3435	Si(2)...H(24)	519.0(26)	20.9(fixed)	—	-2.0	20.9
<i>u</i> 5262	H(64)...H(82)	519.0(76)	23.5(fixed)	—	-7.8	23.5
<i>u</i> 3452	Si(85)...H(119)	519.0(30)	20.3(fixed)	—	-2.5	20.3
<i>u</i> 5181	H(187)...H(197)	519.0(116)	46.1(fixed)	—	-1.4	46.1
<i>u</i> 3518	Si(250)...H(286)	519.1(25)	20.6(fixed)	—	-1.2	20.6
<i>u</i> 3821	H(263)...H(277)	519.1(67)	25.1(fixed)	—	-2.2	25.1

<i>u</i> 3537	Si(126)...H(160)	519.1(28)	28.3(fixed)	—	-1.5	28.3
<i>u</i> 3488	Si(84)...H(106)	519.3(30)	20.3(fixed)	—	-1.7	20.3
<i>u</i> 3475	Si(330)...H(352)	519.3(31)	19.5(fixed)	—	-2.0	19.5
<i>u</i> 2722	Si(251)...H(280)	519.3(45)	18.7(fixed)	—	-3.2	18.7
<i>u</i> 1971	Si(43)...H(74)	519.4(31)	41.8(fixed)	—	-0.9	41.8
<i>u</i> 3171	H(150)...H(163)	519.4(62)	46.6(fixed)	—	5.5	46.6
<i>u</i> 3434	Si(87)...H(111)	519.5(23)	21.6(fixed)	—	-1.0	21.6
<i>u</i> 3478	Si(289)...H(320)	519.5(29)	22.3(fixed)	—	-1.6	22.3
<i>u</i> 3491	Si(125)...H(147)	519.6(30)	20.4(fixed)	—	-2.4	20.4
<i>u</i> 1194	C(88)...H(121)	519.6(91)	32.9(fixed)	—	6.2	32.9
<i>u</i> 820	C(51)...H(65)	519.7(54)	34.4(fixed)	—	12.9	34.4
<i>u</i> 1381	C(216)...H(219)	519.7(53)	31.2(fixed)	—	1.3	31.2
<i>u</i> 3125	H(57)...H(74)	520.1(67)	37.2(fixed)	—	3.7	37.2
<i>u</i> 1920	Si(207)...H(223)	520.1(23)	28.2(fixed)	—	3.1	28.2
<i>u</i> 3108	C(48)...H(57)	520.1(27)	25.3(fixed)	—	-1.8	25.3
<i>u</i> 3591	C(294)...H(324)	520.2(86)	35.2(fixed)	—	0.5	35.2
<i>u</i> 3028	Si(250)...H(265)	520.3(41)	22.4(fixed)	—	-3.6	22.4
<i>u</i> 4625	H(62)...H(81)	520.3(230)	41.6(fixed)	—	-3.8	41.6
<i>u</i> 5050	H(273)...H(277)	520.4(45)	49.8(fixed)	—	-8.4	49.8
<i>u</i> 3131	C(88)...H(119)	520.4(23)	42.8(fixed)	—	0.8	42.8
<i>u</i> 2113	H(68)...H(74)	520.5(107)	38.0(fixed)	—	8.5	38.0
<i>u</i> 3629	H(314)...H(326)	520.5(86)	42.4(fixed)	—	-8.8	42.4
<i>u</i> 3678	H(110)...H(118)	520.6(226)	56.9(fixed)	—	1.9	56.9
<i>u</i> 5374	H(182)...H(191)	520.9(98)	26.6(fixed)	—	-6.8	26.6
<i>u</i> 1943	H(102)...H(107)	520.9(81)	47.4(fixed)	—	12.0	47.4
<i>u</i> 3535	H(232)...H(244)	520.9(245)	38.7(fixed)	—	-5.3	38.7
<i>u</i> 5144	H(117)...H(120)	521.0(141)	28.6(fixed)	—	-5.1	28.6
<i>u</i> 1886	H(61)...H(66)	521.2(83)	50.0(fixed)	—	11.0	50.0
<i>u</i> 3527	Si(290)...H(324)	521.3(32)	19.9(fixed)	—	-2.1	19.9
<i>u</i> 3915	H(150)...H(157)	521.3(86)	40.3(fixed)	—	-14.5	40.3
<i>u</i> 3451	Si(44)...H(78)	521.6(36)	21.8(fixed)	—	-1.8	21.8
<i>u</i> 1288	C(170)...H(179)	521.7(15)	27.5(fixed)	—	3.1	27.5
<i>u</i> 4354	C(91)...H(99)	521.7(16)	15.4(fixed)	—	-2.4	15.4
<i>u</i> 4552	H(64)...H(75)	521.7(84)	37.8(fixed)	—	-1.6	37.8
<i>u</i> 3530	Si(43)...H(65)	521.7(29)	20.9(fixed)	—	-1.8	20.9
<i>u</i> 423	H(104)...H(113)	521.9(106)	41.9(fixed)	—	30.6	41.9
<i>u</i> 3751	H(30)...H(38)	522.0(71)	45.1(fixed)	—	-8.9	45.1
<i>u</i> 3379	C(217)...H(229)	522.1(34)	38.1(fixed)	—	2.4	38.1
<i>u</i> 1996	H(145)...H(164)	522.1(126)	44.1(fixed)	—	5.1	44.1
<i>u</i> 856	C(93)...H(106)	522.1(70)	34.4(fixed)	—	10.2	34.4
<i>u</i> 2833	Si(87)...H(112)	522.2(44)	22.6(fixed)	—	-9.1	22.6
<i>u</i> 1902	Si(126)...H(141)	522.2(24)	26.6(fixed)	—	3.5	26.6
<i>u</i> 1815	H(58)...H(77)	522.2(56)	51.7(fixed)	—	-1.9	51.7
<i>u</i> 2934	H(97)...H(104)	522.3(69)	30.4(fixed)	—	3.7	30.4



<i>u1607</i>	Si(166)...H(193)	522.4(22)	29.9(fixed)	—	4.8	29.9
<i>u3323</i>	H(222)...H(240)	522.4(49)	31.6(fixed)	—	4.5	31.6
<i>u3365</i>	C(295)...C(300)	522.5(46)	22.0(fixed)	—	-1.5	22.0
<i>u3486</i>	Si(210)...H(229)	522.6(32)	21.1(fixed)	—	-1.8	21.1
<i>u3534</i>	Si(330)...H(361)	522.7(31)	21.0(fixed)	—	-1.7	21.0
<i>u4673</i>	H(102)...H(114)	522.8(70)	48.2(fixed)	—	-4.5	48.2
<i>u3645</i>	C(253)...C(254)	522.8(44)	16.6(fixed)	—	-1.3	16.6
<i>u5056</i>	C(93)...H(121)	522.9(143)	24.6(fixed)	—	-2.8	24.6
<i>u3919</i>	H(185)...H(205)	522.9(81)	37.2(fixed)	—	-10.9	37.2
<i>u3326</i>	H(152)...H(164)	522.9(67)	49.6(fixed)	—	2.1	49.6
<i>u4192</i>	H(191)...H(194)	522.9(111)	49.7(fixed)	—	-9.1	49.7
<i>u4787</i>	C(253)...H(280)	522.9(64)	20.7(fixed)	—	-5.1	20.7
<i>u4207</i>	C(134)...H(145)	523.0(62)	33.6(fixed)	—	-1.3	33.6
<i>u3582</i>	C(91)...H(118)	523.0(163)	36.3(fixed)	—	0.4	36.3
<i>u1134</i>	H(260)...H(277)	523.2(29)	61.9(fixed)	—	5.2	61.9
<i>u982</i>	C(133)...H(147)	523.3(48)	42.5(fixed)	—	8.5	42.5
<i>u5235</i>	H(105)...H(123)	523.4(223)	23.1(fixed)	—	-6.2	23.1
<i>u663</i>	H(229)...H(238)	523.5(122)	52.3(fixed)	—	17.3	52.3
<i>u1722</i>	C(211)...C(214)	523.6(61)	21.2(fixed)	—	2.8	21.2
<i>u3975</i>	H(139)...H(143)	523.7(40)	27.0(fixed)	—	-4.3	27.0
<i>u3444</i>	C(295)...H(323)	523.9(49)	34.8(fixed)	—	1.2	34.8
<i>u3548</i>	Si(249)...H(283)	523.9(32)	21.0(fixed)	—	-1.7	21.0
<i>u3049</i>	C(89)...H(98)	524.0(24)	24.3(fixed)	—	-1.5	24.3
<i>u3495</i>	Si(208)...H(242)	524.1(35)	22.6(fixed)	—	-1.6	22.6
<i>u4983</i>	C(215)...H(244)	524.1(152)	25.1(fixed)	—	-1.8	25.1
<i>u1191</i>	C(47)...H(80)	524.2(65)	33.3(fixed)	—	5.8	33.3
<i>u5213</i>	H(236)...H(244)	524.3(99)	36.8(fixed)	—	-2.7	36.8
<i>u3075</i>	Si(127)...H(144)	524.5(42)	26.7(fixed)	—	-4.2	26.7
<i>u2053</i>	Si(208)...H(228)	524.5(27)	36.9(fixed)	—	2.3	36.9
<i>u5071</i>	H(66)...H(75)	524.6(62)	38.9(fixed)	—	-9.3	38.9
<i>u4509</i>	H(228)...H(239)	524.7(70)	36.2(fixed)	—	-1.2	36.2
<i>u1867</i>	Si(43)...H(59)	524.9(23)	28.2(fixed)	—	8.2	28.2
<i>u5057</i>	H(113)...H(123)	525.1(66)	51.6(fixed)	—	-8.4	51.6
<i>u1639</i>	H(239)...H(241)	525.1(129)	52.5(fixed)	—	10.4	52.5
<i>u4391</i>	C(92)...H(98)	525.1(26)	15.3(fixed)	—	-2.2	15.3
<i>u3468</i>	C(258)...H(270)	525.2(28)	38.6(fixed)	—	1.9	38.6
<i>u3533</i>	H(24)...H(30)	525.2(154)	51.4(fixed)	—	1.7	51.4
<i>u2042</i>	Si(85)...H(115)	525.2(33)	34.8(fixed)	—	-0.3	34.8
<i>u3220</i>	C(130)...H(137)	525.5(23)	17.9(fixed)	—	-0.9	17.9
<i>u4046</i>	H(318)...H(326)	525.6(83)	42.0(fixed)	—	4.1	42.0
<i>u1860</i>	Si(84)...H(100)	525.9(22)	27.8(fixed)	—	8.7	27.8
<i>u5209</i>	H(141)...H(164)	525.9(69)	27.5(fixed)	—	-9.5	27.5
<i>u3798</i>	C(296)...H(307)	526.2(56)	29.2(fixed)	—	2.6	29.2
<i>u4535</i>	H(269)...H(271)	526.2(57)	37.9(fixed)	—	-3.1	37.9

<i>u</i> 3170	H(111)...H(123)	526.4(126)	50.0(fixed)	—	5.7	50.0
<i>u</i> 2993	H(14)...H(18)	526.4(639)	34.9(fixed)	—	4.9	34.9
<i>u</i> 4307	C(53)...H(61)	526.4(44)	32.0(fixed)	—	-7.1	32.0
<i>u</i> 3526	C(254)...C(259)	526.4(30)	24.6(fixed)	—	-1.6	24.6
<i>u</i> 2505	H(146)...H(161)	526.6(61)	51.7(fixed)	—	-20.8	51.7
<i>u</i> 4527	C(258)...H(268)	526.6(53)	24.9(fixed)	—	-3.5	24.9
<i>u</i> 2104	Si(44)...H(64)	526.7(30)	31.4(fixed)	—	2.5	31.4
<i>u</i> 4009	C(90)...C(92)	526.7(29)	19.1(fixed)	—	-1.1	19.1
<i>u</i> 3616	H(149)...H(162)	526.9(75)	54.3(fixed)	—	3.0	54.3
<i>u</i> 4628	H(96)...H(105)	527.0(11)	27.7(fixed)	—	-1.8	27.7
<i>u</i> 3949	H(68)...H(75)	527.0(79)	38.0(fixed)	—	-9.9	38.0
<i>u</i> 3637	H(262)...H(285)	527.0(81)	39.4(fixed)	—	-1.7	39.4
<i>u</i> 4563	H(97)...H(103)	527.3(60)	20.8(fixed)	—	-6.5	20.8
<i>u</i> 3413	C(213)...C(218)	527.4(110)	26.1(fixed)	—	-1.7	26.1
<i>u</i> 3340	C(252)...H(260)	527.7(22)	18.2(fixed)	—	-1.5	18.2
<i>u</i> 3818	C(130)...C(134)	527.7(51)	23.6(fixed)	—	-1.3	23.6
<i>u</i> 3023	C(129)...H(139)	527.8(26)	25.2(fixed)	—	-1.7	25.2
<i>u</i> 1452	C(256)...H(260)	527.9(20)	32.7(fixed)	—	1.1	32.7
<i>u</i> 4970	H(102)...H(118)	528.1(175)	35.1(fixed)	—	-8.2	35.1
<i>u</i> 4650	H(220)...H(233)	528.3(60)	27.0(fixed)	—	-2.3	27.0
<i>u</i> 4409	C(214)...H(220)	528.6(36)	15.3(fixed)	—	-2.5	15.3
<i>u</i> 1989	Si(85)...H(105)	529.0(30)	29.6(fixed)	—	4.1	29.6
<i>u</i> 5234	H(62)...H(82)	529.1(136)	31.4(fixed)	—	-7.9	31.4
<i>u</i> 5170	H(182)...H(189)	529.1(68)	27.8(fixed)	—	-10.8	27.8
<i>u</i> 2074	Si(248)...H(269)	529.2(33)	30.7(fixed)	—	2.6	30.7
<i>u</i> 1353	C(49)...H(72)	529.2(50)	38.0(fixed)	—	4.2	38.0
<i>u</i> 5246	H(103)...H(123)	529.2(101)	29.7(fixed)	—	-6.0	29.7
<i>u</i> 3540	C(136)...H(149)	529.6(37)	35.4(fixed)	—	1.0	35.4
<i>u</i> 3266	H(58)...H(76)	529.7(70)	31.3(fixed)	—	3.3	31.3
<i>u</i> 4416	C(217)...H(225)	529.7(84)	24.7(fixed)	—	-4.3	24.7
<i>u</i> 3067	H(139)...H(156)	529.8(51)	42.8(fixed)	—	7.2	42.8
<i>u</i> 1887	C(252)...C(258)	529.8(44)	24.8(fixed)	—	1.0	24.8
<i>u</i> 1738	C(253)...C(255)	529.9(35)	21.9(fixed)	—	1.5	21.9
<i>u</i> 3588	C(335)...C(339)	529.9(50)	20.9(fixed)	—	-1.4	20.9
<i>u</i> 1370	C(133)...H(151)	529.9(45)	40.6(fixed)	—	7.7	40.6
<i>u</i> 3313	H(109)...H(122)	529.9(215)	51.4(fixed)	—	0.9	51.4
<i>u</i> 5276	H(103)...H(120)	530.1(113)	37.2(fixed)	—	-7.0	37.2
<i>u</i> 5109	H(271)...H(281)	530.1(104)	28.9(fixed)	—	-5.2	28.9
<i>u</i> 1772	H(75)...H(77)	530.2(103)	48.9(fixed)	—	11.1	48.9
<i>u</i> 4005	H(231)...H(241)	530.7(241)	40.6(fixed)	—	6.5	40.6
<i>u</i> 4281	H(105)...H(122)	530.8(194)	36.0(fixed)	—	0.9	36.0
<i>u</i> 4074	H(24)...H(31)	531.0(176)	43.8(fixed)	—	-5.2	43.8
<i>u</i> 4137	H(20)...H(28)	531.2(360)	36.8(fixed)	—	3.1	36.8
<i>u</i> 5391	H(266)...H(271)	531.2(45)	25.0(fixed)	—	-5.3	25.0

<i>u672</i>	H(70)...H(74)	531.5(65)	56.0(fixed)	—	14.1	56.0
<i>u5201</i>	H(226)...H(238)	531.5(81)	22.3(fixed)	—	-6.6	22.3
<i>u2082</i>	H(150)...H(156)	531.5(85)	41.6(fixed)	—	16.5	41.6
<i>u1453</i>	C(51)...H(69)	531.6(50)	42.3(fixed)	—	6.5	42.3
<i>u4844</i>	H(183)...H(199)	531.6(56)	35.7(fixed)	—	-3.1	35.7
<i>u3168</i>	C(254)...H(268)	531.7(54)	28.9(fixed)	—	2.3	28.9
<i>u1034</i>	C(92)...H(104)	531.8(95)	30.2(fixed)	—	9.2	30.2
<i>u4271</i>	C(8)...H(31)	531.8(357)	38.7(tied to <i>u3698</i> )	—	-6.7	35.8
<i>u5115</i>	H(148)...H(157)	531.8(57)	43.6(fixed)	—	-11.6	43.6
<i>u5130</i>	H(274)...H(279)	531.8(96)	34.7(fixed)	—	-0.8	34.7
<i>u3606</i>	C(91)...C(94)	531.9(93)	24.3(tied to <i>u3698</i> )	—	-1.8	22.5
<i>u3706</i>	C(294)...C(295)	531.9(19)	18.4(tied to <i>u3698</i> )	—	-1.0	17.0
<i>u3609</i>	H(306)...H(317)	532.3(62)	41.3(fixed)	—	-7.9	41.3
<i>u3510</i>	H(15)...H(37)	532.5(116)	37.7(fixed)	—	-1.2	37.7
<i>u4111</i>	H(308)...H(328)	532.6(81)	43.2(fixed)	—	-9.6	43.2
<i>u1294</i>	C(90)...H(117)	532.7(43)	37.3(fixed)	—	4.9	37.3
<i>u3542</i>	C(337)...H(364)	532.7(29)	32.8(fixed)	—	1.3	32.8
<i>u3631</i>	H(273)...H(287)	532.8(50)	37.4(fixed)	—	-6.8	37.4
<i>u3849</i>	C(293)...C(296)	533.2(35)	19.7(tied to <i>u3698</i> )	—	-1.1	18.3
<i>u3698</i>	C(6)...C(11)	533.3(13)	20.1(17)	—	-1.0	18.6
<i>u1667</i>	H(146)...H(159)	533.5(88)	124.5(fixed)	—	-1.4	124.5
<i>u3692</i>	H(221)...H(244)	533.5(131)	35.3(fixed)	—	-1.7	35.3
<i>u446</i>	H(270)...H(278)	533.6(82)	46.1(fixed)	—	26.0	46.1
<i>u4496</i>	H(223)...H(230)	533.7(118)	37.4(fixed)	—	-2.0	37.4
<i>u5252</i>	H(109)...H(113)	533.7(63)	25.7(fixed)	—	-9.6	25.7
<i>u4006</i>	H(20)...H(35)	534.1(61)	35.6(fixed)	—	7.8	35.6
<i>u4176</i>	H(102)...H(113)	534.2(54)	40.6(fixed)	—	4.5	40.6
<i>u3750</i>	C(211)...C(213)	534.2(55)	20.3(tied to <i>u3698</i> )	—	-1.5	18.8
<i>u3203</i>	H(21)...H(33)	534.4(865)	66.0(fixed)	—	-11.7	66.0
<i>u4470</i>	H(64)...H(81)	534.7(97)	38.8(fixed)	—	-1.1	38.8
<i>u4317</i>	H(264)...H(278)	534.7(83)	38.7(fixed)	—	-2.8	38.7
<i>u3804</i>	C(255)...C(256)	534.8(16)	21.4(tied to <i>u3698</i> )	—	-1.2	19.8
<i>u1490</i>	C(253)...H(285)	534.9(40)	46.1(fixed)	—	5.1	46.1
<i>u3976</i>	H(272)...H(282)	535.1(129)	39.9(fixed)	—	4.8	39.9
<i>u1254</i>	H(140)...H(163)	535.2(60)	61.9(fixed)	—	3.5	61.9
<i>u4709</i>	H(141)...H(158)	535.2(64)	34.3(fixed)	—	-6.5	34.3
<i>u2365</i>	C(51)...H(67)	535.2(99)	47.5(fixed)	—	-2.4	47.5
<i>u1935</i>	H(222)...H(241)	535.3(41)	48.8(fixed)	—	-2.0	48.8
<i>u3576</i>	C(131)...C(136)	535.4(24)	23.5(tied to <i>u3698</i> )	—	-1.3	21.8
<i>u4155</i>	C(47)...H(77)	535.6(60)	38.3(fixed)	—	-6.0	38.3
<i>u3566</i>	H(111)...H(120)	535.7(32)	43.7(fixed)	—	6.6	43.7
<i>u2251</i>	H(99)...H(118)	535.7(163)	41.0(fixed)	—	-0.7	41.0
<i>u3484</i>	H(313)...H(317)	535.9(48)	37.4(fixed)	—	7.7	37.4
<i>u5048</i>	C(255)...H(279)	536.1(70)	24.5(fixed)	—	-2.1	24.5

<i>u2084</i>	H(261)...H(270)	536.1(87)	35.5(fixed)	—	-1.8	35.5
<i>u5074</i>	H(281)...H(287)	536.2(42)	36.6(fixed)	—	-5.8	36.6
<i>u3809</i>	C(9)...H(36)	536.3(77)	31.0(fixed)	—	1.1	31.0
<i>u5149</i>	H(116)...H(120)	536.3(57)	29.2(fixed)	—	-5.0	29.2
<i>u1884</i>	C(216)...C(217)	536.4(57)	21.7(tied to <i>u3698</i> )	—	0.8	20.0
<i>u3855</i>	H(22)...H(36)	536.5(240)	41.6(fixed)	—	9.0	41.6
<i>u3937</i>	C(214)...C(216)	536.8(19)	23.2(tied to <i>u3698</i> )	—	-1.5	21.5
<i>u3792</i>	C(294)...C(299)	536.8(62)	25.4(tied to <i>u3698</i> )	—	-2.0	23.5
<i>u3583</i>	C(294)...C(298)	536.9(34)	25.2(tied to <i>u3698</i> )	—	-1.3	23.3
<i>u5218</i>	H(62)...H(74)	537.0(77)	22.4(fixed)	—	-6.9	22.4
<i>u2010</i>	H(276)...H(282)	537.2(57)	44.8(fixed)	—	3.0	44.8
<i>u2373</i>	H(223)...H(232)	537.3(108)	41.7(fixed)	—	0.9	41.7
<i>u3993</i>	H(343)...H(354)	537.3(49)	26.2(fixed)	—	-3.6	26.2
<i>u4277</i>	C(133)...H(144)	537.4(75)	34.5(fixed)	—	-4.6	34.5
<i>u3260</i>	C(47)...C(53)	537.4(42)	26.2(tied to <i>u3698</i> )	—	-1.6	24.3
<i>u1156</i>	H(220)...H(222)	537.5(25)	34.1(fixed)	—	1.7	34.1
<i>u656</i>	H(152)...H(156)	537.6(80)	56.8(fixed)	—	21.9	56.8
<i>u3935</i>	H(145)...H(158)	537.6(54)	42.8(fixed)	—	10.9	42.8
<i>u3236</i>	H(22)...H(37)	537.6(316)	50.1(fixed)	—	8.5	50.1
<i>u5047</i>	C(51)...H(80)	537.7(115)	24.4(fixed)	—	-2.5	24.4
<i>u1150</i>	H(56)...H(58)	537.7(25)	33.4(fixed)	—	1.6	33.4
<i>u4097</i>	H(26)...H(39)	537.9(100)	40.9(fixed)	—	2.5	40.9
<i>u4778</i>	C(215)...C(218)	538.0(87)	13.7(tied to <i>u3698</i> )	—	-2.2	12.7
<i>u4055</i>	C(253)...H(279)	538.1(51)	32.4(fixed)	—	-1.7	32.4
<i>u3846</i>	H(302)...H(307)	538.3(66)	39.8(fixed)	—	-2.5	39.8
<i>u4058</i>	C(336)...H(359)	538.3(50)	29.5(fixed)	—	1.5	29.5
<i>u3741</i>	C(7)...C(12)	538.6(48)	23.2(tied to <i>u3698</i> )	—	-1.0	21.5
<i>u3302</i>	H(105)...H(114)	538.6(76)	51.5(fixed)	—	-10.2	51.5
<i>u3215</i>	C(173)...H(186)	538.7(35)	36.0(fixed)	—	7.6	36.0
<i>u1784</i>	H(142)...H(149)	538.9(49)	44.7(fixed)	—	5.9	44.7
<i>u2366</i>	H(263)...H(280)	539.0(70)	34.6(fixed)	—	-1.8	34.6
<i>u3835</i>	H(21)...H(25)	539.1(59)	39.2(fixed)	—	-11.3	39.2
<i>u955</i>	C(134)...H(159)	539.1(53)	50.3(fixed)	—	46.3	50.3
<i>u3514</i>	H(148)...H(163)	539.2(69)	40.9(fixed)	—	6.5	40.9
<i>u3594</i>	C(336)...C(341)	539.2(20)	22.8(tied to <i>u3698</i> )	—	-1.1	21.1
<i>u3703</i>	C(170)...C(172)	539.3(20)	20.9(tied to <i>u3698</i> )	—	-1.2	19.3
<i>u1444</i>	C(131)...H(154)	539.3(87)	49.9(fixed)	—	6.2	49.9
<i>u3656</i>	H(232)...H(246)	539.5(90)	35.6(fixed)	—	-5.6	35.6
<i>u1906</i>	C(52)...C(53)	539.5(46)	23.4(tied to <i>u3698</i> )	—	0.7	21.6
<i>u5279</i>	H(265)...H(273)	539.6(82)	30.7(fixed)	—	-6.7	30.7
<i>u4035</i>	H(184)...H(190)	539.7(60)	34.9(fixed)	—	5.9	34.9
<i>u1946</i>	H(231)...H(235)	539.7(64)	48.9(fixed)	—	1.5	48.9
<i>u3724</i>	C(8)...C(13)	539.8(21)	21.5(tied to <i>u3698</i> )	—	-1.3	19.9
<i>u4765</i>	C(93)...C(95)	539.9(80)	13.5(tied to <i>u3698</i> )	—	-2.6	12.5

<i>u4491</i>	C(253)...H(282)	540.0(93)	30.4(fixed)	—	-4.4	30.4
<i>u4996</i>	C(133)...H(162)	540.1(35)	27.1(fixed)	—	-1.9	27.1
<i>u3731</i>	H(25)...H(40)	540.3(73)	40.3(fixed)	—	2.2	40.3
<i>u4529</i>	C(88)...H(110)	540.3(49)	22.4(fixed)	—	-3.3	22.4
<i>u5066</i>	H(265)...H(274)	540.3(61)	34.1(fixed)	—	-5.6	34.1
<i>u5356</i>	H(145)...H(150)	540.4(37)	28.4(fixed)	—	-4.9	28.4
<i>u5196</i>	H(154)...H(162)	540.4(93)	36.7(fixed)	—	-3.4	36.7
<i>u4017</i>	H(21)...H(39)	540.4(90)	43.1(fixed)	—	4.5	43.1
<i>u4028</i>	H(309)...H(313)	540.5(46)	34.5(fixed)	—	1.0	34.5
<i>u3866</i>	C(92)...C(95)	540.5(20)	22.6(tied to <i>u3698</i> )	—	-1.8	20.9
<i>u4398</i>	C(94)...H(102)	540.6(61)	36.2(fixed)	—	-7.3	36.2
<i>u1785</i>	C(49)...C(51)	540.6(36)	26.3(tied to <i>u3698</i> )	—	1.4	24.4
<i>u3708</i>	C(337)...C(338)	540.7(19)	20.3(tied to <i>u3698</i> )	—	-1.0	18.8
<i>u4109</i>	H(319)...H(328)	540.8(41)	37.5(fixed)	—	1.8	37.5
<i>u4081</i>	H(309)...H(311)	540.8(80)	32.3(fixed)	—	-0.6	32.3
<i>u3408</i>	C(211)...C(217)	540.9(77)	25.9(tied to <i>u3698</i> )	—	-1.7	23.9
<i>u2472</i>	C(93)...H(108)	540.9(70)	39.3(fixed)	—	-2.2	39.3
<i>u4268</i>	H(141)...H(163)	541.1(93)	49.7(fixed)	—	0.8	49.7
<i>u3602</i>	H(56)...H(67)	541.1(59)	41.5(fixed)	—	-0.7	41.5
<i>u1127</i>	C(93)...H(110)	541.2(43)	34.2(fixed)	—	12.8	34.2
<i>u4000</i>	H(301)...H(318)	541.3(50)	27.0(fixed)	—	-3.9	27.0
<i>u5250</i>	H(72)...H(80)	541.3(115)	31.3(fixed)	—	-3.5	31.3
<i>u3762</i>	H(301)...H(304)	541.4(20)	17.4(fixed)	—	-2.6	17.4
<i>u3783</i>	C(294)...H(322)	541.6(96)	43.7(fixed)	—	-1.0	43.7
<i>u4182</i>	H(102)...H(110)	541.9(73)	38.1(fixed)	—	3.7	38.1
<i>u3634</i>	C(295)...C(297)	542.0(17)	18.5(tied to <i>u3698</i> )	—	-1.0	17.1
<i>u3877</i>	C(7)...C(13)	542.2(41)	21.8(tied to <i>u3698</i> )	—	-1.5	20.1
<i>u4288</i>	C(211)...H(241)	542.4(22)	35.5(fixed)	—	-5.9	35.5
<i>u4485</i>	C(47)...H(69)	542.4(52)	22.1(fixed)	—	-3.0	22.1
<i>u3864</i>	C(213)...H(241)	542.4(143)	30.2(fixed)	—	3.6	30.2
<i>u4763</i>	C(252)...C(254)	542.5(32)	13.3(tied to <i>u3698</i> )	—	-2.2	12.3
<i>u2931</i>	H(137)...H(145)	542.9(81)	30.8(fixed)	—	3.7	30.8
<i>u3784</i>	H(178)...H(181)	542.9(20)	17.4(fixed)	—	-2.6	17.4
<i>u3775</i>	H(343)...H(345)	543.0(20)	17.3(fixed)	—	-2.1	17.3
<i>u3705</i>	C(95)...H(108)	543.0(62)	29.4(fixed)	—	2.5	29.4
<i>u3790</i>	Si(251)...H(271)	543.1(21)	17.0(fixed)	—	-3.6	17.0
<i>u3630</i>	C(253)...C(258)	543.2(33)	23.3(tied to <i>u3698</i> )	—	-1.5	21.5
<i>u4365</i>	C(92)...H(100)	543.3(68)	25.5(fixed)	—	-1.8	25.5
<i>u4156</i>	H(113)...H(121)	543.4(100)	62.0(fixed)	—	0.1	62.0
<i>u3569</i>	H(25)...H(32)	543.4(178)	45.0(fixed)	—	4.9	45.0
<i>u4499</i>	H(142)...H(163)	543.7(64)	57.5(fixed)	—	-3.5	57.5
<i>u4076</i>	C(334)...C(340)	543.7(35)	21.6(tied to <i>u3698</i> )	—	-1.2	20.0
<i>u2921</i>	H(137)...H(140)	544.0(21)	27.5(fixed)	—	-1.7	27.5
<i>u3836</i>	C(252)...H(277)	544.1(50)	28.5(fixed)	—	5.4	28.5

<i>u3737</i>	H(96)...H(106)	544.1(39)	25.1(fixed)	—	-1.8	25.1
<i>u2945</i>	H(146)...H(155)	544.2(127)	52.7(fixed)	—	4.5	52.7
<i>u2741</i>	Si(166)...H(198)	544.3(23)	24.4(fixed)	—	-6.7	24.4
<i>u2129</i>	H(62)...H(67)	544.3(49)	49.5(fixed)	—	7.7	49.5
<i>u2068</i>	H(103)...H(108)	544.4(54)	46.9(fixed)	—	4.1	46.9
<i>u1858</i>	C(90)...C(93)	544.5(28)	26.6(tied to <i>u3698</i> )	—	1.1	24.6
<i>u2691</i>	C(134)...H(160)	544.5(79)	65.1(fixed)	—	-17.9	65.1
<i>u1900</i>	C(134)...C(135)	544.7(11)	22.2(tied to <i>u3698</i> )	—	1.2	20.6
<i>u3995</i>	H(67)...H(80)	545.0(99)	40.9(fixed)	—	4.3	40.9
<i>u4510</i>	C(214)...H(227)	545.1(60)	26.8(fixed)	—	-4.1	26.8
<i>u3746</i>	H(138)...H(149)	545.1(49)	35.9(fixed)	—	-1.8	35.9
<i>u3681</i>	C(170)...C(175)	545.2(15)	21.8(tied to <i>u3698</i> )	—	-1.3	20.2
<i>u4741</i>	H(234)...H(240)	545.2(57)	47.5(fixed)	—	-1.9	47.5
<i>u2250</i>	C(130)...H(159)	545.2(83)	96.6(fixed)	—	-9.9	96.6
<i>u4160</i>	H(61)...H(69)	545.8(89)	38.6(fixed)	—	3.7	38.6
<i>u5400</i>	H(237)...H(246)	545.8(83)	28.2(fixed)	—	-5.1	28.2
<i>u2439</i>	H(269)...H(273)	545.9(59)	45.7(fixed)	—	-0.5	45.7
<i>u3753</i>	C(54)...H(67)	545.9(43)	29.6(fixed)	—	2.1	29.6
<i>u3980</i>	H(263)...H(274)	546.0(39)	25.1(fixed)	—	-3.7	25.1
<i>u3723</i>	C(335)...C(336)	546.0(14)	18.7(tied to <i>u3698</i> )	—	-1.0	17.3
<i>u4203</i>	H(56)...H(81)	546.0(41)	26.2(fixed)	—	-3.3	26.2
<i>u3841</i>	C(254)...H(282)	546.0(45)	30.7(fixed)	—	2.6	30.7
<i>u3677</i>	H(308)...H(318)	546.0(54)	39.9(fixed)	—	2.4	39.9
<i>u2734</i>	Si(125)...H(157)	546.1(24)	26.1(fixed)	—	-9.7	26.1
<i>u3781</i>	Si(85)...H(120)	546.2(24)	17.1(fixed)	—	-4.3	17.1
<i>u3889</i>	H(96)...H(108)	546.3(57)	28.2(fixed)	—	-2.7	28.2
<i>u1936</i>	C(256)...C(258)	546.3(16)	23.1(tied to <i>u3698</i> )	—	0.6	21.4
<i>u1420</i>	H(178)...H(197)	546.4(21)	62.2(fixed)	—	2.5	62.2
<i>u3711</i>	C(6)...C(9)	546.5(21)	22.6(tied to <i>u3698</i> )	—	-2.0	20.9
<i>u3712</i>	C(10)...C(13)	546.5(21)	22.6(tied to <i>u3698</i> )	—	-2.0	20.9
<i>u4771</i>	C(51)...C(54)	546.5(64)	13.6(tied to <i>u3698</i> )	—	-2.5	12.6
<i>u3899</i>	Si(2)...H(21)	546.5(21)	16.8(fixed)	—	-4.6	16.8
<i>u3699</i>	C(90)...C(95)	546.5(76)	21.4(tied to <i>u3698</i> )	—	-0.7	19.8
<i>u4146</i>	C(7)...H(36)	546.6(138)	33.6(fixed)	—	-1.1	33.6
<i>u3772</i>	Si(126)...H(161)	546.6(17)	18.5(fixed)	—	-7.6	18.5
<i>u3733</i>	H(342)...H(352)	546.7(20)	24.6(fixed)	—	-2.4	24.6
<i>u4079</i>	H(69)...H(77)	546.7(104)	42.0(fixed)	—	5.1	42.0
<i>u3693</i>	C(49)...C(54)	546.7(42)	20.2(tied to <i>u3698</i> )	—	-1.1	18.7
<i>u3720</i>	H(139)...H(160)	546.8(18)	25.9(fixed)	—	-0.1	25.9
<i>u3722</i>	H(342)...H(354)	546.8(26)	28.2(fixed)	—	-2.6	28.2
<i>u2131</i>	H(266)...H(287)	546.9(111)	45.3(fixed)	—	3.3	45.3
<i>u1760</i>	C(129)...C(131)	546.9(12)	25.1(tied to <i>u3698</i> )	—	2.5	23.2
<i>u3828</i>	H(233)...H(240)	547.0(73)	59.9(fixed)	—	3.7	59.9
<i>u3702</i>	C(132)...C(135)	547.0(21)	22.0(tied to <i>u3698</i> )	—	-1.1	20.4

<i>u3859</i>	C(50)...H(77)	547.1(98)	29.4(fixed)	—	2.4	29.4
<i>u3793</i>	H(14)...H(24)	547.1(23)	26.1(fixed)	—	-2.4	26.1
<i>u4920</i>	C(134)...H(142)	547.1(73)	22.7(fixed)	—	-6.0	22.7
<i>u3739</i>	C(50)...C(53)	547.1(57)	20.4(tied to <i>u3698</i> )	—	-1.3	18.9
<i>u3752</i>	C(294)...C(297)	547.1(24)	20.5(tied to <i>u3698</i> )	—	-1.8	19.0
<i>u2710</i>	Si(43)...H(75)	547.2(20)	20.7(fixed)	—	-5.6	20.7
<i>u3717</i>	H(69)...H(81)	547.3(145)	41.8(fixed)	—	-3.0	41.8
<i>u2714</i>	Si(207)...H(239)	547.5(21)	24.0(fixed)	—	-7.0	24.0
<i>u5214</i>	H(266)...H(272)	547.5(47)	29.8(fixed)	—	-2.9	29.8
<i>u4501</i>	H(269)...H(279)	547.7(56)	36.9(fixed)	—	-1.1	36.9
<i>u3133</i>	H(262)...H(281)	547.7(66)	32.8(fixed)	—	1.6	32.8
<i>u3926</i>	H(98)...H(118)	547.8(44)	28.2(fixed)	—	-3.6	28.2
<i>u5062</i>	H(227)...H(233)	547.8(100)	28.4(fixed)	—	-6.0	28.4
<i>u4864</i>	H(275)...H(277)	547.9(51)	48.4(fixed)	—	-3.8	48.4
<i>u1931</i>	C(131)...C(133)	548.0(58)	34.7(tied to <i>u3698</i> )	—	1.5	32.1
<i>u3710</i>	Si(330)...H(353)	548.0(22)	16.9(fixed)	—	-3.4	16.9
<i>u3175</i>	C(253)...H(281)	548.0(53)	29.2(fixed)	—	2.5	29.2
<i>u3716</i>	H(70)...H(80)	548.1(128)	41.4(fixed)	—	-2.5	41.4
<i>u3126</i>	C(133)...H(146)	548.1(66)	42.2(fixed)	—	1.3	42.2
<i>u4043</i>	H(108)...H(121)	548.2(79)	39.3(fixed)	—	3.8	39.3
<i>u4755</i>	C(133)...C(136)	548.2(28)	14.0(tied to <i>u3698</i> )	—	-2.6	12.9
<i>u3924</i>	H(342)...H(359)	548.3(49)	28.0(fixed)	—	-4.3	28.0
<i>u3884</i>	Si(2)...H(25)	548.3(23)	15.9(fixed)	—	-4.0	15.9
<i>u2808</i>	Si(208)...H(235)	548.4(20)	23.5(fixed)	—	-9.3	23.5
<i>u2564</i>	C(133)...H(149)	548.6(131)	41.2(fixed)	—	-1.2	41.2
<i>u3773</i>	C(88)...C(91)	548.7(30)	21.6(tied to <i>u3698</i> )	—	-1.4	20.0
<i>u3231</i>	C(255)...H(278)	548.7(71)	38.0(fixed)	—	10.5	38.0
<i>u4044</i>	C(94)...H(110)	548.8(161)	46.5(fixed)	—	-2.7	46.5
<i>u3833</i>	H(188)...H(198)	548.8(110)	46.4(fixed)	—	4.2	46.4
<i>u1918</i>	H(101)...H(121)	548.8(106)	51.9(fixed)	—	2.5	51.9
<i>u3879</i>	H(316)...H(322)	548.8(60)	37.7(fixed)	—	3.4	37.7
<i>u3763</i>	Si(125)...H(148)	548.9(18)	16.9(fixed)	—	-3.7	16.9
<i>u3874</i>	H(139)...H(159)	548.9(20)	27.6(fixed)	—	-4.8	27.6
<i>u3721</i>	H(21)...H(37)	549.0(65)	47.8(fixed)	—	4.4	47.8
<i>u2027</i>	C(48)...C(49)	549.1(17)	32.4(tied to <i>u3698</i> )	—	1.3	30.0
<i>u4658</i>	H(98)...H(113)	549.1(47)	30.0(fixed)	—	-0.8	30.0
<i>u3801</i>	Si(84)...H(107)	549.2(19)	16.4(fixed)	—	-3.6	16.4
<i>u3916</i>	Si(4)...H(19)	549.3(21)	15.7(fixed)	—	-4.2	15.7
<i>u928</i>	H(57)...H(61)	549.4(49)	57.1(fixed)	—	5.8	57.1
<i>u4224</i>	H(138)...H(163)	549.4(20)	28.8(fixed)	—	-4.0	28.8
<i>u3764</i>	H(343)...H(368)	549.5(20)	26.1(fixed)	—	-1.8	26.1
<i>u3689</i>	C(47)...C(50)	549.6(31)	21.7(tied to <i>u3698</i> )	—	-1.3	20.1
<i>u3493</i>	Si(4)...H(18)	549.8(465)	21.2(fixed)	—	-1.5	21.2
<i>u3956</i>	Si(290)...H(306)	549.8(22)	15.4(fixed)	—	-4.1	15.4

<i>u3794</i>	Si(290)...H(325)	549.9(21)	17.0(fixed)	—	-3.5	17.0
<i>u3909</i>	Si(289)...H(321)	549.9(21)	16.3(fixed)	—	-4.2	16.3
<i>u4250</i>	H(106)...H(112)	549.9(54)	42.3(fixed)	—	1.5	42.3
<i>u2260</i>	H(58)...H(79)	550.0(96)	35.8(fixed)	—	-4.0	35.8
<i>u3800</i>	H(28)...H(40)	550.1(168)	43.7(fixed)	—	-3.2	43.7
<i>u4090</i>	C(257)...C(259)	550.2(11)	21.3(tied to <i>u3698</i> )	—	-1.4	19.7
<i>u3523</i>	H(306)...H(320)	550.2(85)	44.3(fixed)	—	5.0	44.3
<i>u3848</i>	H(137)...H(147)	550.3(19)	25.1(fixed)	—	-3.2	25.1
<i>u3805</i>	C(255)...C(258)	550.4(20)	19.7(tied to <i>u3698</i> )	—	-1.3	18.3
<i>u3440</i>	C(88)...C(94)	550.4(72)	29.5(tied to <i>u3698</i> )	—	-1.9	27.3
<i>u4916</i>	C(95)...H(117)	550.5(9)	24.5(fixed)	—	-1.4	24.5
<i>u3812</i>	H(98)...H(119)	550.5(45)	25.8(fixed)	—	-3.3	25.8
<i>u2572</i>	H(57)...H(60)	550.6(51)	37.4(fixed)	—	-7.2	37.4
<i>u3990</i>	Si(330)...H(347)	550.6(21)	15.0(fixed)	—	-3.5	15.0
<i>u4083</i>	H(14)...H(26)	550.6(62)	26.8(fixed)	—	-3.3	26.8
<i>u3672</i>	H(107)...H(122)	550.7(187)	41.3(fixed)	—	2.8	41.3
<i>u3862</i>	Si(86)...H(123)	550.7(38)	15.3(fixed)	—	-4.1	15.3
<i>u3876</i>	C(213)...C(217)	550.8(86)	23.1(tied to <i>u3698</i> )	—	-1.3	21.4
<i>u3917</i>	H(301)...H(317)	550.8(65)	31.8(fixed)	—	-3.6	31.8
<i>u908</i>	H(98)...H(102)	550.9(53)	55.7(fixed)	—	7.2	55.7
<i>u4750</i>	C(130)...C(132)	550.9(17)	13.9(tied to <i>u3698</i> )	—	-2.8	12.9
<i>u2611</i>	C(216)...H(242)	550.9(41)	38.6(fixed)	—	-4.9	38.6
<i>u3018</i>	Si(43)...H(60)	550.9(18)	25.6(fixed)	—	-5.5	25.6
<i>u1907</i>	C(89)...C(90)	551.0(16)	28.1(tied to <i>u3698</i> )	—	1.2	26.0
<i>u4053</i>	C(295)...H(310)	551.0(66)	32.9(fixed)	—	-1.3	32.9
<i>u4272</i>	C(293)...H(315)	551.1(61)	32.5(fixed)	—	-1.6	32.5
<i>u3735</i>	C(8)...H(35)	551.1(216)	31.5(fixed)	—	5.1	31.5
<i>u3945</i>	H(152)...H(162)	551.2(52)	43.7(fixed)	—	-5.1	43.7
<i>u3404</i>	H(220)...H(244)	551.2(62)	32.4(fixed)	—	0.8	32.4
<i>u3979</i>	Si(210)...H(230)	551.4(25)	16.0(fixed)	—	-3.8	16.0
<i>u1960</i>	C(213)...C(215)	551.5(31)	24.0(tied to <i>u3698</i> )	—	0.7	22.3
<i>u5111</i>	H(271)...H(280)	551.5(51)	28.8(fixed)	—	-5.4	28.8
<i>u4248</i>	H(23)...H(39)	551.6(49)	35.8(fixed)	—	-1.0	35.8
<i>u3896</i>	H(137)...H(149)	551.7(19)	28.6(fixed)	—	-3.6	28.6
<i>u3858</i>	C(214)...C(217)	551.8(31)	20.8(tied to <i>u3698</i> )	—	-1.6	19.2
<i>u3568</i>	H(56)...H(80)	551.8(38)	33.2(fixed)	—	0.3	33.2
<i>u4193</i>	H(220)...H(245)	551.9(38)	26.6(fixed)	—	-3.3	26.6
<i>u3640</i>	H(66)...H(81)	551.9(53)	39.4(fixed)	—	3.7	39.4
<i>u3971</i>	C(131)...H(162)	551.9(63)	44.6(fixed)	—	-1.9	44.6
<i>u2639</i>	H(98)...H(101)	552.1(41)	36.6(fixed)	—	-7.9	36.6
<i>u2431</i>	H(221)...H(227)	552.1(31)	40.1(fixed)	—	-0.9	40.1
<i>u3931</i>	C(334)...H(356)	552.1(36)	28.1(fixed)	—	3.1	28.1
<i>u2584</i>	H(178)...H(198)	552.2(29)	37.6(fixed)	—	-6.8	37.6
<i>u1913</i>	H(224)...H(244)	552.2(64)	45.2(fixed)	—	5.4	45.2



<i>u</i> 1857	C(211)...C(218)	552.2(71)	26.6(tied to <i>u</i> 3698)	—	1.9	24.6
<i>u</i> 3608	H(308)...H(320)	552.4(40)	46.9(fixed)	—	5.2	46.9
<i>u</i> 3401	C(213)...H(225)	552.4(81)	35.0(fixed)	—	1.3	35.0
<i>u</i> 4128	H(274)...H(277)	552.5(46)	58.6(fixed)	—	0.1	58.6
<i>u</i> 3873	Si(209)...H(246)	552.6(18)	15.3(fixed)	—	-3.4	15.3
<i>u</i> 3885	H(151)...H(163)	552.6(48)	39.1(fixed)	—	-1.4	39.1
<i>u</i> 3085	H(260)...H(266)	552.6(60)	33.5(fixed)	—	1.6	33.5
<i>u</i> 4910	C(88)...H(112)	552.7(51)	23.0(fixed)	—	-11.5	23.0
<i>u</i> 2075	H(238)...H(241)	552.7(78)	39.1(fixed)	—	3.9	39.1
<i>u</i> 3934	H(302)...H(327)	552.8(27)	25.6(fixed)	—	-1.8	25.6
<i>u</i> 4434	C(133)...H(145)	552.9(59)	30.5(fixed)	—	-5.0	30.5
<i>u</i> 3697	H(70)...H(79)	552.9(117)	40.5(fixed)	—	4.1	40.5
<i>u</i> 3857	Si(330)...H(362)	553.0(20)	16.6(fixed)	—	-3.6	16.6
<i>u</i> 4026	H(302)...H(326)	553.0(31)	25.3(fixed)	—	-2.6	25.3
<i>u</i> 4458	C(129)...H(157)	553.1(88)	28.4(fixed)	—	-1.3	28.4
<i>u</i> 3891	Si(45)...H(82)	553.2(19)	15.1(fixed)	—	-3.5	15.1
<i>u</i> 3048	Si(84)...H(101)	553.2(18)	24.0(fixed)	—	-6.2	24.0
<i>u</i> 3736	H(57)...H(78)	553.2(52)	25.8(fixed)	—	-1.5	25.8
<i>u</i> 5215	H(269)...H(280)	553.3(93)	22.2(fixed)	—	-6.9	22.2
<i>u</i> 4379	C(334)...H(364)	553.3(87)	32.0(fixed)	—	-1.5	32.0
<i>u</i> 2271	H(143)...H(149)	553.4(39)	39.8(fixed)	—	0.4	39.8
<i>u</i> 1673	C(88)...C(95)	553.4(52)	22.1(tied to <i>u</i> 3698)	—	3.2	20.5
<i>u</i> 4198	H(143)...H(156)	553.5(87)	36.6(fixed)	—	-1.9	36.6
<i>u</i> 3819	H(274)...H(284)	553.6(54)	39.9(fixed)	—	3.1	39.9
<i>u</i> 2106	H(263)...H(279)	553.6(69)	36.6(fixed)	—	-2.0	36.6
<i>u</i> 3887	H(55)...H(65)	553.6(22)	25.4(fixed)	—	-1.6	25.4
<i>u</i> 2836	Si(248)...H(276)	553.7(18)	22.5(fixed)	—	-9.6	22.5
<i>u</i> 4638	H(222)...H(231)	553.7(34)	24.9(fixed)	—	-1.9	24.9
<i>u</i> 3070	Si(207)...H(224)	553.8(22)	22.1(fixed)	—	-3.0	22.1
<i>u</i> 3734	C(334)...H(368)	553.9(66)	46.1(fixed)	—	0.3	46.1
<i>u</i> 3932	C(254)...C(258)	554.0(37)	23.8(tied to <i>u</i> 3698)	—	-1.2	22.1
<i>u</i> 3890	Si(44)...H(79)	554.2(24)	15.8(fixed)	—	-4.2	15.8
<i>u</i> 5226	H(109)...H(112)	554.2(60)	29.8(fixed)	—	-10.2	29.8
<i>u</i> 3912	C(334)...C(337)	554.3(23)	19.0(tied to <i>u</i> 3698)	—	-1.2	17.6
<i>u</i> 4086	C(7)...H(28)	554.4(91)	35.6(fixed)	—	0.0	35.6
<i>u</i> 2107	H(74)...H(77)	554.4(80)	40.0(fixed)	—	5.0	40.0
<i>u</i> 3618	H(152)...H(161)	554.4(72)	51.9(fixed)	—	7.9	51.9
<i>u</i> 3204	Si(208)...H(226)	554.4(17)	25.3(fixed)	—	-3.7	25.3
<i>u</i> 3870	Si(43)...H(66)	554.5(18)	16.1(fixed)	—	-3.8	16.1
<i>u</i> 3376	H(137)...H(154)	554.5(71)	34.2(fixed)	—	1.8	34.2
<i>u</i> 3839	Si(290)...H(317)	554.6(21)	15.2(fixed)	—	-3.3	15.2
<i>u</i> 3601	C(212)...C(214)	554.8(43)	28.5(tied to <i>u</i> 3698)	—	-2.0	26.4
<i>u</i> 3834	H(96)...H(107)	554.9(77)	29.3(fixed)	—	-1.9	29.3
<i>u</i> 3715	H(144)...H(164)	555.0(67)	43.3(fixed)	—	-8.5	43.3

<i>u</i> 3816	Si(250)...H(273)	555.0(18)	15.3(fixed)	—	-3.4	15.3
<i>u</i> 3351	H(55)...H(72)	555.0(81)	32.0(fixed)	—	1.4	32.0
<i>u</i> 1885	H(60)...H(80)	555.2(74)	53.4(fixed)	—	2.9	53.4
<i>u</i> 3797	H(342)...H(358)	555.3(40)	32.5(fixed)	—	-3.6	32.5
<i>u</i> 5399	H(73)...H(82)	555.3(62)	25.2(fixed)	—	-6.0	25.2
<i>u</i> 4707	H(64)...H(76)	555.3(61)	32.8(fixed)	—	-4.0	32.8
<i>u</i> 3946	Si(127)...H(164)	555.5(19)	15.2(fixed)	—	-4.1	15.2
<i>u</i> 4488	H(58)...H(70)	555.5(24)	27.5(fixed)	—	-1.6	27.5
<i>u</i> 5207	H(142)...H(164)	555.6(105)	32.2(fixed)	—	-10.9	32.2
<i>u</i> 3974	Si(208)...H(243)	555.7(35)	16.0(fixed)	—	-4.4	16.0
<i>u</i> 3561	Si(2)...H(23)	555.7(435)	22.8(fixed)	—	-1.9	22.8
<i>u</i> 4686	H(228)...H(240)	555.8(80)	31.8(fixed)	—	-4.4	31.8
<i>u</i> 5230	H(145)...H(151)	555.8(32)	31.1(fixed)	—	-3.3	31.1
<i>u</i> 3984	H(233)...H(243)	555.9(53)	41.1(fixed)	—	3.4	41.1
<i>u</i> 1898	H(278)...H(282)	556.0(60)	56.5(fixed)	—	0.9	56.5
<i>u</i> 4002	H(343)...H(367)	556.1(20)	24.8(fixed)	—	-2.7	24.8
<i>u</i> 2887	Si(44)...H(71)	556.2(20)	19.8(fixed)	—	-4.4	19.8
<i>u</i> 3927	Si(332)...H(369)	556.4(18)	15.2(fixed)	—	-4.3	15.2
<i>u</i> 5402	H(155)...H(164)	556.5(49)	26.4(fixed)	—	-7.6	26.4
<i>u</i> 2886	Si(126)...H(153)	556.5(19)	21.4(fixed)	—	-5.6	21.4
<i>u</i> 2805	Si(85)...H(116)	556.5(20)	18.9(fixed)	—	-4.1	18.9
<i>u</i> 4039	H(99)...H(116)	556.6(68)	31.2(fixed)	—	-4.1	31.2
<i>u</i> 2893	Si(167)...H(205)	556.6(18)	24.7(fixed)	—	-3.6	24.7
<i>u</i> 3943	Si(249)...H(284)	556.6(20)	16.1(fixed)	—	-3.7	16.1
<i>u</i> 4191	H(55)...H(71)	556.7(84)	29.4(fixed)	—	-3.5	29.4
<i>u</i> 3744	C(132)...H(159)	556.7(26)	38.9(fixed)	—	14.1	38.9
<i>u</i> 4402	C(88)...H(118)	556.8(177)	28.0(fixed)	—	-4.3	28.0
<i>u</i> 3704	H(342)...H(353)	556.9(24)	28.4(fixed)	—	-2.4	28.4
<i>u</i> 781	H(178)...H(199)	556.9(35)	50.8(fixed)	—	10.0	50.8
<i>u</i> 4223	C(217)...H(231)	557.0(173)	32.9(fixed)	—	-1.2	32.9
<i>u</i> 4500	C(129)...H(158)	557.1(56)	25.7(fixed)	—	-4.2	25.7
<i>u</i> 3234	Si(44)...H(62)	557.2(17)	22.2(fixed)	—	-3.5	22.2
<i>u</i> 1767	C(47)...C(54)	557.3(55)	24.5(tied to <i>u</i> 3698)	—	2.1	22.7
<i>u</i> 3837	H(270)...H(287)	557.3(72)	48.1(fixed)	—	0.3	48.1
<i>u</i> 4337	H(56)...H(82)	557.4(20)	28.0(fixed)	—	-3.8	28.0
<i>u</i> 4247	H(137)...H(153)	557.4(43)	30.9(fixed)	—	-3.9	30.9
<i>u</i> 2132	H(265)...H(283)	557.5(59)	37.3(fixed)	—	6.5	37.3
<i>u</i> 3966	Si(4)...H(41)	557.7(22)	15.0(fixed)	—	-4.1	15.0
<i>u</i> 3985	H(110)...H(122)	557.7(122)	44.2(fixed)	—	-6.1	44.2
<i>u</i> 3925	Si(128)...H(150)	557.7(20)	15.3(fixed)	—	-3.9	15.3
<i>u</i> 4030	H(343)...H(353)	557.8(54)	29.7(fixed)	—	-3.7	29.7
<i>u</i> 3948	Si(209)...H(232)	557.8(17)	15.0(fixed)	—	-3.7	15.0
<i>u</i> 2112	C(132)...C(133)	557.8(22)	32.4(tied to <i>u</i> 3698)	—	0.3	30.0
<i>u</i> 4141	H(281)...H(285)	558.0(48)	41.2(fixed)	—	3.6	41.2

<i>u</i> 4038	C(7)...C(9)	558.0(50)	23.8(tied to <i>u</i> 3698)	—	-1.9	22.0
<i>u</i> 4010	H(265)...H(287)	558.0(53)	42.5(fixed)	—	-9.3	42.5
<i>u</i> 3635	H(229)...H(246)	558.0(128)	48.3(fixed)	—	1.4	48.3
<i>u</i> 4104	C(336)...H(367)	558.0(58)	44.0(fixed)	—	-2.8	44.0
<i>u</i> 3553	C(214)...H(238)	558.1(70)	39.3(fixed)	—	5.6	39.3
<i>u</i> 4066	H(262)...H(280)	558.1(28)	31.4(fixed)	—	-3.0	31.4
<i>u</i> 5411	H(115)...H(123)	558.2(159)	25.6(fixed)	—	-6.5	25.6
<i>u</i> 4508	H(100)...H(109)	558.2(32)	56.1(fixed)	—	-1.1	56.1
<i>u</i> 3239	Si(248)...H(267)	558.2(23)	21.5(fixed)	—	-3.6	21.5
<i>u</i> 899	H(221)...H(228)	558.3(24)	47.9(fixed)	—	7.9	47.9
<i>u</i> 4007	Si(250)...H(287)	558.3(19)	15.1(fixed)	—	-3.8	15.1
<i>u</i> 2025	H(231)...H(237)	558.4(51)	50.2(fixed)	—	-1.4	50.2
<i>u</i> 2686	C(52)...H(78)	558.4(41)	39.5(fixed)	—	-5.4	39.5
<i>u</i> 3182	Si(85)...H(103)	558.4(17)	21.8(fixed)	—	-4.4	21.8
<i>u</i> 2496	H(99)...H(120)	558.5(44)	41.1(fixed)	—	-1.0	41.1
<i>u</i> 5334	H(107)...H(114)	558.6(54)	29.7(fixed)	—	-9.5	29.7
<i>u</i> 4854	C(256)...H(265)	558.6(50)	23.1(fixed)	—	-5.5	23.1
<i>u</i> 3759	C(130)...H(158)	558.7(52)	33.7(fixed)	—	6.6	33.7
<i>u</i> 3209	H(96)...H(117)	558.7(117)	32.3(fixed)	—	2.5	32.3
<i>u</i> 4033	C(11)...H(29)	558.8(57)	34.0(fixed)	—	-1.2	34.0
<i>u</i> 3147	H(182)...H(199)	558.9(51)	48.1(fixed)	—	7.2	48.1
<i>u</i> 1984	H(224)...H(234)	558.9(108)	32.1(fixed)	—	7.5	32.1
<i>u</i> 2362	H(63)...H(67)	558.9(40)	50.3(fixed)	—	2.3	50.3
<i>u</i> 4014	Si(46)...H(68)	559.0(19)	14.9(fixed)	—	-3.7	14.9
<i>u</i> 3336	H(60)...H(78)	559.0(121)	47.5(fixed)	—	6.9	47.5
<i>u</i> 3555	H(138)...H(162)	559.2(29)	31.7(fixed)	—	2.0	31.7
<i>u</i> 2257	H(104)...H(108)	559.4(44)	47.5(fixed)	—	-0.5	47.5
<i>u</i> 3906	H(98)...H(120)	559.5(24)	27.7(fixed)	—	-4.1	27.7
<i>u</i> 4287	H(59)...H(68)	559.5(35)	56.5(fixed)	—	-0.1	56.5
<i>u</i> 3878	H(14)...H(34)	559.6(44)	36.5(fixed)	—	-6.6	36.5
<i>u</i> 4077	H(57)...H(77)	559.6(35)	25.0(fixed)	—	-3.6	25.0
<i>u</i> 5210	H(274)...H(281)	559.7(77)	29.0(fixed)	—	-2.9	29.0
<i>u</i> 4997	C(218)...H(236)	559.7(52)	28.3(fixed)	—	-0.2	28.3
<i>u</i> 4011	Si(87)...H(109)	559.7(18)	15.0(fixed)	—	-4.4	15.0
<i>u</i> 3940	H(313)...H(318)	559.7(51)	32.3(fixed)	—	4.4	32.3
<i>u</i> 2673	C(256)...H(283)	559.8(59)	35.9(fixed)	—	-4.0	35.9
<i>u</i> 4049	H(14)...H(25)	560.0(59)	27.6(fixed)	—	-3.1	27.6
<i>u</i> 4095	H(55)...H(67)	560.0(48)	25.7(fixed)	—	-3.3	25.7
<i>u</i> 4837	H(113)...H(122)	560.0(36)	48.5(fixed)	—	-4.0	48.5
<i>u</i> 2179	C(50)...C(51)	560.1(27)	34.3(tied to <i>u</i> 3698)	—	-0.2	31.8
<i>u</i> 3050	Si(126)...H(142)	560.4(18)	22.2(fixed)	—	-3.0	22.2
<i>u</i> 4859	H(281)...H(286)	560.6(49)	38.2(fixed)	—	-3.5	38.2
<i>u</i> 4244	C(8)...H(39)	560.6(58)	31.5(fixed)	—	-1.9	31.5
<i>u</i> 2818	C(89)...H(112)	560.7(73)	35.7(fixed)	—	-7.5	35.7

<i>u4483</i>	C(171)...H(192)	560.8(57)	21.6(fixed)	—	-2.6	21.6
<i>u4570</i>	H(222)...H(229)	560.8(34)	28.4(fixed)	—	-1.7	28.4
<i>u4524</i>	H(99)...H(111)	560.9(23)	28.2(fixed)	—	-0.3	28.2
<i>u3676</i>	H(144)...H(155)	560.9(125)	44.8(fixed)	—	2.7	44.8
<i>u3765</i>	H(271)...H(286)	561.1(58)	40.5(fixed)	—	2.9	40.5
<i>u4015</i>	H(184)...H(199)	561.1(66)	41.8(fixed)	—	5.6	41.8
<i>u4063</i>	H(309)...H(318)	561.2(58)	38.2(fixed)	—	0.6	38.2
<i>u3814</i>	H(139)...H(161)	561.2(25)	31.3(fixed)	—	-0.3	31.3
<i>u2284</i>	H(222)...H(243)	561.4(97)	37.5(fixed)	—	-3.4	37.5
<i>u3893</i>	H(111)...H(121)	561.4(88)	37.9(fixed)	—	0.2	37.9
<i>u4236</i>	C(258)...H(272)	561.6(112)	31.5(fixed)	—	-1.2	31.5
<i>u4243</i>	H(220)...H(246)	561.6(25)	28.1(fixed)	—	-3.5	28.1
<i>u4013</i>	C(258)...H(275)	561.7(47)	31.7(fixed)	—	-0.8	31.7
<i>u4752</i>	H(22)...H(29)	561.8(604)	49.3(fixed)	—	-2.1	49.3
<i>u3461</i>	H(219)...H(236)	562.0(112)	31.1(fixed)	—	4.6	31.1
<i>u3933</i>	C(296)...H(320)	562.6(73)	44.5(fixed)	—	-1.6	44.5
<i>u4960</i>	H(22)...H(27)	562.6(782)	57.2(fixed)	—	-6.4	57.2
<i>u3770</i>	H(305)...H(321)	562.6(81)	42.2(fixed)	—	2.5	42.2
<i>u2649</i>	H(221)...H(226)	562.6(32)	41.6(fixed)	—	-1.4	41.6
<i>u5010</i>	H(182)...H(192)	562.7(93)	37.1(fixed)	—	0.1	37.1
<i>u3897</i>	H(222)...H(235)	562.7(64)	38.1(fixed)	—	-6.1	38.1
<i>u424</i>	H(240)...H(241)	563.0(124)	41.1(fixed)	—	27.0	41.1
<i>u5039</i>	C(257)...H(274)	563.2(52)	24.0(fixed)	—	-2.2	24.0
<i>u3653</i>	H(230)...H(245)	563.2(234)	42.3(fixed)	—	1.4	42.3
<i>u4676</i>	H(58)...H(69)	563.2(22)	26.1(fixed)	—	-2.8	26.1
<i>u1987</i>	C(91)...C(93)	563.4(27)	23.4(fixed)	—	0.5	23.4
<i>u4270</i>	H(219)...H(235)	563.5(97)	30.4(fixed)	—	-5.0	30.4
<i>u4615</i>	C(170)...H(197)	563.6(63)	25.5(fixed)	—	-6.0	25.5
<i>u3565</i>	H(156)...H(160)	563.7(99)	58.3(fixed)	—	-30.2	58.3
<i>u2680</i>	H(138)...H(142)	563.8(85)	44.3(fixed)	—	-3.0	44.3
<i>u2142</i>	H(151)...H(153)	563.8(49)	47.6(fixed)	—	4.3	47.6
<i>u4056</i>	H(267)...H(283)	563.8(32)	39.3(fixed)	—	2.9	39.3
<i>u4047</i>	H(227)...H(238)	563.8(74)	32.2(fixed)	—	-0.5	32.2
<i>u3860</i>	C(88)...H(114)	563.9(41)	50.2(fixed)	—	0.6	50.2
<i>u3920</i>	H(137)...H(148)	563.9(20)	28.2(fixed)	—	-3.2	28.2
<i>u4378</i>	H(138)...H(164)	564.2(30)	27.9(fixed)	—	-4.1	27.9
<i>u4147</i>	H(186)...H(201)	564.3(71)	41.4(fixed)	—	-1.3	41.4
<i>u433</i>	H(76)...H(77)	564.3(93)	42.2(fixed)	—	24.0	42.2
<i>u4089</i>	C(294)...H(319)	564.4(58)	34.0(fixed)	—	-1.9	34.0
<i>u4123</i>	H(18)...H(36)	564.4(330)	39.2(fixed)	—	-0.7	39.2
<i>u1525</i>	C(129)...H(147)	564.4(71)	42.6(fixed)	—	4.2	42.6
<i>u4167</i>	C(49)...H(80)	564.4(100)	32.3(fixed)	—	-1.7	32.3
<i>u4054</i>	C(217)...H(234)	564.5(42)	34.4(fixed)	—	-1.2	34.4
<i>u2097</i>	H(106)...H(116)	564.7(39)	36.8(fixed)	—	5.6	36.8

<i>u3560</i>	H(224)...H(242)	564.8(191)	45.8(fixed)	—	5.3	45.8
<i>u3467</i>	C(134)...H(143)	564.8(69)	37.5(fixed)	—	1.2	37.5
<i>u4216</i>	C(53)...H(69)	564.8(66)	33.9(fixed)	—	-1.9	33.9
<i>u3904</i>	H(58)...H(71)	564.9(63)	32.5(fixed)	—	-3.7	32.5
<i>u4057</i>	H(302)...H(328)	565.0(31)	26.9(fixed)	—	-2.2	26.9
<i>u3822</i>	C(136)...H(150)	565.1(54)	34.8(fixed)	—	-3.2	34.8
<i>u2524</i>	H(264)...H(284)	565.3(108)	46.2(fixed)	—	-2.9	46.2
<i>u4929</i>	H(145)...H(152)	565.4(53)	35.8(fixed)	—	0.8	35.8
<i>u3978</i>	H(343)...H(369)	565.4(22)	27.0(fixed)	—	-2.0	27.0
<i>u4278</i>	H(275)...H(278)	565.4(76)	39.7(fixed)	—	6.0	39.7
<i>u4768</i>	C(255)...C(257)	565.5(34)	12.2(fixed)	—	-2.2	12.2
<i>u3963</i>	H(226)...H(234)	565.5(64)	41.6(fixed)	—	0.3	41.6
<i>u1279</i>	H(221)...H(237)	565.5(48)	66.9(fixed)	—	4.4	66.9
<i>u3726</i>	C(54)...H(68)	565.6(110)	36.8(fixed)	—	-3.2	36.8
<i>u1986</i>	C(253)...C(259)	565.6(26)	28.4(fixed)	—	0.8	28.4
<i>u3729</i>	C(50)...H(82)	565.7(96)	37.0(fixed)	—	-3.2	37.0
<i>u4279</i>	C(6)...H(36)	565.8(123)	32.1(fixed)	—	-4.9	32.1
<i>u465</i>	H(141)...H(149)	565.9(66)	43.8(fixed)	—	11.4	43.8
<i>u3322</i>	C(95)...H(114)	565.9(80)	38.2(fixed)	—	9.1	38.2
<i>u5119</i>	H(266)...H(270)	566.0(40)	36.5(fixed)	—	-0.6	36.5
<i>u1696</i>	H(157)...H(159)	566.1(53)	70.7(fixed)	—	44.1	70.7
<i>u4061</i>	H(151)...H(159)	566.1(64)	47.9(fixed)	—	21.5	47.9
<i>u1369</i>	C(88)...H(122)	566.2(49)	37.9(fixed)	—	4.9	37.9
<i>u4078</i>	H(63)...H(74)	566.4(62)	32.2(fixed)	—	-0.6	32.2
<i>u4134</i>	C(132)...H(162)	566.4(47)	36.7(fixed)	—	-6.8	36.7
<i>u3950</i>	C(132)...H(164)	566.6(56)	36.4(fixed)	—	-4.3	36.4
<i>u4928</i>	C(254)...H(264)	566.6(90)	23.9(fixed)	—	-1.0	23.9
<i>u2298</i>	H(69)...H(71)	566.7(54)	50.8(fixed)	—	3.8	50.8
<i>u4094</i>	C(54)...H(69)	566.7(103)	33.7(fixed)	—	-5.2	33.7
<i>u2294</i>	H(225)...H(244)	566.8(81)	41.2(fixed)	—	0.2	41.2
<i>u2655</i>	H(221)...H(235)	567.0(47)	37.7(fixed)	—	-9.8	37.7
<i>u4171</i>	H(274)...H(282)	567.0(53)	38.3(fixed)	—	-0.2	38.3
<i>u4276</i>	H(233)...H(241)	567.1(58)	39.2(fixed)	—	-0.8	39.2
<i>u2151</i>	H(102)...H(121)	567.1(110)	45.5(fixed)	—	-3.3	45.5
<i>u4091</i>	C(50)...H(80)	567.1(118)	32.5(fixed)	—	-4.9	32.5
<i>u4420</i>	H(146)...H(156)	567.1(110)	45.2(fixed)	—	-6.7	45.2
<i>u4654</i>	H(99)...H(110)	567.6(18)	28.7(fixed)	—	-1.6	28.7
<i>u4187</i>	H(310)...H(318)	567.8(47)	34.8(fixed)	—	-0.8	34.8
<i>u5098</i>	H(222)...H(230)	567.9(35)	17.6(fixed)	—	-6.2	17.6
<i>u4129</i>	C(9)...H(39)	568.0(121)	33.4(fixed)	—	-5.2	33.4
<i>u659</i>	H(64)...H(67)	568.1(74)	52.3(fixed)	—	14.2	52.3
<i>u4371</i>	H(305)...H(316)	568.3(73)	35.9(fixed)	—	-1.9	35.9
<i>u1595</i>	C(211)...H(245)	568.6(158)	45.6(fixed)	—	3.6	45.6
<i>u2061</i>	H(65)...H(71)	569.0(74)	36.7(fixed)	—	8.8	36.7

<i>u</i> 4151	C(8)...H(30)	569.0(111)	37.9(fixed)	—	-4.7	37.9
<i>u</i> 4240	C(135)...H(151)	569.0(57)	33.7(fixed)	—	-1.9	33.7
<i>u</i> 2574	H(137)...H(157)	569.0(59)	37.8(fixed)	—	-10.8	37.8
<i>u</i> 1949	C(48)...H(65)	569.1(69)	57.3(fixed)	—	2.3	57.3
<i>u</i> 4635	H(56)...H(66)	569.2(50)	23.1(fixed)	—	-7.5	23.1
<i>u</i> 2667	C(133)...H(152)	569.4(52)	41.7(fixed)	—	-3.0	41.7
<i>u</i> 5323	C(170)...H(191)	569.6(75)	15.8(fixed)	—	-6.6	15.8
<i>u</i> 3820	C(91)...H(123)	569.7(114)	37.4(fixed)	—	-3.5	37.4
<i>u</i> 4940	C(136)...H(154)	569.9(80)	26.7(fixed)	—	-1.7	26.7
<i>u</i> 4791	H(108)...H(114)	569.9(55)	46.0(fixed)	—	-3.8	46.0
<i>u</i> 4050	H(229)...H(243)	570.0(91)	46.8(fixed)	—	2.2	46.8
<i>u</i> 4972	C(54)...H(72)	570.0(73)	25.5(fixed)	—	-1.8	25.5
<i>u</i> 3429	C(91)...H(102)	570.0(58)	40.0(fixed)	—	5.6	40.0
<i>u</i> 4239	C(90)...H(121)	570.1(74)	30.6(fixed)	—	-1.5	30.6
<i>u</i> 4208	H(274)...H(283)	570.2(52)	35.3(fixed)	—	-1.2	35.3
<i>u</i> 3771	H(140)...H(152)	570.2(38)	27.3(fixed)	—	-2.1	27.3
<i>u</i> 1739	C(89)...H(106)	570.3(59)	50.4(fixed)	—	2.6	50.4
<i>u</i> 4179	C(136)...H(151)	570.3(46)	31.4(fixed)	—	-5.5	31.4
<i>u</i> 4302	C(48)...H(75)	570.4(72)	23.7(fixed)	—	-1.1	23.7
<i>u</i> 3691	H(101)...H(119)	570.5(24)	54.4(fixed)	—	0.1	54.4
<i>u</i> 4148	C(95)...H(110)	570.9(60)	37.6(fixed)	—	-7.4	37.6
<i>u</i> 3875	C(341)...H(355)	570.9(52)	34.8(fixed)	—	-3.8	34.8
<i>u</i> 4336	C(212)...H(240)	571.0(73)	23.0(fixed)	—	-2.0	23.0
<i>u</i> 4254	C(212)...H(239)	571.0(61)	24.2(fixed)	—	-0.5	24.2
<i>u</i> 2256	H(147)...H(153)	571.2(59)	46.0(fixed)	—	1.5	46.0
<i>u</i> 2463	H(55)...H(75)	571.2(43)	33.1(fixed)	—	-5.3	33.1
<i>u</i> 4560	H(261)...H(286)	571.2(44)	27.0(fixed)	—	-0.8	27.0
<i>u</i> 4797	C(216)...H(226)	571.3(66)	20.6(fixed)	—	-4.4	20.6
<i>u</i> 3918	C(95)...H(109)	571.5(148)	39.2(fixed)	—	-4.6	39.2
<i>u</i> 4282	C(171)...H(200)	571.5(61)	35.3(fixed)	—	-5.6	35.3
<i>u</i> 3424	H(32)...H(38)	571.6(903)	56.4(fixed)	—	-7.3	56.4
<i>u</i> 526	H(105)...H(108)	571.7(75)	46.0(fixed)	—	15.0	46.0
<i>u</i> 4092	C(335)...H(352)	571.8(59)	33.0(fixed)	—	-1.3	33.0
<i>u</i> 3420	C(50)...H(61)	571.9(68)	41.0(fixed)	—	4.8	41.0
<i>u</i> 4484	H(269)...H(270)	571.9(119)	37.9(fixed)	—	-1.3	37.9
<i>u</i> 2676	C(130)...H(161)	571.9(45)	45.9(fixed)	—	-18.8	45.9
<i>u</i> 5086	H(58)...H(68)	572.1(22)	18.5(fixed)	—	-6.2	18.5
<i>u</i> 4682	H(138)...H(148)	572.1(73)	25.4(fixed)	—	-5.8	25.4
<i>u</i> 2241	H(61)...H(80)	572.1(81)	43.8(fixed)	—	-3.7	43.8
<i>u</i> 3947	H(220)...H(224)	572.1(65)	26.8(fixed)	—	-2.9	26.8
<i>u</i> 3217	C(52)...H(63)	572.2(67)	29.7(fixed)	—	2.7	29.7
<i>u</i> 4612	C(256)...H(275)	572.2(29)	23.5(fixed)	—	-2.9	23.5
<i>u</i> 4072	H(57)...H(79)	572.4(26)	26.8(fixed)	—	-2.4	26.8
<i>u</i> 4206	H(233)...H(242)	572.4(83)	35.5(fixed)	—	-1.3	35.5

<i>u</i> 4185	H(305)...H(322)	572.5(68)	36.4(fixed)	—	-2.2	36.4
<i>u</i> 3195	C(216)...H(227)	572.6(86)	30.6(fixed)	—	2.8	30.6
<i>u</i> 4108	H(55)...H(66)	572.7(42)	27.2(fixed)	—	-2.3	27.2
<i>u</i> 4350	C(48)...H(76)	572.9(59)	22.7(fixed)	—	-1.8	22.7
<i>u</i> 4152	H(342)...H(362)	573.1(36)	30.7(fixed)	—	-3.4	30.7
<i>u</i> 4116	H(270)...H(284)	573.2(43)	47.0(fixed)	—	1.4	47.0
<i>u</i> 4202	C(337)...H(367)	573.2(60)	31.8(fixed)	—	-6.7	31.8
<i>u</i> 4163	H(342)...H(361)	573.3(46)	27.5(fixed)	—	-3.9	27.5
<i>u</i> 2259	H(267)...H(285)	573.5(40)	51.7(fixed)	—	4.4	51.7
<i>u</i> 4263	H(152)...H(160)	573.7(36)	43.3(fixed)	—	-13.9	43.3
<i>u</i> 4186	H(302)...H(316)	573.8(29)	25.8(fixed)	—	-2.9	25.8
<i>u</i> 4808	C(52)...H(62)	573.9(71)	20.4(fixed)	—	-4.8	20.4
<i>u</i> 2600	C(93)...H(111)	574.1(74)	46.1(fixed)	—	-4.3	46.1
<i>u</i> 2443	H(56)...H(62)	574.2(63)	34.8(fixed)	—	-1.6	34.8
<i>u</i> 4557	H(14)...H(22)	574.2(187)	28.6(fixed)	—	0.7	28.6
<i>u</i> 2526	C(89)...H(114)	574.3(56)	51.0(fixed)	—	-5.0	51.0
<i>u</i> 4232	H(100)...H(114)	574.4(66)	52.7(fixed)	—	4.6	52.7
<i>u</i> 1366	H(137)...H(156)	574.4(33)	72.6(fixed)	—	2.3	72.6
<i>u</i> 4211	H(231)...H(245)	574.5(103)	36.0(fixed)	—	-2.2	36.0
<i>u</i> 4269	H(272)...H(286)	574.7(57)	32.8(fixed)	—	-0.4	32.8
<i>u</i> 1994	H(144)...H(160)	574.7(64)	52.1(fixed)	—	42.5	52.1
<i>u</i> 5090	H(237)...H(245)	574.8(156)	42.2(fixed)	—	0.8	42.2
<i>u</i> 4322	C(337)...H(348)	574.9(51)	33.8(fixed)	—	-1.9	33.8
<i>u</i> 1916	H(223)...H(233)	575.1(67)	46.1(fixed)	—	4.2	46.1
<i>u</i> 1535	C(47)...H(81)	575.3(107)	44.2(fixed)	—	3.4	44.2
<i>u</i> 1868	H(264)...H(282)	575.4(48)	59.5(fixed)	—	3.1	59.5
<i>u</i> 4328	H(22)...H(39)	575.5(217)	41.3(fixed)	—	-2.1	41.3
<i>u</i> 4105	H(111)...H(119)	575.7(96)	37.1(fixed)	—	1.5	37.1
<i>u</i> 2752	C(51)...H(70)	575.8(58)	42.4(fixed)	—	-3.2	42.4
<i>u</i> 3494	H(238)...H(242)	575.8(23)	41.4(fixed)	—	-12.8	41.4
<i>u</i> 3473	C(88)...H(113)	575.8(44)	43.6(fixed)	—	6.0	43.6
<i>u</i> 3977	H(56)...H(60)	576.0(57)	26.9(fixed)	—	-1.9	26.9
<i>u</i> 4532	C(212)...H(233)	576.1(84)	27.5(fixed)	—	-4.8	27.5
<i>u</i> 1106	H(55)...H(74)	576.4(63)	57.7(fixed)	—	3.0	57.7
<i>u</i> 4342	C(294)...H(311)	576.5(28)	21.5(fixed)	—	-2.0	21.5
<i>u</i> 2164	H(151)...H(155)	576.6(64)	53.4(fixed)	—	1.6	53.4
<i>u</i> 4183	C(91)...H(121)	576.6(79)	28.6(fixed)	—	-4.8	28.6
<i>u</i> 5104	H(99)...H(109)	576.7(21)	18.0(fixed)	—	-7.1	18.0
<i>u</i> 4663	C(216)...H(234)	576.7(33)	25.0(fixed)	—	-3.4	25.0
<i>u</i> 1942	H(110)...H(116)	576.9(44)	45.2(fixed)	—	10.8	45.2
<i>u</i> 4298	H(223)...H(229)	577.1(58)	36.0(fixed)	—	0.0	36.0
<i>u</i> 529	H(223)...H(244)	577.1(33)	44.6(fixed)	—	11.4	44.6
<i>u</i> 3267	H(278)...H(283)	577.6(64)	54.6(fixed)	—	-10.6	54.6
<i>u</i> 2598	C(217)...H(239)	577.7(72)	41.9(fixed)	—	-4.5	41.9

<i>u</i> 3485	H(18)...H(24)	577.8(612)	44.3(fixed)	—	-9.0	44.3
<i>u</i> 5007	C(170)...H(192)	577.9(79)	25.6(fixed)	—	-2.5	25.6
<i>u</i> 4943	C(132)...H(146)	578.0(77)	28.3(fixed)	—	-2.4	28.3
<i>u</i> 4107	H(147)...H(163)	578.0(39)	36.8(fixed)	—	0.7	36.8
<i>u</i> 2620	C(215)...H(229)	578.1(74)	32.7(fixed)	—	-2.4	32.7
<i>u</i> 2049	H(267)...H(275)	578.1(48)	32.8(fixed)	—	4.2	32.8
<i>u</i> 4422	H(197)...H(204)	578.2(38)	53.8(fixed)	—	0.2	53.8
<i>u</i> 4536	H(234)...H(238)	578.3(93)	40.2(fixed)	—	1.2	40.2
<i>u</i> 4300	H(308)...H(324)	578.3(101)	42.7(fixed)	—	-0.4	42.7
<i>u</i> 3633	C(259)...H(279)	578.3(73)	34.6(fixed)	—	1.7	34.6
<i>u</i> 4120	H(96)...H(116)	578.7(66)	33.1(fixed)	—	-3.1	33.1
<i>u</i> 4267	C(293)...H(322)	578.7(68)	32.1(fixed)	—	-5.1	32.1
<i>u</i> 2664	C(217)...H(238)	578.7(26)	37.0(fixed)	—	-5.8	37.0
<i>u</i> 4865	C(134)...H(144)	578.7(55)	28.8(fixed)	—	-6.3	28.8
<i>u</i> 4150	C(6)...H(38)	578.8(39)	34.0(fixed)	—	-4.0	34.0
<i>u</i> 4291	H(15)...H(19)	578.8(31)	29.8(fixed)	—	-4.2	29.8
<i>u</i> 4145	H(307)...H(320)	579.0(58)	35.0(fixed)	—	-1.9	35.0
<i>u</i> 5223	H(100)...H(112)	579.0(87)	27.4(fixed)	—	-12.6	27.4
<i>u</i> 4406	H(310)...H(311)	579.1(62)	37.8(fixed)	—	0.1	37.8
<i>u</i> 2440	H(220)...H(226)	579.1(63)	36.9(fixed)	—	-1.1	36.9
<i>u</i> 2433	H(268)...H(285)	579.1(35)	51.0(fixed)	—	-0.1	51.0
<i>u</i> 4368	C(294)...H(312)	579.6(28)	24.0(fixed)	—	-1.6	24.0
<i>u</i> 4213	H(24)...H(40)	579.6(37)	33.7(fixed)	—	-1.9	33.7
<i>u</i> 2566	H(219)...H(239)	579.8(41)	34.4(fixed)	—	-7.5	34.4
<i>u</i> 4200	H(301)...H(320)	580.1(48)	28.9(fixed)	—	-4.2	28.9
<i>u</i> 4242	C(295)...H(319)	580.1(23)	23.2(fixed)	—	-1.4	23.2
<i>u</i> 2478	C(258)...H(278)	580.8(18)	53.5(fixed)	—	-4.8	53.5
<i>u</i> 2450	C(252)...H(282)	580.9(41)	43.9(fixed)	—	-2.4	43.9
<i>u</i> 2267	H(69)...H(73)	581.0(51)	47.9(fixed)	—	2.0	47.9
<i>u</i> 4435	C(294)...H(313)	581.1(31)	22.5(fixed)	—	-1.9	22.5
<i>u</i> 4309	H(270)...H(285)	581.2(41)	39.7(fixed)	—	-4.3	39.7
<i>u</i> 2652	C(135)...H(156)	581.2(28)	45.0(fixed)	—	-7.4	45.0
<i>u</i> 1403	H(219)...H(238)	581.3(74)	61.0(fixed)	—	1.9	61.0
<i>u</i> 4331	C(7)...H(30)	581.3(22)	25.3(fixed)	—	-1.2	25.3
<i>u</i> 4614	C(256)...H(273)	581.5(19)	25.4(fixed)	—	-3.6	25.4
<i>u</i> 2073	H(156)...H(159)	581.6(57)	56.1(fixed)	—	30.5	56.1
<i>u</i> 1154	C(135)...H(145)	581.7(78)	34.8(fixed)	—	6.3	34.8
<i>u</i> 5097	H(261)...H(287)	581.7(30)	17.6(fixed)	—	-6.1	17.6
<i>u</i> 4917	C(255)...H(281)	581.7(71)	23.2(fixed)	—	-1.4	23.2
<i>u</i> 427	H(231)...H(236)	581.8(74)	42.4(fixed)	—	27.5	42.4
<i>u</i> 1515	C(130)...H(138)	582.1(20)	33.7(fixed)	—	2.1	33.7
<i>u</i> 4273	H(301)...H(321)	582.1(42)	30.5(fixed)	—	-4.0	30.5
<i>u</i> 1460	C(92)...H(99)	582.1(19)	33.1(fixed)	—	1.1	33.1
<i>u</i> 4266	C(92)...H(108)	582.5(56)	35.4(fixed)	—	-1.2	35.4



<i>u</i> 4303	C(337)...H(360)	582.5(22)	24.2(fixed)	—	-1.4	24.2
<i>u</i> 2646	C(53)...H(74)	582.7(27)	36.7(fixed)	—	-4.4	36.7
<i>u</i> 4921	C(252)...H(272)	582.8(29)	23.4(fixed)	—	-1.4	23.4
<i>u</i> 3307	H(157)...H(160)	582.9(105)	95.0(fixed)	—	-24.9	95.0
<i>u</i> 1735	C(253)...H(286)	582.9(66)	51.1(fixed)	—	3.1	51.1
<i>u</i> 3953	H(140)...H(150)	583.1(37)	28.3(fixed)	—	-2.3	28.3
<i>u</i> 4227	H(303)...H(317)	583.1(29)	27.7(fixed)	—	-3.3	27.7
<i>u</i> 4175	H(229)...H(244)	583.2(162)	39.0(fixed)	—	-3.0	39.0
<i>u</i> 2684	C(53)...H(75)	583.3(58)	37.6(fixed)	—	-3.7	37.6
<i>u</i> 422	H(277)...H(282)	583.4(58)	43.4(fixed)	—	32.5	43.4
<i>u</i> 3328	C(256)...H(264)	583.4(55)	30.7(fixed)	—	3.7	30.7
<i>u</i> 5052	H(73)...H(81)	583.4(105)	36.1(fixed)	—	-0.6	36.1
<i>u</i> 4253	H(145)...H(155)	583.5(112)	37.5(fixed)	—	-1.9	37.5
<i>u</i> 3539	H(74)...H(78)	583.8(45)	41.3(fixed)	—	-11.8	41.3
<i>u</i> 4683	C(216)...H(232)	583.8(25)	26.7(fixed)	—	-4.0	26.7
<i>u</i> 4264	C(6)...H(29)	583.9(51)	27.8(fixed)	—	-2.1	27.8
<i>u</i> 4251	C(253)...H(271)	584.0(39)	23.8(fixed)	—	-2.3	23.8
<i>u</i> 4426	C(171)...H(202)	584.2(81)	33.2(fixed)	—	-6.0	33.2
<i>u</i> 3211	C(254)...H(263)	584.2(14)	24.6(fixed)	—	-1.2	24.6
<i>u</i> 2802	C(135)...H(144)	584.3(45)	28.6(fixed)	—	-2.4	28.6
<i>u</i> 4602	H(220)...H(234)	584.3(35)	26.0(fixed)	—	-1.6	26.0
<i>u</i> 4326	C(7)...H(32)	584.6(148)	25.2(fixed)	—	-1.8	25.2
<i>u</i> 4262	H(311)...H(319)	584.6(72)	48.6(fixed)	—	0.6	48.6
<i>u</i> 5083	H(115)...H(122)	584.7(137)	36.2(fixed)	—	-1.0	36.2
<i>u</i> 3883	C(92)...H(121)	584.7(67)	34.9(fixed)	—	0.0	34.9
<i>u</i> 4380	C(218)...H(231)	584.8(46)	29.6(fixed)	—	-4.4	29.6
<i>u</i> 2134	H(269)...H(274)	585.2(60)	46.9(fixed)	—	1.9	46.9
<i>u</i> 1029	H(260)...H(278)	585.3(30)	62.2(fixed)	—	6.9	62.2
<i>u</i> 2660	C(135)...H(157)	585.3(20)	46.5(fixed)	—	-6.5	46.5
<i>u</i> 4029	H(57)...H(62)	585.3(39)	31.7(fixed)	—	-3.9	31.7
<i>u</i> 4252	C(257)...H(267)	585.3(75)	23.7(fixed)	—	-1.9	23.7
<i>u</i> 437	H(100)...H(121)	585.4(66)	43.2(fixed)	—	22.9	43.2
<i>u</i> 4446	C(259)...H(272)	585.5(67)	26.3(fixed)	—	-3.8	26.3
<i>u</i> 5051	H(155)...H(163)	585.5(55)	39.6(fixed)	—	-0.5	39.6
<i>u</i> 2845	H(139)...H(141)	585.6(32)	32.8(fixed)	—	1.0	32.8
<i>u</i> 3154	C(255)...H(261)	586.0(12)	21.2(fixed)	—	-1.2	21.2
<i>u</i> 4259	H(70)...H(78)	586.0(58)	34.5(fixed)	—	-3.5	34.5
<i>u</i> 4241	H(106)...H(122)	586.0(83)	34.3(fixed)	—	-1.8	34.3
<i>u</i> 4246	H(65)...H(81)	586.3(53)	33.3(fixed)	—	-2.7	33.3
<i>u</i> 2942	H(57)...H(64)	586.5(41)	34.9(fixed)	—	0.6	34.9
<i>u</i> 3212	C(95)...H(97)	586.8(13)	22.0(fixed)	—	-2.0	22.0
<i>u</i> 4364	C(334)...H(342)	586.8(11)	15.2(fixed)	—	-2.3	15.2
<i>u</i> 442	H(59)...H(80)	587.0(51)	43.8(fixed)	—	21.2	43.8
<i>u</i> 3431	H(152)...H(155)	587.3(50)	47.6(fixed)	—	-8.2	47.6

<i>u4401</i>	C(7)...H(14)	587.4(11)	15.1(fixed)	—	-2.4	15.1
<i>u2554</i>	C(211)...H(232)	587.4(82)	31.6(fixed)	—	-0.1	31.6
<i>u4149</i>	C(295)...H(328)	587.6(66)	33.2(fixed)	—	-3.8	33.2
<i>u4360</i>	C(294)...H(302)	587.6(11)	15.1(fixed)	—	-2.3	15.1
<i>u4229</i>	H(182)...H(197)	587.7(80)	36.6(fixed)	—	-3.7	36.6
<i>u4363</i>	C(258)...H(262)	587.7(11)	15.2(fixed)	—	-2.2	15.2
<i>u4448</i>	C(7)...H(31)	587.8(144)	21.2(fixed)	—	-2.6	21.2
<i>u4065</i>	H(269)...H(281)	587.9(67)	31.2(fixed)	—	-0.1	31.2
<i>u2607</i>	C(213)...H(237)	588.1(24)	48.8(fixed)	—	-5.6	48.8
<i>u4315</i>	H(275)...H(283)	588.1(52)	36.3(fixed)	—	0.7	36.3
<i>u2850</i>	C(258)...H(276)	588.1(21)	34.9(fixed)	—	-8.2	34.9
<i>u4466</i>	C(335)...H(363)	588.1(65)	28.6(fixed)	—	-4.1	28.6
<i>u4393</i>	C(9)...H(17)	588.2(11)	15.4(fixed)	—	-3.1	15.4
<i>u3306</i>	C(88)...H(96)	588.3(11)	21.8(fixed)	—	-1.9	21.8
<i>u4617</i>	C(92)...H(122)	588.4(47)	23.4(fixed)	—	-3.5	23.4
<i>u3335</i>	C(51)...H(57)	588.4(12)	19.0(fixed)	—	-1.9	19.0
<i>u3357</i>	C(133)...H(139)	588.5(13)	20.2(fixed)	—	-2.0	20.2
<i>u4205</i>	H(100)...H(111)	588.6(72)	51.7(fixed)	—	3.2	51.7
<i>u534</i>	H(225)...H(234)	588.7(72)	44.0(fixed)	—	12.0	44.0
<i>u3436</i>	C(47)...H(55)	588.7(12)	20.4(fixed)	—	-1.6	20.4
<i>u4157</i>	H(310)...H(320)	588.7(74)	41.6(fixed)	—	0.3	41.6
<i>u3521</i>	C(253)...H(260)	588.8(12)	22.1(fixed)	—	-1.6	22.1
<i>u5416</i>	H(273)...H(279)	588.8(82)	24.4(fixed)	—	-6.2	24.4
<i>u4400</i>	C(295)...H(326)	588.8(44)	28.3(fixed)	—	-5.7	28.3
<i>u4555</i>	H(342)...H(349)	588.8(39)	21.5(fixed)	—	-7.0	21.5
<i>u4662</i>	C(92)...H(123)	588.9(23)	25.9(fixed)	—	-4.2	25.9
<i>u3258</i>	C(93)...H(98)	589.0(13)	17.4(fixed)	—	-1.3	17.4
<i>u2210</i>	H(180)...H(205)	589.1(29)	37.4(fixed)	—	-0.7	37.4
<i>u4082</i>	H(59)...H(70)	589.2(65)	50.7(fixed)	—	3.2	50.7
<i>u3479</i>	H(106)...H(113)	589.3(55)	45.6(fixed)	—	9.5	45.6
<i>u4390</i>	C(91)...H(120)	589.3(55)	30.4(fixed)	—	-4.0	30.4
<i>u3438</i>	C(211)...H(219)	589.3(12)	21.1(fixed)	—	-1.4	21.1
<i>u4280</i>	H(23)...H(40)	589.3(117)	38.7(fixed)	—	2.4	38.7
<i>u3999</i>	H(98)...H(103)	589.3(31)	31.3(fixed)	—	-4.3	31.3
<i>u3130</i>	C(171)...H(196)	589.5(19)	35.4(fixed)	—	3.4	35.4
<i>u4361</i>	C(217)...H(221)	589.6(12)	15.3(fixed)	—	-2.2	15.3
<i>u1922</i>	H(104)...H(114)	589.6(105)	53.8(fixed)	—	0.1	53.8
<i>u4630</i>	H(301)...H(306)	589.7(38)	21.3(fixed)	—	-7.9	21.3
<i>u4427</i>	C(336)...H(350)	589.7(23)	23.1(fixed)	—	-1.9	23.1
<i>u2096</i>	H(110)...H(115)	589.7(45)	39.8(fixed)	—	7.0	39.8
<i>u528</i>	H(178)...H(193)	589.8(32)	37.1(fixed)	—	13.0	37.1
<i>u4450</i>	C(254)...H(285)	589.9(40)	31.0(fixed)	—	-5.3	31.0
<i>u5307</i>	C(252)...H(271)	589.9(38)	15.6(fixed)	—	-5.5	15.6
<i>u4423</i>	C(296)...H(323)	590.1(31)	25.6(fixed)	—	-2.6	25.6

<i>u4352</i>	C(337)...H(358)	590.2(22)	25.7(fixed)	—	-1.7	25.7
<i>u4479</i>	C(337)...H(359)	590.5(29)	21.8(fixed)	—	-2.4	21.8
<i>u3867</i>	C(216)...H(233)	590.6(32)	33.9(fixed)	—	0.6	33.9
<i>u661</i>	H(69)...H(72)	590.7(52)	50.2(fixed)	—	15.7	50.2
<i>u1120</i>	C(255)...H(268)	590.7(58)	34.0(fixed)	—	4.3	34.0
<i>u2860</i>	H(98)...H(105)	590.8(43)	33.1(fixed)	—	2.3	33.1
<i>u4180</i>	H(222)...H(239)	590.8(75)	32.5(fixed)	—	-3.7	32.5
<i>u3161</i>	H(263)...H(272)	590.8(27)	33.9(fixed)	—	1.3	33.9
<i>u2470</i>	C(211)...H(233)	591.3(52)	32.0(fixed)	—	-0.4	32.0
<i>u3728</i>	C(256)...H(274)	591.4(25)	31.7(fixed)	—	0.7	31.7
<i>u4814</i>	C(173)...H(185)	591.5(43)	25.2(fixed)	—	-9.5	25.2
<i>u4550</i>	C(9)...H(35)	591.6(96)	25.0(fixed)	—	-3.9	25.0
<i>u4722</i>	C(90)...H(112)	591.8(44)	27.5(fixed)	—	-5.2	27.5
<i>u2670</i>	H(260)...H(276)	591.8(39)	36.7(fixed)	—	-10.1	36.7
<i>u4226</i>	C(295)...H(317)	591.9(27)	24.1(fixed)	—	-1.6	24.1
<i>u5069</i>	H(266)...H(276)	592.0(91)	39.3(fixed)	—	-9.0	39.3
<i>u4780</i>	C(172)...H(205)	592.0(20)	26.8(fixed)	—	-6.0	26.8
<i>u4431</i>	C(336)...H(351)	592.1(19)	21.4(fixed)	—	-2.0	21.4
<i>u2510</i>	C(253)...H(273)	592.2(47)	32.9(fixed)	—	-0.9	32.9
<i>u4376</i>	C(213)...H(244)	592.2(136)	29.2(fixed)	—	-4.8	29.2
<i>u3166</i>	H(239)...H(242)	592.3(50)	60.2(fixed)	—	-9.1	60.2
<i>u524</i>	H(268)...H(275)	592.3(64)	41.5(fixed)	—	9.2	41.5
<i>u2456</i>	H(97)...H(120)	592.3(26)	38.0(fixed)	—	-1.3	38.0
<i>u2822</i>	C(214)...H(224)	592.4(82)	24.2(fixed)	—	-1.0	24.2
<i>u5192</i>	H(20)...H(31)	592.4(973)	36.8(fixed)	—	-2.8	36.8
<i>u3768</i>	H(260)...H(268)	592.5(42)	33.3(fixed)	—	-1.5	33.3
<i>u4294</i>	H(234)...H(242)	592.8(49)	39.0(fixed)	—	1.3	39.0
<i>u1307</i>	C(214)...H(225)	592.8(51)	36.3(fixed)	—	5.1	36.3
<i>u4571</i>	H(309)...H(324)	592.8(75)	34.4(fixed)	—	-2.8	34.4
<i>u4311</i>	C(136)...H(148)	592.8(42)	28.7(fixed)	—	-3.0	28.7
<i>u2724</i>	C(132)...H(155)	593.0(27)	46.2(fixed)	—	-4.0	46.2
<i>u4725</i>	C(257)...H(286)	593.1(16)	26.1(fixed)	—	-3.8	26.1
<i>u4429</i>	C(255)...H(283)	593.2(26)	22.0(fixed)	—	-2.0	22.0
<i>u4012</i>	H(140)...H(161)	593.2(36)	47.3(fixed)	—	-14.7	47.3
<i>u4515</i>	C(9)...H(34)	593.3(61)	28.1(fixed)	—	-1.8	28.1
<i>u519</i>	H(151)...H(154)	593.3(44)	49.4(fixed)	—	20.6	49.4
<i>u4464</i>	C(296)...H(324)	593.4(27)	22.0(fixed)	—	-2.8	22.0
<i>u4909</i>	H(20)...H(36)	593.4(277)	36.9(fixed)	—	-8.3	36.9
<i>u2776</i>	H(59)...H(78)	593.5(75)	51.5(fixed)	—	9.5	51.5
<i>u2920</i>	H(223)...H(242)	593.7(113)	45.8(fixed)	—	5.9	45.8
<i>u4433</i>	C(9)...H(33)	593.8(147)	22.9(fixed)	—	-1.4	22.9
<i>u1982</i>	H(104)...H(112)	593.8(95)	44.9(fixed)	—	2.5	44.9
<i>u4489</i>	H(310)...H(319)	593.9(68)	38.2(fixed)	—	-1.0	38.2
<i>u2544</i>	C(131)...H(143)	594.0(21)	31.2(fixed)	—	-0.8	31.2

<i>u662</i>	H(266)...H(283)	594.1(88)	49.9(fixed)	—	13.9	49.9
<i>u4399</i>	C(295)...H(318)	594.3(35)	20.6(fixed)	—	-2.3	20.6
<i>u2671</i>	C(49)...H(63)	594.4(24)	37.4(fixed)	—	-1.2	37.4
<i>u930</i>	C(217)...H(240)	594.6(76)	31.6(fixed)	—	14.4	31.6
<i>u4190</i>	C(171)...H(195)	594.6(31)	33.0(fixed)	—	-2.0	33.0
<i>u5019</i>	C(252)...H(270)	594.6(31)	25.9(fixed)	—	-2.2	25.9
<i>u2932</i>	C(258)...H(265)	594.7(41)	27.7(fixed)	—	-4.1	27.7
<i>u5091</i>	H(55)...H(62)	594.8(30)	17.6(fixed)	—	-5.8	17.6
<i>u981</i>	C(53)...H(76)	594.8(57)	31.4(fixed)	—	11.5	31.4
<i>u5092</i>	H(219)...H(226)	594.8(27)	17.8(fixed)	—	-6.2	17.8
<i>u669</i>	H(269)...H(285)	594.8(52)	53.3(fixed)	—	11.4	53.3
<i>u4321</i>	H(114)...H(122)	595.0(130)	38.8(fixed)	—	4.6	38.8
<i>u3989</i>	H(273)...H(278)	595.0(89)	40.9(fixed)	—	10.2	40.9
<i>u2535</i>	C(90)...H(104)	595.1(24)	40.9(fixed)	—	-2.1	40.9
<i>u803</i>	C(131)...H(141)	595.1(24)	31.5(fixed)	—	9.4	31.5
<i>u4627</i>	H(343)...H(347)	595.1(34)	20.1(fixed)	—	-6.5	20.1
<i>u2543</i>	C(131)...H(142)	595.1(20)	33.7(fixed)	—	0.1	33.7
<i>u4545</i>	C(214)...H(241)	595.2(64)	24.3(fixed)	—	-3.2	24.3
<i>u4381</i>	C(254)...H(287)	595.3(55)	34.5(fixed)	—	-4.4	34.5
<i>u4640</i>	H(139)...H(157)	595.3(42)	26.5(fixed)	—	-12.8	26.5
<i>u4421</i>	C(211)...H(230)	595.3(87)	25.8(fixed)	—	-2.4	25.8
<i>u4493</i>	C(255)...H(282)	595.3(21)	23.8(fixed)	—	-2.6	23.8
<i>u4603</i>	C(294)...H(323)	595.4(68)	25.6(fixed)	—	-4.0	25.6
<i>u2782</i>	C(213)...H(235)	595.5(37)	39.3(fixed)	—	-7.0	39.3
<i>u4851</i>	C(130)...H(152)	595.5(18)	26.2(fixed)	—	-1.9	26.2
<i>u3388</i>	H(111)...H(115)	595.6(76)	45.4(fixed)	—	-8.8	45.4
<i>u5035</i>	C(130)...H(151)	595.7(23)	24.9(fixed)	—	-2.6	24.9
<i>u4397</i>	C(214)...H(242)	595.8(58)	22.9(fixed)	—	-1.9	22.9
<i>u4539</i>	H(302)...H(309)	595.9(40)	25.8(fixed)	—	-1.5	25.8
<i>u4521</i>	C(8)...H(34)	596.1(94)	33.6(fixed)	—	-3.2	33.6
<i>u4257</i>	C(213)...H(246)	596.3(89)	35.0(fixed)	—	-3.8	35.0
<i>u4681</i>	C(252)...H(276)	596.5(67)	27.3(fixed)	—	-5.5	27.3
<i>u4370</i>	C(253)...H(270)	596.6(72)	21.1(fixed)	—	-2.5	21.1
<i>u3519</i>	H(70)...H(73)	596.7(52)	43.4(fixed)	—	-6.7	43.4
<i>u4286</i>	C(300)...H(312)	596.7(61)	31.5(fixed)	—	-5.1	31.5
<i>u1142</i>	C(49)...H(64)	596.8(24)	40.5(fixed)	—	7.5	40.5
<i>u4877</i>	H(20)...H(38)	596.9(513)	42.3(fixed)	—	-9.8	42.3
<i>u4358</i>	C(336)...H(349)	596.9(19)	24.1(fixed)	—	-1.5	24.1
<i>u4188</i>	H(58)...H(75)	597.0(51)	31.5(fixed)	—	-3.7	31.5
<i>u4542</i>	C(9)...H(38)	597.0(48)	27.9(fixed)	—	-3.4	27.9
<i>u3622</i>	C(9)...H(23)	597.0(592)	40.1(fixed)	—	6.4	40.1
<i>u4664</i>	C(297)...H(328)	597.1(40)	25.1(fixed)	—	-3.9	25.1
<i>u652</i>	H(141)...H(147)	597.3(67)	47.8(fixed)	—	13.1	47.8
<i>u2937</i>	H(98)...H(117)	597.4(36)	30.5(fixed)	—	3.0	30.5

<i>u4059</i>	C(257)...H(285)	597.5(21)	29.6(fixed)	—	1.9	29.6
<i>u4514</i>	C(6)...H(28)	597.5(31)	22.4(fixed)	—	-3.8	22.4
<i>u4327</i>	C(6)...H(27)	597.6(22)	29.0(fixed)	—	-2.9	29.0
<i>u4340</i>	C(337)...H(366)	597.6(43)	28.9(fixed)	—	-3.0	28.9
<i>u4366</i>	C(295)...H(325)	597.6(59)	31.2(fixed)	—	-3.3	31.2
<i>u2383</i>	C(95)...H(102)	597.6(68)	47.6(fixed)	—	-2.8	47.6
<i>u3347</i>	H(229)...H(237)	597.7(85)	46.9(fixed)	—	-9.9	46.9
<i>u4622</i>	C(296)...H(305)	597.8(45)	26.3(fixed)	—	-3.8	26.3
<i>u4677</i>	H(57)...H(75)	597.9(33)	24.0(fixed)	—	-8.0	24.0
<i>u2553</i>	C(253)...H(274)	598.0(41)	29.4(fixed)	—	-1.6	29.4
<i>u4639</i>	H(178)...H(183)	598.0(32)	21.3(fixed)	—	-7.2	21.3
<i>u2266</i>	H(138)...H(145)	598.1(25)	42.3(fixed)	—	-1.5	42.3
<i>u4407</i>	C(296)...H(325)	598.1(29)	25.9(fixed)	—	-2.8	25.9
<i>u2556</i>	C(218)...H(225)	598.2(65)	32.1(fixed)	—	-0.9	32.1
<i>u2571</i>	C(95)...H(101)	598.2(69)	36.1(fixed)	—	-3.8	36.1
<i>u3727</i>	H(261)...H(275)	598.5(38)	25.2(fixed)	—	-1.7	25.2
<i>u891</i>	H(64)...H(65)	598.5(69)	65.7(fixed)	—	9.4	65.7
<i>u2736</i>	C(50)...H(73)	598.7(18)	40.2(fixed)	—	-2.9	40.2
<i>u2847</i>	C(49)...H(62)	598.8(25)	37.2(fixed)	—	-1.7	37.2
<i>u665</i>	H(223)...H(245)	598.9(131)	51.6(fixed)	—	11.5	51.6
<i>u4440</i>	H(229)...H(242)	599.2(41)	39.5(fixed)	—	-4.0	39.5
<i>u3958</i>	H(55)...H(61)	599.2(44)	43.0(fixed)	—	-3.0	43.0
<i>u4572</i>	H(310)...H(312)	599.2(97)	38.5(fixed)	—	-2.1	38.5
<i>u5103</i>	H(220)...H(232)	599.4(45)	17.5(fixed)	—	-5.8	17.5
<i>u4295</i>	C(130)...H(153)	599.5(66)	36.5(fixed)	—	-4.7	36.5
<i>u1056</i>	H(99)...H(113)	599.6(34)	61.8(fixed)	—	6.0	61.8
<i>u849</i>	C(218)...H(223)	599.6(53)	33.3(fixed)	—	8.5	33.3
<i>u3142</i>	H(228)...H(234)	599.7(59)	48.0(fixed)	—	2.5	48.0
<i>u5107</i>	H(96)...H(103)	599.7(34)	17.5(fixed)	—	-6.6	17.5
<i>u1454</i>	C(258)...H(266)	599.8(68)	42.4(fixed)	—	3.5	42.4
<i>u4062</i>	C(53)...H(60)	599.8(72)	36.0(fixed)	—	-4.0	36.0
<i>u4045</i>	H(268)...H(270)	599.8(52)	30.8(fixed)	—	-0.2	30.8
<i>u2748</i>	C(90)...H(103)	599.8(21)	34.6(fixed)	—	-3.1	34.6
<i>u4583</i>	H(262)...H(282)	599.8(47)	26.2(fixed)	—	-0.8	26.2
<i>u3799</i>	H(139)...H(142)	599.8(35)	33.8(fixed)	—	-3.6	33.8
<i>u660</i>	H(65)...H(73)	599.9(51)	52.2(fixed)	—	14.8	52.2
<i>u4604</i>	H(14)...H(19)	600.0(44)	25.0(fixed)	—	-8.7	25.0
<i>u2490</i>	C(54)...H(61)	600.1(58)	44.8(fixed)	—	-4.2	44.8
<i>u1743</i>	H(67)...H(73)	600.2(114)	65.6(fixed)	—	3.1	65.6
<i>u3543</i>	H(276)...H(283)	600.3(67)	48.1(fixed)	—	-11.3	48.1
<i>u453</i>	H(100)...H(122)	600.3(28)	46.7(fixed)	—	21.9	46.7
<i>u4762</i>	C(257)...H(287)	600.4(17)	26.5(fixed)	—	-4.1	26.5
<i>u913</i>	C(90)...H(105)	600.4(22)	35.7(fixed)	—	10.2	35.7
<i>u4356</i>	C(259)...H(271)	600.7(44)	31.2(fixed)	—	-4.0	31.2

<i>u4584</i>	H(221)...H(241)	600.8(66)	27.5(fixed)	—	-0.3	27.5
<i>u5301</i>	C(130)...H(150)	601.1(23)	16.1(fixed)	—	-6.3	16.1
<i>u5100</i>	H(264)...H(270)	601.3(97)	36.1(fixed)	—	-0.7	36.1
<i>u766</i>	H(105)...H(106)	601.4(61)	57.6(fixed)	—	12.3	57.6
<i>u3997</i>	C(90)...H(113)	601.5(40)	29.1(fixed)	—	4.7	29.1
<i>u432</i>	H(110)...H(117)	601.7(40)	41.0(fixed)	—	23.6	41.0
<i>u2330</i>	H(261)...H(271)	601.7(29)	35.5(fixed)	—	-1.3	35.5
<i>u3081</i>	H(57)...H(72)	601.8(32)	33.9(fixed)	—	1.3	33.9
<i>u3908</i>	H(97)...H(121)	602.0(61)	25.4(fixed)	—	-3.3	25.4
<i>u2631</i>	C(218)...H(224)	602.0(85)	33.9(fixed)	—	-0.7	33.9
<i>u750</i>	H(147)...H(155)	602.4(49)	62.9(fixed)	—	11.8	62.9
<i>u4502</i>	C(335)...H(362)	602.4(60)	29.1(fixed)	—	-4.4	29.1
<i>u4261</i>	C(218)...H(230)	602.5(165)	32.9(fixed)	—	-4.1	32.9
<i>u2677</i>	C(91)...H(115)	602.8(27)	33.7(fixed)	—	-3.0	33.7
<i>u4661</i>	H(178)...H(185)	602.8(31)	24.3(fixed)	—	-9.4	24.3
<i>u4986</i>	C(92)...H(107)	602.9(46)	22.7(fixed)	—	-6.3	22.7
<i>u4598</i>	H(279)...H(286)	602.9(83)	36.9(fixed)	—	-2.6	36.9
<i>u3512</i>	H(268)...H(271)	602.9(92)	35.0(fixed)	—	3.0	35.0
<i>u4517</i>	H(270)...H(283)	603.0(53)	39.2(fixed)	—	-3.3	39.2
<i>u3138</i>	H(269)...H(283)	603.0(70)	41.0(fixed)	—	5.3	41.0
<i>u3339</i>	H(75)...H(78)	603.0(59)	57.2(fixed)	—	-9.4	57.2
<i>u4451</i>	C(255)...H(284)	603.1(27)	25.1(fixed)	—	-1.8	25.1
<i>u4581</i>	H(15)...H(38)	603.2(27)	20.0(fixed)	—	-5.8	20.0
<i>u4969</i>	C(215)...H(245)	603.5(106)	24.6(fixed)	—	-1.6	24.6
<i>u2922</i>	H(100)...H(119)	603.5(33)	52.2(fixed)	—	6.7	52.2
<i>u4668</i>	H(301)...H(308)	603.6(32)	25.0(fixed)	—	-5.6	25.0
<i>u3894</i>	H(219)...H(225)	603.6(66)	33.0(fixed)	—	-1.9	33.0
<i>u4520</i>	C(91)...H(119)	603.6(109)	23.1(fixed)	—	-4.4	23.1
<i>u4538</i>	H(15)...H(40)	603.7(44)	26.7(fixed)	—	-2.0	26.7
<i>u3644</i>	H(96)...H(102)	603.7(23)	47.3(fixed)	—	-2.4	47.3
<i>u2896</i>	C(90)...H(116)	603.8(42)	27.2(fixed)	—	-4.0	27.2
<i>u3627</i>	H(23)...H(28)	603.8(670)	52.3(fixed)	—	8.0	52.3
<i>u2582</i>	C(54)...H(60)	603.9(66)	40.0(fixed)	—	-4.2	40.0
<i>u4459</i>	C(132)...H(161)	604.0(45)	38.9(fixed)	—	-3.5	38.9
<i>u4892</i>	C(93)...H(122)	604.2(58)	24.8(fixed)	—	-1.7	24.8
<i>u4651</i>	H(343)...H(349)	604.3(32)	23.4(fixed)	—	-6.8	23.4
<i>u3572</i>	H(139)...H(155)	604.5(31)	41.7(fixed)	—	-1.9	41.7
<i>u2599</i>	C(259)...H(268)	604.6(36)	36.5(fixed)	—	-1.4	36.5
<i>u4513</i>	C(214)...H(243)	604.7(38)	26.5(fixed)	—	-2.2	26.5
<i>u4100</i>	H(59)...H(77)	604.7(79)	42.5(fixed)	—	-2.4	42.5
<i>u4647</i>	C(132)...H(160)	604.8(33)	35.3(fixed)	—	-12.9	35.3
<i>u4745</i>	H(60)...H(77)	604.8(68)	48.1(fixed)	—	-8.9	48.1
<i>u5328</i>	C(215)...H(246)	604.8(45)	15.3(fixed)	—	-5.5	15.3
<i>u3294</i>	C(134)...H(146)	605.1(66)	42.2(fixed)	—	3.0	42.2

<i>u</i> 5105	H(137)...H(142)	605.1(30)	17.7(fixed)	—	-6.7	17.7
<i>u</i> 4209	H(232)...H(238)	605.2(76)	42.3(fixed)	—	5.7	42.3
<i>u</i> 4475	C(54)...H(66)	605.2(45)	27.8(fixed)	—	-2.7	27.8
<i>u</i> 4238	H(223)...H(241)	605.3(28)	39.1(fixed)	—	-5.0	39.1
<i>u</i> 4534	C(258)...H(267)	605.4(55)	28.6(fixed)	—	-3.8	28.6
<i>u</i> 4653	H(342)...H(348)	605.5(31)	25.9(fixed)	—	-2.0	25.9
<i>u</i> 2826	C(255)...H(267)	605.5(44)	24.5(fixed)	—	-2.5	24.5
<i>u</i> 4558	H(262)...H(287)	605.5(33)	23.8(fixed)	—	-7.0	23.8
<i>u</i> 4525	C(50)...H(79)	605.5(79)	28.3(fixed)	—	-3.0	28.3
<i>u</i> 2874	C(49)...H(71)	605.6(42)	27.2(fixed)	—	-3.6	27.2
<i>u</i> 5017	H(146)...H(152)	605.6(71)	39.8(fixed)	—	-1.2	39.8
<i>u</i> 4506	C(95)...H(107)	605.6(131)	28.9(fixed)	—	-2.7	28.9
<i>u</i> 435	H(145)...H(160)	605.7(71)	59.6(fixed)	—	52.9	59.6
<i>u</i> 4518	C(136)...H(147)	605.9(39)	24.5(fixed)	—	-4.2	24.5
<i>u</i> 3600	H(108)...H(116)	606.1(112)	42.5(fixed)	—	-8.0	42.5
<i>u</i> 767	C(95)...H(100)	606.1(25)	32.4(fixed)	—	19.8	32.4
<i>u</i> 2743	C(252)...H(284)	606.3(81)	32.8(fixed)	—	-4.1	32.8
<i>u</i> 1450	C(49)...H(73)	606.4(49)	45.1(fixed)	—	3.6	45.1
<i>u</i> 5117	H(267)...H(272)	606.6(83)	28.7(fixed)	—	-5.4	28.7
<i>u</i> 3047	H(139)...H(154)	606.6(32)	35.7(fixed)	—	3.0	35.7
<i>u</i> 4195	C(217)...H(224)	606.7(123)	33.4(fixed)	—	-3.7	33.4
<i>u</i> 4369	C(211)...H(229)	606.7(45)	22.2(fixed)	—	-2.3	22.2
<i>u</i> 4706	C(336)...H(360)	606.7(41)	25.3(fixed)	—	-3.2	25.3
<i>u</i> 4714	H(22)...H(40)	606.8(47)	35.0(fixed)	—	-5.7	35.0
<i>u</i> 668	H(106)...H(115)	606.9(93)	54.1(fixed)	—	12.8	54.1
<i>u</i> 4519	C(295)...H(324)	607.0(38)	25.3(fixed)	—	-3.9	25.3
<i>u</i> 4559	H(342)...H(346)	607.1(32)	26.5(fixed)	—	-1.1	26.5
<i>u</i> 4898	H(265)...H(277)	607.2(82)	31.8(fixed)	—	-0.6	31.8
<i>u</i> 3725	H(97)...H(122)	607.3(43)	27.5(fixed)	—	-2.3	27.5
<i>u</i> 3399	H(67)...H(71)	607.3(88)	51.7(fixed)	—	-7.8	51.7
<i>u</i> 4118	C(170)...H(188)	607.5(36)	49.2(fixed)	—	-2.5	49.2
<i>u</i> 3460	H(57)...H(73)	607.8(34)	36.9(fixed)	—	-1.2	36.9
<i>u</i> 5073	H(267)...H(282)	608.1(131)	37.2(fixed)	—	-7.2	37.2
<i>u</i> 2912	C(132)...H(153)	608.1(23)	37.1(fixed)	—	-4.3	37.1
<i>u</i> 3520	H(23)...H(33)	608.1(1462)	44.0(fixed)	—	-16.3	44.0
<i>u</i> 4689	H(15)...H(39)	608.2(41)	26.8(fixed)	—	-3.3	26.8
<i>u</i> 3176	C(217)...H(223)	608.2(43)	34.4(fixed)	—	0.8	34.4
<i>u</i> 4649	H(308)...H(322)	608.3(142)	49.9(fixed)	—	-4.8	49.9
<i>u</i> 4783	H(21)...H(36)	608.3(203)	46.6(fixed)	—	-5.9	46.6
<i>u</i> 933	C(135)...H(158)	608.4(33)	35.8(fixed)	—	20.6	35.8
<i>u</i> 2051	H(145)...H(159)	608.5(105)	81.0(fixed)	—	-12.7	81.0
<i>u</i> 5297	C(93)...H(123)	608.8(93)	16.3(fixed)	—	-5.8	16.3
<i>u</i> 4753	C(336)...H(358)	609.0(44)	26.2(fixed)	—	-3.8	26.2
<i>u</i> 4932	H(117)...H(122)	609.1(32)	35.4(fixed)	—	1.0	35.4

<i>u2732</i>	C(92)...H(103)	609.1(68)	33.6(fixed)	—	-3.2	33.6
<i>u425</i>	H(158)...H(159)	609.2(51)	62.7(fixed)	—	66.1	62.7
<i>u4220</i>	H(100)...H(113)	609.2(61)	49.8(fixed)	—	1.3	49.8
<i>u4528</i>	C(337)...H(365)	609.3(36)	23.6(fixed)	—	-3.7	23.6
<i>u2454</i>	H(142)...H(147)	609.3(82)	48.4(fixed)	—	0.5	48.4
<i>u4585</i>	C(9)...H(37)	609.3(42)	23.2(fixed)	—	-4.1	23.2
<i>u4576</i>	H(302)...H(306)	609.3(35)	25.0(fixed)	—	-7.1	25.0
<i>u654</i>	H(59)...H(81)	609.4(82)	52.4(fixed)	—	20.3	52.4
<i>u792</i>	C(54)...H(59)	609.4(33)	34.0(fixed)	—	17.9	34.0
<i>u3039</i>	C(53)...H(59)	609.7(38)	36.9(fixed)	—	4.7	36.9
<i>u1057</i>	C(258)...H(277)	609.7(22)	35.8(fixed)	—	16.6	35.8
<i>u2408</i>	H(101)...H(122)	609.7(73)	43.6(fixed)	—	-4.1	43.6
<i>u4444</i>	H(269)...H(282)	609.9(54)	36.0(fixed)	—	-3.6	36.0
<i>u4645</i>	H(310)...H(322)	609.9(51)	44.0(fixed)	—	-2.7	44.0
<i>u4660</i>	C(294)...H(325)	610.0(73)	30.5(fixed)	—	-4.4	30.5
<i>u5239</i>	H(142)...H(157)	610.3(103)	31.3(fixed)	—	-5.7	31.3
<i>u5275</i>	H(183)...H(197)	610.4(68)	28.4(fixed)	—	-10.5	28.4
<i>u1446</i>	C(50)...H(72)	610.7(35)	42.6(fixed)	—	6.3	42.6
<i>u4591</i>	H(221)...H(246)	610.7(42)	22.9(fixed)	—	-5.9	22.9
<i>u3280</i>	H(144)...H(159)	610.7(65)	102.3(fixed)	—	-17.2	102.3
<i>u4886</i>	C(51)...H(81)	610.8(70)	24.9(fixed)	—	-1.6	24.9
<i>u3749</i>	H(261)...H(274)	610.8(32)	25.3(fixed)	—	-2.4	25.3
<i>u1064</i>	C(213)...H(236)	611.2(42)	35.5(fixed)	—	16.8	35.5
<i>u2087</i>	H(149)...H(155)	611.4(146)	61.4(fixed)	—	4.6	61.4
<i>u5128</i>	H(275)...H(279)	611.4(55)	34.2(fixed)	—	-0.9	34.2
<i>u1682</i>	C(131)...H(155)	611.4(68)	55.4(fixed)	—	4.0	55.4
<i>u4599</i>	H(21)...H(40)	611.4(86)	41.6(fixed)	—	-2.4	41.6
<i>u4221</i>	H(15)...H(18)	611.4(526)	29.7(fixed)	—	-4.3	29.7
<i>u4798</i>	H(305)...H(315)	611.5(47)	40.6(fixed)	—	-3.8	40.6
<i>u4621</i>	H(262)...H(283)	611.5(45)	27.9(fixed)	—	-1.3	27.9
<i>u3017</i>	C(131)...H(153)	611.8(50)	35.5(fixed)	—	-5.8	35.5
<i>u3034</i>	H(219)...H(223)	611.9(42)	32.8(fixed)	—	2.0	32.8
<i>u2926</i>	H(96)...H(100)	611.9(23)	36.8(fixed)	—	6.3	36.8
<i>u2018</i>	H(108)...H(115)	611.9(44)	60.0(fixed)	—	2.2	60.0
<i>u3036</i>	C(50)...H(71)	611.9(29)	39.5(fixed)	—	-4.0	39.5
<i>u4477</i>	H(311)...H(317)	612.0(83)	51.2(fixed)	—	-2.9	51.2
<i>u4299</i>	C(88)...H(111)	612.0(44)	26.3(fixed)	—	-1.6	26.3
<i>u4726</i>	H(310)...H(313)	612.1(61)	33.2(fixed)	—	-4.1	33.2
<i>u4874</i>	C(133)...H(163)	612.2(33)	25.7(fixed)	—	-1.4	25.7
<i>u5126</i>	H(267)...H(280)	612.3(95)	28.6(fixed)	—	-6.1	28.6
<i>u4742</i>	H(110)...H(120)	612.3(122)	52.1(fixed)	—	-6.7	52.1
<i>u4332</i>	H(23)...H(37)	612.4(400)	39.9(fixed)	—	-5.2	39.9
<i>u4245</i>	C(47)...H(70)	612.5(40)	26.7(fixed)	—	-1.8	26.7
<i>u1105</i>	C(91)...H(117)	612.6(25)	31.9(fixed)	—	7.9	31.9



<i>u</i> 5312	C(51)...H(82)	612.6(48)	15.9(fixed)	—	-5.6	15.9
<i>u</i> 1108	H(99)...H(114)	612.7(30)	60.9(fixed)	—	5.9	60.9
<i>u</i> 4644	C(213)...H(243)	613.2(114)	31.6(fixed)	—	-4.0	31.6
<i>u</i> 4608	C(50)...H(78)	613.2(27)	24.6(fixed)	—	-5.5	24.6
<i>u</i> 4613	C(334)...H(357)	613.2(39)	27.2(fixed)	—	-4.1	27.2
<i>u</i> 1351	C(132)...H(154)	613.2(32)	40.4(fixed)	—	9.8	40.4
<i>u</i> 2628	H(140)...H(164)	613.4(28)	40.7(fixed)	—	-6.3	40.7
<i>u</i> 4609	C(54)...H(65)	613.5(58)	23.5(fixed)	—	-4.8	23.5
<i>u</i> 5327	C(133)...H(164)	613.7(57)	15.8(fixed)	—	-6.8	15.8
<i>u</i> 771	H(269)...H(286)	613.8(57)	58.6(fixed)	—	9.9	58.6
<i>u</i> 3552	H(98)...H(115)	613.9(40)	37.0(fixed)	—	-1.5	37.0
<i>u</i> 3796	H(263)...H(273)	614.1(49)	31.0(fixed)	—	-3.3	31.0
<i>u</i> 4605	C(95)...H(106)	614.2(24)	24.0(fixed)	—	-3.9	24.0
<i>u</i> 4293	C(94)...H(101)	614.2(74)	39.6(fixed)	—	-5.5	39.6
<i>u</i> 1048	C(259)...H(269)	614.3(27)	38.3(fixed)	—	7.1	38.3
<i>u</i> 4088	H(114)...H(123)	614.3(90)	40.9(fixed)	—	8.6	40.9
<i>u</i> 4115	H(263)...H(270)	614.4(39)	26.2(fixed)	—	-3.5	26.2
<i>u</i> 4587	H(221)...H(242)	614.8(60)	30.3(fixed)	—	-0.9	30.3
<i>u</i> 4694	H(148)...H(162)	614.8(62)	50.0(fixed)	—	-5.6	50.0
<i>u</i> 4544	H(275)...H(284)	615.0(51)	37.5(fixed)	—	-1.6	37.5
<i>u</i> 1600	C(90)...H(115)	615.1(51)	47.1(fixed)	—	2.8	47.1
<i>u</i> 5387	H(264)...H(271)	615.2(93)	24.5(fixed)	—	-5.3	24.5
<i>u</i> 2778	C(91)...H(116)	615.4(28)	34.6(fixed)	—	-3.0	34.6
<i>u</i> 4840	H(224)...H(241)	615.4(96)	44.7(fixed)	—	-8.7	44.7
<i>u</i> 4659	C(213)...H(242)	615.8(26)	27.5(fixed)	—	-5.3	27.5
<i>u</i> 4674	H(302)...H(310)	615.9(41)	26.2(fixed)	—	-2.3	26.2
<i>u</i> 3397	C(258)...H(269)	616.0(35)	32.7(fixed)	—	1.1	32.7
<i>u</i> 3003	H(55)...H(59)	616.5(35)	34.7(fixed)	—	6.6	34.7
<i>u</i> 3157	H(260)...H(269)	616.8(43)	36.1(fixed)	—	1.3	36.1
<i>u</i> 4588	H(308)...H(319)	616.9(57)	39.9(fixed)	—	-3.3	39.9
<i>u</i> 4656	C(254)...H(284)	616.9(70)	31.3(fixed)	—	-3.6	31.3
<i>u</i> 4445	C(88)...H(109)	617.0(36)	26.8(fixed)	—	-1.7	26.8
<i>u</i> 4473	C(214)...H(226)	617.0(42)	32.6(fixed)	—	-4.4	32.6
<i>u</i> 4667	C(7)...H(29)	617.4(37)	24.4(fixed)	—	-3.7	24.4
<i>u</i> 2540	H(224)...H(245)	617.4(203)	51.1(fixed)	—	-0.2	51.1
<i>u</i> 4333	C(47)...H(68)	617.4(42)	27.1(fixed)	—	-1.9	27.1
<i>u</i> 4894	H(144)...H(158)	617.6(81)	37.6(fixed)	—	-0.4	37.6
<i>u</i> 4430	C(92)...H(101)	617.9(57)	26.0(fixed)	—	-1.5	26.0
<i>u</i> 4600	H(234)...H(243)	617.9(58)	41.2(fixed)	—	-2.2	41.2
<i>u</i> 3198	H(264)...H(277)	618.8(45)	41.1(fixed)	—	11.4	41.1
<i>u</i> 4968	C(6)...H(31)	618.8(277)	26.5(fixed)	—	-1.2	26.5
<i>u</i> 4704	H(275)...H(282)	618.8(50)	32.5(fixed)	—	-3.8	32.5
<i>u</i> 2824	C(259)...H(267)	619.0(27)	35.6(fixed)	—	-2.4	35.6
<i>u</i> 4690	C(254)...H(283)	619.1(24)	26.5(fixed)	—	-4.5	26.5

<i>u2859</i>	H(62)...H(65)	619.2(100)	62.2(fixed)	—	-2.2	62.2
<i>u4819</i>	H(231)...H(242)	619.3(117)	39.4(fixed)	—	-5.0	39.4
<i>u4737</i>	H(110)...H(119)	619.4(195)	45.6(fixed)	—	-4.4	45.6
<i>u2694</i>	H(103)...H(106)	619.4(89)	54.7(fixed)	—	-3.2	54.7
<i>u3390</i>	H(152)...H(153)	619.6(68)	51.3(fixed)	—	-6.4	51.3
<i>u4718</i>	H(309)...H(319)	619.7(58)	34.2(fixed)	—	-4.0	34.2
<i>u1901</i>	H(103)...H(113)	619.7(74)	47.0(fixed)	—	13.9	47.0
<i>u4736</i>	H(234)...H(241)	619.7(70)	34.9(fixed)	—	-4.8	34.9
<i>u3662</i>	H(149)...H(153)	619.9(116)	44.9(fixed)	—	-8.8	44.9
<i>u5108</i>	H(98)...H(112)	620.1(34)	18.2(fixed)	—	-8.2	18.2
<i>u3114</i>	H(274)...H(278)	620.2(55)	49.7(fixed)	—	13.2	49.7
<i>u4173</i>	H(225)...H(229)	620.4(91)	35.0(fixed)	—	-1.3	35.0
<i>u2083</i>	H(158)...H(160)	620.5(59)	61.9(fixed)	—	-2.0	61.9
<i>u3120</i>	C(94)...H(100)	620.5(71)	37.5(fixed)	—	5.6	37.5
<i>u4691</i>	C(334)...H(355)	620.7(31)	24.6(fixed)	—	-4.3	24.6
<i>u4746</i>	H(109)...H(118)	620.9(163)	41.0(fixed)	—	-8.6	41.0
<i>u764</i>	H(138)...H(146)	621.2(27)	46.0(fixed)	—	11.3	46.0
<i>u5061</i>	H(236)...H(245)	621.3(98)	38.6(fixed)	—	3.0	38.6
<i>u5236</i>	H(142)...H(158)	621.6(76)	29.0(fixed)	—	-8.1	29.0
<i>u2047</i>	H(240)...H(242)	621.6(11)	40.6(fixed)	—	5.7	40.6
<i>u2501</i>	H(60)...H(81)	621.9(140)	51.6(fixed)	—	-5.2	51.6
<i>u4843</i>	H(145)...H(157)	622.0(86)	47.4(fixed)	—	-7.5	47.4
<i>u5186</i>	H(184)...H(189)	622.0(61)	29.7(fixed)	—	-9.8	29.7
<i>u4964</i>	H(264)...H(272)	622.1(76)	32.3(fixed)	—	1.3	32.3
<i>u4724</i>	H(147)...H(162)	622.1(90)	45.4(fixed)	—	-4.2	45.4
<i>u2613</i>	C(134)...H(161)	622.2(40)	72.5(fixed)	—	-14.4	72.5
<i>u5004</i>	H(318)...H(328)	622.3(89)	36.6(fixed)	—	-6.2	36.6
<i>u5222</i>	H(224)...H(231)	622.5(81)	28.4(fixed)	—	-6.3	28.4
<i>u4218</i>	H(100)...H(118)	622.7(153)	35.5(fixed)	—	1.2	35.5
<i>u3748</i>	H(225)...H(230)	622.9(105)	41.1(fixed)	—	2.1	41.1
<i>u3318</i>	H(229)...H(235)	623.1(85)	50.4(fixed)	—	-8.6	50.4
<i>u4926</i>	H(151)...H(160)	623.4(82)	51.2(fixed)	—	-14.5	51.2
<i>u4807</i>	C(6)...H(34)	623.7(38)	26.4(fixed)	—	-10.7	26.4
<i>u4634</i>	H(260)...H(265)	623.9(31)	20.0(fixed)	—	-6.4	20.0
<i>u4546</i>	H(137)...H(144)	623.9(26)	20.0(fixed)	—	-6.1	20.0
<i>u3338</i>	C(214)...H(228)	623.9(59)	41.7(fixed)	—	0.3	41.7
<i>u1724</i>	C(252)...C(257)	623.9(18)	21.0(fixed)	—	1.3	21.0
<i>u4832</i>	H(272)...H(283)	624.2(54)	37.1(fixed)	—	-4.2	37.1
<i>u4903</i>	H(25)...H(39)	624.3(66)	37.5(fixed)	—	-5.3	37.5
<i>u5370</i>	H(235)...H(244)	624.3(169)	27.8(fixed)	—	-7.9	27.8
<i>u4897</i>	H(231)...H(243)	624.7(205)	42.3(fixed)	—	-5.9	42.3
<i>u4578</i>	C(130)...H(157)	624.8(76)	35.8(fixed)	—	-4.2	35.8
<i>u4956</i>	C(257)...H(275)	624.9(32)	23.3(fixed)	—	-1.3	23.3
<i>u4786</i>	C(254)...H(267)	625.0(64)	20.6(fixed)	—	-5.3	20.6

<i>u4699</i>	H(309)...H(321)	625.1(53)	38.1(fixed)	—	-6.8	38.1
<i>u4788</i>	H(197)...H(203)	625.3(83)	45.5(fixed)	—	-5.9	45.5
<i>u4196</i>	H(143)...H(158)	625.4(59)	43.4(fixed)	—	-2.1	43.4
<i>u4829</i>	H(186)...H(200)	625.5(80)	38.8(fixed)	—	-8.3	38.8
<i>u4735</i>	C(7)...H(27)	625.6(61)	26.8(fixed)	—	-4.4	26.8
<i>u1770</i>	H(102)...H(122)	625.7(57)	64.9(fixed)	—	2.5	64.9
<i>u2109</i>	H(76)...H(78)	625.7(46)	41.0(fixed)	—	3.2	41.0
<i>u3465</i>	H(233)...H(238)	626.0(69)	50.6(fixed)	—	7.5	50.6
<i>u3233</i>	H(114)...H(121)	626.0(42)	51.4(fixed)	—	11.3	51.4
<i>u4870</i>	H(184)...H(197)	626.1(66)	38.5(fixed)	—	-6.7	38.5
<i>u4729</i>	C(94)...H(109)	626.1(81)	29.6(fixed)	—	-9.4	29.6
<i>u4130</i>	H(102)...H(111)	626.5(44)	46.1(fixed)	—	1.7	46.1
<i>u4698</i>	H(311)...H(318)	626.5(82)	41.9(fixed)	—	-4.7	41.9
<i>u4815</i>	H(151)...H(161)	626.6(63)	56.3(fixed)	—	-10.2	56.3
<i>u4449</i>	H(27)...H(41)	626.6(211)	49.9(fixed)	—	-4.8	49.9
<i>u5394</i>	H(146)...H(150)	626.7(90)	27.5(fixed)	—	-7.2	27.5
<i>u4900</i>	H(307)...H(314)	627.6(61)	32.0(fixed)	—	-2.7	32.0
<i>u5403</i>	H(116)...H(121)	627.6(163)	26.5(fixed)	—	-6.5	26.5
<i>u3598</i>	H(70)...H(71)	627.6(73)	52.1(fixed)	—	-6.6	52.1
<i>u4789</i>	H(66)...H(80)	627.9(99)	40.5(fixed)	—	-5.0	40.5
<i>u4827</i>	H(69)...H(79)	628.0(84)	42.4(fixed)	—	-5.6	42.4
<i>u2122</i>	H(143)...H(147)	628.1(79)	49.4(fixed)	—	3.2	49.4
<i>u4144</i>	H(61)...H(70)	628.3(49)	46.3(fixed)	—	1.1	46.3
<i>u4569</i>	H(150)...H(164)	628.3(96)	46.5(fixed)	—	-6.4	46.5
<i>u4990</i>	H(101)...H(118)	628.5(191)	38.5(fixed)	—	-8.2	38.5
<i>u4727</i>	H(149)...H(164)	628.6(46)	39.5(fixed)	—	-7.3	39.5
<i>u3245</i>	H(111)...H(116)	628.7(71)	58.0(fixed)	—	-7.1	58.0
<i>u4375</i>	H(279)...H(287)	628.9(83)	40.6(fixed)	—	0.6	40.6
<i>u4830</i>	H(24)...H(39)	629.0(98)	34.9(fixed)	—	-4.4	34.9
<i>u5353</i>	H(117)...H(123)	629.0(52)	27.9(fixed)	—	-4.4	27.9
<i>u2121</i>	H(104)...H(106)	629.2(49)	63.0(fixed)	—	2.3	63.0
<i>u2411</i>	H(63)...H(65)	629.6(57)	62.6(fixed)	—	2.8	62.6
<i>u4833</i>	C(295)...H(308)	629.9(39)	20.2(fixed)	—	-5.0	20.2
<i>u4976</i>	H(72)...H(81)	630.2(77)	36.0(fixed)	—	0.6	36.0
<i>u4911</i>	H(272)...H(284)	630.5(160)	39.3(fixed)	—	-5.3	39.3
<i>u4881</i>	H(19)...H(36)	630.5(165)	41.0(fixed)	—	-8.2	41.0
<i>u2123</i>	H(225)...H(245)	630.5(125)	51.1(fixed)	—	3.3	51.1
<i>u5012</i>	H(61)...H(79)	630.5(49)	39.5(fixed)	—	-11.8	39.5
<i>u4846</i>	H(69)...H(78)	630.5(61)	38.9(fixed)	—	-6.2	38.9
<i>u4498</i>	H(68)...H(82)	630.7(119)	46.3(fixed)	—	-5.3	46.3
<i>u4773</i>	C(90)...C(94)	630.7(10)	12.4(fixed)	—	-2.6	12.4
<i>u4719</i>	C(131)...H(164)	630.7(35)	27.9(fixed)	—	-8.2	27.9
<i>u4812</i>	H(69)...H(80)	630.9(114)	34.6(fixed)	—	-7.7	34.6
<i>u4839</i>	H(65)...H(80)	630.9(114)	36.5(fixed)	—	-5.5	36.5

<i>u3921</i>	H(227)...H(240)	631.0(102)	36.5(fixed)	—	0.8	36.5
<i>u4767</i>	C(6)...C(10)	631.1(12)	12.6(fixed)	—	-2.4	12.6
<i>u4761</i>	C(8)...C(12)	631.1(10)	12.6(fixed)	—	-2.6	12.6
<i>u4766</i>	C(336)...C(340)	631.1(12)	12.3(fixed)	—	-2.3	12.3
<i>u4770</i>	C(131)...C(135)	631.3(11)	12.6(fixed)	—	-2.5	12.6
<i>u4938</i>	H(154)...H(163)	631.3(44)	36.5(fixed)	—	1.9	36.5
<i>u4875</i>	C(293)...H(314)	631.4(44)	22.8(fixed)	—	-5.4	22.8
<i>u4749</i>	C(293)...C(295)	631.5(13)	12.6(fixed)	—	-2.0	12.6
<i>u4848</i>	H(151)...H(162)	631.5(70)	38.0(fixed)	—	-9.0	38.0
<i>u3754</i>	C(214)...C(215)	631.5(15)	19.7(fixed)	—	-1.6	19.7
<i>u4733</i>	H(150)...H(162)	631.6(50)	43.8(fixed)	—	-9.3	43.8
<i>u2648</i>	C(216)...H(243)	631.6(74)	37.2(fixed)	—	-4.2	37.2
<i>u4802</i>	C(255)...H(276)	631.8(27)	32.0(fixed)	—	-10.3	32.0
<i>u5436</i>	H(183)...H(191)	631.9(101)	19.1(fixed)	—	-9.9	19.1
<i>u3907</i>	H(63)...H(76)	631.9(86)	34.5(fixed)	—	1.3	34.5
<i>u4021</i>	C(212)...C(213)	631.9(15)	23.3(fixed)	—	-1.4	23.3
<i>u3898</i>	C(9)...H(18)	632.1(935)	48.9(fixed)	—	-1.6	48.9
<i>u4975</i>	C(214)...H(239)	632.1(37)	24.3(fixed)	—	-9.9	24.3
<i>u2039</i>	H(61)...H(81)	632.1(86)	65.4(fixed)	—	0.5	65.4
<i>u3238</i>	H(146)...H(158)	632.1(45)	54.5(fixed)	—	10.6	54.5
<i>u4852</i>	H(144)...H(153)	632.2(86)	46.0(fixed)	—	-7.8	46.0
<i>u4861</i>	H(28)...H(39)	632.3(90)	32.9(fixed)	—	-7.9	32.9
<i>u5116</i>	H(268)...H(284)	632.3(55)	31.7(fixed)	—	-7.0	31.7
<i>u3638</i>	C(52)...C(54)	632.3(11)	18.0(fixed)	—	-1.2	18.0
<i>u4747</i>	C(335)...C(337)	632.4(12)	12.6(fixed)	—	-2.0	12.6
<i>u3121</i>	C(170)...C(174)	632.4(13)	28.1(fixed)	—	-1.5	28.1
<i>u4553</i>	H(109)...H(123)	632.4(173)	50.1(fixed)	—	-6.7	50.1
<i>u3673</i>	C(216)...C(218)	632.5(16)	17.8(fixed)	—	-1.2	17.8
<i>u4781</i>	C(296)...C(297)	632.6(12)	12.4(fixed)	—	-2.0	12.4
<i>u4754</i>	C(49)...C(53)	632.7(13)	12.6(fixed)	—	-2.1	12.6
<i>u3952</i>	C(129)...C(132)	632.9(13)	19.4(fixed)	—	-1.3	19.4
<i>u3682</i>	C(134)...C(136)	632.9(13)	19.6(fixed)	—	-1.2	19.6
<i>u4140</i>	C(48)...C(50)	632.9(13)	21.3(fixed)	—	-1.7	21.3
<i>u4127</i>	C(10)...H(23)	633.0(819)	51.8(fixed)	—	-2.7	51.8
<i>u4697</i>	C(336)...H(369)	633.0(38)	29.8(fixed)	—	-8.2	29.8
<i>u5295</i>	C(257)...H(273)	633.0(42)	15.9(fixed)	—	-5.2	15.9
<i>u3756</i>	C(256)...C(259)	633.2(14)	19.2(fixed)	—	-1.3	19.2
<i>u2651</i>	C(52)...H(79)	633.2(63)	38.6(fixed)	—	-4.0	38.6
<i>u4060</i>	C(89)...C(91)	633.4(13)	19.4(fixed)	—	-1.4	19.4
<i>u4887</i>	C(213)...H(224)	633.5(60)	21.4(fixed)	—	-5.6	21.4
<i>u1915</i>	C(171)...C(172)	633.9(12)	21.7(fixed)	—	0.9	21.7
<i>u5329</i>	C(218)...H(235)	633.9(100)	16.3(fixed)	—	-8.3	16.3
<i>u2029</i>	H(111)...H(117)	634.0(70)	48.6(fixed)	—	0.7	48.6
<i>u5063</i>	H(225)...H(243)	634.1(93)	32.4(fixed)	—	-8.6	32.4

<i>u4721</i>	H(69)...H(82)	634.2(99)	41.5(fixed)	—	-7.5	41.5
<i>u4716</i>	H(68)...H(80)	634.5(135)	39.9(fixed)	—	-7.1	39.9
<i>u4853</i>	C(95)...H(112)	634.6(43)	29.8(fixed)	—	-10.9	29.8
<i>u2133</i>	H(66)...H(72)	634.7(53)	47.2(fixed)	—	1.0	47.2
<i>u4728</i>	H(27)...H(39)	634.7(144)	42.1(fixed)	—	-7.4	42.1
<i>u4863</i>	H(106)...H(121)	635.2(10)	35.2(fixed)	—	-4.3	35.2
<i>u4740</i>	H(110)...H(123)	635.6(69)	46.5(fixed)	—	-10.3	46.5
<i>u4868</i>	H(110)...H(121)	635.8(51)	36.3(fixed)	—	-9.1	36.3
<i>u4785</i>	C(296)...H(321)	635.8(38)	21.6(fixed)	—	-7.8	21.6
<i>u4869</i>	H(107)...H(121)	636.0(144)	37.7(fixed)	—	-5.0	37.7
<i>u4743</i>	C(294)...H(321)	636.0(36)	28.0(fixed)	—	-8.3	28.0
<i>u2055</i>	H(277)...H(283)	636.1(65)	42.4(fixed)	—	9.4	42.4
<i>u2110</i>	H(152)...H(154)	636.4(45)	49.1(fixed)	—	4.1	49.1
<i>u5375</i>	H(236)...H(246)	636.4(41)	27.9(fixed)	—	-3.2	27.9
<i>u3823</i>	H(143)...H(157)	637.0(101)	44.1(fixed)	—	5.3	44.1
<i>u4876</i>	C(334)...H(369)	637.0(29)	21.0(fixed)	—	-8.8	21.0
<i>u4794</i>	C(8)...H(41)	637.1(35)	25.4(fixed)	—	-5.4	25.4
<i>u2128</i>	H(268)...H(286)	637.5(73)	56.4(fixed)	—	3.9	56.4
<i>u2697</i>	H(267)...H(286)	637.7(67)	56.0(fixed)	—	-1.4	56.0
<i>u4800</i>	H(104)...H(111)	637.8(63)	43.2(fixed)	—	-3.7	43.2
<i>u5081</i>	H(146)...H(151)	637.9(80)	38.3(fixed)	—	-0.6	38.3
<i>u4850</i>	H(63)...H(70)	638.0(68)	37.0(fixed)	—	-3.4	37.0
<i>u4801</i>	H(151)...H(164)	638.0(52)	39.4(fixed)	—	-8.8	39.4
<i>u4991</i>	H(275)...H(281)	638.1(79)	32.3(fixed)	—	0.8	32.3
<i>u4889</i>	H(26)...H(41)	638.2(86)	34.5(fixed)	—	-3.9	34.5
<i>u2269</i>	H(70)...H(72)	638.3(47)	49.8(fixed)	—	1.7	49.8
<i>u5134</i>	H(226)...H(239)	638.7(107)	28.8(fixed)	—	-4.2	28.8
<i>u4927</i>	H(307)...H(322)	638.9(50)	34.9(fixed)	—	-7.7	34.9
<i>u4834</i>	C(7)...H(38)	639.4(35)	26.2(fixed)	—	-5.7	26.2
<i>u4339</i>	C(171)...H(191)	639.6(38)	26.4(fixed)	—	-2.0	26.4
<i>u5147</i>	H(62)...H(75)	639.6(125)	28.1(fixed)	—	-5.1	28.1
<i>u1995</i>	H(107)...H(117)	639.9(55)	46.4(fixed)	—	3.2	46.4
<i>u4235</i>	C(47)...H(79)	639.9(52)	32.1(fixed)	—	-5.5	32.1
<i>u4641</i>	H(278)...H(285)	639.9(28)	49.6(fixed)	—	-3.1	49.6
<i>u5396</i>	H(71)...H(80)	640.1(122)	26.7(fixed)	—	-6.0	26.7
<i>u3570</i>	H(279)...H(285)	640.2(71)	43.1(fixed)	—	5.4	43.1
<i>u5298</i>	C(254)...H(265)	640.2(30)	15.9(fixed)	—	-5.5	15.9
<i>u4965</i>	C(90)...H(118)	640.5(8)	24.1(fixed)	—	-2.0	24.1
<i>u5261</i>	H(101)...H(110)	640.5(57)	26.4(fixed)	—	-10.8	26.4
<i>u3525</i>	H(267)...H(281)	640.7(76)	34.9(fixed)	—	3.5	34.9
<i>u4468</i>	H(228)...H(233)	640.8(112)	39.6(fixed)	—	-3.8	39.6
<i>u4779</i>	H(19)...H(38)	640.9(73)	46.6(fixed)	—	-7.7	46.6
<i>u3967</i>	C(212)...H(231)	641.0(60)	31.8(fixed)	—	1.7	31.8
<i>u4934</i>	C(135)...H(149)	641.1(39)	24.3(fixed)	—	-1.9	24.3

<i>u4162</i>	H(234)...H(236)	641.1(48)	46.6(fixed)	—	3.7	46.6
<i>u4879</i>	C(337)...H(350)	641.1(38)	24.6(fixed)	—	-0.4	24.6
<i>u4963</i>	C(7)...H(41)	641.2(53)	21.8(fixed)	—	-6.0	21.8
<i>u4836</i>	C(335)...H(353)	641.4(38)	20.8(fixed)	—	-5.1	20.8
<i>u5256</i>	H(184)...H(192)	641.4(90)	31.6(fixed)	—	-3.8	31.6
<i>u3743</i>	H(144)...H(161)	641.4(87)	52.9(fixed)	—	-25.2	52.9
<i>u4541</i>	H(267)...H(279)	641.4(74)	37.7(fixed)	—	-2.6	37.7
<i>u5317</i>	C(95)...H(116)	641.4(102)	15.7(fixed)	—	-6.3	15.7
<i>u2045</i>	H(145)...H(161)	641.7(66)	69.0(fixed)	—	-8.9	69.0
<i>u2709</i>	C(51)...H(66)	641.8(38)	32.0(fixed)	—	-4.5	32.0
<i>u4952</i>	H(185)...H(200)	642.0(60)	45.2(fixed)	—	-10.1	45.2
<i>u2550</i>	C(257)...H(266)	642.0(28)	32.0(fixed)	—	-2.4	32.0
<i>u4394</i>	C(215)...H(234)	642.1(42)	25.6(fixed)	—	-2.0	25.6
<i>u5254</i>	H(60)...H(69)	642.1(57)	25.2(fixed)	—	-10.6	25.2
<i>u2369</i>	H(266)...H(282)	642.2(47)	51.8(fixed)	—	-2.9	51.8
<i>u4471</i>	C(50)...H(63)	642.3(42)	32.7(fixed)	—	-1.9	32.7
<i>u5142</i>	H(226)...H(240)	642.5(65)	28.2(fixed)	—	-5.4	28.2
<i>u5274</i>	H(265)...H(276)	642.6(70)	33.6(fixed)	—	-8.9	33.6
<i>u4330</i>	C(211)...H(243)	642.7(90)	33.0(fixed)	—	-5.6	33.0
<i>u3578</i>	H(63)...H(75)	642.8(68)	35.4(fixed)	—	4.8	35.4
<i>u4784</i>	C(135)...H(150)	642.9(35)	27.3(fixed)	—	-6.0	27.3
<i>u5001</i>	H(272)...H(285)	642.9(49)	31.5(fixed)	—	-6.3	31.5
<i>u5386</i>	H(153)...H(162)	643.0(42)	27.4(fixed)	—	-5.8	27.4
<i>u4782</i>	C(90)...H(123)	643.2(78)	25.1(fixed)	—	-4.4	25.1
<i>u3074</i>	C(48)...H(66)	643.3(36)	32.9(fixed)	—	-6.1	32.9
<i>u4977</i>	H(231)...H(244)	643.4(62)	31.3(fixed)	—	-6.4	31.3
<i>u4312</i>	C(91)...H(104)	643.5(40)	35.9(fixed)	—	-1.3	35.9
<i>u4452</i>	C(170)...H(198)	643.6(39)	31.5(fixed)	—	-3.3	31.5
<i>u4902</i>	C(91)...H(101)	643.7(41)	23.1(fixed)	—	-10.0	23.1
<i>u4959</i>	C(336)...H(364)	643.7(40)	23.5(fixed)	—	-1.8	23.5
<i>u2715</i>	C(256)...H(284)	643.8(37)	35.3(fixed)	—	-3.6	35.3
<i>u4982</i>	C(8)...H(36)	643.8(37)	23.9(fixed)	—	-1.9	23.9
<i>u5330</i>	C(54)...H(71)	643.9(69)	15.4(fixed)	—	-6.1	15.4
<i>u4867</i>	C(50)...H(60)	644.1(39)	22.3(fixed)	—	-9.8	22.3
<i>u4652</i>	C(8)...H(33)	644.3(508)	27.9(fixed)	—	-6.5	27.9
<i>u4862</i>	C(9)...H(19)	644.3(25)	23.0(fixed)	—	-9.7	23.0
<i>u4825</i>	H(306)...H(322)	644.4(95)	41.4(fixed)	—	-8.1	41.4
<i>u4908</i>	C(53)...H(67)	644.5(30)	25.4(fixed)	—	-0.6	25.4
<i>u4831</i>	H(108)...H(123)	644.5(64)	32.7(fixed)	—	-2.1	32.7
<i>u4684</i>	C(89)...H(111)	644.6(34)	27.8(fixed)	—	-4.3	27.8
<i>u5381</i>	H(183)...H(192)	644.6(83)	28.3(fixed)	—	-5.9	28.3
<i>u5361</i>	H(154)...H(164)	644.7(123)	28.3(fixed)	—	-5.7	28.3
<i>u4799</i>	H(109)...H(121)	644.7(122)	38.3(fixed)	—	-8.1	38.3
<i>u4813</i>	C(53)...H(68)	644.8(62)	24.3(fixed)	—	-5.9	24.3

<i>u3786</i>	C(259)...H(278)	644.9(38)	51.8(fixed)	—	1.3	51.8
<i>u5031</i>	C(334)...H(366)	644.9(39)	22.6(fixed)	—	-5.2	22.6
<i>u4792</i>	C(49)...H(82)	645.0(40)	23.9(fixed)	—	-5.3	23.9
<i>u4941</i>	C(49)...H(77)	645.0(59)	25.8(fixed)	—	-0.4	25.8
<i>u5003</i>	H(108)...H(112)	645.0(77)	41.5(fixed)	—	-7.8	41.5
<i>u3844</i>	H(76)...H(81)	645.0(44)	38.1(fixed)	—	3.1	38.1
<i>u3545</i>	H(265)...H(282)	645.1(59)	47.7(fixed)	—	-7.8	47.7
<i>u5072</i>	H(309)...H(323)	645.1(84)	28.1(fixed)	—	-5.1	28.1
<i>u4717</i>	C(48)...H(70)	645.3(35)	25.6(fixed)	—	-3.7	25.6
<i>u1132</i>	C(252)...H(281)	645.3(31)	34.2(fixed)	—	4.2	34.2
<i>u3547</i>	H(227)...H(239)	645.4(86)	36.7(fixed)	—	5.6	36.7
<i>u4860</i>	C(294)...H(317)	645.4(35)	22.3(fixed)	—	-6.4	22.3
<i>u3450</i>	H(228)...H(231)	645.7(58)	47.4(fixed)	—	5.0	47.4
<i>u4978</i>	H(102)...H(120)	645.7(52)	43.5(fixed)	—	-10.8	43.5
<i>u2848</i>	C(129)...H(148)	645.8(32)	26.0(fixed)	—	-1.8	26.0
<i>u5362</i>	H(72)...H(82)	645.8(85)	28.2(fixed)	—	-4.8	28.2
<i>u4487</i>	C(256)...H(285)	645.9(29)	21.9(fixed)	—	-2.7	21.9
<i>u4966</i>	H(230)...H(241)	646.0(132)	32.9(fixed)	—	-2.2	32.9
<i>u5331</i>	C(136)...H(153)	646.0(33)	15.4(fixed)	—	-6.6	15.4
<i>u2779</i>	C(215)...H(230)	646.1(47)	31.8(fixed)	—	-2.4	31.8
<i>u5087</i>	H(226)...H(233)	646.2(72)	33.2(fixed)	—	-7.8	33.2
<i>u5049</i>	C(259)...H(280)	646.2(36)	22.2(fixed)	—	-5.4	22.2
<i>u4329</i>	H(23)...H(27)	646.3(511)	42.6(fixed)	—	6.6	42.6
<i>u5319</i>	C(132)...H(144)	646.3(30)	15.7(fixed)	—	-6.8	15.7
<i>u4980</i>	C(94)...H(108)	646.3(65)	23.9(fixed)	—	-1.7	23.9
<i>u5141</i>	H(62)...H(76)	646.4(59)	27.5(fixed)	—	-5.2	27.5
<i>u4161</i>	C(170)...H(195)	646.6(30)	31.2(fixed)	—	-5.0	31.2
<i>u3312</i>	H(141)...H(151)	646.6(36)	42.8(fixed)	—	5.7	42.8
<i>u4981</i>	C(295)...H(307)	646.8(34)	26.5(fixed)	—	-1.3	26.5
<i>u3595</i>	H(186)...H(191)	647.0(48)	41.6(fixed)	—	9.4	41.6
<i>u4575</i>	C(253)...H(284)	647.0(35)	29.7(fixed)	—	-4.8	29.7
<i>u3913</i>	H(158)...H(163)	647.0(77)	47.5(fixed)	—	6.9	47.5
<i>u2688</i>	C(93)...H(107)	647.0(43)	34.0(fixed)	—	-3.1	34.0
<i>u4297</i>	C(213)...H(227)	647.2(35)	31.0(fixed)	—	-1.3	31.0
<i>u3421</i>	C(132)...H(141)	647.3(38)	32.3(fixed)	—	2.5	32.3
<i>u3902</i>	H(182)...H(195)	647.3(24)	39.3(fixed)	—	-2.5	39.3
<i>u2963</i>	C(89)...H(107)	647.3(37)	28.6(fixed)	—	-4.6	28.6
<i>u4260</i>	C(134)...H(163)	647.4(37)	26.1(fixed)	—	-1.8	26.1
<i>u4841</i>	C(335)...H(357)	647.4(31)	26.4(fixed)	—	0.0	26.4
<i>u4637</i>	C(129)...H(152)	647.5(37)	25.0(fixed)	—	-3.6	25.0
<i>u5233</i>	H(101)...H(112)	647.5(77)	31.0(fixed)	—	-12.6	31.0
<i>u3957</i>	C(129)...H(151)	647.6(33)	31.3(fixed)	—	1.4	31.3
<i>u4436</i>	C(216)...H(244)	647.6(28)	20.9(fixed)	—	-2.6	20.9
<i>u4199</i>	C(52)...H(81)	647.9(29)	25.1(fixed)	—	-1.7	25.1

<i>u2275</i>	H(268)...H(274)	648.1(51)	37.3(fixed)	—	-0.5	37.3
<i>u4883</i>	H(67)...H(82)	648.1(47)	32.7(fixed)	—	-3.4	32.7
<i>u3998</i>	C(214)...H(237)	648.1(36)	53.9(fixed)	—	-0.9	53.9
<i>u4922</i>	C(293)...H(313)	648.1(38)	25.1(fixed)	—	-0.2	25.1
<i>u5075</i>	H(227)...H(232)	648.1(61)	35.8(fixed)	—	-6.9	35.8
<i>u3160</i>	C(54)...H(76)	648.2(27)	32.6(fixed)	—	6.0	32.6
<i>u5008</i>	H(145)...H(153)	648.3(69)	38.5(fixed)	—	-8.1	38.5
<i>u5060</i>	H(106)...H(118)	648.4(51)	34.2(fixed)	—	0.7	34.2
<i>u2160</i>	H(148)...H(154)	648.4(85)	54.5(fixed)	—	5.9	54.5
<i>u4948</i>	H(68)...H(77)	648.5(99)	32.8(fixed)	—	-3.7	32.8
<i>u2036</i>	H(229)...H(236)	648.7(70)	40.4(fixed)	—	10.8	40.4
<i>u4979</i>	C(296)...H(319)	648.8(35)	24.3(fixed)	—	-1.3	24.3
<i>u4355</i>	C(256)...H(286)	648.9(34)	25.1(fixed)	—	-1.7	25.1
<i>u3810</i>	H(102)...H(109)	649.7(90)	45.7(fixed)	—	8.6	45.7
<i>u3391</i>	C(214)...H(236)	649.9(37)	41.5(fixed)	—	7.3	41.5
<i>u2794</i>	C(170)...H(196)	650.2(34)	39.7(fixed)	—	2.3	39.7
<i>u3789</i>	H(61)...H(68)	650.4(100)	46.8(fixed)	—	6.6	46.8
<i>u4958</i>	H(271)...H(282)	650.4(43)	32.6(fixed)	—	-2.2	32.6
<i>u4308</i>	C(216)...H(245)	650.4(18)	24.3(fixed)	—	-1.8	24.3
<i>u4764</i>	H(238)...H(244)	650.5(19)	44.1(fixed)	—	-5.9	44.1
<i>u5011</i>	C(296)...H(318)	650.8(29)	24.3(fixed)	—	-1.7	24.3
<i>u2313</i>	H(225)...H(233)	650.8(62)	40.5(fixed)	—	-0.4	40.5
<i>u4467</i>	C(134)...H(162)	650.8(37)	21.7(fixed)	—	-2.9	21.7
<i>u4896</i>	C(337)...H(347)	650.9(35)	22.8(fixed)	—	-5.9	22.8
<i>u2897</i>	C(211)...H(246)	650.9(41)	27.0(fixed)	—	-3.0	27.0
<i>u4918</i>	C(258)...H(273)	651.0(32)	20.8(fixed)	—	-5.5	20.8
<i>u4951</i>	C(131)...H(159)	651.0(42)	36.2(fixed)	—	4.4	36.2
<i>u4184</i>	H(18)...H(29)	651.3(945)	52.6(fixed)	—	1.2	52.6
<i>u2693</i>	C(171)...H(188)	651.4(33)	38.9(fixed)	—	-5.8	38.9
<i>u2784</i>	C(133)...H(148)	651.5(49)	38.4(fixed)	—	-1.7	38.4
<i>u4439</i>	C(52)...H(80)	651.5(36)	20.7(fixed)	—	-2.8	20.7
<i>u4950</i>	C(217)...H(232)	651.7(33)	21.1(fixed)	—	-6.1	21.1
<i>u5070</i>	H(315)...H(319)	651.8(22)	34.3(fixed)	—	0.6	34.3
<i>u4170</i>	C(48)...H(69)	651.9(37)	32.1(fixed)	—	0.7	32.1
<i>u4071</i>	C(136)...H(156)	651.9(43)	57.1(fixed)	—	-2.7	57.1
<i>u4113</i>	C(218)...H(238)	651.9(18)	48.1(fixed)	—	-2.6	48.1
<i>u4912</i>	C(217)...H(230)	652.1(63)	25.4(fixed)	—	-5.8	25.4
<i>u4751</i>	H(156)...H(162)	652.1(79)	53.0(fixed)	—	-7.0	53.0
<i>u5085</i>	H(21)...H(28)	652.1(100)	37.1(fixed)	—	-11.3	37.1
<i>u4893</i>	C(295)...H(305)	652.5(34)	25.8(fixed)	—	-0.4	25.8
<i>u4835</i>	H(143)...H(152)	652.6(24)	37.8(fixed)	—	-3.8	37.8
<i>u4085</i>	C(89)...H(110)	652.7(35)	29.5(fixed)	—	2.8	29.5
<i>u4946</i>	H(67)...H(78)	652.8(42)	37.6(fixed)	—	3.9	37.6
<i>u4455</i>	C(212)...H(232)	652.9(42)	36.4(fixed)	—	-4.2	36.4



<i>u</i> 5009	H(24)...H(36)	653.0(31)	35.6(fixed)	—	0.6	35.6
<i>u</i> 4388	C(132)...H(143)	653.0(31)	32.2(fixed)	—	-2.0	32.2
<i>u</i> 5022	H(65)...H(77)	653.1(45)	36.8(fixed)	—	3.7	36.8
<i>u</i> 3202	C(136)...H(158)	653.2(51)	40.9(fixed)	—	11.2	40.9
<i>u</i> 3660	H(103)...H(112)	653.3(101)	45.9(fixed)	—	-12.7	45.9
<i>u</i> 4068	H(108)...H(113)	653.3(48)	44.1(fixed)	—	7.6	44.1
<i>u</i> 4283	C(88)...H(120)	653.4(46)	34.2(fixed)	—	-4.4	34.2
<i>u</i> 4891	H(22)...H(38)	653.5(200)	34.9(fixed)	—	-1.2	34.9
<i>u</i> 5028	C(9)...H(21)	653.5(62)	24.6(fixed)	—	-11.4	24.6
<i>u</i> 4856	H(150)...H(159)	653.6(37)	44.2(fixed)	—	4.5	44.2
<i>u</i> 5037	C(335)...H(356)	653.6(31)	26.4(fixed)	—	-1.4	26.4
<i>u</i> 3564	C(213)...H(228)	653.6(25)	40.9(fixed)	—	1.6	40.9
<i>u</i> 3930	H(240)...H(245)	653.6(29)	40.4(fixed)	—	5.2	40.4
<i>u</i> 4939	C(293)...H(311)	654.1(32)	28.4(fixed)	—	-1.1	28.4
<i>u</i> 4712	H(233)...H(237)	654.1(25)	49.8(fixed)	—	-4.7	49.8
<i>u</i> 3172	C(218)...H(240)	654.1(19)	34.6(fixed)	—	8.3	34.6
<i>u</i> 2674	H(99)...H(112)	654.2(37)	36.6(fixed)	—	-9.7	36.6
<i>u</i> 4967	H(231)...H(246)	654.3(53)	37.9(fixed)	—	-7.0	37.9
<i>u</i> 4486	C(215)...H(233)	654.3(32)	22.1(fixed)	—	-3.0	22.1
<i>u</i> 5000	C(94)...H(106)	654.4(59)	25.3(fixed)	—	-1.7	25.3
<i>u</i> 3610	H(224)...H(232)	654.4(119)	36.2(fixed)	—	-3.8	36.2
<i>u</i> 2789	C(88)...H(123)	654.6(61)	23.3(fixed)	—	-0.3	23.3
<i>u</i> 5076	H(185)...H(202)	654.6(128)	42.6(fixed)	—	-11.7	42.6
<i>u</i> 4942	H(305)...H(313)	655.0(63)	35.5(fixed)	—	3.9	35.5
<i>u</i> 4255	H(277)...H(286)	655.0(25)	49.6(fixed)	—	1.6	49.6
<i>u</i> 4803	H(227)...H(229)	655.2(31)	35.0(fixed)	—	-3.1	35.0
<i>u</i> 5046	H(307)...H(311)	655.2(55)	38.9(fixed)	—	2.1	38.9
<i>u</i> 5041	H(272)...H(287)	655.3(98)	34.9(fixed)	—	-6.9	34.9
<i>u</i> 4412	H(141)...H(152)	655.4(81)	34.6(fixed)	—	-1.5	34.6
<i>u</i> 4945	C(258)...H(271)	655.6(29)	25.1(fixed)	—	-5.3	25.1
<i>u</i> 3910	C(54)...H(74)	655.6(30)	46.4(fixed)	—	-1.8	46.4
<i>u</i> 2861	C(47)...H(82)	655.6(43)	25.0(fixed)	—	-2.3	25.0
<i>u</i> 3679	H(146)...H(153)	655.7(74)	50.7(fixed)	—	1.3	50.7
<i>u</i> 4944	C(49)...H(78)	655.7(50)	28.2(fixed)	—	-0.9	28.2
<i>u</i> 4994	C(53)...H(65)	655.7(26)	26.6(fixed)	—	-1.2	26.6
<i>u</i> 4919	C(8)...H(37)	656.3(28)	26.6(fixed)	—	-1.8	26.6
<i>u</i> 4685	C(212)...H(229)	656.3(39)	25.8(fixed)	—	-3.8	25.8
<i>u</i> 2117	H(186)...H(188)	656.5(24)	41.8(fixed)	—	4.3	41.8
<i>u</i> 3614	C(91)...H(105)	656.5(35)	35.3(fixed)	—	2.8	35.3
<i>u</i> 5026	C(336)...H(365)	656.6(33)	24.1(fixed)	—	-2.0	24.1
<i>u</i> 3713	C(50)...H(64)	656.6(37)	36.3(fixed)	—	1.4	36.3
<i>u</i> 5054	H(149)...H(160)	656.8(26)	41.3(fixed)	—	10.3	41.3
<i>u</i> 1750	H(268)...H(273)	657.1(73)	43.7(fixed)	—	4.3	43.7
<i>u</i> 2973	C(133)...H(150)	657.3(28)	36.8(fixed)	—	-3.6	36.8

<i>u4318</i>	H(234)...H(237)	657.3(83)	56.3(fixed)	—	2.2	56.3
<i>u5027</i>	C(135)...H(147)	657.5(33)	25.3(fixed)	—	-2.2	25.3
<i>u1474</i>	C(252)...H(279)	657.6(25)	39.1(fixed)	—	3.0	39.1
<i>u5036</i>	C(131)...H(160)	657.7(33)	36.4(fixed)	—	2.8	36.4
<i>u4989</i>	C(337)...H(351)	657.7(35)	26.7(fixed)	—	-1.5	26.7
<i>u2460</i>	H(138)...H(144)	657.8(38)	42.3(fixed)	—	-1.8	42.3
<i>u4711</i>	H(74)...H(80)	657.8(51)	42.9(fixed)	—	-5.2	42.9
<i>u3301</i>	H(157)...H(161)	657.9(55)	78.6(fixed)	—	-25.8	78.6
<i>u5067</i>	H(108)...H(119)	657.9(76)	36.6(fixed)	—	0.4	36.6
<i>u4999</i>	C(90)...H(119)	657.9(8)	26.1(fixed)	—	-2.3	26.1
<i>u3508</i>	C(259)...H(277)	658.5(33)	44.4(fixed)	—	5.9	44.4
<i>u996</i>	C(171)...H(190)	658.5(40)	33.3(fixed)	—	13.9	33.3
<i>u3599</i>	H(105)...H(110)	658.6(60)	45.6(fixed)	—	7.3	45.6
<i>u3027</i>	C(51)...H(68)	658.7(32)	37.8(fixed)	—	-3.8	37.8
<i>u5352</i>	H(273)...H(281)	658.9(66)	26.7(fixed)	—	-4.2	26.7
<i>u3671</i>	H(64)...H(69)	659.1(65)	45.1(fixed)	—	4.3	45.1
<i>u4178</i>	H(278)...H(286)	659.1(82)	53.1(fixed)	—	4.8	53.1
<i>u2831</i>	C(93)...H(109)	659.3(27)	34.1(fixed)	—	-5.5	34.1
<i>u4805</i>	H(306)...H(321)	660.5(74)	44.3(fixed)	—	-8.1	44.3
<i>u796</i>	C(257)...H(264)	660.5(27)	29.6(fixed)	—	9.4	29.6
<i>u1909</i>	H(225)...H(232)	660.6(65)	45.9(fixed)	—	4.8	45.9
<i>u2124</i>	H(266)...H(279)	660.8(41)	49.6(fixed)	—	1.2	49.6
<i>u5021</i>	H(18)...H(31)	660.9(297)	37.2(fixed)	—	2.7	37.2
<i>u3054</i>	C(253)...H(287)	661.6(26)	31.5(fixed)	—	-5.8	31.5
<i>u2640</i>	H(182)...H(196)	661.9(81)	51.6(fixed)	—	4.1	51.6
<i>u4675</i>	H(14)...H(23)	662.1(489)	30.7(fixed)	—	-1.1	30.7
<i>u5106</i>	H(316)...H(319)	662.3(77)	35.0(fixed)	—	-0.3	35.0
<i>u3586</i>	H(224)...H(233)	662.3(69)	35.0(fixed)	—	-4.5	35.0
<i>u525</i>	H(264)...H(281)	663.1(42)	42.6(fixed)	—	10.3	42.6
<i>u4828</i>	H(23)...H(36)	663.3(698)	40.2(fixed)	—	-6.8	40.2
<i>u4551</i>	H(105)...H(111)	663.3(41)	38.8(fixed)	—	-2.7	38.8
<i>u5044</i>	H(312)...H(326)	663.5(77)	36.4(fixed)	—	-10.0	36.4
<i>u5024</i>	H(271)...H(285)	663.6(76)	37.4(fixed)	—	-8.3	37.4
<i>u5131</i>	H(67)...H(77)	663.7(86)	37.5(fixed)	—	-1.2	37.5
<i>u5148</i>	H(149)...H(159)	664.6(91)	48.8(fixed)	—	-0.7	48.8
<i>u5065</i>	H(147)...H(159)	665.1(29)	49.0(fixed)	—	10.8	49.0
<i>u5211</i>	H(26)...H(36)	665.3(101)	30.5(fixed)	—	-2.8	30.5
<i>u4620</i>	H(64)...H(70)	665.3(41)	37.1(fixed)	—	-2.4	37.1
<i>u5300</i>	C(255)...H(280)	665.3(40)	15.7(fixed)	—	-5.2	15.7
<i>u5195</i>	H(108)...H(118)	665.6(89)	30.3(fixed)	—	-2.7	30.3
<i>u3188</i>	H(156)...H(161)	665.9(37)	96.0(fixed)	—	-18.7	96.0
<i>u4325</i>	H(156)...H(163)	666.6(40)	61.5(fixed)	—	0.7	61.5
<i>u3546</i>	H(267)...H(273)	667.0(58)	37.3(fixed)	—	-4.7	37.3
<i>u4565</i>	H(23)...H(29)	667.2(597)	40.4(fixed)	—	1.7	40.4

<i>u4973</i>	H(230)...H(244)	667.3(198)	35.5(fixed)	—	-7.6	35.5
<i>u4476</i>	H(18)...H(33)	667.3(966)	56.7(fixed)	—	0.4	56.7
<i>u3585</i>	H(187)...H(188)	667.9(87)	43.0(fixed)	—	-13.6	43.0
<i>u5110</i>	H(14)...H(21)	667.9(24)	18.5(fixed)	—	-8.5	18.5
<i>u5385</i>	H(274)...H(280)	668.0(58)	25.6(fixed)	—	-5.2	25.6
<i>u4460</i>	H(238)...H(245)	668.0(38)	52.8(fixed)	—	-0.2	52.8
<i>u5150</i>	H(19)...H(34)	668.4(46)	34.3(fixed)	—	-11.2	34.3
<i>u4106</i>	H(263)...H(271)	668.4(24)	32.1(fixed)	—	-3.4	32.1
<i>u4454</i>	H(101)...H(114)	668.7(60)	57.7(fixed)	—	0.0	57.7
<i>u3308</i>	H(239)...H(243)	668.8(100)	52.3(fixed)	—	-10.9	52.3
<i>u4954</i>	H(271)...H(287)	668.9(53)	42.9(fixed)	—	-7.3	42.9
<i>u5342</i>	H(107)...H(112)	668.9(58)	31.8(fixed)	—	-9.8	31.8
<i>u4568</i>	H(96)...H(101)	669.0(25)	26.5(fixed)	—	-9.8	26.5
<i>u4069</i>	H(227)...H(231)	669.4(98)	39.5(fixed)	—	3.3	39.5
<i>u5151</i>	H(308)...H(323)	669.6(66)	31.7(fixed)	—	-6.8	31.7
<i>u4214</i>	H(74)...H(81)	669.9(40)	51.3(fixed)	—	0.5	51.3
<i>u4597</i>	H(55)...H(60)	670.4(23)	27.1(fixed)	—	-8.6	27.1
<i>u4935</i>	H(112)...H(121)	670.7(108)	39.8(fixed)	—	-10.7	39.8
<i>u5096</i>	H(342)...H(347)	670.7(23)	17.8(fixed)	—	-5.8	17.8
<i>u4842</i>	H(230)...H(246)	670.9(144)	43.4(fixed)	—	-6.7	43.4
<i>u3961</i>	H(265)...H(284)	671.1(77)	37.2(fixed)	—	-9.5	37.2
<i>u5260</i>	H(144)...H(157)	671.2(83)	40.4(fixed)	—	-8.3	40.4
<i>u3719</i>	H(261)...H(273)	671.6(25)	26.9(fixed)	—	-2.2	26.9
<i>u5273</i>	H(275)...H(276)	671.6(41)	30.4(fixed)	—	-12.1	30.4
<i>u5059</i>	H(305)...H(311)	671.7(38)	41.6(fixed)	—	0.7	41.6
<i>u5089</i>	H(302)...H(308)	672.0(23)	17.5(fixed)	—	-5.5	17.5
<i>u5099</i>	H(262)...H(284)	672.5(23)	17.5(fixed)	—	-6.2	17.5
<i>u3394</i>	H(75)...H(79)	672.6(86)	49.0(fixed)	—	-9.7	49.0
<i>u4626</i>	H(139)...H(153)	672.6(23)	22.1(fixed)	—	-8.2	22.1
<i>u3830</i>	H(101)...H(113)	672.8(65)	49.4(fixed)	—	9.6	49.4
<i>u3831</i>	H(97)...H(123)	673.2(25)	27.8(fixed)	—	-3.3	27.8
<i>u5183</i>	H(322)...H(326)	673.2(45)	35.4(fixed)	—	-2.1	35.4
<i>u5112</i>	H(221)...H(243)	673.2(24)	17.7(fixed)	—	-7.3	17.7
<i>u5354</i>	H(265)...H(272)	673.5(50)	27.0(fixed)	—	-4.5	27.0
<i>u5095</i>	H(15)...H(41)	673.5(22)	18.4(fixed)	—	-6.5	18.4
<i>u5174</i>	H(308)...H(313)	673.7(50)	26.8(fixed)	—	-5.3	26.8
<i>u5182</i>	H(308)...H(312)	673.8(51)	28.0(fixed)	—	-5.8	28.0
<i>u4562</i>	H(98)...H(116)	673.8(24)	20.4(fixed)	—	-6.3	20.4
<i>u2281</i>	H(266)...H(281)	673.9(39)	38.7(fixed)	—	-1.5	38.7
<i>u4629</i>	H(57)...H(71)	674.0(24)	20.6(fixed)	—	-6.9	20.6
<i>u4606</i>	H(219)...H(224)	674.2(22)	23.8(fixed)	—	-5.1	23.8
<i>u4284</i>	H(63)...H(69)	674.3(46)	43.5(fixed)	—	2.0	43.5
<i>u4880</i>	H(184)...H(195)	674.6(69)	33.0(fixed)	—	-7.5	33.0
<i>u4533</i>	H(228)...H(229)	674.7(87)	39.9(fixed)	—	-2.7	39.9

<i>u4688</i>	H(260)...H(267)	675.2(25)	23.7(fixed)	—	-5.5	23.7
<i>u3135</i>	H(103)...H(114)	675.4(68)	62.1(fixed)	—	-7.6	62.1
<i>u3655</i>	H(267)...H(274)	675.4(60)	31.9(fixed)	—	-6.1	31.9
<i>u5161</i>	H(20)...H(34)	675.8(192)	31.1(fixed)	—	-10.7	31.1
<i>u5338</i>	H(234)...H(239)	676.4(44)	26.3(fixed)	—	-11.3	26.3
<i>u5030</i>	H(107)...H(113)	676.7(68)	31.5(fixed)	—	-1.9	31.5
<i>u4133</i>	H(104)...H(110)	676.9(48)	44.8(fixed)	—	5.6	44.8
<i>u5336</i>	H(232)...H(239)	677.0(46)	31.0(fixed)	—	-12.3	31.0
<i>u5237</i>	H(273)...H(276)	677.2(37)	40.5(fixed)	—	-12.0	40.5
<i>u5133</i>	H(65)...H(78)	678.1(89)	42.3(fixed)	—	-0.9	42.3
<i>u5135</i>	H(109)...H(120)	678.1(46)	39.4(fixed)	—	-11.4	39.4
<i>u4119</i>	H(264)...H(276)	678.6(75)	39.9(fixed)	—	0.9	39.9
<i>u4988</i>	H(233)...H(239)	678.7(58)	35.7(fixed)	—	-9.2	35.7
<i>u2244</i>	H(266)...H(284)	678.7(107)	50.6(fixed)	—	1.0	50.6
<i>u3293</i>	H(238)...H(243)	678.7(42)	55.6(fixed)	—	-10.0	55.6
<i>u5155</i>	H(312)...H(319)	678.8(42)	24.9(fixed)	—	-9.0	24.9
<i>u5202</i>	H(308)...H(311)	678.8(44)	22.7(fixed)	—	-6.8	22.7
<i>u5240</i>	H(315)...H(318)	679.6(65)	30.7(fixed)	—	-2.9	30.7
<i>u5189</i>	H(18)...H(34)	680.2(162)	28.2(fixed)	—	-12.8	28.2
<i>u5137</i>	H(106)...H(119)	680.3(99)	37.2(fixed)	—	-1.4	37.2
<i>u4776</i>	H(20)...H(33)	680.4(703)	48.0(fixed)	—	-6.7	48.0
<i>u3981</i>	H(76)...H(80)	680.5(38)	32.6(fixed)	—	4.4	32.6
<i>u5064</i>	H(24)...H(37)	681.0(92)	38.8(fixed)	—	-1.1	38.8
<i>u5187</i>	H(147)...H(160)	681.2(90)	52.3(fixed)	—	1.8	52.3
<i>u3847</i>	H(63)...H(66)	681.8(45)	40.2(fixed)	—	-9.2	40.2
<i>u5271</i>	H(112)...H(123)	681.9(56)	37.8(fixed)	—	-12.8	37.8
<i>u5124</i>	H(267)...H(271)	682.1(57)	28.7(fixed)	—	-6.6	28.7
<i>u3221</i>	H(74)...H(79)	682.3(43)	55.4(fixed)	—	-8.0	55.4
<i>u3664</i>	H(276)...H(284)	682.3(45)	47.1(fixed)	—	-13.9	47.1
<i>u4824</i>	H(274)...H(276)	682.3(46)	39.7(fixed)	—	-10.0	39.7
<i>u5164</i>	H(309)...H(317)	682.4(49)	30.2(fixed)	—	-6.7	30.2
<i>u5120</i>	H(312)...H(317)	682.4(48)	29.2(fixed)	—	-8.9	29.2
<i>u4177</i>	H(143)...H(151)	682.5(67)	43.1(fixed)	—	2.2	43.1
<i>u1628</i>	H(158)...H(161)	682.6(66)	86.7(fixed)	—	10.0	86.7
<i>u3954</i>	H(240)...H(244)	682.7(41)	33.8(fixed)	—	6.5	33.8
<i>u5158</i>	H(312)...H(318)	682.8(52)	26.7(fixed)	—	-8.4	26.7
<i>u5185</i>	H(308)...H(325)	683.1(113)	38.6(fixed)	—	-7.3	38.6
<i>u5118</i>	H(148)...H(164)	683.2(61)	36.3(fixed)	—	-9.7	36.3
<i>u1700</i>	H(76)...H(79)	683.6(77)	48.6(fixed)	—	9.1	48.6
<i>u3051</i>	H(278)...H(284)	683.8(38)	64.7(fixed)	—	-7.4	64.7
<i>u5393</i>	H(144)...H(151)	683.9(38)	26.4(fixed)	—	-6.4	26.4
<i>u5173</i>	H(19)...H(29)	684.1(51)	28.8(fixed)	—	-10.4	28.8
<i>u4032</i>	H(158)...H(162)	684.1(43)	38.8(fixed)	—	9.4	38.8
<i>u4795</i>	H(184)...H(198)	684.2(59)	43.4(fixed)	—	-6.2	43.4

<i>u4624</i>	H(19)...H(33)	684.3(869)	58.3(fixed)	—	-3.7	58.3
<i>u3641</i>	H(104)...H(107)	684.9(46)	43.9(fixed)	—	-8.5	43.9
<i>u5068</i>	H(280)...H(285)	685.2(53)	31.0(fixed)	—	-3.0	31.0
<i>u1701</i>	H(240)...H(243)	685.4(99)	48.9(fixed)	—	12.0	48.9
<i>u5422</i>	H(265)...H(271)	685.5(40)	20.5(fixed)	—	-8.3	20.5
<i>u5157</i>	H(183)...H(189)	685.7(66)	33.1(fixed)	—	-10.8	33.1
<i>u5282</i>	H(112)...H(122)	686.1(42)	28.4(fixed)	—	-12.4	28.4
<i>u3642</i>	H(143)...H(148)	686.1(37)	34.0(fixed)	—	-5.5	34.0
<i>u4189</i>	H(277)...H(285)	686.3(67)	41.1(fixed)	—	5.0	41.1
<i>u3663</i>	H(230)...H(235)	686.6(54)	46.3(fixed)	—	-11.4	46.3
<i>u4124</i>	H(233)...H(236)	686.9(66)	39.1(fixed)	—	6.3	39.1
<i>u4443</i>	H(18)...H(27)	687.5(1000)	58.3(fixed)	—	-2.8	58.3
<i>u5268</i>	H(22)...H(41)	687.9(103)	27.5(fixed)	—	-7.9	27.5
<i>u3297</i>	H(230)...H(237)	688.3(38)	59.9(fixed)	—	-8.2	59.9
<i>u5146</i>	H(183)...H(198)	688.7(47)	37.9(fixed)	—	-7.3	37.9
<i>u4713</i>	H(18)...H(28)	689.3(832)	44.8(fixed)	—	-5.4	44.8
<i>u5225</i>	H(224)...H(230)	689.3(96)	29.4(fixed)	—	-6.8	29.4
<i>u5270</i>	H(21)...H(41)	689.4(75)	30.4(fixed)	—	-6.3	30.4
<i>u5198</i>	H(25)...H(41)	689.5(63)	34.5(fixed)	—	-7.0	34.5
<i>u4051</i>	H(62)...H(66)	689.5(47)	42.0(fixed)	—	-9.1	42.0
<i>u5263</i>	H(232)...H(241)	689.6(62)	26.9(fixed)	—	-7.2	26.9
<i>u3658</i>	H(225)...H(246)	690.1(42)	34.9(fixed)	—	-6.2	34.9
<i>u5285</i>	H(306)...H(314)	690.3(46)	30.9(fixed)	—	-7.6	30.9
<i>u5232</i>	H(273)...H(282)	690.5(39)	27.2(fixed)	—	-6.4	27.2
<i>u5253</i>	H(19)...H(28)	690.7(59)	26.6(fixed)	—	-10.7	26.6
<i>u3611</i>	H(61)...H(82)	691.4(52)	47.7(fixed)	—	-9.5	47.7
<i>u3577</i>	H(142)...H(148)	692.1(40)	38.2(fixed)	—	-4.1	38.2
<i>u4949</i>	C(6)...H(32)	692.5(535)	26.5(fixed)	—	-1.2	26.5
<i>u3430</i>	H(102)...H(123)	692.6(79)	51.4(fixed)	—	-6.9	51.4
<i>u3905</i>	H(103)...H(107)	693.0(48)	39.0(fixed)	—	-9.0	39.0
<i>u5160</i>	H(308)...H(321)	693.3(47)	37.6(fixed)	—	-10.3	37.6
<i>u5190</i>	H(19)...H(27)	693.5(35)	31.5(fixed)	—	-11.4	31.5
<i>u3714</i>	H(268)...H(287)	693.8(36)	40.0(fixed)	—	-8.3	40.0
<i>u5193</i>	H(308)...H(317)	693.8(47)	30.4(fixed)	—	-7.7	30.4
<i>u5220</i>	H(25)...H(34)	694.2(65)	37.8(fixed)	—	-7.2	37.8
<i>u5347</i>	H(280)...H(286)	694.3(35)	26.1(fixed)	—	-7.7	26.1
<i>u430</i>	H(186)...H(190)	694.4(85)	43.8(fixed)	—	27.2	43.8
<i>u531</i>	H(264)...H(279)	694.5(34)	44.1(fixed)	—	13.3	44.1
<i>u5431</i>	H(144)...H(150)	694.9(37)	20.1(fixed)	—	-9.8	20.1
<i>u5351</i>	H(280)...H(287)	694.9(41)	30.0(fixed)	—	-7.8	30.0
<i>u5368</i>	H(144)...H(152)	695.3(37)	26.3(fixed)	—	-7.0	26.3
<i>u5257</i>	H(310)...H(317)	695.3(40)	23.2(fixed)	—	-7.9	23.2
<i>u3613</i>	H(189)...H(204)	695.5(36)	44.4(fixed)	—	4.0	44.4
<i>u3584</i>	H(150)...H(155)	695.7(38)	55.7(fixed)	—	-7.4	55.7

<i>u5413</i>	H(265)...H(270)	696.1(35)	25.4(fixed)	—	-6.7	25.4
<i>u2386</i>	H(64)...H(66)	696.3(40)	43.2(fixed)	—	0.3	43.2
<i>u5429</i>	H(235)...H(246)	696.5(71)	19.7(fixed)	—	-10.4	19.7
<i>u5243</i>	H(273)...H(283)	696.5(41)	23.1(fixed)	—	-6.6	23.1
<i>u5289</i>	H(305)...H(314)	696.7(58)	27.0(fixed)	—	-8.2	27.0
<i>u5248</i>	H(23)...H(41)	696.8(140)	23.8(fixed)	—	-6.4	23.8
<i>u3624</i>	H(101)...H(123)	697.5(85)	41.3(fixed)	—	-7.6	41.3
<i>u5169</i>	H(107)...H(123)	697.5(134)	35.0(fixed)	—	-5.8	35.0
<i>u4777</i>	H(60)...H(79)	697.9(93)	46.0(fixed)	—	-9.0	46.0
<i>u5143</i>	H(150)...H(161)	698.1(63)	41.1(fixed)	—	-5.7	41.1
<i>u2820</i>	C(252)...H(280)	698.2(35)	23.8(fixed)	—	-2.7	23.8
<i>u5249</i>	H(109)...H(119)	698.2(92)	27.3(fixed)	—	-11.8	27.3
<i>u2044</i>	H(141)...H(148)	698.2(42)	34.3(fixed)	—	5.4	34.3
<i>u5229</i>	H(232)...H(242)	698.5(69)	23.8(fixed)	—	-7.0	23.8
<i>u5206</i>	H(267)...H(270)	698.6(87)	22.3(fixed)	—	-7.1	22.3
<i>u5405</i>	H(235)...H(245)	698.7(105)	25.5(fixed)	—	-9.7	25.5
<i>u3659</i>	H(224)...H(246)	699.0(50)	38.0(fixed)	—	-5.6	38.0
<i>u1934</i>	H(230)...H(236)	699.3(68)	44.7(fixed)	—	15.2	44.7
<i>u5200</i>	H(68)...H(79)	699.5(91)	33.9(fixed)	—	-7.0	33.9
<i>u2488</i>	C(257)...H(265)	699.5(35)	33.6(fixed)	—	-1.7	33.6
<i>u5171</i>	H(66)...H(82)	699.6(53)	33.2(fixed)	—	-6.3	33.2
<i>u3626</i>	H(60)...H(82)	700.1(54)	45.4(fixed)	—	-8.7	45.4
<i>u5255</i>	H(147)...H(164)	701.1(47)	27.6(fixed)	—	-11.0	27.6
<i>u3575</i>	H(68)...H(73)	701.1(32)	48.4(fixed)	—	-5.9	48.4
<i>u5284</i>	H(150)...H(160)	701.2(44)	34.9(fixed)	—	-17.0	34.9
<i>u1894</i>	H(277)...H(284)	701.2(48)	49.8(fixed)	—	13.5	49.8
<i>u5241</i>	H(273)...H(284)	701.8(46)	28.5(fixed)	—	-6.2	28.5
<i>u2158</i>	H(105)...H(107)	702.1(39)	38.2(fixed)	—	4.9	38.2
<i>u2101</i>	H(223)...H(246)	702.3(47)	35.6(fixed)	—	4.0	35.6
<i>u5269</i>	H(232)...H(243)	702.7(45)	29.2(fixed)	—	-7.0	29.2
<i>u2288</i>	H(68)...H(72)	702.9(47)	49.5(fixed)	—	3.6	49.5
<i>u2005</i>	H(109)...H(117)	703.2(37)	43.3(fixed)	—	3.3	43.3
<i>u3852</i>	H(66)...H(71)	703.5(61)	36.4(fixed)	—	-9.8	36.4
<i>u3456</i>	H(109)...H(115)	703.7(35)	45.6(fixed)	—	-7.7	45.6
<i>u3758</i>	H(107)...H(116)	703.7(48)	38.4(fixed)	—	-8.3	38.4
<i>u4858</i>	H(224)...H(243)	704.5(143)	43.8(fixed)	—	-8.2	43.8
<i>u5377</i>	H(116)...H(122)	705.0(72)	25.4(fixed)	—	-6.5	25.4
<i>u5428</i>	H(71)...H(82)	705.1(55)	19.2(fixed)	—	-8.8	19.2
<i>u4025</i>	H(150)...H(153)	705.6(41)	43.5(fixed)	—	-9.1	43.5
<i>u5266</i>	H(310)...H(321)	705.6(56)	27.5(fixed)	—	-10.8	27.5
<i>u3872</i>	H(146)...H(157)	705.6(87)	52.0(fixed)	—	3.7	52.0
<i>u2523</i>	H(66)...H(73)	705.7(53)	48.0(fixed)	—	-3.7	48.0
<i>u5221</i>	H(224)...H(229)	705.8(53)	23.3(fixed)	—	-6.8	23.3
<i>u5188</i>	H(101)...H(111)	705.9(56)	27.9(fixed)	—	-10.9	27.9

<i>u5123</i>	H(267)...H(284)	706.1(49)	37.5(fixed)	—	-7.8	37.5
<i>u5296</i>	C(131)...H(161)	706.1(19)	19.2(fixed)	—	-14.5	19.2
<i>u5267</i>	H(24)...H(41)	706.3(49)	25.8(fixed)	—	-8.2	25.8
<i>u5162</i>	H(60)...H(70)	706.4(53)	28.2(fixed)	—	-10.6	28.2
<i>u5208</i>	H(60)...H(68)	706.5(45)	30.1(fixed)	—	-11.2	30.1
<i>u5238</i>	H(101)...H(109)	706.9(43)	30.9(fixed)	—	-11.0	30.9
<i>u4601</i>	H(183)...H(188)	706.9(48)	56.4(fixed)	—	-3.7	56.4
<i>u5424</i>	H(116)...H(123)	707.0(125)	20.5(fixed)	—	-9.2	20.5
<i>u2212</i>	H(150)...H(154)	707.2(43)	47.6(fixed)	—	7.3	47.6
<i>u5435</i>	H(153)...H(164)	707.4(49)	19.1(fixed)	—	-9.8	19.1
<i>u5379</i>	H(71)...H(81)	707.8(72)	25.0(fixed)	—	-6.4	25.0
<i>u4122</i>	H(68)...H(71)	708.5(46)	45.5(fixed)	—	-8.5	45.5
<i>u5369</i>	H(19)...H(31)	708.6(197)	27.5(fixed)	—	-5.6	27.5
<i>u3690</i>	H(109)...H(116)	708.8(38)	43.5(fixed)	—	-10.1	43.5
<i>u5376</i>	H(153)...H(163)	708.9(49)	25.8(fixed)	—	-7.0	25.8
<i>u4806</i>	C(136)...H(157)	709.3(22)	26.8(fixed)	—	-12.6	26.8
<i>u5014</i>	H(226)...H(232)	709.7(54)	44.2(fixed)	—	-6.9	44.2
<i>u5277</i>	H(68)...H(78)	710.2(41)	26.7(fixed)	—	-9.8	26.7
<i>u5272</i>	H(106)...H(123)	710.5(46)	26.4(fixed)	—	-7.7	26.4
<i>u4793</i>	C(218)...H(239)	710.9(27)	25.0(fixed)	—	-9.5	25.0
<i>u5280</i>	H(65)...H(82)	710.9(58)	25.8(fixed)	—	-8.8	25.8
<i>u4884</i>	C(214)...H(235)	711.1(21)	24.3(fixed)	—	-12.1	24.3
<i>u3895</i>	H(223)...H(243)	711.3(58)	43.2(fixed)	—	-0.7	43.2
<i>u1917</i>	H(100)...H(123)	711.5(40)	34.6(fixed)	—	17.2	34.6
<i>u4913</i>	C(259)...H(276)	711.6(22)	23.1(fixed)	—	-11.9	23.1
<i>u5335</i>	H(21)...H(29)	711.9(46)	26.0(fixed)	—	-12.5	26.0
<i>u4020</i>	H(148)...H(153)	711.9(56)	43.5(fixed)	—	-9.2	43.5
<i>u5286</i>	H(230)...H(243)	712.2(86)	36.1(fixed)	—	-8.1	36.1
<i>u2675</i>	H(148)...H(155)	712.3(63)	60.0(fixed)	—	-0.7	60.0
<i>u4790</i>	C(54)...H(75)	712.5(22)	21.6(fixed)	—	-8.2	21.6
<i>u2009</i>	H(59)...H(82)	712.6(37)	36.0(fixed)	—	14.1	36.0
<i>u4873</i>	H(101)...H(120)	713.0(41)	48.6(fixed)	—	-8.7	48.6
<i>u5302</i>	C(94)...H(107)	713.2(23)	15.9(fixed)	—	-6.4	15.9
<i>u4073</i>	H(267)...H(287)	713.3(36)	40.4(fixed)	—	-9.2	40.4
<i>u2666</i>	C(172)...H(185)	713.5(22)	41.6(fixed)	—	-4.3	41.6
<i>u5325</i>	C(293)...H(312)	713.6(21)	15.6(fixed)	—	-6.6	15.6
<i>u5332</i>	C(6)...H(30)	713.7(21)	15.6(fixed)	—	-6.9	15.6
<i>u5306</i>	C(90)...H(120)	713.9(19)	15.8(fixed)	—	-6.0	15.8
<i>u3686</i>	H(59)...H(79)	714.0(49)	44.8(fixed)	—	4.1	44.8
<i>u5320</i>	C(8)...H(38)	714.3(22)	15.4(fixed)	—	-6.1	15.4
<i>u5293</i>	C(336)...H(366)	714.4(22)	16.0(fixed)	—	-5.5	16.0
<i>u2297</i>	H(269)...H(287)	714.6(41)	41.3(fixed)	—	0.9	41.3
<i>u5305</i>	C(135)...H(148)	715.2(20)	15.8(fixed)	—	-5.8	15.8
<i>u5314</i>	C(295)...H(306)	715.3(21)	15.6(fixed)	—	-6.2	15.6

<i>u2594</i>	H(107)...H(115)	715.3(67)	51.5(fixed)	—	-2.9	51.5
<i>u4995</i>	C(213)...H(226)	715.5(22)	26.2(fixed)	—	-5.4	26.2
<i>u5303</i>	C(335)...H(355)	715.9(20)	16.2(fixed)	—	-6.5	16.2
<i>u5291</i>	H(271)...H(284)	716.0(50)	35.3(fixed)	—	-7.4	35.3
<i>u5309</i>	H(230)...H(242)	716.2(27)	28.4(fixed)	—	-9.7	28.4
<i>u5326</i>	C(49)...H(79)	716.6(21)	15.5(fixed)	—	-6.8	15.5
<i>u5313</i>	C(337)...H(349)	716.9(21)	15.6(fixed)	—	-5.9	15.6
<i>u5318</i>	C(53)...H(66)	717.1(21)	15.5(fixed)	—	-6.3	15.5
<i>u4732</i>	C(212)...H(230)	717.1(23)	31.9(fixed)	—	-4.0	31.9
<i>u5359</i>	H(149)...H(161)	717.3(30)	30.0(fixed)	—	-15.3	30.0
<i>u5322</i>	C(296)...H(317)	717.7(21)	15.4(fixed)	—	-5.3	15.4
<i>u3652</i>	H(266)...H(280)	717.8(38)	34.5(fixed)	—	-7.1	34.5
<i>u4907</i>	C(132)...H(142)	717.8(22)	23.5(fixed)	—	-5.2	23.5
<i>u5349</i>	H(21)...H(27)	718.0(85)	30.9(fixed)	—	-13.9	30.9
<i>u5033</i>	C(91)...H(103)	718.0(21)	22.4(fixed)	—	-6.6	22.4
<i>u4392</i>	C(215)...H(232)	718.1(24)	27.2(fixed)	—	-2.6	27.2
<i>u5078</i>	C(50)...H(62)	718.4(21)	23.1(fixed)	—	-5.7	23.1
<i>u4231</i>	C(52)...H(82)	718.7(19)	25.0(fixed)	—	-1.8	25.0
<i>u3825</i>	C(170)...H(194)	719.3(20)	36.8(fixed)	—	-3.3	36.8
<i>u5341</i>	H(271)...H(283)	719.3(46)	27.1(fixed)	—	-8.5	27.1
<i>u4296</i>	C(216)...H(246)	719.7(20)	24.8(fixed)	—	-1.7	24.8
<i>u4822</i>	C(48)...H(68)	719.9(19)	26.8(fixed)	—	-4.3	26.8
<i>u4153</i>	H(269)...H(284)	720.1(53)	41.1(fixed)	—	-0.3	41.1
<i>u4748</i>	C(89)...H(109)	720.6(20)	26.0(fixed)	—	-4.5	26.0
<i>u4323</i>	C(134)...H(164)	720.7(21)	26.5(fixed)	—	-1.4	26.5
<i>u4702</i>	C(129)...H(150)	720.7(20)	25.3(fixed)	—	-3.8	25.3
<i>u5392</i>	H(275)...H(280)	722.4(38)	23.9(fixed)	—	-5.3	23.9
<i>u4425</i>	C(256)...H(287)	722.7(20)	26.0(fixed)	—	-1.8	26.0
<i>u4008</i>	H(228)...H(232)	723.0(57)	51.6(fixed)	—	-0.1	51.6
<i>u5251</i>	H(276)...H(285)	723.8(33)	26.4(fixed)	—	-12.2	26.4
<i>u3665</i>	H(100)...H(120)	724.1(59)	44.8(fixed)	—	5.7	44.8
<i>u1737</i>	H(265)...H(281)	724.8(45)	45.7(fixed)	—	3.8	45.7
<i>u5363</i>	H(107)...H(118)	725.3(52)	27.0(fixed)	—	-5.8	27.0
<i>u5015</i>	H(226)...H(231)	725.8(49)	33.9(fixed)	—	-2.9	33.9
<i>u5152</i>	H(239)...H(244)	727.3(36)	30.2(fixed)	—	-9.7	30.2
<i>u5121</i>	H(63)...H(68)	728.8(42)	36.4(fixed)	—	-5.8	36.4
<i>u5228</i>	H(234)...H(235)	729.0(42)	27.9(fixed)	—	-13.1	27.9
<i>u5053</i>	H(104)...H(109)	729.4(40)	41.0(fixed)	—	-6.5	41.0
<i>u5419</i>	H(273)...H(280)	729.8(64)	20.5(fixed)	—	-7.9	20.5
<i>u5184</i>	H(157)...H(162)	729.8(44)	31.2(fixed)	—	-12.9	31.2
<i>u5382</i>	H(307)...H(312)	730.2(42)	27.1(fixed)	—	-5.9	27.1
<i>u5378</i>	H(25)...H(36)	730.2(29)	25.8(fixed)	—	-5.4	25.8
<i>u5159</i>	H(157)...H(163)	730.3(45)	28.8(fixed)	—	-14.6	28.8
<i>u4974</i>	H(142)...H(151)	730.5(35)	33.6(fixed)	—	-3.4	33.6



<i>u5364</i>	H(67)...H(79)	731.3(30)	26.0(fixed)	—	-6.0	26.0
<i>u5372</i>	H(66)...H(77)	732.4(55)	25.7(fixed)	—	-5.3	25.7
<i>u5367</i>	H(108)...H(120)	732.6(48)	25.2(fixed)	—	-5.2	25.2
<i>u4760</i>	H(183)...H(195)	732.6(30)	39.3(fixed)	—	-7.6	39.3
<i>u5358</i>	H(306)...H(313)	732.9(39)	26.7(fixed)	—	-4.2	26.7
<i>u5179</i>	H(75)...H(80)	733.5(44)	26.6(fixed)	—	-9.0	26.6
<i>u5023</i>	H(227)...H(230)	733.8(27)	37.6(fixed)	—	-5.2	37.6
<i>u5410</i>	H(147)...H(161)	734.7(36)	30.2(fixed)	—	-18.4	30.2
<i>u5227</i>	H(233)...H(235)	734.8(36)	28.7(fixed)	—	-12.3	28.7
<i>u5140</i>	H(75)...H(81)	735.3(37)	26.1(fixed)	—	-9.4	26.1
<i>u5219</i>	H(276)...H(286)	735.6(39)	27.7(fixed)	—	-12.7	27.7
<i>u5178</i>	H(239)...H(245)	736.4(30)	27.0(fixed)	—	-11.1	27.0
<i>u3507</i>	H(76)...H(82)	736.6(34)	37.9(fixed)	—	7.6	37.9
<i>u5373</i>	H(314)...H(318)	736.6(32)	26.5(fixed)	—	-4.8	26.5
<i>u5339</i>	H(103)...H(111)	736.7(41)	27.6(fixed)	—	-9.3	27.6
<i>u5079</i>	H(103)...H(110)	737.7(42)	31.3(fixed)	—	-3.7	31.3
<i>u3701</i>	H(232)...H(236)	737.7(42)	47.1(fixed)	—	9.3	47.1
<i>u5346</i>	H(62)...H(70)	737.9(43)	25.6(fixed)	—	-7.6	25.6
<i>u5366</i>	H(148)...H(159)	738.2(34)	30.7(fixed)	—	0.1	30.7
<i>u3285</i>	H(185)...H(188)	738.2(36)	58.9(fixed)	—	-10.0	58.9
<i>u5122</i>	H(62)...H(69)	738.4(46)	33.0(fixed)	—	-4.0	33.0
<i>u5077</i>	H(143)...H(150)	739.3(32)	35.5(fixed)	—	-5.9	35.5
<i>u2412</i>	H(265)...H(279)	740.8(43)	45.5(fixed)	—	-1.5	45.5
<i>u5299</i>	H(23)...H(38)	740.9(436)	29.3(fixed)	—	-10.9	29.3
<i>u5404</i>	H(314)...H(319)	741.0(36)	24.4(fixed)	—	-5.6	24.4
<i>u5288</i>	H(142)...H(152)	741.0(40)	26.0(fixed)	—	-7.7	26.0
<i>u5384</i>	H(305)...H(312)	741.0(42)	26.2(fixed)	—	-6.7	26.2
<i>u4386</i>	H(278)...H(287)	741.8(38)	59.4(fixed)	—	0.5	59.4
<i>u4503</i>	H(232)...H(237)	742.4(41)	62.7(fixed)	—	-2.4	62.7
<i>u1707</i>	H(185)...H(190)	743.2(34)	53.1(fixed)	—	11.5	53.1
<i>u5407</i>	H(106)...H(120)	743.4(51)	25.4(fixed)	—	-6.2	25.4
<i>u3538</i>	H(240)...H(246)	743.8(30)	39.8(fixed)	—	10.5	39.8
<i>u2024</i>	H(264)...H(280)	743.8(45)	32.2(fixed)	—	5.6	32.2
<i>u5395</i>	H(306)...H(311)	744.0(44)	28.1(fixed)	—	-7.1	28.1
<i>u4168</i>	H(141)...H(150)	744.1(39)	37.5(fixed)	—	1.2	37.5
<i>u5408</i>	H(65)...H(79)	744.2(32)	26.5(fixed)	—	-7.5	26.5
<i>u3593</i>	H(158)...H(164)	744.4(58)	45.7(fixed)	—	14.4	45.7
<i>u5390</i>	H(66)...H(78)	744.7(49)	27.8(fixed)	—	-6.6	27.8
<i>u5388</i>	H(24)...H(38)	745.0(32)	26.2(fixed)	—	-6.5	26.2
<i>u5414</i>	H(148)...H(160)	745.4(34)	33.3(fixed)	—	-3.5	33.3
<i>u4594</i>	H(238)...H(246)	746.4(36)	55.0(fixed)	—	-3.9	55.0
<i>u5406</i>	H(107)...H(119)	746.6(27)	25.9(fixed)	—	-7.2	25.9
<i>u4579</i>	H(156)...H(164)	746.7(52)	63.9(fixed)	—	-3.7	63.9
<i>u4274</i>	H(228)...H(230)	746.8(35)	49.1(fixed)	—	0.4	49.1

<i>u</i> 3196	H(183)...H(196)	747.3(36)	47.7(fixed)	—	2.7	47.7
<i>u</i> 5340	H(226)...H(229)	747.4(43)	26.6(fixed)	—	-8.0	26.6
<i>u</i> 4447	H(74)...H(82)	749.6(43)	53.7(fixed)	—	-2.7	53.7
<i>u</i> 3892	H(277)...H(287)	750.1(32)	50.3(fixed)	—	8.4	50.3
<i>u</i> 4523	H(64)...H(68)	752.2(49)	41.7(fixed)	—	0.1	41.7
<i>u</i> 4341	H(105)...H(109)	753.1(47)	40.5(fixed)	—	2.0	40.5
<i>u</i> 3532	H(265)...H(280)	764.9(55)	38.4(fixed)	—	-5.6	38.4
<i>u</i> 5080	H(18)...H(32)	772.9(1296)	41.3(fixed)	—	0.1	41.3
<i>u</i> 5401	H(18)...H(30)	777.9(471)	26.6(fixed)	—	-7.6	26.6
<i>u</i> 3352	H(185)...H(189)	784.8(39)	55.4(fixed)	—	-11.0	55.4
<i>u</i> 5418	H(148)...H(161)	786.4(34)	22.6(fixed)	—	-14.4	22.6
<i>u</i> 5420	H(107)...H(120)	789.8(35)	20.8(fixed)	—	-9.3	20.8
<i>u</i> 5156	H(157)...H(164)	790.3(36)	34.8(fixed)	—	-13.3	34.8
<i>u</i> 5432	H(25)...H(38)	790.8(39)	19.5(fixed)	—	-9.2	19.5
<i>u</i> 5204	H(232)...H(235)	791.1(37)	32.5(fixed)	—	-14.0	32.5
<i>u</i> 5132	H(239)...H(246)	791.4(36)	32.8(fixed)	—	-10.5	32.8
<i>u</i> 5433	H(19)...H(30)	791.5(38)	19.2(fixed)	—	-10.2	19.2
<i>u</i> 5434	H(306)...H(312)	791.8(37)	19.5(fixed)	—	-9.9	19.5
<i>u</i> 5127	H(75)...H(82)	792.0(35)	29.1(fixed)	—	-9.3	29.1
<i>u</i> 5345	H(226)...H(230)	794.2(37)	36.1(fixed)	—	-8.0	36.1
<i>u</i> 5242	H(276)...H(287)	794.9(37)	30.8(fixed)	—	-13.4	30.8
<i>u</i> 5430	H(66)...H(79)	795.7(36)	19.5(fixed)	—	-9.7	19.5
<i>u</i> 5426	H(314)...H(317)	797.5(38)	19.2(fixed)	—	-8.1	19.2
<i>u</i> 5360	H(62)...H(68)	799.6(34)	29.9(fixed)	—	-8.0	29.9
<i>u</i> 5350	H(103)...H(109)	799.9(35)	30.0(fixed)	—	-9.2	30.0
<i>u</i> 4526	H(183)...H(194)	800.1(36)	47.7(fixed)	—	-5.4	47.7
<i>u</i> 5292	H(142)...H(150)	800.8(37)	30.8(fixed)	—	-7.2	30.8

<sup>a</sup> Distances in pm. Values in parentheses are the standard deviations on the last digits. See Figure 1 for atom numbering.

**Table S10** Refined and calculated [B3LYP/6-31G(d)] amplitudes of vibration ( $u_{h1}$ ), associated  $r_a$  distances and corresponding correction values ( $k_{h1}$ ) for the refinement of C(SiFMe<sub>2</sub>)<sub>4</sub> (**2**).<sup>a</sup>

	Atom pair	$r_a$	$u_{GED}$	Restraint	$k_{h1}$	$u_{calc.}$
<i>u</i> 55	C(173)-H(192)	108.8(3)	9.9(tied to <i>u</i> 47)	—	0.4	10.6
<i>u</i> 66	C(88)-H(102)	108.8(3)	9.9(tied to <i>u</i> 47)	—	0.4	10.5
<i>u</i> 17	C(173)-H(193)	108.8(3)	9.7(tied to <i>u</i> 47)	—	0.4	10.3
<i>u</i> 9	C(88)-H(100)	108.8(3)	9.7(tied to <i>u</i> 47)	—	0.4	10.3
<i>u</i> 56	C(174)-H(195)	108.9(3)	9.5(tied to <i>u</i> 47)	—	0.4	10.1
<i>u</i> 15	C(170)-H(182)	108.9(3)	9.3(tied to <i>u</i> 47)	—	0.4	9.9
<i>u</i> 129	C(173)-H(191)	108.9(3)	9.1(tied to <i>u</i> 47)	—	0.4	9.7
<i>u</i> 128	C(88)-H(101)	109.0(3)	9.0(tied to <i>u</i> 47)	—	0.4	9.6
<i>u</i> 130	C(174)-H(194)	109.0(3)	8.6(tied to <i>u</i> 47)	—	0.4	9.2
<i>u</i> 127	C(9)-H(27)	109.0(3)	8.5(tied to <i>u</i> 47)	—	0.4	9.0

<i>u8</i>	C(9)-H(29)	109.0(3)	8.4(tied to <i>u47</i> )	—	0.4	8.9
<i>u72</i>	C(9)-H(28)	109.1(3)	8.3(tied to <i>u47</i> )	—	0.4	8.9
<i>u89</i>	C(254)-H(271)	109.1(3)	8.2(tied to <i>u47</i> )	—	0.4	8.8
<i>u85</i>	C(254)-H(270)	109.1(3)	8.1(tied to <i>u47</i> )	—	0.4	8.7
<i>u7</i>	C(254)-H(272)	109.1(3)	8.0(tied to <i>u47</i> )	—	0.4	8.5
<i>u22</i>	C(214)-H(234)	109.1(3)	7.9(tied to <i>u47</i> )	—	0.4	8.4
<i>u132</i>	C(214)-H(232)	109.1(3)	7.8(tied to <i>u47</i> )	—	0.4	8.4
<i>u50</i>	C(89)-H(105)	109.1(3)	7.8(tied to <i>u47</i> )	—	0.4	8.3
<i>u5</i>	C(89)-H(104)	109.1(3)	7.8(tied to <i>u47</i> )	—	0.4	8.3
<i>u49</i>	C(8)-H(24)	109.1(3)	7.8(tied to <i>u47</i> )	—	0.4	8.3
<i>u68</i>	C(214)-H(233)	109.1(3)	7.8(tied to <i>u47</i> )	—	0.4	8.3
<i>u10</i>	C(8)-H(26)	109.1(3)	7.7(tied to <i>u47</i> )	—	0.4	8.2
<i>u126</i>	C(8)-H(25)	109.2(3)	7.7(tied to <i>u47</i> )	—	0.4	8.2
<i>u122</i>	C(89)-H(103)	109.2(3)	7.5(tied to <i>u47</i> )	—	0.4	8.0
<i>u54</i>	C(50)-H(69)	109.2(3)	7.4(tied to <i>u47</i> )	—	0.4	7.9
<i>u4</i>	C(50)-H(70)	109.2(3)	7.4(tied to <i>u47</i> )	—	0.4	7.8
<i>u6</i>	C(132)-H(152)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.8
<i>u1</i>	C(258)-H(282)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u21</i>	C(51)-H(73)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u45</i>	C(132)-H(151)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.8
<i>u62</i>	C(258)-H(283)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.8
<i>u14</i>	C(53)-H(77)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u125</i>	C(258)-H(284)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.8
<i>u52</i>	C(130)-H(146)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.8
<i>u119</i>	C(50)-H(68)	109.2(3)	7.4(tied to <i>u47</i> )	—	0.4	7.8
<i>u41</i>	C(51)-H(72)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.8
<i>u53</i>	C(211)-H(225)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.8
<i>u120</i>	C(51)-H(71)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.7
<i>u124</i>	C(133)-H(153)	109.2(3)	7.3(tied to <i>u47</i> )	—	0.4	7.7
<i>u51</i>	C(53)-H(78)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u42</i>	C(130)-H(145)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u112</i>	C(211)-H(224)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u121</i>	C(53)-H(79)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u19</i>	C(211)-H(223)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u71</i>	C(253)-H(269)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u114</i>	C(213)-H(230)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u96</i>	C(253)-H(267)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u67</i>	C(213)-H(229)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u76</i>	C(212)-H(228)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u105</i>	C(257)-H(280)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u94</i>	C(216)-H(239)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u88</i>	C(175)-H(197)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u109</i>	C(49)-H(66)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u97</i>	C(6)-H(19)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7

<i>u100</i>	C(52)-H(75)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u92</i>	C(92)-H(112)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u93</i>	C(129)-H(142)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u118</i>	C(47)-H(60)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u98</i>	C(10)-H(30)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u106</i>	C(259)-H(287)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u99</i>	C(11)-H(34)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u90</i>	C(13)-H(41)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u117</i>	C(256)-H(276)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u107</i>	C(7)-H(21)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u95</i>	C(218)-H(246)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u101</i>	C(54)-H(82)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u110</i>	C(93)-H(116)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u104</i>	C(215)-H(235)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u86</i>	C(48)-H(64)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u103</i>	C(175)-H(198)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u84</i>	C(49)-H(65)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u91</i>	C(48)-H(62)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u83</i>	C(54)-H(80)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u82</i>	C(259)-H(285)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u87</i>	C(171)-H(187)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u102</i>	C(171)-H(185)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u79</i>	C(93)-H(115)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u64</i>	C(47)-H(61)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u77</i>	C(215)-H(236)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u78</i>	C(216)-H(238)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u80</i>	C(255)-H(274)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u81</i>	C(129)-H(143)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u69</i>	C(252)-H(266)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u111</i>	C(130)-H(144)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.7
<i>u65</i>	C(52)-H(74)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u46</i>	C(252)-H(264)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u75</i>	C(12)-H(37)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u47</i>	C(6)-H(20)	109.2(3)	7.2(3)	—	0.4	7.6
<i>u73</i>	C(10)-H(31)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u70</i>	C(217)-H(242)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u58</i>	C(11)-H(33)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u74</i>	C(13)-H(39)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u61</i>	C(256)-H(277)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u63</i>	C(218)-H(244)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u60</i>	C(131)-H(147)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u36</i>	C(47)-H(59)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u44</i>	C(92)-H(114)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6
<i>u57</i>	C(257)-H(279)	109.2(3)	7.2(tied to <i>u47</i> )	—	0.4	7.6

<i>u</i> 24	C(212)-H(227)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 39	C(259)-H(286)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 38	C(218)-H(245)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 59	C(92)-H(113)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 48	C(7)-H(23)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 3	C(253)-H(268)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 23	C(6)-H(18)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 33	C(13)-H(40)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 40	C(11)-H(35)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 43	C(255)-H(275)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 32	C(257)-H(281)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 34	C(129)-H(141)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 2	C(213)-H(231)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 28	C(131)-H(149)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 25	C(7)-H(22)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 31	C(54)-H(81)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 26	C(10)-H(32)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 35	C(216)-H(240)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 37	C(215)-H(237)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 27	C(49)-H(67)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 29	C(217)-H(241)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 30	C(256)-H(278)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 16	C(171)-H(186)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 13	C(52)-H(76)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 12	C(12)-H(36)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 18	C(176)-H(200)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 113	C(212)-H(226)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.7
<i>u</i> 20	C(48)-H(63)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 11	C(93)-H(117)	109.2(3)	7.1(tied to <i>u</i> 47)	—	0.4	7.6
<i>u</i> 131	C(255)-H(273)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.7
<i>u</i> 116	C(252)-H(265)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.7
<i>u</i> 115	C(217)-H(243)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.7
<i>u</i> 108	C(12)-H(38)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.7
<i>u</i> 123	C(131)-H(148)	109.2(3)	7.2(tied to <i>u</i> 47)	—	0.4	7.7
<i>u</i> 2771	H(141)...H(152)	156.2(156)	68.4(fixed)	—	6.4	68.4
<i>u</i> 1724	H(266)...H(273)	159.3(140)	37.7(fixed)	—	10.1	37.7
<i>u</i> 150	Si(2)-F(14)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 149	Si(85)-F(98)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 144	Si(84)-F(96)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 145	Si(208)-F(221)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 143	Si(126)-F(139)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 138	Si(3)-F(16)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 140	Si(251)-F(263)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 153	Si(248)-F(260)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5

<i>u</i> 152	Si(210)-F(222)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 151	Si(4)-F(15)	160.6(1)	4.7(2)	—	0.1	4.5
<i>u</i> 148	Si(45)-F(56)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 141	Si(166)-F(178)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 137	Si(46)-F(58)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 142	Si(168)-F(179)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 135	Si(250)-F(261)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 139	Si(207)-F(219)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 136	Si(44)-F(57)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.1	4.5
<i>u</i> 134	Si(249)-F(262)	160.6(1)	4.6(tied to <i>u</i> 151)	—	0.1	4.4
<i>u</i> 133	Si(209)-F(220)	160.6(1)	4.6(tied to <i>u</i> 151)	—	0.1	4.4
<i>u</i> 154	Si(5)-F(17)	160.6(1)	4.8(tied to <i>u</i> 151)	—	0.2	4.6
<i>u</i> 146	Si(125)-F(137)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.2	4.5
<i>u</i> 147	Si(43)-F(55)	160.6(1)	4.7(tied to <i>u</i> 151)	—	0.2	4.5
<i>u</i> 228	H(100)...H(101)	172.4(7)	15.2(fixed)	—	-4.5	15.2
<i>u</i> 194	H(101)...H(102)	172.8(7)	15.4(fixed)	—	-4.0	15.4
<i>u</i> 234	H(270)...H(272)	173.5(7)	13.7(fixed)	—	-3.7	13.7
<i>u</i> 231	H(191)...H(193)	173.6(7)	14.6(fixed)	—	-3.4	14.6
<i>u</i> 230	H(182)...H(183)	173.6(7)	14.4(fixed)	—	-3.4	14.4
<i>u</i> 160	H(100)...H(102)	174.0(7)	16.1(fixed)	—	-2.7	16.1
<i>u</i> 213	H(191)...H(192)	174.0(7)	15.1(fixed)	—	-2.9	15.1
<i>u</i> 214	H(194)...H(195)	174.1(7)	14.7(fixed)	—	-2.9	14.7
<i>u</i> 181	H(27)...H(28)	174.2(7)	14.0(fixed)	—	-2.9	14.0
<i>u</i> 166	H(28)...H(29)	174.2(7)	13.8(fixed)	—	-2.9	13.8
<i>u</i> 169	H(270)...H(271)	174.3(7)	13.7(fixed)	—	-2.9	13.7
<i>u</i> 239	H(271)...H(272)	174.3(7)	13.7(fixed)	—	-2.8	13.7
<i>u</i> 248	H(27)...H(29)	174.7(7)	14.0(fixed)	—	-2.4	14.0
<i>u</i> 156	H(192)...H(193)	174.9(7)	15.9(fixed)	—	-1.9	15.9
<i>u</i> 157	H(195)...H(196)	174.9(7)	15.5(fixed)	—	-1.9	15.5
<i>u</i> 204	H(25)...H(26)	176.3(7)	13.0(fixed)	—	-0.9	13.0
<i>u</i> 219	H(103)...H(105)	176.4(7)	13.1(fixed)	—	-0.8	13.1
<i>u</i> 220	H(24)...H(25)	176.5(7)	13.2(fixed)	—	-0.8	13.2
<i>u</i> 176	H(232)...H(233)	176.5(7)	13.3(fixed)	—	-0.7	13.3
<i>u</i> 172	H(24)...H(26)	176.5(7)	13.2(fixed)	—	-0.7	13.2
<i>u</i> 171	H(233)...H(234)	176.5(7)	13.2(fixed)	—	-0.7	13.2
<i>u</i> 237	H(103)...H(104)	176.5(7)	13.1(fixed)	—	-0.7	13.1
<i>u</i> 245	H(232)...H(234)	176.6(7)	13.3(fixed)	—	-0.6	13.3
<i>u</i> 158	H(104)...H(105)	176.7(7)	13.4(fixed)	—	-0.5	13.4
<i>u</i> 233	H(150)...H(152)	176.8(7)	12.6(fixed)	—	-0.5	12.6
<i>u</i> 211	H(283)...H(284)	176.9(7)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 222	H(68)...H(70)	176.9(7)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 250	H(282)...H(284)	176.9(7)	12.6(fixed)	—	-0.4	12.6
<i>u</i> 190	H(78)...H(79)	176.9(7)	12.6(fixed)	—	-0.4	12.6
<i>u</i> 253	H(77)...H(79)	176.9(7)	12.5(fixed)	—	-0.4	12.5

<i>u</i> 224	H(68)...H(69)	176.9(7)	12.8(fixed)	—	-0.4	12.8
<i>u</i> 162	H(282)...H(283)	176.9(7)	12.7(fixed)	—	-0.4	12.7
<i>u</i> 225	H(71)...H(73)	176.9(7)	12.6(fixed)	—	-0.4	12.6
<i>u</i> 155	H(69)...H(70)	176.9(7)	12.8(fixed)	—	-0.4	12.8
<i>u</i> 168	H(77)...H(78)	176.9(7)	12.6(fixed)	—	-0.4	12.6
<i>u</i> 180	H(151)...H(152)	176.9(7)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 265	H(150)...H(151)	177.0(7)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 182	H(72)...H(73)	177.0(7)	12.7(fixed)	—	-0.3	12.7
<i>u</i> 262	H(71)...H(72)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 184	H(144)...H(145)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 238	H(267)...H(269)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 207	H(268)...H(269)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 226	H(223)...H(224)	177.0(7)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 159	H(223)...H(225)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 240	H(224)...H(225)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 164	H(144)...H(146)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 280	H(267)...H(268)	177.0(7)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 243	H(145)...H(146)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 186	H(229)...H(231)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 244	H(229)...H(230)	177.0(7)	12.6(fixed)	—	-0.3	12.6
<i>u</i> 281	H(230)...H(231)	177.1(7)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 227	H(18)...H(19)	177.1(7)	12.5(fixed)	—	-0.3	12.5
<i>u</i> 198	H(226)...H(227)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 174	H(286)...H(287)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 170	H(226)...H(228)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 242	H(227)...H(228)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 201	H(18)...H(20)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 188	H(60)...H(61)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 179	H(197)...H(198)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 193	H(285)...H(287)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 178	H(185)...H(187)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 161	H(264)...H(265)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 167	H(59)...H(60)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 252	H(285)...H(286)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 217	H(59)...H(61)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 200	H(21)...H(22)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 261	H(19)...H(20)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 218	H(21)...H(23)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 187	H(265)...H(266)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 241	H(264)...H(266)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 185	H(238)...H(239)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 173	H(112)...H(114)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 177	H(40)...H(41)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 271	H(22)...H(23)	177.1(7)	12.4(fixed)	—	-0.2	12.4

<i>u</i> 163	H(65)...H(66)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 183	H(62)...H(64)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 199	H(273)...H(274)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 192	H(147)...H(148)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 235	H(30)...H(31)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 175	H(245)...H(246)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 203	H(66)...H(67)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 256	H(65)...H(67)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 189	H(148)...H(149)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 195	H(115)...H(116)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 197	H(80)...H(82)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 212	H(142)...H(143)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 247	H(39)...H(41)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 210	H(74)...H(75)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 209	H(235)...H(236)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 221	H(33)...H(34)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 236	H(276)...H(277)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 254	H(112)...H(113)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 267	H(63)...H(64)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 269	H(238)...H(240)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 257	H(39)...H(40)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 249	H(244)...H(246)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 165	H(273)...H(275)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 260	H(113)...H(114)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 251	H(239)...H(240)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 266	H(244)...H(245)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 229	H(141)...H(142)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 202	H(276)...H(278)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 215	H(235)...H(237)	177.1(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 255	H(274)...H(275)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 196	H(241)...H(243)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 191	H(34)...H(35)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 205	H(36)...H(38)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 284	H(115)...H(117)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 273	H(197)...H(199)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 272	H(186)...H(187)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 208	H(242)...H(243)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 206	H(37)...H(38)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 216	H(279)...H(280)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 232	H(81)...H(82)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 246	H(280)...H(281)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 223	H(30)...H(32)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 259	H(75)...H(76)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 268	H(62)...H(63)	177.2(7)	12.4(fixed)	—	-0.2	12.4



<i>u</i> 277	H(80)...H(81)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 279	H(236)...H(237)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 270	H(36)...H(37)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 275	H(241)...H(242)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 285	H(31)...H(32)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 283	H(277)...H(278)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 274	H(33)...H(35)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 276	H(147)...H(149)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 278	H(141)...H(143)	177.2(7)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 258	H(116)...H(117)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 282	H(74)...H(76)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 286	H(279)...H(281)	177.2(7)	12.4(fixed)	—	-0.2	12.4
<i>u</i> 1357	H(271)...H(277)	177.2(135)	138.3(fixed)	—	-8.9	138.3
<i>u</i> 264	H(198)...H(199)	177.2(7)	12.5(fixed)	—	-0.1	12.5
<i>u</i> 263	H(185)...H(186)	177.2(7)	12.5(fixed)	—	-0.1	12.5
<i>u</i> 319	Si(85)-C(91)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 329	Si(251)-C(252)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 315	Si(166)-C(177)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 316	Si(168)-C(174)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 320	Si(3)-C(8)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 327	Si(125)-C(135)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 326	Si(46)-C(47)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 322	Si(210)-C(212)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 323	Si(249)-C(255)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 321	Si(248)-C(259)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 324	Si(44)-C(49)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 330	Si(249)-C(254)	186.5(2)	6.2(tied to <i>u</i> 325)	—	0.2	5.7
<i>u</i> 317	Si(43)-C(53)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 314	Si(84)-C(95)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 312	Si(209)-C(216)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 318	Si(126)-C(131)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 313	Si(4)-C(11)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 310	Si(44)-C(50)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 309	Si(85)-C(90)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 306	Si(207)-C(218)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 311	Si(207)-C(217)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 304	Si(248)-C(258)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 307	Si(5)-C(7)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 308	Si(2)-C(13)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 296	Si(126)-C(132)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 298	Si(45)-C(51)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 297	Si(46)-C(48)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 305	Si(2)-C(12)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 301	Si(43)-C(54)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6

<i>u</i> 302	Si(210)-C(211)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 300	Si(168)-C(175)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 303	Si(209)-C(215)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 299	Si(166)-C(176)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 294	Si(250)-C(256)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 291	Si(5)-C(6)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 293	Si(125)-C(136)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 295	Si(250)-C(257)	186.5(2)	6.1(tied to <i>u</i> 325)	—	0.2	5.6
<i>u</i> 290	Si(208)-C(213)	186.5(2)	6.0(tied to <i>u</i> 325)	—	0.2	5.5
<i>u</i> 288	Si(84)-C(94)	186.5(2)	6.0(tied to <i>u</i> 325)	—	0.2	5.5
<i>u</i> 292	Si(45)-C(52)	186.5(2)	6.0(tied to <i>u</i> 325)	—	0.2	5.5
<i>u</i> 289	Si(4)-C(10)	186.5(2)	6.0(tied to <i>u</i> 325)	—	0.2	5.5
<i>u</i> 287	Si(251)-C(253)	186.5(2)	6.0(tied to <i>u</i> 325)	—	0.2	5.5
<i>u</i> 328	Si(208)-C(214)	186.5(2)	6.2(tied to <i>u</i> 325)	—	0.2	5.7
<i>u</i> 325	Si(3)-C(9)	186.5(2)	6.2(2)	—	0.2	5.7
<i>u</i> 346	C(1)-Si(4)	189.2(2)	6.6(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 339	C(247)-Si(251)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 337	C(42)-Si(44)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	5.9
<i>u</i> 335	C(42)-Si(46)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	5.9
<i>u</i> 336	C(247)-Si(249)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	5.9
<i>u</i> 334	C(124)-Si(125)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	5.9
<i>u</i> 333	C(1)-Si(2)	189.3(2)	6.4(tied to <i>u</i> 325)	—	0.2	5.9
<i>u</i> 332	C(206)-Si(210)	189.3(2)	6.4(tied to <i>u</i> 325)	—	0.2	5.9
<i>u</i> 349	C(206)-Si(208)	189.3(2)	6.6(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 352	C(247)-Si(250)	189.3(2)	6.7(tied to <i>u</i> 325)	—	0.2	6.2
<i>u</i> 331	C(247)-Si(248)	189.3(2)	6.4(tied to <i>u</i> 325)	—	0.2	5.9
<i>u</i> 348	C(206)-Si(209)	189.3(2)	6.6(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 347	C(83)-Si(84)	189.3(2)	6.6(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 345	C(1)-Si(5)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 343	C(165)-Si(168)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 344	C(42)-Si(43)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 342	C(165)-Si(166)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 341	C(206)-Si(207)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 340	C(1)-Si(3)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	6.0
<i>u</i> 338	C(83)-Si(85)	189.3(2)	6.5(tied to <i>u</i> 325)	—	0.2	5.9
<i>u</i> 350	C(124)-Si(126)	189.3(2)	6.6(tied to <i>u</i> 325)	—	0.2	6.1
<i>u</i> 351	C(42)-Si(45)	189.3(2)	6.7(tied to <i>u</i> 325)	—	0.2	6.1
<i>u</i> 784	H(272)...H(286)	197.6(102)	122.9(fixed)	—	2.4	122.9
<i>u</i> 580	H(28)...H(39)	212.5(192)	93.5(fixed)	—	26.3	93.5
<i>u</i> 576	H(233)...H(244)	213.9(166)	76.6(fixed)	—	20.0	76.6
<i>u</i> 362	H(228)...H(238)	214.6(116)	41.5(fixed)	—	25.0	41.5
<i>u</i> 2558	H(145)...H(159)	217.8(417)	74.9(fixed)	—	-13.5	74.9
<i>u</i> 2128	F(260)...H(271)	220.4(78)	62.5(fixed)	—	-23.3	62.5
<i>u</i> 372	H(18)...H(29)	221.8(146)	66.6(fixed)	—	49.9	66.6

<i>u578</i>	H(227)...H(236)	222.1(303)	62.2(fixed)	—	12.5	62.2
<i>u373</i>	H(223)...H(234)	222.7(148)	56.8(fixed)	—	40.9	56.8
<i>u2548</i>	H(272)...H(275)	226.8(48)	26.9(fixed)	—	-16.9	26.9
<i>u4206</i>	H(145)...H(155)	227.7(181)	40.5(fixed)	—	10.8	40.5
<i>u543</i>	H(237)...H(241)	230.6(154)	47.0(fixed)	—	10.0	47.0
<i>u374</i>	H(233)...H(245)	230.8(160)	54.4(fixed)	—	39.1	54.4
<i>u547</i>	H(22)...H(35)	235.3(393)	52.3(fixed)	—	12.1	52.3
<i>u357</i>	H(70)...H(73)	235.7(232)	48.9(fixed)	—	44.5	48.9
<i>u1995</i>	H(270)...H(278)	236.7(95)	45.9(fixed)	—	-22.3	45.9
<i>u1271</i>	F(99)...H(110)	237.1(103)	145.4(fixed)	—	-1.0	145.4
<i>u1269</i>	F(98)...H(102)	237.3(102)	145.3(fixed)	—	-0.9	145.3
<i>u1487</i>	H(146)...H(159)	239.1(385)	64.8(fixed)	—	7.4	64.8
<i>u574</i>	H(228)...H(236)	239.2(290)	59.9(fixed)	—	12.2	59.9
<i>u2416</i>	C(252)...H(273)	239.7(120)	26.3(fixed)	—	-3.8	26.3
<i>u388</i>	F(58)...H(76)	239.9(166)	26.5(tied to <i>u454</i> )	—	10.8	30.1
<i>u366</i>	H(35)...H(36)	240.1(382)	40.2(fixed)	—	14.6	40.2
<i>u385</i>	H(61)...H(65)	240.3(341)	47.2(fixed)	—	22.1	47.2
<i>u384</i>	F(56)...H(63)	240.4(166)	29.8(fixed)	—	12.0	29.8
<i>u354</i>	H(59)...H(78)	240.6(213)	55.5(fixed)	—	48.4	55.5
<i>u380</i>	H(67)...H(80)	241.6(133)	43.4(fixed)	—	17.6	43.4
<i>u365</i>	F(261)...H(268)	241.7(142)	33.5(fixed)	—	21.5	33.5
<i>u557</i>	H(67)...H(81)	241.8(207)	50.5(fixed)	—	10.9	50.5
<i>u514</i>	H(74)...H(77)	242.0(377)	56.1(fixed)	—	25.6	56.1
<i>u361</i>	H(24)...H(40)	242.5(157)	57.1(fixed)	—	45.5	57.1
<i>u568</i>	H(23)...H(35)	243.2(415)	54.1(fixed)	—	9.3	54.1
<i>u481</i>	H(236)...H(241)	243.4(121)	45.8(fixed)	—	13.4	45.8
<i>u375</i>	H(229)...H(245)	244.0(119)	47.2(fixed)	—	27.4	47.2
<i>u364</i>	H(26)...H(31)	244.6(125)	55.1(fixed)	—	43.3	55.1
<i>u4297</i>	H(147)...H(158)	245.0(368)	35.0(fixed)	—	1.3	35.0
<i>u498</i>	Si(250)...H(278)	245.0(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.8
<i>u405</i>	Si(125)...H(164)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u390</i>	Si(4)...H(30)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u416</i>	Si(249)...H(273)	245.0(5)	11.4(tied to <i>u454</i> )	—	-0.4	13.0
<i>u404</i>	Si(43)...H(82)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u418</i>	Si(166)...H(202)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u419</i>	Si(168)...H(198)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u455</i>	Si(2)...H(37)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u476</i>	Si(209)...H(237)	245.0(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.8
<i>u391</i>	Si(250)...H(276)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u410</i>	Si(209)...H(235)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u463</i>	Si(126)...H(147)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u453</i>	Si(207)...H(244)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u472</i>	Si(125)...H(163)	245.0(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.7
<i>u451</i>	Si(209)...H(240)	245.0(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.7

<i>u395</i>	Si(207)...H(243)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u446</i>	Si(2)...H(39)	245.0(5)	11.4(tied to <i>u454</i> )	—	-0.4	12.9
<i>u394</i>	Si(2)...H(38)	245.0(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u413</i>	Si(44)...H(66)	245.0(5)	11.4(tied to <i>u454</i> )	—	-0.4	12.9
<i>u467</i>	Si(207)...H(242)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u490</i>	Si(125)...H(162)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.8
<i>u493</i>	Si(43)...H(80)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.8
<i>u396</i>	Si(126)...H(148)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.4	12.9
<i>u464</i>	Si(4)...H(31)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u449</i>	Si(84)...H(121)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u497</i>	Si(44)...H(65)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u438</i>	Si(84)...H(123)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u431</i>	Si(46)...H(62)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u480</i>	Si(43)...H(81)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.7
<i>u400</i>	Si(4)...H(34)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u479</i>	Si(4)...H(33)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u421</i>	Si(207)...H(246)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u430</i>	Si(251)...H(265)	245.1(5)	11.5(tied to <i>u454</i> )	—	-0.3	13.0
<i>u482</i>	Si(4)...H(32)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.4	12.6
<i>u495</i>	Si(46)...H(64)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.7
<i>u461</i>	Si(250)...H(277)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.9
<i>u468</i>	Si(84)...H(119)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.7
<i>u462</i>	Si(250)...H(281)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.4	12.6
<i>u403</i>	Si(45)...H(75)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u499</i>	Si(249)...H(274)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.4	12.8
<i>u429</i>	Si(46)...H(60)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	13.0
<i>u526</i>	Si(84)...H(122)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.8
<i>u465</i>	Si(45)...H(74)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.7
<i>u427</i>	Si(209)...H(239)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.9
<i>u511</i>	Si(4)...H(35)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.4	12.6
<i>u484</i>	Si(46)...H(61)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	13.0
<i>u502</i>	Si(209)...H(236)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.7
<i>u428</i>	Si(2)...H(41)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.8
<i>u491</i>	Si(166)...H(201)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.8
<i>u492</i>	Si(168)...H(197)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.8
<i>u485</i>	Si(250)...H(279)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.4	12.7
<i>u393</i>	Si(84)...H(120)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.8
<i>u392</i>	Si(250)...H(280)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.8
<i>u519</i>	Si(249)...H(275)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.4	12.7
<i>u471</i>	Si(168)...H(199)	245.1(5)	11.0(tied to <i>u454</i> )	—	-0.4	12.5
<i>u470</i>	Si(166)...H(200)	245.1(5)	11.0(tied to <i>u454</i> )	—	-0.4	12.5
<i>u478</i>	Si(84)...H(118)	245.1(5)	11.0(tied to <i>u454</i> )	—	-0.4	12.5
<i>u521</i>	Si(248)...H(286)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.9
<i>u533</i>	Si(251)...H(264)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.9

<i>u399</i>	Si(5)...H(21)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.9
<i>u452</i>	Si(5)...H(23)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.9
<i>u500</i>	Si(251)...H(266)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	12.9
<i>u516</i>	Si(207)...H(241)	245.1(5)	11.0(tied to <i>u454</i> )	—	-0.4	12.5
<i>u459</i>	Si(46)...H(63)	245.1(5)	11.0(tied to <i>u454</i> )	—	-0.4	12.5
<i>u477</i>	Si(45)...H(76)	245.1(5)	11.0(tied to <i>u454</i> )	—	-0.4	12.5
<i>u522</i>	Si(2)...H(36)	245.1(5)	11.0(tied to <i>u454</i> )	—	-0.4	12.5
<i>u518</i>	Si(207)...H(245)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.3	12.6
<i>u414</i>	Si(125)...H(161)	245.1(5)	11.5(tied to <i>u454</i> )	—	-0.3	13.1
<i>u528</i>	Si(2)...H(40)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.3	12.6
<i>u435</i>	Si(248)...H(287)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	13.0
<i>u527</i>	Si(126)...H(149)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.3	12.6
<i>u402</i>	Si(85)...H(107)	245.1(5)	11.7(tied to <i>u454</i> )	—	-0.3	13.3
<i>u415</i>	Si(210)...H(226)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	13.0
<i>u524</i>	Si(44)...H(67)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.3	12.6
<i>u515</i>	Si(5)...H(18)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.8
<i>u486</i>	Si(248)...H(285)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	12.9
<i>u512</i>	Si(210)...H(227)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.3	12.8
<i>u536</i>	Si(46)...H(59)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.9
<i>u520</i>	Si(209)...H(238)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.3	12.7
<i>u437</i>	Si(5)...H(19)	245.1(5)	11.3(tied to <i>u454</i> )	—	-0.3	12.8
<i>u436</i>	Si(208)...H(230)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	13.0
<i>u503</i>	Si(210)...H(228)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	13.0
<i>u523</i>	Si(5)...H(22)	245.1(5)	11.1(tied to <i>u454</i> )	—	-0.3	12.6
<i>u443</i>	Si(5)...H(20)	245.1(5)	11.5(tied to <i>u454</i> )	—	-0.3	13.0
<i>u448</i>	Si(208)...H(231)	245.1(5)	11.2(tied to <i>u454</i> )	—	-0.3	12.7
<i>u420</i>	Si(210)...H(224)	245.1(5)	11.4(tied to <i>u454</i> )	—	-0.3	13.0
<i>u513</i>	Si(210)...H(223)	245.2(5)	11.5(tied to <i>u454</i> )	—	-0.2	13.1
<i>u407</i>	Si(44)...H(68)	245.2(5)	11.5(tied to <i>u454</i> )	—	-0.2	13.1
<i>u509</i>	Si(125)...H(159)	245.2(5)	11.5(tied to <i>u454</i> )	—	-0.2	13.1
<i>u445</i>	Si(251)...H(268)	245.2(5)	11.3(tied to <i>u454</i> )	—	-0.2	12.8
<i>u517</i>	Si(125)...H(160)	245.2(5)	11.6(tied to <i>u454</i> )	—	-0.2	13.2
<i>u423</i>	Si(45)...H(71)	245.2(5)	11.4(tied to <i>u454</i> )	—	-0.2	13.0
<i>u466</i>	Si(210)...H(225)	245.2(5)	11.5(tied to <i>u454</i> )	—	-0.2	13.1
<i>u432</i>	Si(251)...H(267)	245.2(5)	11.4(tied to <i>u454</i> )	—	-0.2	12.9
<i>u425</i>	Si(126)...H(150)	245.2(5)	11.4(tied to <i>u454</i> )	—	-0.2	13.0
<i>u488</i>	Si(208)...H(229)	245.2(5)	11.2(tied to <i>u454</i> )	—	-0.2	12.7
<i>u398</i>	Si(43)...H(79)	245.2(5)	11.5(tied to <i>u454</i> )	—	-0.2	13.1
<i>u401</i>	Si(248)...H(284)	245.2(5)	11.5(tied to <i>u454</i> )	—	-0.2	13.1
<i>u487</i>	Si(251)...H(269)	245.3(5)	11.3(tied to <i>u454</i> )	—	-0.1	12.8
<i>u525</i>	Si(44)...H(70)	245.3(5)	11.6(tied to <i>u454</i> )	—	-0.1	13.2
<i>u444</i>	Si(45)...H(72)	245.3(5)	11.6(tied to <i>u454</i> )	—	-0.1	13.2
<i>u475</i>	Si(44)...H(69)	245.3(5)	11.8(tied to <i>u454</i> )	—	-0.1	13.4
<i>u504</i>	Si(43)...H(77)	245.3(5)	11.4(tied to <i>u454</i> )	—	-0.1	13.0

<i>u</i> 506	Si(43)...H(78)	245.3(5)	11.6(tied to <i>u</i> 454)	—	-0.1	13.1
<i>u</i> 483	Si(248)...H(283)	245.3(5)	11.7(tied to <i>u</i> 454)	—	0.0	13.3
<i>u</i> 532	Si(45)...H(73)	245.3(5)	11.3(tied to <i>u</i> 454)	—	-0.1	12.8
<i>u</i> 442	Si(126)...H(151)	245.4(5)	11.7(tied to <i>u</i> 454)	—	0.0	13.3
<i>u</i> 507	Si(248)...H(282)	245.4(5)	11.5(tied to <i>u</i> 454)	—	0.0	13.0
<i>u</i> 529	Si(126)...H(152)	245.4(5)	11.4(tied to <i>u</i> 454)	—	0.0	12.9
<i>u</i> 460	Si(208)...H(233)	245.6(5)	12.0(tied to <i>u</i> 454)	—	0.2	13.6
<i>u</i> 424	Si(208)...H(232)	245.6(5)	12.4(tied to <i>u</i> 454)	—	0.3	14.1
<i>u</i> 417	Si(3)...H(25)	245.6(5)	12.2(tied to <i>u</i> 454)	—	0.3	13.8
<i>u</i> 501	Si(3)...H(26)	245.7(5)	12.3(tied to <i>u</i> 454)	—	0.4	14.0
<i>u</i> 542	Si(208)...H(234)	245.8(5)	11.7(tied to <i>u</i> 454)	—	0.5	13.3
<i>u</i> 508	Si(85)...H(108)	245.9(5)	12.4(tied to <i>u</i> 454)	—	0.5	14.1
<i>u</i> 496	Si(85)...H(106)	245.9(5)	12.5(tied to <i>u</i> 454)	—	0.6	14.2
<i>u</i> 510	Si(3)...H(24)	246.0(5)	12.4(tied to <i>u</i> 454)	—	0.7	14.1
<i>u</i> 408	Si(166)...H(205)	246.5(5)	13.5(tied to <i>u</i> 454)	—	1.3	15.4
<i>u</i> 409	Si(168)...H(194)	246.6(5)	12.8(tied to <i>u</i> 454)	—	1.3	14.6
<i>u</i> 411	Si(85)...H(109)	247.8(5)	14.0(tied to <i>u</i> 454)	—	2.6	15.9
<i>u</i> 412	Si(87)...H(101)	247.8(5)	13.2(tied to <i>u</i> 454)	—	2.6	15.0
<i>u</i> 378	H(26)...H(32)	247.9(160)	54.7(fixed)	—	40.6	54.7
<i>u</i> 439	H(22)...H(36)	248.1(402)	46.0(fixed)	—	14.9	46.0
<i>u</i> 454	Si(3)...H(28)	248.4(5)	13.0(6)	—	3.2	14.8
<i>u</i> 4310	H(149)...H(158)	248.5(392)	36.8(fixed)	—	0.3	36.8
<i>u</i> 539	H(264)...H(285)	248.5(172)	53.8(fixed)	—	18.8	53.8
<i>u</i> 360	H(104)...H(119)	248.7(410)	61.6(fixed)	—	51.5	61.6
<i>u</i> 433	H(279)...H(282)	248.7(383)	54.6(fixed)	—	29.3	54.6
<i>u</i> 426	Si(3)...H(27)	248.9(5)	14.2(tied to <i>u</i> 454)	—	3.8	16.2
<i>u</i> 534	Si(249)...H(272)	249.1(5)	12.4(tied to <i>u</i> 454)	—	3.8	14.1
<i>u</i> 367	H(105)...H(114)	249.1(307)	61.3(fixed)	—	48.3	61.3
<i>u</i> 1031	F(138)...H(151)	249.2(65)	79.1(fixed)	—	2.5	79.1
<i>u</i> 530	Si(166)...H(204)	249.2(5)	18.0(tied to <i>u</i> 454)	—	4.6	20.5
<i>u</i> 540	Si(3)...H(29)	249.4(5)	13.0(tied to <i>u</i> 454)	—	4.1	14.8
<i>u</i> 473	Si(166)...H(203)	249.4(5)	18.2(tied to <i>u</i> 454)	—	4.8	20.7
<i>u</i> 531	Si(168)...H(196)	249.5(5)	16.0(tied to <i>u</i> 454)	—	4.6	18.2
<i>u</i> 368	H(106)...H(122)	249.5(306)	60.7(fixed)	—	48.3	60.7
<i>u</i> 469	Si(249)...H(270)	249.6(5)	12.8(tied to <i>u</i> 454)	—	4.3	14.5
<i>u</i> 474	Si(168)...H(195)	249.7(5)	15.9(tied to <i>u</i> 454)	—	4.8	18.1
<i>u</i> 441	Si(249)...H(271)	250.7(5)	13.8(tied to <i>u</i> 454)	—	5.5	15.6
<i>u</i> 555	F(15)...H(23)	250.8(123)	34.9(fixed)	—	8.6	34.9
<i>u</i> 538	Si(85)...H(111)	251.5(5)	17.3(tied to <i>u</i> 454)	—	6.8	19.7
<i>u</i> 537	Si(87)...H(100)	251.5(5)	16.7(tied to <i>u</i> 454)	—	6.7	19.0
<i>u</i> 457	Si(85)...H(110)	251.5(5)	17.1(tied to <i>u</i> 454)	—	6.8	19.4
<i>u</i> 458	Si(87)...H(102)	251.6(5)	16.2(tied to <i>u</i> 454)	—	6.8	18.5
<i>u</i> 1151	F(178)...H(192)	252.7(167)	147.0(fixed)	—	0.6	147.0
<i>u</i> 1150	F(179)...H(184)	252.7(167)	147.0(fixed)	—	0.6	147.0

<i>u406</i>	H(64)...H(69)	252.7(310)	51.2(fixed)	—	31.9	51.2
<i>u379</i>	H(227)...H(241)	252.8(376)	44.9(fixed)	—	19.3	44.9
<i>u546</i>	F(263)...H(281)	253.5(131)	33.9(fixed)	—	8.0	33.9
<i>u3148</i>	C(129)...H(152)	253.5(117)	59.0(fixed)	—	-0.1	59.0
<i>u1492</i>	F(262)...H(270)	253.7(19)	35.4(fixed)	—	-12.3	35.4
<i>u1775</i>	H(271)...H(286)	254.2(123)	40.1(fixed)	—	-13.2	40.1
<i>u550</i>	H(33)...H(36)	254.4(411)	47.9(fixed)	—	9.9	47.9
<i>u358</i>	H(264)...H(283)	255.1(179)	55.7(fixed)	—	46.7	55.7
<i>u553</i>	H(61)...H(67)	255.3(292)	57.7(fixed)	—	16.7	57.7
<i>u381</i>	H(28)...H(40)	255.7(164)	63.7(fixed)	—	54.1	63.7
<i>u551</i>	H(225)...H(240)	256.7(281)	53.8(fixed)	—	23.0	53.8
<i>u548</i>	F(57)...H(81)	256.7(115)	34.3(fixed)	—	7.8	34.3
<i>u369</i>	H(281)...H(282)	256.9(417)	54.6(fixed)	—	37.2	54.6
<i>u434</i>	F(96)...H(117)	257.2(153)	31.2(fixed)	—	11.1	31.2
<i>u564</i>	F(16)...H(32)	257.4(75)	37.9(fixed)	—	7.0	37.9
<i>u450</i>	H(22)...H(37)	257.5(396)	45.0(fixed)	—	13.2	45.0
<i>u571</i>	H(59)...H(80)	258.8(189)	58.9(fixed)	—	17.6	58.9
<i>u363</i>	F(220)...H(231)	259.6(101)	34.6(fixed)	—	21.1	34.6
<i>u552</i>	H(64)...H(65)	260.8(217)	47.9(fixed)	—	17.5	47.9
<i>u359</i>	H(182)...H(196)	261.1(298)	87.1(fixed)	—	101.1	87.1
<i>u544</i>	H(225)...H(238)	261.7(293)	52.7(fixed)	—	23.1	52.7
<i>u559</i>	F(262)...H(278)	262.9(97)	36.3(fixed)	—	8.1	36.3
<i>u560</i>	F(219)...H(237)	263.0(72)	37.0(fixed)	—	7.3	37.0
<i>u567</i>	H(187)...H(201)	263.1(249)	57.4(fixed)	—	22.1	57.4
<i>u356</i>	H(100)...H(111)	263.6(433)	81.1(fixed)	—	105.5	81.1
<i>u2797</i>	C(132)...H(141)	263.8(114)	34.5(fixed)	—	1.6	34.5
<i>u440</i>	H(227)...H(242)	264.1(388)	45.2(fixed)	—	16.7	45.2
<i>u489</i>	F(221)...H(240)	264.6(89)	31.6(fixed)	—	10.5	31.6
<i>u2160</i>	H(273)...H(285)	264.6(293)	56.5(fixed)	—	-1.5	56.5
<i>u456</i>	F(55)...H(72)	265.1(140)	41.2(fixed)	—	25.6	41.2
<i>u1458</i>	C(256)...H(271)	265.4(94)	118.6(fixed)	—	-2.9	118.6
<i>u2038</i>	H(275)...H(286)	265.5(206)	50.6(fixed)	—	0.3	50.6
<i>u714</i>	C(218)...H(233)	265.6(103)	54.5(fixed)	—	25.3	54.5
<i>u2691</i>	F(137)...H(143)	266.0(61)	38.9(fixed)	—	1.8	38.9
<i>u561</i>	F(15)...H(20)	266.6(98)	38.7(fixed)	—	16.5	38.7
<i>u648</i>	F(222)...H(242)	267.0(114)	41.2(fixed)	—	6.0	41.2
<i>u687</i>	H(271)...H(278)	267.0(155)	114.2(fixed)	—	16.1	114.2
<i>u575</i>	H(63)...H(69)	269.3(313)	61.3(fixed)	—	24.6	61.3
<i>u1578</i>	F(262)...H(274)	269.9(23)	12.3(fixed)	—	-3.5	12.3
<i>u386</i>	F(178)...H(199)	270.3(159)	38.0(fixed)	—	24.5	38.0
<i>u387</i>	F(179)...H(200)	270.3(159)	38.0(fixed)	—	24.5	38.0
<i>u693</i>	H(266)...H(285)	271.1(177)	68.1(fixed)	—	14.3	68.1
<i>u1037</i>	H(61)...H(80)	271.1(183)	73.4(fixed)	—	9.3	73.4
<i>u677</i>	F(16)...H(18)	271.2(102)	47.7(fixed)	—	7.9	47.7

<i>u577</i>	F(14)...H(33)	271.4(145)	38.9(fixed)	—	6.9	38.9
<i>u633</i>	F(221)...H(223)	271.5(116)	51.5(fixed)	—	10.0	51.5
<i>u549</i>	F(98)...H(113)	272.4(172)	36.7(fixed)	—	16.2	36.7
<i>u2058</i>	C(130)...H(159)	272.6(110)	57.6(fixed)	—	-5.5	57.6
<i>u815</i>	F(221)...H(225)	273.6(107)	67.5(fixed)	—	3.7	67.5
<i>u447</i>	H(104)...H(118)	273.7(501)	64.2(fixed)	—	47.6	64.2
<i>u587</i>	F(56)...H(70)	274.5(157)	52.8(fixed)	—	13.8	52.8
<i>u590</i>	C(216)...F(220)	274.5(12)	10.4(tied to <i>u646</i> )	—	-0.2	10.2
<i>u377</i>	H(102)...H(114)	274.9(274)	76.2(fixed)	—	75.6	76.2
<i>u610</i>	C(48)...F(58)	275.1(11)	10.4(tied to <i>u646</i> )	—	-0.1	10.2
<i>u840</i>	C(212)...H(236)	275.2(85)	39.4(fixed)	—	8.2	39.4
<i>u572</i>	H(102)...H(113)	275.4(233)	79.4(fixed)	—	58.1	79.4
<i>u602</i>	C(49)...F(57)	275.5(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u612</i>	C(175)...F(179)	275.6(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u593</i>	C(257)...F(261)	275.6(11)	10.4(tied to <i>u646</i> )	—	-0.2	10.2
<i>u645</i>	C(254)...F(262)	275.6(11)	10.5(tied to <i>u646</i> )	—	-0.1	10.3
<i>u682</i>	F(17)...H(37)	275.8(141)	41.2(fixed)	—	6.1	41.2
<i>u611</i>	C(171)...F(181)	275.9(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u640</i>	C(253)...F(263)	275.9(11)	10.5(tied to <i>u646</i> )	—	-0.1	10.3
<i>u604</i>	C(8)...F(16)	276.0(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u609</i>	C(217)...F(219)	276.0(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u614</i>	C(93)...F(97)	276.0(11)	10.4(tied to <i>u646</i> )	—	-0.2	10.3
<i>u697</i>	C(255)...H(266)	276.0(137)	35.7(fixed)	—	14.7	35.7
<i>u636</i>	C(1)...F(17)	276.1(10)	10.0(tied to <i>u646</i> )	—	-0.1	9.8
<i>u573</i>	H(110)...H(121)	276.1(232)	78.5(fixed)	—	58.2	78.5
<i>u545</i>	H(76)...H(77)	276.2(439)	58.9(fixed)	—	32.2	58.9
<i>u627</i>	C(213)...F(221)	276.4(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u376</i>	H(110)...H(122)	276.5(272)	74.2(fixed)	—	75.8	74.2
<i>u616</i>	C(258)...F(260)	276.6(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u591</i>	C(53)...F(55)	276.7(11)	10.4(tied to <i>u646</i> )	—	-0.2	10.2
<i>u598</i>	C(212)...F(222)	276.7(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u588</i>	C(130)...F(140)	276.8(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u603</i>	C(131)...F(139)	276.8(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u600</i>	C(215)...F(220)	276.9(13)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u608</i>	C(52)...F(56)	277.0(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u629</i>	C(12)...F(14)	277.0(11)	10.6(tied to <i>u646</i> )	—	-0.2	10.4
<i>u607</i>	C(89)...F(99)	277.0(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u597</i>	C(11)...F(15)	277.2(11)	10.5(tied to <i>u646</i> )	—	-0.1	10.3
<i>u643</i>	C(1)...F(15)	277.2(10)	9.9(tied to <i>u646</i> )	—	-0.1	9.8
<i>u1774</i>	C(255)...H(272)	277.2(27)	29.7(fixed)	—	-14.0	29.7
<i>u615</i>	C(47)...F(58)	277.4(13)	10.5(tied to <i>u646</i> )	—	-0.1	10.3
<i>u644</i>	C(83)...F(98)	277.5(10)	10.0(tied to <i>u646</i> )	—	-0.1	9.8
<i>u635</i>	C(1)...F(14)	277.5(10)	10.0(tied to <i>u646</i> )	—	-0.1	9.8
<i>u660</i>	C(42)...F(56)	277.6(10)	10.1(tied to <i>u646</i> )	—	-0.1	9.9



<i>u606</i>	C(7)...F(17)	277.8(11)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u601</i>	F(260)...H(277)	277.8(85)	40.9(fixed)	—	9.4	40.9
<i>u641</i>	C(50)...F(57)	277.8(13)	10.5(tied to <i>u646</i> )	—	-0.1	10.3
<i>u596</i>	C(255)...F(262)	277.9(13)	10.7(tied to <i>u646</i> )	—	-0.2	10.5
<i>u631</i>	C(174)...F(179)	277.9(13)	10.7(tied to <i>u646</i> )	—	-0.2	10.5
<i>u619</i>	C(256)...F(261)	277.9(13)	10.6(tied to <i>u646</i> )	—	-0.2	10.5
<i>u639</i>	C(206)...F(222)	278.1(10)	9.8(tied to <i>u646</i> )	—	-0.1	9.7
<i>u658</i>	C(42)...F(55)	278.1(10)	10.1(tied to <i>u646</i> )	—	-0.1	9.9
<i>u630</i>	C(170)...F(181)	278.1(13)	10.7(tied to <i>u646</i> )	—	-0.2	10.5
<i>u599</i>	C(252)...F(263)	278.2(12)	10.4(tied to <i>u646</i> )	—	-0.1	10.3
<i>u637</i>	C(218)...F(219)	278.2(12)	10.6(tied to <i>u646</i> )	—	-0.1	10.4
<i>u638</i>	C(92)...F(97)	278.2(12)	10.7(tied to <i>u646</i> )	—	-0.2	10.5
<i>u646</i>	C(9)...F(16)	278.3(12)	10.7(3)	—	-0.1	10.5
<i>u642</i>	C(247)...F(260)	278.4(10)	9.9(tied to <i>u646</i> )	—	-0.1	9.7
<i>u960</i>	F(56)...H(69)	278.4(136)	79.1(fixed)	—	2.8	79.1
<i>u1376</i>	H(182)...H(200)	278.6(313)	163.5(fixed)	—	2.2	163.5
<i>u1374</i>	H(193)...H(199)	278.6(313)	163.4(fixed)	—	2.2	163.4
<i>u632</i>	C(214)...F(221)	278.7(12)	10.4(tied to <i>u646</i> )	—	-0.1	10.3
<i>u652</i>	C(206)...F(221)	278.7(10)	9.9(tied to <i>u646</i> )	—	-0.1	9.8
<i>u625</i>	C(259)...F(260)	278.8(12)	10.7(tied to <i>u646</i> )	—	-0.2	10.5
<i>u2885</i>	F(138)...H(147)	278.8(104)	30.5(fixed)	—	1.3	30.5
<i>u653</i>	C(124)...F(137)	278.8(10)	9.9(tied to <i>u646</i> )	—	-0.1	9.7
<i>u654</i>	C(124)...F(138)	278.8(10)	10.1(tied to <i>u646</i> )	—	-0.1	9.9
<i>u621</i>	C(54)...F(55)	278.9(12)	10.6(tied to <i>u646</i> )	—	-0.2	10.4
<i>u647</i>	C(211)...F(222)	278.9(12)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u622</i>	C(129)...F(140)	279.0(12)	10.6(tied to <i>u646</i> )	—	-0.2	10.4
<i>u667</i>	C(132)...F(139)	279.0(12)	10.6(tied to <i>u646</i> )	—	-0.1	10.4
<i>u605</i>	F(260)...H(279)	279.0(128)	41.6(fixed)	—	6.0	41.6
<i>u649</i>	C(51)...F(56)	279.1(12)	10.5(tied to <i>u646</i> )	—	-0.2	10.3
<i>u688</i>	C(215)...H(241)	279.2(69)	31.9(fixed)	—	8.9	31.9
<i>u650</i>	C(13)...F(14)	279.2(12)	10.7(tied to <i>u646</i> )	—	-0.2	10.6
<i>u651</i>	C(88)...F(99)	279.2(12)	10.8(tied to <i>u646</i> )	—	-0.1	10.6
<i>u623</i>	C(10)...F(15)	279.3(12)	10.8(tied to <i>u646</i> )	—	-0.2	10.6
<i>u738</i>	C(13)...H(28)	279.4(84)	66.9(fixed)	—	34.7	66.9
<i>u657</i>	C(83)...F(96)	279.4(10)	10.0(tied to <i>u646</i> )	—	-0.1	9.8
<i>u662</i>	C(206)...F(219)	279.4(10)	10.0(tied to <i>u646</i> )	—	-0.1	9.8
<i>u655</i>	C(1)...F(16)	279.4(10)	10.1(tied to <i>u646</i> )	—	-0.1	9.9
<i>u656</i>	C(247)...F(263)	279.6(10)	9.9(tied to <i>u646</i> )	—	-0.1	9.7
<i>u664</i>	C(165)...F(180)	279.6(10)	10.1(tied to <i>u646</i> )	—	-0.1	9.9
<i>u668</i>	C(6)...F(17)	279.8(12)	10.7(tied to <i>u646</i> )	—	-0.2	10.5
<i>u673</i>	C(247)...F(261)	280.1(10)	10.1(tied to <i>u646</i> )	—	-0.1	9.9
<i>u665</i>	C(165)...F(179)	280.1(10)	10.1(tied to <i>u646</i> )	—	-0.1	9.9
<i>u659</i>	C(247)...F(262)	280.1(10)	10.0(tied to <i>u646</i> )	—	-0.1	9.8
<i>u661</i>	C(42)...F(57)	280.3(10)	10.0(tied to <i>u646</i> )	—	-0.1	9.8

<i>u670</i>	C(42)...F(58)	281.1(10)	9.8(tied to <i>u646</i> )	—	-0.1	9.7
<i>u2684</i>	F(137)...H(146)	281.2(105)	42.1(fixed)	—	6.7	42.1
<i>u748</i>	C(7)...H(35)	281.5(135)	36.7(fixed)	—	7.5	36.7
<i>u758</i>	F(16)...H(20)	281.6(109)	62.6(fixed)	—	3.9	62.6
<i>u932</i>	F(58)...H(78)	282.0(313)	78.0(fixed)	—	4.0	78.0
<i>u675</i>	C(206)...F(220)	282.1(10)	10.0(tied to <i>u646</i> )	—	-0.1	9.8
<i>u579</i>	F(222)...H(244)	283.6(81)	38.6(fixed)	—	8.6	38.6
<i>u681</i>	C(54)...H(67)	283.7(104)	32.6(fixed)	—	11.3	32.6
<i>u807</i>	F(263)...H(283)	284.5(291)	75.3(fixed)	—	7.7	75.3
<i>u383</i>	H(188)...H(195)	284.8(383)	76.7(fixed)	—	72.7	76.7
<i>u2937</i>	H(264)...H(273)	285.2(200)	49.7(fixed)	—	-8.8	49.7
<i>u910</i>	C(214)...H(245)	285.9(124)	37.8(fixed)	—	4.8	37.8
<i>u4212</i>	C(131)...H(158)	286.4(106)	25.0(fixed)	—	-0.9	25.0
<i>u705</i>	C(9)...H(18)	287.0(110)	37.1(fixed)	—	14.8	37.1
<i>u2352</i>	Si(248)...H(271)	287.2(53)	39.4(fixed)	—	-22.2	39.4
<i>u582</i>	F(17)...H(39)	287.2(125)	38.8(fixed)	—	9.4	38.8
<i>u2356</i>	Si(251)...H(273)	287.4(95)	19.1(fixed)	—	-4.1	19.1
<i>u674</i>	C(11)...H(36)	287.7(142)	30.6(fixed)	—	9.6	30.6
<i>u586</i>	C(10)...H(26)	288.1(43)	45.4(fixed)	—	39.1	45.4
<i>u634</i>	F(55)...H(74)	289.0(148)	42.2(fixed)	—	6.9	42.2
<i>u691</i>	C(49)...H(61)	289.0(139)	37.6(fixed)	—	16.1	37.6
<i>u382</i>	H(187)...H(203)	289.8(375)	68.6(fixed)	—	72.7	68.6
<i>u952</i>	C(212)...H(238)	290.4(98)	33.1(fixed)	—	8.5	33.1
<i>u1769</i>	H(269)...H(274)	290.7(327)	43.4(fixed)	—	11.0	43.4
<i>u1863</i>	C(254)...H(275)	291.0(38)	13.7(fixed)	—	-3.4	13.7
<i>u620</i>	F(57)...H(73)	291.5(131)	53.5(fixed)	—	15.5	53.5
<i>u698</i>	C(254)...H(286)	291.8(94)	36.7(fixed)	—	10.8	36.7
<i>u877</i>	F(14)...H(31)	291.8(72)	47.1(fixed)	—	7.3	47.1
<i>u1399</i>	H(111)...H(121)	291.9(214)	159.2(fixed)	—	-0.9	159.2
<i>u1400</i>	H(100)...H(113)	292.0(213)	159.0(fixed)	—	-0.9	159.0
<i>u746</i>	F(262)...H(269)	292.2(253)	57.7(fixed)	—	9.4	57.7
<i>u890</i>	F(99)...H(119)	292.4(218)	61.7(fixed)	—	5.6	61.7
<i>u833</i>	F(16)...H(25)	292.8(120)	43.1(fixed)	—	2.0	43.1
<i>u959</i>	C(216)...H(228)	292.8(108)	35.1(fixed)	—	12.6	35.1
<i>u1046</i>	C(131)...H(163)	293.0(109)	36.8(fixed)	—	4.6	36.8
<i>u710</i>	F(220)...H(239)	293.0(118)	24.4(fixed)	—	0.7	24.4
<i>u1188</i>	F(16)...H(29)	293.1(38)	53.9(fixed)	—	1.5	53.9
<i>u4189</i>	C(130)...H(155)	293.3(108)	28.5(fixed)	—	3.1	28.5
<i>u707</i>	C(214)...H(223)	293.5(111)	36.9(fixed)	—	18.4	36.9
<i>u669</i>	C(12)...H(22)	293.7(114)	31.0(fixed)	—	11.4	31.0
<i>u1565</i>	F(17)...H(28)	294.0(110)	95.7(fixed)	—	-8.7	95.7
<i>u724</i>	F(58)...H(62)	294.3(118)	24.0(fixed)	—	0.8	24.0
<i>u1042</i>	F(99)...H(100)	294.4(38)	66.7(fixed)	—	7.6	66.7
<i>u592</i>	C(257)...H(282)	294.4(108)	44.7(fixed)	—	31.2	44.7

<i>u822</i>	H(25)...H(27)	294.5(144)	88.2(fixed)	—	26.2	88.2
<i>u1158</i>	F(221)...H(234)	294.6(38)	42.9(fixed)	—	-0.7	42.9
<i>u914</i>	H(230)...H(232)	294.9(139)	65.8(fixed)	—	14.9	65.8
<i>u717</i>	F(261)...H(280)	295.1(118)	23.2(fixed)	—	0.5	23.2
<i>u929</i>	F(178)...H(204)	295.1(39)	62.7(fixed)	—	7.1	62.7
<i>u922</i>	C(9)...H(40)	295.1(119)	40.4(fixed)	—	4.8	40.4
<i>u930</i>	F(180)...H(193)	295.3(39)	62.5(fixed)	—	7.1	62.5
<i>u1035</i>	Si(126)...H(163)	295.3(72)	28.2(fixed)	—	4.3	28.2
<i>u711</i>	F(57)...H(66)	295.4(118)	24.3(fixed)	—	1.1	24.3
<i>u721</i>	F(179)...H(198)	295.4(118)	24.9(fixed)	—	1.1	24.9
<i>u811</i>	F(221)...H(230)	295.6(119)	31.5(fixed)	—	1.1	31.5
<i>u943</i>	C(8)...H(32)	295.7(98)	32.7(fixed)	—	4.8	32.7
<i>u806</i>	Si(5)...F(15)	295.8(50)	17.8(tied to <i>u838</i> )	—	0.4	17.9
<i>u770</i>	F(263)...H(267)	295.8(119)	30.5(fixed)	—	1.9	30.5
<i>u722</i>	F(180)...H(189)	295.9(118)	24.9(fixed)	—	1.1	24.9
<i>u725</i>	F(219)...H(243)	296.0(118)	23.2(fixed)	—	0.7	23.2
<i>u843</i>	C(8)...H(40)	296.1(120)	31.7(fixed)	—	8.5	31.7
<i>u706</i>	F(96)...H(120)	296.3(118)	24.1(fixed)	—	1.0	24.1
<i>u727</i>	F(138)...H(157)	296.7(118)	24.1(fixed)	—	0.9	24.1
<i>u595</i>	F(58)...H(77)	296.7(288)	60.6(fixed)	—	13.4	60.6
<i>u695</i>	H(276)...H(280)	296.8(134)	33.9(fixed)	—	6.0	33.9
<i>u704</i>	F(137)...H(161)	296.9(119)	30.4(fixed)	—	2.3	30.4
<i>u740</i>	F(222)...H(226)	297.2(119)	27.8(fixed)	—	1.3	27.8
<i>u894</i>	F(55)...H(77)	297.2(125)	38.4(fixed)	—	0.9	38.4
<i>u709</i>	H(235)...H(239)	297.2(134)	34.4(fixed)	—	6.6	34.4
<i>u762</i>	F(99)...H(103)	297.2(120)	39.1(fixed)	—	3.2	39.1
<i>u663</i>	H(243)...H(246)	297.3(134)	34.3(fixed)	—	6.6	34.3
<i>u696</i>	H(120)...H(123)	297.3(135)	35.9(fixed)	—	7.0	35.9
<i>u666</i>	H(30)...H(34)	297.6(134)	32.9(fixed)	—	6.5	32.9
<i>u751</i>	F(220)...H(235)	297.7(38)	24.3(fixed)	—	0.2	24.3
<i>u913</i>	F(260)...H(282)	297.7(125)	39.3(fixed)	—	1.7	39.3
<i>u735</i>	F(56)...H(75)	297.8(118)	23.9(fixed)	—	0.7	23.9
<i>u732</i>	F(263)...H(282)	297.8(288)	69.5(fixed)	—	9.8	69.5
<i>u742</i>	F(14)...H(38)	297.9(118)	23.5(fixed)	—	0.6	23.5
<i>u747</i>	F(15)...H(34)	297.9(118)	23.6(fixed)	—	0.4	23.6
<i>u1789</i>	C(247)...H(271)	297.9(29)	37.9(fixed)	—	-11.0	37.9
<i>u628</i>	H(38)...H(41)	298.0(134)	34.4(fixed)	—	7.3	34.4
<i>u1038</i>	F(97)...H(104)	298.0(321)	100.0(fixed)	—	6.4	100.0
<i>u933</i>	F(58)...H(59)	298.1(38)	31.1(fixed)	—	0.5	31.1
<i>u908</i>	F(57)...H(70)	298.2(38)	36.9(fixed)	—	1.6	36.9
<i>u774</i>	F(220)...H(240)	298.2(127)	25.4(fixed)	—	0.1	25.4
<i>u1475</i>	H(101)...H(105)	298.4(218)	114.7(fixed)	—	-11.7	114.7
<i>u851</i>	F(58)...H(63)	298.4(126)	24.8(fixed)	—	0.0	24.8
<i>u864</i>	F(178)...H(200)	298.5(126)	26.0(fixed)	—	0.1	26.0

<i>u805</i>	F(140)...H(145)	298.6(124)	34.1(fixed)	—	1.2	34.1
<i>u896</i>	F(57)...H(67)	298.6(126)	25.8(fixed)	—	0.1	25.8
<i>u741</i>	H(60)...H(62)	298.6(135)	39.7(fixed)	—	9.3	39.7
<i>u865</i>	F(181)...H(186)	298.6(125)	26.0(fixed)	—	0.1	26.0
<i>u898</i>	F(96)...H(118)	298.7(125)	25.1(fixed)	—	-0.1	25.1
<i>u813</i>	F(263)...H(268)	298.7(126)	32.0(fixed)	—	1.2	32.0
<i>u781</i>	F(220)...H(237)	298.8(38)	24.4(fixed)	—	0.2	24.4
<i>u874</i>	F(222)...H(223)	298.9(37)	33.9(fixed)	—	1.2	33.9
<i>u715</i>	F(260)...H(284)	298.9(119)	33.7(fixed)	—	4.5	33.7
<i>u786</i>	F(261)...H(281)	298.9(125)	23.5(fixed)	—	0.0	23.5
<i>u876</i>	F(219)...H(241)	298.9(125)	24.3(fixed)	—	0.0	24.3
<i>u826</i>	F(261)...H(278)	299.0(38)	25.4(fixed)	—	0.1	25.4
<i>u873</i>	F(138)...H(158)	299.1(124)	25.3(fixed)	—	0.2	25.3
<i>u836</i>	F(263)...H(264)	299.2(37)	29.2(fixed)	—	0.8	29.2
<i>u613</i>	C(217)...H(227)	299.3(99)	31.6(fixed)	—	15.5	31.6
<i>u935</i>	F(138)...H(155)	299.3(37)	36.3(fixed)	—	2.3	36.3
<i>u814</i>	F(222)...H(227)	299.3(124)	28.9(fixed)	—	0.9	28.9
<i>u736</i>	F(17)...H(21)	299.4(118)	24.5(fixed)	—	0.9	24.5
<i>u885</i>	F(14)...H(36)	299.5(123)	24.4(fixed)	—	0.1	24.4
<i>u810</i>	F(137)...H(163)	299.5(37)	24.3(fixed)	—	0.1	24.3
<i>u827</i>	F(56)...H(76)	299.5(123)	24.4(fixed)	—	0.1	24.4
<i>u570</i>	H(190)...H(195)	299.5(301)	78.8(fixed)	—	55.1	78.8
<i>u923</i>	F(56)...H(73)	299.5(37)	35.4(fixed)	—	2.1	35.4
<i>u683</i>	F(55)...H(79)	299.6(119)	32.0(fixed)	—	4.5	32.0
<i>u816</i>	F(260)...H(286)	299.6(37)	27.5(fixed)	—	0.7	27.5
<i>u809</i>	F(55)...H(81)	299.7(37)	24.1(fixed)	—	0.1	24.1
<i>u728</i>	H(79)...H(82)	299.7(136)	45.8(fixed)	—	12.1	45.8
<i>u794</i>	F(96)...H(122)	299.7(37)	25.9(fixed)	—	0.8	25.9
<i>u618</i>	F(98)...H(100)	299.8(201)	79.1(fixed)	—	47.4	79.1
<i>u792</i>	F(15)...H(35)	299.8(123)	23.8(fixed)	—	0.2	23.8
<i>u838</i>	Si(4)...Si(5)	299.8(36)	9.1(3)	—	0.0	9.2
<i>u802</i>	F(98)...H(108)	299.8(125)	42.6(fixed)	—	4.4	42.6
<i>u750</i>	F(261)...H(276)	299.8(38)	24.7(fixed)	—	0.4	24.7
<i>u800</i>	F(219)...H(245)	299.9(37)	24.4(fixed)	—	0.6	24.4
<i>u850</i>	F(17)...H(22)	299.9(122)	25.8(fixed)	—	0.4	25.8
<i>u761</i>	F(221)...H(231)	300.0(125)	30.9(fixed)	—	2.1	30.9
<i>u808</i>	F(15)...H(32)	300.0(37)	23.7(fixed)	—	0.2	23.7
<i>u855</i>	F(17)...H(18)	300.1(37)	30.7(fixed)	—	1.3	30.7
<i>u713</i>	F(58)...H(60)	300.1(38)	27.6(fixed)	—	2.2	27.6
<i>u617</i>	F(99)...H(111)	300.2(201)	78.6(fixed)	—	47.5	78.6
<i>u812</i>	F(219)...H(246)	300.2(38)	24.7(fixed)	—	0.1	24.7
<i>u821</i>	F(14)...H(40)	300.3(37)	25.0(fixed)	—	0.8	25.0
<i>u835</i>	F(96)...H(123)	300.3(38)	25.0(fixed)	—	0.2	25.0
<i>u694</i>	H(142)...H(144)	300.3(135)	39.7(fixed)	—	11.0	39.7

<i>u752</i>	F(57)...H(68)	300.5(38)	32.7(fixed)	—	2.8	32.7
<i>u907</i>	Si(209)...Si(210)	300.5(36)	9.5(tied to <i>u838</i> )	—	0.0	9.5
<i>u739</i>	F(263)...H(265)	300.6(38)	27.8(fixed)	—	1.2	27.8
<i>u790</i>	C(254)...H(278)	300.6(108)	39.5(fixed)	—	5.8	39.5
<i>u880</i>	H(18)...H(27)	300.7(148)	118.3(fixed)	—	8.9	118.3
<i>u692</i>	C(52)...H(77)	300.8(115)	45.1(fixed)	—	26.4	45.1
<i>u731</i>	C(216)...H(225)	300.8(91)	39.2(fixed)	—	19.9	39.2
<i>u749</i>	F(137)...H(164)	300.9(38)	24.6(fixed)	—	0.2	24.6
<i>u680</i>	H(19)...H(21)	301.1(135)	37.4(fixed)	—	11.1	37.4
<i>u1055</i>	Si(3)...H(40)	301.3(75)	30.6(fixed)	—	4.8	30.6
<i>u743</i>	F(16)...H(26)	301.4(126)	41.4(fixed)	—	6.2	41.4
<i>u1078</i>	Si(208)...H(245)	301.4(71)	29.9(fixed)	—	4.4	29.9
<i>u773</i>	F(260)...H(287)	301.5(38)	26.6(fixed)	—	0.6	26.6
<i>u857</i>	Si(250)...Si(251)	301.6(36)	8.9(tied to <i>u838</i> )	—	0.0	9.0
<i>u753</i>	F(55)...H(82)	301.6(38)	24.4(fixed)	—	0.2	24.4
<i>u791</i>	F(138)...H(153)	301.9(38)	33.5(fixed)	—	2.9	33.5
<i>u730</i>	F(179)...H(194)	301.9(39)	48.6(fixed)	—	8.3	48.6
<i>u729</i>	F(178)...H(205)	301.9(39)	48.4(fixed)	—	8.3	48.4
<i>u828</i>	F(14)...H(41)	302.1(38)	25.3(fixed)	—	0.2	25.3
<i>u716</i>	C(48)...H(69)	302.1(103)	43.1(fixed)	—	24.9	43.1
<i>u755</i>	F(15)...H(30)	302.1(38)	25.5(fixed)	—	0.0	25.5
<i>u771</i>	F(222)...H(224)	302.2(38)	30.3(fixed)	—	1.8	30.3
<i>u718</i>	H(71)...H(75)	302.3(135)	42.5(fixed)	—	13.8	42.5
<i>u2035</i>	H(270)...H(277)	302.4(111)	49.5(fixed)	—	-20.9	49.5
<i>u569</i>	H(186)...H(203)	302.4(298)	73.7(fixed)	—	55.1	73.7
<i>u1968</i>	C(247)...H(273)	302.4(36)	12.7(fixed)	—	-3.3	12.7
<i>u939</i>	C(89)...H(114)	302.5(225)	35.3(fixed)	—	9.5	35.3
<i>u993</i>	Si(3)...H(32)	302.5(73)	27.6(fixed)	—	4.3	27.6
<i>u775</i>	C(53)...H(59)	302.7(167)	35.0(fixed)	—	15.2	35.0
<i>u754</i>	C(51)...H(70)	302.8(167)	36.8(fixed)	—	23.1	36.8
<i>u589</i>	C(93)...H(108)	302.8(163)	52.4(fixed)	—	46.6	52.4
<i>u788</i>	C(172)...C(173)	303.1(19)	11.4(tied to <i>u838</i> )	—	-0.2	11.5
<i>u789</i>	C(174)...C(175)	303.1(19)	11.4(tied to <i>u838</i> )	—	-0.2	11.5
<i>u772</i>	C(88)...C(89)	303.1(19)	11.3(tied to <i>u838</i> )	—	-0.2	11.4
<i>u782</i>	C(6)...C(7)	303.1(19)	11.5(tied to <i>u838</i> )	—	-0.1	11.6
<i>u797</i>	C(129)...C(130)	303.1(19)	11.3(tied to <i>u838</i> )	—	-0.2	11.4
<i>u783</i>	C(92)...C(93)	303.1(19)	11.3(tied to <i>u838</i> )	—	-0.1	11.4
<i>u776</i>	C(211)...C(212)	303.1(19)	11.3(tied to <i>u838</i> )	—	-0.1	11.4
<i>u801</i>	C(256)...C(257)	303.1(19)	11.4(tied to <i>u838</i> )	—	-0.1	11.5
<i>u796</i>	C(51)...C(52)	303.1(19)	11.3(tied to <i>u838</i> )	—	-0.1	11.3
<i>u769</i>	C(131)...C(132)	303.1(19)	11.2(tied to <i>u838</i> )	—	-0.1	11.3
<i>u777</i>	C(258)...C(259)	303.1(19)	11.4(tied to <i>u838</i> )	—	-0.1	11.5
<i>u798</i>	C(53)...C(54)	303.1(19)	11.1(tied to <i>u838</i> )	—	-0.1	11.2
<i>u767</i>	C(49)...C(50)	303.1(19)	11.1(tied to <i>u838</i> )	—	-0.1	11.2

<i>u799</i>	C(252)...C(253)	303.1(19)	11.1(tied to <i>u838</i> )	—	-0.1	11.2
<i>u817</i>	C(215)...C(216)	303.1(19)	11.2(tied to <i>u838</i> )	—	-0.1	11.3
<i>u779</i>	C(10)...C(11)	303.1(19)	11.1(tied to <i>u838</i> )	—	-0.1	11.2
<i>u787</i>	C(47)...C(48)	303.1(19)	11.1(tied to <i>u838</i> )	—	-0.1	11.2
<i>u768</i>	C(217)...C(218)	303.1(19)	11.0(tied to <i>u838</i> )	—	-0.1	11.1
<i>u897</i>	Si(45)...Si(46)	303.1(36)	8.9(tied to <i>u838</i> )	—	0.0	9.0
<i>u793</i>	C(254)...C(255)	303.2(19)	11.7(tied to <i>u838</i> )	—	-0.1	11.8
<i>u760</i>	C(12)...C(13)	303.2(19)	11.0(tied to <i>u838</i> )	—	-0.1	11.1
<i>u803</i>	C(213)...C(214)	303.2(19)	11.2(tied to <i>u838</i> )	—	-0.1	11.3
<i>u780</i>	C(8)...C(9)	303.2(19)	11.5(tied to <i>u838</i> )	—	-0.1	11.6
<i>u690</i>	H(66)...H(68)	303.2(135)	41.8(fixed)	—	14.5	41.8
<i>u763</i>	F(56)...H(71)	303.2(38)	33.1(fixed)	—	3.0	33.1
<i>u1022</i>	C(91)...H(122)	303.3(177)	39.8(fixed)	—	6.8	39.8
<i>u4209</i>	C(130)...H(154)	303.3(96)	34.6(fixed)	—	0.2	34.6
<i>u685</i>	H(284)...H(287)	303.5(136)	47.8(fixed)	—	16.6	47.8
<i>u856</i>	C(252)...H(285)	303.6(110)	40.3(fixed)	—	11.7	40.3
<i>u906</i>	C(253)...F(261)	303.6(106)	19.5(tied to <i>u838</i> )	—	2.3	19.7
<i>u844</i>	F(17)...H(19)	303.6(38)	28.6(fixed)	—	1.0	28.6
<i>u701</i>	H(265)...H(267)	303.6(135)	40.8(fixed)	—	14.6	40.8
<i>u684</i>	H(148)...H(150)	303.8(135)	42.5(fixed)	—	15.2	42.5
<i>u1067</i>	C(217)...H(237)	304.0(102)	37.9(fixed)	—	4.6	37.9
<i>u978</i>	C(89)...H(119)	304.0(288)	33.4(fixed)	—	6.0	33.4
<i>u585</i>	F(179)...H(182)	304.4(192)	73.5(fixed)	—	44.1	73.5
<i>u678</i>	H(224)...H(226)	304.5(135)	39.4(fixed)	—	15.1	39.4
<i>u2557</i>	Si(126)...H(141)	304.9(70)	23.4(fixed)	—	-0.3	23.4
<i>u942</i>	C(213)...H(245)	305.2(88)	33.2(fixed)	—	7.6	33.2
<i>u1660</i>	H(269)...H(273)	305.4(333)	47.8(fixed)	—	16.0	47.8
<i>u584</i>	F(178)...H(193)	305.4(191)	71.4(fixed)	—	44.1	71.4
<i>u832</i>	Si(43)...Si(45)	305.7(5)	9.1(tied to <i>u838</i> )	—	-0.1	9.2
<i>u1033</i>	C(214)...H(244)	306.0(117)	43.4(fixed)	—	4.1	43.4
<i>u766</i>	C(50)...H(73)	306.0(178)	39.0(fixed)	—	23.4	39.0
<i>u924</i>	Si(125)...Si(126)	306.2(5)	9.4(tied to <i>u838</i> )	—	-0.1	9.5
<i>u1218</i>	C(8)...H(27)	306.5(43)	63.4(fixed)	—	2.2	63.4
<i>u975</i>	Si(251)...F(261)	306.7(51)	18.1(tied to <i>u838</i> )	—	0.4	18.2
<i>u967</i>	Si(3)...H(18)	307.1(73)	33.3(fixed)	—	9.2	33.3
<i>u893</i>	Si(249)...H(278)	307.1(72)	27.8(fixed)	—	5.3	27.8
<i>u686</i>	F(96)...H(106)	307.2(318)	69.3(fixed)	—	20.8	69.3
<i>u1036</i>	Si(249)...H(286)	307.3(71)	32.6(fixed)	—	6.4	32.6
<i>u1095</i>	Si(85)...H(122)	307.5(83)	29.9(fixed)	—	6.0	29.9
<i>u862</i>	Si(248)...Si(250)	307.8(5)	9.4(tied to <i>u838</i> )	—	-0.1	9.4
<i>u712</i>	F(98)...H(109)	307.9(38)	49.1(fixed)	—	11.8	49.1
<i>u819</i>	Si(125)...Si(127)	308.0(6)	9.0(tied to <i>u838</i> )	—	-0.1	9.0
<i>u879</i>	Si(166)...Si(168)	308.0(6)	9.0(tied to <i>u838</i> )	—	-0.1	9.1
<i>u886</i>	Si(84)...Si(86)	308.0(6)	9.0(tied to <i>u838</i> )	—	0.0	9.0

<i>u</i> 999	Si(44)...H(81)	308.1(72)	27.9(fixed)	—	4.3	27.9
<i>u</i> 888	Si(44)...Si(46)	308.1(4)	9.3(tied to <i>u</i> 838)	—	0.0	9.4
<i>u</i> 837	C(211)...H(234)	308.1(114)	47.2(fixed)	—	29.8	47.2
<i>u</i> 881	Si(84)...Si(87)	308.2(6)	9.3(tied to <i>u</i> 838)	—	-0.1	9.4
<i>u</i> 1019	Si(207)...H(237)	308.3(69)	28.4(fixed)	—	4.2	28.4
<i>u</i> 878	Si(85)...Si(87)	308.3(6)	9.7(tied to <i>u</i> 838)	—	-0.1	9.8
<i>u</i> 726	F(219)...H(229)	308.3(247)	58.2(fixed)	—	12.0	58.2
<i>u</i> 901	Si(166)...Si(169)	308.5(6)	9.4(tied to <i>u</i> 838)	—	0.0	9.4
<i>u</i> 858	Si(2)...Si(3)	308.7(4)	9.5(tied to <i>u</i> 838)	—	-0.1	9.5
<i>u</i> 883	Si(207)...Si(208)	308.8(4)	9.5(tied to <i>u</i> 838)	—	0.0	9.5
<i>u</i> 905	Si(249)...Si(251)	308.9(4)	9.5(tied to <i>u</i> 838)	—	0.0	9.6
<i>u</i> 1044	C(8)...H(31)	308.9(91)	40.1(fixed)	—	5.1	40.1
<i>u</i> 823	Si(45)...F(55)	308.9(30)	19.1(tied to <i>u</i> 838)	—	0.3	19.2
<i>u</i> 1162	C(47)...H(80)	309.1(116)	43.8(fixed)	—	7.7	43.8
<i>u</i> 863	Si(166)...Si(167)	309.2(4)	9.5(tied to <i>u</i> 838)	—	0.0	9.5
<i>u</i> 1062	C(211)...F(221)	309.3(64)	26.0(tied to <i>u</i> 838)	—	1.3	26.2
<i>u</i> 859	Si(207)...Si(210)	309.3(4)	9.2(tied to <i>u</i> 838)	—	-0.1	9.3
<i>u</i> 3896	H(142)...H(152)	309.6(135)	66.4(fixed)	—	-5.8	66.4
<i>u</i> 1225	C(213)...H(232)	309.8(42)	48.1(fixed)	—	0.1	48.1
<i>u</i> 3926	H(141)...H(150)	309.8(132)	41.0(fixed)	—	-13.9	41.0
<i>u</i> 871	Si(84)...Si(85)	309.8(4)	9.4(tied to <i>u</i> 838)	—	0.0	9.5
<i>u</i> 848	Si(208)...Si(209)	309.9(4)	8.8(tied to <i>u</i> 838)	—	0.0	8.8
<i>u</i> 941	Si(125)...Si(128)	309.9(6)	10.1(tied to <i>u</i> 838)	—	0.0	10.1
<i>u</i> 845	Si(126)...Si(127)	310.0(6)	9.4(tied to <i>u</i> 838)	—	0.0	9.5
<i>u</i> 861	Si(3)...Si(5)	310.0(4)	9.4(tied to <i>u</i> 838)	—	-0.1	9.5
<i>u</i> 1087	C(9)...H(39)	310.5(129)	47.1(fixed)	—	3.7	47.1
<i>u</i> 895	Si(3)...Si(4)	310.5(4)	9.2(tied to <i>u</i> 838)	—	0.0	9.2
<i>u</i> 1039	C(48)...F(56)	310.5(123)	20.4(tied to <i>u</i> 838)	—	2.2	20.5
<i>u</i> 903	H(29)...H(39)	310.6(99)	121.0(fixed)	—	5.8	121.0
<i>u</i> 671	F(221)...H(232)	310.6(38)	32.3(fixed)	—	11.2	32.3
<i>u</i> 963	Si(208)...H(223)	310.7(72)	34.6(fixed)	—	11.9	34.6
<i>u</i> 902	Si(43)...Si(46)	310.8(4)	9.7(tied to <i>u</i> 838)	—	0.0	9.8
<i>u</i> 853	Si(44)...Si(45)	310.9(5)	9.4(tied to <i>u</i> 838)	—	0.0	9.5
<i>u</i> 884	Si(248)...Si(249)	311.0(4)	9.4(tied to <i>u</i> 838)	—	-0.1	9.5
<i>u</i> 860	Si(249)...Si(250)	311.0(5)	9.3(tied to <i>u</i> 838)	—	-0.1	9.4
<i>u</i> 1093	C(49)...H(81)	311.0(131)	39.5(fixed)	—	4.4	39.5
<i>u</i> 1050	C(52)...F(58)	311.1(122)	21.0(tied to <i>u</i> 838)	—	2.1	21.1
<i>u</i> 909	Si(2)...Si(4)	311.1(4)	9.6(tied to <i>u</i> 838)	—	0.0	9.7
<i>u</i> 1409	C(215)...H(227)	311.3(287)	55.2(fixed)	—	4.3	55.2
<i>u</i> 869	Si(208)...Si(210)	311.4(5)	9.5(tied to <i>u</i> 838)	—	-0.1	9.5
<i>u</i> 1120	F(261)...F(263)	311.4(112)	31.6(tied to <i>u</i> 838)	—	0.0	31.8
<i>u</i> 1187	H(107)...H(110)	311.4(196)	127.5(fixed)	—	-0.1	127.5
<i>u</i> 1189	H(102)...H(103)	311.5(196)	127.3(fixed)	—	-0.1	127.3
<i>u</i> 1138	Si(4)...H(23)	311.8(176)	31.4(fixed)	—	4.5	31.4

<i>u</i> 899	Si(248)...Si(251)	311.8(4)	9.6(tied to <i>u</i> 838)	—	0.0	9.6
<i>u</i> 889	Si(2)...Si(5)	311.8(4)	9.4(tied to <i>u</i> 838)	—	-0.1	9.4
<i>u</i> 1263	C(215)...H(228)	311.9(268)	52.5(fixed)	—	6.1	52.5
<i>u</i> 962	C(258)...H(279)	312.1(270)	35.3(fixed)	—	4.5	35.3
<i>u</i> 1073	C(6)...F(16)	312.1(48)	26.8(tied to <i>u</i> 838)	—	1.4	27.0
<i>u</i> 1213	C(11)...H(23)	312.2(276)	45.6(fixed)	—	4.3	45.6
<i>u</i> 1207	Si(209)...H(228)	312.2(181)	37.4(fixed)	—	6.8	37.4
<i>u</i> 1106	C(7)...F(15)	312.3(97)	25.9(tied to <i>u</i> 838)	—	0.6	26.1
<i>u</i> 912	Si(207)...Si(209)	312.3(4)	9.4(tied to <i>u</i> 838)	—	0.0	9.5
<i>u</i> 868	C(258)...H(264)	312.4(138)	33.7(fixed)	—	12.5	33.7
<i>u</i> 820	C(47)...H(78)	312.4(165)	43.8(fixed)	—	23.6	43.8
<i>u</i> 1065	C(53)...H(74)	312.5(263)	38.4(fixed)	—	5.2	38.4
<i>u</i> 1103	C(47)...H(65)	312.7(293)	38.5(fixed)	—	4.8	38.5
<i>u</i> 733	H(183)...H(185)	312.8(137)	56.4(fixed)	—	28.9	56.4
<i>u</i> 3202	H(265)...H(273)	312.8(128)	39.1(fixed)	—	-10.1	39.1
<i>u</i> 1336	F(14)...H(26)	312.9(285)	83.9(fixed)	—	1.3	83.9
<i>u</i> 1149	F(57)...H(72)	313.1(140)	77.8(fixed)	—	1.4	77.8
<i>u</i> 1180	C(255)...H(286)	313.1(120)	45.6(fixed)	—	6.3	45.6
<i>u</i> 1016	C(1)...C(9)	313.1(22)	10.3(tied to <i>u</i> 838)	—	-0.1	10.4
<i>u</i> 1034	C(247)...C(256)	313.1(22)	10.5(tied to <i>u</i> 838)	—	-0.1	10.6
<i>u</i> 987	C(1)...C(13)	313.1(22)	10.4(tied to <i>u</i> 838)	—	-0.1	10.5
<i>u</i> 980	C(83)...C(92)	313.1(22)	10.5(tied to <i>u</i> 838)	—	-0.1	10.5
<i>u</i> 1000	C(206)...C(218)	313.1(22)	10.5(tied to <i>u</i> 838)	—	-0.1	10.5
<i>u</i> 990	C(247)...C(259)	313.2(22)	10.4(tied to <i>u</i> 838)	—	-0.1	10.4
<i>u</i> 981	C(1)...C(6)	313.2(22)	10.2(tied to <i>u</i> 838)	—	-0.1	10.3
<i>u</i> 1027	C(247)...C(255)	313.2(22)	10.3(tied to <i>u</i> 838)	—	-0.1	10.4
<i>u</i> 988	C(42)...C(47)	313.2(22)	10.3(tied to <i>u</i> 838)	—	-0.1	10.4
<i>u</i> 984	C(247)...C(252)	313.2(22)	10.3(tied to <i>u</i> 838)	—	-0.1	10.4
<i>u</i> 1017	C(206)...C(214)	313.2(22)	10.1(tied to <i>u</i> 838)	—	-0.1	10.2
<i>u</i> 1004	C(42)...C(51)	313.2(22)	10.4(tied to <i>u</i> 838)	—	-0.1	10.5
<i>u</i> 1002	C(165)...C(174)	313.2(22)	10.4(tied to <i>u</i> 838)	—	-0.1	10.5
<i>u</i> 1001	C(165)...C(170)	313.2(22)	10.4(tied to <i>u</i> 838)	—	-0.1	10.5
<i>u</i> 2430	C(259)...H(271)	313.2(95)	30.9(fixed)	—	-24.0	30.9
<i>u</i> 1061	C(1)...C(10)	313.2(22)	10.3(tied to <i>u</i> 838)	—	-0.1	10.4
<i>u</i> 1009	C(124)...C(132)	313.2(22)	10.3(tied to <i>u</i> 838)	—	-0.1	10.4
<i>u</i> 1011	C(206)...C(215)	313.2(22)	10.1(tied to <i>u</i> 838)	—	-0.1	10.2
<i>u</i> 1040	C(124)...C(129)	313.2(22)	10.2(tied to <i>u</i> 838)	—	0.0	10.3
<i>u</i> 1020	C(83)...C(88)	313.2(22)	10.2(tied to <i>u</i> 838)	—	0.0	10.2
<i>u</i> 1018	C(206)...C(211)	313.2(22)	10.0(tied to <i>u</i> 838)	—	-0.1	10.1
<i>u</i> 1023	C(42)...C(50)	313.2(22)	10.1(tied to <i>u</i> 838)	—	0.0	10.2
<i>u</i> 1045	C(42)...C(54)	313.2(22)	10.2(tied to <i>u</i> 838)	—	0.0	10.2
<i>u</i> 734	H(202)...H(205)	313.3(137)	55.1(fixed)	—	28.9	55.1
<i>u</i> 953	H(113)...H(115)	313.3(154)	42.3(fixed)	—	4.9	42.3
<i>u</i> 965	Si(207)...F(222)	313.4(27)	18.1(tied to <i>u</i> 838)	—	0.2	18.2



<i>u</i> 916	Si(43)...Si(44)	313.5(4)	9.4(tied to <i>u</i> 838)	—	-0.1	9.4
<i>u</i> 1028	H(277)...H(279)	313.6(153)	38.8(fixed)	—	4.3	38.8
<i>u</i> 1084	C(50)...F(56)	313.7(106)	29.0(tied to <i>u</i> 838)	—	1.3	29.2
<i>u</i> 1147	F(137)...F(139)	313.7(61)	26.6(tied to <i>u</i> 838)	—	1.1	26.8
<i>u</i> 957	H(242)...H(244)	313.8(153)	37.8(fixed)	—	4.2	37.8
<i>u</i> 928	H(37)...H(39)	313.8(153)	38.9(fixed)	—	4.6	38.9
<i>u</i> 1133	H(236)...H(238)	313.9(153)	38.7(fixed)	—	4.6	38.7
<i>u</i> 2928	C(133)...F(140)	313.9(72)	19.3(tied to <i>u</i> 838)	—	-1.0	19.4
<i>u</i> 1052	H(31)...H(33)	314.0(153)	37.0(fixed)	—	4.3	37.0
<i>u</i> 946	H(20)...H(23)	314.0(154)	47.1(fixed)	—	7.0	47.1
<i>u</i> 1116	F(262)...H(268)	314.0(293)	63.6(fixed)	—	3.7	63.6
<i>u</i> 689	F(14)...H(24)	314.1(280)	72.2(fixed)	—	22.8	72.2
<i>u</i> 1739	H(24)...H(27)	314.2(209)	86.5(fixed)	—	-12.2	86.5
<i>u</i> 830	H(234)...H(244)	314.4(122)	95.9(fixed)	—	6.7	95.9
<i>u</i> 2274	C(256)...H(270)	314.5(51)	35.4(fixed)	—	-24.0	35.4
<i>u</i> 1156	Si(210)...H(238)	314.5(170)	32.2(fixed)	—	4.6	32.2
<i>u</i> 1097	C(170)...H(201)	314.6(263)	39.0(fixed)	—	9.5	39.0
<i>u</i> 1264	F(178)...F(179)	314.6(267)	50.7(tied to <i>u</i> 838)	—	-0.5	51.0
<i>u</i> 1115	Si(250)...F(263)	314.9(66)	17.6(tied to <i>u</i> 838)	—	0.1	17.8
<i>u</i> 834	C(6)...H(29)	314.9(105)	54.4(fixed)	—	43.6	54.4
<i>u</i> 1462	Si(126)...F(138)	315.0(28)	17.8(tied to <i>u</i> 838)	—	-0.3	17.9
<i>u</i> 1060	C(89)...H(101)	315.0(42)	56.1(fixed)	—	8.0	56.1
<i>u</i> 1137	Si(46)...F(56)	315.3(73)	17.7(tied to <i>u</i> 838)	—	0.2	17.8
<i>u</i> 1077	H(143)...H(146)	315.3(154)	46.6(fixed)	—	8.2	46.6
<i>u</i> 1793	H(275)...H(285)	315.4(287)	60.4(fixed)	—	3.7	60.4
<i>u</i> 954	Si(45)...H(70)	316.0(72)	36.8(fixed)	—	15.8	36.8
<i>u</i> 1049	C(48)...H(60)	316.1(42)	29.0(fixed)	—	1.8	29.0
<i>u</i> 948	C(53)...H(82)	316.1(41)	23.5(fixed)	—	0.9	23.5
<i>u</i> 950	C(130)...H(142)	316.1(41)	23.6(fixed)	—	0.9	23.6
<i>u</i> 966	Si(250)...F(260)	316.1(33)	19.1(tied to <i>u</i> 838)	—	0.2	19.2
<i>u</i> 977	C(216)...H(235)	316.2(41)	23.3(fixed)	—	1.0	23.3
<i>u</i> 915	C(11)...H(30)	316.3(41)	23.0(fixed)	—	1.0	23.0
<i>u</i> 958	C(257)...H(276)	316.3(41)	23.2(fixed)	—	1.0	23.2
<i>u</i> 672	F(16)...H(27)	316.3(38)	37.8(fixed)	—	18.9	37.8
<i>u</i> 1135	C(174)...F(181)	316.4(57)	41.6(tied to <i>u</i> 838)	—	3.0	41.8
<i>u</i> 994	H(225)...H(228)	316.5(155)	50.5(fixed)	—	10.5	50.5
<i>u</i> 841	C(217)...H(246)	316.5(41)	23.7(fixed)	—	1.3	23.7
<i>u</i> 1026	Si(2)...F(17)	316.6(32)	18.3(tied to <i>u</i> 838)	—	0.1	18.4
<i>u</i> 831	C(12)...H(41)	316.7(41)	24.1(fixed)	—	1.5	24.1
<i>u</i> 911	C(258)...H(287)	316.7(41)	25.5(fixed)	—	1.8	25.5
<i>u</i> 986	C(253)...H(265)	316.7(41)	26.7(fixed)	—	2.0	26.7
<i>u</i> 875	C(93)...H(112)	316.8(41)	23.8(fixed)	—	1.6	23.8
<i>u</i> 852	H(61)...H(64)	316.9(154)	43.0(fixed)	—	8.7	43.0
<i>u</i> 969	F(261)...F(262)	316.9(58)	28.1(tied to <i>u</i> 838)	—	1.4	28.3

<i>u818</i>	H(147)...H(151)	317.0(155)	51.6(fixed)	—	11.3	51.6
<i>u1128</i>	C(50)...H(64)	317.1(269)	37.9(fixed)	—	5.3	37.9
<i>u1059</i>	H(266)...H(269)	317.2(155)	49.1(fixed)	—	10.8	49.1
<i>u566</i>	F(222)...H(234)	317.3(112)	58.2(fixed)	—	32.5	58.2
<i>u842</i>	H(65)...H(69)	317.3(155)	51.3(fixed)	—	11.6	51.3
<i>u1007</i>	C(52)...H(71)	317.4(42)	32.8(fixed)	—	3.9	32.8
<i>u887</i>	H(72)...H(74)	317.5(155)	48.9(fixed)	—	11.0	48.9
<i>u1697</i>	H(273)...H(286)	317.5(316)	52.5(fixed)	—	5.9	52.5
<i>u900</i>	C(7)...H(19)	317.8(41)	26.3(fixed)	—	3.0	26.3
<i>u925</i>	C(212)...H(224)	317.9(42)	28.1(fixed)	—	3.5	28.1
<i>u1025</i>	C(175)...H(194)	317.9(42)	48.9(fixed)	—	8.5	48.9
<i>u1024</i>	C(171)...H(183)	317.9(42)	48.9(fixed)	—	8.5	48.9
<i>u927</i>	C(49)...H(68)	318.0(42)	31.6(fixed)	—	4.2	31.6
<i>u1164</i>	Si(45)...F(58)	318.0(71)	17.8(tied to <i>u838</i> )	—	0.2	17.9
<i>u974</i>	C(247)...C(254)	318.1(19)	10.1(tied to <i>u838</i> )	—	-0.1	10.1
<i>u956</i>	C(206)...C(216)	318.1(19)	10.3(tied to <i>u838</i> )	—	-0.1	10.3
<i>u931</i>	C(131)...H(150)	318.1(42)	32.7(fixed)	—	4.5	32.7
<i>u989</i>	C(42)...C(49)	318.1(19)	10.3(tied to <i>u838</i> )	—	-0.1	10.3
<i>u968</i>	C(42)...C(48)	318.1(19)	10.2(tied to <i>u838</i> )	—	-0.1	10.2
<i>u976</i>	C(124)...C(130)	318.1(19)	10.3(tied to <i>u838</i> )	—	-0.1	10.4
<i>u982</i>	C(165)...C(171)	318.1(19)	10.3(tied to <i>u838</i> )	—	-0.1	10.4
<i>u983</i>	C(165)...C(175)	318.1(19)	10.3(tied to <i>u838</i> )	—	-0.1	10.4
<i>u998</i>	C(247)...C(257)	318.1(19)	10.3(tied to <i>u838</i> )	—	-0.1	10.3
<i>u996</i>	C(1)...C(11)	318.1(19)	10.1(tied to <i>u838</i> )	—	-0.1	10.2
<i>u1012</i>	C(1)...C(8)	318.1(19)	10.3(tied to <i>u838</i> )	—	-0.1	10.4
<i>u972</i>	C(247)...C(253)	318.1(19)	10.2(tied to <i>u838</i> )	—	-0.1	10.3
<i>u1010</i>	C(83)...C(93)	318.1(19)	10.1(tied to <i>u838</i> )	—	-0.1	10.2
<i>u1006</i>	C(42)...C(52)	318.2(19)	10.2(tied to <i>u838</i> )	—	-0.1	10.2
<i>u1030</i>	C(124)...C(131)	318.2(19)	10.2(tied to <i>u838</i> )	—	-0.1	10.2
<i>u992</i>	C(206)...C(213)	318.2(19)	10.3(tied to <i>u838</i> )	—	0.0	10.3
<i>u997</i>	C(206)...C(212)	318.2(19)	10.2(tied to <i>u838</i> )	—	0.0	10.3
<i>u1029</i>	C(1)...C(12)	318.2(19)	9.9(tied to <i>u838</i> )	—	-0.1	10.0
<i>u985</i>	C(42)...C(53)	318.2(19)	10.1(tied to <i>u838</i> )	—	0.0	10.1
<i>u1021</i>	C(206)...C(217)	318.2(19)	10.0(tied to <i>u838</i> )	—	0.0	10.1
<i>u1015</i>	C(83)...C(89)	318.2(19)	10.1(tied to <i>u838</i> )	—	0.0	10.2
<i>u1032</i>	C(1)...C(7)	318.2(19)	10.1(tied to <i>u838</i> )	—	0.0	10.1
<i>u556</i>	F(17)...H(29)	318.2(122)	71.0(fixed)	—	46.9	71.0
<i>u1014</i>	C(247)...C(258)	318.2(19)	10.0(tied to <i>u838</i> )	—	0.0	10.1
<i>u971</i>	C(51)...F(55)	318.3(111)	21.7(tied to <i>u838</i> )	—	2.0	21.9
<i>u1074</i>	Si(4)...F(14)	318.3(42)	18.6(tied to <i>u838</i> )	—	0.2	18.7
<i>u1076</i>	Si(84)...F(99)	318.5(51)	21.6(tied to <i>u838</i> )	—	0.6	21.7
<i>u1083</i>	Si(248)...H(264)	318.5(75)	31.4(fixed)	—	8.4	31.4
<i>u973</i>	C(50)...H(66)	318.5(116)	26.4(fixed)	—	0.7	26.4
<i>u1058</i>	C(174)...H(198)	318.5(116)	26.8(fixed)	—	0.8	26.8

<i>u</i> 1057	C(173)...H(189)	318.5(116)	26.8(fixed)	—	0.8	26.8
<i>u</i> 961	C(132)...H(148)	318.5(116)	26.1(fixed)	—	0.7	26.1
<i>u</i> 1630	F(222)...H(233)	318.6(112)	77.2(fixed)	—	-6.5	77.2
<i>u</i> 947	C(218)...H(243)	318.7(116)	24.3(fixed)	—	0.6	24.3
<i>u</i> 1041	C(51)...H(75)	318.7(116)	24.9(fixed)	—	0.7	24.9
<i>u</i> 1005	C(256)...H(280)	318.7(116)	24.2(fixed)	—	0.6	24.2
<i>u</i> 1368	H(24)...H(31)	318.8(292)	102.5(fixed)	—	-2.7	102.5
<i>u</i> 970	C(6)...H(21)	318.8(116)	26.1(fixed)	—	0.9	26.1
<i>u</i> 1075	C(95)...H(120)	318.8(116)	24.9(fixed)	—	0.7	24.9
<i>u</i> 1119	Si(84)...F(97)	318.8(61)	17.7(tied to <i>u</i> 838)	—	0.2	17.8
<i>u</i> 1048	C(47)...H(62)	318.8(116)	25.1(fixed)	—	0.8	25.1
<i>u</i> 926	C(13)...H(38)	318.8(116)	24.2(fixed)	—	0.7	24.2
<i>u</i> 964	H(78)...H(80)	319.0(154)	48.3(fixed)	—	12.3	48.3
<i>u</i> 1089	C(54)...H(79)	319.0(117)	35.0(fixed)	—	2.9	35.0
<i>u</i> 1071	Si(43)...H(59)	319.1(80)	33.1(fixed)	—	10.8	33.1
<i>u</i> 917	C(10)...H(34)	319.1(116)	23.6(fixed)	—	0.8	23.6
<i>u</i> 1064	C(215)...H(239)	319.1(116)	24.4(fixed)	—	1.0	24.4
<i>u</i> 703	C(175)...H(192)	319.1(60)	62.9(fixed)	—	60.4	62.9
<i>u</i> 1241	C(9)...H(24)	319.3(138)	49.4(fixed)	—	0.8	49.4
<i>u</i> 945	H(283)...H(285)	319.6(155)	52.7(fixed)	—	14.3	52.7
<i>u</i> 936	C(211)...H(226)	319.6(116)	27.6(fixed)	—	2.0	27.6
<i>u</i> 1008	C(259)...H(284)	319.6(117)	36.8(fixed)	—	3.9	36.8
<i>u</i> 1261	F(96)...F(97)	319.7(258)	31.6(tied to <i>u</i> 838)	—	-0.1	31.8
<i>u</i> 1126	C(259)...H(264)	319.7(128)	44.6(fixed)	—	8.7	44.6
<i>u</i> 1047	F(219)...F(220)	319.8(33)	27.4(tied to <i>u</i> 838)	—	1.4	27.5
<i>u</i> 1124	Si(166)...F(179)	319.8(64)	20.6(tied to <i>u</i> 838)	—	0.9	20.8
<i>u</i> 1125	Si(168)...F(178)	319.8(64)	20.6(tied to <i>u</i> 838)	—	0.9	20.8
<i>u</i> 1231	C(170)...H(200)	319.8(299)	70.4(fixed)	—	5.4	70.4
<i>u</i> 1013	C(129)...H(144)	320.1(116)	29.8(fixed)	—	2.9	29.8
<i>u</i> 1216	C(88)...F(98)	320.2(93)	37.2(tied to <i>u</i> 838)	—	2.6	37.4
<i>u</i> 991	C(252)...H(267)	320.6(116)	29.3(fixed)	—	3.3	29.3
<i>u</i> 708	C(92)...H(102)	320.6(159)	65.2(fixed)	—	62.4	65.2
<i>u</i> 892	C(91)...H(107)	320.9(117)	39.2(fixed)	—	5.7	39.2
<i>u</i> 1185	C(211)...H(238)	320.9(263)	42.1(fixed)	—	4.7	42.1
<i>u</i> 1165	C(6)...F(15)	321.3(78)	25.2(tied to <i>u</i> 838)	—	1.8	25.4
<i>u</i> 934	C(214)...H(230)	321.3(116)	28.7(fixed)	—	3.9	28.7
<i>u</i> 870	C(213)...F(220)	322.1(60)	19.9(tied to <i>u</i> 838)	—	2.3	20.0
<i>u</i> 1152	Si(125)...H(156)	322.3(182)	31.5(fixed)	—	4.1	31.5
<i>u</i> 1168	C(88)...H(105)	322.7(138)	45.5(fixed)	—	3.1	45.5
<i>u</i> 1051	Si(250)...F(262)	322.7(23)	18.2(tied to <i>u</i> 838)	—	0.3	18.3
<i>u</i> 1223	C(214)...H(229)	322.9(137)	34.7(fixed)	—	0.6	34.7
<i>u</i> 1117	Si(248)...H(279)	322.9(181)	31.1(fixed)	—	3.5	31.1
<i>u</i> 1066	Si(209)...F(219)	323.1(28)	18.2(tied to <i>u</i> 838)	—	0.3	18.3
<i>u</i> 1166	C(129)...H(146)	323.3(137)	35.8(fixed)	—	1.3	35.8

<i>u</i> 1102	C(254)...H(277)	323.5(102)	47.0(fixed)	—	3.7	47.0
<i>u</i> 1184	C(252)...H(269)	323.5(137)	35.0(fixed)	—	1.3	35.0
<i>u</i> 1195	F(15)...F(16)	323.5(50)	27.6(tied to <i>u</i> 838)	—	1.0	27.8
<i>u</i> 1131	C(258)...H(281)	323.6(285)	37.1(fixed)	—	4.0	37.1
<i>u</i> 1163	C(257)...F(263)	323.7(103)	24.2(tied to <i>u</i> 838)	—	1.4	24.3
<i>u</i> 1145	C(211)...H(228)	323.7(136)	31.1(fixed)	—	0.8	31.1
<i>u</i> 951	Si(44)...H(73)	323.9(79)	37.8(fixed)	—	16.6	37.8
<i>u</i> 1092	C(259)...H(283)	323.9(137)	41.3(fixed)	—	3.2	41.3
<i>u</i> 1236	C(91)...H(121)	323.9(180)	59.6(fixed)	—	4.4	59.6
<i>u</i> 1159	C(10)...H(33)	324.0(136)	25.6(fixed)	—	0.0	25.6
<i>u</i> 1098	C(6)...H(23)	324.1(136)	27.6(fixed)	—	0.5	27.6
<i>u</i> 1302	C(11)...H(22)	324.1(311)	46.8(fixed)	—	3.7	46.8
<i>u</i> 1043	Si(208)...F(220)	324.1(23)	18.0(tied to <i>u</i> 838)	—	0.3	18.1
<i>u</i> 1081	C(13)...H(37)	324.1(136)	26.1(fixed)	—	0.3	26.1
<i>u</i> 1201	C(215)...H(238)	324.2(136)	26.7(fixed)	—	0.4	26.7
<i>u</i> 1086	C(218)...H(242)	324.2(136)	25.7(fixed)	—	0.3	25.7
<i>u</i> 1155	C(256)...H(279)	324.2(136)	25.1(fixed)	—	0.2	25.1
<i>u</i> 1130	C(51)...H(74)	324.3(136)	26.0(fixed)	—	0.4	26.0
<i>u</i> 1079	C(132)...H(147)	324.3(136)	26.6(fixed)	—	0.6	26.6
<i>u</i> 1467	C(259)...H(272)	324.4(76)	109.9(fixed)	—	3.2	109.9
<i>u</i> 1072	C(92)...H(115)	324.4(136)	27.3(fixed)	—	0.7	27.3
<i>u</i> 1121	C(47)...H(64)	324.5(136)	26.0(fixed)	—	0.6	26.0
<i>u</i> 1080	C(50)...H(65)	324.5(136)	26.6(fixed)	—	0.7	26.6
<i>u</i> 720	C(91)...H(100)	324.5(297)	66.9(fixed)	—	64.5	66.9
<i>u</i> 1167	Si(210)...H(242)	324.5(181)	31.4(fixed)	—	3.4	31.4
<i>u</i> 1104	C(54)...H(78)	324.7(137)	38.6(fixed)	—	3.3	38.6
<i>u</i> 1110	C(174)...H(197)	324.7(136)	26.7(fixed)	—	1.0	26.7
<i>u</i> 1109	C(170)...H(187)	324.7(136)	26.7(fixed)	—	1.0	26.7
<i>u</i> 1197	C(49)...H(80)	324.8(110)	38.0(fixed)	—	4.6	38.0
<i>u</i> 1129	Si(4)...F(16)	325.1(16)	18.1(tied to <i>u</i> 838)	—	0.1	18.2
<i>u</i> 1100	C(172)...H(192)	325.2(44)	66.3(fixed)	—	9.3	66.3
<i>u</i> 1101	C(175)...H(195)	325.3(44)	66.1(fixed)	—	9.3	66.1
<i>u</i> 1419	H(106)...H(117)	325.3(203)	107.9(fixed)	—	-3.1	107.9
<i>u</i> 1708	H(229)...H(232)	325.3(204)	67.6(fixed)	—	-9.5	67.6
<i>u</i> 1233	Si(46)...H(78)	325.3(189)	53.9(fixed)	—	9.5	53.9
<i>u</i> 1420	H(105)...H(118)	325.3(203)	107.9(fixed)	—	-3.1	107.9
<i>u</i> 719	C(88)...H(111)	325.5(297)	65.3(fixed)	—	64.7	65.3
<i>u</i> 1107	C(12)...H(35)	325.5(284)	35.3(fixed)	—	4.7	35.3
<i>u</i> 1096	C(174)...H(188)	325.6(299)	39.0(fixed)	—	9.5	39.0
<i>u</i> 1170	C(7)...H(20)	325.7(43)	34.8(fixed)	—	0.1	34.8
<i>u</i> 1070	C(93)...F(96)	325.7(102)	21.6(tied to <i>u</i> 838)	—	2.1	21.8
<i>u</i> 846	H(184)...H(187)	325.7(159)	73.6(fixed)	—	28.8	73.6
<i>u</i> 825	C(9)...H(25)	325.7(117)	35.6(fixed)	—	9.7	35.6
<i>u</i> 1143	C(212)...H(225)	325.7(43)	37.5(fixed)	—	0.8	37.5

<i>u</i> 1091	C(131)...H(151)	325.7(43)	41.0(fixed)	—	1.6	41.0
<i>u</i> 847	H(188)...H(192)	325.8(159)	73.4(fixed)	—	28.8	73.4
<i>u</i> 1112	Si(2)...H(33)	325.8(188)	31.1(fixed)	—	3.6	31.1
<i>u</i> 1113	C(49)...H(69)	325.9(43)	40.6(fixed)	—	1.7	40.6
<i>u</i> 1272	Si(87)...H(119)	326.0(174)	38.0(fixed)	—	3.4	38.0
<i>u</i> 558	H(266)...H(274)	326.1(289)	55.5(fixed)	—	17.0	55.5
<i>u</i> 904	H(223)...H(232)	326.1(140)	92.4(fixed)	—	14.8	92.4
<i>u</i> 1643	H(25)...H(32)	326.3(219)	68.1(fixed)	—	-6.4	68.1
<i>u</i> 1123	Si(209)...F(221)	326.3(28)	17.4(tied to <i>u</i> 838)	—	0.1	17.5
<i>u</i> 1343	H(201)...H(205)	326.3(208)	83.1(fixed)	—	-1.8	83.1
<i>u</i> 1342	H(183)...H(187)	326.3(208)	83.0(fixed)	—	-1.8	83.0
<i>u</i> 1094	Si(43)...F(57)	326.4(34)	17.3(tied to <i>u</i> 838)	—	0.3	17.4
<i>u</i> 1088	C(53)...F(58)	326.4(106)	28.8(tied to <i>u</i> 838)	—	1.5	29.0
<i>u</i> 699	H(101)...H(103)	326.4(140)	69.5(fixed)	—	48.1	69.5
<i>u</i> 1053	C(171)...F(180)	326.5(39)	24.3(tied to <i>u</i> 838)	—	6.7	24.4
<i>u</i> 1199	C(93)...H(113)	326.6(43)	27.8(fixed)	—	-0.3	27.8
<i>u</i> 1118	C(52)...H(72)	326.7(43)	38.4(fixed)	—	1.9	38.4
<i>u</i> 765	C(174)...H(182)	326.7(191)	66.6(fixed)	—	60.1	66.6
<i>u</i> 1127	C(12)...H(33)	326.8(293)	39.7(fixed)	—	3.9	39.7
<i>u</i> 1378	H(189)...H(192)	326.8(187)	98.8(fixed)	—	-2.9	98.8
<i>u</i> 1172	C(258)...H(285)	326.8(43)	29.4(fixed)	—	0.2	29.4
<i>u</i> 1148	C(12)...H(39)	326.9(43)	26.9(fixed)	—	-0.2	26.9
<i>u</i> 2265	C(259)...H(273)	326.9(279)	35.5(fixed)	—	-2.1	35.5
<i>u</i> 1379	H(184)...H(185)	326.9(187)	98.6(fixed)	—	-2.9	98.6
<i>u</i> 1178	C(217)...H(244)	326.9(43)	25.9(fixed)	—	-0.2	25.9
<i>u</i> 700	H(107)...H(109)	327.0(140)	68.3(fixed)	—	48.2	68.3
<i>u</i> 1153	C(253)...H(266)	327.0(43)	30.8(fixed)	—	0.7	30.8
<i>u</i> 1171	C(257)...H(277)	327.1(43)	27.0(fixed)	—	0.1	27.0
<i>u</i> 995	C(218)...H(229)	327.1(96)	37.8(fixed)	—	17.7	37.8
<i>u</i> 1219	C(216)...H(236)	327.3(43)	25.4(fixed)	—	0.0	25.4
<i>u</i> 1191	C(130)...H(143)	327.3(43)	25.4(fixed)	—	0.0	25.4
<i>u</i> 1367	C(255)...H(285)	327.3(118)	52.0(fixed)	—	3.7	52.0
<i>u</i> 1154	C(11)...H(31)	327.4(43)	25.1(fixed)	—	0.1	25.1
<i>u</i> 1192	C(53)...H(80)	327.4(43)	25.0(fixed)	—	0.1	25.0
<i>u</i> 1173	Si(43)...H(74)	327.4(166)	31.8(fixed)	—	4.1	31.8
<i>u</i> 1090	C(48)...H(61)	327.5(43)	32.0(fixed)	—	1.4	32.0
<i>u</i> 918	C(252)...H(283)	327.7(145)	44.9(fixed)	—	26.3	44.9
<i>u</i> 764	C(173)...H(204)	328.0(210)	59.3(fixed)	—	60.1	59.3
<i>u</i> 1003	C(90)...H(110)	328.0(45)	69.3(fixed)	—	13.3	69.3
<i>u</i> 1176	F(55)...F(57)	328.0(63)	27.7(tied to <i>u</i> 838)	—	1.1	27.9
<i>u</i> 849	H(229)...H(233)	328.1(156)	55.9(fixed)	—	24.0	55.9
<i>u</i> 1134	C(170)...F(179)	328.3(139)	41.6(tied to <i>u</i> 838)	—	3.0	41.8
<i>u</i> 1082	C(7)...H(37)	328.3(284)	37.6(fixed)	—	4.3	37.6
<i>u</i> 1200	Si(5)...H(37)	328.6(182)	31.9(fixed)	—	3.5	31.9

<i>u</i> 1230	Si(46)...H(65)	328.6(173)	33.0(fixed)	—	4.2	33.0
<i>u</i> 1063	C(212)...H(242)	328.6(273)	36.3(fixed)	—	4.2	36.3
<i>u</i> 1136	C(258)...F(263)	328.6(86)	28.1(tied to <i>u</i> 838)	—	1.2	28.3
<i>u</i> 1146	C(54)...F(57)	328.7(93)	25.0(tied to <i>u</i> 838)	—	1.1	25.2
<i>u</i> 1242	C(217)...H(236)	329.1(89)	40.7(fixed)	—	3.8	40.7
<i>u</i> 872	H(24)...H(28)	329.4(160)	77.1(fixed)	—	34.2	77.1
<i>u</i> 979	C(255)...H(269)	329.4(137)	37.7(fixed)	—	17.8	37.7
<i>u</i> 891	C(13)...H(24)	329.6(115)	46.8(fixed)	—	34.5	46.8
<i>u</i> 1198	C(10)...F(16)	329.8(55)	27.6(tied to <i>u</i> 838)	—	0.9	27.8
<i>u</i> 1217	C(54)...H(59)	329.8(134)	49.4(fixed)	—	11.4	49.4
<i>u</i> 1332	F(56)...F(58)	330.2(150)	33.0(tied to <i>u</i> 838)	—	-0.4	33.2
<i>u</i> 1235	Si(44)...H(64)	330.4(169)	32.6(fixed)	—	4.2	32.6
<i>u</i> 1327	C(206)...H(245)	330.6(46)	21.8(fixed)	—	0.5	21.8
<i>u</i> 1285	C(206)...H(237)	330.7(46)	21.2(fixed)	—	0.6	21.2
<i>u</i> 1320	C(1)...H(40)	330.7(46)	22.1(fixed)	—	0.7	22.1
<i>u</i> 1317	C(83)...H(114)	330.7(46)	22.3(fixed)	—	0.8	22.3
<i>u</i> 1289	C(42)...H(81)	330.8(46)	20.9(fixed)	—	0.7	20.9
<i>u</i> 1287	C(124)...H(141)	330.8(46)	20.9(fixed)	—	0.7	20.9
<i>u</i> 1304	C(1)...H(32)	330.9(46)	20.5(fixed)	—	0.7	20.5
<i>u</i> 1249	C(211)...H(240)	331.0(271)	45.7(fixed)	—	3.7	45.7
<i>u</i> 1290	C(247)...H(278)	331.0(46)	20.9(fixed)	—	0.9	20.9
<i>u</i> 1299	C(247)...H(286)	331.2(46)	23.0(fixed)	—	1.3	23.0
<i>u</i> 3906	H(143)...H(152)	331.3(139)	57.1(fixed)	—	-1.0	57.1
<i>u</i> 1282	C(217)...F(222)	331.3(68)	30.2(tied to <i>u</i> 838)	—	0.2	30.4
<i>u</i> 1139	C(90)...H(117)	331.3(331)	42.7(fixed)	—	5.9	42.7
<i>u</i> 1141	C(89)...H(118)	331.3(331)	42.7(fixed)	—	5.9	42.7
<i>u</i> 1870	H(232)...H(245)	331.4(92)	47.1(fixed)	—	-11.2	47.1
<i>u</i> 1054	C(175)...F(178)	331.4(102)	24.3(tied to <i>u</i> 838)	—	6.7	24.5
<i>u</i> 1511	C(1)...H(28)	331.5(42)	46.6(fixed)	—	1.1	46.6
<i>u</i> 1308	F(219)...H(231)	331.5(276)	63.8(fixed)	—	1.8	63.8
<i>u</i> 1244	Si(125)...H(146)	331.7(173)	45.0(fixed)	—	9.2	45.0
<i>u</i> 1203	C(7)...H(36)	331.7(291)	40.6(fixed)	—	3.7	40.6
<i>u</i> 1276	C(247)...H(264)	331.8(46)	23.8(fixed)	—	2.1	23.8
<i>u</i> 1301	C(1)...H(18)	331.9(46)	24.0(fixed)	—	2.2	24.0
<i>u</i> 1509	C(206)...H(233)	332.1(42)	37.3(fixed)	—	-0.6	37.3
<i>u</i> 3767	C(129)...F(139)	332.3(54)	12.6(fixed)	—	-2.2	12.6
<i>u</i> 1194	C(47)...H(67)	332.3(280)	48.5(fixed)	—	3.9	48.5
<i>u</i> 1177	C(256)...F(262)	332.4(75)	26.6(fixed)	—	0.8	26.6
<i>u</i> 1250	C(42)...H(59)	332.4(46)	24.9(fixed)	—	2.8	24.9
<i>u</i> 1144	C(212)...H(241)	332.7(280)	38.8(fixed)	—	3.9	38.8
<i>u</i> 1114	C(216)...F(221)	332.8(43)	22.2(fixed)	—	1.5	22.2
<i>u</i> 1296	C(206)...H(223)	332.8(46)	24.7(fixed)	—	3.2	24.7
<i>u</i> 1186	C(215)...F(219)	333.1(58)	27.4(fixed)	—	0.7	27.4
<i>u</i> 1220	C(48)...H(65)	333.1(166)	40.7(fixed)	—	7.5	40.7

<i>u1887</i>	H(27)...H(40)	333.2(81)	55.5(fixed)	—	-14.8	55.5
<i>u1329</i>	C(214)...C(218)	333.5(85)	24.3(tied to <i>u1442</i> )	—	1.8	23.9
<i>u940</i>	C(92)...H(105)	333.5(222)	50.8(fixed)	—	36.2	50.8
<i>u1229</i>	Si(251)...H(283)	333.6(183)	51.8(fixed)	—	12.6	51.8
<i>u1169</i>	C(92)...F(98)	333.6(139)	24.7(tied to <i>u1442</i> )	—	3.9	24.2
<i>u1221</i>	C(49)...H(64)	333.6(170)	40.4(fixed)	—	7.2	40.4
<i>u1293</i>	C(42)...H(70)	333.7(46)	27.1(fixed)	—	4.4	27.1
<i>u1295</i>	C(124)...H(152)	333.7(46)	28.5(fixed)	—	4.7	28.5
<i>u1278</i>	C(42)...H(73)	333.8(46)	28.5(fixed)	—	4.8	28.5
<i>u1451</i>	H(29)...H(40)	334.1(175)	111.3(fixed)	—	-10.1	111.3
<i>u1815</i>	Si(85)...H(102)	334.2(121)	105.6(fixed)	—	-8.6	105.6
<i>u1183</i>	F(220)...F(221)	334.6(54)	32.0(fixed)	—	-0.2	32.0
<i>u1247</i>	H(283)...H(287)	334.6(203)	64.4(fixed)	—	-1.4	64.4
<i>u4038</i>	C(130)...C(133)	334.8(49)	12.9(fixed)	—	-1.8	12.9
<i>u1283</i>	C(171)...H(201)	334.8(201)	48.4(fixed)	—	10.4	48.4
<i>u1991</i>	H(272)...H(274)	334.9(187)	59.9(fixed)	—	-13.8	59.9
<i>u2975</i>	C(129)...F(137)	334.9(46)	22.7(tied to <i>u1442</i> )	—	-1.4	22.3
<i>u702</i>	C(172)...H(195)	335.0(182)	67.4(fixed)	—	60.4	67.4
<i>u1068</i>	C(132)...F(140)	335.0(54)	23.2(tied to <i>u1442</i> )	—	1.7	22.8
<i>u882</i>	C(213)...H(233)	335.0(43)	37.4(fixed)	—	10.1	37.4
<i>u1347</i>	C(1)...H(31)	335.1(42)	25.1(fixed)	—	0.2	25.1
<i>u535</i>	F(140)...H(151)	335.1(85)	41.6(fixed)	—	26.4	41.6
<i>u1215</i>	C(11)...F(14)	335.2(98)	28.1(tied to <i>u838</i> )	—	0.7	28.3
<i>u1228</i>	C(247)...H(281)	335.2(115)	22.3(fixed)	—	0.6	22.3
<i>u4559</i>	H(144)...H(155)	335.2(219)	30.0(fixed)	—	-2.8	30.0
<i>u1316</i>	C(247)...H(277)	335.3(42)	24.5(fixed)	—	0.2	24.5
<i>u1280</i>	C(1)...H(35)	335.3(115)	21.8(fixed)	—	0.7	21.8
<i>u1406</i>	Si(126)...C(136)	335.3(41)	15.9(tied to <i>u1442</i> )	—	0.6	15.6
<i>u1227</i>	C(42)...H(76)	335.5(115)	22.6(fixed)	—	0.9	22.6
<i>u1303</i>	C(42)...H(72)	335.5(42)	34.2(fixed)	—	2.1	34.2
<i>u1351</i>	C(124)...H(143)	335.5(42)	23.9(fixed)	—	0.3	23.9
<i>u1204</i>	C(206)...H(240)	335.5(115)	22.8(fixed)	—	1.0	22.8
<i>u1373</i>	C(42)...H(61)	335.5(42)	27.3(fixed)	—	0.9	27.3
<i>u1270</i>	C(206)...H(241)	335.5(115)	22.0(fixed)	—	0.9	22.0
<i>u1349</i>	C(42)...H(80)	335.5(42)	23.6(fixed)	—	0.3	23.6
<i>u1251</i>	Si(166)...H(187)	335.5(160)	34.3(fixed)	—	7.1	34.3
<i>u1252</i>	Si(168)...H(188)	335.5(160)	34.3(fixed)	—	7.1	34.3
<i>u1208</i>	C(42)...H(63)	335.5(115)	22.6(fixed)	—	1.0	22.6
<i>u1288</i>	C(1)...H(36)	335.6(115)	21.7(fixed)	—	0.9	21.7
<i>u1323</i>	C(247)...H(266)	335.6(42)	26.9(fixed)	—	0.9	26.9
<i>u1274</i>	C(124)...H(149)	335.6(115)	23.1(fixed)	—	1.2	23.1
<i>u1309</i>	C(206)...H(236)	335.6(42)	23.3(fixed)	—	0.4	23.3
<i>u1257</i>	C(1)...H(39)	335.7(42)	24.6(fixed)	—	0.7	24.6
<i>u1240</i>	C(42)...H(67)	335.7(115)	23.4(fixed)	—	1.3	23.4

<i>u</i> 1260	C(206)...H(244)	335.7(42)	24.0(fixed)	—	0.6	24.0
<i>u</i> 1211	C(165)...H(186)	335.7(115)	23.2(fixed)	—	1.3	23.2
<i>u</i> 1212	C(165)...H(199)	335.7(115)	23.2(fixed)	—	1.3	23.2
<i>u</i> 1279	C(1)...H(22)	335.7(115)	23.1(fixed)	—	1.3	23.1
<i>u</i> 1305	C(247)...H(285)	335.7(42)	25.6(fixed)	—	0.8	25.6
<i>u</i> 1234	C(83)...H(113)	335.8(42)	24.7(fixed)	—	0.7	24.7
<i>u</i> 1255	C(253)...F(262)	335.8(61)	29.8(fixed)	—	1.2	29.8
<i>u</i> 1214	C(83)...H(117)	335.9(115)	22.3(fixed)	—	1.3	22.3
<i>u</i> 1294	C(124)...H(151)	335.9(42)	34.3(fixed)	—	2.6	34.3
<i>u</i> 1248	C(1)...H(20)	336.0(42)	28.3(fixed)	—	1.5	28.3
<i>u</i> 1275	C(206)...H(231)	336.1(115)	27.5(fixed)	—	2.3	27.5
<i>u</i> 1683	H(111)...H(122)	336.1(257)	111.5(fixed)	—	-12.8	111.5
<i>u</i> 1439	H(234)...H(245)	336.1(174)	87.8(fixed)	—	-7.6	87.8
<i>u</i> 1311	C(206)...H(225)	336.1(42)	29.5(fixed)	—	1.9	29.5
<i>u</i> 1326	C(42)...H(69)	336.2(42)	32.7(fixed)	—	2.6	32.7
<i>u</i> 1684	H(100)...H(114)	336.2(257)	111.3(fixed)	—	-12.8	111.3
<i>u</i> 1277	C(206)...H(227)	336.2(115)	24.5(fixed)	—	2.0	24.5
<i>u</i> 1412	C(83)...H(102)	336.3(42)	53.7(fixed)	—	8.0	53.7
<i>u</i> 1765	H(101)...H(114)	336.3(131)	73.7(fixed)	—	-12.6	73.7
<i>u</i> 1766	H(109)...H(122)	336.4(131)	73.5(fixed)	—	-12.6	73.5
<i>u</i> 1132	C(132)...F(138)	336.5(46)	29.3(tied to <i>u</i> 1442)	—	1.2	28.8
<i>u</i> 2194	C(259)...H(275)	336.6(228)	37.7(fixed)	—	-1.7	37.7
<i>u</i> 1222	C(247)...H(268)	336.6(115)	26.9(fixed)	—	2.7	26.9
<i>u</i> 1284	C(175)...H(188)	336.8(180)	48.4(fixed)	—	10.4	48.4
<i>u</i> 1418	H(265)...H(269)	336.8(202)	56.0(fixed)	—	-2.1	56.0
<i>u</i> 1193	Si(249)...H(269)	336.8(168)	40.1(fixed)	—	10.3	40.1
<i>u</i> 1361	C(165)...H(192)	336.9(42)	52.1(fixed)	—	8.1	52.1
<i>u</i> 1362	C(165)...H(195)	337.0(42)	51.8(fixed)	—	8.1	51.8
<i>u</i> 1181	C(51)...F(57)	337.1(88)	29.4(tied to <i>u</i> 1442)	—	1.3	28.9
<i>u</i> 1237	H(100)...H(109)	337.2(297)	133.2(fixed)	—	56.5	133.2
<i>u</i> 1344	C(1)...H(26)	337.4(115)	35.1(fixed)	—	5.0	35.1
<i>u</i> 1226	C(124)...H(145)	337.4(115)	26.5(fixed)	—	3.5	26.5
<i>u</i> 1292	F(262)...H(272)	337.5(14)	53.2(fixed)	—	-4.3	53.2
<i>u</i> 1256	H(78)...H(82)	337.6(202)	58.0(fixed)	—	-0.6	58.0
<i>u</i> 1331	C(12)...F(17)	338.3(99)	30.5(fixed)	—	0.1	30.5
<i>u</i> 1224	C(9)...F(17)	338.3(78)	25.6(tied to <i>u</i> 1442)	—	0.9	25.2
<i>u</i> 1330	H(142)...H(146)	338.5(201)	52.0(fixed)	—	-1.7	52.0
<i>u</i> 1321	H(224)...H(228)	338.6(201)	54.5(fixed)	—	-0.8	54.5
<i>u</i> 1300	C(50)...H(63)	338.7(292)	47.9(fixed)	—	3.0	47.9
<i>u</i> 1297	C(83)...H(104)	338.8(115)	34.3(fixed)	—	6.2	34.3
<i>u</i> 1652	H(103)...H(119)	338.8(122)	71.2(fixed)	—	-6.9	71.2
<i>u</i> 1267	H(147)...H(150)	339.0(201)	55.4(fixed)	—	-0.1	55.4
<i>u</i> 1345	H(71)...H(74)	339.1(201)	53.7(fixed)	—	-0.6	53.7
<i>u</i> 1239	C(247)...H(282)	339.1(115)	30.6(fixed)	—	5.9	30.6



<i>u</i> 824	C(8)...H(28)	339.3(44)	45.8(fixed)	—	16.4	45.8
<i>u</i> 854	Si(210)...H(234)	339.3(69)	41.7(fixed)	—	28.9	41.7
<i>u</i> 1268	H(65)...H(68)	339.5(201)	54.2(fixed)	—	0.0	54.2
<i>u</i> 1196	C(42)...H(77)	339.5(115)	28.8(fixed)	—	6.0	28.8
<i>u</i> 1160	C(206)...H(234)	339.6(46)	33.3(fixed)	—	11.5	33.3
<i>u</i> 1341	C(8)...C(10)	340.0(42)	21.3(tied to <i>u</i> 1442)	—	2.5	20.9
<i>u</i> 4591	H(145)...H(153)	340.1(76)	29.5(fixed)	—	-10.1	29.5
<i>u</i> 1392	H(60)...H(64)	340.2(200)	47.1(fixed)	—	-1.3	47.1
<i>u</i> 397	H(266)...H(275)	340.2(196)	46.1(fixed)	—	18.8	46.1
<i>u</i> 1371	C(9)...C(13)	340.4(70)	26.9(tied to <i>u</i> 1442)	—	1.4	26.4
<i>u</i> 1281	C(256)...F(260)	340.4(66)	29.5(tied to <i>u</i> 1442)	—	1.4	29.1
<i>u</i> 1175	C(89)...F(97)	340.5(139)	35.3(tied to <i>u</i> 1442)	—	2.6	34.7
<i>u</i> 1232	C(174)...H(190)	341.4(293)	70.4(fixed)	—	5.4	70.4
<i>u</i> 1262	C(257)...F(260)	341.4(85)	31.1(tied to <i>u</i> 1442)	—	0.3	30.6
<i>u</i> 1631	H(281)...H(283)	341.5(120)	79.5(fixed)	—	-4.4	79.5
<i>u</i> 1437	H(25)...H(40)	341.5(235)	74.7(fixed)	—	-0.5	74.7
<i>u</i> 1337	Si(3)...C(13)	341.6(51)	16.7(tied to <i>u</i> 1442)	—	0.5	16.4
<i>u</i> 1355	Si(3)...C(10)	341.8(40)	15.4(tied to <i>u</i> 1442)	—	0.9	15.2
<i>u</i> 1759	Si(168)...H(184)	341.8(78)	105.4(fixed)	—	-7.7	105.4
<i>u</i> 1760	Si(166)...H(192)	341.8(77)	105.3(fixed)	—	-7.7	105.3
<i>u</i> 1243	H(19)...H(23)	341.8(200)	47.1(fixed)	—	0.3	47.1
<i>u</i> 1469	Si(209)...C(212)	342.1(65)	17.9(tied to <i>u</i> 1442)	—	0.3	17.6
<i>u</i> 804	C(135)...H(146)	342.1(267)	36.2(fixed)	—	20.2	36.2
<i>u</i> 1363	Si(208)...C(218)	342.2(39)	16.4(tied to <i>u</i> 1442)	—	0.7	16.2
<i>u</i> 2378	C(253)...H(273)	342.4(238)	34.6(fixed)	—	-3.2	34.6
<i>u</i> 1335	H(30)...H(33)	342.5(199)	39.4(fixed)	—	-1.0	39.4
<i>u</i> 1259	C(165)...H(196)	342.5(47)	40.3(fixed)	—	15.9	40.3
<i>u</i> 1258	C(165)...H(182)	342.5(47)	40.2(fixed)	—	15.9	40.2
<i>u</i> 1364	H(148)...H(151)	342.6(179)	61.4(fixed)	—	-3.9	61.4
<i>u</i> 1381	H(235)...H(238)	342.6(199)	40.2(fixed)	—	-0.7	40.2
<i>u</i> 1205	H(37)...H(41)	342.6(199)	41.9(fixed)	—	-0.3	41.9
<i>u</i> 2869	C(131)...F(138)	342.7(69)	21.2(tied to <i>u</i> 1442)	—	-1.1	20.9
<i>u</i> 1390	H(66)...H(69)	342.8(179)	61.1(fixed)	—	-3.8	61.1
<i>u</i> 1333	Si(3)...C(6)	342.8(44)	17.9(tied to <i>u</i> 1442)	—	0.3	17.6
<i>u</i> 1427	C(42)...H(78)	343.0(123)	33.1(fixed)	—	1.5	33.1
<i>u</i> 938	Si(168)...H(182)	343.0(68)	57.5(fixed)	—	46.8	57.5
<i>u</i> 1356	Si(46)...H(76)	343.0(133)	27.5(fixed)	—	4.3	27.5
<i>u</i> 1206	H(242)...H(246)	343.0(199)	40.6(fixed)	—	-0.2	40.6
<i>u</i> 2888	C(130)...F(137)	343.0(69)	16.6(tied to <i>u</i> 1442)	—	-1.3	16.4
<i>u</i> 1405	C(83)...H(119)	343.1(122)	23.7(fixed)	—	0.1	23.7
<i>u</i> 1318	C(53)...H(76)	343.2(303)	44.8(fixed)	—	2.9	44.8
<i>u</i> 1338	H(276)...H(279)	343.2(199)	37.9(fixed)	—	-0.6	37.9
<i>u</i> 2402	H(141)...H(151)	343.2(140)	64.6(fixed)	—	13.6	64.6
<i>u</i> 1372	Si(208)...C(211)	343.3(40)	17.1(tied to <i>u</i> 1442)	—	0.3	16.8

<i>u</i> 1383	C(165)...H(197)	343.3(122)	23.9(fixed)	—	0.3	23.9
<i>u</i> 1382	C(165)...H(187)	343.3(122)	23.9(fixed)	—	0.3	23.9
<i>u</i> 1161	Si(207)...H(229)	343.3(158)	39.0(fixed)	—	11.7	39.0
<i>u</i> 1359	C(42)...H(64)	343.3(122)	23.3(fixed)	—	0.3	23.3
<i>u</i> 921	Si(85)...H(100)	343.3(81)	58.2(fixed)	—	51.3	58.2
<i>u</i> 1348	C(42)...H(74)	343.4(122)	22.8(fixed)	—	0.2	22.8
<i>u</i> 1340	C(247)...H(279)	343.4(122)	22.1(fixed)	—	0.2	22.1
<i>u</i> 1315	C(1)...H(33)	343.4(122)	22.3(fixed)	—	0.2	22.3
<i>u</i> 1353	C(1)...H(37)	343.4(122)	22.1(fixed)	—	0.2	22.1
<i>u</i> 1384	C(42)...H(65)	343.4(122)	23.0(fixed)	—	0.4	23.0
<i>u</i> 1360	C(206)...H(242)	343.4(122)	21.8(fixed)	—	0.2	21.8
<i>u</i> 1424	Si(4)...C(7)	343.5(67)	16.4(tied to <i>u</i> 1442)	—	0.3	16.1
<i>u</i> 1328	C(206)...H(238)	343.5(122)	23.5(fixed)	—	0.4	23.5
<i>u</i> 1366	C(124)...H(147)	343.5(122)	22.6(fixed)	—	0.3	22.6
<i>u</i> 1354	C(1)...H(23)	343.5(122)	23.0(fixed)	—	0.5	23.0
<i>u</i> 1174	H(112)...H(115)	343.6(199)	41.3(fixed)	—	0.5	41.3
<i>u</i> 1346	C(206)...H(228)	343.7(122)	26.2(fixed)	—	1.0	26.2
<i>u</i> 1385	C(124)...H(146)	343.7(123)	29.5(fixed)	—	1.6	29.5
<i>u</i> 1398	C(247)...H(283)	343.9(123)	33.4(fixed)	—	2.5	33.4
<i>u</i> 920	Si(87)...H(111)	343.9(81)	57.1(fixed)	—	51.5	57.1
<i>u</i> 937	Si(166)...H(193)	343.9(68)	54.8(fixed)	—	46.8	54.8
<i>u</i> 1306	C(247)...H(269)	344.0(123)	29.7(fixed)	—	2.0	29.7
<i>u</i> 756	F(262)...H(273)	344.1(114)	25.4(fixed)	—	0.2	25.4
<i>u</i> 1365	H(225)...H(226)	344.2(179)	59.5(fixed)	—	-2.9	59.5
<i>u</i> 2213	Si(250)...H(271)	344.3(57)	83.5(fixed)	—	-9.0	83.5
<i>u</i> 1246	C(218)...F(222)	344.3(62)	27.8(tied to <i>u</i> 1442)	—	1.3	27.3
<i>u</i> 1444	H(284)...H(285)	344.3(179)	60.0(fixed)	—	-2.7	60.0
<i>u</i> 1286	C(206)...H(229)	344.6(123)	29.9(fixed)	—	2.6	29.9
<i>u</i> 867	H(102)...H(105)	344.6(159)	74.7(fixed)	—	48.3	74.7
<i>u</i> 1453	H(59)...H(77)	344.7(284)	73.5(fixed)	—	0.9	73.5
<i>u</i> 1157	C(1)...H(29)	344.7(47)	41.2(fixed)	—	18.4	41.2
<i>u</i> 1388	H(72)...H(75)	344.9(178)	57.5(fixed)	—	-2.9	57.5
<i>u</i> 1785	H(18)...H(28)	345.2(123)	41.3(fixed)	—	-9.5	41.3
<i>u</i> 1520	H(156)...H(161)	345.4(300)	61.6(fixed)	—	1.1	61.6
<i>u</i> 866	H(106)...H(110)	345.5(159)	73.3(fixed)	—	48.5	73.3
<i>u</i> 1481	C(252)...C(255)	345.5(113)	23.9(tied to <i>u</i> 1442)	—	1.4	23.5
<i>u</i> 2986	C(129)...C(132)	345.6(93)	22.6(tied to <i>u</i> 1442)	—	-1.1	22.3
<i>u</i> 1314	C(83)...H(105)	345.7(123)	35.9(fixed)	—	4.8	35.9
<i>u</i> 1238	C(83)...H(111)	345.9(47)	41.9(fixed)	—	19.7	41.9
<i>u</i> 1394	Si(249)...C(259)	346.0(41)	18.0(tied to <i>u</i> 1442)	—	0.3	17.7
<i>u</i> 1358	Si(45)...H(63)	346.1(131)	26.6(fixed)	—	4.7	26.6
<i>u</i> 1253	C(52)...F(55)	346.3(108)	32.6(tied to <i>u</i> 1442)	—	0.1	32.0
<i>u</i> 1436	H(20)...H(21)	346.4(178)	51.6(fixed)	—	-3.2	51.6
<i>u</i> 1313	Si(249)...C(256)	346.4(43)	16.5(tied to <i>u</i> 1442)	—	0.6	16.2

<i>u</i> 1416	Si(85)...C(88)	346.6(60)	20.6(tied to <i>u</i> 1442)	—	1.1	20.3
<i>u</i> 1422	Si(210)...C(216)	346.6(52)	16.9(tied to <i>u</i> 1442)	—	0.4	16.6
<i>u</i> 1395	Si(45)...C(50)	346.7(45)	17.1(tied to <i>u</i> 1442)	—	0.4	16.8
<i>u</i> 1245	C(254)...F(260)	346.7(64)	25.8(tied to <i>u</i> 1442)	—	1.1	25.4
<i>u</i> 1377	H(70)...H(71)	346.8(170)	65.8(fixed)	—	18.3	65.8
<i>u</i> 1350	H(191)...H(204)	346.9(229)	118.1(fixed)	—	51.1	118.1
<i>u</i> 1386	Si(44)...C(54)	346.9(41)	15.3(tied to <i>u</i> 1442)	—	0.8	15.0
<i>u</i> 839	Si(5)...H(29)	346.9(66)	48.4(fixed)	—	42.9	48.4
<i>u</i> 1298	C(8)...F(14)	347.0(93)	31.0(tied to <i>u</i> 1442)	—	1.0	30.5
<i>u</i> 1142	Si(86)...H(105)	347.0(173)	47.9(fixed)	—	23.1	47.9
<i>u</i> 1140	Si(84)...H(106)	347.1(173)	47.8(fixed)	—	23.1	47.8
<i>u</i> 1266	C(13)...F(17)	347.1(96)	27.7(tied to <i>u</i> 1442)	—	1.3	27.2
<i>u</i> 1497	H(79)...H(80)	347.2(178)	51.7(fixed)	—	-2.4	51.7
<i>u</i> 1404	Si(85)...C(95)	347.4(69)	17.1(tied to <i>u</i> 1442)	—	0.7	16.8
<i>u</i> 1375	H(266)...H(267)	347.6(178)	54.7(fixed)	—	-1.1	54.7
<i>u</i> 2428	Si(126)...C(129)	347.6(38)	11.8(tied to <i>u</i> 1442)	—	-1.2	11.6
<i>u</i> 1265	C(1)...H(24)	347.7(123)	37.5(fixed)	—	7.2	37.5
<i>u</i> 1273	C(214)...F(222)	347.8(72)	26.2(tied to <i>u</i> 1442)	—	0.9	25.8
<i>u</i> 1322	H(59)...H(67)	348.0(304)	75.0(fixed)	—	4.2	75.0
<i>u</i> 1432	Si(251)...C(255)	348.0(41)	16.3(tied to <i>u</i> 1442)	—	0.4	16.1
<i>u</i> 1325	Si(250)...H(268)	348.2(124)	28.6(fixed)	—	10.7	28.6
<i>u</i> 1401	Si(207)...C(215)	348.4(35)	15.9(tied to <i>u</i> 1442)	—	0.5	15.6
<i>u</i> 1502	H(63)...H(70)	348.6(298)	85.0(fixed)	—	1.2	85.0
<i>u</i> 1339	H(61)...H(62)	348.6(177)	49.5(fixed)	—	-1.6	49.5
<i>u</i> 1460	H(279)...H(284)	348.7(86)	72.3(fixed)	—	-1.4	72.3
<i>u</i> 1632	C(212)...C(215)	348.8(78)	29.7(tied to <i>u</i> 1442)	—	1.1	29.2
<i>u</i> 1352	H(182)...H(194)	349.2(187)	120.6(fixed)	—	51.1	120.6
<i>u</i> 1105	Si(2)...H(24)	349.4(164)	49.2(fixed)	—	24.2	49.2
<i>u</i> 1310	C(254)...C(256)	349.6(57)	26.2(tied to <i>u</i> 1442)	—	1.8	25.8
<i>u</i> 1435	H(161)...H(162)	350.1(177)	46.5(fixed)	—	-1.0	46.5
<i>u</i> 1324	C(213)...F(219)	350.3(56)	33.0(tied to <i>u</i> 1442)	—	1.0	32.5
<i>u</i> 1784	H(26)...H(40)	350.3(215)	53.5(fixed)	—	-9.0	53.5
<i>u</i> 1415	H(38)...H(39)	350.3(176)	40.7(fixed)	—	-2.2	40.7
<i>u</i> 1555	C(259)...H(266)	350.4(137)	59.9(fixed)	—	2.5	59.9
<i>u</i> 1515	H(120)...H(121)	350.5(176)	39.1(fixed)	—	-2.3	39.1
<i>u</i> 1548	F(261)...H(269)	350.5(235)	53.2(fixed)	—	-5.0	53.2
<i>u</i> 1464	C(91)...C(95)	350.6(124)	34.6(tied to <i>u</i> 1442)	—	2.3	34.0
<i>u</i> 1410	Si(166)...C(173)	350.6(36)	22.0(tied to <i>u</i> 1442)	—	1.2	21.7
<i>u</i> 1411	Si(168)...C(170)	350.6(36)	22.0(tied to <i>u</i> 1442)	—	1.2	21.7
<i>u</i> 1441	H(243)...H(244)	350.6(176)	39.4(fixed)	—	-2.2	39.4
<i>u</i> 1750	H(104)...H(114)	350.9(327)	70.7(fixed)	—	-7.3	70.7
<i>u</i> 1751	H(108)...H(122)	350.9(327)	70.6(fixed)	—	-7.3	70.6
<i>u</i> 1414	H(277)...H(280)	351.1(176)	40.3(fixed)	—	-1.5	40.3
<i>u</i> 1752	H(106)...H(115)	351.3(492)	69.4(fixed)	—	-16.2	69.4

<i>u</i> 1470	H(236)...H(239)	351.5(176)	39.0(fixed)	—	-1.3	39.0
<i>u</i> 1334	H(31)...H(34)	351.5(176)	39.4(fixed)	—	-1.2	39.4
<i>u</i> 1679	H(226)...H(238)	351.6(257)	46.9(fixed)	—	4.0	46.9
<i>u</i> 1430	Si(125)...C(134)	351.6(38)	17.2(tied to <i>u</i> 1442)	—	0.2	16.9
<i>u</i> 1423	Si(210)...F(221)	351.9(31)	17.7(tied to <i>u</i> 1442)	—	-0.3	17.4
<i>u</i> 1706	H(227)...H(238)	352.1(225)	46.3(fixed)	—	1.5	46.3
<i>u</i> 2881	Si(127)...H(145)	352.2(86)	23.1(fixed)	—	-0.7	23.1
<i>u</i> 1413	C(90)...C(93)	352.5(124)	23.4(tied to <i>u</i> 1442)	—	3.3	23.1
<i>u</i> 1773	H(227)...H(237)	352.5(263)	60.9(fixed)	—	5.3	60.9
<i>u</i> 785	F(262)...H(275)	352.5(95)	24.8(fixed)	—	0.5	24.8
<i>u</i> 1615	H(107)...H(122)	353.0(279)	62.1(fixed)	—	-1.5	62.1
<i>u</i> 1639	Si(208)...H(225)	353.0(84)	53.4(fixed)	—	-1.4	53.4
<i>u</i> 1479	C(170)...C(176)	353.1(49)	38.7(tied to <i>u</i> 1442)	—	3.6	38.0
<i>u</i> 1512	C(10)...F(14)	353.2(56)	33.6(tied to <i>u</i> 1442)	—	1.0	33.0
<i>u</i> 1408	C(257)...C(258)	353.5(81)	21.2(tied to <i>u</i> 1442)	—	2.0	20.9
<i>u</i> 1474	C(215)...C(217)	353.8(54)	23.4(tied to <i>u</i> 1442)	—	1.7	23.0
<i>u</i> 1673	Si(209)...H(227)	353.8(243)	41.4(fixed)	—	0.2	41.4
<i>u</i> 1431	Si(44)...F(56)	353.8(61)	18.7(tied to <i>u</i> 1442)	—	-0.3	18.4
<i>u</i> 1495	C(94)...F(99)	353.8(166)	45.9(tied to <i>u</i> 1442)	—	-0.4	45.1
<i>u</i> 1396	Si(248)...C(257)	353.8(38)	16.7(tied to <i>u</i> 1442)	—	0.5	16.4
<i>u</i> 1421	H(68)...H(73)	353.8(184)	66.5(fixed)	—	18.5	66.5
<i>u</i> 1442	Si(5)...F(16)	354.0(17)	17.7(14)	—	-0.3	17.4
<i>u</i> 944	H(230)...H(233)	354.0(180)	65.2(fixed)	—	8.8	65.2
<i>u</i> 1448	H(74)...H(79)	354.2(89)	71.8(fixed)	—	1.0	71.8
<i>u</i> 1380	Si(46)...C(53)	354.3(34)	17.0(tied to <i>u</i> 1442)	—	0.5	16.8
<i>u</i> 1892	C(175)...H(193)	354.5(90)	125.9(fixed)	—	-8.4	125.9
<i>u</i> 1546	C(7)...C(11)	354.6(115)	27.7(tied to <i>u</i> 1442)	—	1.1	27.2
<i>u</i> 2034	H(272)...H(273)	354.7(133)	31.2(fixed)	—	-19.9	31.2
<i>u</i> 1429	Si(5)...C(9)	354.7(36)	16.6(tied to <i>u</i> 1442)	—	0.2	16.4
<i>u</i> 1425	Si(210)...C(217)	354.8(34)	17.2(tied to <i>u</i> 1442)	—	0.3	16.9
<i>u</i> 1393	Si(2)...C(11)	354.8(34)	16.2(tied to <i>u</i> 1442)	—	0.6	16.0
<i>u</i> 1466	Si(43)...C(47)	355.0(59)	16.9(tied to <i>u</i> 1442)	—	0.4	16.6
<i>u</i> 1498	C(88)...C(91)	355.0(226)	20.8(tied to <i>u</i> 1442)	—	1.6	20.5
<i>u</i> 1403	Si(44)...C(51)	355.1(57)	17.2(tied to <i>u</i> 1442)	—	0.4	17.0
<i>u</i> 1519	H(237)...H(243)	355.1(219)	47.0(fixed)	—	4.3	47.0
<i>u</i> 1457	C(49)...C(54)	355.2(80)	23.1(tied to <i>u</i> 1442)	—	2.0	22.8
<i>u</i> 1792	C(54)...H(61)	355.4(144)	63.5(fixed)	—	1.5	63.5
<i>u</i> 1695	H(228)...H(239)	355.6(277)	44.2(fixed)	—	10.2	44.2
<i>u</i> 1468	Si(251)...H(281)	356.1(110)	29.2(fixed)	—	3.2	29.2
<i>u</i> 1445	Si(248)...C(252)	356.1(52)	16.5(tied to <i>u</i> 1442)	—	0.3	16.2
<i>u</i> 1685	H(23)...H(34)	356.1(134)	52.8(fixed)	—	4.4	52.8
<i>u</i> 1472	Si(168)...F(181)	356.3(23)	23.9(tied to <i>u</i> 1442)	—	-0.3	23.5
<i>u</i> 1471	Si(166)...F(180)	356.3(23)	23.9(tied to <i>u</i> 1442)	—	-0.3	23.5
<i>u</i> 1494	C(6)...C(9)	356.3(88)	25.8(tied to <i>u</i> 1442)	—	0.5	25.3

<i>u</i> 1716	H(188)...H(196)	356.3(363)	102.4(fixed)	—	-10.9	102.4
<i>u</i> 1537	Si(3)...H(20)	356.3(91)	49.5(fixed)	—	-0.9	49.5
<i>u</i> 1787	H(223)...H(233)	356.7(127)	41.1(fixed)	—	-1.1	41.1
<i>u</i> 1319	Si(209)...H(231)	356.7(100)	29.9(fixed)	—	10.3	29.9
<i>u</i> 1715	H(187)...H(204)	356.8(363)	101.6(fixed)	—	-10.9	101.6
<i>u</i> 1527	Si(125)...H(149)	356.8(87)	27.4(fixed)	—	4.6	27.4
<i>u</i> 1722	Si(207)...H(233)	356.9(61)	49.2(fixed)	—	11.6	49.2
<i>u</i> 1543	Si(3)...H(31)	357.0(80)	32.2(fixed)	—	0.5	32.2
<i>u</i> 1496	Si(87)...F(98)	357.0(62)	21.9(tied to <i>u</i> 1442)	—	-0.4	21.5
<i>u</i> 1881	C(95)...H(111)	357.3(193)	128.3(fixed)	—	-9.9	128.3
<i>u</i> 1883	C(92)...H(100)	357.4(193)	128.1(fixed)	—	-9.9	128.1
<i>u</i> 1452	Si(248)...F(263)	357.5(50)	18.4(tied to <i>u</i> 1442)	—	-0.3	18.1
<i>u</i> 1455	C(47)...C(49)	357.5(115)	24.9(tied to <i>u</i> 1442)	—	1.5	24.5
<i>u</i> 1556	C(255)...C(259)	357.6(80)	27.6(tied to <i>u</i> 1442)	—	1.4	27.1
<i>u</i> 1545	F(16)...H(28)	357.6(11)	25.4(fixed)	—	-12.8	25.4
<i>u</i> 1459	Si(43)...F(58)	357.6(61)	19.0(tied to <i>u</i> 1442)	—	-0.3	18.7
<i>u</i> 795	H(25)...H(28)	357.9(182)	79.0(fixed)	—	18.3	79.0
<i>u</i> 1593	F(178)...H(203)	357.9(11)	18.4(fixed)	—	-13.1	18.4
<i>u</i> 1454	Si(5)...C(12)	358.0(43)	17.7(tied to <i>u</i> 1442)	—	0.2	17.4
<i>u</i> 1620	Si(4)...H(22)	358.0(244)	36.3(fixed)	—	0.1	36.3
<i>u</i> 1594	F(180)...H(192)	358.0(11)	19.1(fixed)	—	-13.1	19.1
<i>u</i> 1558	F(55)...H(73)	358.1(163)	59.2(fixed)	—	-5.6	59.2
<i>u</i> 1689	Si(45)...H(69)	358.1(92)	58.9(fixed)	—	-2.3	58.9
<i>u</i> 1634	F(56)...H(64)	358.2(257)	38.1(fixed)	—	-1.5	38.1
<i>u</i> 1661	C(212)...C(216)	358.3(84)	24.2(tied to <i>u</i> 1442)	—	0.5	23.8
<i>u</i> 1598	F(16)...H(24)	358.3(11)	15.7(fixed)	—	-11.4	15.7
<i>u</i> 1397	Si(84)...H(117)	358.5(135)	27.6(fixed)	—	4.6	27.6
<i>u</i> 1478	Si(87)...C(94)	358.7(70)	20.3(tied to <i>u</i> 1442)	—	0.2	20.0
<i>u</i> 1763	H(24)...H(32)	358.9(192)	63.3(fixed)	—	-12.9	63.3
<i>u</i> 1541	C(170)...C(174)	358.9(154)	21.6(tied to <i>u</i> 1442)	—	1.3	21.3
<i>u</i> 1433	Si(210)...C(214)	359.0(42)	16.3(tied to <i>u</i> 1442)	—	0.2	16.0
<i>u</i> 1579	H(264)...H(282)	359.2(245)	69.3(fixed)	—	-1.6	69.3
<i>u</i> 1604	F(58)...H(74)	359.2(255)	37.8(fixed)	—	-1.1	37.8
<i>u</i> 1449	Si(43)...C(52)	359.3(53)	18.2(tied to <i>u</i> 1442)	—	0.2	17.9
<i>u</i> 1507	H(66)...H(81)	359.4(225)	50.7(fixed)	—	4.0	50.7
<i>u</i> 1443	Si(251)...C(258)	359.4(36)	17.5(tied to <i>u</i> 1442)	—	0.3	17.2
<i>u</i> 1597	F(98)...H(110)	359.5(11)	20.4(fixed)	—	-12.3	20.4
<i>u</i> 1687	H(228)...H(240)	359.6(205)	42.3(fixed)	—	6.9	42.3
<i>u</i> 1434	H(60)...H(78)	359.7(167)	68.1(fixed)	—	19.2	68.1
<i>u</i> 1505	C(211)...C(214)	359.8(90)	24.0(tied to <i>u</i> 1442)	—	0.4	23.6
<i>u</i> 1691	Si(210)...H(236)	359.8(61)	30.9(fixed)	—	3.3	30.9
<i>u</i> 1516	Si(251)...F(262)	359.8(29)	18.4(tied to <i>u</i> 1442)	—	-0.3	18.1
<i>u</i> 1465	Si(46)...C(49)	359.8(47)	18.3(tied to <i>u</i> 1442)	—	0.2	18.0
<i>u</i> 1530	Si(3)...H(39)	359.8(101)	35.3(fixed)	—	0.2	35.3

<i>u</i> 2223	H(271)...H(275)	359.9(42)	60.2(fixed)	—	-3.4	60.2
<i>u</i> 1606	F(98)...H(106)	359.9(10)	14.9(fixed)	—	-10.8	14.9
<i>u</i> 1547	F(221)...H(233)	360.0(11)	21.2(fixed)	—	-11.3	21.2
<i>u</i> 1450	Si(125)...C(130)	360.3(33)	17.3(tied to <i>u</i> 1442)	—	0.5	17.0
<i>u</i> 1602	F(260)...H(283)	360.6(10)	16.1(fixed)	—	-9.5	16.1
<i>u</i> 1369	Si(166)...H(199)	361.0(141)	29.4(fixed)	—	6.8	29.4
<i>u</i> 1370	Si(168)...H(200)	361.0(141)	29.4(fixed)	—	6.8	29.4
<i>u</i> 1725	H(233)...H(246)	361.0(111)	53.8(fixed)	—	22.6	53.8
<i>u</i> 1531	C(211)...C(216)	361.1(75)	26.5(tied to <i>u</i> 1442)	—	1.4	26.0
<i>u</i> 1524	Si(208)...H(244)	361.1(77)	33.7(fixed)	—	0.5	33.7
<i>u</i> 1544	H(230)...H(245)	361.2(223)	52.9(fixed)	—	3.1	52.9
<i>u</i> 2070	Si(5)...H(28)	361.3(72)	67.2(fixed)	—	-12.4	67.2
<i>u</i> 1557	H(223)...H(240)	361.4(270)	76.3(fixed)	—	1.6	76.3
<i>u</i> 1389	Si(46)...H(77)	361.4(237)	54.2(fixed)	—	4.4	54.2
<i>u</i> 1647	Si(125)...H(158)	361.5(232)	35.3(fixed)	—	0.1	35.3
<i>u</i> 1563	F(55)...H(78)	361.6(10)	15.9(fixed)	—	-8.7	15.9
<i>u</i> 1482	Si(44)...C(48)	361.6(56)	18.8(tied to <i>u</i> 1442)	—	0.2	18.5
<i>u</i> 1438	C(11)...C(12)	361.8(108)	22.2(tied to <i>u</i> 1442)	—	1.9	21.8
<i>u</i> 1440	F(220)...H(229)	362.0(233)	58.0(fixed)	—	-4.1	58.0
<i>u</i> 1577	Si(44)...H(80)	362.1(84)	32.2(fixed)	—	0.4	32.2
<i>u</i> 1417	Si(208)...H(240)	362.2(89)	27.8(fixed)	—	4.4	27.8
<i>u</i> 1518	C(48)...C(50)	362.2(84)	25.9(tied to <i>u</i> 1442)	—	1.4	25.5
<i>u</i> 1501	C(52)...C(53)	362.3(89)	25.2(tied to <i>u</i> 1442)	—	1.4	24.8
<i>u</i> 1426	Si(248)...C(254)	362.4(35)	16.9(tied to <i>u</i> 1442)	—	0.2	16.6
<i>u</i> 1461	Si(87)...F(97)	362.6(84)	20.6(tied to <i>u</i> 1442)	—	-0.4	20.2
<i>u</i> 1536	C(50)...C(51)	362.8(136)	20.8(tied to <i>u</i> 1442)	—	0.6	20.5
<i>u</i> 1901	H(76)...H(78)	362.9(136)	77.3(fixed)	—	-5.0	77.3
<i>u</i> 1456	Si(86)...C(89)	363.0(53)	21.7(tied to <i>u</i> 1442)	—	0.9	21.3
<i>u</i> 1642	Si(5)...H(35)	363.0(100)	28.8(fixed)	—	3.1	28.8
<i>u</i> 1609	F(57)...H(69)	363.1(11)	13.6(fixed)	—	-8.2	13.6
<i>u</i> 1190	C(254)...H(274)	363.2(133)	26.2(fixed)	—	0.1	26.2
<i>u</i> 1551	Si(210)...H(240)	363.2(230)	34.5(fixed)	—	0.3	34.5
<i>u</i> 1624	F(263)...H(269)	363.3(11)	13.2(fixed)	—	-6.5	13.2
<i>u</i> 1532	C(13)...H(29)	363.3(106)	110.1(fixed)	—	-3.8	110.1
<i>u</i> 1522	Si(2)...H(35)	363.3(228)	30.5(fixed)	—	0.8	30.5
<i>u</i> 1678	H(59)...H(79)	363.4(238)	46.7(fixed)	—	4.6	46.7
<i>u</i> 1566	F(137)...H(160)	363.4(10)	13.7(fixed)	—	-6.7	13.7
<i>u</i> 1638	Si(249)...H(285)	363.4(82)	40.6(fixed)	—	-0.5	40.6
<i>u</i> 1608	F(138)...H(154)	363.5(11)	14.6(fixed)	—	-8.3	14.6
<i>u</i> 1486	Si(249)...C(253)	363.5(49)	18.8(tied to <i>u</i> 1442)	—	0.2	18.5
<i>u</i> 1616	F(221)...H(229)	363.5(10)	13.6(fixed)	—	-6.6	13.6
<i>u</i> 1491	H(224)...H(234)	363.8(130)	67.4(fixed)	—	27.8	67.4
<i>u</i> 1619	Si(249)...H(266)	364.0(82)	31.5(fixed)	—	6.6	31.5
<i>u</i> 1804	H(188)...H(194)	364.2(279)	74.6(fixed)	—	-8.4	74.6

<i>u</i> 1589	F(56)...H(72)	364.3(11)	14.4(fixed)	—	-8.0	14.4
<i>u</i> 3204	H(271)...H(287)	364.3(108)	42.7(fixed)	—	-31.3	42.7
<i>u</i> 1484	Si(166)...C(171)	364.4(31)	23.6(tied to <i>u</i> 1442)	—	0.9	23.2
<i>u</i> 1485	Si(168)...C(172)	364.4(31)	23.6(tied to <i>u</i> 1442)	—	0.9	23.2
<i>u</i> 1743	Si(2)...H(28)	364.5(49)	60.5(fixed)	—	16.8	60.5
<i>u</i> 1803	H(187)...H(205)	364.6(278)	73.4(fixed)	—	-8.4	73.4
<i>u</i> 1559	Si(249)...H(277)	364.7(84)	35.7(fixed)	—	-0.3	35.7
<i>u</i> 1463	Si(43)...H(72)	364.7(93)	37.0(fixed)	—	12.6	37.0
<i>u</i> 1483	Si(2)...C(8)	364.8(29)	18.2(tied to <i>u</i> 1442)	—	0.2	17.9
<i>u</i> 1625	Si(44)...H(61)	365.0(95)	32.1(fixed)	—	7.4	32.1
<i>u</i> 1488	C(254)...C(259)	365.1(72)	26.9(tied to <i>u</i> 1442)	—	0.6	26.4
<i>u</i> 1677	F(15)...H(22)	365.1(239)	40.9(fixed)	—	-2.9	40.9
<i>u</i> 1571	F(220)...H(238)	365.2(12)	12.2(fixed)	—	-3.5	12.2
<i>u</i> 1500	C(218)...H(234)	365.2(126)	85.3(fixed)	—	-2.2	85.3
<i>u</i> 1517	Si(3)...F(14)	365.3(53)	18.8(tied to <i>u</i> 1442)	—	-0.4	18.5
<i>u</i> 1583	F(58)...H(61)	365.4(11)	13.7(fixed)	—	-5.6	13.7
<i>u</i> 1618	F(222)...H(225)	365.5(11)	13.1(fixed)	—	-6.7	13.1
<i>u</i> 1599	F(222)...H(228)	365.5(10)	12.7(fixed)	—	-5.0	12.7
<i>u</i> 1447	C(7)...C(12)	365.5(89)	22.8(tied to <i>u</i> 1442)	—	1.5	22.4
<i>u</i> 1600	F(58)...H(64)	365.7(11)	12.3(fixed)	—	-3.5	12.3
<i>u</i> 1595	F(178)...H(201)	365.8(11)	12.5(fixed)	—	-3.9	12.5
<i>u</i> 1929	H(226)...H(236)	365.8(94)	43.2(fixed)	—	0.3	43.2
<i>u</i> 1553	Si(4)...H(36)	365.8(109)	26.6(fixed)	—	3.9	26.6
<i>u</i> 2887	Si(126)...H(158)	365.8(91)	20.3(fixed)	—	-1.0	20.3
<i>u</i> 1582	F(57)...H(65)	365.9(11)	12.5(fixed)	—	-3.7	12.5
<i>u</i> 1596	F(180)...H(188)	366.0(11)	12.5(fixed)	—	-3.9	12.5
<i>u</i> 1428	C(212)...C(217)	366.0(78)	21.5(tied to <i>u</i> 1442)	—	1.7	21.2
<i>u</i> 1499	Si(3)...F(17)	366.0(43)	16.9(tied to <i>u</i> 1442)	—	-0.3	16.6
<i>u</i> 1568	Si(210)...H(241)	366.3(228)	31.9(fixed)	—	0.4	31.9
<i>u</i> 829	Si(126)...F(140)	366.3(24)	19.0(tied to <i>u</i> 1442)	—	0.2	18.7
<i>u</i> 1564	Si(209)...H(241)	366.3(94)	27.4(fixed)	—	3.7	27.4
<i>u</i> 1576	F(96)...H(119)	366.4(11)	12.4(fixed)	—	-3.5	12.4
<i>u</i> 4057	C(131)...C(134)	366.5(82)	12.8(tied to <i>u</i> 1442)	—	-1.9	12.6
<i>u</i> 1701	Si(86)...H(104)	366.5(243)	75.3(fixed)	—	-1.2	75.3
<i>u</i> 1585	F(263)...H(266)	366.6(11)	12.9(fixed)	—	-5.0	12.9
<i>u</i> 1540	Si(248)...H(281)	366.7(227)	30.1(fixed)	—	0.4	30.1
<i>u</i> 1569	F(138)...H(156)	366.7(10)	12.4(fixed)	—	-3.5	12.4
<i>u</i> 1542	Si(208)...F(219)	366.7(28)	19.5(tied to <i>u</i> 1442)	—	-0.4	19.2
<i>u</i> 1567	F(261)...H(279)	366.7(11)	12.0(fixed)	—	-2.9	12.0
<i>u</i> 1538	Si(251)...H(282)	366.8(233)	58.6(fixed)	—	2.4	58.6
<i>u</i> 1575	F(219)...H(242)	366.9(11)	12.2(fixed)	—	-3.1	12.2
<i>u</i> 1753	H(65)...H(80)	366.9(286)	49.6(fixed)	—	2.0	49.6
<i>u</i> 1526	Si(249)...F(260)	367.0(33)	17.1(tied to <i>u</i> 1442)	—	-0.3	16.9
<i>u</i> 1525	Si(4)...H(20)	367.2(68)	32.2(fixed)	—	8.0	32.2

<i>u1617</i>	F(17)...H(20)	367.4(11)	13.0(fixed)	—	-5.6	13.0
<i>u1629</i>	Si(207)...H(236)	367.4(71)	33.2(fixed)	—	0.1	33.2
<i>u1581</i>	F(56)...H(74)	367.4(10)	12.1(fixed)	—	-3.3	12.1
<i>u1490</i>	Si(45)...F(57)	367.5(47)	18.5(tied to <i>u1442</i> )	—	-0.3	18.2
<i>u1603</i>	F(220)...H(236)	367.5(12)	12.1(fixed)	—	-3.2	12.1
<i>u1858</i>	H(228)...H(235)	367.6(264)	57.8(fixed)	—	6.3	57.8
<i>u1592</i>	F(14)...H(37)	367.6(10)	12.2(fixed)	—	-3.2	12.2
<i>u1493</i>	Si(85)...H(113)	367.6(116)	30.8(fixed)	—	4.8	30.8
<i>u1572</i>	F(17)...H(23)	367.8(10)	12.2(fixed)	—	-3.6	12.2
<i>u1480</i>	C(172)...C(174)	367.9(143)	38.7(tied to <i>u1442</i> )	—	3.6	38.0
<i>u1610</i>	F(260)...H(285)	367.9(11)	12.3(fixed)	—	-4.2	12.3
<i>u1570</i>	F(15)...H(33)	367.9(10)	12.0(fixed)	—	-3.0	12.0
<i>u1391</i>	C(255)...H(271)	368.0(19)	65.9(fixed)	—	-1.8	65.9
<i>u1612</i>	H(35)...H(37)	368.0(158)	45.0(fixed)	—	3.3	45.0
<i>u1588</i>	Si(85)...H(121)	368.0(130)	38.4(fixed)	—	0.0	38.4
<i>u1591</i>	F(261)...H(277)	368.1(11)	12.1(fixed)	—	-3.4	12.1
<i>u1648</i>	Si(126)...F(137)	368.2(36)	17.0(tied to <i>u1442</i> )	—	-0.3	16.8
<i>u1584</i>	F(96)...H(121)	368.2(11)	12.3(fixed)	—	-3.6	12.3
<i>u1539</i>	C(47)...C(53)	368.2(122)	22.1(tied to <i>u1442</i> )	—	0.8	21.8
<i>u1523</i>	Si(43)...H(67)	368.4(103)	27.6(fixed)	—	4.8	27.6
<i>u1590</i>	F(219)...H(244)	368.5(11)	12.1(fixed)	—	-3.3	12.1
<i>u1099</i>	Si(128)...F(138)	368.5(36)	18.0(tied to <i>u1442</i> )	—	0.1	17.7
<i>u2949</i>	Si(126)...H(143)	368.5(75)	20.5(fixed)	—	-2.3	20.5
<i>u1646</i>	Si(5)...H(36)	368.5(237)	32.8(fixed)	—	0.3	32.8
<i>u2662</i>	H(144)...H(159)	368.6(112)	60.1(fixed)	—	-11.1	60.1
<i>u1504</i>	Si(207)...C(213)	368.6(37)	19.0(tied to <i>u1442</i> )	—	0.2	18.7
<i>u1550</i>	C(130)...C(135)	368.6(82)	22.5(tied to <i>u1442</i> )	—	1.1	22.1
<i>u1754</i>	H(225)...H(234)	368.6(140)	53.1(fixed)	—	15.4	53.1
<i>u1549</i>	Si(249)...F(261)	368.7(34)	18.0(tied to <i>u1442</i> )	—	-0.3	17.7
<i>u1611</i>	F(137)...H(162)	368.7(11)	12.1(fixed)	—	-3.2	12.1
<i>u1699</i>	H(69)...H(73)	368.9(208)	50.2(fixed)	—	9.4	50.2
<i>u1607</i>	F(14)...H(39)	368.9(11)	12.2(fixed)	—	-3.5	12.2
<i>u1613</i>	F(55)...H(80)	369.1(11)	12.1(fixed)	—	-3.2	12.1
<i>u1682</i>	H(264)...H(284)	369.2(233)	52.8(fixed)	—	1.9	52.8
<i>u1605</i>	F(15)...H(31)	369.3(11)	12.1(fixed)	—	-3.2	12.1
<i>u1521</i>	Si(2)...H(22)	369.4(97)	26.9(fixed)	—	5.1	26.9
<i>u1703</i>	H(70)...H(72)	369.6(201)	49.3(fixed)	—	9.4	49.3
<i>u1756</i>	H(236)...H(242)	369.7(273)	47.9(fixed)	—	2.6	47.9
<i>u594</i>	F(262)...H(271)	369.8(11)	36.0(fixed)	—	27.7	36.0
<i>u1510</i>	Si(4)...H(26)	369.9(91)	40.4(fixed)	—	20.0	40.4
<i>u1833</i>	Si(125)...H(143)	369.9(51)	34.6(fixed)	—	2.9	34.6
<i>u1779</i>	H(224)...H(238)	369.9(257)	57.4(fixed)	—	0.8	57.4
<i>u1623</i>	C(8)...C(13)	370.5(89)	22.9(tied to <i>u1442</i> )	—	0.7	22.5
<i>u2252</i>	C(253)...H(274)	370.7(277)	35.5(fixed)	—	-2.9	35.5



<i>u1645</i>	C(252)...C(259)	370.8(91)	29.4(tied to <i>u1442</i> )	—	1.2	28.9
<i>u1636</i>	H(23)...H(36)	371.0(128)	54.0(fixed)	—	2.6	54.0
<i>u1651</i>	Si(169)...H(200)	371.3(249)	47.4(fixed)	—	0.0	47.4
<i>u1786</i>	H(64)...H(68)	371.4(253)	57.4(fixed)	—	-1.9	57.4
<i>u1654</i>	Si(3)...F(15)	371.4(29)	17.4(tied to <i>u1442</i> )	—	-0.4	17.1
<i>u1506</i>	Si(250)...H(282)	371.5(96)	33.8(fixed)	—	17.6	33.8
<i>u1811</i>	H(60)...H(65)	371.5(274)	49.3(fixed)	—	-0.1	49.3
<i>u1554</i>	H(228)...H(241)	371.6(109)	61.3(fixed)	—	1.3	61.3
<i>u1802</i>	H(231)...H(245)	371.7(184)	48.0(fixed)	—	-2.0	48.0
<i>u1958</i>	H(25)...H(31)	371.9(154)	43.9(fixed)	—	-14.5	43.9
<i>u1720</i>	H(235)...H(241)	372.0(77)	34.7(fixed)	—	4.7	34.7
<i>u1893</i>	C(172)...H(196)	372.0(230)	126.2(fixed)	—	-8.5	126.2
<i>u1533</i>	Si(208)...F(222)	372.0(36)	17.3(tied to <i>u1442</i> )	—	-0.3	17.1
<i>u1489</i>	Si(84)...H(104)	372.1(120)	37.2(fixed)	—	23.0	37.2
<i>u1574</i>	Si(207)...F(220)	372.1(15)	17.8(tied to <i>u1442</i> )	—	-0.3	17.6
<i>u2098</i>	H(27)...H(39)	372.1(165)	53.4(fixed)	—	-22.4	53.4
<i>u1529</i>	H(19)...H(29)	372.3(120)	69.0(fixed)	—	43.1	69.0
<i>u1560</i>	H(226)...H(242)	372.6(83)	53.3(fixed)	—	1.6	53.3
<i>u2655</i>	Si(248)...H(273)	372.6(157)	21.9(fixed)	—	-3.9	21.9
<i>u1514</i>	Si(207)...H(227)	372.6(88)	27.2(fixed)	—	7.4	27.2
<i>u1635</i>	Si(46)...H(69)	372.8(73)	35.7(fixed)	—	12.8	35.7
<i>u1719</i>	Si(44)...H(72)	372.8(106)	58.1(fixed)	—	-3.1	58.1
<i>u1552</i>	Si(125)...H(145)	373.0(227)	47.8(fixed)	—	1.7	47.8
<i>u2232</i>	H(272)...H(285)	373.2(125)	109.3(fixed)	—	-6.4	109.3
<i>u2072</i>	Si(210)...H(233)	373.5(80)	53.7(fixed)	—	-9.9	53.7
<i>u2306</i>	H(271)...H(276)	373.5(95)	122.7(fixed)	—	-5.3	122.7
<i>u1770</i>	F(261)...H(267)	373.6(200)	35.9(fixed)	—	-6.2	35.9
<i>u1894</i>	Si(2)...H(26)	373.8(220)	62.5(fixed)	—	-3.5	62.5
<i>u1663</i>	Si(248)...H(277)	373.9(62)	33.4(fixed)	—	3.2	33.4
<i>u4601</i>	H(144)...H(154)	373.9(170)	34.4(fixed)	—	-9.6	34.4
<i>u1670</i>	Si(209)...H(225)	373.9(64)	32.3(fixed)	—	9.9	32.3
<i>u1534</i>	Si(45)...H(77)	374.0(91)	32.8(fixed)	—	15.2	32.8
<i>u1790</i>	H(64)...H(70)	374.3(303)	60.2(fixed)	—	-6.3	60.2
<i>u1659</i>	C(89)...C(92)	374.4(173)	26.8(tied to <i>u1442</i> )	—	1.0	26.4
<i>u2068</i>	H(232)...H(244)	374.5(142)	48.7(fixed)	—	-16.8	48.7
<i>u1649</i>	Si(44)...F(55)	374.6(36)	17.4(tied to <i>u1442</i> )	—	-0.3	17.2
<i>u1735</i>	H(59)...H(65)	374.6(329)	55.8(fixed)	—	-3.6	55.8
<i>u1788</i>	H(22)...H(33)	374.9(137)	52.6(fixed)	—	3.2	52.6
<i>u1827</i>	H(21)...H(35)	375.0(143)	39.8(fixed)	—	1.9	39.8
<i>u1628</i>	Si(85)...H(117)	375.8(254)	32.1(fixed)	—	0.6	32.1
<i>u1586</i>	H(33)...H(38)	375.9(112)	49.1(fixed)	—	3.6	49.1
<i>u1637</i>	Si(46)...H(67)	376.4(227)	37.2(fixed)	—	0.3	37.2
<i>u1755</i>	H(28)...H(41)	376.8(91)	65.1(fixed)	—	31.4	65.1
<i>u1707</i>	H(67)...H(82)	376.9(115)	35.3(fixed)	—	7.2	35.3

<i>u</i> 1723	H(20)...H(29)	377.0(135)	58.2(fixed)	—	27.8	58.2
<i>u</i> 1933	H(270)...H(275)	377.4(96)	36.9(fixed)	—	15.9	36.9
<i>u</i> 1573	H(21)...H(37)	377.4(96)	49.5(fixed)	—	3.0	49.5
<i>u</i> 1895	Si(43)...H(61)	377.5(107)	43.3(fixed)	—	-2.2	43.3
<i>u</i> 1921	C(93)...H(106)	377.5(278)	84.2(fixed)	—	-12.0	84.2
<i>u</i> 1776	C(47)...C(54)	377.9(94)	32.2(tied to <i>u</i> 1442)	—	1.2	31.7
<i>u</i> 1580	Si(210)...H(244)	378.0(58)	32.1(fixed)	—	3.4	32.1
<i>u</i> 1641	C(252)...C(258)	378.1(103)	23.0(tied to <i>u</i> 1442)	—	0.4	22.6
<i>u</i> 1667	F(178)...H(197)	378.3(283)	52.8(fixed)	—	-1.2	52.8
<i>u</i> 1668	F(179)...H(201)	378.3(283)	52.8(fixed)	—	-1.2	52.8
<i>u</i> 1822	F(15)...H(18)	378.4(105)	44.8(fixed)	—	-3.9	44.8
<i>u</i> 1535	H(265)...H(283)	378.5(152)	61.9(fixed)	—	22.8	61.9
<i>u</i> 2011	H(74)...H(78)	378.6(441)	49.1(fixed)	—	-9.6	49.1
<i>u</i> 1665	Si(43)...H(76)	378.6(234)	34.1(fixed)	—	-0.2	34.1
<i>u</i> 1747	F(98)...H(114)	378.6(202)	41.5(fixed)	—	-0.9	41.5
<i>u</i> 1692	Si(249)...H(268)	378.7(232)	48.7(fixed)	—	-0.4	48.7
<i>u</i> 4441	H(146)...H(155)	378.7(188)	42.2(fixed)	—	-0.6	42.2
<i>u</i> 1919	H(279)...H(283)	378.7(430)	48.9(fixed)	—	-11.5	48.9
<i>u</i> 1890	C(10)...H(24)	378.8(227)	78.4(fixed)	—	-9.8	78.4
<i>u</i> 1688	Si(250)...C(253)	378.9(71)	14.5(tied to <i>u</i> 1442)	—	-0.1	14.3
<i>u</i> 1669	C(213)...C(218)	379.1(69)	24.4(tied to <i>u</i> 1442)	—	0.7	24.0
<i>u</i> 1640	C(247)...H(270)	379.2(18)	48.3(fixed)	—	-3.1	48.3
<i>u</i> 1777	Si(248)...H(266)	379.2(96)	42.4(fixed)	—	-1.4	42.4
<i>u</i> 1704	F(57)...H(80)	379.4(126)	37.4(fixed)	—	-2.1	37.4
<i>u</i> 1658	Si(44)...H(63)	379.4(238)	36.0(fixed)	—	-0.1	36.0
<i>u</i> 1700	Si(46)...C(52)	379.8(78)	15.9(tied to <i>u</i> 1442)	—	-0.1	15.7
<i>u</i> 1733	H(61)...H(78)	379.9(195)	46.1(fixed)	—	12.4	46.1
<i>u</i> 1818	F(222)...H(241)	380.2(229)	37.9(fixed)	—	-2.3	37.9
<i>u</i> 1721	F(14)...H(35)	380.3(244)	38.0(fixed)	—	-1.9	38.0
<i>u</i> 1698	F(97)...H(119)	380.3(290)	33.3(fixed)	—	-1.6	33.3
<i>u</i> 1987	H(266)...H(286)	380.6(126)	72.1(fixed)	—	2.4	72.1
<i>u</i> 1711	Si(251)...H(285)	380.8(64)	32.2(fixed)	—	5.1	32.2
<i>u</i> 1650	Si(166)...H(186)	381.0(221)	47.4(fixed)	—	0.0	47.4
<i>u</i> 2228	C(88)...H(110)	381.2(277)	82.5(fixed)	—	-23.9	82.5
<i>u</i> 1705	H(264)...H(287)	381.2(95)	52.5(fixed)	—	7.5	52.5
<i>u</i> 2227	C(91)...H(102)	381.2(278)	82.5(fixed)	—	-23.9	82.5
<i>u</i> 4599	H(148)...H(158)	381.4(110)	25.2(fixed)	—	-5.9	25.2
<i>u</i> 1477	Si(128)...H(151)	381.7(76)	36.7(fixed)	—	13.4	36.7
<i>u</i> 1714	Si(45)...C(48)	381.9(79)	15.4(tied to <i>u</i> 1442)	—	-0.1	15.1
<i>u</i> 1312	C(247)...H(275)	382.0(104)	21.6(fixed)	—	0.8	21.6
<i>u</i> 1621	Si(5)...H(39)	382.1(81)	32.6(fixed)	—	3.9	32.6
<i>u</i> 1681	C(253)...C(255)	382.2(98)	24.9(tied to <i>u</i> 1442)	—	0.5	24.5
<i>u</i> 2648	H(102)...H(109)	382.2(293)	172.4(fixed)	—	-41.5	172.4
<i>u</i> 2649	H(101)...H(110)	382.3(293)	172.3(fixed)	—	-41.5	172.3

<i>u</i> 1768	F(263)...H(279)	382.5(213)	34.1(fixed)	—	-1.4	34.1
<i>u</i> 1741	H(182)...H(195)	382.6(239)	73.1(fixed)	—	34.8	73.1
<i>u</i> 1742	H(192)...H(204)	382.7(233)	73.2(fixed)	—	34.8	73.2
<i>u</i> 1696	F(221)...H(238)	382.7(209)	38.5(fixed)	—	-2.2	38.5
<i>u</i> 1737	F(16)...H(31)	382.8(89)	35.0(fixed)	—	-2.1	35.0
<i>u</i> 1672	H(34)...H(36)	382.9(150)	32.9(fixed)	—	6.0	32.9
<i>u</i> 919	C(254)...H(273)	383.2(90)	25.0(fixed)	—	1.3	25.0
<i>u</i> 1561	H(26)...H(30)	383.3(54)	46.7(fixed)	—	37.0	46.7
<i>u</i> 2239	C(170)...H(195)	383.5(213)	83.3(fixed)	—	-24.1	83.3
<i>u</i> 1824	C(8)...H(29)	383.6(15)	20.8(fixed)	—	-13.3	20.8
<i>u</i> 1709	H(100)...H(110)	383.6(345)	66.7(fixed)	—	38.8	66.7
<i>u</i> 1710	H(102)...H(111)	383.7(345)	67.0(fixed)	—	39.0	67.0
<i>u</i> 2173	H(101)...H(113)	383.9(209)	56.2(fixed)	—	-27.7	56.2
<i>u</i> 1712	H(61)...H(66)	383.9(153)	39.7(fixed)	—	11.8	39.7
<i>u</i> 1872	C(171)...H(182)	383.9(15)	16.9(fixed)	—	-13.3	16.9
<i>u</i> 1873	C(175)...H(196)	383.9(15)	16.8(fixed)	—	-13.3	16.8
<i>u</i> 2174	H(109)...H(121)	384.0(209)	55.4(fixed)	—	-27.8	55.4
<i>u</i> 1891	Si(2)...H(31)	384.3(53)	37.1(fixed)	—	2.4	37.1
<i>u</i> 1871	Si(46)...H(80)	384.5(66)	33.5(fixed)	—	2.8	33.5
<i>u</i> 1307	C(247)...H(274)	384.6(114)	24.1(fixed)	—	0.6	24.1
<i>u</i> 1860	C(90)...H(111)	384.6(15)	16.2(fixed)	—	-12.7	16.2
<i>u</i> 1859	C(89)...H(100)	384.6(15)	15.8(fixed)	—	-12.7	15.8
<i>u</i> 1626	Si(166)...H(184)	385.1(50)	52.0(fixed)	—	34.7	52.0
<i>u</i> 1864	C(213)...H(234)	385.3(15)	18.4(fixed)	—	-11.9	18.4
<i>u</i> 1805	C(9)...H(26)	385.3(14)	19.9(fixed)	—	-12.0	19.9
<i>u</i> 1627	Si(168)...H(192)	385.5(50)	50.6(fixed)	—	34.7	50.6
<i>u</i> 1772	Si(207)...C(214)	385.5(41)	16.5(tied to <i>u</i> 1442)	—	-0.2	16.2
<i>u</i> 1998	H(237)...H(242)	385.5(190)	41.8(fixed)	—	-0.8	41.8
<i>u</i> 1690	H(229)...H(246)	385.7(114)	46.3(fixed)	—	16.4	46.3
<i>u</i> 1907	F(17)...H(36)	386.3(255)	38.9(fixed)	—	-2.5	38.9
<i>u</i> 1814	Si(207)...H(231)	386.4(218)	47.2(fixed)	—	-1.6	47.2
<i>u</i> 1820	C(88)...H(104)	386.5(14)	17.7(fixed)	—	-11.0	17.7
<i>u</i> 1821	C(91)...H(108)	386.5(14)	17.4(fixed)	—	-11.0	17.4
<i>u</i> 2240	C(174)...H(184)	387.0(170)	83.3(fixed)	—	-24.1	83.3
<i>u</i> 2169	H(183)...H(200)	387.1(308)	61.5(fixed)	—	-25.4	61.5
<i>u</i> 1783	F(262)...H(277)	387.3(106)	38.7(fixed)	—	-3.1	38.7
<i>u</i> 1662	Si(209)...C(213)	387.5(39)	14.6(tied to <i>u</i> 1442)	—	0.0	14.4
<i>u</i> 1846	C(259)...H(282)	387.7(14)	16.4(fixed)	—	-9.9	16.4
<i>u</i> 1717	Si(167)...C(171)	388.0(32)	18.5(tied to <i>u</i> 1442)	—	0.3	18.2
<i>u</i> 1718	Si(169)...C(172)	388.0(32)	18.5(tied to <i>u</i> 1442)	—	0.3	18.2
<i>u</i> 1736	Si(43)...C(51)	388.2(69)	15.8(tied to <i>u</i> 1874)	—	-0.1	15.2
<i>u</i> 3685	F(140)...H(153)	388.5(79)	33.0(fixed)	—	-6.4	33.0
<i>u</i> 1764	F(219)...H(236)	388.5(79)	38.5(fixed)	—	-2.5	38.5
<i>u</i> 1847	C(131)...H(152)	388.6(15)	15.5(fixed)	—	-8.8	15.5

<i>u1869</i>	C(54)...H(77)	388.8(14)	15.6(fixed)	—	-8.8	15.6
<i>u1885</i>	C(52)...H(73)	389.0(15)	15.3(fixed)	—	-8.4	15.3
<i>u1830</i>	C(49)...H(70)	389.1(15)	14.5(fixed)	—	-8.4	14.5
<i>u2104</i>	C(88)...H(109)	389.1(222)	93.8(fixed)	—	-18.6	93.8
<i>u1666</i>	H(22)...H(38)	389.1(121)	33.5(fixed)	—	7.5	33.5
<i>u757</i>	C(255)...H(270)	389.2(18)	38.9(fixed)	—	25.3	38.9
<i>u1949</i>	Si(210)...C(215)	389.2(47)	18.4(tied to <i>u1874</i> )	—	-0.3	17.7
<i>u1922</i>	H(264)...H(286)	389.3(178)	53.8(fixed)	—	1.1	53.8
<i>u2718</i>	H(183)...H(195)	389.4(245)	163.5(fixed)	—	-42.0	163.5
<i>u2147</i>	F(180)...H(205)	389.4(60)	38.5(fixed)	—	-31.1	38.5
<i>u1622</i>	H(24)...H(41)	389.5(119)	54.9(fixed)	—	34.1	54.9
<i>u1782</i>	Si(2)...C(9)	389.6(30)	18.3(tied to <i>u1874</i> )	—	-0.4	17.6
<i>u1877</i>	F(56)...H(62)	389.7(202)	30.4(fixed)	—	-2.2	30.4
<i>u1843</i>	Si(168)...C(173)	389.9(31)	20.9(tied to <i>u1874</i> )	—	0.2	20.1
<i>u1842</i>	Si(166)...C(170)	389.9(31)	20.9(tied to <i>u1874</i> )	—	0.2	20.1
<i>u1780</i>	Si(251)...C(257)	390.0(65)	16.9(tied to <i>u1442</i> )	—	-0.3	16.6
<i>u1935</i>	C(83)...H(101)	390.1(17)	19.6(fixed)	—	-15.5	19.6
<i>u1936</i>	C(83)...H(109)	390.1(17)	19.2(fixed)	—	-15.6	19.2
<i>u1767</i>	Si(84)...C(89)	390.2(66)	17.8(tied to <i>u1874</i> )	—	0.2	17.2
<i>u1947</i>	C(165)...H(194)	390.2(17)	18.6(fixed)	—	-15.5	18.6
<i>u1946</i>	C(165)...H(183)	390.2(17)	18.5(fixed)	—	-15.5	18.5
<i>u2030</i>	C(255)...H(264)	390.2(161)	46.1(fixed)	—	-2.9	46.1
<i>u2719</i>	H(191)...H(203)	390.3(245)	162.0(fixed)	—	-42.0	162.0
<i>u1808</i>	Si(125)...C(131)	390.6(32)	16.2(tied to <i>u1874</i> )	—	-0.2	15.6
<i>u1848</i>	C(212)...H(223)	390.7(15)	14.2(fixed)	—	-6.8	14.2
<i>u1889</i>	F(55)...H(71)	390.7(101)	38.7(fixed)	—	-8.7	38.7
<i>u3028</i>	H(271)...H(285)	390.9(109)	47.0(fixed)	—	-26.3	47.0
<i>u1900</i>	F(58)...H(75)	391.0(204)	28.6(fixed)	—	-1.8	28.6
<i>u1867</i>	C(129)...H(145)	391.1(14)	14.2(fixed)	—	-6.7	14.2
<i>u1614</i>	H(280)...H(282)	391.2(110)	47.1(fixed)	—	28.5	47.1
<i>u1826</i>	C(214)...H(231)	391.3(14)	15.0(fixed)	—	-6.5	15.0
<i>u1825</i>	Si(4)...C(6)	391.3(51)	17.5(tied to <i>u1874</i> )	—	-0.2	16.8
<i>u1587</i>	F(260)...H(270)	391.3(71)	103.1(fixed)	—	-9.3	103.1
<i>u1839</i>	C(252)...H(268)	391.3(14)	14.0(fixed)	—	-6.4	14.0
<i>u1799</i>	H(59)...H(82)	391.4(96)	53.4(fixed)	—	11.5	53.4
<i>u1674</i>	Si(86)...H(102)	391.4(91)	53.7(fixed)	—	34.3	53.7
<i>u2196</i>	F(98)...H(101)	391.5(107)	41.8(fixed)	—	-31.9	41.8
<i>u1914</i>	H(281)...H(284)	391.5(433)	50.1(fixed)	—	-10.7	50.1
<i>u1653</i>	H(105)...H(112)	391.6(206)	60.4(fixed)	—	36.1	60.4
<i>u2197</i>	F(99)...H(109)	391.6(107)	40.7(fixed)	—	-32.0	40.7
<i>u2067</i>	H(228)...H(237)	391.6(271)	56.6(fixed)	—	0.1	56.6
<i>u1749</i>	Si(4)...C(8)	391.7(29)	15.7(tied to <i>u1874</i> )	—	-0.1	15.1
<i>u1849</i>	C(7)...H(18)	391.7(15)	14.2(fixed)	—	-5.8	14.2
<i>u1675</i>	Si(251)...H(274)	391.7(230)	35.5(fixed)	—	-0.2	35.5

<i>u1875</i>	C(48)...H(59)	391.8(15)	13.9(fixed)	—	-5.8	13.9
<i>u1857</i>	Si(249)...C(252)	391.8(60)	16.5(tied to <i>u1874</i> )	—	-0.2	15.9
<i>u3164</i>	F(137)...H(141)	391.8(83)	33.2(fixed)	—	-1.3	33.2
<i>u1809</i>	Si(44)...C(47)	391.9(69)	16.7(tied to <i>u1874</i> )	—	-0.1	16.1
<i>u1898</i>	C(1)...H(27)	392.1(17)	26.1(fixed)	—	-12.8	26.1
<i>u2212</i>	H(227)...H(235)	392.2(295)	59.9(fixed)	—	-0.6	59.9
<i>u1980</i>	F(15)...H(21)	392.3(160)	31.9(fixed)	—	-3.4	31.9
<i>u1734</i>	Si(84)...C(93)	392.4(85)	16.1(tied to <i>u1874</i> )	—	-0.1	15.5
<i>u2023</i>	F(139)...H(164)	392.4(79)	33.8(fixed)	—	-2.3	33.8
<i>u1882</i>	C(253)...H(264)	392.5(15)	13.7(fixed)	—	-5.1	13.7
<i>u1879</i>	C(6)...H(27)	392.6(112)	105.9(fixed)	—	-10.2	105.9
<i>u1841</i>	C(211)...H(227)	392.7(14)	13.7(fixed)	—	-5.1	13.7
<i>u1910</i>	F(15)...H(19)	392.8(86)	38.3(fixed)	—	-3.9	38.3
<i>u1798</i>	F(260)...H(281)	392.8(226)	35.9(fixed)	—	-2.2	35.9
<i>u2047</i>	H(65)...H(81)	393.0(216)	44.3(fixed)	—	-2.2	44.3
<i>u1797</i>	Si(250)...C(258)	393.2(41)	15.7(tied to <i>u1874</i> )	—	-0.1	15.1
<i>u1840</i>	C(258)...H(286)	393.3(15)	13.4(fixed)	—	-4.3	13.4
<i>u1977</i>	H(223)...H(238)	393.7(275)	55.9(fixed)	—	-4.9	55.9
<i>u1844</i>	C(93)...H(114)	393.8(15)	13.4(fixed)	—	-3.7	13.4
<i>u1924</i>	H(265)...H(285)	393.9(121)	43.4(fixed)	—	3.9	43.4
<i>u1806</i>	C(12)...H(40)	393.9(15)	13.3(fixed)	—	-3.6	13.3
<i>u1861</i>	C(6)...H(22)	394.0(14)	13.1(fixed)	—	-3.9	13.1
<i>u2154</i>	C(10)...H(25)	394.0(164)	45.5(fixed)	—	-14.0	45.5
<i>u1828</i>	C(50)...H(67)	394.0(14)	13.0(fixed)	—	-3.8	13.0
<i>u1702</i>	H(24)...H(39)	394.0(152)	50.7(fixed)	—	24.0	50.7
<i>u1838</i>	C(174)...H(199)	394.0(14)	13.1(fixed)	—	-3.8	13.1
<i>u1837</i>	C(173)...H(190)	394.0(14)	13.1(fixed)	—	-3.8	13.1
<i>u1845</i>	C(132)...H(149)	394.1(14)	13.1(fixed)	—	-3.8	13.1
<i>u1834</i>	C(92)...H(117)	394.1(14)	13.0(fixed)	—	-3.7	13.0
<i>u1888</i>	Si(46)...C(50)	394.1(51)	17.1(tied to <i>u1874</i> )	—	-0.2	16.4
<i>u1812</i>	C(217)...H(245)	394.2(15)	13.3(fixed)	—	-3.3	13.3
<i>u1866</i>	C(257)...H(278)	394.3(15)	12.9(fixed)	—	-3.3	12.9
<i>u1904</i>	C(206)...H(232)	394.3(17)	22.1(fixed)	—	-11.1	22.1
<i>u1865</i>	C(215)...H(240)	394.4(14)	12.9(fixed)	—	-3.5	12.9
<i>u1899</i>	Si(5)...C(11)	394.4(61)	17.7(tied to <i>u1874</i> )	—	-0.3	17.0
<i>u1829</i>	C(47)...H(63)	394.4(14)	12.8(fixed)	—	-3.4	12.8
<i>u1855</i>	C(51)...H(76)	394.5(14)	12.8(fixed)	—	-3.4	12.8
<i>u1850</i>	C(130)...H(141)	394.5(15)	13.0(fixed)	—	-3.1	13.0
<i>u1868</i>	C(216)...H(237)	394.5(15)	13.0(fixed)	—	-3.1	13.0
<i>u1817</i>	C(13)...H(36)	394.5(14)	12.8(fixed)	—	-3.3	12.8
<i>u1823</i>	C(11)...H(32)	394.6(15)	12.8(fixed)	—	-3.0	12.8
<i>u1854</i>	C(53)...H(81)	394.6(15)	12.9(fixed)	—	-3.0	12.9
<i>u1831</i>	C(218)...H(241)	394.6(14)	12.8(fixed)	—	-3.3	12.8
<i>u3123</i>	H(267)...H(273)	394.6(123)	48.3(fixed)	—	-11.7	48.3

<i>u</i> 1832	C(10)...H(35)	394.7(14)	12.9(fixed)	—	-3.2	12.9
<i>u</i> 1851	C(256)...H(281)	394.8(14)	12.8(fixed)	—	-3.1	12.8
<i>u</i> 1897	F(260)...H(278)	394.9(100)	38.5(fixed)	—	-1.4	38.5
<i>u</i> 2201	H(61)...H(81)	394.9(130)	68.3(fixed)	—	2.4	68.3
<i>u</i> 2059	H(272)...H(287)	395.1(87)	117.7(fixed)	—	2.9	117.7
<i>u</i> 1923	Si(209)...C(211)	395.1(47)	17.5(tied to <i>u</i> 1874)	—	-0.2	16.8
<i>u</i> 1644	H(227)...H(243)	395.2(105)	34.0(fixed)	—	12.1	34.0
<i>u</i> 1748	H(229)...H(244)	395.3(113)	43.5(fixed)	—	10.5	43.5
<i>u</i> 1874	Si(84)...C(91)	395.3(66)	20.8(20)	—	-0.1	20.0
<i>u</i> 2016	H(100)...H(103)	395.4(90)	35.0(fixed)	—	-19.0	35.0
<i>u</i> 1746	Si(208)...C(216)	395.6(28)	16.5(tied to <i>u</i> 1874)	—	-0.2	15.9
<i>u</i> 1794	Si(85)...C(92)	395.6(85)	17.6(tied to <i>u</i> 1874)	—	-0.1	17.0
<i>u</i> 1807	F(220)...H(230)	395.7(158)	31.8(fixed)	—	-7.0	31.8
<i>u</i> 1801	C(48)...C(49)	395.8(129)	31.0(tied to <i>u</i> 1874)	—	0.0	29.8
<i>u</i> 1852	Si(45)...C(53)	395.8(43)	16.9(tied to <i>u</i> 1874)	—	-0.2	16.2
<i>u</i> 3581	F(138)...H(149)	395.9(222)	25.6(fixed)	—	-3.2	25.6
<i>u</i> 2182	C(177)...H(191)	396.0(171)	84.1(fixed)	—	-18.9	84.1
<i>u</i> 2056	H(103)...H(118)	396.1(459)	49.1(fixed)	—	-17.8	49.1
<i>u</i> 2055	H(107)...H(117)	396.1(459)	48.9(fixed)	—	-17.9	48.9
<i>u</i> 3025	F(137)...H(145)	396.1(224)	45.9(fixed)	—	0.6	45.9
<i>u</i> 1917	H(62)...H(65)	396.2(294)	49.2(fixed)	—	5.0	49.2
<i>u</i> 1886	C(171)...C(176)	396.2(146)	37.4(tied to <i>u</i> 1874)	—	0.4	36.0
<i>u</i> 1738	H(75)...H(77)	396.3(117)	47.8(fixed)	—	22.1	47.8
<i>u</i> 2064	H(196)...H(198)	396.3(90)	34.3(fixed)	—	-18.2	34.3
<i>u</i> 2063	H(182)...H(185)	396.3(90)	34.3(fixed)	—	-18.2	34.3
<i>u</i> 1778	H(225)...H(239)	396.5(96)	41.8(fixed)	—	15.9	41.8
<i>u</i> 2277	C(218)...H(232)	396.8(89)	32.5(fixed)	—	-17.4	32.5
<i>u</i> 1952	H(64)...H(66)	396.8(293)	49.6(fixed)	—	4.3	49.6
<i>u</i> 1758	H(266)...H(283)	396.8(165)	49.4(fixed)	—	16.3	49.4
<i>u</i> 2302	C(13)...H(27)	397.0(84)	37.5(fixed)	—	-22.4	37.5
<i>u</i> 2008	H(189)...H(197)	397.1(325)	57.8(fixed)	—	7.9	57.8
<i>u</i> 2007	H(185)...H(201)	397.1(325)	57.7(fixed)	—	7.9	57.7
<i>u</i> 1757	Si(250)...C(254)	397.2(36)	17.8(tied to <i>u</i> 1874)	—	-0.4	17.1
<i>u</i> 2088	C(257)...H(283)	397.3(224)	57.3(fixed)	—	-10.2	57.3
<i>u</i> 1862	C(49)...H(59)	397.5(171)	54.6(fixed)	—	-2.5	54.6
<i>u</i> 2009	C(48)...H(70)	398.0(129)	63.3(fixed)	—	-5.0	63.3
<i>u</i> 1974	C(124)...H(150)	398.0(17)	14.8(fixed)	—	-8.0	14.8
<i>u</i> 2078	H(26)...H(27)	398.1(66)	65.9(fixed)	—	-8.3	65.9
<i>u</i> 1973	C(42)...H(71)	398.1(17)	14.9(fixed)	—	-7.9	14.9
<i>u</i> 3318	H(270)...H(276)	398.2(64)	37.2(fixed)	—	-30.8	37.2
<i>u</i> 1762	H(62)...H(69)	398.2(113)	44.6(fixed)	—	21.0	44.6
<i>u</i> 2085	H(22)...H(34)	398.5(478)	52.1(fixed)	—	-0.4	52.1
<i>u</i> 1957	C(1)...H(25)	398.5(19)	15.8(fixed)	—	-11.0	15.8
<i>u</i> 2110	H(60)...H(80)	398.5(127)	47.5(fixed)	—	-1.9	47.5

<i>u</i> 2183	C(173)...H(205)	398.6(145)	83.6(fixed)	—	-19.0	83.6
<i>u</i> 1964	C(42)...H(68)	398.7(17)	13.9(fixed)	—	-7.4	13.9
<i>u</i> 1955	C(83)...H(103)	398.8(19)	16.1(fixed)	—	-10.6	16.1
<i>u</i> 1956	C(83)...H(107)	398.8(19)	15.8(fixed)	—	-10.6	15.8
<i>u</i> 1853	Si(4)...C(12)	398.9(57)	15.9(tied to <i>u</i> 1874)	—	-0.1	15.3
<i>u</i> 2046	Si(125)...C(129)	399.1(33)	20.8(tied to <i>u</i> 1874)	—	-0.4	20.0
<i>u</i> 1971	F(263)...H(280)	399.3(209)	31.9(fixed)	—	-1.6	31.9
<i>u</i> 2076	H(23)...H(33)	399.3(405)	48.9(fixed)	—	-1.0	48.9
<i>u</i> 1927	Si(248)...C(255)	399.5(37)	17.8(tied to <i>u</i> 1874)	—	-0.3	17.1
<i>u</i> 1291	C(252)...H(274)	399.5(274)	46.3(fixed)	—	3.2	46.3
<i>u</i> 1884	Si(209)...C(217)	399.7(36)	16.5(tied to <i>u</i> 1874)	—	-0.1	15.9
<i>u</i> 1913	H(66)...H(80)	399.7(175)	46.2(fixed)	—	-0.6	46.2
<i>u</i> 1963	C(206)...H(224)	400.3(17)	13.4(fixed)	—	-5.8	13.4
<i>u</i> 2368	C(6)...H(28)	400.5(100)	42.4(fixed)	—	-22.9	42.4
<i>u</i> 2146	F(178)...H(191)	400.5(148)	40.9(fixed)	—	-31.1	40.9
<i>u</i> 1819	Si(43)...C(49)	400.6(48)	16.4(tied to <i>u</i> 1874)	—	-0.2	15.8
<i>u</i> 1939	C(247)...H(284)	400.7(19)	16.2(fixed)	—	-8.8	16.2
<i>u</i> 1601	H(104)...H(120)	400.7(161)	54.7(fixed)	—	44.7	54.7
<i>u</i> 1796	Si(2)...C(7)	400.8(45)	16.0(tied to <i>u</i> 1874)	—	-0.2	15.4
<i>u</i> 1934	C(42)...H(60)	400.8(17)	13.9(fixed)	—	-5.3	13.9
<i>u</i> 1791	Si(207)...C(212)	400.9(38)	15.5(tied to <i>u</i> 1874)	—	-0.1	14.9
<i>u</i> 1960	C(1)...H(19)	401.1(17)	13.3(fixed)	—	-5.1	13.3
<i>u</i> 2057	H(230)...H(234)	401.1(89)	32.3(fixed)	—	-13.8	32.3
<i>u</i> 2491	Si(126)...C(134)	401.2(41)	11.0(tied to <i>u</i> 1874)	—	-0.9	10.6
<i>u</i> 1909	Si(248)...C(256)	401.3(42)	19.5(tied to <i>u</i> 1874)	—	-0.4	18.7
<i>u</i> 1920	C(42)...H(79)	401.3(19)	16.4(fixed)	—	-8.1	16.4
<i>u</i> 1940	C(247)...H(265)	401.4(17)	13.3(fixed)	—	-4.7	13.3
<i>u</i> 1816	F(96)...H(116)	401.7(168)	34.1(fixed)	—	-1.7	34.1
<i>u</i> 1916	F(222)...H(245)	401.8(94)	36.0(fixed)	—	-1.8	36.0
<i>u</i> 1906	H(64)...H(67)	401.9(260)	46.6(fixed)	—	2.4	46.6
<i>u</i> 1728	H(105)...H(113)	401.9(273)	52.3(fixed)	—	26.4	52.3
<i>u</i> 1911	F(17)...H(40)	401.9(136)	37.2(fixed)	—	-1.9	37.2
<i>u</i> 1729	H(106)...H(121)	402.0(273)	51.9(fixed)	—	26.5	51.9
<i>u</i> 1944	C(247)...H(287)	402.2(17)	12.8(fixed)	—	-3.9	12.8
<i>u</i> 626	F(138)...H(152)	402.4(84)	55.3(fixed)	—	14.2	55.3
<i>u</i> 3058	H(156)...H(164)	402.5(272)	39.8(fixed)	—	3.6	39.8
<i>u</i> 1905	H(35)...H(38)	402.5(438)	41.5(fixed)	—	0.4	41.5
<i>u</i> 1993	H(188)...H(199)	402.7(290)	54.2(fixed)	—	4.2	54.2
<i>u</i> 1915	H(63)...H(65)	402.7(257)	46.3(fixed)	—	2.9	46.3
<i>u</i> 1953	C(83)...H(112)	402.7(17)	12.8(fixed)	—	-3.4	12.8
<i>u</i> 1945	C(1)...H(41)	402.8(17)	12.7(fixed)	—	-3.4	12.7
<i>u</i> 2005	H(25)...H(29)	402.8(90)	38.1(fixed)	—	-11.1	38.1
<i>u</i> 1962	C(206)...H(246)	403.0(17)	12.7(fixed)	—	-3.1	12.7
<i>u</i> 1978	C(247)...H(276)	403.0(17)	12.7(fixed)	—	-3.1	12.7

<i>u</i> 1928	C(47)...H(77)	403.0(268)	66.3(fixed)	—	-5.7	66.3
<i>u</i> 2010	H(282)...H(287)	403.1(65)	30.5(fixed)	—	-11.5	30.5
<i>u</i> 1982	C(1)...H(30)	403.2(17)	12.6(fixed)	—	-3.0	12.6
<i>u</i> 1926	C(124)...H(144)	403.2(19)	14.2(fixed)	—	-6.4	14.2
<i>u</i> 1975	C(124)...H(142)	403.2(17)	12.6(fixed)	—	-3.0	12.6
<i>u</i> 1970	C(206)...H(235)	403.2(17)	12.6(fixed)	—	-3.0	12.6
<i>u</i> 1979	C(42)...H(82)	403.3(17)	12.6(fixed)	—	-2.9	12.6
<i>u</i> 1972	C(206)...H(230)	403.4(19)	13.8(fixed)	—	-6.2	13.8
<i>u</i> 1943	C(247)...H(267)	403.6(19)	13.6(fixed)	—	-6.0	13.6
<i>u</i> 1992	H(186)...H(201)	403.6(265)	54.2(fixed)	—	4.2	54.2
<i>u</i> 2298	C(92)...H(101)	403.8(120)	48.2(fixed)	—	-24.6	48.2
<i>u</i> 1878	F(55)...H(76)	403.8(239)	39.7(fixed)	—	-3.0	39.7
<i>u</i> 2299	C(95)...H(109)	403.9(120)	47.6(fixed)	—	-24.7	47.6
<i>u</i> 2099	F(221)...H(224)	404.0(69)	29.8(fixed)	—	-9.7	29.8
<i>u</i> 2042	H(77)...H(82)	404.1(65)	28.2(fixed)	—	-10.8	28.2
<i>u</i> 2036	H(101)...H(104)	404.1(65)	42.5(fixed)	—	-8.3	42.5
<i>u</i> 2032	H(59)...H(81)	404.4(183)	55.3(fixed)	—	5.0	55.3
<i>u</i> 1896	Si(210)...C(218)	404.4(40)	18.8(tied to <i>u</i> 1874)	—	-0.3	18.1
<i>u</i> 3820	C(132)...H(143)	404.6(116)	25.4(fixed)	—	-4.1	25.4
<i>u</i> 2022	H(148)...H(152)	404.9(89)	30.0(fixed)	—	-10.3	30.0
<i>u</i> 624	H(272)...H(278)	404.9(110)	96.6(fixed)	—	19.4	96.6
<i>u</i> 1942	C(206)...H(226)	405.0(19)	13.2(fixed)	—	-4.7	13.2
<i>u</i> 1835	F(178)...H(198)	405.0(171)	33.7(fixed)	—	0.4	33.7
<i>u</i> 4468	H(147)...H(156)	405.0(426)	32.1(fixed)	—	-3.0	32.1
<i>u</i> 1761	Si(125)...C(133)	405.1(42)	16.1(tied to <i>u</i> 1874)	—	-0.2	15.5
<i>u</i> 1836	F(180)...H(185)	405.1(156)	33.7(fixed)	—	0.4	33.7
<i>u</i> 2053	H(73)...H(75)	405.3(89)	29.3(fixed)	—	-9.9	29.3
<i>u</i> 2149	F(138)...H(150)	405.4(58)	33.5(fixed)	—	-13.6	33.5
<i>u</i> 2029	H(66)...H(70)	405.4(89)	29.5(fixed)	—	-9.8	29.5
<i>u</i> 2130	C(214)...H(225)	405.5(117)	52.3(fixed)	—	-7.4	52.3
<i>u</i> 2112	F(56)...H(68)	405.6(112)	32.3(fixed)	—	-12.5	32.3
<i>u</i> 1983	Si(251)...C(259)	405.8(44)	18.9(tied to <i>u</i> 1874)	—	-0.2	18.1
<i>u</i> 1937	C(165)...H(185)	406.0(19)	13.3(fixed)	—	-3.6	13.3
<i>u</i> 1938	C(165)...H(198)	406.0(19)	13.3(fixed)	—	-3.6	13.3
<i>u</i> 1932	C(42)...H(66)	406.1(19)	13.1(fixed)	—	-3.5	13.1
<i>u</i> 1996	H(226)...H(241)	406.2(442)	44.1(fixed)	—	-3.8	44.1
<i>u</i> 1966	C(1)...H(21)	406.2(19)	12.8(fixed)	—	-3.5	12.8
<i>u</i> 1965	C(124)...H(148)	406.3(19)	13.0(fixed)	—	-3.4	13.0
<i>u</i> 1925	C(206)...H(239)	406.3(19)	12.9(fixed)	—	-3.3	12.9
<i>u</i> 1941	C(83)...H(116)	406.3(19)	13.1(fixed)	—	-3.3	13.1
<i>u</i> 1930	C(42)...H(62)	406.3(19)	12.9(fixed)	—	-3.3	12.9
<i>u</i> 2109	H(231)...H(232)	406.5(66)	45.3(fixed)	—	-5.4	45.3
<i>u</i> 1969	C(42)...H(75)	406.5(19)	12.8(fixed)	—	-3.1	12.8
<i>u</i> 2118	H(24)...H(29)	406.6(112)	61.3(fixed)	—	-12.0	61.3



<i>u</i> 1954	C(1)...H(38)	406.7(19)	12.6(fixed)	—	-2.9	12.6
<i>u</i> 1948	C(206)...H(243)	406.8(19)	12.7(fixed)	—	-2.9	12.7
<i>u</i> 1959	C(247)...H(280)	406.8(19)	12.7(fixed)	—	-2.8	12.7
<i>u</i> 1950	C(1)...H(34)	406.8(19)	12.6(fixed)	—	-2.8	12.6
<i>u</i> 2103	H(196)...H(197)	406.9(110)	33.0(fixed)	—	-17.9	33.0
<i>u</i> 2102	H(182)...H(187)	406.9(110)	33.0(fixed)	—	-17.9	33.0
<i>u</i> 2080	C(9)...H(20)	407.0(121)	49.9(fixed)	—	-5.6	49.9
<i>u</i> 1918	H(228)...H(242)	407.1(421)	44.6(fixed)	—	-4.3	44.6
<i>u</i> 2193	C(212)...H(237)	407.1(88)	37.8(fixed)	—	-1.5	37.8
<i>u</i> 2126	H(224)...H(240)	407.1(275)	48.4(fixed)	—	-6.3	48.4
<i>u</i> 1951	H(23)...H(37)	407.3(441)	43.2(fixed)	—	-2.0	43.2
<i>u</i> 4016	C(129)...H(150)	407.4(106)	31.6(fixed)	—	-14.8	31.6
<i>u</i> 2020	H(142)...H(145)	407.5(65)	27.1(fixed)	—	-7.6	27.1
<i>u</i> 1912	Si(5)...C(13)	407.6(57)	18.9(tied to <i>u</i> 1874)	—	-0.3	18.1
<i>u</i> 2028	H(236)...H(243)	407.7(155)	47.2(fixed)	—	-0.3	47.2
<i>u</i> 2207	C(216)...H(227)	407.7(237)	42.2(fixed)	—	-4.0	42.2
<i>u</i> 2219	C(52)...H(78)	407.8(231)	53.1(fixed)	—	-10.1	53.1
<i>u</i> 2527	Si(250)...H(270)	408.0(35)	42.5(fixed)	—	-17.7	42.5
<i>u</i> 2031	H(33)...H(37)	408.5(440)	43.4(fixed)	—	-1.7	43.4
<i>u</i> 1056	C(247)...H(272)	408.5(17)	35.2(fixed)	—	23.3	35.2
<i>u</i> 2127	H(100)...H(105)	408.5(110)	38.8(fixed)	—	-15.4	38.8
<i>u</i> 1903	C(211)...H(232)	408.5(107)	81.5(fixed)	—	-7.8	81.5
<i>u</i> 2003	H(223)...H(226)	408.6(89)	28.4(fixed)	—	-6.8	28.4
<i>u</i> 2019	H(265)...H(268)	408.6(65)	28.2(fixed)	—	-6.3	28.2
<i>u</i> 2170	H(190)...H(194)	408.7(282)	61.5(fixed)	—	-25.4	61.5
<i>u</i> 2111	F(16)...H(19)	408.7(53)	30.5(fixed)	—	-7.7	30.5
<i>u</i> 1997	F(57)...H(82)	408.8(98)	31.1(fixed)	—	-2.0	31.1
<i>u</i> 2062	H(59)...H(62)	409.0(89)	27.0(fixed)	—	-6.6	27.0
<i>u</i> 2192	C(93)...H(107)	409.1(211)	48.2(fixed)	—	-15.6	48.2
<i>u</i> 2191	C(94)...H(103)	409.1(211)	48.4(fixed)	—	-15.6	48.4
<i>u</i> 2033	H(21)...H(36)	409.2(447)	45.8(fixed)	—	-1.9	45.8
<i>u</i> 2040	F(16)...H(30)	409.3(68)	35.3(fixed)	—	-1.8	35.3
<i>u</i> 2006	H(18)...H(21)	409.5(89)	28.0(fixed)	—	-6.0	28.0
<i>u</i> 1988	F(262)...H(276)	409.6(83)	32.9(fixed)	—	-2.3	32.9
<i>u</i> 2243	C(92)...H(104)	409.6(293)	73.3(fixed)	—	-13.0	73.3
<i>u</i> 2050	Si(46)...C(54)	409.9(46)	20.0(tied to <i>u</i> 1874)	—	-0.4	19.3
<i>u</i> 2071	H(108)...H(110)	410.1(67)	61.5(fixed)	—	-9.9	61.5
<i>u</i> 2061	Si(2)...C(10)	410.3(35)	21.0(tied to <i>u</i> 1874)	—	-0.5	20.2
<i>u</i> 2041	F(99)...H(118)	410.5(291)	43.6(fixed)	—	-3.1	43.6
<i>u</i> 2373	C(211)...H(233)	410.5(110)	37.2(fixed)	—	-17.9	37.2
<i>u</i> 2012	F(219)...H(235)	410.5(76)	33.5(fixed)	—	-2.4	33.5
<i>u</i> 2190	Si(168)...H(193)	410.6(70)	84.9(fixed)	—	-2.4	84.9
<i>u</i> 2189	Si(166)...H(182)	410.6(70)	84.9(fixed)	—	-2.4	84.9
<i>u</i> 2204	C(51)...H(69)	410.8(163)	49.8(fixed)	—	-9.7	49.8

<i>u</i> 1908	F(221)...H(239)	411.5(164)	31.1(fixed)	—	-2.6	31.1
<i>u</i> 2108	H(229)...H(234)	411.6(110)	43.0(fixed)	—	-11.5	43.0
<i>u</i> 1999	H(224)...H(227)	411.6(65)	27.8(fixed)	—	-3.3	27.8
<i>u</i> 2134	F(14)...H(32)	411.7(87)	36.2(fixed)	—	-1.5	36.2
<i>u</i> 2039	H(264)...H(267)	411.9(89)	28.7(fixed)	—	-3.4	28.7
<i>u</i> 2026	H(235)...H(240)	411.9(65)	24.2(fixed)	—	-3.4	24.2
<i>u</i> 2081	H(63)...H(76)	412.0(287)	50.7(fixed)	—	4.8	50.7
<i>u</i> 2002	H(112)...H(117)	412.2(65)	24.3(fixed)	—	-3.2	24.3
<i>u</i> 2313	C(175)...H(191)	412.2(76)	44.8(fixed)	—	-22.4	44.8
<i>u</i> 1976	H(38)...H(40)	412.4(89)	25.8(fixed)	—	-3.4	25.8
<i>u</i> 1981	H(241)...H(246)	412.4(65)	24.2(fixed)	—	-3.0	24.2
<i>u</i> 1986	H(30)...H(35)	412.4(65)	23.9(fixed)	—	-3.0	23.9
<i>u</i> 2052	H(60)...H(63)	412.4(65)	27.6(fixed)	—	-2.5	27.6
<i>u</i> 2075	C(216)...H(223)	412.5(101)	55.5(fixed)	—	-4.3	55.5
<i>u</i> 1967	H(36)...H(41)	412.5(65)	24.5(fixed)	—	-2.8	24.5
<i>u</i> 2024	H(120)...H(122)	412.5(89)	27.1(fixed)	—	-3.0	27.1
<i>u</i> 2027	H(278)...H(280)	412.6(89)	24.7(fixed)	—	-3.3	24.7
<i>u</i> 1985	H(243)...H(245)	412.6(89)	25.7(fixed)	—	-3.1	25.7
<i>u</i> 2013	H(276)...H(281)	412.7(65)	24.0(fixed)	—	-2.8	24.0
<i>u</i> 2069	C(257)...H(284)	412.7(195)	52.5(fixed)	—	-9.2	52.5
<i>u</i> 2004	H(19)...H(22)	413.0(65)	25.9(fixed)	—	-2.2	25.9
<i>u</i> 2831	H(268)...H(273)	413.1(364)	61.1(fixed)	—	-8.9	61.1
<i>u</i> 2121	F(17)...H(27)	413.1(86)	61.0(fixed)	—	-23.3	61.0
<i>u</i> 1984	H(32)...H(34)	413.2(89)	24.1(fixed)	—	-2.8	24.1
<i>u</i> 2037	H(237)...H(239)	413.2(89)	25.1(fixed)	—	-2.6	25.1
<i>u</i> 2308	C(13)...H(26)	413.3(215)	55.0(fixed)	—	-13.3	55.0
<i>u</i> 2014	H(67)...H(68)	413.5(65)	29.4(fixed)	—	-1.2	29.4
<i>u</i> 2017	H(284)...H(286)	413.6(90)	33.2(fixed)	—	-1.1	33.2
<i>u</i> 2015	H(149)...H(150)	413.9(65)	29.9(fixed)	—	-0.7	29.9
<i>u</i> 2181	C(212)...H(240)	413.9(223)	36.0(fixed)	—	-2.5	36.0
<i>u</i> 2043	H(71)...H(76)	413.9(65)	29.6(fixed)	—	-0.8	29.6
<i>u</i> 4002	F(137)...H(142)	414.4(58)	23.8(fixed)	—	-5.8	23.8
<i>u</i> 2048	H(183)...H(186)	414.5(65)	39.7(fixed)	—	1.5	39.7
<i>u</i> 2049	H(194)...H(199)	414.5(65)	39.7(fixed)	—	1.5	39.7
<i>u</i> 2090	H(147)...H(152)	414.5(110)	29.5(fixed)	—	-10.9	29.5
<i>u</i> 2136	H(282)...H(285)	414.6(66)	32.4(fixed)	—	-11.8	32.4
<i>u</i> 2065	H(76)...H(79)	414.7(446)	58.0(fixed)	—	-10.0	58.0
<i>u</i> 2051	H(79)...H(81)	414.7(89)	31.7(fixed)	—	-0.2	31.7
<i>u</i> 2164	C(215)...H(242)	414.8(219)	31.6(fixed)	—	-1.6	31.6
<i>u</i> 2018	H(141)...H(144)	414.8(89)	28.1(fixed)	—	-0.6	28.1
<i>u</i> 2094	C(252)...H(282)	414.9(243)	65.8(fixed)	—	-7.8	65.8
<i>u</i> 1994	F(98)...H(112)	415.0(123)	34.4(fixed)	—	-0.7	34.4
<i>u</i> 2122	H(73)...H(74)	415.1(110)	29.0(fixed)	—	-10.3	29.0
<i>u</i> 2091	H(65)...H(70)	415.4(110)	28.5(fixed)	—	-10.1	28.5

<i>u</i> 2117	F(222)...H(243)	415.5(150)	36.3(fixed)	—	-3.0	36.3
<i>u</i> 2125	H(60)...H(67)	415.7(281)	50.9(fixed)	—	-5.7	50.9
<i>u</i> 1731	H(184)...H(202)	416.0(66)	69.4(fixed)	—	57.6	69.4
<i>u</i> 2144	H(77)...H(80)	416.2(66)	30.2(fixed)	—	-10.5	30.2
<i>u</i> 2535	C(129)...H(151)	416.3(117)	50.5(fixed)	—	12.2	50.5
<i>u</i> 2180	C(54)...H(65)	416.5(235)	34.6(fixed)	—	-2.5	34.6
<i>u</i> 2145	H(223)...H(228)	417.1(110)	30.5(fixed)	—	-8.1	30.5
<i>u</i> 1069	C(252)...H(275)	417.1(189)	37.0(fixed)	—	5.0	37.0
<i>u</i> 2218	C(50)...H(72)	417.1(169)	48.7(fixed)	—	-9.9	48.7
<i>u</i> 1726	H(102)...H(112)	417.4(170)	65.5(fixed)	—	59.1	65.5
<i>u</i> 2120	F(58)...H(79)	417.7(109)	35.0(fixed)	—	-13.9	35.0
<i>u</i> 2202	H(63)...H(68)	417.9(299)	51.9(fixed)	—	-10.5	51.9
<i>u</i> 2273	Si(85)...H(101)	418.2(55)	46.2(fixed)	—	-25.6	46.2
<i>u</i> 1931	Si(207)...H(234)	418.2(78)	62.7(fixed)	—	3.8	62.7
<i>u</i> 1727	H(110)...H(123)	418.2(170)	63.6(fixed)	—	59.3	63.6
<i>u</i> 2272	Si(87)...H(109)	418.2(55)	45.7(fixed)	—	-25.6	45.7
<i>u</i> 2167	F(263)...H(284)	418.3(90)	35.8(fixed)	—	-15.7	35.8
<i>u</i> 2119	H(18)...H(23)	418.4(110)	27.9(fixed)	—	-7.2	27.9
<i>u</i> 1111	Si(248)...H(272)	418.5(33)	73.6(fixed)	—	26.5	73.6
<i>u</i> 3974	F(137)...H(144)	418.5(151)	21.2(fixed)	—	-11.3	21.2
<i>u</i> 2171	Si(84)...H(111)	418.6(105)	88.7(fixed)	—	0.4	88.7
<i>u</i> 2172	Si(86)...H(100)	418.6(105)	88.5(fixed)	—	0.3	88.5
<i>u</i> 2096	C(254)...H(285)	418.7(106)	42.9(fixed)	—	-4.0	42.9
<i>u</i> 3650	C(132)...H(142)	418.8(106)	31.5(fixed)	—	-3.5	31.5
<i>u</i> 2161	H(143)...H(145)	419.0(66)	27.1(fixed)	—	-8.2	27.1
<i>u</i> 2133	H(266)...H(268)	419.0(66)	29.8(fixed)	—	-7.8	29.8
<i>u</i> 2890	H(268)...H(274)	419.1(158)	48.3(fixed)	—	-10.3	48.3
<i>u</i> 2113	H(59)...H(64)	419.1(110)	27.4(fixed)	—	-6.5	27.4
<i>u</i> 2165	H(264)...H(269)	419.5(110)	32.8(fixed)	—	-5.4	32.8
<i>u</i> 2079	F(260)...H(276)	419.8(72)	36.0(fixed)	—	-2.2	36.0
<i>u</i> 2222	C(7)...H(34)	419.9(237)	35.9(fixed)	—	-1.6	35.9
<i>u</i> 2137	H(225)...H(227)	420.0(66)	34.6(fixed)	—	-6.1	34.6
<i>u</i> 2001	H(26)...H(28)	420.2(67)	47.5(fixed)	—	-3.4	47.5
<i>u</i> 2114	H(283)...H(286)	420.5(110)	37.8(fixed)	—	-3.5	37.8
<i>u</i> 1961	Si(2)...H(29)	420.6(68)	80.8(fixed)	—	6.2	80.8
<i>u</i> 2203	C(252)...H(286)	421.1(126)	43.8(fixed)	—	-2.6	43.8
<i>u</i> 2195	C(50)...H(71)	421.1(136)	50.4(fixed)	—	-8.3	50.4
<i>u</i> 3031	H(102)...H(110)	421.2(286)	67.7(fixed)	—	-68.4	67.7
<i>u</i> 2163	Si(250)...H(269)	421.2(196)	44.7(fixed)	—	-3.7	44.7
<i>u</i> 2100	H(37)...H(40)	421.3(110)	25.8(fixed)	—	-4.5	25.8
<i>u</i> 2073	F(14)...H(34)	421.3(161)	33.5(fixed)	—	-2.4	33.5
<i>u</i> 2101	H(114)...H(115)	421.5(110)	26.8(fixed)	—	-4.3	26.8
<i>u</i> 2141	Si(43)...H(73)	421.7(104)	47.6(fixed)	—	-2.2	47.6
<i>u</i> 2106	H(242)...H(245)	421.7(110)	25.3(fixed)	—	-4.2	25.3

<i>u</i> 2142	H(20)...H(22)	421.8(66)	32.3(fixed)	—	-4.7	32.3
<i>u</i> 2153	H(141)...H(146)	421.8(110)	32.8(fixed)	—	-3.1	32.8
<i>u</i> 2258	C(255)...H(265)	421.9(109)	34.5(fixed)	—	-4.8	34.5
<i>u</i> 2025	F(222)...H(246)	421.9(69)	35.7(fixed)	—	-1.9	35.7
<i>u</i> 3159	H(275)...H(287)	422.0(225)	41.2(fixed)	—	-9.0	41.2
<i>u</i> 2151	H(278)...H(279)	422.1(110)	24.7(fixed)	—	-3.9	24.7
<i>u</i> 2150	H(32)...H(33)	422.2(110)	24.7(fixed)	—	-3.8	24.7
<i>u</i> 2178	H(237)...H(238)	422.3(110)	25.6(fixed)	—	-3.6	25.6
<i>u</i> 2089	H(149)...H(151)	422.4(66)	36.8(fixed)	—	-3.3	36.8
<i>u</i> 2097	H(67)...H(69)	422.5(66)	36.6(fixed)	—	-3.3	36.6
<i>u</i> 2138	H(113)...H(117)	422.6(66)	28.3(fixed)	—	-4.4	28.3
<i>u</i> 2107	C(11)...H(37)	422.8(241)	32.2(fixed)	—	-1.5	32.2
<i>u</i> 2159	F(17)...H(38)	422.9(155)	36.2(fixed)	—	-3.2	36.2
<i>u</i> 2205	C(7)...H(33)	423.0(206)	34.8(fixed)	—	-1.9	34.8
<i>u</i> 2116	H(78)...H(81)	423.0(110)	35.0(fixed)	—	-1.6	35.0
<i>u</i> 2284	Si(168)...H(183)	423.0(43)	39.1(fixed)	—	-25.4	39.1
<i>u</i> 2344	C(212)...H(235)	423.1(100)	36.4(fixed)	—	-2.1	36.4
<i>u</i> 2177	H(236)...H(240)	423.1(66)	24.9(fixed)	—	-4.3	24.9
<i>u</i> 2132	H(36)...H(39)	423.2(66)	26.4(fixed)	—	-4.1	26.4
<i>u</i> 2283	Si(166)...H(191)	423.2(43)	37.9(fixed)	—	-25.4	37.9
<i>u</i> 3207	H(273)...H(287)	423.2(288)	40.7(fixed)	—	-9.0	40.7
<i>u</i> 2148	H(241)...H(244)	423.3(66)	25.6(fixed)	—	-4.0	25.6
<i>u</i> 2092	C(54)...H(66)	423.4(175)	36.3(fixed)	—	-1.4	36.3
<i>u</i> 2152	H(31)...H(35)	423.5(66)	24.6(fixed)	—	-4.0	24.6
<i>u</i> 2095	H(72)...H(76)	423.5(66)	34.2(fixed)	—	-2.7	34.2
<i>u</i> 2143	H(277)...H(281)	423.5(66)	26.0(fixed)	—	-3.8	26.0
<i>u</i> 2084	H(61)...H(63)	423.7(66)	29.7(fixed)	—	-3.1	29.7
<i>u</i> 2216	Si(86)...H(106)	423.8(205)	63.5(fixed)	—	-6.9	63.5
<i>u</i> 2087	H(195)...H(199)	424.0(67)	55.0(fixed)	—	2.2	55.0
<i>u</i> 2086	H(184)...H(186)	424.0(67)	55.0(fixed)	—	2.2	55.0
<i>u</i> 2082	C(12)...H(23)	424.1(228)	36.9(fixed)	—	-2.3	36.9
<i>u</i> 2140	C(215)...H(243)	424.3(169)	34.0(fixed)	—	-1.1	34.0
<i>u</i> 2060	C(217)...H(228)	424.4(214)	43.4(fixed)	—	-3.9	43.4
<i>u</i> 2105	C(52)...H(79)	424.4(199)	54.5(fixed)	—	-8.0	54.5
<i>u</i> 2021	H(231)...H(233)	424.5(66)	35.9(fixed)	—	-1.4	35.9
<i>u</i> 2185	F(97)...H(103)	424.6(146)	40.5(fixed)	—	-20.5	40.5
<i>u</i> 2186	F(96)...H(107)	424.6(146)	40.1(fixed)	—	-20.6	40.1
<i>u</i> 2093	F(260)...H(280)	424.7(163)	37.3(fixed)	—	-2.6	37.3
<i>u</i> 2066	F(55)...H(75)	424.7(171)	38.2(fixed)	—	-3.1	38.2
<i>u</i> 2337	Si(248)...H(275)	425.0(183)	28.1(fixed)	—	-1.5	28.1
<i>u</i> 3613	F(138)...H(148)	425.6(151)	26.8(fixed)	—	-3.6	26.8
<i>u</i> 2208	C(51)...H(68)	425.7(144)	49.0(fixed)	—	-8.5	49.0
<i>u</i> 2054	F(17)...H(41)	425.7(89)	36.3(fixed)	—	-2.4	36.3
<i>u</i> 2199	Si(46)...H(74)	425.8(203)	30.0(fixed)	—	-2.0	30.0

<i>u</i> 3013	H(184)...H(195)	426.0(204)	73.2(fixed)	—	-66.4	73.2
<i>u</i> 2166	C(8)...H(39)	426.1(136)	35.0(fixed)	—	-2.6	35.0
<i>u</i> 562	H(274)...H(286)	426.3(110)	54.1(fixed)	—	12.9	54.1
<i>u</i> 2230	C(9)...H(19)	426.4(97)	36.6(fixed)	—	-5.7	36.6
<i>u</i> 2260	C(53)...H(61)	426.5(164)	38.2(fixed)	—	-6.6	38.2
<i>u</i> 370	H(270)...H(286)	426.7(96)	77.6(fixed)	—	48.0	77.6
<i>u</i> 2312	C(171)...H(205)	427.0(123)	43.3(fixed)	—	-22.4	43.3
<i>u</i> 2074	Si(209)...H(229)	427.1(197)	47.2(fixed)	—	-2.9	47.2
<i>u</i> 2175	Si(5)...H(27)	427.4(44)	67.3(fixed)	—	-18.2	67.3
<i>u</i> 2221	Si(249)...H(264)	427.7(94)	34.8(fixed)	—	-1.5	34.8
<i>u</i> 2176	F(57)...H(71)	427.7(93)	33.6(fixed)	—	-13.1	33.6
<i>u</i> 2168	Si(44)...H(59)	427.7(104)	39.8(fixed)	—	-1.2	39.8
<i>u</i> 2123	Si(4)...H(24)	428.2(192)	63.1(fixed)	—	-3.2	63.1
<i>u</i> 2226	Si(45)...H(64)	428.3(202)	30.4(fixed)	—	-2.1	30.4
<i>u</i> 2242	Si(46)...H(70)	428.6(85)	45.4(fixed)	—	-2.3	45.4
<i>u</i> 1179	H(271)...H(273)	428.7(126)	92.5(fixed)	—	6.1	92.5
<i>u</i> 2214	C(214)...H(224)	429.2(104)	40.2(fixed)	—	-7.1	40.2
<i>u</i> 4537	C(130)...H(153)	429.6(56)	17.5(fixed)	—	-9.8	17.5
<i>u</i> 4251	C(131)...H(156)	429.8(221)	24.8(fixed)	—	-1.5	24.8
<i>u</i> 2280	C(216)...H(224)	430.0(88)	37.5(fixed)	—	-6.3	37.5
<i>u</i> 2156	F(222)...H(232)	430.7(78)	48.5(fixed)	—	-18.1	48.5
<i>u</i> 2220	C(13)...H(25)	430.7(193)	62.8(fixed)	—	-11.0	62.8
<i>u</i> 2249	F(14)...H(30)	431.1(68)	41.1(fixed)	—	-2.2	41.1
<i>u</i> 2326	Si(210)...H(237)	431.2(68)	26.9(fixed)	—	-1.5	26.9
<i>u</i> 2139	C(217)...H(226)	431.3(196)	36.2(fixed)	—	-4.2	36.2
<i>u</i> 2124	C(11)...H(38)	431.6(202)	32.6(fixed)	—	-1.0	32.6
<i>u</i> 2250	F(262)...H(267)	431.6(67)	34.0(fixed)	—	-9.9	34.0
<i>u</i> 2269	Si(4)...H(18)	431.9(77)	36.1(fixed)	—	-2.4	36.1
<i>u</i> 2224	Si(4)...F(17)	431.9(30)	11.5(5)	—	-1.0	10.3
<i>u</i> 2158	C(53)...H(60)	432.1(116)	44.7(fixed)	—	-4.6	44.7
<i>u</i> 2303	C(214)...H(246)	432.2(92)	26.9(fixed)	—	-2.7	26.9
<i>u</i> 2179	H(199)...H(200)	432.2(437)	85.3(fixed)	—	-0.3	85.3
<i>u</i> 1856	H(271)...H(274)	432.3(101)	72.9(fixed)	—	-12.3	72.9
<i>u</i> 3293	Si(128)...H(153)	432.5(43)	17.9(fixed)	—	-6.3	17.9
<i>u</i> 2248	Si(209)...F(222)	432.7(30)	11.5(tied to <i>u</i> 2224)	—	-1.1	10.4
<i>u</i> 2339	Si(250)...H(283)	432.8(185)	47.3(fixed)	—	-6.3	47.3
<i>u</i> 2211	C(89)...H(113)	432.9(223)	34.9(fixed)	—	-3.2	34.9
<i>u</i> 2268	Si(85)...H(114)	433.4(121)	30.6(fixed)	—	-1.9	30.6
<i>u</i> 2257	F(14)...H(25)	433.4(101)	41.3(fixed)	—	-19.0	41.3
<i>u</i> 2311	C(218)...H(231)	433.5(199)	45.1(fixed)	—	-6.6	45.1
<i>u</i> 2379	C(216)...H(226)	433.5(166)	36.8(fixed)	—	-5.2	36.8
<i>u</i> 2358	C(130)...H(161)	433.6(195)	33.6(fixed)	—	-7.9	33.6
<i>u</i> 2233	C(255)...H(268)	433.7(226)	49.4(fixed)	—	-5.8	49.4
<i>u</i> 2294	F(99)...H(120)	433.7(195)	53.5(fixed)	—	-4.1	53.5

<i>u</i> 2393	C(212)...H(239)	434.0(174)	32.5(fixed)	—	-3.2	32.5
<i>u</i> 2285	C(49)...H(60)	434.1(108)	32.4(fixed)	—	-6.5	32.4
<i>u</i> 2359	H(266)...H(287)	434.2(167)	64.6(fixed)	—	-4.3	64.6
<i>u</i> 3856	H(271)...H(279)	434.3(103)	96.0(fixed)	—	-19.4	96.0
<i>u</i> 2330	C(47)...H(81)	434.5(128)	38.4(fixed)	—	-1.4	38.4
<i>u</i> 2319	C(48)...H(68)	434.6(90)	39.7(fixed)	—	-9.6	39.7
<i>u</i> 2157	C(12)...H(21)	435.1(197)	34.0(fixed)	—	-2.6	34.0
<i>u</i> 2331	Si(126)...H(164)	435.4(43)	18.8(fixed)	—	-3.3	18.8
<i>u</i> 2200	C(213)...H(244)	435.4(96)	34.6(fixed)	—	-2.3	34.6
<i>u</i> 2295	Si(209)...H(223)	435.6(72)	40.4(fixed)	—	-2.1	40.4
<i>u</i> 745	H(270)...H(274)	435.9(161)	50.4(fixed)	—	39.4	50.4
<i>u</i> 2385	C(131)...H(164)	436.3(56)	24.8(fixed)	—	-2.4	24.8
<i>u</i> 2210	C(254)...H(287)	436.8(83)	36.7(fixed)	—	-4.0	36.7
<i>u</i> 2254	Si(210)...F(220)	436.9(25)	11.9(tied to <i>u</i> 2224)	—	-1.1	10.7
<i>u</i> 2853	H(267)...H(274)	437.1(464)	51.4(fixed)	—	-8.3	51.4
<i>u</i> 2238	Si(168)...H(201)	437.1(209)	37.8(fixed)	—	-3.3	37.8
<i>u</i> 2237	Si(166)...H(197)	437.1(209)	37.8(fixed)	—	-3.3	37.8
<i>u</i> 1732	H(185)...H(203)	437.3(196)	61.3(fixed)	—	57.6	61.3
<i>u</i> 2296	Si(45)...H(68)	437.5(46)	25.2(fixed)	—	-11.1	25.2
<i>u</i> 2271	C(258)...H(266)	437.6(138)	38.8(fixed)	—	-5.5	38.8
<i>u</i> 2209	Si(2)...F(15)	437.6(12)	12.2(tied to <i>u</i> 2224)	—	-1.2	11.0
<i>u</i> 2225	Si(125)...F(138)	437.9(14)	11.3(tied to <i>u</i> 2224)	—	-1.0	10.1
<i>u</i> 2342	C(95)...H(107)	437.9(227)	50.5(fixed)	—	-13.0	50.5
<i>u</i> 4534	C(131)...H(157)	437.9(194)	15.8(fixed)	—	-5.5	15.8
<i>u</i> 2300	Si(208)...H(224)	438.0(43)	22.4(fixed)	—	-8.8	22.4
<i>u</i> 2215	Si(46)...F(55)	438.1(14)	12.6(tied to <i>u</i> 2224)	—	-1.3	11.3
<i>u</i> 2129	H(231)...H(240)	438.1(181)	50.6(fixed)	—	10.4	50.6
<i>u</i> 2304	Si(125)...H(147)	438.2(183)	28.0(fixed)	—	-2.1	28.0
<i>u</i> 2382	Si(125)...H(141)	438.3(67)	27.1(fixed)	—	-1.4	27.1
<i>u</i> 2275	H(20)...H(27)	438.3(124)	121.1(fixed)	—	-9.6	121.1
<i>u</i> 2407	Si(45)...H(78)	438.4(182)	42.8(fixed)	—	-6.7	42.8
<i>u</i> 2293	Si(3)...H(19)	438.8(45)	20.9(fixed)	—	-7.3	20.9
<i>u</i> 2582	H(101)...H(109)	438.8(227)	82.4(fixed)	—	-47.1	82.4
<i>u</i> 2537	H(61)...H(82)	439.1(177)	68.5(fixed)	—	-3.6	68.5
<i>u</i> 2188	Si(210)...H(232)	439.1(47)	51.3(fixed)	—	-14.3	51.3
<i>u</i> 2324	C(9)...H(41)	439.2(76)	29.4(fixed)	—	-3.7	29.4
<i>u</i> 2270	Si(84)...H(115)	439.3(214)	27.0(fixed)	—	-2.2	27.0
<i>u</i> 2234	Si(43)...F(56)	439.3(13)	11.5(tied to <i>u</i> 2224)	—	-1.1	10.4
<i>u</i> 2314	C(8)...H(30)	439.4(49)	23.9(fixed)	—	-1.3	23.9
<i>u</i> 2229	Si(248)...F(261)	439.4(13)	12.0(tied to <i>u</i> 2224)	—	-1.2	10.8
<i>u</i> 554	F(260)...H(272)	439.4(75)	71.4(fixed)	—	49.4	71.4
<i>u</i> 2231	Si(210)...F(219)	439.5(11)	11.6(tied to <i>u</i> 2224)	—	-1.2	10.4
<i>u</i> 2235	Si(5)...F(14)	439.8(18)	11.6(tied to <i>u</i> 2224)	—	-1.1	10.4
<i>u</i> 1800	H(264)...H(275)	440.0(245)	49.8(fixed)	—	-2.8	49.8

<i>u2389</i>	Si(209)...H(226)	440.1(76)	21.6(fixed)	—	-6.7	21.6
<i>u2544</i>	Si(128)...H(150)	440.1(43)	27.7(fixed)	—	-10.3	27.7
<i>u2305</i>	Si(3)...H(41)	440.4(49)	19.2(fixed)	—	-4.1	19.2
<i>u2245</i>	Si(84)...F(98)	440.4(15)	12.3(tied to <i>u2224</i> )	—	-2.0	11.1
<i>u2383</i>	C(47)...H(79)	440.6(189)	35.6(fixed)	—	-11.7	35.6
<i>u2244</i>	Si(125)...F(140)	440.7(10)	12.0(tied to <i>u2224</i> )	—	-1.2	10.8
<i>u3943</i>	F(263)...H(273)	440.7(78)	18.6(fixed)	—	-6.0	18.6
<i>u2253</i>	Si(85)...F(97)	440.9(20)	11.6(tied to <i>u2224</i> )	—	-1.3	10.4
<i>u2276</i>	Si(251)...H(279)	441.0(178)	26.5(fixed)	—	-1.9	26.5
<i>u2236</i>	Si(251)...F(260)	441.0(12)	11.6(tied to <i>u2224</i> )	—	-1.1	10.5
<i>u2316</i>	Si(208)...H(246)	441.3(43)	18.7(fixed)	—	-3.5	18.7
<i>u2281</i>	C(48)...H(76)	441.6(178)	38.3(fixed)	—	2.5	38.3
<i>u2187</i>	Si(125)...H(155)	441.6(74)	46.8(fixed)	—	-2.7	46.8
<i>u2263</i>	Si(168)...F(180)	441.8(8)	11.9(tied to <i>u2224</i> )	—	-2.1	10.7
<i>u2262</i>	Si(166)...F(181)	441.8(8)	11.9(tied to <i>u2224</i> )	—	-2.1	10.7
<i>u2255</i>	Si(208)...H(238)	441.8(180)	30.6(fixed)	—	-2.3	30.6
<i>u2246</i>	H(268)...H(281)	441.9(228)	48.8(fixed)	—	8.6	48.8
<i>u2251</i>	Si(46)...F(57)	442.0(13)	11.4(tied to <i>u2224</i> )	—	-1.1	10.2
<i>u2301</i>	Si(248)...H(278)	442.1(73)	27.9(fixed)	—	-1.4	27.9
<i>u565</i>	H(274)...H(285)	442.1(136)	57.8(fixed)	—	13.8	57.8
<i>u2310</i>	Si(3)...H(30)	442.4(43)	17.9(fixed)	—	-2.8	17.9
<i>u2348</i>	C(171)...H(190)	442.4(87)	59.8(fixed)	—	-0.1	59.8
<i>u1656</i>	Si(248)...H(270)	442.6(39)	85.3(fixed)	—	1.2	85.3
<i>u2261</i>	Si(249)...F(263)	442.8(12)	11.3(tied to <i>u2224</i> )	—	-1.0	10.2
<i>u2247</i>	Si(2)...F(16)	442.9(8)	11.3(tied to <i>u2224</i> )	—	-1.0	10.2
<i>u2360</i>	Si(4)...H(21)	443.0(79)	18.7(fixed)	—	-4.7	18.7
<i>u2286</i>	C(52)...H(63)	443.0(179)	38.0(fixed)	—	2.5	38.0
<i>u2264</i>	Si(44)...F(58)	443.0(13)	11.5(tied to <i>u2224</i> )	—	-1.1	10.4
<i>u2291</i>	Si(44)...H(71)	443.1(53)	27.4(fixed)	—	-11.3	27.4
<i>u2256</i>	Si(207)...F(221)	443.2(8)	11.3(tied to <i>u2224</i> )	—	-1.0	10.2
<i>u1122</i>	Si(251)...H(275)	443.2(115)	29.0(fixed)	—	4.7	29.0
<i>u2241</i>	Si(248)...F(262)	443.3(10)	11.3(tied to <i>u2224</i> )	—	-1.1	10.2
<i>u2318</i>	Si(249)...H(287)	443.4(44)	21.2(fixed)	—	-5.3	21.2
<i>u2350</i>	C(8)...H(41)	443.6(88)	32.2(fixed)	—	-3.0	32.2
<i>u2266</i>	C(258)...H(265)	443.7(103)	40.4(fixed)	—	-4.8	40.4
<i>u2354</i>	Si(251)...H(286)	444.2(75)	31.6(fixed)	—	-1.8	31.6
<i>u2329</i>	H(225)...H(232)	444.5(111)	105.2(fixed)	—	-10.8	105.2
<i>u2336</i>	Si(210)...H(245)	444.6(70)	27.7(fixed)	—	-1.8	27.7
<i>u2334</i>	Si(85)...H(123)	444.8(59)	19.1(fixed)	—	-4.2	19.1
<i>u2372</i>	C(89)...H(112)	444.9(161)	38.7(fixed)	—	-2.8	38.7
<i>u2267</i>	Si(249)...H(276)	445.4(45)	18.8(fixed)	—	-3.5	18.8
<i>u2529</i>	C(215)...H(226)	446.0(82)	32.9(fixed)	—	-7.3	32.9
<i>u2292</i>	F(219)...H(230)	446.0(68)	37.9(fixed)	—	-10.1	37.9
<i>u2366</i>	Si(210)...H(239)	446.0(73)	19.1(fixed)	—	-4.2	19.1

<i>u</i> 2315	Si(4)...H(37)	446.1(192)	26.2(fixed)	—	-1.8	26.2
<i>u</i> 2333	Si(43)...H(65)	446.2(190)	28.1(fixed)	—	-2.2	28.1
<i>u</i> 2365	F(98)...F(99)	446.3(146)	24.1(tied to <i>u</i> 2224)	—	-1.9	21.6
<i>u</i> 2346	Si(209)...H(242)	446.6(181)	25.5(fixed)	—	-1.8	25.5
<i>u</i> 2351	Si(46)...H(79)	446.7(52)	23.6(fixed)	—	-12.8	23.6
<i>u</i> 2217	H(117)...H(118)	446.8(432)	46.4(fixed)	—	4.5	46.4
<i>u</i> 2345	Si(5)...H(40)	446.8(87)	29.0(fixed)	—	-1.8	29.0
<i>u</i> 2717	H(191)...H(205)	446.9(179)	71.2(fixed)	—	-46.9	71.2
<i>u</i> 2322	Si(44)...H(82)	447.2(43)	18.2(fixed)	—	-3.2	18.2
<i>u</i> 2340	C(171)...H(200)	447.2(281)	46.9(fixed)	—	-4.5	46.9
<i>u</i> 2328	Si(43)...H(60)	447.2(55)	26.3(fixed)	—	-7.1	26.3
<i>u</i> 2289	Si(2)...H(23)	447.3(186)	29.5(fixed)	—	-2.2	29.5
<i>u</i> 2279	Si(207)...H(228)	447.4(180)	35.3(fixed)	—	-3.0	35.3
<i>u</i> 2357	Si(5)...H(33)	447.5(171)	26.1(fixed)	—	-1.9	26.1
<i>u</i> 2325	Si(207)...H(235)	447.5(41)	18.6(fixed)	—	-3.5	18.6
<i>u</i> 3131	Si(126)...H(142)	447.6(43)	18.0(fixed)	—	-3.7	18.0
<i>u</i> 2347	C(252)...H(287)	447.7(96)	38.2(fixed)	—	-3.4	38.2
<i>u</i> 2400	C(252)...H(284)	447.7(186)	41.4(fixed)	—	-12.4	41.4
<i>u</i> 2307	C(218)...H(230)	447.9(186)	42.9(fixed)	—	-5.6	42.9
<i>u</i> 2288	F(178)...F(180)	448.0(100)	24.8(tied to <i>u</i> 2224)	—	-2.2	22.2
<i>u</i> 2278	C(254)...H(276)	448.0(64)	28.8(fixed)	—	-3.3	28.8
<i>u</i> 2375	Si(84)...H(107)	448.5(71)	28.3(fixed)	—	-16.9	28.3
<i>u</i> 2287	F(56)...F(57)	448.6(93)	23.7(tied to <i>u</i> 2224)	—	-1.4	21.3
<i>u</i> 371	H(269)...H(275)	448.7(142)	45.5(fixed)	—	29.0	45.5
<i>u</i> 2395	C(91)...H(123)	449.3(132)	36.4(fixed)	—	-3.3	36.4
<i>u</i> 2323	F(16)...F(17)	449.6(49)	23.0(tied to <i>u</i> 2224)	—	-1.3	20.7
<i>u</i> 2343	Si(248)...H(265)	449.7(50)	22.6(fixed)	—	-6.5	22.6
<i>u</i> 2355	Si(2)...H(25)	449.8(69)	36.0(fixed)	—	-15.7	36.0
<i>u</i> 2386	Si(251)...H(284)	449.8(58)	25.6(fixed)	—	-13.9	25.6
<i>u</i> 2297	C(48)...H(67)	450.3(249)	40.1(fixed)	—	-2.9	40.1
<i>u</i> 2332	H(20)...H(32)	450.4(120)	55.3(fixed)	—	10.9	55.3
<i>u</i> 2403	Si(46)...H(81)	451.0(75)	26.6(fixed)	—	-1.5	26.6
<i>u</i> 2341	C(175)...H(190)	451.3(245)	46.9(fixed)	—	-4.5	46.9
<i>u</i> 2320	F(221)...F(222)	451.4(53)	23.1(tied to <i>u</i> 2224)	—	-1.2	20.8
<i>u</i> 2317	C(49)...H(63)	451.8(255)	39.2(fixed)	—	-3.0	39.2
<i>u</i> 2423	Si(2)...H(32)	451.9(67)	24.7(fixed)	—	-1.4	24.7
<i>u</i> 2417	C(170)...H(202)	452.0(56)	40.2(fixed)	—	-3.6	40.2
<i>u</i> 2792	Si(126)...H(156)	452.2(180)	21.1(fixed)	—	-0.5	21.1
<i>u</i> 2767	H(182)...H(202)	452.5(97)	134.3(fixed)	—	-19.6	134.3
<i>u</i> 2364	Si(125)...H(157)	452.5(57)	19.4(fixed)	—	-4.5	19.4
<i>u</i> 2396	C(213)...H(246)	452.7(84)	32.6(fixed)	—	-2.7	32.6
<i>u</i> 2405	C(217)...H(235)	452.9(61)	26.0(fixed)	—	-2.8	26.0
<i>u</i> 2380	C(255)...H(267)	453.0(190)	40.0(fixed)	—	-6.6	40.0
<i>u</i> 2362	C(90)...H(116)	453.1(132)	25.4(fixed)	—	-0.7	25.4



<i>u</i> 2363	C(89)...H(120)	453.1(132)	25.4(fixed)	—	-0.7	25.4
<i>u</i> 2401	F(15)...F(17)	453.4(46)	19.5(tied to <i>u</i> 2224)	—	-1.0	17.5
<i>u</i> 2454	C(11)...H(21)	454.0(120)	30.3(fixed)	—	-4.9	30.3
<i>u</i> 2391	Si(125)...H(144)	454.3(60)	22.2(fixed)	—	-9.7	22.2
<i>u</i> 2437	C(47)...H(82)	454.6(98)	38.8(fixed)	—	-2.0	38.8
<i>u</i> 2353	C(258)...H(280)	454.7(86)	23.7(fixed)	—	-1.9	23.7
<i>u</i> 2399	C(49)...H(82)	455.0(87)	25.8(fixed)	—	-2.4	25.8
<i>u</i> 2335	Si(248)...H(280)	455.2(61)	19.0(fixed)	—	-3.2	19.0
<i>u</i> 2462	C(255)...H(287)	455.5(86)	30.4(fixed)	—	-5.4	30.4
<i>u</i> 4489	H(143)...H(150)	456.1(105)	31.0(fixed)	—	-17.5	31.0
<i>u</i> 2367	Si(210)...H(243)	456.3(57)	19.1(fixed)	—	-3.6	19.1
<i>u</i> 2583	H(26)...H(29)	456.4(17)	27.2(fixed)	—	-24.8	27.2
<i>u</i> 2162	H(265)...H(274)	456.4(289)	51.1(fixed)	—	-4.7	51.1
<i>u</i> 2434	F(262)...H(266)	456.8(109)	31.2(fixed)	—	4.8	31.2
<i>u</i> 2675	H(69)...H(71)	456.9(155)	82.4(fixed)	—	-16.9	82.4
<i>u</i> 2338	Si(2)...H(34)	457.1(53)	18.5(fixed)	—	-3.2	18.5
<i>u</i> 3059	H(19)...H(28)	457.2(83)	63.9(fixed)	—	-31.0	63.9
<i>u</i> 2397	Si(249)...H(267)	457.5(72)	23.5(fixed)	—	-8.7	23.5
<i>u</i> 2394	C(47)...H(66)	457.6(125)	27.4(fixed)	—	-4.1	27.4
<i>u</i> 2376	Si(43)...H(75)	458.0(75)	20.2(fixed)	—	-4.1	20.2
<i>u</i> 353	H(146)...H(160)	458.3(431)	53.2(fixed)	—	54.6	53.2
<i>u</i> 2408	Si(85)...H(116)	458.3(77)	22.1(fixed)	—	-4.2	22.1
<i>u</i> 2757	H(111)...H(123)	458.5(194)	135.0(fixed)	—	-19.3	135.0
<i>u</i> 2758	H(100)...H(112)	458.6(194)	134.9(fixed)	—	-19.3	134.9
<i>u</i> 2392	Si(46)...H(66)	458.7(71)	19.8(fixed)	—	-4.7	19.8
<i>u</i> 2370	H(104)...H(121)	458.7(259)	74.0(fixed)	—	15.2	74.0
<i>u</i> 2369	H(108)...H(113)	458.8(259)	73.9(fixed)	—	15.2	73.9
<i>u</i> 2327	H(60)...H(77)	459.1(294)	78.2(fixed)	—	-8.1	78.2
<i>u</i> 2384	Si(5)...H(38)	459.5(58)	19.6(fixed)	—	-3.8	19.6
<i>u</i> 2444	Si(250)...H(267)	459.9(136)	25.8(fixed)	—	-7.7	25.8
<i>u</i> 2404	Si(44)...H(62)	460.4(74)	20.1(fixed)	—	-4.4	20.1
<i>u</i> 2517	F(16)...H(40)	460.5(76)	31.1(fixed)	—	3.3	31.1
<i>u</i> 2534	F(221)...H(245)	460.5(72)	30.4(fixed)	—	3.0	30.4
<i>u</i> 2426	Si(5)...C(10)	460.9(33)	12.3(tied to <i>u</i> 2449)	—	-1.3	11.8
<i>u</i> 2472	H(19)...H(27)	461.1(148)	110.1(fixed)	—	-19.1	110.1
<i>u</i> 2431	H(268)...H(278)	461.2(222)	53.8(fixed)	—	10.5	53.8
<i>u</i> 2387	Si(207)...H(230)	461.2(74)	26.3(fixed)	—	-8.6	26.3
<i>u</i> 3347	F(138)...H(145)	461.4(66)	23.3(fixed)	—	-1.9	23.3
<i>u</i> 2410	Si(168)...H(189)	461.7(67)	22.8(fixed)	—	-5.1	22.8
<i>u</i> 2409	Si(166)...H(185)	461.7(67)	22.8(fixed)	—	-5.1	22.8
<i>u</i> 2438	C(211)...H(239)	461.8(80)	29.0(fixed)	—	-3.9	29.0
<i>u</i> 2653	F(222)...H(236)	462.0(89)	35.9(fixed)	—	2.3	35.9
<i>u</i> 2633	Si(166)...H(183)	462.0(34)	32.3(fixed)	—	-21.6	32.3
<i>u</i> 2634	Si(168)...H(191)	462.1(34)	31.4(fixed)	—	-21.6	31.4

<i>u</i> 2425	C(53)...H(75)	462.3(99)	27.5(fixed)	—	-3.7	27.5
<i>u</i> 2435	C(50)...H(62)	462.7(93)	28.0(fixed)	—	-3.9	28.0
<i>u</i> 2388	C(257)...H(268)	462.9(139)	35.9(fixed)	—	8.1	35.9
<i>u</i> 2985	H(20)...H(28)	463.0(133)	48.4(fixed)	—	-32.1	48.4
<i>u</i> 2381	C(12)...H(34)	463.2(114)	24.7(fixed)	—	-2.2	24.7
<i>u</i> 2659	Si(2)...H(27)	463.6(33)	22.9(fixed)	—	-21.2	22.9
<i>u</i> 3823	C(257)...H(271)	463.8(79)	90.9(fixed)	—	-17.5	90.9
<i>u</i> 2647	Si(207)...H(232)	464.1(40)	22.6(fixed)	—	-17.3	22.6
<i>u</i> 2457	F(219)...H(233)	464.2(74)	41.4(fixed)	—	14.8	41.4
<i>u</i> 2371	C(213)...H(240)	464.3(70)	36.6(fixed)	—	2.3	36.6
<i>u</i> 2433	C(253)...H(281)	464.3(130)	35.8(fixed)	—	1.4	35.8
<i>u</i> 2531	Si(84)...H(103)	464.4(121)	31.5(fixed)	—	-13.9	31.5
<i>u</i> 2532	Si(86)...H(107)	464.4(121)	31.3(fixed)	—	-13.9	31.3
<i>u</i> 4109	C(258)...H(271)	464.7(52)	44.1(fixed)	—	-25.7	44.1
<i>u</i> 2440	Si(251)...C(256)	464.9(32)	11.8(tied to <i>u</i> 2449)	—	-1.3	11.4
<i>u</i> 2349	C(175)...H(200)	464.9(306)	59.9(fixed)	—	-0.1	59.9
<i>u</i> 4050	H(145)...H(156)	464.9(244)	48.9(fixed)	—	-5.2	48.9
<i>u</i> 2419	F(15)...H(36)	465.0(159)	33.0(fixed)	—	2.9	33.0
<i>u</i> 2521	F(137)...H(149)	465.1(66)	29.7(fixed)	—	2.5	29.7
<i>u</i> 2321	C(216)...H(231)	465.2(78)	36.2(fixed)	—	8.8	36.2
<i>u</i> 2568	Si(4)...H(25)	465.3(108)	29.8(fixed)	—	-15.5	29.8
<i>u</i> 2413	F(55)...F(56)	465.3(30)	19.3(tied to <i>u</i> 2449)	—	-1.3	18.5
<i>u</i> 2581	H(231)...H(234)	465.6(16)	20.3(fixed)	—	-16.3	20.3
<i>u</i> 2445	Si(46)...H(75)	465.8(137)	21.5(fixed)	—	-3.7	21.5
<i>u</i> 2669	Si(86)...H(101)	465.9(56)	31.1(fixed)	—	-22.9	31.1
<i>u</i> 2668	Si(84)...H(109)	465.9(56)	30.4(fixed)	—	-22.9	30.4
<i>u</i> 2420	F(55)...F(58)	466.0(56)	23.9(tied to <i>u</i> 2449)	—	-1.5	23.0
<i>u</i> 2506	F(262)...H(286)	466.0(71)	32.6(fixed)	—	4.6	32.6
<i>u</i> 1562	H(264)...H(274)	466.2(270)	66.3(fixed)	—	2.2	66.3
<i>u</i> 2398	H(72)...H(81)	466.4(128)	63.9(fixed)	—	12.2	63.9
<i>u</i> 2562	F(17)...H(35)	466.6(161)	33.0(fixed)	—	2.4	33.0
<i>u</i> 2520	C(259)...H(265)	466.7(98)	32.1(fixed)	—	-7.1	32.1
<i>u</i> 2390	C(7)...H(38)	466.8(94)	25.3(fixed)	—	-3.0	25.3
<i>u</i> 2559	F(98)...H(122)	466.8(86)	30.4(fixed)	—	4.2	30.4
<i>u</i> 2427	H(29)...H(41)	466.9(102)	114.4(fixed)	—	-9.4	114.4
<i>u</i> 2446	Si(45)...H(62)	467.0(137)	22.2(fixed)	—	-3.9	22.2
<i>u</i> 2418	C(174)...H(189)	467.1(154)	40.2(fixed)	—	-3.6	40.2
<i>u</i> 2406	H(234)...H(246)	467.4(126)	89.2(fixed)	—	-6.8	89.2
<i>u</i> 2374	C(212)...H(243)	467.6(82)	24.1(fixed)	—	-2.5	24.1
<i>u</i> 2429	Si(45)...C(54)	467.6(19)	12.3(tied to <i>u</i> 2449)	—	-1.3	11.8
<i>u</i> 3040	H(225)...H(233)	467.7(135)	49.7(fixed)	—	-28.8	49.7
<i>u</i> 2861	H(104)...H(112)	468.1(317)	91.6(fixed)	—	-16.7	91.6
<i>u</i> 2597	H(108)...H(111)	468.2(16)	21.1(fixed)	—	-13.6	21.1
<i>u</i> 2596	H(100)...H(104)	468.3(16)	20.0(fixed)	—	-13.6	20.0

<i>u</i> 3037	H(224)...H(233)	468.4(103)	62.6(fixed)	—	-26.2	62.6
<i>u</i> 2523	F(220)...H(241)	468.4(62)	30.5(fixed)	—	1.6	30.5
<i>u</i> 2467	Si(250)...C(252)	468.9(34)	11.2(tied to <i>u</i> 2449)	—	-0.9	10.8
<i>u</i> 2590	H(182)...H(186)	469.5(16)	18.9(fixed)	—	-12.5	18.9
<i>u</i> 2591	H(196)...H(199)	469.5(16)	18.8(fixed)	—	-12.5	18.8
<i>u</i> 2504	Si(250)...H(284)	469.6(115)	35.4(fixed)	—	-10.3	35.4
<i>u</i> 2507	Si(45)...C(47)	469.7(36)	11.2(tied to <i>u</i> 2449)	—	-1.0	10.8
<i>u</i> 2450	Si(209)...H(230)	469.7(110)	23.3(fixed)	—	-8.3	23.3
<i>u</i> 2743	H(68)...H(72)	469.7(173)	79.9(fixed)	—	-17.7	79.9
<i>u</i> 2452	F(219)...F(222)	469.8(27)	18.4(tied to <i>u</i> 2449)	—	-1.7	17.7
<i>u</i> 3681	C(129)...H(155)	470.1(68)	23.7(fixed)	—	-1.5	23.7
<i>u</i> 2447	Si(207)...C(211)	470.1(19)	11.8(tied to <i>u</i> 2449)	—	-1.1	11.3
<i>u</i> 2637	F(220)...H(228)	470.1(177)	37.2(fixed)	—	5.0	37.2
<i>u</i> 2489	Si(46)...C(51)	470.1(35)	11.2(tied to <i>u</i> 2449)	—	-1.0	10.8
<i>u</i> 2585	H(282)...H(286)	470.2(16)	18.5(fixed)	—	-11.8	18.5
<i>u</i> 3382	F(138)...H(160)	470.2(173)	50.3(fixed)	—	-3.2	50.3
<i>u</i> 2482	Si(125)...C(132)	470.4(15)	11.3(tied to <i>u</i> 2449)	—	-1.0	10.8
<i>u</i> 2474	Si(166)...C(174)	470.5(29)	13.2(tied to <i>u</i> 2449)	—	-2.1	12.7
<i>u</i> 2475	Si(168)...C(177)	470.5(29)	13.2(tied to <i>u</i> 2449)	—	-2.1	12.7
<i>u</i> 4249	H(273)...H(283)	470.7(149)	34.3(fixed)	—	2.6	34.3
<i>u</i> 2377	C(93)...H(118)	470.9(301)	36.2(fixed)	—	2.4	36.2
<i>u</i> 2554	C(176)...H(185)	470.9(216)	44.8(fixed)	—	-4.2	44.8
<i>u</i> 2448	Si(250)...C(259)	471.0(18)	12.4(tied to <i>u</i> 2449)	—	-1.3	11.9
<i>u</i> 2453	F(260)...F(263)	471.0(47)	21.6(tied to <i>u</i> 2449)	—	-1.4	20.7
<i>u</i> 2766	H(185)...H(204)	471.3(234)	134.0(fixed)	—	-19.6	134.0
<i>u</i> 3416	F(137)...F(140)	471.3(27)	12.9(tied to <i>u</i> 2449)	—	-2.2	12.4
<i>u</i> 2536	H(265)...H(282)	471.4(273)	79.6(fixed)	—	-11.2	79.6
<i>u</i> 2542	Si(43)...H(71)	471.5(59)	26.3(fixed)	—	-10.2	26.3
<i>u</i> 2309	F(138)...F(139)	471.6(27)	21.7(tied to <i>u</i> 2449)	—	-1.4	20.8
<i>u</i> 2600	H(149)...H(152)	471.6(16)	17.4(fixed)	—	-10.5	17.4
<i>u</i> 2466	Si(84)...C(92)	471.6(30)	11.5(tied to <i>u</i> 2449)	—	-1.2	11.0
<i>u</i> 2546	Si(5)...H(32)	471.6(45)	24.0(fixed)	—	-0.1	24.0
<i>u</i> 1387	Si(126)...C(133)	471.7(20)	17.8(tied to <i>u</i> 2449)	—	0.4	17.1
<i>u</i> 2469	Si(84)...C(88)	471.7(23)	13.3(tied to <i>u</i> 2449)	—	-1.9	12.7
<i>u</i> 2577	H(77)...H(81)	471.8(16)	17.7(fixed)	—	-10.2	17.7
<i>u</i> 2595	H(67)...H(70)	471.8(16)	17.0(fixed)	—	-10.3	17.0
<i>u</i> 2505	F(263)...H(285)	472.0(99)	34.2(fixed)	—	2.9	34.2
<i>u</i> 2481	F(14)...F(17)	472.0(31)	18.4(tied to <i>u</i> 2449)	—	-1.6	17.6
<i>u</i> 2584	H(223)...H(227)	472.2(16)	17.6(fixed)	—	-9.8	17.6
<i>u</i> 2594	H(73)...H(76)	472.3(16)	17.2(fixed)	—	-9.8	17.2
<i>u</i> 2514	C(49)...H(62)	472.3(193)	37.3(fixed)	—	-3.7	37.3
<i>u</i> 4019	F(138)...H(162)	472.3(58)	25.9(fixed)	—	-2.3	25.9
<i>u</i> 2459	Si(45)...H(79)	472.4(115)	36.1(fixed)	—	-8.7	36.1
<i>u</i> 2571	H(264)...H(268)	472.5(16)	17.5(fixed)	—	-9.5	17.5

<i>u2443</i>	Si(208)...C(215)	472.6(15)	11.8(tied to <i>u2449</i> )	—	-1.1	11.3
<i>u2522</i>	C(48)...H(66)	472.6(196)	38.0(fixed)	—	-4.2	38.0
<i>u2455</i>	F(260)...F(261)	472.6(31)	19.3(tied to <i>u2449</i> )	—	-1.6	18.5
<i>u2656</i>	C(54)...H(60)	472.7(101)	36.3(fixed)	—	-8.6	36.3
<i>u2848</i>	H(227)...H(239)	472.7(124)	51.9(fixed)	—	-7.0	51.9
<i>u2613</i>	F(222)...H(238)	472.8(163)	32.3(fixed)	—	3.0	32.3
<i>u2449</i>	Si(2)...C(6)	472.9(20)	11.9(6)	—	-1.2	11.4
<i>u2465</i>	Si(4)...C(13)	473.0(24)	11.6(tied to <i>u2449</i> )	—	-1.1	11.1
<i>u2512</i>	F(14)...H(22)	473.0(167)	32.4(fixed)	—	3.9	32.4
<i>u2510</i>	Si(251)...H(280)	473.1(137)	22.5(fixed)	—	-3.3	22.5
<i>u2509</i>	F(14)...F(15)	473.2(40)	18.6(tied to <i>u2449</i> )	—	-1.7	17.9
<i>u422</i>	H(272)...H(277)	473.2(104)	68.2(fixed)	—	57.1	68.2
<i>u2511</i>	F(96)...F(99)	473.3(45)	20.1(tied to <i>u2449</i> )	—	-2.2	19.3
<i>u2461</i>	Si(250)...C(255)	473.4(17)	11.4(tied to <i>u2449</i> )	—	-0.9	10.9
<i>u2499</i>	Si(126)...C(135)	473.5(16)	11.4(tied to <i>u2449</i> )	—	-0.9	10.9
<i>u2688</i>	C(132)...H(163)	473.5(68)	29.7(fixed)	—	2.7	29.7
<i>u1676</i>	H(151)...H(155)	473.6(122)	51.1(fixed)	—	10.3	51.1
<i>u2570</i>	H(141)...H(145)	473.6(16)	17.3(fixed)	—	-8.5	17.3
<i>u2553</i>	C(171)...H(202)	473.6(193)	44.8(fixed)	—	-4.3	44.8
<i>u2593</i>	H(18)...H(22)	473.8(16)	16.9(fixed)	—	-8.3	16.9
<i>u2460</i>	Si(209)...C(218)	473.9(17)	11.7(tied to <i>u2449</i> )	—	-1.1	11.2
<i>u778</i>	C(259)...H(274)	474.1(85)	36.5(fixed)	—	9.5	36.5
<i>u2588</i>	H(59)...H(63)	474.3(16)	16.3(fixed)	—	-7.9	16.3
<i>u2498</i>	H(72)...H(77)	474.5(181)	53.2(fixed)	—	17.6	53.2
<i>u737</i>	H(270)...H(273)	474.7(46)	64.4(fixed)	—	23.9	64.4
<i>u2496</i>	Si(4)...C(9)	474.7(14)	10.9(tied to <i>u2449</i> )	—	-0.9	10.5
<i>u2539</i>	Si(125)...H(148)	474.9(112)	23.0(fixed)	—	-3.9	23.0
<i>u2598</i>	H(223)...H(244)	474.9(116)	51.7(fixed)	—	10.5	51.7
<i>u2485</i>	Si(43)...C(50)	475.1(20)	11.2(tied to <i>u2449</i> )	—	-0.9	10.8
<i>u2490</i>	F(219)...H(227)	475.2(149)	34.3(fixed)	—	6.1	34.3
<i>u2473</i>	Si(209)...C(214)	475.3(15)	10.8(tied to <i>u2449</i> )	—	-0.9	10.4
<i>u2572</i>	H(114)...H(117)	475.3(16)	16.3(fixed)	—	-6.9	16.3
<i>u2545</i>	F(55)...H(67)	475.6(97)	30.0(fixed)	—	2.3	30.0
<i>u2586</i>	Si(5)...H(34)	475.8(136)	22.6(fixed)	—	-3.3	22.6
<i>u2492</i>	C(256)...H(268)	476.0(177)	38.5(fixed)	—	9.2	38.5
<i>u2667</i>	H(61)...H(77)	476.0(251)	69.0(fixed)	—	-14.1	69.0
<i>u2580</i>	H(36)...H(40)	476.1(16)	16.0(fixed)	—	-6.1	16.0
<i>u2574</i>	Si(4)...H(19)	476.2(54)	24.9(fixed)	—	-6.1	24.9
<i>u2576</i>	H(241)...H(245)	476.3(16)	15.9(fixed)	—	-5.8	15.9
<i>u2458</i>	Si(3)...C(11)	476.4(15)	11.6(tied to <i>u2449</i> )	—	-1.1	11.2
<i>u2549</i>	H(237)...H(240)	476.4(16)	16.3(fixed)	—	-5.8	16.3
<i>u2996</i>	H(26)...H(41)	476.5(241)	67.5(fixed)	—	-17.3	67.5
<i>u2470</i>	Si(3)...C(12)	476.5(17)	11.3(tied to <i>u2449</i> )	—	-1.0	10.8
<i>u2565</i>	H(278)...H(281)	476.5(16)	15.9(fixed)	—	-5.6	15.9

<i>u2486</i>	Si(208)...C(217)	476.6(14)	11.3(tied to <i>u2449</i> )	—	-1.0	10.8
<i>u2561</i>	H(32)...H(35)	476.8(16)	15.9(fixed)	—	-5.3	15.9
<i>u2456</i>	F(15)...H(26)	476.9(52)	35.2(fixed)	—	17.5	35.2
<i>u2464</i>	H(224)...H(232)	477.0(146)	84.6(fixed)	—	-17.5	84.6
<i>u2439</i>	Si(84)...H(116)	477.1(125)	24.6(fixed)	—	-3.7	24.6
<i>u2442</i>	Si(168)...H(202)	477.3(130)	22.7(fixed)	—	-4.0	22.7
<i>u2441</i>	Si(166)...H(198)	477.3(130)	22.7(fixed)	—	-4.0	22.7
<i>u2497</i>	Si(85)...C(89)	477.3(16)	11.4(tied to <i>u2449</i> )	—	-1.6	10.9
<i>u2479</i>	Si(3)...C(7)	477.4(15)	11.1(tied to <i>u2449</i> )	—	-0.9	10.7
<i>u2791</i>	H(227)...H(240)	477.4(360)	43.7(fixed)	—	-8.1	43.7
<i>u2929</i>	H(69)...H(72)	477.5(180)	51.3(fixed)	—	-23.3	51.3
<i>u2184</i>	C(133)...H(151)	477.6(83)	50.7(fixed)	—	-9.8	50.7
<i>u2487</i>	Si(208)...C(212)	477.6(15)	11.2(tied to <i>u2449</i> )	—	-0.9	10.8
<i>u2526</i>	F(55)...H(59)	477.8(84)	32.3(fixed)	—	8.6	32.3
<i>u2679</i>	Si(210)...H(235)	477.9(55)	21.6(fixed)	—	-3.5	21.6
<i>u2543</i>	F(260)...H(264)	477.9(76)	31.3(fixed)	—	6.5	31.3
<i>u2513</i>	C(90)...H(113)	477.9(194)	45.6(fixed)	—	1.1	45.6
<i>u3637</i>	C(130)...H(152)	478.0(75)	40.5(fixed)	—	-7.6	40.5
<i>u4391</i>	H(142)...H(150)	478.0(144)	42.8(fixed)	—	-17.0	42.8
<i>u2636</i>	Si(46)...H(68)	478.0(46)	25.5(fixed)	—	-9.5	25.5
<i>u2484</i>	Si(168)...C(171)	478.1(12)	11.6(tied to <i>u2449</i> )	—	-2.0	11.2
<i>u2483</i>	Si(166)...C(172)	478.1(12)	11.6(tied to <i>u2449</i> )	—	-2.0	11.2
<i>u2763</i>	H(24)...H(30)	478.2(233)	84.3(fixed)	—	-15.6	84.3
<i>u2495</i>	Si(85)...C(94)	478.3(20)	11.1(tied to <i>u2449</i> )	—	-1.3	10.7
<i>u2508</i>	C(10)...H(20)	478.4(90)	43.3(fixed)	—	7.7	43.3
<i>u2676</i>	Si(209)...H(224)	478.5(52)	23.7(fixed)	—	-7.2	23.7
<i>u2432</i>	H(61)...H(69)	478.5(173)	46.9(fixed)	—	18.6	46.9
<i>u2503</i>	Si(251)...C(254)	478.5(13)	10.9(tied to <i>u2449</i> )	—	-1.0	10.4
<i>u2451</i>	Si(249)...C(257)	478.5(15)	11.3(tied to <i>u2449</i> )	—	-1.1	10.8
<i>u2619</i>	Si(251)...H(278)	478.6(47)	22.9(fixed)	—	-0.3	22.9
<i>u2805</i>	H(106)...H(116)	478.7(266)	89.5(fixed)	—	-17.7	89.5
<i>u2494</i>	Si(249)...C(258)	478.7(14)	11.1(tied to <i>u2449</i> )	—	-0.9	10.6
<i>u2488</i>	Si(45)...C(49)	478.8(15)	11.2(tied to <i>u2449</i> )	—	-1.0	10.7
<i>u2478</i>	F(14)...H(28)	478.8(75)	45.1(fixed)	—	21.5	45.1
<i>u2608</i>	C(252)...F(262)	478.9(73)	21.8(tied to <i>u2449</i> )	—	-1.3	20.9
<i>u2644</i>	F(58)...H(80)	479.0(113)	34.8(fixed)	—	0.7	34.8
<i>u2468</i>	Si(44)...C(53)	479.0(15)	11.2(tied to <i>u2449</i> )	—	-1.0	10.8
<i>u2587</i>	H(25)...H(39)	479.1(237)	71.0(fixed)	—	-10.6	71.0
<i>u2626</i>	Si(44)...H(60)	479.2(60)	21.0(fixed)	—	-7.0	21.0
<i>u2567</i>	C(48)...C(52)	479.4(135)	27.5(tied to <i>u2449</i> )	—	-1.4	26.4
<i>u2436</i>	F(261)...H(282)	479.4(154)	43.4(fixed)	—	16.6	43.4
<i>u3224</i>	Si(250)...H(273)	479.5(39)	16.6(fixed)	—	-3.5	16.6
<i>u2518</i>	F(97)...F(99)	479.6(81)	28.9(tied to <i>u2449</i> )	—	-2.3	27.7
<i>u2477</i>	Si(207)...C(216)	479.6(12)	11.1(tied to <i>u2449</i> )	—	-0.9	10.7

<i>u</i> 2552	Si(45)...H(81)	479.9(42)	23.5(fixed)	—	-0.3	23.5
<i>u</i> 1810	Si(126)...C(130)	480.2(13)	16.6(tied to <i>u</i> 2449)	—	-0.2	15.9
<i>u</i> 2774	H(226)...H(240)	480.2(96)	48.9(fixed)	—	-6.9	48.9
<i>u</i> 2463	Si(208)...H(239)	480.3(112)	22.4(fixed)	—	-4.0	22.4
<i>u</i> 2500	Si(5)...C(8)	480.3(12)	10.8(tied to <i>u</i> 2449)	—	-0.9	10.4
<i>u</i> 2623	Si(249)...H(265)	480.4(52)	22.0(fixed)	—	-5.9	22.0
<i>u</i> 2617	F(220)...H(225)	480.4(68)	41.3(fixed)	—	8.2	41.3
<i>u</i> 2515	Si(43)...C(48)	480.6(13)	11.1(tied to <i>u</i> 2449)	—	-1.0	10.6
<i>u</i> 2476	Si(44)...C(52)	480.6(12)	11.0(tied to <i>u</i> 2449)	—	-1.1	10.6
<i>u</i> 2599	C(214)...F(219)	480.7(53)	22.2(tied to <i>u</i> 2449)	—	-1.4	21.3
<i>u</i> 2604	H(117)...H(122)	480.7(256)	46.1(fixed)	—	6.3	46.1
<i>u</i> 3128	H(28)...H(37)	480.8(136)	88.2(fixed)	—	8.2	88.2
<i>u</i> 2686	F(57)...H(61)	480.8(98)	39.5(fixed)	—	5.2	39.5
<i>u</i> 2480	H(231)...H(237)	480.9(194)	54.0(fixed)	—	8.9	54.0
<i>u</i> 2501	Si(248)...C(253)	481.3(13)	10.9(tied to <i>u</i> 2449)	—	-1.0	10.5
<i>u</i> 2895	F(261)...H(271)	481.4(65)	75.9(fixed)	—	-1.3	75.9
<i>u</i> 2493	Si(210)...C(213)	481.4(12)	10.8(tied to <i>u</i> 2449)	—	-0.9	10.4
<i>u</i> 2788	H(68)...H(71)	482.0(167)	61.8(fixed)	—	-20.1	61.8
<i>u</i> 2528	Si(207)...H(226)	482.1(113)	24.4(fixed)	—	-5.7	24.4
<i>u</i> 2642	H(277)...H(286)	482.1(117)	55.2(fixed)	—	6.6	55.2
<i>u</i> 3272	Si(251)...H(271)	482.4(25)	22.4(fixed)	—	-11.1	22.4
<i>u</i> 2921	H(26)...H(39)	482.5(197)	51.3(fixed)	—	-18.0	51.3
<i>u</i> 581	F(137)...H(156)	482.7(172)	39.9(fixed)	—	7.4	39.9
<i>u</i> 2541	F(260)...F(262)	482.9(38)	20.7(tied to <i>u</i> 2449)	—	-1.1	19.9
<i>u</i> 2671	C(9)...H(32)	482.9(68)	29.8(fixed)	—	3.0	29.8
<i>u</i> 2871	H(104)...H(113)	482.9(277)	61.6(fixed)	—	-19.5	61.6
<i>u</i> 2611	C(171)...C(172)	482.9(65)	43.3(tied to <i>u</i> 2449)	—	-3.3	41.6
<i>u</i> 2607	F(262)...F(263)	483.3(50)	21.2(tied to <i>u</i> 2449)	—	-1.2	20.3
<i>u</i> 3654	F(261)...H(270)	483.3(66)	29.8(fixed)	—	-19.7	29.8
<i>u</i> 3008	H(142)...H(151)	483.6(105)	53.8(fixed)	—	14.1	53.8
<i>u</i> 2609	H(62)...H(76)	483.7(236)	45.5(fixed)	—	2.5	45.5
<i>u</i> 2737	H(59)...H(76)	483.7(250)	43.5(fixed)	—	6.4	43.5
<i>u</i> 2666	Si(207)...H(223)	483.9(41)	22.1(fixed)	—	2.1	22.1
<i>u</i> 2556	Si(4)...H(38)	483.9(116)	22.1(fixed)	—	-3.4	22.1
<i>u</i> 3121	H(233)...H(242)	484.1(90)	71.0(fixed)	—	6.1	71.0
<i>u</i> 2632	H(18)...H(39)	484.3(129)	51.6(fixed)	—	9.3	51.6
<i>u</i> 2630	H(277)...H(282)	484.3(124)	51.2(fixed)	—	11.9	51.2
<i>u</i> 3051	H(25)...H(30)	484.4(184)	51.7(fixed)	—	-18.8	51.7
<i>u</i> 2872	H(31)...H(40)	484.6(152)	51.6(fixed)	—	6.2	51.6
<i>u</i> 2651	H(199)...H(204)	484.8(251)	83.2(fixed)	—	21.1	83.2
<i>u</i> 2533	Si(2)...H(21)	484.9(112)	22.7(fixed)	—	-4.1	22.7
<i>u</i> 723	C(256)...H(272)	485.0(61)	67.0(fixed)	—	36.8	67.0
<i>u</i> 2550	Si(85)...H(112)	485.0(71)	22.5(fixed)	—	-4.1	22.5
<i>u</i> 2563	Si(209)...H(243)	485.2(112)	22.7(fixed)	—	-3.3	22.7

<i>u3622</i>	C(131)...H(141)	485.2(74)	24.9(fixed)	—	-2.4	24.9
<i>u2603</i>	C(9)...F(14)	485.4(65)	21.9(tied to <i>u2449</i> )	—	-1.5	21.0
<i>u2530</i>	Si(43)...H(66)	485.5(112)	24.3(fixed)	—	-4.0	24.3
<i>u1182</i>	C(259)...H(270)	485.5(74)	78.3(fixed)	—	22.9	78.3
<i>u2624</i>	H(26)...H(33)	485.6(248)	69.9(fixed)	—	16.8	69.9
<i>u2569</i>	C(88)...F(97)	485.7(125)	23.4(tied to <i>u2449</i> )	—	-2.0	22.5
<i>u2631</i>	H(63)...H(75)	485.7(235)	46.4(fixed)	—	2.3	46.4
<i>u3256</i>	Si(126)...H(157)	485.9(114)	15.4(fixed)	—	-3.5	15.4
<i>u2578</i>	F(96)...H(104)	486.0(184)	47.9(fixed)	—	18.6	47.9
<i>u2579</i>	F(97)...H(108)	486.0(184)	47.7(fixed)	—	18.7	47.7
<i>u2650</i>	C(47)...H(76)	486.1(192)	30.0(fixed)	—	3.2	30.0
<i>u2665</i>	Si(250)...H(286)	486.2(40)	23.7(fixed)	—	0.2	23.7
<i>u3496</i>	H(143)...H(151)	486.4(140)	51.1(fixed)	—	5.6	51.1
<i>u2730</i>	Si(4)...H(40)	486.4(53)	21.9(fixed)	—	0.0	21.9
<i>u2622</i>	Si(208)...H(237)	486.7(32)	22.8(fixed)	—	-0.4	22.8
<i>u2602</i>	F(14)...F(16)	486.7(43)	21.6(tied to <i>u2449</i> )	—	-1.3	20.8
<i>u2753</i>	Si(86)...H(122)	486.8(72)	22.0(fixed)	—	-0.2	22.0
<i>u2690</i>	Si(2)...H(18)	487.1(46)	22.6(fixed)	—	1.3	22.6
<i>u2700</i>	Si(209)...H(245)	487.3(38)	22.3(fixed)	—	-0.1	22.3
<i>u3290</i>	H(232)...H(246)	487.5(96)	36.7(fixed)	—	-22.7	36.7
<i>u3320</i>	H(27)...H(41)	487.5(87)	42.5(fixed)	—	-28.5	42.5
<i>u2660</i>	C(50)...H(81)	487.7(70)	28.9(fixed)	—	2.8	28.9
<i>u2673</i>	C(8)...H(18)	487.7(79)	35.1(fixed)	—	7.7	35.1
<i>u2695</i>	F(58)...H(65)	487.8(176)	33.4(fixed)	—	2.4	33.4
<i>u2519</i>	C(54)...H(72)	487.8(100)	50.3(fixed)	—	11.2	50.3
<i>u4630</i>	H(144)...H(153)	487.9(191)	21.8(fixed)	—	-14.2	21.8
<i>u2806</i>	H(266)...H(282)	487.9(222)	65.9(fixed)	—	-15.2	65.9
<i>u2605</i>	C(255)...H(278)	488.0(69)	29.0(fixed)	—	3.9	29.0
<i>u2778</i>	H(103)...H(113)	488.3(289)	65.4(fixed)	—	-13.4	65.4
<i>u2525</i>	C(95)...H(104)	488.3(176)	50.9(fixed)	—	16.3	50.9
<i>u2685</i>	H(264)...H(281)	488.3(224)	42.0(fixed)	—	7.0	42.0
<i>u2625</i>	C(259)...F(263)	488.4(76)	23.9(tied to <i>u2449</i> )	—	-1.4	22.9
<i>u2524</i>	C(92)...H(108)	488.4(176)	50.8(fixed)	—	16.3	50.8
<i>u2744</i>	C(10)...H(23)	488.9(163)	31.8(fixed)	—	2.8	31.8
<i>u2677</i>	C(8)...F(15)	488.9(41)	20.9(tied to <i>u2449</i> )	—	-1.4	20.0
<i>u2783</i>	Si(125)...H(142)	489.1(34)	23.3(fixed)	—	-3.7	23.3
<i>u2674</i>	C(218)...H(237)	489.1(64)	29.7(fixed)	—	2.7	29.7
<i>u2735</i>	Si(250)...H(264)	489.1(55)	21.3(fixed)	—	1.0	21.3
<i>u2714</i>	C(131)...F(137)	489.2(51)	21.4(tied to <i>u2449</i> )	—	-1.3	20.5
<i>u2749</i>	Si(45)...H(59)	489.3(61)	21.5(fixed)	—	1.2	21.5
<i>u2808</i>	C(130)...F(138)	489.3(51)	18.7(tied to <i>u2449</i> )	—	-1.3	18.0
<i>u2716</i>	F(180)...H(197)	489.3(181)	34.6(fixed)	—	4.8	34.6
<i>u2551</i>	C(53)...H(72)	489.4(134)	35.3(fixed)	—	11.2	35.3
<i>u2725</i>	F(58)...H(69)	489.6(99)	44.7(fixed)	—	10.2	44.7

<i>u</i> 2701	F(57)...H(64)	489.7(171)	33.0(fixed)	—	2.3	33.0
<i>u</i> 2610	C(254)...F(261)	489.7(54)	22.4(tied to <i>u</i> 2449)	—	-1.6	21.5
<i>u</i> 2724	Si(125)...H(152)	489.7(34)	22.3(fixed)	—	4.0	22.3
<i>u</i> 2643	Si(248)...H(276)	489.8(40)	22.2(fixed)	—	-3.9	22.2
<i>u</i> 2638	C(51)...H(63)	490.0(185)	31.0(fixed)	—	3.2	31.0
<i>u</i> 2710	H(63)...H(73)	490.8(241)	49.2(fixed)	—	10.0	49.2
<i>u</i> 2646	C(50)...H(61)	490.9(140)	33.1(fixed)	—	6.7	33.1
<i>u</i> 2663	C(213)...H(223)	491.3(79)	36.4(fixed)	—	10.2	36.4
<i>u</i> 4230	C(258)...H(273)	491.6(144)	23.4(fixed)	—	-5.9	23.4
<i>u</i> 2614	C(177)...H(199)	491.6(150)	35.8(fixed)	—	2.9	35.8
<i>u</i> 2736	C(252)...F(261)	491.6(48)	19.2(tied to <i>u</i> 2449)	—	-1.1	18.4
<i>u</i> 2692	H(20)...H(35)	491.9(126)	43.5(fixed)	—	5.9	43.5
<i>u</i> 2654	F(219)...F(221)	492.1(35)	21.6(tied to <i>u</i> 2449)	—	-1.3	20.8
<i>u</i> 2713	Si(43)...H(70)	492.2(47)	21.7(fixed)	—	3.7	21.7
<i>u</i> 2540	C(215)...H(231)	492.4(153)	39.6(fixed)	—	8.3	39.6
<i>u</i> 2683	H(185)...H(190)	492.5(173)	59.2(fixed)	—	3.2	59.2
<i>u</i> 3299	H(101)...H(112)	492.6(125)	56.1(fixed)	—	-32.2	56.1
<i>u</i> 3300	H(109)...H(123)	492.7(125)	55.3(fixed)	—	-32.3	55.3
<i>u</i> 2747	Si(46)...H(73)	492.7(59)	22.1(fixed)	—	3.2	22.1
<i>u</i> 2538	F(56)...H(77)	492.7(153)	38.6(fixed)	—	14.8	38.6
<i>u</i> 2616	C(95)...H(117)	492.8(153)	33.3(fixed)	—	3.4	33.3
<i>u</i> 3062	H(61)...H(79)	492.8(241)	46.8(fixed)	—	-17.3	46.8
<i>u</i> 2606	Si(210)...H(246)	492.8(39)	23.2(fixed)	—	-3.8	23.2
<i>u</i> 2694	C(51)...H(77)	492.9(114)	38.6(fixed)	—	9.8	38.6
<i>u</i> 2693	C(253)...C(257)	493.0(105)	24.6(tied to <i>u</i> 2449)	—	-1.4	23.6
<i>u</i> 2422	F(97)...H(102)	493.2(163)	44.7(fixed)	—	33.0	44.7
<i>u</i> 2696	C(217)...F(220)	493.4(39)	22.2(tied to <i>u</i> 2449)	—	-1.3	21.3
<i>u</i> 2421	F(96)...H(110)	493.4(163)	43.8(fixed)	—	33.1	43.8
<i>u</i> 2697	Si(251)...H(287)	493.8(41)	23.2(fixed)	—	-4.7	23.2
<i>u</i> 2859	H(18)...H(32)	493.9(135)	58.7(fixed)	—	4.0	58.7
<i>u</i> 583	H(143)...H(159)	493.9(117)	63.7(fixed)	—	18.1	63.7
<i>u</i> 2731	C(54)...F(58)	494.0(89)	22.7(tied to <i>u</i> 2820)	—	-1.6	23.2
<i>u</i> 2547	H(22)...H(39)	494.2(155)	43.8(fixed)	—	5.0	43.8
<i>u</i> 2726	H(100)...H(121)	494.2(171)	86.6(fixed)	—	21.7	86.6
<i>u</i> 2727	H(111)...H(113)	494.4(171)	86.4(fixed)	—	21.8	86.4
<i>u</i> 2715	F(178)...H(187)	494.6(162)	34.6(fixed)	—	4.8	34.6
<i>u</i> 2721	F(178)...H(184)	494.9(113)	62.5(fixed)	—	28.0	62.5
<i>u</i> 2761	H(225)...H(236)	494.9(80)	42.8(fixed)	—	9.1	42.8
<i>u</i> 2723	C(255)...F(260)	494.9(51)	20.2(tied to <i>u</i> 2820)	—	-1.3	20.7
<i>u</i> 2722	F(179)...H(192)	495.1(113)	61.7(fixed)	—	28.0	61.7
<i>u</i> 2670	H(73)...H(81)	495.3(154)	68.6(fixed)	—	7.1	68.6
<i>u</i> 2706	C(252)...H(281)	495.4(171)	31.7(fixed)	—	2.7	31.7
<i>u</i> 4385	H(142)...H(155)	495.4(70)	29.3(fixed)	—	-4.7	29.3
<i>u</i> 2787	C(6)...H(32)	495.4(87)	36.3(fixed)	—	1.9	36.3



<i>u</i> 2680	H(230)...H(244)	495.4(211)	52.2(fixed)	—	-6.5	52.2
<i>u</i> 2781	Si(126)...H(160)	495.5(67)	23.1(fixed)	—	1.5	23.1
<i>u</i> 2728	Si(166)...H(196)	495.5(71)	25.9(fixed)	—	9.1	25.9
<i>u</i> 2729	Si(168)...H(204)	495.6(71)	25.6(fixed)	—	9.1	25.6
<i>u</i> 2672	Si(3)...H(33)	495.7(69)	23.2(fixed)	—	-0.5	23.2
<i>u</i> 2618	Si(5)...H(41)	495.9(50)	23.5(fixed)	—	-4.1	23.5
<i>u</i> 2615	C(173)...H(186)	496.2(151)	35.8(fixed)	—	2.9	35.8
<i>u</i> 2361	Si(126)...H(146)	496.4(68)	40.5(fixed)	—	-4.7	40.5
<i>u</i> 2612	C(213)...C(216)	496.4(54)	25.0(tied to <i>u</i> 2449)	—	-1.4	24.0
<i>u</i> 3133	C(217)...H(233)	496.5(74)	60.1(fixed)	—	7.4	60.1
<i>u</i> 2800	F(221)...H(228)	496.6(59)	29.6(fixed)	—	3.2	29.6
<i>u</i> 949	Si(126)...H(155)	496.6(43)	38.8(fixed)	—	16.5	38.8
<i>u</i> 4423	H(271)...H(284)	496.8(70)	49.5(fixed)	—	-30.0	49.5
<i>u</i> 2661	C(47)...H(69)	496.8(123)	34.8(fixed)	—	11.3	34.8
<i>u</i> 3027	H(280)...H(283)	496.8(199)	61.7(fixed)	—	-16.0	61.7
<i>u</i> 2720	C(211)...H(244)	496.9(83)	37.7(fixed)	—	2.9	37.7
<i>u</i> 2865	H(31)...H(36)	496.9(138)	43.6(fixed)	—	2.8	43.6
<i>u</i> 2657	C(52)...H(70)	497.1(79)	38.7(fixed)	—	14.3	38.7
<i>u</i> 955	C(253)...H(275)	497.3(101)	32.9(fixed)	—	7.9	32.9
<i>u</i> 3490	F(260)...H(273)	497.5(159)	28.0(fixed)	—	-3.8	28.0
<i>u</i> 2765	F(220)...H(245)	497.6(57)	32.1(fixed)	—	1.8	32.1
<i>u</i> 2741	H(59)...H(66)	497.6(178)	59.6(fixed)	—	-8.5	59.6
<i>u</i> 2775	C(258)...H(277)	497.7(82)	35.9(fixed)	—	1.3	35.9
<i>u</i> 2776	Si(46)...H(82)	498.0(42)	22.5(fixed)	—	-3.6	22.5
<i>u</i> 2560	H(227)...H(244)	498.1(112)	44.8(fixed)	—	6.1	44.8
<i>u</i> 2740	Si(3)...H(37)	498.2(72)	22.1(fixed)	—	-0.6	22.1
<i>u</i> 2785	Si(2)...H(30)	498.2(35)	24.3(fixed)	—	-3.9	24.3
<i>u</i> 2772	Si(208)...H(228)	498.3(68)	22.1(fixed)	—	0.4	22.1
<i>u</i> 2555	H(67)...H(78)	498.3(239)	47.6(fixed)	—	16.1	47.6
<i>u</i> 2738	C(49)...F(55)	498.5(68)	20.4(tied to <i>u</i> 2820)	—	-1.4	20.8
<i>u</i> 2882	H(62)...H(70)	498.5(136)	67.8(fixed)	—	-11.5	67.8
<i>u</i> 2751	Si(208)...H(242)	498.6(67)	22.1(fixed)	—	-0.6	22.1
<i>u</i> 2759	Si(3)...H(23)	498.9(69)	21.3(fixed)	—	-0.3	21.3
<i>u</i> 3152	C(12)...H(28)	498.9(92)	75.2(fixed)	—	10.9	75.2
<i>u</i> 2964	C(215)...F(222)	499.0(61)	20.5(tied to <i>u</i> 2820)	—	-1.2	21.0
<i>u</i> 2798	C(218)...F(221)	499.1(38)	15.6(tied to <i>u</i> 2820)	—	-0.7	16.0
<i>u</i> 2652	H(186)...H(193)	499.1(201)	83.5(fixed)	—	21.1	83.5
<i>u</i> 2832	C(47)...F(56)	499.2(66)	17.1(tied to <i>u</i> 2820)	—	-1.5	17.5
<i>u</i> 3014	H(231)...H(246)	499.2(233)	55.2(fixed)	—	-9.9	55.2
<i>u</i> 2810	C(256)...F(263)	499.2(63)	17.6(tied to <i>u</i> 2820)	—	-1.9	18.0
<i>u</i> 2794	C(13)...F(16)	499.4(47)	15.9(tied to <i>u</i> 2820)	—	-0.9	16.3
<i>u</i> 3594	C(132)...H(158)	499.5(76)	24.2(fixed)	—	-1.4	24.2
<i>u</i> 563	F(138)...H(141)	499.6(53)	37.1(fixed)	—	7.2	37.1
<i>u</i> 1694	H(265)...H(275)	500.1(181)	48.4(fixed)	—	1.7	48.4

<i>u</i> 2920	C(211)...H(236)	500.1(60)	32.5(fixed)	—	1.6	32.5
<i>u</i> 2712	Si(209)...H(234)	500.1(39)	23.2(fixed)	—	6.6	23.2
<i>u</i> 4307	H(141)...H(163)	500.2(133)	28.6(fixed)	—	-4.6	28.6
<i>u</i> 2769	H(238)...H(241)	500.3(222)	41.2(fixed)	—	6.4	41.2
<i>u</i> 2813	F(16)...H(23)	500.4(68)	29.9(fixed)	—	1.5	29.9
<i>u</i> 2708	Si(84)...H(100)	500.4(57)	27.5(fixed)	—	11.8	27.5
<i>u</i> 4369	H(271)...H(282)	500.5(78)	56.7(fixed)	—	-22.9	56.7
<i>u</i> 2709	Si(86)...H(111)	500.5(57)	27.2(fixed)	—	11.8	27.2
<i>u</i> 2793	C(212)...F(221)	500.5(40)	19.6(tied to <i>u</i> 2820)	—	-1.1	20.1
<i>u</i> 2995	H(60)...H(79)	500.7(191)	58.6(fixed)	—	-19.3	58.6
<i>u</i> 2796	C(259)...H(277)	500.7(85)	42.5(fixed)	—	2.2	42.5
<i>u</i> 2711	C(88)...H(121)	500.8(126)	39.7(fixed)	—	2.3	39.7
<i>u</i> 4594	H(146)...H(153)	500.8(220)	29.8(fixed)	—	-8.1	29.8
<i>u</i> 2734	Si(249)...H(279)	500.9(72)	22.1(fixed)	—	-0.7	22.1
<i>u</i> 3015	H(266)...H(284)	500.9(227)	54.5(fixed)	—	-16.0	54.5
<i>u</i> 4120	H(144)...H(152)	500.9(87)	53.9(fixed)	—	-12.7	53.9
<i>u</i> 3099	H(107)...H(116)	500.9(176)	55.8(fixed)	—	-21.3	55.8
<i>u</i> 2924	C(212)...F(220)	500.9(62)	16.8(tied to <i>u</i> 2820)	—	-1.3	17.2
<i>u</i> 3098	H(103)...H(120)	500.9(176)	55.9(fixed)	—	-21.2	55.9
<i>u</i> 2777	Si(44)...H(78)	501.0(69)	25.3(fixed)	—	2.5	25.3
<i>u</i> 2959	H(25)...H(41)	501.1(203)	70.3(fixed)	—	-16.8	70.3
<i>u</i> 1680	Si(248)...H(274)	501.2(78)	30.1(fixed)	—	3.7	30.1
<i>u</i> 3333	H(183)...H(202)	501.2(97)	54.4(fixed)	—	-32.7	54.4
<i>u</i> 2899	H(231)...H(244)	501.4(170)	44.7(fixed)	—	-10.3	44.7
<i>u</i> 2845	C(6)...H(35)	501.4(87)	32.2(fixed)	—	1.0	32.2
<i>u</i> 2818	C(174)...F(178)	501.6(61)	19.4(tied to <i>u</i> 2820)	—	-3.6	19.9
<i>u</i> 2842	C(51)...F(58)	501.9(64)	17.1(tied to <i>u</i> 2820)	—	-1.6	17.5
<i>u</i> 2799	Si(45)...H(65)	502.0(71)	21.6(fixed)	—	-0.4	21.6
<i>u</i> 2779	Si(207)...H(238)	502.2(68)	21.4(fixed)	—	-0.3	21.4
<i>u</i> 2821	Si(85)...H(119)	502.3(83)	23.2(fixed)	—	-1.1	23.2
<i>u</i> 2864	F(137)...H(152)	502.5(53)	31.8(fixed)	—	9.4	31.8
<i>u</i> 2746	C(256)...H(282)	502.6(82)	37.3(fixed)	—	12.6	37.3
<i>u</i> 2627	C(93)...C(94)	502.7(223)	24.4(tied to <i>u</i> 2820)	—	-1.3	25.0
<i>u</i> 2755	C(11)...H(20)	502.9(87)	34.3(fixed)	—	5.3	34.3
<i>u</i> 2739	C(11)...H(26)	502.9(153)	55.4(fixed)	—	17.0	55.4
<i>u</i> 2745	H(268)...H(280)	503.1(209)	44.8(fixed)	—	8.9	44.8
<i>u</i> 3157	H(226)...H(237)	503.1(107)	41.8(fixed)	—	-10.4	41.8
<i>u</i> 2703	Si(4)...H(29)	503.1(34)	26.2(fixed)	—	12.2	26.2
<i>u</i> 2812	C(92)...F(96)	503.2(56)	17.3(tied to <i>u</i> 2820)	—	-1.5	17.7
<i>u</i> 2847	H(234)...H(240)	503.2(198)	51.1(fixed)	—	10.9	51.1
<i>u</i> 2837	F(55)...H(70)	503.5(82)	31.8(fixed)	—	8.9	31.8
<i>u</i> 2839	C(92)...F(99)	503.7(60)	16.5(tied to <i>u</i> 2820)	—	-1.5	16.9
<i>u</i> 2824	C(259)...F(262)	503.9(39)	16.8(tied to <i>u</i> 2820)	—	-1.2	17.2
<i>u</i> 2790	Si(249)...H(283)	504.0(70)	24.3(fixed)	—	2.6	24.3

<i>u</i> 2809	C(211)...H(242)	504.1(168)	33.4(fixed)	—	1.8	33.4
<i>u</i> 2702	C(53)...H(67)	504.2(156)	34.8(fixed)	—	4.1	34.8
<i>u</i> 2764	C(259)...H(279)	504.2(174)	33.3(fixed)	—	1.8	33.3
<i>u</i> 1407	C(129)...H(159)	504.4(77)	56.3(fixed)	—	8.7	56.3
<i>u</i> 2820	C(7)...F(16)	504.5(40)	19.8(12)	—	-1.1	20.3
<i>u</i> 2858	C(216)...F(222)	504.6(48)	15.8(tied to <i>u</i> 2820)	—	-1.0	16.2
<i>u</i> 2816	Si(168)...H(187)	504.9(68)	22.5(fixed)	—	-1.8	22.5
<i>u</i> 2815	Si(166)...H(188)	504.9(68)	22.5(fixed)	—	-1.8	22.5
<i>u</i> 2868	C(255)...F(263)	504.9(40)	15.5(tied to <i>u</i> 2820)	—	-1.0	15.8
<i>u</i> 2768	C(6)...H(39)	505.0(96)	39.0(fixed)	—	3.0	39.0
<i>u</i> 2852	F(56)...H(65)	505.0(79)	30.8(fixed)	—	1.6	30.8
<i>u</i> 2756	C(12)...F(15)	505.2(55)	19.6(tied to <i>u</i> 2820)	—	-1.2	20.1
<i>u</i> 2760	C(51)...H(81)	505.2(98)	34.4(fixed)	—	1.7	34.4
<i>u</i> 3485	F(260)...H(275)	505.7(154)	25.1(fixed)	—	-3.6	25.1
<i>u</i> 1671	Si(126)...H(154)	505.7(33)	60.1(fixed)	—	-2.6	60.1
<i>u</i> 2748	C(13)...H(33)	505.8(177)	32.7(fixed)	—	1.9	32.7
<i>u</i> 3092	H(107)...H(123)	506.1(226)	55.8(fixed)	—	-19.4	55.8
<i>u</i> 3093	H(103)...H(112)	506.1(226)	55.9(fixed)	—	-19.4	55.9
<i>u</i> 2935	H(269)...H(278)	506.2(275)	64.2(fixed)	—	4.0	64.2
<i>u</i> 2938	Si(5)...H(31)	506.2(38)	21.1(fixed)	—	-2.5	21.1
<i>u</i> 2817	C(170)...F(180)	506.3(17)	19.4(tied to <i>u</i> 2820)	—	-3.6	19.9
<i>u</i> 2780	Si(85)...H(105)	506.4(74)	23.4(fixed)	—	2.7	23.4
<i>u</i> 2681	C(214)...H(240)	506.4(149)	30.8(fixed)	—	3.8	30.8
<i>u</i> 2664	C(49)...H(73)	506.4(85)	39.3(fixed)	—	15.1	39.3
<i>u</i> 2893	C(253)...H(278)	506.5(84)	33.8(fixed)	—	1.3	33.8
<i>u</i> 2802	C(90)...C(92)	506.6(134)	30.0(tied to <i>u</i> 2820)	—	-2.3	30.7
<i>u</i> 2910	H(267)...H(281)	506.8(191)	49.3(fixed)	—	-0.4	49.3
<i>u</i> 3072	F(178)...H(182)	506.8(127)	98.6(fixed)	—	2.9	98.6
<i>u</i> 2822	C(49)...F(56)	506.9(60)	21.0(tied to <i>u</i> 2820)	—	-1.2	21.5
<i>u</i> 3938	C(129)...H(163)	506.9(89)	26.6(fixed)	—	-3.8	26.6
<i>u</i> 2925	H(280)...H(284)	507.2(170)	59.5(fixed)	—	-13.5	59.5
<i>u</i> 2704	C(13)...H(22)	507.2(100)	32.3(fixed)	—	2.9	32.3
<i>u</i> 3046	C(13)...H(31)	507.3(103)	43.4(fixed)	—	1.9	43.4
<i>u</i> 2754	C(257)...F(262)	507.4(23)	18.3(tied to <i>u</i> 2820)	—	-1.3	18.7
<i>u</i> 3196	H(226)...H(239)	507.4(331)	44.4(fixed)	—	-10.1	44.4
<i>u</i> 2966	C(170)...F(178)	507.5(86)	25.5(tied to <i>u</i> 2820)	—	-1.7	26.1
<i>u</i> 2967	C(173)...F(179)	507.5(86)	25.5(tied to <i>u</i> 2820)	—	-1.7	26.1
<i>u</i> 2898	C(10)...H(36)	507.6(106)	31.7(fixed)	—	1.6	31.7
<i>u</i> 3217	H(75)...H(78)	507.7(224)	56.0(fixed)	—	-17.0	56.0
<i>u</i> 2918	C(11)...F(17)	507.8(70)	19.6(tied to <i>u</i> 2820)	—	-1.2	20.0
<i>u</i> 3538	H(266)...H(272)	507.8(102)	62.2(fixed)	—	1.3	62.2
<i>u</i> 2969	C(88)...H(119)	507.8(174)	40.8(fixed)	—	0.3	40.8
<i>u</i> 2770	C(216)...F(219)	507.9(27)	18.1(tied to <i>u</i> 2820)	—	-1.1	18.6
<i>u</i> 2933	Si(251)...H(277)	507.9(37)	21.0(fixed)	—	-2.5	21.0

<i>u</i> 2917	C(48)...H(78)	507.9(195)	56.4(fixed)	—	7.3	56.4
<i>u</i> 2762	C(214)...F(220)	508.1(24)	17.8(tied to <i>u</i> 2820)	—	-1.3	18.2
<i>u</i> 2841	C(255)...F(261)	508.2(44)	20.5(tied to <i>u</i> 2820)	—	-1.0	20.9
<i>u</i> 2962	Si(250)...H(266)	508.3(35)	21.9(fixed)	—	-1.7	21.9
<i>u</i> 2840	C(258)...F(261)	508.3(50)	19.6(tied to <i>u</i> 2820)	—	-1.1	20.0
<i>u</i> 2902	Si(46)...H(72)	508.4(35)	26.2(fixed)	—	-1.9	26.2
<i>u</i> 3091	F(220)...H(227)	508.5(242)	41.4(fixed)	—	-0.7	41.4
<i>u</i> 2955	F(180)...H(201)	508.5(138)	42.6(fixed)	—	0.4	42.6
<i>u</i> 2803	Si(44)...H(74)	508.5(76)	21.1(fixed)	—	-0.9	21.1
<i>u</i> 2846	H(230)...H(240)	508.6(155)	48.7(fixed)	—	-0.1	48.7
<i>u</i> 2844	Si(43)...H(64)	508.6(77)	21.3(fixed)	—	-0.7	21.3
<i>u</i> 2883	F(221)...H(244)	508.9(78)	34.8(fixed)	—	-0.3	34.8
<i>u</i> 2834	C(216)...H(241)	509.0(143)	32.2(fixed)	—	3.1	32.2
<i>u</i> 3001	Si(45)...H(61)	509.1(35)	22.0(fixed)	—	-1.9	22.0
<i>u</i> 1202	C(129)...F(138)	509.1(40)	26.7(tied to <i>u</i> 2820)	—	0.7	27.3
<i>u</i> 2971	Si(168)...H(203)	509.1(31)	36.0(fixed)	—	-2.9	36.0
<i>u</i> 2970	Si(166)...H(195)	509.2(31)	35.6(fixed)	—	-2.9	35.6
<i>u</i> 2851	C(6)...H(37)	509.3(171)	33.5(fixed)	—	1.7	33.5
<i>u</i> 2635	H(231)...H(239)	509.4(169)	44.7(fixed)	—	9.8	44.7
<i>u</i> 2811	C(54)...H(74)	509.6(160)	33.8(fixed)	—	2.3	33.8
<i>u</i> 2823	C(11)...F(16)	509.7(16)	18.0(tied to <i>u</i> 2820)	—	-1.6	18.5
<i>u</i> 3011	Si(86)...H(110)	509.7(31)	37.0(fixed)	—	-2.1	37.0
<i>u</i> 3010	Si(84)...H(102)	509.8(31)	36.8(fixed)	—	-2.2	36.8
<i>u</i> 2879	C(175)...F(181)	509.9(77)	30.7(tied to <i>u</i> 2820)	—	-2.1	31.4
<i>u</i> 2819	C(215)...F(221)	510.0(26)	17.3(tied to <i>u</i> 2820)	—	-1.7	17.7
<i>u</i> 2953	Si(45)...H(80)	510.1(32)	20.4(fixed)	—	-2.4	20.4
<i>u</i> 2874	C(215)...H(225)	510.1(71)	32.8(fixed)	—	7.6	32.8
<i>u</i> 2915	Si(125)...H(151)	510.2(30)	27.1(fixed)	—	-2.0	27.1
<i>u</i> 3079	H(265)...H(284)	510.3(192)	56.4(fixed)	—	-20.0	56.4
<i>u</i> 2807	Si(248)...H(269)	510.3(76)	22.8(fixed)	—	0.8	22.8
<i>u</i> 2826	Si(169)...H(199)	510.5(82)	20.4(fixed)	—	-2.8	20.4
<i>u</i> 2825	Si(167)...H(200)	510.5(82)	20.4(fixed)	—	-2.8	20.4
<i>u</i> 4346	H(141)...H(148)	510.5(87)	29.9(fixed)	—	-6.9	29.9
<i>u</i> 2919	F(16)...H(39)	510.5(91)	36.5(fixed)	—	-0.7	36.5
<i>u</i> 2866	C(51)...C(53)	510.7(90)	20.6(tied to <i>u</i> 2820)	—	-1.3	21.0
<i>u</i> 3052	Si(209)...H(233)	510.7(30)	25.8(fixed)	—	-2.8	25.8
<i>u</i> 2705	C(212)...H(244)	510.8(72)	35.6(fixed)	—	1.6	35.6
<i>u</i> 2862	C(7)...F(14)	510.9(65)	18.3(tied to <i>u</i> 2820)	—	-1.1	18.7
<i>u</i> 2916	Si(85)...H(104)	510.9(81)	25.1(fixed)	—	-1.3	25.1
<i>u</i> 2856	Si(210)...H(231)	511.0(75)	21.8(fixed)	—	-0.5	21.8
<i>u</i> 2838	C(218)...F(220)	511.0(36)	21.2(tied to <i>u</i> 2820)	—	-1.2	21.7
<i>u</i> 3047	H(189)...H(199)	511.1(221)	63.2(fixed)	—	-8.4	63.2
<i>u</i> 3070	Si(4)...H(28)	511.1(31)	31.2(fixed)	—	-2.5	31.2
<i>u</i> 2904	C(47)...F(55)	511.2(55)	15.6(tied to <i>u</i> 2820)	—	-1.3	16.0

<i>u</i> 2948	C(211)...F(220)	511.2(43)	20.8(tied to <i>u</i> 2820)	—	-1.2	21.3
<i>u</i> 3458	C(171)...H(195)	511.2(121)	113.7(fixed)	—	-9.2	113.7
<i>u</i> 2804	C(53)...F(57)	511.2(33)	17.3(tied to <i>u</i> 2820)	—	-1.2	17.7
<i>u</i> 2950	Si(250)...H(285)	511.2(31)	21.9(fixed)	—	-2.3	21.9
<i>u</i> 3459	C(172)...H(203)	511.2(121)	113.5(fixed)	—	-9.2	113.5
<i>u</i> 2830	Si(44)...H(76)	511.3(78)	20.4(fixed)	—	-1.2	20.4
<i>u</i> 2939	Si(207)...H(225)	511.3(32)	24.1(fixed)	—	-2.6	24.1
<i>u</i> 2698	C(218)...H(227)	511.3(72)	32.7(fixed)	—	4.8	32.7
<i>u</i> 2827	Si(43)...H(63)	511.3(77)	20.4(fixed)	—	-1.2	20.4
<i>u</i> 2699	C(7)...H(39)	511.4(114)	35.7(fixed)	—	2.1	35.7
<i>u</i> 3584	F(261)...H(273)	511.5(124)	29.2(fixed)	—	-3.6	29.2
<i>u</i> 2907	C(50)...F(55)	511.6(53)	19.4(tied to <i>u</i> 2820)	—	-1.1	19.8
<i>u</i> 1633	Si(127)...H(143)	511.7(31)	32.9(fixed)	—	0.1	32.9
<i>u</i> 2884	C(89)...F(98)	511.8(16)	27.0(tied to <i>u</i> 2820)	—	-1.7	27.6
<i>u</i> 2863	Si(84)...H(113)	511.8(31)	21.5(fixed)	—	-1.8	21.5
<i>u</i> 2947	Si(5)...H(26)	512.1(75)	24.7(fixed)	—	0.6	24.7
<i>u</i> 2901	C(47)...F(57)	512.1(74)	18.7(tied to <i>u</i> 2820)	—	-1.0	19.2
<i>u</i> 2850	C(212)...F(219)	512.1(46)	18.5(tied to <i>u</i> 2820)	—	-1.2	18.9
<i>u</i> 3153	H(21)...H(34)	512.2(217)	40.9(fixed)	—	-7.7	40.9
<i>u</i> 2903	Si(208)...H(241)	512.3(85)	20.0(fixed)	—	-1.2	20.0
<i>u</i> 2914	Si(3)...H(36)	512.3(85)	19.7(fixed)	—	-1.3	19.7
<i>u</i> 2836	Si(248)...H(268)	512.4(78)	21.9(fixed)	—	-0.5	21.9
<i>u</i> 2894	C(252)...F(260)	512.5(48)	15.5(tied to <i>u</i> 2820)	—	-1.3	15.9
<i>u</i> 2789	Si(210)...H(229)	512.6(74)	22.7(fixed)	—	0.9	22.7
<i>u</i> 2908	C(89)...F(96)	512.6(90)	17.6(tied to <i>u</i> 2820)	—	-0.9	18.0
<i>u</i> 2940	Si(208)...H(236)	512.7(31)	20.4(fixed)	—	-2.0	20.4
<i>u</i> 3005	H(223)...H(239)	512.7(112)	60.3(fixed)	—	-10.7	60.3
<i>u</i> 2829	Si(85)...H(118)	512.7(82)	20.4(fixed)	—	-0.9	20.4
<i>u</i> 2867	Si(2)...H(20)	512.8(32)	23.9(fixed)	—	-2.4	23.9
<i>u</i> 2911	Si(3)...H(35)	512.9(90)	19.9(fixed)	—	-1.5	19.9
<i>u</i> 2896	Si(3)...H(22)	513.0(86)	20.4(fixed)	—	-1.1	20.4
<i>u</i> 2843	Si(249)...H(281)	513.0(85)	20.3(fixed)	—	-1.4	20.3
<i>u</i> 2892	C(170)...C(177)	513.1(111)	23.7(tied to <i>u</i> 2820)	—	-1.6	24.3
<i>u</i> 2972	C(254)...H(266)	513.1(86)	39.3(fixed)	—	5.3	39.3
<i>u</i> 2876	Si(45)...H(67)	513.2(84)	20.6(fixed)	—	-1.1	20.6
<i>u</i> 2960	H(186)...H(200)	513.3(376)	43.9(fixed)	—	-10.7	43.9
<i>u</i> 2889	Si(4)...H(39)	513.3(32)	21.6(fixed)	—	-1.8	21.6
<i>u</i> 2922	C(47)...C(50)	513.5(97)	20.7(tied to <i>u</i> 2820)	—	-1.2	21.2
<i>u</i> 2782	Si(5)...H(24)	513.6(71)	24.8(fixed)	—	4.3	24.8
<i>u</i> 2973	Si(43)...H(69)	513.6(32)	25.9(fixed)	—	-2.2	25.9
<i>u</i> 2833	Si(207)...H(240)	513.8(86)	20.7(fixed)	—	-1.2	20.7
<i>u</i> 2905	Si(208)...H(227)	513.8(89)	21.1(fixed)	—	-0.9	21.1
<i>u</i> 2932	C(175)...F(180)	513.9(58)	21.8(tied to <i>u</i> 2820)	—	-1.8	22.3
<i>u</i> 2891	Si(209)...H(244)	513.9(32)	21.2(fixed)	—	-1.8	21.2

<i>u3536</i>	C(89)...H(110)	514.2(85)	112.7(fixed)	—	-10.7	112.7
<i>u3377</i>	H(226)...H(235)	514.2(113)	42.1(fixed)	—	-10.8	42.1
<i>u3535</i>	C(90)...H(102)	514.2(85)	112.6(fixed)	—	-10.7	112.6
<i>u2976</i>	C(9)...F(15)	514.3(35)	18.8(tied to <i>u2820</i> )	—	-1.0	19.3
<i>u2873</i>	Si(249)...H(282)	514.4(85)	24.7(fixed)	—	0.4	24.7
<i>u3035</i>	C(12)...H(31)	514.6(83)	38.4(fixed)	—	0.5	38.4
<i>u3351</i>	H(274)...H(278)	514.7(68)	32.0(fixed)	—	0.8	32.0
<i>u3182</i>	F(222)...H(237)	514.8(89)	33.5(fixed)	—	-1.3	33.5
<i>u2689</i>	H(116)...H(118)	514.9(329)	46.7(fixed)	—	2.0	46.7
<i>u2687</i>	H(151)...H(153)	514.9(68)	82.3(fixed)	—	-17.8	82.3
<i>u2682</i>	H(198)...H(200)	514.9(343)	59.2(fixed)	—	3.2	59.2
<i>u2621</i>	C(174)...H(192)	515.0(126)	48.3(fixed)	—	34.6	48.3
<i>u3114</i>	H(235)...H(242)	515.2(225)	34.3(fixed)	—	-6.5	34.3
<i>u1781</i>	F(137)...H(158)	515.5(223)	39.5(fixed)	—	-3.0	39.5
<i>u3020</i>	H(235)...H(243)	515.6(190)	38.7(fixed)	—	-5.5	38.7
<i>u2835</i>	Si(44)...H(77)	515.7(91)	25.1(fixed)	—	0.5	25.1
<i>u1657</i>	F(137)...H(155)	515.9(76)	58.2(fixed)	—	-6.5	58.2
<i>u2906</i>	C(253)...H(283)	516.0(190)	54.3(fixed)	—	10.3	54.3
<i>u3334</i>	H(189)...H(194)	516.0(154)	54.6(fixed)	—	-32.7	54.6
<i>u2968</i>	H(66)...H(82)	516.0(194)	41.0(fixed)	—	-5.6	41.0
<i>u3012</i>	C(50)...F(58)	516.1(73)	19.2(tied to <i>u2820</i> )	—	-1.2	19.7
<i>u3249</i>	H(141)...H(155)	516.1(67)	37.8(fixed)	—	1.4	37.8
<i>u2897</i>	C(49)...F(58)	516.2(44)	17.0(tied to <i>u2820</i> )	—	-1.4	17.3
<i>u2909</i>	C(130)...F(139)	516.8(16)	18.6(tied to <i>u2820</i> )	—	-1.1	19.0
<i>u3140</i>	H(65)...H(82)	516.8(243)	37.4(fixed)	—	-7.4	37.4
<i>u2930</i>	H(63)...H(67)	516.8(369)	41.4(fixed)	—	-6.8	41.4
<i>u1209</i>	C(131)...F(140)	517.0(16)	29.0(tied to <i>u2820</i> )	—	0.2	29.7
<i>u3023</i>	H(23)...H(30)	517.1(168)	38.4(fixed)	—	3.3	38.4
<i>u2977</i>	H(75)...H(79)	517.2(153)	61.7(fixed)	—	-12.9	61.7
<i>u3057</i>	F(262)...H(285)	517.2(79)	40.8(fixed)	—	-1.7	40.8
<i>u3007</i>	F(181)...H(200)	517.6(236)	49.3(fixed)	—	-2.0	49.3
<i>u3009</i>	F(98)...H(121)	517.7(112)	41.2(fixed)	—	-1.9	41.2
<i>u2982</i>	F(222)...H(240)	517.8(226)	34.8(fixed)	—	-0.6	34.8
<i>u2936</i>	C(48)...F(57)	517.8(49)	17.2(tied to <i>u2820</i> )	—	-1.4	17.6
<i>u2980</i>	H(62)...H(67)	517.8(153)	50.1(fixed)	—	-5.9	50.1
<i>u3003</i>	C(6)...C(10)	518.2(68)	23.7(tied to <i>u2820</i> )	—	-1.2	24.3
<i>u2870</i>	C(254)...H(269)	518.4(176)	41.9(fixed)	—	8.2	41.9
<i>u3214</i>	H(223)...H(245)	518.5(135)	47.4(fixed)	—	9.5	47.4
<i>u3088</i>	H(102)...H(115)	518.7(186)	84.7(fixed)	—	29.7	84.7
<i>u2900</i>	F(98)...H(105)	518.8(67)	40.0(fixed)	—	8.7	40.0
<i>u3089</i>	H(110)...H(119)	518.8(186)	84.7(fixed)	—	29.7	84.7
<i>u3074</i>	C(218)...H(223)	518.8(87)	36.1(fixed)	—	6.3	36.1
<i>u3186</i>	H(265)...H(286)	519.1(130)	46.8(fixed)	—	-11.9	46.8
<i>u3048</i>	H(186)...H(202)	519.1(138)	63.1(fixed)	—	-8.4	63.1

<i>u</i> 2993	C(253)...C(256)	519.2(72)	19.6(tied to <i>u</i> 2820)	—	-1.2	20.1
<i>u</i> 2984	C(53)...F(56)	519.3(64)	18.9(tied to <i>u</i> 2820)	—	-1.2	19.3
<i>u</i> 2931	C(171)...F(178)	519.6(32)	21.8(tied to <i>u</i> 2820)	—	-1.8	22.3
<i>u</i> 2620	C(170)...H(203)	519.7(174)	46.6(fixed)	—	34.6	46.6
<i>u</i> 3066	H(230)...H(246)	519.7(203)	50.5(fixed)	—	-10.2	50.5
<i>u</i> 2923	H(268)...H(276)	519.8(177)	43.2(fixed)	—	10.3	43.2
<i>u</i> 3030	H(63)...H(66)	519.9(175)	49.8(fixed)	—	-6.7	49.8
<i>u</i> 2878	C(171)...F(179)	519.9(63)	30.7(tied to <i>u</i> 2820)	—	-2.1	31.4
<i>u</i> 2991	F(15)...H(29)	520.0(49)	35.7(fixed)	—	19.1	35.7
<i>u</i> 3108	C(129)...C(133)	520.1(42)	16.1(tied to <i>u</i> 2820)	—	-1.0	16.4
<i>u</i> 2814	H(229)...H(237)	520.2(264)	63.9(fixed)	—	5.3	63.9
<i>u</i> 2994	C(256)...C(258)	520.4(57)	21.4(tied to <i>u</i> 2820)	—	-1.5	21.9
<i>u</i> 3208	H(144)...H(161)	520.8(165)	48.4(fixed)	—	-18.9	48.4
<i>u</i> 2954	F(178)...H(188)	521.7(58)	42.6(fixed)	—	0.4	42.6
<i>u</i> 2990	H(237)...H(246)	521.7(63)	35.7(fixed)	—	3.5	35.7
<i>u</i> 3034	C(6)...C(11)	521.7(66)	21.0(tied to <i>u</i> 2820)	—	-1.5	21.5
<i>u</i> 3073	F(180)...H(196)	521.8(119)	98.6(fixed)	—	2.9	98.6
<i>u</i> 2639	C(171)...H(196)	521.9(91)	58.0(fixed)	—	44.7	58.0
<i>u</i> 2965	H(18)...H(25)	522.0(89)	42.4(fixed)	—	14.7	42.4
<i>u</i> 2886	C(213)...H(237)	522.2(37)	32.6(fixed)	—	1.2	32.6
<i>u</i> 2601	C(212)...H(234)	522.4(74)	41.9(fixed)	—	26.8	41.9
<i>u</i> 3184	H(21)...H(33)	522.4(189)	37.9(fixed)	—	-8.2	37.9
<i>u</i> 3094	C(211)...C(215)	522.5(54)	20.4(tied to <i>u</i> 2820)	—	-1.4	20.9
<i>u</i> 2912	H(27)...H(32)	522.6(68)	38.6(fixed)	—	12.9	38.6
<i>u</i> 3045	H(34)...H(37)	522.9(212)	35.1(fixed)	—	-5.9	35.1
<i>u</i> 2941	C(51)...C(54)	522.9(80)	21.6(tied to <i>u</i> 2820)	—	-1.0	22.1
<i>u</i> 2957	Si(250)...H(274)	523.2(100)	20.7(fixed)	—	-1.8	20.7
<i>u</i> 2979	H(223)...H(230)	523.2(88)	42.0(fixed)	—	14.3	42.0
<i>u</i> 3231	H(18)...H(40)	523.3(150)	49.5(fixed)	—	7.4	49.5
<i>u</i> 2944	H(68)...H(81)	523.6(72)	36.1(fixed)	—	7.2	36.1
<i>u</i> 2412	H(184)...H(203)	523.9(202)	68.5(fixed)	—	69.5	68.5
<i>u</i> 3112	H(278)...H(286)	524.0(135)	46.3(fixed)	—	5.4	46.3
<i>u</i> 3029	F(57)...H(59)	524.3(118)	45.5(fixed)	—	0.8	45.5
<i>u</i> 3268	H(187)...H(190)	524.4(135)	60.6(fixed)	—	-8.5	60.6
<i>u</i> 3026	H(23)...H(38)	524.4(200)	40.1(fixed)	—	-7.2	40.1
<i>u</i> 3549	C(130)...H(156)	524.4(80)	35.5(fixed)	—	-1.8	35.5
<i>u</i> 3278	H(224)...H(239)	524.4(107)	43.0(fixed)	—	-12.2	43.0
<i>u</i> 3065	C(256)...H(286)	524.5(88)	37.8(fixed)	—	2.7	37.8
<i>u</i> 2997	F(58)...H(67)	524.6(224)	37.9(fixed)	—	-0.6	37.9
<i>u</i> 3370	H(29)...H(32)	524.6(62)	38.4(fixed)	—	-0.5	38.4
<i>u</i> 3253	F(261)...H(283)	524.8(225)	59.3(fixed)	—	-3.8	59.3
<i>u</i> 1528	Si(126)...H(145)	524.9(86)	29.4(fixed)	—	11.0	29.4
<i>u</i> 4232	H(146)...H(152)	524.9(77)	43.6(fixed)	—	-11.4	43.6
<i>u</i> 2981	H(228)...H(243)	524.9(186)	47.1(fixed)	—	-8.8	47.1

<i>u</i> 3110	C(13)...H(18)	525.3(100)	36.2(fixed)	—	4.7	36.2
<i>u</i> 2945	C(8)...F(17)	525.4(43)	18.2(tied to <i>u</i> 2820)	—	-1.0	18.6
<i>u</i> 2629	C(90)...H(100)	525.9(85)	57.4(fixed)	—	48.3	57.4
<i>u</i> 1476	Si(250)...H(272)	525.9(34)	43.8(fixed)	—	33.8	43.8
<i>u</i> 2828	C(217)...H(229)	526.0(162)	40.8(fixed)	—	9.5	40.8
<i>u</i> 3250	C(213)...H(225)	526.0(87)	56.5(fixed)	—	-1.3	56.5
<i>u</i> 3024	H(107)...H(113)	526.0(254)	50.4(fixed)	—	1.4	50.4
<i>u</i> 3595	F(261)...H(274)	526.2(147)	25.9(fixed)	—	-3.7	25.9
<i>u</i> 2628	C(89)...H(111)	526.3(84)	56.2(fixed)	—	48.4	56.2
<i>u</i> 3870	F(138)...H(163)	526.3(75)	24.7(fixed)	—	-1.2	24.7
<i>u</i> 3145	C(93)...H(122)	526.4(118)	30.7(fixed)	—	1.6	30.7
<i>u</i> 3064	C(211)...C(213)	526.4(41)	17.4(tied to <i>u</i> 2820)	—	-1.0	17.8
<i>u</i> 3054	C(6)...C(8)	526.4(44)	18.1(tied to <i>u</i> 2820)	—	-1.0	18.5
<i>u</i> 3056	F(15)...H(37)	526.5(229)	34.3(fixed)	—	-1.5	34.3
<i>u</i> 2640	C(175)...H(182)	526.6(73)	57.8(fixed)	—	44.7	57.8
<i>u</i> 3071	C(9)...C(10)	526.8(41)	15.8(tied to <i>u</i> 2820)	—	-0.7	16.2
<i>u</i> 1730	C(129)...C(135)	526.8(50)	32.5(tied to <i>u</i> 2820)	—	1.3	33.2
<i>u</i> 3191	H(70)...H(81)	526.9(80)	38.1(fixed)	—	1.2	38.1
<i>u</i> 3113	C(7)...C(10)	526.9(67)	16.7(tied to <i>u</i> 2820)	—	-1.7	17.0
<i>u</i> 3041	H(226)...H(243)	526.9(177)	41.4(fixed)	—	-8.7	41.4
<i>u</i> 3323	C(10)...H(40)	527.2(117)	33.2(fixed)	—	2.3	33.2
<i>u</i> 2946	C(52)...F(57)	527.4(57)	20.9(tied to <i>u</i> 2820)	—	-1.3	21.3
<i>u</i> 3165	H(64)...H(76)	527.5(192)	39.9(fixed)	—	-2.7	39.9
<i>u</i> 2742	H(234)...H(242)	527.6(109)	77.1(fixed)	—	18.2	77.1
<i>u</i> 3021	H(34)...H(38)	527.7(193)	37.2(fixed)	—	-5.2	37.2
<i>u</i> 4405	H(147)...H(153)	527.7(160)	33.4(fixed)	—	-14.4	33.4
<i>u</i> 3036	F(57)...H(63)	527.8(231)	36.2(fixed)	—	-1.2	36.2
<i>u</i> 3304	H(60)...H(66)	528.0(138)	36.9(fixed)	—	-12.6	36.9
<i>u</i> 3043	H(60)...H(76)	528.2(196)	39.7(fixed)	—	4.3	39.7
<i>u</i> 3434	H(32)...H(40)	528.2(155)	38.9(fixed)	—	3.9	38.9
<i>u</i> 3193	F(58)...H(70)	528.2(115)	52.8(fixed)	—	0.4	52.8
<i>u</i> 2951	H(70)...H(75)	528.3(88)	43.9(fixed)	—	17.2	43.9
<i>u</i> 2575	C(7)...H(29)	528.3(71)	47.8(fixed)	—	38.8	47.8
<i>u</i> 3016	H(20)...H(30)	528.6(89)	50.5(fixed)	—	7.6	50.5
<i>u</i> 3332	H(62)...H(68)	528.7(116)	45.2(fixed)	—	-15.6	45.2
<i>u</i> 2987	C(8)...H(33)	528.8(72)	33.7(fixed)	—	1.2	33.7
<i>u</i> 3120	C(214)...H(242)	528.8(58)	32.4(fixed)	—	1.1	32.4
<i>u</i> 3146	H(63)...H(74)	528.8(196)	38.3(fixed)	—	-2.6	38.3
<i>u</i> 3170	F(97)...H(106)	528.9(243)	67.2(fixed)	—	-1.3	67.2
<i>u</i> 3006	F(178)...H(186)	529.0(222)	49.3(fixed)	—	-2.0	49.3
<i>u</i> 3141	F(220)...H(223)	529.1(83)	49.8(fixed)	—	-0.4	49.8
<i>u</i> 2801	C(93)...H(105)	529.3(178)	49.7(fixed)	—	20.3	49.7
<i>u</i> 3199	F(96)...H(111)	529.3(116)	68.2(fixed)	—	-12.2	68.2
<i>u</i> 3194	C(52)...H(59)	529.4(129)	30.4(fixed)	—	3.4	30.4



<i>u</i> 3104	C(172)...C(177)	529.4(63)	23.0(tied to <i>u</i> 2820)	—	-0.8	23.5
<i>u</i> 2516	F(138)...H(159)	529.4(223)	35.2(fixed)	—	10.3	35.2
<i>u</i> 3215	H(23)...H(32)	529.6(135)	35.2(fixed)	—	2.2	35.2
<i>u</i> 3987	H(143)...H(155)	529.7(80)	34.7(fixed)	—	-5.5	34.7
<i>u</i> 4460	H(271)...H(283)	529.7(54)	38.6(fixed)	—	-27.3	38.6
<i>u</i> 3218	H(64)...H(80)	529.7(132)	45.4(fixed)	—	5.3	45.4
<i>u</i> 3154	C(8)...H(20)	529.9(90)	52.3(fixed)	—	-1.2	52.3
<i>u</i> 3075	C(50)...C(52)	530.0(46)	17.8(tied to <i>u</i> 2820)	—	-1.0	18.2
<i>u</i> 3124	C(9)...H(37)	530.0(98)	33.5(fixed)	—	1.0	33.5
<i>u</i> 2860	H(24)...H(33)	530.3(297)	83.8(fixed)	—	9.1	83.8
<i>u</i> 4205	H(271)...H(280)	530.4(158)	102.5(fixed)	—	-16.5	102.5
<i>u</i> 3060	C(54)...H(73)	530.5(131)	59.6(fixed)	—	0.6	59.6
<i>u</i> 3345	C(129)...C(136)	530.6(62)	25.0(tied to <i>u</i> 2820)	—	-1.9	25.5
<i>u</i> 4494	H(145)...H(157)	530.8(68)	31.0(fixed)	—	-10.5	31.0
<i>u</i> 3002	F(57)...H(74)	530.8(93)	31.3(fixed)	—	0.8	31.3
<i>u</i> 3055	H(21)...H(38)	530.8(179)	38.8(fixed)	—	-7.2	38.8
<i>u</i> 3115	C(88)...C(90)	530.9(49)	21.0(tied to <i>u</i> 2820)	—	-0.5	21.5
<i>u</i> 3083	C(93)...H(102)	531.2(124)	67.7(fixed)	—	28.6	67.7
<i>u</i> 3084	C(94)...H(110)	531.3(124)	67.5(fixed)	—	28.7	67.5
<i>u</i> 2958	C(212)...C(218)	531.3(50)	21.9(tied to <i>u</i> 2820)	—	-1.5	22.4
<i>u</i> 3087	C(50)...C(54)	531.3(43)	15.6(tied to <i>u</i> 2820)	—	-0.8	15.9
<i>u</i> 3049	C(255)...C(256)	531.3(44)	16.7(tied to <i>u</i> 2820)	—	-0.8	17.1
<i>u</i> 2961	C(7)...C(13)	531.4(76)	22.0(tied to <i>u</i> 2820)	—	-1.5	22.5
<i>u</i> 3421	H(60)...H(81)	531.5(132)	41.6(fixed)	—	-12.0	41.6
<i>u</i> 3235	F(260)...H(266)	531.5(86)	43.1(fixed)	—	-2.4	43.1
<i>u</i> 3401	H(114)...H(119)	531.5(259)	39.8(fixed)	—	3.0	39.8
<i>u</i> 2752	H(29)...H(37)	531.6(137)	94.9(fixed)	—	23.6	94.9
<i>u</i> 3395	F(55)...H(61)	531.6(93)	43.1(fixed)	—	-3.7	43.1
<i>u</i> 3127	C(47)...C(52)	531.6(96)	17.0(tied to <i>u</i> 2820)	—	-1.0	17.4
<i>u</i> 3077	H(269)...H(285)	531.8(115)	47.3(fixed)	—	10.3	47.3
<i>u</i> 3357	C(52)...H(69)	532.1(98)	63.9(fixed)	—	-2.2	63.9
<i>u</i> 3069	H(63)...H(71)	532.2(189)	42.6(fixed)	—	4.1	42.6
<i>u</i> 3096	C(253)...H(285)	532.2(84)	37.1(fixed)	—	4.0	37.1
<i>u</i> 3126	Si(5)...H(30)	532.2(41)	18.7(fixed)	—	-4.1	18.7
<i>u</i> 3177	H(237)...H(245)	532.4(58)	34.5(fixed)	—	1.9	34.5
<i>u</i> 3189	F(14)...H(23)	532.4(225)	36.5(fixed)	—	-1.7	36.5
<i>u</i> 4582	H(148)...H(156)	532.5(202)	26.8(fixed)	—	-5.0	26.8
<i>u</i> 2773	C(12)...H(24)	532.5(165)	50.7(fixed)	—	21.8	50.7
<i>u</i> 2989	C(213)...C(215)	532.5(37)	19.1(tied to <i>u</i> 2820)	—	-1.1	19.6
<i>u</i> 3149	C(131)...H(160)	532.7(79)	31.1(fixed)	—	6.0	31.1
<i>u</i> 2988	C(213)...F(222)	533.0(42)	18.6(tied to <i>u</i> 2820)	—	-1.1	19.1
<i>u</i> 3039	F(219)...H(234)	533.0(69)	55.7(fixed)	—	-4.1	55.7
<i>u</i> 3101	C(215)...C(218)	533.0(37)	16.2(tied to <i>u</i> 2820)	—	-1.1	16.5
<i>u</i> 3241	F(261)...H(266)	533.2(52)	22.4(fixed)	—	-1.9	22.4

<i>u3285</i>	C(10)...H(18)	533.2(109)	48.0(fixed)	—	-1.3	48.0
<i>u3135</i>	C(129)...C(131)	533.3(37)	17.5(tied to <i>u2820</i> )	—	-1.6	17.9
<i>u3139</i>	C(10)...C(12)	533.3(67)	22.7(tied to <i>u2820</i> )	—	-1.7	23.2
<i>u3676</i>	C(129)...H(154)	533.4(83)	21.7(fixed)	—	-3.3	21.7
<i>u1513</i>	C(132)...C(133)	533.5(62)	19.5(tied to <i>u2820</i> )	—	0.6	19.9
<i>u2877</i>	C(130)...C(132)	533.5(37)	20.1(tied to <i>u2820</i> )	—	-1.3	20.6
<i>u744</i>	C(132)...H(155)	533.5(90)	38.8(fixed)	—	24.4	38.8
<i>u2875</i>	H(72)...H(79)	533.6(204)	52.6(fixed)	—	13.8	52.6
<i>u3319</i>	H(59)...H(74)	533.9(286)	45.4(fixed)	—	6.4	45.4
<i>u3393</i>	C(132)...H(162)	534.1(83)	33.9(fixed)	—	-1.3	33.9
<i>u3103</i>	C(170)...C(175)	534.6(39)	23.0(tied to <i>u2820</i> )	—	-0.8	23.5
<i>u3044</i>	F(14)...H(29)	534.7(69)	70.8(fixed)	—	-3.8	70.8
<i>u3271</i>	C(48)...H(80)	534.7(91)	37.7(fixed)	—	1.9	37.7
<i>u3831</i>	H(266)...H(271)	534.8(79)	52.8(fixed)	—	-8.0	52.8
<i>u4622</i>	H(148)...H(157)	534.9(164)	19.5(fixed)	—	-8.4	19.5
<i>u4321</i>	H(271)...H(281)	534.9(148)	80.4(fixed)	—	-20.7	80.4
<i>u3144</i>	C(48)...C(51)	535.0(91)	17.0(tied to <i>u2820</i> )	—	-1.1	17.4
<i>u3175</i>	F(219)...H(228)	535.2(219)	43.6(fixed)	—	-1.9	43.6
<i>u3274</i>	H(111)...H(119)	535.2(196)	117.3(fixed)	—	19.4	117.3
<i>u3275</i>	H(100)...H(115)	535.2(196)	117.2(fixed)	—	19.3	117.2
<i>u3173</i>	C(214)...C(217)	535.4(45)	20.7(tied to <i>u2820</i> )	—	-1.2	21.2
<i>u3125</i>	H(275)...H(278)	535.4(99)	33.6(fixed)	—	2.6	33.6
<i>u3169</i>	C(211)...C(218)	535.4(63)	22.2(tied to <i>u2820</i> )	—	-1.2	22.7
<i>u2290</i>	Si(126)...H(153)	535.5(20)	26.7(fixed)	—	-11.8	26.7
<i>u3118</i>	C(174)...C(176)	535.6(38)	20.0(tied to <i>u2820</i> )	—	-2.1	20.5
<i>u3259</i>	H(18)...H(26)	535.7(98)	44.4(fixed)	—	3.7	44.4
<i>u3176</i>	C(257)...H(264)	536.1(110)	29.5(fixed)	—	3.6	29.5
<i>u3329</i>	H(265)...H(287)	536.5(97)	43.9(fixed)	—	-11.7	43.9
<i>u3185</i>	Si(251)...H(276)	536.8(40)	17.2(fixed)	—	-3.7	17.2
<i>u3134</i>	C(92)...C(94)	536.9(39)	18.4(tied to <i>u2820</i> )	—	-1.1	18.9
<i>u3050</i>	H(279)...H(287)	537.0(176)	39.3(fixed)	—	3.4	39.3
<i>u3313</i>	F(56)...H(61)	537.0(67)	22.8(fixed)	—	-1.4	22.8
<i>u3691</i>	H(190)...H(203)	537.1(111)	117.6(fixed)	—	-1.6	117.6
<i>u3238</i>	C(256)...H(269)	537.1(248)	54.8(fixed)	—	-2.1	54.8
<i>u3195</i>	C(48)...H(73)	537.2(122)	31.9(fixed)	—	6.9	31.9
<i>u3343</i>	F(262)...H(264)	537.2(83)	30.8(fixed)	—	-4.6	30.8
<i>u3438</i>	F(178)...H(196)	537.3(118)	29.2(fixed)	—	-10.1	29.2
<i>u3190</i>	C(131)...C(135)	537.3(54)	19.0(tied to <i>u2820</i> )	—	-1.1	19.4
<i>u3346</i>	F(261)...H(264)	537.5(56)	24.1(fixed)	—	-2.4	24.1
<i>u3286</i>	F(17)...H(33)	537.5(215)	33.0(fixed)	—	-1.8	33.0
<i>u2978</i>	H(72)...H(82)	537.6(103)	53.5(fixed)	—	13.2	53.5
<i>u2963</i>	C(48)...H(77)	537.7(240)	53.8(fixed)	—	5.3	53.8
<i>u3068</i>	C(48)...C(53)	537.9(37)	17.6(tied to <i>u2820</i> )	—	-0.9	18.0
<i>u2999</i>	F(17)...H(24)	537.9(55)	31.3(fixed)	—	10.8	31.3

<i>u3836</i>	H(104)...H(110)	537.9(104)	123.3(fixed)	—	-4.4	123.3
<i>u3835</i>	H(102)...H(108)	538.0(104)	123.2(fixed)	—	-4.4	123.2
<i>u3187</i>	C(9)...C(12)	538.0(60)	22.0(tied to <i>u2820</i> )	—	-1.4	22.5
<i>u3297</i>	C(9)...H(31)	538.0(82)	33.9(fixed)	—	-0.9	33.9
<i>u3167</i>	C(88)...C(95)	538.1(101)	22.3(tied to <i>u2820</i> )	—	-1.9	22.8
<i>u2983</i>	H(231)...H(235)	538.2(147)	43.5(fixed)	—	9.5	43.5
<i>u3067</i>	C(8)...C(11)	538.3(50)	21.0(tied to <i>u2820</i> )	—	-1.1	21.5
<i>u3105</i>	C(257)...C(259)	538.4(36)	16.9(tied to <i>u2820</i> )	—	-1.4	17.3
<i>u3197</i>	C(52)...H(62)	538.5(217)	34.4(fixed)	—	-3.5	34.4
<i>u3053</i>	H(33)...H(41)	538.6(181)	39.0(fixed)	—	2.9	39.0
<i>u3209</i>	H(223)...H(231)	538.8(101)	43.9(fixed)	—	6.1	43.9
<i>u3325</i>	H(141)...H(147)	538.8(77)	37.3(fixed)	—	1.6	37.3
<i>u3117</i>	C(170)...C(172)	538.9(29)	20.0(tied to <i>u2820</i> )	—	-2.1	20.5
<i>u3138</i>	C(211)...C(217)	538.9(32)	17.3(tied to <i>u2820</i> )	—	-1.4	17.7
<i>u3147</i>	H(117)...H(123)	539.0(136)	38.6(fixed)	—	2.9	38.6
<i>u3237</i>	H(62)...H(78)	539.0(199)	63.4(fixed)	—	10.0	63.4
<i>u3097</i>	H(224)...H(242)	539.2(170)	39.4(fixed)	—	5.4	39.4
<i>u3400</i>	H(18)...H(24)	539.2(77)	37.7(fixed)	—	1.9	37.7
<i>u3179</i>	C(256)...C(259)	539.2(64)	24.7(tied to <i>u2820</i> )	—	-1.5	25.3
<i>u3100</i>	C(11)...C(13)	539.2(32)	16.5(tied to <i>u2820</i> )	—	-1.1	16.8
<i>u3230</i>	C(48)...H(75)	539.3(217)	35.1(fixed)	—	-3.6	35.1
<i>u3156</i>	C(176)...H(196)	539.5(118)	53.6(fixed)	—	18.9	53.6
<i>u3280</i>	Si(46)...H(71)	539.5(41)	17.3(fixed)	—	-6.0	17.3
<i>u2956</i>	H(66)...H(73)	539.7(98)	44.6(fixed)	—	18.1	44.6
<i>u3261</i>	F(58)...H(72)	539.7(63)	23.2(fixed)	—	-1.3	23.2
<i>u3232</i>	Si(250)...H(265)	539.7(41)	16.8(fixed)	—	-4.1	16.8
<i>u3107</i>	C(49)...C(51)	539.8(54)	17.5(tied to <i>u2820</i> )	—	-0.9	17.9
<i>u3132</i>	C(7)...C(9)	539.8(36)	16.7(tied to <i>u2820</i> )	—	-1.1	17.1
<i>u3233</i>	Si(166)...H(194)	540.0(27)	19.7(fixed)	—	-8.1	19.7
<i>u3234</i>	Si(168)...H(205)	540.0(27)	19.3(fixed)	—	-8.1	19.3
<i>u2077</i>	H(143)...H(161)	540.0(153)	49.7(fixed)	—	-4.3	49.7
<i>u3368</i>	F(263)...H(278)	540.1(66)	24.7(fixed)	—	-2.8	24.7
<i>u3955</i>	H(141)...H(149)	540.2(88)	35.8(fixed)	—	-4.0	35.8
<i>u3498</i>	F(56)...H(78)	540.2(221)	52.8(fixed)	—	-5.0	52.8
<i>u3160</i>	H(265)...H(281)	540.2(171)	41.7(fixed)	—	2.1	41.7
<i>u3181</i>	C(252)...C(257)	540.4(82)	18.3(tied to <i>u2820</i> )	—	-0.9	18.7
<i>u3142</i>	Si(45)...H(82)	540.4(18)	18.0(fixed)	—	-3.7	18.0
<i>u3573</i>	H(145)...H(152)	540.5(88)	42.5(fixed)	—	-2.7	42.5
<i>u3260</i>	Si(45)...H(60)	540.6(42)	16.9(fixed)	—	-4.4	16.9
<i>u3821</i>	C(7)...H(28)	540.8(75)	73.4(fixed)	—	-13.4	73.4
<i>u3257</i>	F(261)...H(265)	540.9(63)	25.0(fixed)	—	-1.7	25.0
<i>u3338</i>	H(28)...H(32)	540.9(82)	35.6(fixed)	—	-0.2	35.6
<i>u3201</i>	Si(86)...H(109)	540.9(21)	22.1(fixed)	—	-8.0	22.1
<i>u3042</i>	F(222)...H(229)	541.2(65)	28.8(fixed)	—	4.5	28.8

<i>u</i> 3198	C(6)...C(13)	541.3(75)	22.8(tied to <i>u</i> 2820)	—	-1.4	23.3
<i>u</i> 3174	H(229)...H(240)	541.6(130)	45.7(fixed)	—	-6.7	45.7
<i>u</i> 3223	C(88)...C(94)	541.7(64)	19.5(tied to <i>u</i> 2820)	—	-3.2	20.0
<i>u</i> 3419	H(223)...H(242)	541.7(135)	41.1(fixed)	—	-0.3	41.1
<i>u</i> 3402	C(10)...H(22)	542.0(245)	37.2(fixed)	—	-1.9	37.2
<i>u</i> 3364	H(146)...H(156)	542.2(291)	45.3(fixed)	—	8.3	45.3
<i>u</i> 3404	H(149)...H(161)	542.2(68)	40.6(fixed)	—	2.2	40.6
<i>u</i> 3180	C(6)...C(12)	542.3(42)	17.5(tied to <i>u</i> 2820)	—	-1.6	17.9
<i>u</i> 3468	H(60)...H(82)	542.3(98)	45.7(fixed)	—	-11.7	45.7
<i>u</i> 3129	C(253)...H(282)	542.4(237)	59.2(fixed)	—	3.7	59.2
<i>u</i> 3143	C(253)...C(258)	542.5(38)	17.8(tied to <i>u</i> 2820)	—	-1.0	18.2
<i>u</i> 3166	Si(4)...H(27)	542.5(12)	26.7(fixed)	—	-8.4	26.7
<i>u</i> 3162	C(95)...H(100)	542.6(136)	57.2(fixed)	—	21.2	57.2
<i>u</i> 3203	Si(207)...H(224)	542.7(18)	17.5(fixed)	—	-4.7	17.5
<i>u</i> 3095	H(74)...H(82)	542.7(162)	40.2(fixed)	—	3.2	40.2
<i>u</i> 3163	C(92)...H(111)	542.8(136)	56.8(fixed)	—	21.3	56.8
<i>u</i> 3242	H(61)...H(68)	542.8(159)	47.8(fixed)	—	4.7	47.8
<i>u</i> 3380	H(269)...H(281)	542.8(156)	42.7(fixed)	—	-7.4	42.7
<i>u</i> 4285	H(264)...H(271)	542.9(91)	45.0(fixed)	—	-21.2	45.0
<i>u</i> 3365	F(263)...H(277)	543.0(52)	23.1(fixed)	—	-3.0	23.1
<i>u</i> 3568	H(199)...H(203)	543.1(146)	48.5(fixed)	—	-27.1	48.5
<i>u</i> 3227	H(277)...H(284)	543.3(171)	55.3(fixed)	—	0.4	55.3
<i>u</i> 3102	C(254)...H(279)	543.3(80)	33.0(fixed)	—	0.9	33.0
<i>u</i> 3575	F(219)...H(232)	543.5(60)	33.3(fixed)	—	-15.6	33.3
<i>u</i> 3225	H(70)...H(76)	543.5(109)	45.1(fixed)	—	9.9	45.1
<i>u</i> 2732	Si(251)...H(272)	543.5(20)	30.6(fixed)	—	11.8	30.6
<i>u</i> 3171	C(52)...C(54)	543.6(51)	18.4(tied to <i>u</i> 2820)	—	-1.8	18.8
<i>u</i> 3213	Si(250)...H(287)	543.7(17)	17.4(fixed)	—	-4.2	17.4
<i>u</i> 3452	H(106)...H(113)	543.9(205)	62.4(fixed)	—	-16.2	62.4
<i>u</i> 3454	H(105)...H(121)	543.9(205)	62.4(fixed)	—	-16.2	62.4
<i>u</i> 3436	F(96)...H(109)	544.0(135)	48.0(fixed)	—	-15.9	48.0
<i>u</i> 3317	Si(126)...H(161)	544.0(27)	15.8(fixed)	—	-5.3	15.8
<i>u</i> 3435	F(97)...H(101)	544.0(135)	48.1(fixed)	—	-15.9	48.1
<i>u</i> 3150	C(212)...C(214)	544.2(41)	16.4(tied to <i>u</i> 2820)	—	-1.0	16.7
<i>u</i> 2998	Si(251)...H(270)	544.2(12)	38.9(fixed)	—	1.4	38.9
<i>u</i> 3572	F(14)...H(27)	544.2(79)	35.7(fixed)	—	-18.5	35.7
<i>u</i> 3151	Si(209)...H(232)	544.2(12)	21.9(fixed)	—	-7.4	21.9
<i>u</i> 3111	C(49)...H(78)	544.3(75)	32.8(fixed)	—	9.0	32.8
<i>u</i> 3348	F(15)...H(24)	544.4(145)	52.7(fixed)	—	-9.1	52.7
<i>u</i> 3183	H(19)...H(37)	544.4(175)	39.7(fixed)	—	4.1	39.7
<i>u</i> 3287	Si(84)...H(112)	544.7(28)	15.7(fixed)	—	-3.8	15.7
<i>u</i> 1664	H(144)...H(160)	544.8(204)	50.9(fixed)	—	10.8	50.9
<i>u</i> 3080	C(131)...C(133)	544.8(31)	17.7(tied to <i>u</i> 2820)	—	-0.9	18.1
<i>u</i> 3267	H(199)...H(201)	544.8(286)	60.6(fixed)	—	-8.5	60.6

<i>u3398</i>	C(91)...H(119)	544.9(147)	36.5(fixed)	—	2.7	36.5
<i>u3441</i>	F(96)...H(114)	544.9(113)	23.5(fixed)	—	-2.6	23.5
<i>u3466</i>	F(56)...H(59)	544.9(71)	23.0(fixed)	—	-3.4	23.0
<i>u3414</i>	C(10)...C(13)	545.1(78)	22.9(tied to <i>u2820</i> )	—	-1.3	23.4
<i>u3252</i>	F(96)...H(113)	545.2(31)	23.3(fixed)	—	-2.2	23.3
<i>u3366</i>	C(50)...H(80)	545.2(84)	33.2(fixed)	—	-1.1	33.2
<i>u3369</i>	H(64)...H(73)	545.2(282)	44.2(fixed)	—	11.4	44.2
<i>u3425</i>	H(69)...H(81)	545.4(78)	32.9(fixed)	—	-3.4	32.9
<i>u3307</i>	F(180)...H(184)	545.4(20)	25.2(fixed)	—	-0.9	25.2
<i>u2707</i>	Si(250)...H(275)	545.5(57)	21.2(fixed)	—	0.1	21.2
<i>u3376</i>	C(94)...H(108)	545.7(242)	78.1(fixed)	—	-0.7	78.1
<i>u3375</i>	C(93)...H(104)	545.7(242)	78.1(fixed)	—	-0.7	78.1
<i>u3306</i>	H(33)...H(40)	545.9(149)	37.1(fixed)	—	1.1	37.1
<i>u3383</i>	H(223)...H(229)	545.9(74)	35.9(fixed)	—	6.8	35.9
<i>u3363</i>	H(71)...H(77)	545.9(123)	52.6(fixed)	—	8.0	52.6
<i>u3439</i>	F(180)...H(182)	546.0(30)	29.3(fixed)	—	-10.1	29.3
<i>u3243</i>	C(13)...H(35)	546.0(228)	31.2(fixed)	—	-0.7	31.2
<i>u3019</i>	H(104)...H(123)	546.0(184)	57.2(fixed)	—	20.6	57.2
<i>u2855</i>	H(151)...H(154)	546.1(99)	54.0(fixed)	—	-23.4	54.0
<i>u3018</i>	H(108)...H(112)	546.1(184)	57.1(fixed)	—	20.6	57.1
<i>u3254</i>	Si(2)...H(19)	546.2(18)	16.7(fixed)	—	-4.7	16.7
<i>u3569</i>	H(186)...H(192)	546.2(141)	49.2(fixed)	—	-27.1	49.2
<i>u3200</i>	Si(208)...H(235)	546.3(14)	16.7(fixed)	—	-3.5	16.7
<i>u3284</i>	Si(85)...H(103)	546.5(15)	16.7(fixed)	—	-6.7	16.7
<i>u3283</i>	Si(4)...H(41)	546.6(21)	16.5(fixed)	—	-3.9	16.5
<i>u3219</i>	C(253)...C(254)	546.7(46)	18.6(tied to <i>u2820</i> )	—	-1.2	19.0
<i>u3771</i>	C(131)...H(143)	546.7(74)	22.0(fixed)	—	-2.9	22.0
<i>u3548</i>	F(15)...H(25)	546.7(138)	39.6(fixed)	—	-12.5	39.6
<i>u3161</i>	C(49)...C(53)	546.8(56)	19.3(tied to <i>u2820</i> )	—	-1.1	19.7
<i>u3281</i>	C(217)...H(238)	546.8(51)	28.7(fixed)	—	2.0	28.7
<i>u1740</i>	H(268)...H(275)	546.8(230)	51.3(fixed)	—	-1.1	51.3
<i>u3158</i>	C(89)...C(93)	546.9(52)	21.5(tied to <i>u2820</i> )	—	-0.8	22.0
<i>u3251</i>	H(20)...H(34)	547.0(169)	43.2(fixed)	—	5.9	43.2
<i>u3337</i>	C(255)...H(277)	547.1(84)	36.9(fixed)	—	-1.7	36.9
<i>u3226</i>	F(262)...H(281)	547.1(32)	24.3(fixed)	—	-1.8	24.3
<i>u3258</i>	Si(43)...H(68)	547.2(18)	18.2(fixed)	—	-5.8	18.2
<i>u3130</i>	C(254)...C(258)	547.3(35)	16.9(tied to <i>u2820</i> )	—	-1.1	17.3
<i>u3248</i>	C(171)...H(189)	547.3(172)	41.1(fixed)	—	-4.0	41.1
<i>u3309</i>	F(179)...H(203)	547.3(28)	25.6(fixed)	—	-0.9	25.6
<i>u3216</i>	F(219)...H(240)	547.3(23)	23.9(fixed)	—	-1.7	23.9
<i>u3295</i>	C(259)...H(281)	547.4(228)	31.1(fixed)	—	-1.3	31.1
<i>u3172</i>	C(214)...C(216)	547.5(44)	17.1(tied to <i>u2820</i> )	—	-0.9	17.5
<i>u3422</i>	F(263)...H(286)	547.7(75)	28.1(fixed)	—	-4.5	28.1
<i>u3266</i>	Si(5)...H(25)	547.7(8)	16.9(fixed)	—	-7.6	16.9

<i>u</i> 3426	H(237)...H(244)	547.7(78)	31.9(fixed)	—	-0.3	31.9
<i>u</i> 3495	H(185)...H(202)	547.7(349)	50.0(fixed)	—	-10.3	50.0
<i>u</i> 2502	Si(126)...H(144)	547.8(17)	28.9(fixed)	—	-7.4	28.9
<i>u</i> 1745	H(270)...H(285)	547.9(105)	72.1(fixed)	—	23.2	72.1
<i>u</i> 3273	Si(209)...H(246)	548.0(16)	16.5(fixed)	—	-3.8	16.5
<i>u</i> 3379	H(264)...H(279)	548.0(269)	41.5(fixed)	—	5.5	41.5
<i>u</i> 3336	C(255)...H(283)	548.1(69)	32.5(fixed)	—	9.2	32.5
<i>u</i> 3362	C(255)...C(258)	548.1(46)	20.0(tied to <i>u</i> 2820)	—	-1.2	20.4
<i>u</i> 3298	Si(249)...H(284)	548.1(19)	16.5(fixed)	—	-6.9	16.5
<i>u</i> 3033	H(183)...H(190)	548.1(143)	54.4(fixed)	—	13.2	54.4
<i>u</i> 3308	C(252)...C(254)	548.1(60)	18.7(tied to <i>u</i> 2820)	—	-0.9	19.1
<i>u</i> 3032	H(186)...H(191)	548.2(143)	54.3(fixed)	—	13.2	54.3
<i>u</i> 3205	H(231)...H(238)	548.3(114)	37.1(fixed)	—	2.6	37.1
<i>u</i> 3367	C(91)...C(94)	548.3(93)	23.8(tied to <i>u</i> 2820)	—	-0.9	24.4
<i>u</i> 3473	F(58)...H(73)	548.3(70)	22.9(fixed)	—	-3.3	22.9
<i>u</i> 3359	H(279)...H(286)	548.3(145)	39.2(fixed)	—	0.4	39.2
<i>u</i> 3116	C(215)...H(229)	548.3(242)	56.0(fixed)	—	-0.7	56.0
<i>u</i> 3324	H(268)...H(279)	548.4(141)	34.4(fixed)	—	3.1	34.4
<i>u</i> 3228	F(220)...H(233)	548.4(36)	23.3(fixed)	—	0.8	23.3
<i>u</i> 2849	H(273)...H(278)	548.4(66)	35.2(fixed)	—	5.4	35.2
<i>u</i> 3455	H(62)...H(66)	548.6(345)	44.9(fixed)	—	-8.8	44.9
<i>u</i> 3480	H(225)...H(231)	548.9(112)	60.1(fixed)	—	4.1	60.1
<i>u</i> 3137	C(254)...C(257)	548.9(55)	21.3(tied to <i>u</i> 2820)	—	-1.3	21.8
<i>u</i> 3017	C(217)...H(234)	548.9(90)	69.9(fixed)	—	9.6	69.9
<i>u</i> 355	H(152)...H(155)	549.0(134)	50.8(fixed)	—	47.7	50.8
<i>u</i> 3244	Si(3)...H(38)	549.1(22)	15.4(fixed)	—	-3.5	15.4
<i>u</i> 3633	H(111)...H(115)	549.1(162)	60.0(fixed)	—	-6.1	60.0
<i>u</i> 3632	H(100)...H(119)	549.1(162)	59.9(fixed)	—	-6.2	59.9
<i>u</i> 3451	H(18)...H(37)	549.1(145)	39.5(fixed)	—	0.2	39.5
<i>u</i> 3282	Si(208)...H(243)	549.1(21)	15.3(fixed)	—	-3.5	15.3
<i>u</i> 3516	C(211)...H(245)	549.3(105)	36.0(fixed)	—	-1.5	36.0
<i>u</i> 3311	Si(44)...H(79)	549.4(24)	16.4(fixed)	—	-7.0	16.4
<i>u</i> 3381	F(221)...H(236)	549.4(22)	22.3(fixed)	—	-2.5	22.3
<i>u</i> 3262	H(224)...H(244)	549.5(73)	48.1(fixed)	—	1.9	48.1
<i>u</i> 3220	C(8)...C(12)	549.5(32)	18.2(tied to <i>u</i> 2820)	—	-1.2	18.6
<i>u</i> 3155	C(172)...H(182)	549.5(43)	53.5(fixed)	—	18.9	53.5
<i>u</i> 3371	C(253)...H(280)	549.6(199)	32.6(fixed)	—	-3.5	32.6
<i>u</i> 3690	H(184)...H(199)	549.6(149)	117.6(fixed)	—	-1.6	117.6
<i>u</i> 3444	F(262)...H(265)	549.6(73)	29.8(fixed)	—	-5.1	29.8
<i>u</i> 3390	F(263)...H(276)	549.7(81)	24.9(fixed)	—	-3.0	24.9
<i>u</i> 3394	C(218)...H(236)	549.7(73)	34.1(fixed)	—	-1.5	34.1
<i>u</i> 3322	C(216)...H(234)	549.7(67)	33.6(fixed)	—	9.7	33.6
<i>u</i> 3342	C(211)...H(241)	549.7(227)	32.8(fixed)	—	-1.0	32.8
<i>u</i> 3255	Si(3)...H(34)	549.8(26)	15.6(fixed)	—	-3.5	15.6

<i>u</i> 3263	H(100)...H(122)	550.1(187)	61.0(fixed)	—	35.0	61.0
<i>u</i> 3288	Si(85)...H(120)	550.1(18)	15.3(fixed)	—	-4.3	15.3
<i>u</i> 3270	Si(3)...H(21)	550.2(22)	15.4(fixed)	—	-3.5	15.4
<i>u</i> 3279	Si(208)...H(226)	550.3(24)	15.6(fixed)	—	-4.2	15.6
<i>u</i> 3880	H(189)...H(203)	550.3(162)	125.5(fixed)	—	-11.1	125.5
<i>u</i> 3264	H(111)...H(114)	550.4(187)	60.2(fixed)	—	35.1	60.2
<i>u</i> 3291	Si(166)...H(189)	550.4(10)	15.3(fixed)	—	-3.9	15.3
<i>u</i> 3292	Si(168)...H(185)	550.4(10)	15.3(fixed)	—	-3.9	15.3
<i>u</i> 3534	H(224)...H(236)	550.4(75)	44.1(fixed)	—	0.2	44.1
<i>u</i> 3694	H(233)...H(243)	550.5(167)	62.1(fixed)	—	10.6	62.1
<i>u</i> 3245	H(267)...H(283)	550.7(185)	60.6(fixed)	—	15.4	60.6
<i>u</i> 4530	H(273)...H(282)	550.8(82)	34.3(fixed)	—	-10.7	34.3
<i>u</i> 3388	C(6)...H(36)	551.0(233)	33.5(fixed)	—	-1.2	33.5
<i>u</i> 3433	F(56)...H(60)	551.2(86)	24.3(fixed)	—	-2.3	24.3
<i>u</i> 3399	F(16)...H(35)	551.2(29)	23.3(fixed)	—	-2.1	23.3
<i>u</i> 3431	C(49)...H(72)	551.2(100)	62.0(fixed)	—	-3.2	62.0
<i>u</i> 3446	C(257)...H(267)	551.3(199)	38.3(fixed)	—	-6.2	38.3
<i>u</i> 3277	Si(45)...H(66)	551.3(18)	15.5(fixed)	—	-3.7	15.5
<i>u</i> 3372	F(221)...H(237)	551.4(32)	24.6(fixed)	—	-2.8	24.6
<i>u</i> 3361	H(60)...H(69)	551.5(131)	44.5(fixed)	—	10.3	44.5
<i>u</i> 3239	Si(249)...H(280)	551.5(20)	15.2(fixed)	—	-3.5	15.2
<i>u</i> 3289	C(216)...C(217)	551.6(41)	18.2(tied to <i>u</i> 2820)	—	-0.9	18.7
<i>u</i> 3063	F(263)...H(274)	551.7(229)	36.6(fixed)	—	-1.0	36.6
<i>u</i> 3296	Si(210)...H(230)	551.7(7)	15.5(fixed)	—	-5.0	15.5
<i>u</i> 3385	H(65)...H(78)	551.8(297)	46.2(fixed)	—	11.3	46.2
<i>u</i> 3384	H(277)...H(287)	551.8(76)	49.6(fixed)	—	1.2	49.6
<i>u</i> 3492	C(88)...H(122)	551.8(150)	34.2(fixed)	—	-1.1	34.2
<i>u</i> 3509	C(171)...H(188)	552.1(153)	49.0(fixed)	—	-9.2	49.0
<i>u</i> 3316	Si(248)...H(267)	552.1(8)	15.3(fixed)	—	-4.9	15.3
<i>u</i> 3038	C(12)...H(29)	552.2(99)	88.5(fixed)	—	13.3	88.5
<i>u</i> 3331	C(91)...H(117)	552.3(247)	33.9(fixed)	—	-2.3	33.9
<i>u</i> 4067	C(252)...H(271)	552.4(49)	27.9(fixed)	—	-16.6	27.9
<i>u</i> 3392	C(254)...H(268)	552.4(237)	50.2(fixed)	—	-0.6	50.2
<i>u</i> 3389	F(220)...H(234)	552.4(25)	22.4(fixed)	—	-3.2	22.4
<i>u</i> 3518	H(23)...H(31)	552.5(186)	35.0(fixed)	—	-0.4	35.0
<i>u</i> 3321	Si(43)...H(62)	552.5(8)	15.2(fixed)	—	-3.5	15.2
<i>u</i> 3445	C(48)...H(74)	552.7(185)	31.0(fixed)	—	-4.9	31.0
<i>u</i> 3276	Si(44)...H(75)	552.7(8)	15.2(fixed)	—	-3.4	15.2
<i>u</i> 3247	C(213)...C(217)	552.7(37)	19.0(tied to <i>u</i> 2820)	—	-1.3	19.4
<i>u</i> 3315	Si(207)...H(239)	552.8(18)	15.1(fixed)	—	-3.5	15.1
<i>u</i> 3470	C(52)...H(64)	552.9(183)	32.4(fixed)	—	-5.1	32.4
<i>u</i> 3830	C(212)...H(233)	553.1(80)	58.6(fixed)	—	-10.6	58.6
<i>u</i> 3463	C(94)...H(111)	553.3(140)	101.5(fixed)	—	6.2	101.5
<i>u</i> 3464	C(93)...H(100)	553.4(140)	101.3(fixed)	—	6.2	101.3

<i>u</i> 3453	F(58)...H(71)	553.4(84)	24.4(fixed)	—	-2.4	24.4
<i>u</i> 1876	H(270)...H(287)	553.5(89)	89.7(fixed)	—	16.8	89.7
<i>u</i> 3374	F(16)...H(33)	553.5(27)	24.1(fixed)	—	-2.5	24.1
<i>u</i> 3314	H(67)...H(73)	553.5(97)	45.3(fixed)	—	10.7	45.3
<i>u</i> 3356	F(57)...H(77)	553.6(33)	22.9(fixed)	—	-1.7	22.9
<i>u</i> 3567	H(69)...H(76)	553.7(134)	67.2(fixed)	—	2.1	67.2
<i>u</i> 3447	H(269)...H(270)	553.7(206)	42.9(fixed)	—	11.2	42.9
<i>u</i> 3450	H(19)...H(35)	553.8(109)	42.0(fixed)	—	0.1	42.0
<i>u</i> 3354	F(262)...H(279)	553.9(34)	23.1(fixed)	—	-2.5	23.1
<i>u</i> 3483	C(47)...H(74)	553.9(251)	35.3(fixed)	—	-1.7	35.3
<i>u</i> 3360	H(70)...H(74)	554.0(83)	36.9(fixed)	—	12.5	36.9
<i>u</i> 3585	C(12)...H(26)	554.0(224)	64.4(tied to <i>u</i> 2820)	—	-3.3	65.8
<i>u</i> 3387	F(57)...H(78)	554.0(46)	23.2(fixed)	—	-2.1	23.2
<i>u</i> 3305	H(101)...H(119)	554.2(179)	49.0(fixed)	—	14.5	49.0
<i>u</i> 3391	F(219)...H(238)	554.2(35)	23.1(fixed)	—	-2.4	23.1
<i>u</i> 3327	H(115)...H(118)	554.2(287)	35.7(fixed)	—	-2.2	35.7
<i>u</i> 3519	C(6)...H(40)	554.4(118)	38.0(fixed)	—	-1.7	38.0
<i>u</i> 3477	F(58)...H(81)	554.5(81)	24.9(fixed)	—	-3.7	24.9
<i>u</i> 3500	F(137)...H(147)	554.7(140)	25.6(fixed)	—	-4.2	25.6
<i>u</i> 3462	C(259)...H(278)	554.8(106)	35.7(fixed)	—	-1.1	35.7
<i>u</i> 3543	H(63)...H(78)	554.8(261)	61.8(fixed)	—	1.7	61.8
<i>u</i> 3469	F(137)...H(148)	554.8(141)	30.2(fixed)	—	-3.8	30.2
<i>u</i> 3429	F(178)...F(181)	554.8(20)	12.8(tied to <i>u</i> 2820)	—	-4.7	13.1
<i>u</i> 3423	H(67)...H(79)	554.8(75)	44.6(fixed)	—	-0.2	44.6
<i>u</i> 3471	H(238)...H(242)	554.8(284)	40.6(fixed)	—	3.0	40.6
<i>u</i> 3408	F(96)...H(112)	554.9(77)	23.8(fixed)	—	-2.5	23.8
<i>u</i> 2206	H(142)...H(159)	554.9(96)	63.0(fixed)	—	3.0	63.0
<i>u</i> 3687	H(102)...H(121)	554.9(121)	52.3(fixed)	—	-23.1	52.3
<i>u</i> 3688	H(110)...H(113)	554.9(121)	52.1(fixed)	—	-23.1	52.1
<i>u</i> 3178	C(11)...H(24)	555.1(237)	74.9(fixed)	—	1.6	74.9
<i>u</i> 3373	H(74)...H(81)	555.1(137)	37.9(fixed)	—	1.1	37.9
<i>u</i> 2415	F(137)...F(138)	555.3(19)	17.7(tied to <i>u</i> 2820)	—	-1.3	18.2
<i>u</i> 3597	C(174)...H(193)	555.4(100)	66.5(fixed)	—	-15.0	66.5
<i>u</i> 3082	H(101)...H(121)	555.6(136)	60.1(fixed)	—	10.9	60.1
<i>u</i> 3081	H(109)...H(113)	555.6(136)	60.2(fixed)	—	11.0	60.2
<i>u</i> 3432	F(220)...F(222)	555.7(19)	12.3(fixed)	—	-2.2	12.3
<i>u</i> 3424	C(216)...H(230)	556.1(163)	36.7(fixed)	—	-7.0	36.7
<i>u</i> 3265	C(213)...H(239)	556.1(162)	32.7(fixed)	—	-3.6	32.7
<i>u</i> 3413	F(138)...H(146)	556.3(140)	23.5(fixed)	—	-2.8	23.5
<i>u</i> 2942	H(189)...H(204)	556.3(102)	57.6(fixed)	—	50.0	57.6
<i>u</i> 3310	F(262)...H(280)	556.6(30)	24.9(fixed)	—	-2.3	24.9
<i>u</i> 2913	H(232)...H(240)	556.8(141)	49.2(fixed)	—	9.2	49.2
<i>u</i> 3448	H(268)...H(277)	556.9(168)	38.8(fixed)	—	3.3	38.8
<i>u</i> 3440	H(20)...H(26)	557.1(104)	58.0(fixed)	—	7.9	58.0



<i>u3341</i>	H(276)...H(282)	557.1(99)	44.3(fixed)	—	14.2	44.3
<i>u3386</i>	F(138)...H(144)	557.4(140)	24.4(fixed)	—	-1.7	24.4
<i>u3705</i>	H(28)...H(38)	557.4(171)	75.9(fixed)	—	15.7	75.9
<i>u3598</i>	C(173)...H(196)	557.5(118)	66.8(fixed)	—	-15.0	66.8
<i>u3344</i>	F(219)...H(239)	557.6(34)	24.6(fixed)	—	-1.9	24.6
<i>u3457</i>	H(20)...H(31)	557.6(103)	43.6(fixed)	—	2.0	43.6
<i>u3411</i>	F(263)...H(287)	557.7(85)	30.6(fixed)	—	-4.3	30.6
<i>u4547</i>	H(273)...H(284)	558.0(297)	34.4(fixed)	—	-11.0	34.4
<i>u3355</i>	H(196)...H(201)	558.0(265)	56.1(fixed)	—	32.7	56.1
<i>u3210</i>	H(226)...H(244)	558.0(151)	46.9(fixed)	—	0.8	46.9
<i>u2880</i>	H(226)...H(234)	558.2(86)	47.0(fixed)	—	30.9	47.0
<i>u2926</i>	H(100)...H(107)	558.2(95)	61.3(fixed)	—	52.3	61.3
<i>u3396</i>	H(19)...H(39)	558.3(96)	47.1(fixed)	—	1.8	47.1
<i>u3494</i>	H(268)...H(283)	558.4(258)	61.8(fixed)	—	3.7	61.8
<i>u3962</i>	H(103)...H(110)	558.5(120)	117.7(fixed)	—	-10.7	117.7
<i>u3960</i>	H(102)...H(107)	558.6(120)	117.6(fixed)	—	-10.6	117.6
<i>u2927</i>	H(103)...H(111)	558.7(94)	59.6(fixed)	—	52.5	59.6
<i>u3565</i>	H(269)...H(272)	558.8(152)	45.3(fixed)	—	3.4	45.3
<i>u3522</i>	C(174)...H(201)	558.9(228)	34.8(fixed)	—	-2.3	34.8
<i>u3515</i>	C(51)...H(64)	558.9(248)	34.2(fixed)	—	-1.6	34.2
<i>u3558</i>	H(61)...H(70)	559.0(122)	42.4(fixed)	—	-3.6	42.4
<i>u3430</i>	F(57)...F(58)	559.0(18)	12.4(fixed)	—	-2.1	12.4
<i>u3294</i>	H(26)...H(34)	559.0(59)	56.4(fixed)	—	19.9	56.4
<i>u3523</i>	F(221)...H(227)	559.2(117)	26.9(fixed)	—	-4.0	26.9
<i>u3428</i>	F(220)...H(243)	559.4(137)	30.1(fixed)	—	-3.5	30.1
<i>u3443</i>	C(54)...H(76)	559.4(230)	34.7(fixed)	—	-2.1	34.7
<i>u3501</i>	F(220)...H(242)	559.4(135)	24.5(fixed)	—	-3.8	24.5
<i>u3512</i>	C(257)...H(269)	559.5(165)	40.2(fixed)	—	-8.2	40.2
<i>u3328</i>	F(220)...H(232)	559.5(28)	26.9(fixed)	—	-3.0	26.9
<i>u2592</i>	C(130)...H(151)	559.6(74)	34.9(fixed)	—	11.3	34.9
<i>u3564</i>	C(92)...H(119)	559.7(228)	31.4(fixed)	—	-1.9	31.4
<i>u3412</i>	F(16)...H(34)	559.8(21)	24.5(fixed)	—	-2.8	24.5
<i>u3136</i>	H(229)...H(243)	560.1(156)	45.8(fixed)	—	11.7	45.8
<i>u3465</i>	H(234)...H(238)	560.2(254)	47.3(fixed)	—	16.0	47.3
<i>u3521</i>	C(170)...H(188)	560.2(228)	34.8(fixed)	—	-2.3	34.8
<i>u3467</i>	H(30)...H(36)	560.3(127)	37.9(fixed)	—	0.6	37.9
<i>u3488</i>	H(104)...H(122)	560.5(156)	48.3(fixed)	—	6.5	48.3
<i>u3556</i>	H(110)...H(115)	560.5(201)	38.2(fixed)	—	-1.7	38.2
<i>u3555</i>	H(102)...H(119)	560.5(201)	37.9(fixed)	—	-1.7	37.9
<i>u3487</i>	H(108)...H(114)	560.5(156)	48.1(fixed)	—	6.5	48.1
<i>u2943</i>	H(182)...H(198)	560.6(83)	63.5(fixed)	—	50.0	63.5
<i>u3352</i>	H(65)...H(73)	560.7(95)	37.6(fixed)	—	13.4	37.6
<i>u3409</i>	F(178)...H(194)	560.8(81)	28.7(fixed)	—	3.2	28.7
<i>u3486</i>	H(279)...H(285)	561.0(198)	34.5(fixed)	—	-1.4	34.5

<i>u3188</i>	H(21)...H(39)	561.0(178)	45.1(fixed)	—	1.8	45.1
<i>u3405</i>	C(216)...H(229)	561.1(155)	43.5(fixed)	—	-7.8	43.5
<i>u3553</i>	H(73)...H(77)	561.2(105)	44.7(fixed)	—	-0.3	44.7
<i>u3206</i>	H(22)...H(41)	561.3(112)	41.0(fixed)	—	2.4	41.0
<i>u3601</i>	C(92)...H(106)	561.5(188)	59.8(fixed)	—	-15.0	59.8
<i>u3668</i>	C(13)...H(32)	561.5(114)	29.6(fixed)	—	-1.1	29.6
<i>u3708</i>	H(31)...H(41)	561.6(89)	51.1(fixed)	—	0.3	51.1
<i>u3546</i>	F(55)...H(65)	561.6(149)	26.3(fixed)	—	-4.3	26.3
<i>u3222</i>	H(63)...H(77)	561.7(197)	52.0(fixed)	—	9.5	52.0
<i>u3378</i>	F(57)...H(79)	561.7(41)	24.2(fixed)	—	-2.1	24.2
<i>u3484</i>	C(254)...H(264)	561.8(103)	41.1(fixed)	—	-0.1	41.1
<i>u3552</i>	H(63)...H(72)	562.0(166)	35.8(fixed)	—	-7.2	35.8
<i>u3303</i>	H(191)...H(195)	562.1(202)	73.6(fixed)	—	24.3	73.6
<i>u3481</i>	H(239)...H(241)	562.2(54)	37.4(fixed)	—	2.1	37.4
<i>u3502</i>	C(211)...H(231)	562.2(53)	24.8(fixed)	—	-0.8	24.8
<i>u3600</i>	H(61)...H(76)	562.4(172)	32.1(fixed)	—	-3.9	32.1
<i>u3476</i>	F(58)...H(82)	562.5(99)	29.2(fixed)	—	-3.9	29.2
<i>u3610</i>	F(99)...H(108)	562.5(106)	43.3(fixed)	—	-8.0	43.3
<i>u3609</i>	F(98)...H(104)	562.5(106)	43.2(fixed)	—	-8.0	43.2
<i>u3302</i>	H(183)...H(203)	562.6(202)	71.7(fixed)	—	24.2	71.7
<i>u3606</i>	H(145)...H(158)	562.8(240)	40.6(fixed)	—	-3.3	40.6
<i>u3848</i>	F(15)...H(28)	562.9(44)	33.4(fixed)	—	-13.1	33.4
<i>u3246</i>	C(175)...H(202)	563.1(275)	41.1(fixed)	—	-4.0	41.1
<i>u3576</i>	H(72)...H(78)	563.2(150)	39.7(fixed)	—	-1.5	39.7
<i>u3517</i>	C(217)...H(231)	563.2(222)	49.3(fixed)	—	-2.2	49.3
<i>u3542</i>	F(16)...H(22)	563.3(115)	25.7(fixed)	—	-3.4	25.7
<i>u3240</i>	C(94)...H(116)	563.3(263)	36.0(fixed)	—	-3.5	36.0
<i>u3879</i>	H(184)...H(198)	563.5(112)	125.6(fixed)	—	-11.1	125.6
<i>u3456</i>	C(253)...C(259)	563.5(55)	20.0(fixed)	—	-1.2	20.0
<i>u3514</i>	H(225)...H(242)	563.6(193)	35.3(fixed)	—	-2.9	35.3
<i>u3406</i>	F(221)...H(235)	563.6(33)	24.1(fixed)	—	-2.8	24.1
<i>u2854</i>	H(21)...H(29)	563.9(81)	51.7(fixed)	—	43.8	51.7
<i>u3588</i>	C(7)...H(32)	563.9(65)	24.3(fixed)	—	-2.1	24.3
<i>u3629</i>	F(137)...H(151)	564.2(46)	35.8(fixed)	—	-7.3	35.8
<i>u4041</i>	H(268)...H(270)	564.2(259)	51.4(fixed)	—	-10.7	51.4
<i>u3335</i>	H(147)...H(155)	564.4(128)	38.5(fixed)	—	13.5	38.5
<i>u3541</i>	H(74)...H(80)	564.8(187)	35.2(fixed)	—	-0.4	35.2
<i>u3527</i>	C(6)...H(26)	564.8(46)	26.4(fixed)	—	0.7	26.4
<i>u3768</i>	H(225)...H(230)	564.8(117)	64.7(fixed)	—	-3.0	64.7
<i>u3528</i>	F(56)...H(67)	564.9(116)	26.1(fixed)	—	-3.3	26.1
<i>u3537</i>	H(64)...H(78)	564.9(130)	50.4(fixed)	—	7.4	50.4
<i>u3353</i>	H(182)...H(188)	565.1(251)	56.0(fixed)	—	32.7	56.0
<i>u3589</i>	H(31)...H(38)	565.1(156)	47.5(fixed)	—	-0.1	47.5
<i>u3560</i>	C(174)...H(186)	565.2(47)	30.7(fixed)	—	-1.9	30.7

<i>u3531</i>	C(50)...H(76)	565.3(71)	25.2(fixed)	—	-1.4	25.2
<i>u3513</i>	F(221)...H(226)	565.4(101)	27.3(fixed)	—	-4.0	27.3
<i>u3545</i>	C(92)...H(107)	565.4(195)	39.7(fixed)	—	-8.8	39.7
<i>u3472</i>	F(55)...H(66)	565.5(139)	30.4(fixed)	—	-3.9	30.4
<i>u3397</i>	H(268)...H(282)	565.5(196)	59.7(fixed)	—	10.4	59.7
<i>u3085</i>	H(105)...H(116)	565.6(178)	55.7(fixed)	—	26.4	55.7
<i>u3086</i>	H(106)...H(120)	565.7(178)	55.5(fixed)	—	26.4	55.5
<i>u3482</i>	H(225)...H(235)	565.8(88)	40.4(fixed)	—	8.3	40.4
<i>u3969</i>	C(257)...H(270)	566.0(51)	62.0(fixed)	—	-19.0	62.0
<i>u3192</i>	H(227)...H(246)	566.0(89)	41.0(fixed)	—	4.8	41.0
<i>u3663</i>	F(55)...H(69)	566.0(56)	34.7(fixed)	—	-7.6	34.7
<i>u3475</i>	H(33)...H(39)	566.2(200)	34.5(fixed)	—	-1.3	34.5
<i>u3211</i>	H(190)...H(204)	566.2(99)	58.3(fixed)	—	36.0	58.3
<i>u3529</i>	H(59)...H(69)	566.4(113)	41.4(fixed)	—	2.8	41.4
<i>u3489</i>	H(72)...H(80)	566.7(105)	50.6(fixed)	—	5.0	50.6
<i>u3592</i>	C(53)...H(73)	566.8(99)	41.9(fixed)	—	-7.3	41.9
<i>u3540</i>	F(180)...H(200)	566.9(119)	33.7(fixed)	—	-4.8	33.7
<i>u3741</i>	C(170)...H(205)	566.9(100)	53.3(fixed)	—	-16.0	53.3
<i>u3533</i>	C(48)...C(54)	566.9(62)	21.4(fixed)	—	-1.3	21.4
<i>u3579</i>	C(54)...H(64)	567.0(106)	31.3(fixed)	—	1.3	31.3
<i>u3526</i>	H(20)...H(37)	567.3(196)	35.4(fixed)	—	-2.5	35.4
<i>u3510</i>	C(175)...H(201)	567.3(243)	49.0(fixed)	—	-9.2	49.0
<i>u3460</i>	C(51)...H(79)	567.3(165)	41.6(fixed)	—	-5.0	41.6
<i>u3474</i>	C(259)...H(269)	567.4(91)	29.8(fixed)	—	4.8	29.8
<i>u1655</i>	H(267)...H(275)	567.4(161)	49.8(fixed)	—	2.4	49.8
<i>u3410</i>	F(180)...H(183)	567.5(24)	28.8(fixed)	—	3.2	28.8
<i>u3871</i>	H(270)...H(279)	567.6(86)	77.0(fixed)	—	-15.5	77.0
<i>u4029</i>	H(22)...H(28)	567.6(94)	81.3(fixed)	—	-7.7	81.3
<i>u3061</i>	H(24)...H(38)	567.9(167)	55.8(fixed)	—	26.2	55.8
<i>u3675</i>	C(252)...H(272)	568.0(77)	52.2(fixed)	—	3.5	52.2
<i>u3648</i>	H(225)...H(244)	568.2(100)	43.2(fixed)	—	-6.2	43.2
<i>u3728</i>	H(151)...H(162)	568.2(79)	39.9(fixed)	—	0.2	39.9
<i>u3566</i>	C(253)...H(279)	568.2(146)	25.9(fixed)	—	-4.2	25.9
<i>u3754</i>	H(277)...H(283)	568.3(124)	42.2(fixed)	—	-11.0	42.2
<i>u3499</i>	C(213)...H(238)	568.3(139)	29.9(fixed)	—	-5.0	29.9
<i>u3697</i>	H(20)...H(25)	568.3(122)	63.1(fixed)	—	-3.2	63.1
<i>u3634</i>	C(88)...H(108)	568.3(51)	31.0(fixed)	—	-1.6	31.0
<i>u3635</i>	C(91)...H(104)	568.4(51)	30.8(fixed)	—	-1.6	30.8
<i>u1771</i>	F(138)...H(143)	568.8(47)	37.8(fixed)	—	-2.5	37.8
<i>u3636</i>	C(90)...H(114)	568.8(131)	35.4(fixed)	—	-5.9	35.4
<i>u3561</i>	C(252)...H(279)	569.1(232)	32.1(fixed)	—	-1.6	32.1
<i>u3570</i>	C(53)...H(65)	569.1(229)	34.7(fixed)	—	-1.8	34.7
<i>u3631</i>	C(54)...H(70)	569.5(61)	24.2(fixed)	—	-1.6	24.2
<i>u3551</i>	H(269)...H(286)	569.5(134)	46.7(fixed)	—	8.2	46.7

<i>u3677</i>	C(47)...H(70)	569.6(94)	38.4(fixed)	—	-7.3	38.4
<i>u3563</i>	F(16)...H(21)	569.7(96)	26.5(fixed)	—	-3.6	26.5
<i>u3742</i>	C(174)...H(191)	569.8(131)	53.7(fixed)	—	-16.0	53.7
<i>u3590</i>	C(211)...H(230)	570.2(53)	25.6(fixed)	—	-1.3	25.6
<i>u3807</i>	H(223)...H(236)	570.2(57)	37.2(fixed)	—	-5.7	37.2
<i>u3683</i>	C(10)...H(29)	570.3(47)	22.3(fixed)	—	-0.6	22.3
<i>u3562</i>	C(6)...H(25)	570.5(57)	28.1(fixed)	—	-0.9	28.1
<i>u3212</i>	H(182)...H(199)	570.6(110)	61.4(fixed)	—	36.0	61.4
<i>u3511</i>	H(117)...H(121)	570.7(147)	35.0(fixed)	—	-1.5	35.0
<i>u4316</i>	F(263)...H(271)	570.8(36)	39.8(fixed)	—	-16.1	39.8
<i>u3326</i>	H(228)...H(234)	570.8(71)	40.2(fixed)	—	21.9	40.2
<i>u3503</i>	H(184)...H(204)	570.9(118)	71.7(fixed)	—	15.1	71.7
<i>u3554</i>	C(214)...H(238)	570.9(225)	35.6(fixed)	—	-1.7	35.6
<i>u3704</i>	H(64)...H(81)	570.9(147)	42.2(fixed)	—	2.6	42.2
<i>u3493</i>	H(231)...H(236)	571.0(145)	39.7(fixed)	—	3.0	39.7
<i>u3959</i>	H(233)...H(241)	571.2(86)	58.4(fixed)	—	2.1	58.4
<i>u3507</i>	H(67)...H(77)	571.3(252)	46.0(fixed)	—	-4.1	46.0
<i>u3649</i>	H(266)...H(281)	571.3(158)	34.4(fixed)	—	-3.5	34.4
<i>u3604</i>	C(7)...H(30)	571.4(87)	25.0(fixed)	—	-3.2	25.0
<i>u3602</i>	C(50)...H(59)	571.4(102)	35.9(fixed)	—	-5.1	35.9
<i>u3229</i>	H(100)...H(108)	571.7(101)	62.0(fixed)	—	40.7	62.0
<i>u4001</i>	H(151)...H(156)	571.7(113)	59.1(fixed)	—	-6.7	59.1
<i>u3119</i>	H(227)...H(234)	571.7(88)	49.1(fixed)	—	23.1	49.1
<i>u3577</i>	F(56)...H(66)	571.8(111)	27.6(fixed)	—	-3.8	27.6
<i>u3559</i>	C(170)...H(199)	571.9(77)	30.7(fixed)	—	-1.9	30.7
<i>u3461</i>	H(229)...H(241)	571.9(226)	47.3(fixed)	—	6.2	47.3
<i>u3420</i>	H(105)...H(117)	572.0(250)	58.0(fixed)	—	12.9	58.0
<i>u3824</i>	H(143)...H(149)	572.2(88)	40.8(fixed)	—	-0.8	40.8
<i>u1880</i>	H(274)...H(287)	572.3(87)	40.1(fixed)	—	3.2	40.1
<i>u3544</i>	F(220)...H(244)	572.4(46)	25.6(fixed)	—	-3.6	25.6
<i>u3766</i>	H(18)...H(35)	572.4(77)	35.2(fixed)	—	-5.0	35.2
<i>u3621</i>	C(215)...H(245)	572.4(45)	23.5(fixed)	—	-1.9	23.5
<i>u4443</i>	H(142)...H(154)	572.5(99)	23.3(fixed)	—	-9.0	23.3
<i>u3679</i>	H(233)...H(240)	572.6(140)	33.1(fixed)	—	-10.3	33.1
<i>u3571</i>	H(269)...H(283)	572.6(131)	49.0(fixed)	—	8.3	49.0
<i>u3977</i>	H(28)...H(36)	572.7(106)	72.5(fixed)	—	4.6	72.5
<i>u3808</i>	H(69)...H(75)	572.9(126)	72.1(fixed)	—	-3.9	72.1
<i>u3703</i>	F(17)...H(26)	573.0(104)	31.3(fixed)	—	-7.5	31.3
<i>u3525</i>	C(256)...H(273)	573.1(47)	24.6(fixed)	—	-1.3	24.6
<i>u3504</i>	H(182)...H(203)	573.3(150)	72.9(fixed)	—	15.1	72.9
<i>u3520</i>	C(53)...H(63)	573.3(71)	24.7(fixed)	—	-1.5	24.7
<i>u3547</i>	C(93)...H(119)	573.5(248)	28.3(fixed)	—	-4.8	28.3
<i>u3090</i>	H(143)...H(162)	573.6(99)	46.5(fixed)	—	2.8	46.5
<i>u3586</i>	H(104)...H(117)	574.0(222)	73.9(fixed)	—	7.4	73.9

<i>u3418</i>	C(129)...H(149)	574.1(36)	36.3(fixed)	—	-1.7	36.3
<i>u3539</i>	F(178)...H(190)	574.4(110)	33.7(fixed)	—	-4.8	33.7
<i>u3811</i>	C(51)...H(78)	574.4(150)	33.6(fixed)	—	-10.3	33.6
<i>u3652</i>	C(256)...H(274)	574.4(54)	21.7(fixed)	—	-2.2	21.7
<i>u4110</i>	C(129)...H(148)	574.4(48)	21.5(fixed)	—	-6.9	21.5
<i>u3587</i>	C(50)...H(75)	574.5(59)	25.2(fixed)	—	-1.6	25.2
<i>u3784</i>	C(132)...H(146)	574.6(43)	32.6(fixed)	—	-8.1	32.6
<i>u3647</i>	C(10)...H(28)	574.6(46)	22.0(fixed)	—	0.6	22.0
<i>u3530</i>	C(132)...H(144)	574.8(48)	36.6(fixed)	—	-5.0	36.6
<i>u3710</i>	C(217)...H(223)	574.8(39)	25.2(fixed)	—	-2.9	25.2
<i>u3550</i>	C(10)...H(27)	575.3(35)	25.4(fixed)	—	0.7	25.4
<i>u3109</i>	H(22)...H(29)	575.4(92)	57.9(fixed)	—	33.3	57.9
<i>u3717</i>	H(67)...H(72)	575.4(108)	64.7(fixed)	—	0.8	64.7
<i>u3524</i>	C(90)...H(112)	575.5(133)	35.6(fixed)	—	-4.3	35.6
<i>u3731</i>	H(277)...H(285)	575.7(96)	43.9(fixed)	—	-3.8	43.9
<i>u3709</i>	C(53)...H(71)	575.9(90)	36.0(fixed)	—	-8.2	36.0
<i>u3656</i>	F(180)...H(202)	575.9(108)	33.4(fixed)	—	-3.9	33.4
<i>u3617</i>	F(98)...H(103)	575.9(87)	30.4(fixed)	—	-5.8	30.4
<i>u3506</i>	F(15)...H(27)	576.0(48)	53.4(fixed)	—	-5.2	53.4
<i>u3657</i>	H(281)...H(285)	576.0(218)	37.1(fixed)	—	-0.3	37.1
<i>u3626</i>	C(253)...H(276)	576.0(95)	28.6(fixed)	—	-3.1	28.6
<i>u3644</i>	C(216)...H(242)	576.0(221)	31.4(fixed)	—	-1.5	31.4
<i>u3557</i>	C(258)...H(268)	576.2(64)	25.5(fixed)	—	-1.0	25.5
<i>u3616</i>	H(28)...H(31)	576.2(80)	41.5(fixed)	—	8.5	41.5
<i>u3638</i>	H(278)...H(282)	576.3(76)	35.2(fixed)	—	6.9	35.2
<i>u3661</i>	H(26)...H(35)	576.3(241)	54.6(fixed)	—	10.5	54.6
<i>u3653</i>	F(55)...H(68)	576.7(62)	34.1(fixed)	—	-6.1	34.1
<i>u3640</i>	H(20)...H(39)	576.8(106)	43.3(fixed)	—	-4.5	43.3
<i>u3619</i>	F(220)...H(246)	576.9(45)	29.6(fixed)	—	-4.0	29.6
<i>u3660</i>	C(11)...H(40)	577.5(48)	23.6(fixed)	—	-2.0	23.6
<i>u3945</i>	H(275)...H(277)	577.5(93)	36.7(fixed)	—	-4.3	36.7
<i>u3627</i>	C(88)...H(107)	577.5(63)	27.4(fixed)	—	0.9	27.4
<i>u3715</i>	H(264)...H(272)	577.6(127)	76.1(fixed)	—	8.3	76.1
<i>u3269</i>	H(23)...H(29)	577.7(65)	43.3(fixed)	—	33.4	43.3
<i>u3614</i>	C(51)...H(67)	577.8(51)	23.8(fixed)	—	-1.3	23.8
<i>u3713</i>	C(54)...H(69)	577.9(49)	21.4(fixed)	—	-3.5	21.4
<i>u3714</i>	C(6)...H(24)	578.3(46)	22.2(fixed)	—	-4.8	22.2
<i>u3625</i>	H(35)...H(39)	578.4(218)	35.7(fixed)	—	-0.1	35.7
<i>u3415</i>	H(62)...H(77)	578.5(340)	62.6(fixed)	—	4.7	62.6
<i>u3417</i>	H(24)...H(36)	578.6(231)	58.5(fixed)	—	16.1	58.5
<i>u3774</i>	C(7)...H(31)	578.7(57)	22.4(fixed)	—	-3.1	22.4
<i>u3761</i>	H(69)...H(80)	578.9(90)	38.9(fixed)	—	0.1	38.9
<i>u3832</i>	H(22)...H(31)	578.9(233)	41.2(fixed)	—	-1.2	41.2
<i>u3350</i>	H(187)...H(196)	579.1(108)	55.4(fixed)	—	43.0	55.4

<i>u3722</i>	C(47)...H(68)	579.1(109)	35.6(fixed)	—	-7.1	35.6
<i>u3651</i>	H(22)...H(40)	579.3(89)	32.4(fixed)	—	-1.5	32.4
<i>u2645</i>	C(129)...H(161)	579.3(137)	37.6(fixed)	—	-11.3	37.6
<i>u3667</i>	C(257)...H(286)	579.3(41)	25.1(fixed)	—	-2.6	25.1
<i>u3659</i>	C(256)...H(284)	579.4(147)	44.1(fixed)	—	-7.2	44.1
<i>u3844</i>	C(256)...H(283)	579.4(146)	39.0(fixed)	—	-11.0	39.0
<i>u3699</i>	C(215)...H(244)	579.4(44)	21.5(fixed)	—	-2.3	21.5
<i>u3491</i>	H(229)...H(242)	579.7(107)	38.2(fixed)	—	7.5	38.2
<i>u4032</i>	H(227)...H(233)	579.8(89)	66.1(fixed)	—	-5.8	66.1
<i>u3670</i>	C(9)...H(22)	579.8(41)	23.1(fixed)	—	-1.6	23.1
<i>u3869</i>	H(26)...H(36)	579.9(206)	68.5(fixed)	—	2.2	68.5
<i>u3745</i>	C(12)...H(18)	580.0(53)	24.8(fixed)	—	-2.7	24.8
<i>u4107</i>	H(102)...H(106)	580.2(106)	102.2(fixed)	—	-18.0	102.2
<i>u3727</i>	C(253)...H(286)	580.3(93)	37.1(fixed)	—	-1.2	37.1
<i>u3725</i>	C(211)...H(229)	580.4(43)	21.4(fixed)	—	-3.5	21.4
<i>u3583</i>	C(54)...H(68)	580.5(39)	23.8(fixed)	—	-0.1	23.8
<i>u4074</i>	H(188)...H(203)	580.6(125)	100.8(fixed)	—	-15.9	100.8
<i>u3772</i>	H(236)...H(244)	580.6(79)	38.4(fixed)	—	-0.8	38.4
<i>u3706</i>	C(6)...H(30)	580.7(81)	34.8(fixed)	—	-3.9	34.8
<i>u3593</i>	C(256)...H(275)	580.7(42)	23.1(fixed)	—	-1.8	23.1
<i>u2282</i>	C(130)...H(163)	580.7(37)	40.0(fixed)	—	-1.4	40.0
<i>u3833</i>	C(215)...H(223)	580.8(64)	33.7(fixed)	—	-6.1	33.7
<i>u3339</i>	H(100)...H(106)	580.9(128)	56.6(fixed)	—	46.2	56.6
<i>u3591</i>	F(57)...H(76)	580.9(106)	25.1(fixed)	—	-3.2	25.1
<i>u3798</i>	H(32)...H(36)	580.9(93)	30.6(fixed)	—	-1.4	30.6
<i>u3607</i>	C(173)...H(202)	581.0(49)	30.3(fixed)	—	-0.5	30.3
<i>u3608</i>	C(170)...H(198)	581.0(49)	30.3(fixed)	—	-0.5	30.3
<i>u3684</i>	H(240)...H(241)	581.1(233)	34.4(fixed)	—	-1.0	34.4
<i>u3615</i>	C(215)...H(246)	581.1(27)	23.6(fixed)	—	-2.1	23.6
<i>u3340</i>	H(105)...H(111)	581.2(128)	55.8(fixed)	—	46.3	55.8
<i>u3729</i>	C(6)...H(34)	581.3(153)	30.4(fixed)	—	-3.6	30.4
<i>u3804</i>	C(11)...H(18)	581.3(68)	31.4(fixed)	—	-5.7	31.4
<i>u4076</i>	C(131)...H(153)	581.4(45)	27.8(fixed)	—	-14.6	27.8
<i>u3802</i>	H(27)...H(31)	581.4(97)	44.2(fixed)	—	-2.8	44.2
<i>u3746</i>	C(88)...H(106)	581.5(86)	22.7(fixed)	—	-2.8	22.7
<i>u3782</i>	C(50)...H(60)	581.7(98)	30.4(fixed)	—	-6.1	30.4
<i>u3866</i>	H(31)...H(39)	581.9(114)	43.1(fixed)	—	-2.7	43.1
<i>u1795</i>	H(272)...H(276)	581.9(68)	68.6(fixed)	—	28.8	68.6
<i>u3779</i>	H(225)...H(237)	581.9(66)	32.5(fixed)	—	2.6	32.5
<i>u3624</i>	C(258)...H(275)	582.1(210)	34.4(fixed)	—	-1.3	34.4
<i>u3666</i>	F(222)...H(231)	582.1(102)	27.4(fixed)	—	-4.6	27.4
<i>u3758</i>	C(177)...H(188)	582.1(75)	23.6(fixed)	—	-2.8	23.6
<i>u3916</i>	C(175)...H(203)	582.3(44)	42.7(fixed)	—	-21.8	42.7
<i>u3695</i>	H(20)...H(33)	582.5(108)	33.2(fixed)	—	0.8	33.2

<i>u3826</i>	C(94)...H(100)	582.6(75)	29.2(fixed)	—	-6.9	29.2
<i>u3825</i>	C(93)...H(111)	582.6(75)	29.4(fixed)	—	-6.9	29.4
<i>u3702</i>	C(257)...H(285)	582.6(33)	21.7(fixed)	—	-2.7	21.7
<i>u3686</i>	H(20)...H(36)	582.6(217)	38.9(fixed)	—	0.0	38.9
<i>u3843</i>	C(211)...H(237)	582.8(63)	24.5(fixed)	—	-3.6	24.5
<i>u3849</i>	C(253)...H(270)	582.8(49)	23.9(fixed)	—	-2.6	23.9
<i>u3582</i>	C(53)...H(62)	582.8(46)	25.1(fixed)	—	-1.4	25.1
<i>u3221</i>	H(269)...H(271)	582.8(174)	51.2(fixed)	—	13.9	51.2
<i>u3753</i>	C(258)...H(278)	582.9(63)	26.0(fixed)	—	-3.9	26.0
<i>u3349</i>	H(193)...H(201)	582.9(80)	52.4(fixed)	—	42.9	52.4
<i>u3645</i>	H(227)...H(245)	583.0(66)	32.0(fixed)	—	0.4	32.0
<i>u759</i>	H(143)...H(160)	583.1(115)	84.1(fixed)	—	10.9	84.1
<i>u3669</i>	C(52)...H(81)	583.2(55)	25.6(fixed)	—	-2.5	25.6
<i>u1813</i>	H(141)...H(159)	583.2(71)	57.9(fixed)	—	10.5	57.9
<i>u2678</i>	C(132)...H(145)	583.2(36)	35.2(fixed)	—	7.4	35.2
<i>u4008</i>	F(179)...H(191)	583.3(79)	31.1(fixed)	—	-29.6	31.1
<i>u3478</i>	H(105)...H(115)	583.4(132)	45.1(fixed)	—	17.9	45.1
<i>u3479</i>	H(106)...H(119)	583.4(132)	45.0(fixed)	—	17.9	45.0
<i>u3764</i>	C(10)...F(17)	583.5(24)	12.4(fixed)	—	-2.3	12.4
<i>u3596</i>	C(89)...H(117)	583.7(82)	26.0(fixed)	—	-0.5	26.0
<i>u3737</i>	C(50)...H(74)	583.9(51)	21.1(fixed)	—	-2.6	21.1
<i>u3689</i>	H(225)...H(241)	584.0(215)	38.8(fixed)	—	0.4	38.8
<i>u4151</i>	H(21)...H(28)	584.1(89)	79.5(fixed)	—	-17.3	79.5
<i>u3599</i>	C(51)...H(82)	584.2(95)	30.9(fixed)	—	-3.2	30.9
<i>u3954</i>	C(95)...H(102)	584.3(88)	47.4(fixed)	—	-19.2	47.4
<i>u3358</i>	C(131)...H(154)	584.5(30)	64.1(fixed)	—	-2.5	64.1
<i>u3680</i>	C(214)...H(227)	584.5(38)	22.8(fixed)	—	-1.4	22.8
<i>u3437</i>	H(24)...H(37)	584.5(102)	45.4(fixed)	—	19.2	45.4
<i>u3915</i>	C(172)...H(184)	584.6(34)	43.7(fixed)	—	-21.8	43.7
<i>u3757</i>	C(170)...H(197)	584.6(52)	23.6(fixed)	—	-2.8	23.6
<i>u3800</i>	H(231)...H(241)	584.7(201)	52.1(fixed)	—	1.1	52.1
<i>u3639</i>	H(267)...H(282)	584.7(339)	69.1(fixed)	—	2.4	69.1
<i>u3813</i>	C(6)...H(31)	584.9(70)	25.8(fixed)	—	-4.2	25.8
<i>u4482</i>	H(143)...H(148)	585.1(92)	23.3(fixed)	—	-8.8	23.3
<i>u3574</i>	H(110)...H(117)	585.2(236)	49.1(fixed)	—	10.4	49.1
<i>u2784</i>	C(129)...H(147)	585.3(43)	33.3(fixed)	—	2.6	33.3
<i>u3628</i>	H(149)...H(154)	585.3(214)	66.6(fixed)	—	1.8	66.6
<i>u3721</i>	C(94)...H(102)	585.9(60)	25.1(fixed)	—	0.6	25.1
<i>u3720</i>	C(93)...H(110)	586.0(60)	25.3(fixed)	—	0.6	25.3
<i>u3834</i>	H(22)...H(30)	586.0(279)	43.4(fixed)	—	-3.8	43.4
<i>u3662</i>	H(228)...H(244)	586.0(117)	38.0(fixed)	—	-4.8	38.0
<i>u3671</i>	C(11)...H(39)	586.2(37)	21.8(fixed)	—	-2.4	21.8
<i>u3655</i>	F(178)...H(189)	586.4(115)	33.4(fixed)	—	-3.9	33.4
<i>u3822</i>	C(48)...H(81)	586.4(98)	31.9(fixed)	—	-1.5	31.9

<i>u3603</i>	C(51)...H(66)	586.5(69)	25.0(fixed)	—	-1.6	25.0
<i>u3664</i>	C(254)...H(282)	586.6(46)	23.4(fixed)	—	-1.4	23.4
<i>u3719</i>	C(217)...H(225)	586.7(29)	22.1(fixed)	—	-3.2	22.1
<i>u3765</i>	C(54)...F(56)	586.7(24)	10.2(tied to <i>u3756</i> )	—	-2.3	12.6
<i>u3618</i>	C(257)...H(287)	586.8(51)	24.8(fixed)	—	-2.0	24.8
<i>u3740</i>	C(9)...H(23)	586.9(40)	21.6(fixed)	—	-2.5	21.6
<i>u3641</i>	C(9)...H(21)	586.9(45)	24.0(fixed)	—	-1.7	24.0
<i>u3809</i>	H(104)...H(116)	587.0(338)	94.6(fixed)	—	-3.1	94.6
<i>u3726</i>	H(267)...H(285)	587.1(158)	43.5(fixed)	—	3.2	43.5
<i>u3837</i>	H(76)...H(80)	587.3(219)	39.3(fixed)	—	-1.3	39.3
<i>u3875</i>	C(215)...H(224)	587.4(65)	32.2(fixed)	—	-5.8	32.2
<i>u3611</i>	C(11)...H(41)	587.4(46)	24.2(fixed)	—	-2.0	24.2
<i>u3734</i>	C(52)...H(60)	587.4(114)	29.1(fixed)	—	-2.8	29.1
<i>u3756</i>	C(13)...F(15)	587.6(22)	10.2(18)	—	-2.3	12.7
<i>u3732</i>	C(8)...H(36)	587.7(57)	24.3(fixed)	—	-1.6	24.3
<i>u2471</i>	H(145)...H(151)	587.8(88)	50.3(fixed)	—	16.3	50.3
<i>u3795</i>	C(52)...H(80)	587.8(40)	22.4(fixed)	—	-2.9	22.4
<i>u3707</i>	C(12)...H(20)	588.0(35)	22.6(fixed)	—	-3.2	22.6
<i>u4073</i>	H(184)...H(197)	588.1(87)	101.0(fixed)	—	-15.9	101.0
<i>u3646</i>	H(23)...H(39)	588.1(145)	36.3(fixed)	—	-2.8	36.3
<i>u3748</i>	C(258)...H(276)	588.1(68)	27.6(fixed)	—	-4.0	27.6
<i>u3701</i>	C(253)...H(271)	588.2(47)	28.3(fixed)	—	-0.6	28.3
<i>u3797</i>	C(11)...H(19)	588.2(82)	32.1(fixed)	—	-5.2	32.1
<i>u3755</i>	C(6)...F(14)	588.3(23)	10.2(tied to <i>u3756</i> )	—	-2.2	12.7
<i>u2198</i>	C(132)...H(153)	588.3(67)	49.7(fixed)	—	-9.0	49.7
<i>u3814</i>	C(253)...H(277)	588.4(63)	23.9(fixed)	—	-4.5	23.9
<i>u3658</i>	C(217)...H(224)	588.4(47)	25.0(fixed)	—	-0.9	25.0
<i>u3747</i>	C(51)...H(65)	588.9(63)	21.5(fixed)	—	-2.2	21.5
<i>u3692</i>	C(258)...H(267)	589.0(48)	25.6(fixed)	—	-1.3	25.6
<i>u3735</i>	C(213)...H(241)	589.1(45)	24.9(fixed)	—	-1.6	24.9
<i>u4149</i>	H(102)...H(122)	589.1(117)	65.1(fixed)	—	-21.1	65.1
<i>u4150</i>	H(110)...H(114)	589.1(117)	65.0(fixed)	—	-21.2	65.0
<i>u3605</i>	F(17)...H(25)	589.1(92)	32.8(fixed)	—	-5.9	32.8
<i>u3759</i>	H(273)...H(277)	589.3(95)	42.9(fixed)	—	-2.3	42.9
<i>u3773</i>	C(214)...H(228)	589.4(46)	21.3(fixed)	—	-2.6	21.3
<i>u3786</i>	C(211)...F(219)	589.5(22)	9.9(tied to <i>u3756</i> )	—	-2.1	12.4
<i>u3788</i>	C(51)...H(80)	589.6(76)	25.3(fixed)	—	-4.0	25.3
<i>u3792</i>	C(48)...H(71)	589.8(111)	31.6(fixed)	—	-4.1	31.6
<i>u3789</i>	C(88)...F(96)	589.8(23)	10.1(tied to <i>u3756</i> )	—	-2.4	12.6
<i>u3794</i>	C(259)...F(261)	590.0(22)	10.1(tied to <i>u3756</i> )	—	-2.4	12.6
<i>u3578</i>	C(132)...H(157)	590.4(137)	25.2(fixed)	—	-1.5	25.2
<i>u3778</i>	C(7)...H(40)	590.8(78)	26.4(fixed)	—	-4.3	26.4
<i>u3739</i>	C(53)...H(64)	590.9(44)	21.2(fixed)	—	-2.5	21.2
<i>u3780</i>	C(212)...H(245)	591.1(58)	25.5(fixed)	—	-4.1	25.5



<i>u3738</i>	C(48)...F(55)	591.1(25)	10.7(tied to <i>u3756</i> )	—	-2.3	13.3
<i>u3623</i>	C(213)...H(235)	591.1(57)	27.6(fixed)	—	-3.1	27.6
<i>u3892</i>	H(62)...H(80)	591.3(162)	43.1(fixed)	—	0.6	43.1
<i>u3403</i>	H(141)...H(154)	591.3(77)	33.1(fixed)	—	-3.1	33.1
<i>u3905</i>	H(31)...H(37)	591.3(129)	37.8(fixed)	—	-3.5	37.8
<i>u3839</i>	C(6)...H(33)	591.5(129)	24.0(fixed)	—	-4.1	24.0
<i>u3449</i>	H(275)...H(283)	591.6(254)	45.9(fixed)	—	12.8	45.9
<i>u3776</i>	C(93)...F(99)	591.8(20)	10.3(tied to <i>u3756</i> )	—	-3.6	12.9
<i>u3897</i>	H(19)...H(32)	591.9(89)	40.9(fixed)	—	-7.6	40.9
<i>u3696</i>	H(268)...H(271)	591.9(210)	63.1(fixed)	—	4.5	63.1
<i>u3730</i>	C(12)...H(19)	592.1(57)	25.1(fixed)	—	-1.8	25.1
<i>u2589</i>	F(260)...H(274)	592.3(46)	31.0(fixed)	—	1.8	31.0
<i>u3861</i>	C(211)...H(235)	592.3(68)	28.0(fixed)	—	-3.7	28.0
<i>u3878</i>	F(17)...H(32)	592.4(48)	24.7(fixed)	—	-1.1	24.7
<i>u3673</i>	C(214)...H(226)	592.4(52)	23.9(fixed)	—	-1.6	23.9
<i>u3718</i>	H(35)...H(41)	592.6(258)	37.1(fixed)	—	-1.6	37.1
<i>u4009</i>	F(180)...H(194)	592.6(60)	32.5(fixed)	—	-29.6	32.5
<i>u3899</i>	H(20)...H(24)	592.7(95)	51.0(fixed)	—	-9.8	51.0
<i>u3925</i>	H(29)...H(31)	592.7(73)	36.4(fixed)	—	-5.9	36.4
<i>u3698</i>	C(52)...H(82)	592.8(69)	26.5(fixed)	—	-2.9	26.5
<i>u3873</i>	F(261)...H(284)	592.9(97)	35.2(fixed)	—	-14.9	35.2
<i>u3796</i>	H(68)...H(80)	592.9(98)	38.9(fixed)	—	-0.3	38.9
<i>u3749</i>	C(253)...F(260)	593.0(22)	10.3(tied to <i>u3756</i> )	—	-2.0	12.9
<i>u3961</i>	H(225)...H(229)	593.0(91)	53.7(fixed)	—	-7.2	53.7
<i>u3858</i>	F(56)...H(81)	593.1(58)	24.9(fixed)	—	-1.2	24.9
<i>u3952</i>	F(97)...H(107)	593.4(118)	31.5(fixed)	—	-18.9	31.5
<i>u3951</i>	F(96)...H(103)	593.4(118)	31.8(fixed)	—	-18.9	31.8
<i>u3678</i>	C(218)...H(226)	593.5(133)	34.9(fixed)	—	-4.9	34.9
<i>u3711</i>	H(102)...H(116)	593.6(188)	62.7(fixed)	—	35.3	62.7
<i>u3700</i>	F(57)...H(75)	593.7(97)	26.4(fixed)	—	-3.5	26.4
<i>u3914</i>	C(218)...H(225)	593.8(68)	33.8(fixed)	—	-7.4	33.8
<i>u3939</i>	H(18)...H(31)	593.8(83)	47.2(fixed)	—	-2.8	47.2
<i>u3712</i>	H(110)...H(120)	593.8(188)	62.1(fixed)	—	35.4	62.1
<i>u3750</i>	C(254)...H(283)	593.8(43)	22.2(fixed)	—	-3.2	22.2
<i>u3674</i>	C(89)...H(116)	593.8(64)	31.5(fixed)	—	-1.5	31.5
<i>u3787</i>	C(217)...F(221)	594.1(20)	10.1(tied to <i>u3756</i> )	—	-2.0	12.5
<i>u4411</i>	H(149)...H(153)	594.1(252)	29.2(fixed)	—	-16.2	29.2
<i>u3937</i>	H(22)...H(32)	594.2(215)	37.0(fixed)	—	-3.9	37.0
<i>u3876</i>	C(12)...H(32)	594.4(65)	23.8(fixed)	—	-3.5	23.8
<i>u3783</i>	C(218)...H(228)	594.8(141)	31.7(fixed)	—	-6.2	31.7
<i>u3793</i>	C(12)...F(16)	594.9(20)	10.1(tied to <i>u3756</i> )	—	-2.1	12.6
<i>u3723</i>	C(132)...H(156)	594.9(139)	21.5(fixed)	—	-2.4	21.5
<i>u3883</i>	H(102)...H(117)	594.9(124)	70.3(fixed)	—	16.2	70.3
<i>u3884</i>	H(110)...H(118)	595.0(124)	70.2(fixed)	—	16.2	70.2

<i>u3803</i>	C(258)...H(269)	595.0(45)	21.7(fixed)	—	-3.5	21.7
<i>u3855</i>	H(62)...H(75)	595.1(412)	44.6(fixed)	—	-6.2	44.6
<i>u4012</i>	C(129)...H(164)	595.2(67)	31.7(fixed)	—	-4.6	31.7
<i>u3854</i>	H(73)...H(80)	595.2(98)	58.0(fixed)	—	-0.5	58.0
<i>u3777</i>	C(254)...F(263)	595.2(20)	12.7(fixed)	—	-2.0	12.7
<i>u1503</i>	C(129)...H(160)	595.3(141)	72.6(fixed)	—	6.1	72.6
<i>u2573</i>	F(263)...H(275)	595.3(131)	29.4(fixed)	—	3.1	29.4
<i>u3643</i>	C(254)...H(284)	595.3(35)	24.8(fixed)	—	-1.0	24.8
<i>u3769</i>	H(281)...H(287)	595.4(258)	36.6(fixed)	—	-2.1	36.6
<i>u3744</i>	C(175)...H(205)	595.7(48)	44.6(fixed)	—	-2.4	44.6
<i>u3785</i>	C(13)...H(23)	595.8(155)	27.7(fixed)	—	-4.8	27.7
<i>u3790</i>	C(258)...F(262)	595.9(20)	12.5(fixed)	—	-1.9	12.5
<i>u3928</i>	C(52)...H(61)	596.1(76)	23.9(fixed)	—	-6.1	23.9
<i>u3672</i>	C(13)...H(21)	596.1(146)	32.7(fixed)	—	-4.0	32.7
<i>u3862</i>	H(66)...H(72)	596.1(129)	69.9(fixed)	—	-5.0	69.9
<i>u3872</i>	C(131)...H(159)	596.1(123)	31.6(fixed)	—	-5.3	31.6
<i>u3819</i>	C(89)...H(115)	596.2(65)	23.8(fixed)	—	-3.3	23.8
<i>u3891</i>	C(48)...H(72)	596.2(73)	28.9(fixed)	—	-8.1	28.9
<i>u2424</i>	C(135)...H(142)	596.3(64)	40.1(fixed)	—	-1.9	40.1
<i>u3886</i>	C(214)...H(241)	596.6(99)	24.5(fixed)	—	-3.1	24.5
<i>u3743</i>	C(171)...H(191)	596.6(47)	44.6(fixed)	—	-2.4	44.6
<i>u3958</i>	H(70)...H(80)	596.8(78)	34.3(fixed)	—	-5.5	34.3
<i>u3847</i>	C(93)...H(123)	596.8(48)	26.4(fixed)	—	-3.4	26.4
<i>u3888</i>	H(268)...H(285)	596.9(94)	40.9(fixed)	—	-2.8	40.9
<i>u3812</i>	C(8)...H(37)	596.9(41)	22.1(fixed)	—	-2.5	22.1
<i>u3736</i>	C(8)...H(38)	597.2(30)	25.8(fixed)	—	-2.1	25.8
<i>u2658</i>	C(131)...H(155)	597.2(37)	40.5(fixed)	—	15.1	40.5
<i>u3829</i>	H(236)...H(246)	597.3(83)	39.8(fixed)	—	-2.5	39.8
<i>u3990</i>	F(222)...H(235)	597.4(63)	22.6(fixed)	—	-5.4	22.6
<i>u3900</i>	H(71)...H(81)	597.6(97)	40.1(fixed)	—	-13.4	40.1
<i>u3894</i>	C(10)...H(37)	597.7(155)	26.4(fixed)	—	-4.4	26.4
<i>u3999</i>	H(26)...H(38)	597.8(307)	75.0(fixed)	—	-6.5	75.0
<i>u3763</i>	C(93)...H(109)	597.9(87)	29.3(fixed)	—	2.6	29.3
<i>u3978</i>	F(220)...H(226)	598.0(73)	21.0(fixed)	—	-8.7	21.0
<i>u3841</i>	H(73)...H(82)	598.1(167)	66.7(fixed)	—	-4.8	66.7
<i>u3805</i>	H(224)...H(241)	598.1(257)	38.7(fixed)	—	-0.8	38.7
<i>u4101</i>	H(193)...H(196)	598.1(109)	60.2(fixed)	—	-30.1	60.2
<i>u3898</i>	C(9)...H(36)	598.2(111)	25.6(fixed)	—	-3.3	25.6
<i>u3903</i>	F(16)...H(41)	598.2(46)	18.8(fixed)	—	-5.9	18.8
<i>u3840</i>	C(257)...H(265)	598.4(99)	29.7(fixed)	—	-3.5	29.7
<i>u1108</i>	C(130)...H(162)	598.4(30)	45.7(fixed)	—	8.1	45.7
<i>u3882</i>	C(214)...H(243)	598.6(123)	27.3(fixed)	—	-3.6	27.3
<i>u4115</i>	C(130)...H(157)	598.7(114)	24.3(fixed)	—	-6.0	24.3
<i>u3913</i>	F(221)...H(246)	598.8(40)	18.2(fixed)	—	-5.3	18.2

<i>u3817</i>	F(55)...H(63)	598.9(107)	25.4(fixed)	—	-1.0	25.4
<i>u3168</i>	C(129)...H(162)	598.9(68)	38.0(fixed)	—	0.8	38.0
<i>u3770</i>	C(92)...H(109)	599.0(115)	48.4(fixed)	—	-3.4	48.4
<i>u4173</i>	H(226)...H(233)	599.0(96)	64.2(fixed)	—	-13.7	64.2
<i>u4159</i>	H(195)...H(201)	599.1(223)	57.0(fixed)	—	-23.9	57.0
<i>u3815</i>	C(213)...H(236)	599.1(39)	23.4(fixed)	—	-4.0	23.4
<i>u3874</i>	C(10)...H(38)	599.3(138)	32.7(fixed)	—	-4.1	32.7
<i>u3716</i>	F(222)...H(230)	599.4(85)	26.9(fixed)	—	-4.4	26.9
<i>u3921</i>	C(131)...H(161)	599.4(114)	27.2(fixed)	—	-5.0	27.2
<i>u3922</i>	H(35)...H(40)	599.5(204)	32.6(fixed)	—	-3.4	32.6
<i>u4061</i>	C(90)...H(101)	599.6(53)	48.6(fixed)	—	-31.6	48.6
<i>u4083</i>	H(225)...H(245)	599.6(82)	49.5(fixed)	—	-7.2	49.5
<i>u4060</i>	C(89)...H(109)	599.6(53)	47.8(fixed)	—	-31.7	47.8
<i>u3845</i>	C(8)...H(35)	599.7(120)	24.7(fixed)	—	-3.2	24.7
<i>u4015</i>	H(69)...H(74)	599.7(97)	58.4(fixed)	—	-6.6	58.4
<i>u3850</i>	H(19)...H(36)	599.7(267)	39.7(fixed)	—	-1.5	39.7
<i>u3889</i>	C(13)...H(20)	599.8(74)	32.9(fixed)	—	-6.3	32.9
<i>u4070</i>	C(171)...H(194)	599.8(59)	41.6(fixed)	—	-32.1	41.6
<i>u3949</i>	H(223)...H(241)	599.9(202)	33.4(fixed)	—	-5.2	33.4
<i>u3682</i>	C(7)...H(41)	600.0(81)	31.3(fixed)	—	-4.1	31.3
<i>u3665</i>	C(212)...H(246)	600.3(62)	30.7(fixed)	—	-3.9	30.7
<i>u3988</i>	H(267)...H(278)	600.3(106)	38.3(fixed)	—	-10.2	38.3
<i>u3932</i>	F(98)...H(123)	600.4(55)	19.0(fixed)	—	-7.4	19.0
<i>u3865</i>	C(218)...H(224)	600.4(69)	33.5(fixed)	—	-4.6	33.5
<i>u3909</i>	F(262)...H(287)	600.5(42)	20.8(fixed)	—	-7.3	20.8
<i>u3927</i>	H(269)...H(276)	600.5(258)	60.5(fixed)	—	-6.5	60.5
<i>u3979</i>	F(15)...H(40)	600.5(51)	23.9(fixed)	—	-1.7	23.9
<i>u3936</i>	F(17)...H(34)	600.6(124)	22.9(fixed)	—	-5.1	22.9
<i>u3919</i>	C(256)...H(285)	600.6(66)	30.2(fixed)	—	-5.2	30.2
<i>u3929</i>	F(14)...H(18)	600.7(53)	25.7(fixed)	—	0.1	25.7
<i>u3863</i>	C(12)...H(30)	601.0(82)	29.4(fixed)	—	-4.4	29.4
<i>u3838</i>	C(213)...H(242)	601.0(45)	22.5(fixed)	—	-2.6	22.5
<i>u3846</i>	F(15)...H(38)	601.1(95)	23.5(fixed)	—	-5.5	23.5
<i>u3775</i>	C(213)...H(243)	601.2(41)	26.5(fixed)	—	-2.5	26.5
<i>u3933</i>	C(255)...H(282)	601.3(108)	36.4(fixed)	—	-5.8	36.4
<i>u2786</i>	F(261)...H(275)	601.5(42)	30.2(fixed)	—	2.1	30.2
<i>u3950</i>	H(63)...H(80)	601.7(102)	38.3(fixed)	—	-1.9	38.3
<i>u3930</i>	F(219)...H(223)	601.8(49)	25.4(fixed)	—	0.9	25.4
<i>u3944</i>	H(141)...H(162)	601.9(83)	36.5(fixed)	—	-2.6	36.5
<i>u3902</i>	F(55)...H(60)	601.9(54)	26.7(fixed)	—	-9.2	26.7
<i>u3947</i>	H(111)...H(117)	602.1(217)	38.1(fixed)	—	-11.3	38.1
<i>u3948</i>	H(100)...H(118)	602.1(217)	37.9(fixed)	—	-11.3	37.9
<i>u3864</i>	C(93)...H(121)	602.2(44)	24.1(fixed)	—	-4.0	24.1
<i>u3818</i>	C(49)...H(77)	602.2(129)	36.3(fixed)	—	-5.3	36.3

<i>u4158</i>	H(184)...H(188)	602.4(216)	56.9(fixed)	—	-23.9	56.9
<i>u3924</i>	H(281)...H(286)	602.4(202)	32.2(fixed)	—	-4.2	32.2
<i>u3810</i>	C(8)...H(34)	602.4(115)	27.4(fixed)	—	-3.3	27.4
<i>u4276</i>	H(23)...H(28)	602.4(82)	64.5(fixed)	—	-17.0	64.5
<i>u3994</i>	C(216)...H(233)	602.5(42)	24.8(fixed)	—	-11.4	24.8
<i>u3942</i>	F(261)...H(286)	602.5(49)	25.2(fixed)	—	-1.1	25.2
<i>u1902</i>	F(137)...H(153)	602.5(34)	41.9(fixed)	—	-9.0	41.9
<i>u3887</i>	C(9)...H(38)	602.7(123)	28.4(fixed)	—	-3.8	28.4
<i>u3946</i>	F(222)...H(239)	602.7(70)	18.4(fixed)	—	-6.1	18.4
<i>u3985</i>	F(220)...H(224)	602.9(45)	24.6(fixed)	—	-10.4	24.6
<i>u3852</i>	F(260)...H(268)	602.9(108)	27.7(fixed)	—	1.1	27.7
<i>u3912</i>	F(138)...H(161)	603.0(61)	28.1(fixed)	—	-10.6	28.1
<i>u3986</i>	H(18)...H(36)	603.0(209)	33.9(fixed)	—	-4.7	33.9
<i>u3791</i>	H(64)...H(77)	603.0(190)	53.3(fixed)	—	-0.1	53.3
<i>u3881</i>	C(256)...H(287)	603.2(71)	33.6(fixed)	—	-4.4	33.6
<i>u3972</i>	H(236)...H(245)	603.4(64)	34.7(fixed)	—	-3.9	34.7
<i>u4071</i>	C(175)...H(183)	603.4(43)	41.4(fixed)	—	-32.1	41.4
<i>u3935</i>	C(257)...H(266)	603.5(67)	25.6(fixed)	—	-5.1	25.6
<i>u3904</i>	F(219)...H(226)	603.6(97)	24.4(fixed)	—	-8.4	24.4
<i>u3004</i>	H(144)...H(151)	603.7(93)	49.4(fixed)	—	13.0	49.4
<i>u3976</i>	H(267)...H(280)	603.7(399)	48.6(fixed)	—	-9.0	48.6
<i>u3920</i>	F(56)...H(79)	604.2(105)	35.6(fixed)	—	-12.6	35.6
<i>u3992</i>	H(18)...H(30)	604.5(139)	55.8(fixed)	—	-6.2	55.8
<i>u3965</i>	H(269)...H(277)	604.9(234)	54.7(fixed)	—	-4.3	54.7
<i>u2750</i>	C(130)...H(158)	605.1(123)	33.6(fixed)	—	3.9	33.6
<i>u4214</i>	H(182)...H(205)	605.1(81)	103.1(fixed)	—	-29.5	103.1
<i>u3931</i>	F(260)...H(265)	605.3(48)	22.5(fixed)	—	-8.6	22.5
<i>u2564</i>	F(261)...H(272)	605.3(47)	48.6(fixed)	—	20.1	48.6
<i>u3975</i>	C(10)...H(39)	605.4(80)	27.2(fixed)	—	-3.8	27.2
<i>u3911</i>	F(14)...H(21)	605.6(103)	22.7(fixed)	—	-6.4	22.7
<i>u4043</i>	H(20)...H(40)	605.6(91)	48.9(fixed)	—	-5.9	48.9
<i>u3868</i>	F(99)...H(117)	605.7(115)	25.9(fixed)	—	-1.3	25.9
<i>u3908</i>	H(269)...H(282)	606.0(177)	57.1(fixed)	—	-3.5	57.1
<i>u3923</i>	C(88)...H(117)	606.1(120)	24.4(fixed)	—	-3.0	24.4
<i>u3907</i>	F(15)...H(39)	606.2(46)	27.4(fixed)	—	-1.4	27.4
<i>u4586</i>	H(273)...H(281)	606.5(128)	25.3(fixed)	—	-6.0	25.3
<i>u4020</i>	F(58)...H(68)	606.9(66)	24.7(fixed)	—	-13.1	24.7
<i>u2733</i>	C(258)...H(272)	607.0(32)	70.9(fixed)	—	25.6	70.9
<i>u4025</i>	H(104)...H(115)	607.0(178)	70.6(fixed)	—	-8.2	70.6
<i>u3733</i>	H(274)...H(277)	607.0(88)	40.8(fixed)	—	-0.9	40.8
<i>u3630</i>	C(216)...H(232)	607.0(56)	40.2(fixed)	—	-2.1	40.2
<i>u3982</i>	F(57)...H(60)	607.0(66)	21.9(fixed)	—	-9.5	21.9
<i>u3918</i>	C(13)...H(19)	607.1(85)	31.9(fixed)	—	-4.8	31.9
<i>u3857</i>	H(101)...H(118)	607.1(287)	41.1(fixed)	—	0.8	41.1

<i>u3917</i>	F(14)...H(20)	607.5(45)	30.0(fixed)	—	-1.1	30.0
<i>u3851</i>	C(254)...H(281)	608.0(116)	24.2(fixed)	—	-3.3	24.2
<i>u4156</i>	H(27)...H(37)	608.1(98)	46.7(fixed)	—	-27.2	46.7
<i>u4352</i>	F(138)...H(164)	608.3(33)	16.0(fixed)	—	-5.7	16.0
<i>u3724</i>	C(253)...H(272)	608.3(57)	24.3(fixed)	—	3.5	24.3
<i>u4010</i>	F(17)...H(31)	608.7(43)	27.1(fixed)	—	-2.5	27.1
<i>u4006</i>	C(256)...H(267)	608.7(120)	27.8(fixed)	—	-11.3	27.8
<i>u3934</i>	C(49)...H(79)	608.9(114)	29.9(fixed)	—	-7.5	29.9
<i>u2044</i>	F(137)...H(157)	609.1(62)	36.6(fixed)	—	-3.5	36.6
<i>u3893</i>	C(217)...H(240)	609.5(117)	24.2(fixed)	—	-3.1	24.2
<i>u4022</i>	F(56)...H(80)	609.8(45)	25.6(fixed)	—	-2.4	25.6
<i>u3953</i>	F(221)...H(242)	609.8(115)	25.5(fixed)	—	-1.6	25.5
<i>u3895</i>	H(76)...H(82)	609.9(264)	40.9(fixed)	—	-3.8	40.9
<i>u4033</i>	H(109)...H(114)	609.9(185)	70.5(fixed)	—	-11.8	70.5
<i>u3993</i>	F(261)...H(285)	610.0(44)	27.1(fixed)	—	-1.8	27.1
<i>u3752</i>	H(234)...H(241)	610.1(158)	63.3(fixed)	—	9.1	63.3
<i>u3941</i>	F(221)...H(241)	610.2(119)	24.5(fixed)	—	-1.2	24.5
<i>u4026</i>	H(278)...H(285)	610.3(82)	41.9(fixed)	—	-4.2	41.9
<i>u3956</i>	F(16)...H(36)	610.6(117)	24.2(fixed)	—	-1.2	24.2
<i>u3967</i>	H(231)...H(243)	610.6(309)	57.5(fixed)	—	-4.4	57.5
<i>u4213</i>	H(183)...H(204)	611.0(138)	102.9(fixed)	—	-29.5	102.9
<i>u4013</i>	C(255)...H(284)	611.0(117)	30.9(fixed)	—	-7.5	30.9
<i>u3989</i>	F(219)...H(225)	611.3(44)	29.9(fixed)	—	-0.8	29.9
<i>u4296</i>	H(228)...H(233)	611.5(87)	52.9(fixed)	—	-14.5	52.9
<i>u4017</i>	F(98)...H(119)	611.6(120)	28.5(fixed)	—	-3.8	28.5
<i>u4031</i>	F(97)...H(110)	611.7(48)	50.3(fixed)	—	3.6	50.3
<i>u4030</i>	F(96)...H(102)	611.7(48)	50.2(fixed)	—	3.6	50.2
<i>u4005</i>	C(10)...H(19)	611.7(67)	30.4(fixed)	—	-9.4	30.4
<i>u3996</i>	F(180)...H(198)	611.7(64)	22.1(fixed)	—	-8.8	22.1
<i>u4052</i>	H(25)...H(33)	611.8(100)	40.4(fixed)	—	-20.5	40.4
<i>u4047</i>	C(10)...H(41)	612.0(78)	31.9(fixed)	—	-4.4	31.9
<i>u3968</i>	C(7)...H(27)	612.0(44)	69.6(fixed)	—	-22.3	69.6
<i>u3966</i>	F(16)...H(37)	612.0(114)	25.4(fixed)	—	-1.7	25.4
<i>u4063</i>	H(187)...H(191)	612.1(238)	73.0(fixed)	—	-12.7	73.0
<i>u4457</i>	H(270)...H(280)	612.1(116)	58.7(fixed)	—	-25.5	58.7
<i>u3973</i>	H(76)...H(81)	612.2(200)	34.5(fixed)	—	-4.2	34.5
<i>u4003</i>	C(91)...H(120)	612.3(139)	32.3(fixed)	—	-4.3	32.3
<i>u4004</i>	H(62)...H(74)	612.5(142)	38.9(fixed)	—	-7.5	38.9
<i>u3532</i>	H(143)...H(147)	612.5(80)	35.1(fixed)	—	-0.4	35.1
<i>u3964</i>	H(230)...H(239)	612.5(365)	46.7(fixed)	—	-10.2	46.7
<i>u3859</i>	H(229)...H(235)	612.6(253)	62.4(fixed)	—	-5.2	62.4
<i>u4049</i>	H(65)...H(72)	613.0(103)	57.3(fixed)	—	-7.3	57.3
<i>u4000</i>	C(54)...H(71)	613.0(73)	30.1(fixed)	—	-14.5	30.1
<i>u4513</i>	C(257)...H(273)	613.0(27)	15.9(fixed)	—	-5.6	15.9

<i>u3580</i>	H(146)...H(151)	613.3(81)	38.4(fixed)	—	0.8	38.4
<i>u3910</i>	F(262)...H(282)	613.4(112)	30.5(fixed)	—	3.5	30.5
<i>u3867</i>	C(254)...H(280)	613.4(110)	28.0(fixed)	—	-3.7	28.0
<i>u3781</i>	H(29)...H(36)	613.6(173)	79.0(fixed)	—	13.5	79.0
<i>u4027</i>	H(64)...H(75)	613.6(141)	40.8(fixed)	—	-7.9	40.8
<i>u4148</i>	H(232)...H(242)	613.6(56)	43.4(fixed)	—	-21.1	43.4
<i>u3890</i>	F(96)...H(100)	613.7(62)	36.9(fixed)	—	12.7	36.9
<i>u4064</i>	H(194)...H(201)	614.0(240)	73.1(fixed)	—	-12.7	73.1
<i>u4121</i>	H(26)...H(37)	614.5(161)	59.3(fixed)	—	-7.4	59.3
<i>u4092</i>	H(32)...H(39)	614.5(97)	35.9(fixed)	—	-2.7	35.9
<i>u4304</i>	H(101)...H(115)	614.7(145)	44.1(fixed)	—	-34.2	44.1
<i>u3901</i>	H(229)...H(236)	614.8(227)	54.9(fixed)	—	-2.7	54.9
<i>u4303</i>	H(109)...H(119)	614.8(144)	42.7(fixed)	—	-34.2	42.7
<i>u3983</i>	F(58)...H(66)	614.9(61)	19.0(fixed)	—	-6.9	19.0
<i>u3984</i>	C(259)...H(268)	614.9(99)	29.0(fixed)	—	-4.6	29.0
<i>u2952</i>	H(266)...H(270)	615.1(90)	59.2(fixed)	—	26.9	59.2
<i>u4196</i>	C(12)...H(27)	615.2(59)	31.2(fixed)	—	-27.2	31.2
<i>u4434</i>	H(141)...H(164)	615.5(130)	31.9(fixed)	—	-6.9	31.9
<i>u4055</i>	H(187)...H(189)	615.6(70)	51.1(fixed)	—	-10.9	51.1
<i>u4018</i>	H(60)...H(74)	615.7(265)	45.1(fixed)	—	-5.5	45.1
<i>u3995</i>	F(178)...H(185)	615.8(57)	22.1(fixed)	—	-8.8	22.1
<i>u3885</i>	H(24)...H(35)	616.0(86)	70.5(fixed)	—	2.3	70.5
<i>u4129</i>	H(111)...H(120)	616.3(187)	115.6(fixed)	—	-6.6	115.6
<i>u4130</i>	H(100)...H(116)	616.4(187)	115.4(fixed)	—	-6.6	115.4
<i>u3991</i>	F(57)...H(62)	616.4(63)	19.1(fixed)	—	-6.5	19.1
<i>u3963</i>	C(217)...H(239)	616.7(100)	24.8(fixed)	—	-3.3	24.8
<i>u4056</i>	H(269)...H(280)	616.8(118)	49.2(fixed)	—	-11.5	49.2
<i>u4135</i>	H(61)...H(74)	616.8(232)	40.6(fixed)	—	-7.1	40.6
<i>u3997</i>	H(230)...H(237)	616.9(56)	36.3(fixed)	—	-10.7	36.3
<i>u3816</i>	H(234)...H(243)	617.2(161)	78.9(fixed)	—	3.0	78.9
<i>u4011</i>	F(262)...H(283)	617.4(116)	33.2(fixed)	—	0.4	33.2
<i>u3970</i>	H(111)...H(118)	617.7(188)	81.3(fixed)	—	8.0	81.3
<i>u4093</i>	C(11)...H(25)	618.1(98)	31.0(fixed)	—	-20.7	31.0
<i>u4117</i>	H(64)...H(72)	618.1(228)	44.4(fixed)	—	-9.1	44.4
<i>u4095</i>	C(132)...H(164)	618.2(46)	20.4(fixed)	—	-5.4	20.4
<i>u4079</i>	H(64)...H(71)	618.3(262)	48.4(fixed)	—	-7.8	48.4
<i>u4182</i>	C(217)...H(232)	618.6(44)	29.8(fixed)	—	-21.7	29.8
<i>u4007</i>	H(65)...H(77)	618.6(82)	53.4(fixed)	—	-4.6	53.4
<i>u4166</i>	H(187)...H(188)	618.8(259)	51.5(fixed)	—	-12.4	51.5
<i>u4023</i>	F(55)...H(64)	618.8(121)	24.8(fixed)	—	-2.5	24.8
<i>u4014</i>	C(54)...H(63)	619.0(103)	25.6(fixed)	—	-3.2	25.6
<i>u3981</i>	F(260)...H(269)	619.3(122)	30.8(fixed)	—	-0.8	30.8
<i>u4090</i>	H(223)...H(246)	619.7(86)	38.7(fixed)	—	0.3	38.7
<i>u3828</i>	H(29)...H(38)	620.2(157)	99.1(fixed)	—	5.0	99.1

<i>u3957</i>	H(229)...H(239)	620.6(75)	52.4(fixed)	—	-10.9	52.4
<i>u4075</i>	C(52)...H(68)	620.7(46)	25.9(fixed)	—	-14.1	25.9
<i>u4266</i>	C(93)...H(101)	620.8(84)	32.0(fixed)	—	-30.6	32.0
<i>u4267</i>	C(94)...H(109)	620.9(84)	30.7(fixed)	—	-30.7	30.7
<i>u4274</i>	H(233)...H(238)	621.2(212)	41.1(fixed)	—	-14.4	41.1
<i>u4035</i>	C(252)...C(256)	621.3(40)	13.2(tied to <i>u4053</i> )	—	-2.0	12.8
<i>u3312</i>	H(149)...H(155)	621.3(196)	46.7(fixed)	—	10.5	46.7
<i>u4187</i>	H(106)...H(114)	621.4(166)	56.5(fixed)	—	-14.5	56.5
<i>u4102</i>	H(64)...H(74)	621.4(269)	34.4(fixed)	—	-7.8	34.4
<i>u4077</i>	C(213)...H(224)	621.5(43)	23.0(fixed)	—	-11.2	23.0
<i>u4228</i>	H(144)...H(156)	621.6(117)	39.7(fixed)	—	-8.4	39.7
<i>u3827</i>	H(116)...H(120)	621.8(411)	45.8(fixed)	—	-5.8	45.8
<i>u4097</i>	H(113)...H(119)	622.1(219)	35.9(fixed)	—	-4.2	35.9
<i>u4145</i>	H(224)...H(245)	622.1(131)	44.0(fixed)	—	-7.6	44.0
<i>u4127</i>	H(59)...H(70)	622.2(104)	40.9(fixed)	—	-9.2	40.9
<i>u3620</i>	C(129)...H(153)	622.5(46)	24.1(fixed)	—	-0.8	24.1
<i>u4078</i>	C(8)...H(19)	622.7(45)	21.8(fixed)	—	-9.6	21.8
<i>u3853</i>	H(198)...H(202)	622.8(425)	45.3(fixed)	—	-5.8	45.3
<i>u4021</i>	C(215)...H(230)	622.8(84)	25.5(fixed)	—	-11.6	25.5
<i>u4028</i>	C(92)...C(95)	623.1(41)	13.3(tied to <i>u4053</i> )	—	-2.2	12.9
<i>u4045</i>	C(47)...C(51)	623.1(41)	13.3(tied to <i>u4053</i> )	—	-1.7	12.9
<i>u4046</i>	C(170)...C(173)	623.4(41)	14.4(tied to <i>u4053</i> )	—	-2.5	14.0
<i>u4087</i>	H(231)...H(242)	623.8(154)	45.7(fixed)	—	-5.3	45.7
<i>u4036</i>	C(214)...C(215)	623.8(41)	12.9(tied to <i>u4053</i> )	—	-1.8	12.5
<i>u4099</i>	C(10)...H(21)	623.8(88)	20.5(fixed)	—	-7.0	20.5
<i>u3980</i>	C(212)...H(232)	623.8(46)	53.4(fixed)	—	-17.1	53.4
<i>u4058</i>	H(73)...H(79)	624.6(157)	56.8(fixed)	—	-12.5	56.8
<i>u3940</i>	H(24)...H(34)	625.1(360)	80.8(fixed)	—	-4.9	80.8
<i>u4118</i>	H(116)...H(122)	625.7(145)	36.1(fixed)	—	-4.1	36.1
<i>u4294</i>	H(275)...H(284)	625.8(129)	42.0(fixed)	—	-11.0	42.0
<i>u4081</i>	C(9)...H(30)	625.9(44)	19.7(fixed)	—	-5.1	19.7
<i>u4098</i>	H(276)...H(286)	625.9(86)	40.1(fixed)	—	-3.0	40.1
<i>u4231</i>	H(73)...H(78)	626.1(140)	45.8(fixed)	—	-12.7	45.8
<i>u4116</i>	H(18)...H(41)	626.3(98)	38.4(fixed)	—	-1.6	38.4
<i>u4089</i>	C(47)...H(75)	626.4(133)	21.7(fixed)	—	-5.7	21.7
<i>u4104</i>	H(278)...H(287)	627.0(132)	42.9(fixed)	—	-5.9	42.9
<i>u4183</i>	H(112)...H(119)	627.0(240)	37.8(fixed)	—	-5.7	37.8
<i>u4136</i>	H(268)...H(286)	627.0(156)	45.2(fixed)	—	-4.0	45.2
<i>u4080</i>	C(49)...H(71)	627.3(53)	28.5(fixed)	—	-13.9	28.5
<i>u4318</i>	H(183)...H(205)	627.6(137)	52.0(fixed)	—	-30.9	52.0
<i>u4188</i>	H(19)...H(40)	628.1(147)	43.8(fixed)	—	-7.4	43.8
<i>u4040</i>	C(255)...C(257)	628.2(12)	13.1(tied to <i>u4053</i> )	—	-2.1	12.7
<i>u4024</i>	C(216)...C(218)	628.3(12)	13.3(tied to <i>u4053</i> )	—	-2.1	12.9
<i>u4042</i>	C(9)...C(11)	628.3(11)	13.1(tied to <i>u4053</i> )	—	-2.0	12.7

<i>u</i> 3427	C(258)...H(270)	628.5(40)	87.4(fixed)	—	0.0	87.4
<i>u</i> 4069	C(177)...H(198)	628.5(98)	29.3(fixed)	—	-8.2	29.3
<i>u</i> 4048	C(255)...H(276)	628.5(47)	20.4(fixed)	—	-5.4	20.4
<i>u</i> 4155	H(266)...H(279)	628.6(219)	39.1(fixed)	—	-5.6	39.1
<i>u</i> 4164	H(106)...H(112)	628.6(211)	68.6(fixed)	—	-19.5	68.6
<i>u</i> 3693	C(130)...H(150)	628.6(43)	36.3(fixed)	—	-7.8	36.3
<i>u</i> 4243	H(30)...H(40)	628.8(116)	35.9(fixed)	—	-2.9	35.9
<i>u</i> 4086	C(51)...H(62)	628.9(130)	23.5(fixed)	—	-6.0	23.5
<i>u</i> 4044	C(50)...C(53)	628.9(12)	13.0(tied to <i>u</i> 4053)	—	-1.8	12.6
<i>u</i> 4072	H(229)...H(238)	628.9(255)	43.6(fixed)	—	-9.8	43.6
<i>u</i> 4059	C(259)...H(267)	629.0(109)	27.6(fixed)	—	-4.7	27.6
<i>u</i> 4141	H(269)...H(279)	629.2(249)	39.5(fixed)	—	-9.4	39.5
<i>u</i> 4184	H(59)...H(75)	629.2(143)	32.3(fixed)	—	-2.7	32.3
<i>u</i> 4088	H(240)...H(242)	629.2(74)	36.6(fixed)	—	-3.1	36.6
<i>u</i> 4084	H(71)...H(79)	629.2(185)	56.8(fixed)	—	-13.1	56.8
<i>u</i> 4082	C(50)...H(82)	629.7(47)	19.8(fixed)	—	-5.1	19.8
<i>u</i> 4153	H(267)...H(279)	629.7(100)	38.2(fixed)	—	-9.2	38.2
<i>u</i> 4126	H(230)...H(238)	629.8(52)	40.6(fixed)	—	-10.7	40.6
<i>u</i> 4096	H(103)...H(123)	629.9(211)	51.5(fixed)	—	-13.2	51.5
<i>u</i> 4146	C(252)...H(278)	629.9(66)	23.9(fixed)	—	-0.9	23.9
<i>u</i> 4034	C(171)...C(175)	630.0(33)	13.9(tied to <i>u</i> 4053)	—	-5.1	13.5
<i>u</i> 4085	C(218)...H(235)	630.3(44)	20.4(fixed)	—	-5.5	20.4
<i>u</i> 4111	C(48)...H(79)	630.3(48)	24.6(fixed)	—	-15.1	24.6
<i>u</i> 4143	H(196)...H(202)	630.4(141)	61.2(fixed)	—	4.9	61.2
<i>u</i> 1446	C(129)...C(134)	630.6(11)	22.5(tied to <i>u</i> 4053)	—	1.9	21.8
<i>u</i> 4200	H(103)...H(122)	630.9(187)	40.8(fixed)	—	-11.9	40.8
<i>u</i> 4051	C(89)...C(90)	631.2(33)	13.3(tied to <i>u</i> 4053)	—	-3.9	12.9
<i>u</i> 4065	C(95)...H(116)	631.3(101)	26.6(fixed)	—	-5.8	26.6
<i>u</i> 1402	H(150)...H(155)	631.4(90)	66.6(fixed)	—	19.1	66.6
<i>u</i> 4140	C(94)...H(107)	631.5(67)	29.2(fixed)	—	-20.3	29.2
<i>u</i> 4139	C(93)...H(103)	631.5(67)	29.5(fixed)	—	-20.3	29.5
<i>u</i> 4138	C(214)...H(237)	631.7(65)	24.1(fixed)	—	-1.0	24.1
<i>u</i> 4037	C(212)...C(213)	631.9(35)	13.3(tied to <i>u</i> 4053)	—	-1.8	12.9
<i>u</i> 4054	H(198)...H(201)	632.0(226)	51.1(fixed)	—	-10.9	51.1
<i>u</i> 2641	H(146)...H(158)	632.2(87)	45.8(fixed)	—	11.7	45.8
<i>u</i> 4258	H(223)...H(237)	632.3(88)	33.5(fixed)	—	-6.5	33.5
<i>u</i> 4068	C(173)...H(185)	632.5(90)	29.3(fixed)	—	-8.2	29.3
<i>u</i> 4053	C(7)...C(8)	632.6(34)	13.0(31)	—	-1.8	12.6
<i>u</i> 4152	H(63)...H(81)	632.8(160)	36.3(fixed)	—	-2.8	36.3
<i>u</i> 4160	C(253)...H(284)	632.9(52)	26.3(fixed)	—	-16.5	26.3
<i>u</i> 4039	C(49)...C(52)	633.0(35)	13.2(tied to <i>u</i> 4053)	—	-2.1	12.8
<i>u</i> 4103	C(252)...H(280)	633.3(131)	23.0(fixed)	—	-4.9	23.0
<i>u</i> 4108	C(211)...H(246)	633.5(59)	26.1(fixed)	—	-5.8	26.1
<i>u</i> 4122	C(12)...H(25)	633.6(66)	36.9(fixed)	—	-18.9	36.9



<i>u3971</i>	H(232)...H(238)	633.8(233)	61.5(fixed)	—	-6.6	61.5
<i>u3751</i>	H(268)...H(272)	634.0(239)	53.6(fixed)	—	8.7	53.6
<i>u4163</i>	H(240)...H(245)	634.3(83)	34.8(fixed)	—	1.5	34.8
<i>u3508</i>	H(272)...H(283)	634.5(56)	74.7(fixed)	—	12.3	74.7
<i>u3642</i>	C(131)...H(142)	634.7(43)	25.7(fixed)	—	-2.8	25.7
<i>u4154</i>	C(54)...H(62)	634.7(111)	26.9(fixed)	—	-4.0	26.9
<i>u4128</i>	H(265)...H(279)	634.7(238)	40.8(fixed)	—	-6.1	40.8
<i>u4217</i>	C(92)...H(122)	634.8(63)	24.4(fixed)	—	-1.4	24.4
<i>u4157</i>	H(264)...H(280)	634.9(134)	31.9(fixed)	—	-1.5	31.9
<i>u4229</i>	H(266)...H(278)	635.1(86)	34.8(fixed)	—	2.9	34.8
<i>u4180</i>	H(62)...H(73)	635.4(137)	35.5(fixed)	—	-0.3	35.5
<i>u4113</i>	C(88)...H(123)	635.6(90)	28.4(fixed)	—	-7.3	28.4
<i>u4283</i>	H(278)...H(283)	635.8(138)	38.9(fixed)	—	-10.5	38.9
<i>u4062</i>	H(116)...H(119)	635.9(225)	39.7(fixed)	—	-7.6	39.7
<i>u1473</i>	C(130)...C(131)	636.1(34)	24.5(tied to <i>u4053</i> )	—	1.2	23.8
<i>u4176</i>	C(216)...H(245)	636.1(42)	25.1(fixed)	—	-1.2	25.1
<i>u4308</i>	H(233)...H(237)	636.1(76)	43.6(fixed)	—	6.0	43.6
<i>u4583</i>	H(273)...H(279)	636.1(202)	26.1(fixed)	—	-5.4	26.1
<i>u4171</i>	C(51)...H(59)	636.8(71)	26.0(fixed)	—	1.1	26.0
<i>u4137</i>	C(259)...H(276)	636.9(59)	27.8(fixed)	—	-6.3	27.8
<i>u4306</i>	H(32)...H(41)	637.4(133)	35.9(fixed)	—	-5.5	35.9
<i>u4202</i>	H(115)...H(119)	637.8(299)	29.4(fixed)	—	-7.7	29.4
<i>u4124</i>	C(211)...H(243)	638.1(66)	20.5(fixed)	—	-5.9	20.5
<i>u4106</i>	C(259)...H(280)	638.3(65)	20.6(fixed)	—	-5.8	20.6
<i>u4275</i>	H(60)...H(70)	638.4(89)	49.2(fixed)	—	-12.5	49.2
<i>u4272</i>	H(65)...H(79)	638.5(344)	40.9(fixed)	—	-11.4	40.9
<i>u4191</i>	H(59)...H(68)	638.5(110)	48.2(fixed)	—	-10.6	48.2
<i>u4348</i>	H(270)...H(281)	638.5(82)	65.4(fixed)	—	-17.3	65.4
<i>u4168</i>	H(100)...H(123)	638.6(134)	61.1(fixed)	—	9.2	61.1
<i>u4169</i>	H(111)...H(112)	638.8(134)	60.8(fixed)	—	9.3	60.8
<i>u4410</i>	H(101)...H(108)	638.8(47)	42.6(fixed)	—	-37.2	42.6
<i>u4134</i>	C(6)...H(41)	639.1(68)	26.4(fixed)	—	-6.5	26.4
<i>u4215</i>	C(256)...H(264)	639.4(63)	24.8(fixed)	—	-0.3	24.8
<i>u4199</i>	C(88)...H(120)	639.7(74)	23.2(fixed)	—	-8.9	23.2
<i>u4105</i>	C(13)...H(34)	639.8(60)	19.8(fixed)	—	-5.3	19.8
<i>u4235</i>	H(113)...H(122)	639.9(73)	35.6(fixed)	—	0.9	35.6
<i>u4320</i>	C(215)...H(233)	640.0(62)	35.7(fixed)	—	-0.4	35.7
<i>u4186</i>	C(47)...H(73)	640.0(70)	28.4(fixed)	—	3.0	28.4
<i>u4125</i>	C(54)...H(75)	640.5(78)	22.1(fixed)	—	-6.6	22.1
<i>u4112</i>	C(218)...H(240)	640.5(93)	25.1(fixed)	—	-1.0	25.1
<i>u4342</i>	H(71)...H(78)	640.6(169)	45.8(fixed)	—	-18.9	45.8
<i>u4203</i>	H(228)...H(231)	640.7(95)	38.8(fixed)	—	5.8	38.8
<i>u4131</i>	H(146)...H(157)	640.7(347)	34.3(fixed)	—	-0.5	34.3
<i>u4174</i>	C(255)...H(281)	640.7(96)	24.8(fixed)	—	-1.3	24.8

<i>u4234</i>	C(256)...H(266)	640.7(62)	27.2(fixed)	—	-0.9	27.2
<i>u4091</i>	C(53)...H(66)	640.8(103)	26.3(fixed)	—	-6.2	26.3
<i>u2857</i>	H(274)...H(283)	641.1(207)	48.1(fixed)	—	14.6	48.1
<i>u4167</i>	C(212)...H(231)	641.1(111)	27.7(fixed)	—	0.6	27.7
<i>u2259</i>	H(141)...H(160)	641.2(132)	75.7(fixed)	—	-0.9	75.7
<i>u4185</i>	C(254)...H(267)	641.2(65)	23.5(fixed)	—	-11.0	23.5
<i>u4142</i>	H(182)...H(189)	641.2(68)	61.1(fixed)	—	4.9	61.1
<i>u4100</i>	C(214)...H(239)	641.4(96)	23.0(fixed)	—	-5.8	23.0
<i>u4133</i>	C(175)...H(186)	641.7(114)	25.5(fixed)	—	-5.3	25.5
<i>u4361</i>	H(189)...H(205)	641.8(78)	45.2(fixed)	—	-33.2	45.2
<i>u3330</i>	H(141)...H(161)	641.8(118)	43.7(fixed)	—	-13.9	43.7
<i>u4161</i>	C(6)...H(38)	641.9(64)	20.5(fixed)	—	-6.2	20.5
<i>u4094</i>	H(66)...H(78)	642.0(103)	37.2(fixed)	—	2.2	37.2
<i>u4277</i>	H(18)...H(33)	642.1(125)	32.4(fixed)	—	-6.5	32.4
<i>u4190</i>	C(53)...H(70)	642.3(46)	26.8(fixed)	—	2.7	26.8
<i>u4259</i>	C(13)...H(30)	642.7(73)	26.7(fixed)	—	-5.8	26.7
<i>u4170</i>	C(92)...H(121)	642.9(60)	26.7(fixed)	—	-1.8	26.7
<i>u4386</i>	H(105)...H(109)	643.1(94)	59.7(fixed)	—	-33.6	59.7
<i>u4223</i>	C(254)...H(265)	643.4(54)	23.0(fixed)	—	-8.4	23.0
<i>u4220</i>	C(47)...H(72)	643.6(64)	34.1(fixed)	—	0.3	34.1
<i>u4381</i>	H(183)...H(199)	643.6(67)	39.5(fixed)	—	-36.1	39.5
<i>u4147</i>	C(49)...H(76)	643.7(117)	25.0(fixed)	—	-1.3	25.0
<i>u4227</i>	C(9)...H(35)	643.8(102)	24.5(fixed)	—	-1.4	24.5
<i>u3442</i>	C(252)...H(270)	643.8(58)	49.6(fixed)	—	14.0	49.6
<i>u4382</i>	H(191)...H(200)	643.8(67)	37.5(fixed)	—	-36.1	37.5
<i>u4239</i>	H(186)...H(197)	643.9(91)	36.7(fixed)	—	-3.9	36.7
<i>u4201</i>	C(213)...H(228)	644.1(118)	27.7(fixed)	—	-0.3	27.7
<i>u4204</i>	H(276)...H(284)	644.1(176)	52.9(fixed)	—	-10.8	52.9
<i>u4293</i>	H(18)...H(34)	644.2(129)	40.1(fixed)	—	-9.0	40.1
<i>u4270</i>	C(51)...H(61)	644.4(63)	28.5(fixed)	—	-0.7	28.5
<i>u4260</i>	C(214)...H(236)	644.4(62)	25.3(fixed)	—	-1.6	25.3
<i>u4250</i>	H(19)...H(34)	644.6(190)	42.7(fixed)	—	-7.8	42.7
<i>u2155</i>	C(131)...H(146)	644.6(119)	50.5(fixed)	—	-6.9	50.5
<i>u4233</i>	H(65)...H(76)	644.6(104)	35.5(fixed)	—	1.2	35.5
<i>u1744</i>	H(146)...H(149)	644.7(81)	73.5(fixed)	—	-1.3	73.5
<i>u4132</i>	C(171)...H(199)	644.8(122)	25.5(fixed)	—	-5.3	25.5
<i>u4211</i>	H(59)...H(72)	645.1(93)	42.4(fixed)	—	8.4	42.4
<i>u4175</i>	C(217)...H(230)	645.3(70)	26.5(fixed)	—	-11.0	26.5
<i>u4179</i>	C(174)...H(204)	645.3(62)	32.8(fixed)	—	9.9	32.8
<i>u2974</i>	C(258)...H(274)	645.4(130)	36.0(fixed)	—	2.9	36.0
<i>u4314</i>	H(60)...H(68)	645.5(126)	43.9(fixed)	—	-13.7	43.9
<i>u4242</i>	H(278)...H(284)	645.6(128)	42.5(fixed)	—	-10.0	42.5
<i>u4257</i>	C(252)...H(277)	645.6(59)	26.5(fixed)	—	-2.2	26.5
<i>u4178</i>	C(170)...H(193)	645.7(64)	33.2(fixed)	—	9.9	33.2

<i>u4119</i>	C(215)...H(234)	645.8(66)	32.7(fixed)	—	7.2	32.7
<i>u3076</i>	H(272)...H(284)	645.8(36)	82.3(fixed)	—	28.8	82.3
<i>u4281</i>	H(228)...H(245)	645.8(134)	33.0(fixed)	—	-7.3	33.0
<i>u4263</i>	C(173)...H(184)	645.8(61)	49.1(fixed)	—	4.7	49.1
<i>u4195</i>	C(9)...H(33)	646.0(119)	25.5(fixed)	—	-1.6	25.5
<i>u4162</i>	C(216)...H(243)	646.0(98)	23.4(fixed)	—	-5.1	23.4
<i>u2135</i>	C(129)...H(156)	646.0(113)	33.7(fixed)	—	-2.0	33.7
<i>u4360</i>	H(183)...H(198)	646.1(60)	48.8(fixed)	—	-33.1	48.8
<i>u4241</i>	C(7)...H(26)	646.1(111)	33.2(fixed)	—	3.5	33.2
<i>u4340</i>	H(103)...H(109)	646.2(70)	56.3(fixed)	—	-27.5	56.3
<i>u4172</i>	C(132)...H(159)	646.2(95)	27.7(fixed)	—	1.4	27.7
<i>u4207</i>	H(238)...H(243)	646.2(84)	31.5(fixed)	—	-3.1	31.5
<i>u4144</i>	C(50)...H(77)	646.3(98)	29.3(fixed)	—	3.4	29.3
<i>u4219</i>	C(8)...H(23)	646.4(115)	25.0(fixed)	—	-1.1	25.0
<i>u4278</i>	H(23)...H(40)	646.6(143)	30.5(fixed)	—	-6.5	30.5
<i>u3505</i>	H(142)...H(161)	646.7(167)	47.1(fixed)	—	-15.2	47.1
<i>u4329</i>	C(11)...H(28)	646.8(35)	44.3(fixed)	—	0.3	44.3
<i>u4264</i>	C(174)...H(203)	646.8(61)	49.2(fixed)	—	4.7	49.2
<i>u4247</i>	C(171)...H(197)	647.1(122)	26.3(fixed)	—	-5.1	26.3
<i>u4331</i>	H(276)...H(283)	647.2(169)	46.8(fixed)	—	-15.3	46.8
<i>u4066</i>	H(275)...H(282)	647.2(264)	53.1(fixed)	—	-5.0	53.1
<i>u4238</i>	H(234)...H(239)	647.2(88)	35.7(fixed)	—	1.7	35.7
<i>u3998</i>	H(270)...H(282)	647.3(55)	87.4(fixed)	—	-10.2	87.4
<i>u4222</i>	C(90)...H(104)	647.4(115)	31.6(fixed)	—	-1.1	31.6
<i>u4256</i>	C(132)...H(160)	648.2(113)	29.6(fixed)	—	-0.3	29.6
<i>u4236</i>	C(52)...H(65)	648.6(122)	25.5(fixed)	—	-1.5	25.5
<i>u4413</i>	H(183)...H(197)	648.9(71)	51.0(fixed)	—	-31.4	51.0
<i>u4279</i>	H(61)...H(73)	648.9(90)	40.4(fixed)	—	9.2	40.4
<i>u4414</i>	H(188)...H(205)	649.1(68)	48.6(fixed)	—	-31.4	48.6
<i>u4192</i>	H(70)...H(77)	649.2(91)	40.2(fixed)	—	12.4	40.2
<i>u4244</i>	C(53)...H(69)	649.4(38)	32.9(fixed)	—	0.1	32.9
<i>u4284</i>	H(23)...H(26)	649.4(87)	39.8(fixed)	—	9.7	39.8
<i>u4194</i>	C(216)...H(244)	649.5(37)	26.6(fixed)	—	-1.6	26.6
<i>u4311</i>	H(32)...H(37)	649.5(143)	28.0(fixed)	—	-5.0	28.0
<i>u4286</i>	C(50)...H(78)	649.5(121)	32.7(fixed)	—	0.0	32.7
<i>u4197</i>	C(52)...H(67)	649.5(124)	25.6(fixed)	—	-1.2	25.6
<i>u4301</i>	H(264)...H(277)	649.5(73)	37.1(fixed)	—	1.9	37.1
<i>u1254</i>	C(130)...H(149)	649.9(118)	45.7(fixed)	—	3.4	45.7
<i>u4288</i>	H(239)...H(242)	650.0(331)	35.3(fixed)	—	-5.4	35.3
<i>u4246</i>	C(255)...H(279)	650.2(122)	24.5(fixed)	—	-1.9	24.5
<i>u4435</i>	H(195)...H(203)	650.4(106)	98.3(fixed)	—	2.3	98.3
<i>u4254</i>	C(218)...H(238)	650.5(121)	25.1(fixed)	—	-1.8	25.1
<i>u4341</i>	H(224)...H(237)	650.7(53)	33.1(fixed)	—	-8.3	33.1
<i>u4224</i>	C(8)...H(22)	650.8(126)	25.4(fixed)	—	-0.8	25.4

<i>u541</i>	H(141)...H(158)	650.9(89)	46.1(fixed)	—	11.4	46.1
<i>u4216</i>	C(213)...H(227)	651.2(131)	26.5(fixed)	—	-0.3	26.5
<i>u4248</i>	C(175)...H(187)	651.6(121)	26.3(fixed)	—	-5.1	26.3
<i>u4561</i>	H(265)...H(271)	651.7(43)	32.7(fixed)	—	-23.4	32.7
<i>u4240</i>	H(188)...H(200)	651.7(96)	36.7(fixed)	—	-3.9	36.7
<i>u4193</i>	F(263)...H(270)	652.3(28)	50.5(fixed)	—	-5.0	50.5
<i>u4324</i>	H(223)...H(235)	652.7(59)	42.2(fixed)	—	-9.4	42.2
<i>u4208</i>	H(186)...H(199)	653.1(296)	36.3(fixed)	—	-5.4	36.3
<i>u4471</i>	H(28)...H(35)	653.1(139)	58.4(fixed)	—	-1.6	58.4
<i>u4114</i>	C(11)...H(29)	653.3(43)	39.5(fixed)	—	12.3	39.5
<i>u1210</i>	C(134)...H(143)	653.4(35)	39.6(fixed)	—	4.2	39.6
<i>u4313</i>	H(267)...H(286)	653.6(142)	43.2(fixed)	—	-7.5	43.2
<i>u4226</i>	C(89)...H(106)	654.0(116)	32.1(fixed)	—	-0.1	32.1
<i>u4327</i>	H(21)...H(32)	654.1(107)	29.0(fixed)	—	-6.5	29.0
<i>u4225</i>	H(234)...H(236)	654.6(73)	43.8(fixed)	—	13.0	43.8
<i>u4255</i>	H(21)...H(27)	654.7(62)	81.6(fixed)	—	-23.5	81.6
<i>u4490</i>	H(233)...H(236)	655.2(106)	48.4(fixed)	—	-2.5	48.4
<i>u4355</i>	H(224)...H(235)	655.2(104)	40.4(fixed)	—	-9.0	40.4
<i>u676</i>	C(129)...H(158)	655.3(95)	31.2(fixed)	—	10.8	31.2
<i>u4309</i>	H(227)...H(231)	655.6(301)	42.4(fixed)	—	1.7	42.4
<i>u1713</i>	H(143)...H(156)	655.8(149)	51.0(fixed)	—	2.4	51.0
<i>u4339</i>	H(28)...H(33)	656.0(154)	51.1(fixed)	—	7.7	51.1
<i>u4289</i>	H(23)...H(27)	656.1(50)	72.9(fixed)	—	-19.8	72.9
<i>u4343</i>	H(22)...H(27)	656.2(38)	60.3(fixed)	—	-26.4	60.3
<i>u4253</i>	C(49)...H(74)	656.3(122)	25.0(fixed)	—	-2.0	25.0
<i>u4237</i>	H(240)...H(244)	656.6(133)	37.3(fixed)	—	-0.1	37.3
<i>u4265</i>	H(67)...H(76)	656.8(299)	37.0(fixed)	—	-0.2	37.0
<i>u4290</i>	H(226)...H(245)	656.9(114)	35.9(fixed)	—	-8.0	35.9
<i>u1085</i>	C(130)...H(147)	657.6(118)	38.8(fixed)	—	4.6	38.8
<i>u4302</i>	H(238)...H(244)	658.1(155)	37.1(fixed)	—	0.3	37.1
<i>u4437</i>	H(114)...H(122)	658.3(101)	31.6(fixed)	—	-2.3	31.6
<i>u4269</i>	H(104)...H(106)	658.5(79)	47.6(fixed)	—	7.5	47.6
<i>u4356</i>	H(22)...H(26)	658.6(299)	48.7(fixed)	—	3.6	48.7
<i>u4287</i>	H(67)...H(74)	658.6(79)	35.6(fixed)	—	0.7	35.6
<i>u4280</i>	H(21)...H(40)	658.7(130)	35.3(fixed)	—	-7.4	35.3
<i>u4332</i>	H(104)...H(108)	658.7(294)	48.9(fixed)	—	1.3	48.9
<i>u4295</i>	C(253)...H(287)	658.9(50)	23.1(fixed)	—	-7.0	23.1
<i>u4334</i>	H(182)...H(193)	659.0(106)	66.2(fixed)	—	5.1	66.2
<i>u4372</i>	H(68)...H(76)	659.0(64)	28.2(fixed)	—	-15.6	28.2
<i>u4379</i>	H(264)...H(278)	659.1(97)	32.2(fixed)	—	-1.4	32.2
<i>u4273</i>	H(113)...H(121)	659.1(104)	39.2(fixed)	—	-1.2	39.2
<i>u4165</i>	H(29)...H(35)	659.2(97)	50.5(fixed)	—	19.5	50.5
<i>u4359</i>	H(224)...H(231)	659.3(49)	27.0(fixed)	—	-12.2	27.0
<i>u4353</i>	H(267)...H(276)	659.3(168)	38.2(fixed)	—	-13.0	38.2

<i>u4345</i>	H(69)...H(78)	659.6(160)	48.1(fixed)	—	6.4	48.1
<i>u4221</i>	C(212)...H(229)	660.1(124)	30.6(fixed)	—	0.0	30.6
<i>u4177</i>	H(226)...H(246)	660.3(163)	44.4(fixed)	—	-8.0	44.4
<i>u4300</i>	H(151)...H(160)	660.5(148)	45.5(fixed)	—	6.4	45.5
<i>u4409</i>	H(61)...H(72)	660.9(103)	51.1(fixed)	—	-0.5	51.1
<i>u4292</i>	H(69)...H(77)	661.0(137)	50.7(fixed)	—	6.6	50.7
<i>u4335</i>	H(59)...H(73)	661.1(102)	42.3(fixed)	—	2.1	42.3
<i>u4399</i>	H(142)...H(153)	661.4(51)	29.0(fixed)	—	-5.3	29.0
<i>u4398</i>	H(266)...H(277)	661.4(102)	40.2(fixed)	—	-1.2	40.2
<i>u4373</i>	F(96)...H(101)	661.6(17)	23.2(fixed)	—	-17.6	23.2
<i>u4333</i>	H(19)...H(33)	661.7(150)	32.1(fixed)	—	-8.3	32.1
<i>u4354</i>	H(70)...H(82)	662.0(70)	29.5(fixed)	—	-4.7	29.5
<i>u4298</i>	H(234)...H(237)	662.1(104)	44.6(fixed)	—	4.5	44.6
<i>u4362</i>	H(68)...H(75)	662.1(62)	33.6(fixed)	—	-15.7	33.6
<i>u4210</i>	C(7)...H(24)	662.4(122)	36.4(fixed)	—	3.9	36.4
<i>u4299</i>	H(151)...H(159)	662.4(133)	51.2(fixed)	—	3.8	51.2
<i>u4319</i>	H(146)...H(150)	662.4(50)	45.1(fixed)	—	-15.7	45.1
<i>u4383</i>	H(19)...H(26)	662.8(42)	27.9(fixed)	—	-9.6	27.9
<i>u4323</i>	C(48)...H(82)	663.0(56)	23.0(fixed)	—	-5.5	23.0
<i>u4380</i>	H(224)...H(230)	663.0(58)	31.2(fixed)	—	-11.9	31.2
<i>u4181</i>	H(21)...H(41)	663.1(170)	42.8(fixed)	—	-7.1	42.8
<i>u4344</i>	H(235)...H(245)	663.2(55)	28.6(fixed)	—	-5.6	28.6
<i>u4394</i>	H(62)...H(81)	663.6(142)	35.5(fixed)	—	-5.6	35.5
<i>u4436</i>	H(274)...H(276)	663.8(69)	22.9(fixed)	—	-7.5	22.9
<i>u4404</i>	H(29)...H(30)	663.9(52)	27.6(fixed)	—	-4.0	27.6
<i>u4370</i>	H(32)...H(38)	663.9(116)	31.6(fixed)	—	-6.5	31.6
<i>u4438</i>	H(265)...H(272)	664.3(75)	49.2(fixed)	—	-4.8	49.2
<i>u3000</i>	H(141)...H(153)	664.6(56)	36.7(fixed)	—	6.7	36.7
<i>u4371</i>	H(19)...H(25)	664.6(62)	31.1(fixed)	—	-9.6	31.1
<i>u4305</i>	H(228)...H(232)	664.9(51)	56.9(fixed)	—	-15.7	56.9
<i>u4347</i>	F(17)...H(30)	665.1(25)	16.1(fixed)	—	-6.0	16.1
<i>u4326</i>	H(30)...H(38)	665.3(169)	40.6(fixed)	—	-7.1	40.6
<i>u4282</i>	H(228)...H(246)	665.8(162)	39.4(fixed)	—	-9.6	39.4
<i>u4388</i>	H(21)...H(30)	666.3(114)	29.6(fixed)	—	-9.0	29.6
<i>u4291</i>	H(23)...H(41)	666.3(176)	35.3(fixed)	—	-8.1	35.3
<i>u4328</i>	H(269)...H(287)	666.4(87)	31.5(fixed)	—	-2.9	31.5
<i>u4123</i>	H(144)...H(150)	666.6(61)	52.3(fixed)	—	-12.8	52.3
<i>u4365</i>	H(63)...H(79)	667.1(67)	30.0(fixed)	—	-15.5	30.0
<i>u4268</i>	H(227)...H(229)	667.2(73)	41.4(fixed)	—	5.2	41.4
<i>u4358</i>	H(30)...H(37)	667.5(180)	31.6(fixed)	—	-7.6	31.6
<i>u4416</i>	H(223)...H(243)	667.6(92)	29.6(fixed)	—	-6.7	29.6
<i>u4349</i>	H(227)...H(232)	667.6(35)	47.9(fixed)	—	-20.8	47.9
<i>u679</i>	C(131)...H(145)	667.7(118)	38.1(fixed)	—	20.2	38.1
<i>u4401</i>	H(268)...H(284)	667.9(60)	31.2(fixed)	—	-17.1	31.2

<i>u4390</i>	H(64)...H(82)	668.0(101)	32.2(fixed)	—	-3.7	32.2
<i>u3497</i>	H(264)...H(270)	668.0(97)	71.2(fixed)	—	16.7	71.2
<i>u4325</i>	H(273)...H(276)	668.5(47)	28.6(fixed)	—	-6.0	28.6
<i>u4392</i>	H(19)...H(30)	668.6(70)	42.4(fixed)	—	-11.8	42.4
<i>u4417</i>	H(67)...H(71)	669.3(45)	29.1(fixed)	—	-15.7	29.1
<i>u4271</i>	H(226)...H(232)	669.4(66)	63.1(fixed)	—	-17.6	63.1
<i>u4377</i>	H(71)...H(82)	669.5(78)	40.8(fixed)	—	-16.7	40.8
<i>u4245</i>	H(22)...H(24)	669.5(77)	47.7(fixed)	—	10.2	47.7
<i>u4418</i>	H(103)...H(117)	670.2(75)	32.2(fixed)	—	-21.0	32.2
<i>u4445</i>	H(238)...H(245)	670.6(146)	32.3(fixed)	—	-2.8	32.3
<i>u4374</i>	F(219)...H(224)	670.6(15)	16.0(fixed)	—	-7.8	16.0
<i>u4421</i>	H(68)...H(74)	670.6(56)	31.7(fixed)	—	-14.3	31.7
<i>u505</i>	H(145)...H(147)	670.6(80)	52.1(fixed)	—	20.5	52.1
<i>u4357</i>	F(56)...H(82)	670.7(17)	16.1(fixed)	—	-5.7	16.1
<i>u4375</i>	F(14)...H(19)	670.8(17)	15.7(fixed)	—	-7.4	15.7
<i>u2414</i>	H(272)...H(279)	670.9(91)	57.3(fixed)	—	46.7	57.3
<i>u4351</i>	F(15)...H(41)	670.9(15)	15.7(fixed)	—	-6.1	15.7
<i>u4364</i>	H(66)...H(71)	670.9(72)	36.1(fixed)	—	-15.6	36.1
<i>u4430</i>	H(19)...H(24)	670.9(46)	26.5(fixed)	—	-11.8	26.5
<i>u4412</i>	H(65)...H(71)	671.5(64)	34.1(fixed)	—	-13.5	34.1
<i>u4461</i>	H(70)...H(78)	671.7(143)	42.0(fixed)	—	-1.3	42.0
<i>u3122</i>	H(272)...H(282)	671.8(39)	63.6(fixed)	—	32.1	63.6
<i>u4336</i>	F(55)...H(62)	671.8(38)	17.4(fixed)	—	-5.9	17.4
<i>u4427</i>	H(224)...H(229)	672.1(45)	27.7(fixed)	—	-12.4	27.7
<i>u1989</i>	H(141)...H(156)	672.1(136)	41.2(fixed)	—	-1.4	41.2
<i>u4367</i>	F(260)...H(267)	672.1(33)	16.7(fixed)	—	-8.1	16.7
<i>u4400</i>	H(34)...H(40)	672.2(94)	27.5(fixed)	—	-5.7	27.5
<i>u4378</i>	F(261)...H(287)	672.5(15)	15.8(fixed)	—	-6.6	15.8
<i>u4338</i>	H(27)...H(30)	672.6(46)	29.8(fixed)	—	-3.4	29.8
<i>u4477</i>	H(100)...H(120)	672.7(98)	36.0(fixed)	—	-14.0	36.0
<i>u2083</i>	H(142)...H(160)	672.8(164)	76.2(fixed)	—	7.4	76.2
<i>u4376</i>	F(262)...H(284)	673.0(18)	18.2(fixed)	—	-10.7	18.2
<i>u4363</i>	F(98)...H(120)	673.1(21)	17.7(fixed)	—	-8.3	17.7
<i>u4395</i>	H(280)...H(286)	673.1(89)	29.7(fixed)	—	-6.5	29.7
<i>u4420</i>	H(62)...H(79)	673.3(45)	32.2(fixed)	—	-17.2	32.2
<i>u4368</i>	H(75)...H(81)	673.4(96)	30.2(fixed)	—	-6.6	30.2
<i>u4433</i>	H(18)...H(38)	673.6(91)	29.0(fixed)	—	-6.6	29.0
<i>u4402</i>	H(142)...H(148)	673.6(61)	30.6(fixed)	—	-8.5	30.6
<i>u2795</i>	H(150)...H(153)	673.8(51)	62.7(fixed)	—	-21.4	62.7
<i>u4453</i>	H(25)...H(36)	674.0(53)	34.4(fixed)	—	-21.1	34.4
<i>u4542</i>	H(27)...H(38)	674.2(123)	34.0(fixed)	—	-31.2	34.0
<i>u4429</i>	H(103)...H(116)	674.9(81)	38.0(fixed)	—	-24.1	38.0
<i>u4442</i>	H(28)...H(30)	675.1(45)	23.1(fixed)	—	-6.3	23.1
<i>u3842</i>	H(143)...H(153)	675.3(44)	39.7(fixed)	—	-1.1	39.7

<i>u389</i>	H(143)...H(158)	675.4(133)	44.4(fixed)	—	15.8	44.4
<i>u4479</i>	H(25)...H(34)	675.7(43)	39.9(fixed)	—	-23.3	39.9
<i>u4393</i>	H(235)...H(246)	675.9(47)	28.2(fixed)	—	-6.8	28.2
<i>u4389</i>	H(230)...H(235)	676.3(128)	34.9(fixed)	—	-13.7	34.9
<i>u4539</i>	H(232)...H(243)	676.5(122)	33.6(fixed)	—	-25.3	33.6
<i>u4261</i>	H(184)...H(193)	676.6(70)	56.8(fixed)	—	43.0	56.8
<i>u4366</i>	H(68)...H(82)	676.8(52)	28.7(fixed)	—	-4.6	28.7
<i>u4512</i>	H(27)...H(36)	676.9(98)	35.8(fixed)	—	-27.4	35.8
<i>u4424</i>	H(25)...H(37)	677.1(95)	41.3(fixed)	—	-17.5	41.3
<i>u4454</i>	H(267)...H(284)	677.3(48)	34.4(fixed)	—	-18.5	34.4
<i>u4406</i>	H(60)...H(75)	677.4(178)	33.0(fixed)	—	-6.8	33.0
<i>u4387</i>	F(221)...H(243)	677.5(13)	15.2(fixed)	—	-5.5	15.2
<i>u4384</i>	F(16)...H(38)	677.8(14)	15.3(fixed)	—	-5.4	15.3
<i>u3762</i>	F(263)...H(272)	678.3(21)	35.6(fixed)	—	18.6	35.6
<i>u2000</i>	H(146)...H(147)	678.4(263)	49.2(fixed)	—	-6.8	49.2
<i>u4452</i>	H(267)...H(271)	678.5(48)	32.2(fixed)	—	-13.6	32.2
<i>u4464</i>	H(107)...H(119)	678.6(103)	33.0(fixed)	—	-19.1	33.0
<i>u4465</i>	H(103)...H(115)	678.6(103)	33.2(fixed)	—	-19.0	33.2
<i>u2566</i>	C(257)...H(272)	678.8(57)	46.5(fixed)	—	39.2	46.5
<i>u4315</i>	H(29)...H(33)	678.8(143)	53.5(fixed)	—	7.5	53.5
<i>u4480</i>	H(267)...H(277)	678.8(94)	28.2(fixed)	—	-14.4	28.2
<i>u4481</i>	H(21)...H(31)	678.9(61)	23.6(fixed)	—	-9.0	23.6
<i>u4459</i>	H(69)...H(82)	678.9(45)	22.9(fixed)	—	-9.1	22.9
<i>u4419</i>	H(25)...H(38)	679.0(86)	46.7(fixed)	—	-21.1	46.7
<i>u4499</i>	H(195)...H(202)	679.0(73)	43.3(fixed)	—	-24.9	43.3
<i>u3860</i>	H(142)...H(149)	679.1(34)	42.4(fixed)	—	-3.3	42.4
<i>u4262</i>	H(195)...H(204)	679.2(74)	55.8(fixed)	—	43.0	55.8
<i>u4426</i>	H(62)...H(71)	679.4(176)	35.4(fixed)	—	-7.9	35.4
<i>u494</i>	H(145)...H(149)	679.4(298)	53.7(fixed)	—	25.3	53.7
<i>u4476</i>	H(187)...H(197)	679.9(266)	33.0(fixed)	—	-6.9	33.0
<i>u4466</i>	H(64)...H(79)	680.1(80)	27.3(fixed)	—	-15.5	27.3
<i>u4483</i>	H(19)...H(31)	680.2(71)	29.1(fixed)	—	-12.4	29.1
<i>u4550</i>	H(101)...H(116)	680.4(131)	38.6(fixed)	—	-34.1	38.6
<i>u4484</i>	H(71)...H(80)	680.4(72)	30.1(fixed)	—	-17.2	30.1
<i>u4551</i>	H(109)...H(120)	680.5(131)	37.6(fixed)	—	-34.2	37.6
<i>u4448</i>	H(235)...H(244)	680.7(43)	22.9(fixed)	—	-7.3	22.9
<i>u4505</i>	H(232)...H(241)	681.0(88)	33.3(fixed)	—	-22.0	33.3
<i>u4500</i>	H(184)...H(189)	681.1(71)	43.2(fixed)	—	-24.9	43.2
<i>u4497</i>	H(25)...H(35)	681.4(164)	30.8(fixed)	—	-22.0	30.8
<i>u4415</i>	H(228)...H(229)	681.4(270)	43.0(fixed)	—	-1.9	43.0
<i>u4350</i>	H(148)...H(153)	681.6(87)	35.5(fixed)	—	-16.1	35.5
<i>u4532</i>	H(101)...H(117)	682.4(102)	32.0(fixed)	—	-28.5	32.0
<i>u4533</i>	H(109)...H(118)	682.4(102)	30.9(fixed)	—	-28.6	30.9
<i>u4486</i>	H(267)...H(270)	682.6(59)	30.4(fixed)	—	-10.1	30.4

<i>u4330</i>	H(275)...H(276)	682.6(47)	27.8(fixed)	—	-5.6	27.8
<i>u3760</i>	H(270)...H(284)	682.6(54)	96.8(fixed)	—	3.8	96.8
<i>u4478</i>	H(269)...H(284)	682.7(85)	29.2(fixed)	—	-17.0	29.2
<i>u4467</i>	H(65)...H(74)	682.7(271)	32.8(fixed)	—	-3.2	32.8
<i>u4407</i>	H(23)...H(24)	683.6(267)	47.9(fixed)	—	-0.3	47.9
<i>u4543</i>	H(102)...H(123)	684.1(78)	44.5(fixed)	—	-23.0	44.5
<i>u4428</i>	H(105)...H(106)	684.3(264)	46.5(fixed)	—	-1.3	46.5
<i>u4463</i>	H(230)...H(241)	684.6(43)	28.3(fixed)	—	-12.2	28.3
<i>u4458</i>	H(280)...H(285)	684.8(35)	22.9(fixed)	—	-7.7	22.9
<i>u4469</i>	H(102)...H(120)	685.6(55)	25.3(fixed)	—	-7.0	25.3
<i>u4470</i>	H(110)...H(116)	685.6(55)	25.5(fixed)	—	-7.0	25.5
<i>u4403</i>	H(280)...H(287)	685.7(88)	29.0(fixed)	—	-6.5	29.0
<i>u4446</i>	H(265)...H(280)	685.7(178)	34.2(fixed)	—	-6.8	34.2
<i>u4439</i>	H(116)...H(123)	686.1(137)	34.7(fixed)	—	-7.5	34.7
<i>u4440</i>	H(112)...H(120)	686.1(137)	34.6(fixed)	—	-7.5	34.6
<i>u4425</i>	H(224)...H(243)	686.8(86)	28.7(fixed)	—	-5.6	28.7
<i>u3877</i>	H(270)...H(283)	687.0(52)	82.5(fixed)	—	4.6	82.5
<i>u3301</i>	H(145)...H(150)	687.2(34)	49.4(fixed)	—	5.8	49.4
<i>u3801</i>	H(274)...H(282)	687.2(49)	45.5(fixed)	—	-6.0	45.5
<i>u4491</i>	H(144)...H(157)	687.3(48)	33.5(fixed)	—	-8.9	33.5
<i>u4408</i>	H(34)...H(41)	687.3(80)	28.0(fixed)	—	-6.5	28.0
<i>u4462</i>	H(225)...H(243)	687.9(35)	23.1(fixed)	—	-8.6	23.1
<i>u4422</i>	H(75)...H(82)	688.1(104)	31.1(fixed)	—	-8.0	31.1
<i>u4487</i>	H(75)...H(80)	688.2(46)	23.6(fixed)	—	-8.4	23.6
<i>u3799</i>	H(148)...H(154)	688.4(37)	72.2(fixed)	—	-4.1	72.2
<i>u4451</i>	H(230)...H(242)	688.5(95)	30.5(fixed)	—	-10.7	30.5
<i>u4447</i>	H(34)...H(39)	688.7(36)	23.0(fixed)	—	-7.0	23.0
<i>u4456</i>	H(20)...H(38)	689.5(36)	23.6(fixed)	—	-8.5	23.6
<i>u4488</i>	H(230)...H(236)	689.6(65)	26.8(fixed)	—	-14.1	26.8
<i>u4252</i>	C(257)...H(274)	689.7(120)	25.8(fixed)	—	-1.7	25.8
<i>u4495</i>	H(62)...H(72)	690.1(98)	29.9(fixed)	—	-12.4	29.9
<i>u4397</i>	H(183)...H(189)	690.3(132)	41.3(fixed)	—	-5.0	41.3
<i>u4396</i>	H(185)...H(191)	690.3(132)	41.3(fixed)	—	-5.0	41.3
<i>u4506</i>	H(61)...H(75)	690.5(100)	25.5(fixed)	—	-10.5	25.5
<i>u4455</i>	H(19)...H(38)	691.0(84)	28.6(fixed)	—	-6.8	28.6
<i>u4449</i>	H(230)...H(243)	692.3(88)	34.8(fixed)	—	-12.8	34.8
<i>u4507</i>	H(225)...H(246)	692.9(67)	32.7(fixed)	—	-12.2	32.7
<i>u4520</i>	C(174)...H(205)	693.4(33)	19.3(fixed)	—	-18.1	19.3
<i>u4472</i>	H(224)...H(246)	694.7(52)	38.1(fixed)	—	-8.2	38.1
<i>u4519</i>	C(170)...H(191)	695.0(29)	20.7(fixed)	—	-18.1	20.7
<i>u4198</i>	C(257)...H(275)	695.2(100)	23.9(fixed)	—	-1.0	23.9
<i>u2934</i>	H(148)...H(155)	695.8(90)	45.7(fixed)	—	18.2	45.7
<i>u4473</i>	H(101)...H(120)	696.1(102)	31.5(fixed)	—	-2.1	31.5
<i>u4474</i>	H(109)...H(116)	696.1(102)	31.6(fixed)	—	-2.1	31.6



<i>u4431</i>	H(109)...H(112)	696.4(97)	46.7(fixed)	—	-5.9	46.7
<i>u4432</i>	H(101)...H(123)	696.4(97)	46.5(fixed)	—	-5.9	46.5
<i>u4509</i>	H(266)...H(280)	696.6(98)	26.7(fixed)	—	-9.1	26.7
<i>u4492</i>	H(276)...H(287)	696.6(54)	37.3(fixed)	—	-8.9	37.3
<i>u4485</i>	H(116)...H(121)	697.0(74)	27.8(fixed)	—	-8.6	27.8
<i>u4544</i>	H(233)...H(239)	697.0(72)	27.4(fixed)	—	-14.9	27.4
<i>u4450</i>	H(267)...H(272)	697.1(102)	26.2(fixed)	—	-6.9	26.2
<i>u4475</i>	H(66)...H(77)	697.3(171)	35.4(fixed)	—	-11.0	35.4
<i>u4337</i>	H(232)...H(239)	697.4(137)	40.2(fixed)	—	-6.0	40.2
<i>u4502</i>	H(20)...H(41)	698.1(70)	32.0(fixed)	—	-11.6	32.0
<i>u4493</i>	H(66)...H(79)	698.4(53)	37.2(fixed)	—	-11.3	37.2
<i>u4518</i>	H(276)...H(285)	698.7(64)	30.0(fixed)	—	-9.9	30.0
<i>u4501</i>	C(215)...H(232)	698.9(28)	22.4(fixed)	—	-13.4	22.4
<i>u4503</i>	C(11)...H(27)	699.7(10)	26.4(fixed)	—	-16.4	26.4
<i>u4508</i>	C(256)...H(265)	700.7(33)	16.4(fixed)	—	-6.8	16.4
<i>u4538</i>	C(47)...H(71)	700.9(35)	17.4(fixed)	—	-9.5	17.4
<i>u4496</i>	H(19)...H(41)	701.1(68)	36.6(fixed)	—	-9.2	36.6
<i>u4444</i>	H(275)...H(279)	701.1(48)	30.5(fixed)	—	-2.6	30.5
<i>u4317</i>	H(274)...H(281)	701.3(102)	36.6(fixed)	—	-0.7	36.6
<i>u3806</i>	H(142)...H(162)	701.5(66)	44.9(fixed)	—	-0.2	44.9
<i>u4619</i>	H(273)...H(280)	702.0(62)	20.2(fixed)	—	-8.3	20.2
<i>u4511</i>	C(252)...H(276)	703.1(34)	16.0(fixed)	—	-5.4	16.0
<i>u4525</i>	C(51)...H(60)	703.5(34)	16.7(fixed)	—	-7.1	16.7
<i>u4546</i>	H(30)...H(39)	703.6(74)	27.7(fixed)	—	-8.5	27.7
<i>u4498</i>	H(240)...H(243)	704.6(162)	25.8(fixed)	—	-7.3	25.8
<i>u4526</i>	C(132)...H(161)	704.8(12)	17.0(fixed)	—	-8.1	17.0
<i>u4549</i>	H(30)...H(41)	705.2(64)	36.6(fixed)	—	-8.7	36.6
<i>u4536</i>	C(7)...H(25)	705.5(34)	18.2(fixed)	—	-12.7	18.2
<i>u4504</i>	H(239)...H(243)	705.6(46)	30.8(fixed)	—	-7.0	30.8
<i>u4557</i>	H(232)...H(237)	705.7(47)	28.2(fixed)	—	-14.8	28.2
<i>u4524</i>	C(92)...H(123)	706.0(33)	15.7(fixed)	—	-5.8	15.7
<i>u4515</i>	C(50)...H(79)	706.1(15)	18.6(fixed)	—	-9.9	18.6
<i>u4517</i>	C(214)...H(235)	708.1(29)	15.7(fixed)	—	-5.2	15.7
<i>u4540</i>	C(89)...H(107)	708.2(25)	17.4(fixed)	—	-11.5	17.4
<i>u4521</i>	C(53)...H(68)	708.7(11)	16.9(fixed)	—	-9.2	16.9
<i>u4514</i>	C(255)...H(280)	709.6(17)	15.9(fixed)	—	-5.3	15.9
<i>u4510</i>	C(218)...H(239)	709.6(15)	16.2(fixed)	—	-5.6	16.2
<i>u4553</i>	H(265)...H(278)	709.7(53)	26.5(fixed)	—	-5.9	26.5
<i>u4535</i>	C(212)...H(230)	709.8(39)	16.5(fixed)	—	-8.0	16.5
<i>u4545</i>	H(268)...H(287)	709.9(84)	28.5(fixed)	—	-10.1	28.5
<i>u2115</i>	C(129)...H(157)	710.2(12)	34.2(fixed)	—	-1.5	34.2
<i>u4531</i>	C(9)...H(34)	710.6(11)	15.4(fixed)	—	-5.3	15.4
<i>u4523</i>	C(175)...H(185)	711.8(30)	16.4(fixed)	—	-7.8	16.4
<i>u4563</i>	H(183)...H(193)	712.0(47)	32.9(fixed)	—	-13.4	32.9

<i>u4564</i>	H(182)...H(191)	712.0(47)	32.6(fixed)	—	-13.4	32.6
<i>u2131</i>	C(131)...H(144)	712.1(25)	43.5(fixed)	—	-6.6	43.5
<i>u4516</i>	C(216)...H(246)	712.1(11)	15.7(fixed)	—	-5.8	15.7
<i>u4608</i>	H(183)...H(192)	712.5(46)	43.6(fixed)	—	-24.5	43.6
<i>u4607</i>	H(184)...H(191)	712.5(46)	43.1(fixed)	—	-24.5	43.1
<i>u4522</i>	C(171)...H(198)	712.6(22)	16.4(fixed)	—	-7.8	16.4
<i>u4529</i>	C(213)...H(226)	714.2(25)	15.7(fixed)	—	-6.7	15.7
<i>u4527</i>	C(49)...H(75)	714.3(33)	15.9(fixed)	—	-5.5	15.9
<i>u4548</i>	H(63)...H(82)	714.5(87)	25.5(fixed)	—	-7.4	25.5
<i>u4562</i>	H(27)...H(33)	715.1(96)	29.1(fixed)	—	-18.2	29.1
<i>u4541</i>	C(8)...H(21)	715.2(23)	15.4(fixed)	—	-5.5	15.4
<i>u4566</i>	H(59)...H(71)	715.3(65)	27.5(fixed)	—	-8.2	27.5
<i>u4528</i>	C(52)...H(66)	715.4(23)	15.8(fixed)	—	-6.0	15.8
<i>u4218</i>	H(275)...H(281)	715.6(243)	34.4(fixed)	—	1.3	34.4
<i>u4555</i>	H(239)...H(245)	715.9(61)	28.0(fixed)	—	-4.5	28.0
<i>u2411</i>	C(130)...H(148)	716.2(25)	26.6(fixed)	—	-4.2	26.6
<i>u3612</i>	H(274)...H(284)	717.1(195)	46.4(fixed)	—	-0.7	46.4
<i>u4577</i>	H(23)...H(25)	717.1(50)	29.1(fixed)	—	-13.0	29.1
<i>u4554</i>	H(70)...H(79)	718.3(64)	31.5(fixed)	—	-4.5	31.5
<i>u4573</i>	H(112)...H(122)	718.5(56)	26.2(fixed)	—	-4.9	26.2
<i>u4578</i>	H(27)...H(35)	719.5(95)	40.9(fixed)	—	-19.4	40.9
<i>u4567</i>	H(228)...H(230)	720.1(50)	29.0(fixed)	—	-6.9	29.0
<i>u4552</i>	H(267)...H(287)	720.6(103)	31.6(fixed)	—	-9.9	31.6
<i>u4568</i>	H(60)...H(73)	721.4(62)	27.5(fixed)	—	-3.9	27.5
<i>u3106</i>	H(146)...H(148)	721.7(52)	54.1(fixed)	—	-13.7	54.1
<i>u4574</i>	H(264)...H(276)	722.7(56)	25.0(fixed)	—	-4.0	25.0
<i>u1508</i>	H(141)...H(157)	724.3(55)	48.3(fixed)	—	4.0	48.3
<i>u4593</i>	H(232)...H(236)	724.5(48)	35.6(fixed)	—	-15.7	35.6
<i>u4322</i>	H(274)...H(279)	725.6(191)	35.5(fixed)	—	0.0	35.5
<i>u3078</i>	H(142)...H(156)	725.6(89)	36.7(fixed)	—	-7.0	36.7
<i>u4581</i>	H(62)...H(82)	726.3(104)	29.8(fixed)	—	-7.9	29.8
<i>u3407</i>	H(272)...H(281)	726.6(138)	45.5(fixed)	—	32.6	45.5
<i>u4612</i>	H(61)...H(71)	727.4(50)	29.7(fixed)	—	-11.0	29.7
<i>u4587</i>	H(185)...H(197)	728.4(75)	29.0(fixed)	—	-7.7	29.0
<i>u4576</i>	H(65)...H(75)	729.2(61)	27.7(fixed)	—	-4.7	27.7
<i>u4605</i>	H(266)...H(276)	729.4(49)	27.0(fixed)	—	-5.6	27.0
<i>u4595</i>	H(60)...H(72)	729.5(51)	32.9(fixed)	—	-7.4	32.9
<i>u4598</i>	H(68)...H(78)	729.6(97)	31.7(fixed)	—	-6.6	31.7
<i>u4600</i>	H(22)...H(25)	729.8(118)	28.8(fixed)	—	-15.0	28.8
<i>u4585</i>	H(226)...H(231)	729.8(74)	27.4(fixed)	—	-6.3	27.4
<i>u4580</i>	H(105)...H(107)	730.3(52)	32.8(fixed)	—	-8.1	32.8
<i>u4579</i>	H(103)...H(106)	730.3(52)	32.9(fixed)	—	-8.1	32.9
<i>u4603</i>	H(104)...H(107)	730.4(93)	33.0(fixed)	—	-11.8	33.0
<i>u4602</i>	H(103)...H(108)	730.5(93)	33.1(fixed)	—	-11.7	33.1

<i>u4560</i>	H(234)...H(235)	730.6(51)	29.1(fixed)	—	2.1	29.1
<i>u4613</i>	H(233)...H(235)	730.8(48)	32.9(fixed)	—	-5.1	32.9
<i>u4571</i>	H(68)...H(77)	731.1(92)	30.4(fixed)	—	-7.9	30.4
<i>u4565</i>	H(240)...H(246)	731.5(85)	25.5(fixed)	—	-5.8	25.5
<i>u4610</i>	H(69)...H(79)	732.1(36)	34.5(fixed)	—	-12.1	34.5
<i>u4609</i>	H(265)...H(277)	732.2(46)	26.9(fixed)	—	-8.5	26.9
<i>u4590</i>	H(112)...H(121)	732.8(46)	26.6(fixed)	—	-6.5	26.6
<i>u2045</i>	H(144)...H(149)	733.4(101)	52.5(fixed)	—	-7.2	52.5
<i>u4575</i>	H(66)...H(76)	733.4(86)	25.3(fixed)	—	-6.4	25.3
<i>u4312</i>	H(265)...H(270)	733.6(53)	49.6(fixed)	—	5.2	49.6
<i>u4556</i>	H(29)...H(34)	733.8(55)	33.8(fixed)	—	7.5	33.8
<i>u4588</i>	H(188)...H(202)	734.2(61)	29.0(fixed)	—	-7.7	29.0
<i>u4569</i>	H(185)...H(199)	734.6(103)	25.6(fixed)	—	-9.3	25.6
<i>u4570</i>	H(189)...H(200)	734.6(103)	25.6(fixed)	—	-9.3	25.6
<i>u4592</i>	H(238)...H(246)	734.6(96)	26.0(fixed)	—	-5.3	26.0
<i>u4606</i>	H(21)...H(26)	734.9(77)	31.0(fixed)	—	-3.1	31.0
<i>u4604</i>	H(227)...H(230)	736.5(128)	27.0(fixed)	—	-8.6	27.0
<i>u4614</i>	H(28)...H(34)	736.7(37)	39.7(fixed)	—	-5.2	39.7
<i>u4596</i>	H(67)...H(75)	738.8(111)	25.6(fixed)	—	-5.9	25.6
<i>u4597</i>	H(239)...H(244)	738.9(35)	26.6(fixed)	—	-6.5	26.6
<i>u4589</i>	H(66)...H(74)	739.0(69)	27.0(fixed)	—	-5.7	27.0
<i>u1990</i>	H(143)...H(157)	741.3(35)	45.5(fixed)	—	-0.8	45.5
<i>u4584</i>	H(226)...H(229)	742.6(75)	29.5(fixed)	—	-5.2	29.5
<i>u4572</i>	H(21)...H(24)	745.2(69)	32.5(fixed)	—	-0.2	32.5
<i>u1686</i>	H(142)...H(158)	745.6(88)	33.9(fixed)	—	6.9	33.9
<i>u3236</i>	H(272)...H(280)	749.6(111)	52.5(fixed)	—	36.3	52.5
<i>u1693</i>	H(145)...H(148)	757.7(101)	40.9(fixed)	—	15.6	40.9
<i>u4611</i>	H(274)...H(280)	761.5(87)	25.7(fixed)	—	-6.1	25.7
<i>u4618</i>	H(183)...H(191)	775.4(20)	25.2(fixed)	—	-18.4	25.2
<i>u4617</i>	H(265)...H(276)	776.3(40)	21.2(fixed)	—	-9.2	21.2
<i>u4621</i>	H(60)...H(71)	776.5(41)	21.5(fixed)	—	-12.6	21.5
<i>u4616</i>	H(27)...H(34)	778.7(17)	29.2(fixed)	—	-16.8	29.2
<i>u4615</i>	H(232)...H(235)	779.1(19)	24.8(fixed)	—	-14.2	24.8
<i>u4558</i>	H(275)...H(280)	779.6(64)	26.6(fixed)	—	-4.1	26.6
<i>u4626</i>	H(103)...H(107)	780.9(18)	21.2(fixed)	—	-17.1	21.2
<i>u4620</i>	H(68)...H(79)	781.8(17)	22.9(fixed)	—	-15.6	22.9
<i>u4627</i>	H(112)...H(123)	782.7(35)	19.4(fixed)	—	-8.8	19.4
<i>u4623</i>	H(21)...H(25)	784.3(17)	21.2(fixed)	—	-14.1	21.2
<i>u2992</i>	H(142)...H(157)	784.6(17)	39.1(fixed)	—	-5.7	39.1
<i>u3022</i>	H(144)...H(148)	785.7(19)	49.7(fixed)	—	-12.2	49.7
<i>u4629</i>	H(226)...H(230)	787.5(17)	19.9(fixed)	—	-11.3	19.9
<i>u4625</i>	H(239)...H(246)	787.8(16)	19.8(fixed)	—	-8.8	19.8
<i>u4628</i>	H(185)...H(198)	788.7(18)	19.4(fixed)	—	-10.0	19.4
<i>u4624</i>	H(66)...H(75)	791.1(16)	19.4(fixed)	—	-8.7	19.4

<sup>a</sup> Distances in pm. Values in parentheses are the standard deviations on the last digits. See Figure 1 for atom numbering.

**Table S11** Refined and calculated [B3LYP/6-31G(d)] amplitudes of vibration ( $u_{h1}$ ), associated  $r_a$  distances and corresponding correction values ( $k_{h1}$ ) for the refinement of C(SiClMe<sub>2</sub>)<sub>4</sub> (**3**).<sup>a</sup>

	Atom pair	$r_a$	$u_{GED}$	Restraint	$k_{h1}$	$u_{calc.}$
$u_{22}$	C(10)-H(31)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_2$	C(10)-H(32)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.6
$u_{19}$	C(51)-H(72)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.6
$u_{24}$	C(50)-H(69)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.6
$u_{18}$	C(11)-H(33)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.6
$u_{16}$	C(48)-H(64)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{20}$	C(6)-H(20)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{23}$	C(9)-H(28)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{21}$	C(13)-H(39)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_3$	C(47)-H(59)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{11}$	C(12)-H(37)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{14}$	C(8)-H(24)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{10}$	C(8)-H(26)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{12}$	C(49)-H(67)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_4$	C(12)-H(36)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{17}$	C(49)-H(65)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{15}$	C(7)-H(23)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{13}$	C(6)-H(18)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{31}$	C(47)-H(60)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{34}$	C(10)-H(30)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_7$	C(48)-H(63)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_8$	C(13)-H(40)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_5$	C(11)-H(35)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_9$	C(7)-H(22)	110.7(6)	7.5(6)	0.8	0.4	7.6
$u_{35}$	C(12)-H(38)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_6$	C(9)-H(29)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{30}$	C(11)-H(34)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_1$	C(50)-H(70)	110.7(6)	7.5(tied to $u_9$ )	—	0.4	7.6
$u_{28}$	C(50)-H(68)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{29}$	C(7)-H(21)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{27}$	C(13)-H(41)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{26}$	C(9)-H(27)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{25}$	C(6)-H(19)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{36}$	C(49)-H(66)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{32}$	C(48)-H(62)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{33}$	C(8)-H(25)	110.7(6)	7.6(tied to $u_9$ )	—	0.4	7.7
$u_{61}$	H(60)...H(61)	178.7(12)	12.6(fixed)	—	-0.2	12.6
$u_{58}$	H(30)...H(31)	178.8(12)	12.6(fixed)	—	-0.2	12.6

<i>u</i> 39	H(59)...H(61)	178.8(12)	12.6(fixed)	—	-0.2	12.6
<i>u</i> 47	H(30)...H(32)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 53	H(59)...H(60)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 51	H(36)...H(38)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 54	H(71)...H(73)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 42	H(31)...H(32)	178.8(12)	12.6(fixed)	—	-0.2	12.6
<i>u</i> 48	H(36)...H(37)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 65	H(37)...H(38)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 40	H(33)...H(35)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 49	H(34)...H(35)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 59	H(33)...H(34)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 41	H(63)...H(64)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 50	H(62)...H(63)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 62	H(62)...H(64)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 55	H(39)...H(41)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 37	H(66)...H(67)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 38	H(25)...H(26)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 44	H(40)...H(41)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 43	H(18)...H(19)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 46	H(27)...H(29)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 56	H(27)...H(28)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 64	H(24)...H(25)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 60	H(65)...H(66)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 45	H(21)...H(22)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 63	H(21)...H(23)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 52	H(19)...H(20)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 57	H(68)...H(70)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 68	H(39)...H(40)	178.8(12)	12.5(fixed)	—	-0.2	12.5
<i>u</i> 66	H(65)...H(67)	178.9(12)	12.5(fixed)	—	-0.1	12.5
<i>u</i> 67	H(24)...H(26)	178.9(12)	12.5(fixed)	—	-0.1	12.5
<i>u</i> 69	H(28)...H(29)	178.9(12)	12.5(fixed)	—	-0.1	12.5
<i>u</i> 70	H(18)...H(20)	178.9(12)	12.5(fixed)	—	-0.1	12.5
<i>u</i> 71	H(69)...H(70)	178.9(12)	12.4(fixed)	—	-0.1	12.4
<i>u</i> 72	H(22)...H(23)	178.9(12)	12.5(fixed)	—	-0.1	12.5
<i>u</i> 84	Si(43)-C(53)	188.8(4)	7.3(tied to <i>u</i> 73)	—	0.2	5.8
<i>u</i> 73	Si(2)-C(12)	189.0(4)	7.2(6)	1.0	0.2	5.8
<i>u</i> 74	Si(5)-C(7)	189.1(4)	7.2(tied to <i>u</i> 73)	—	0.2	5.8
<i>u</i> 76	Si(3)-C(9)	189.3(4)	7.2(tied to <i>u</i> 73)	—	0.2	5.8
<i>u</i> 77	Si(45)-C(51)	189.4(4)	7.2(tied to <i>u</i> 73)	—	0.2	5.8
<i>u</i> 78	Si(45)-C(52)	189.4(4)	7.2(tied to <i>u</i> 73)	—	0.2	5.8
<i>u</i> 79	Si(2)-C(13)	189.5(4)	7.2(tied to <i>u</i> 73)	—	0.2	5.8
<i>u</i> 82	Si(4)-C(10)	189.5(4)	7.2(tied to <i>u</i> 73)	—	0.2	5.8
<i>u</i> 81	Si(4)-C(11)	189.5(4)	7.2(tied to <i>u</i> 73)	—	0.2	5.8
<i>u</i> 80	Si(3)-C(8)	189.6(4)	7.3(tied to <i>u</i> 73)	—	0.2	5.8

<i>u83</i>	Si(5)-C(6)	189.7(4)	7.3(tied to <i>u73</i> )	—	0.2	5.8
<i>u75</i>	Si(43)-C(54)	189.7(4)	7.2(tied to <i>u73</i> )	—	0.2	5.8
<i>u90</i>	C(42)-Si(43)	191.4(4)	6.7(tied to <i>u86</i> )	—	0.3	6.6
<i>u86</i>	C(1)-Si(4)	191.7(4)	6.5(10)	1.0	0.3	6.5
<i>u87</i>	C(1)-Si(3)	191.8(4)	6.6(tied to <i>u86</i> )	—	0.3	6.6
<i>u88</i>	C(1)-Si(2)	192.0(4)	6.6(tied to <i>u86</i> )	—	0.3	6.6
<i>u89</i>	C(1)-Si(5)	192.5(4)	6.7(tied to <i>u86</i> )	—	0.3	6.6
<i>u85</i>	C(42)-Si(45)	192.5(4)	6.6(tied to <i>u86</i> )	—	0.3	6.5
<i>u91</i>	Si(4)-Cl(15)	206.9(2)	4.2(3)	0.6	0.2	5.9
<i>u92</i>	Si(43)-Cl(55)	207.5(2)	4.2(tied to <i>u91</i> )	—	0.2	6.0
<i>u93</i>	Si(5)-Cl(17)	208.2(2)	4.3(tied to <i>u91</i> )	—	0.3	6.1
<i>u94</i>	Si(45)-Cl(56)	208.3(2)	4.3(tied to <i>u91</i> )	—	0.3	6.1
<i>u95</i>	Si(3)-Cl(16)	208.8(2)	4.3(tied to <i>u91</i> )	—	0.3	6.1
<i>u96</i>	Si(2)-Cl(14)	209.2(2)	4.4(tied to <i>u91</i> )	—	0.3	6.2
<i>u105</i>	H(64)...H(67)	214.6(91)	44.5(fixed)	—	16.5	44.5
<i>u101</i>	H(23)...H(32)	218.8(104)	46.0(fixed)	—	19.9	46.0
<i>u99</i>	H(26)...H(31)	222.6(51)	40.1(fixed)	—	24.7	40.1
<i>u102</i>	H(59)...H(80)	223.2(94)	44.6(fixed)	—	19.8	44.6
<i>u97</i>	H(35)...H(36)	225.1(103)	42.8(fixed)	—	30.9	42.8
<i>u106</i>	H(22)...H(32)	238.5(99)	44.8(fixed)	—	18.5	44.8
<i>u121</i>	H(29)...H(40)	239.8(87)	46.0(fixed)	—	13.0	46.0
<i>u115</i>	H(28)...H(40)	241.6(110)	43.9(fixed)	—	12.0	43.9
<i>u104</i>	H(18)...H(29)	242.2(107)	43.1(fixed)	—	12.3	43.1
<i>u103</i>	H(26)...H(33)	244.9(101)	45.6(fixed)	—	19.7	45.6
<i>u100</i>	H(63)...H(76)	246.7(114)	42.8(fixed)	—	27.9	42.8
<i>u142</i>	H(18)...H(39)	246.8(104)	47.1(fixed)	—	10.0	47.1
<i>u98</i>	H(61)...H(67)	247.3(46)	40.3(fixed)	—	25.9	40.3
<i>u109</i>	Si(43)...H(79)	249.0(8)	14.7(tied to <i>u160</i> )	—	-0.3	13.0
<i>u131</i>	Si(43)...H(78)	249.0(8)	14.5(tied to <i>u160</i> )	—	-0.3	12.9
<i>u150</i>	Si(43)...H(77)	249.0(8)	14.3(tied to <i>u160</i> )	—	-0.3	12.7
<i>u125</i>	Si(2)...H(37)	249.2(8)	14.6(tied to <i>u160</i> )	—	-0.3	12.9
<i>u111</i>	Si(2)...H(38)	249.2(8)	14.6(tied to <i>u160</i> )	—	-0.3	13.0
<i>u108</i>	Si(5)...H(21)	249.2(8)	14.5(tied to <i>u160</i> )	—	-0.4	12.9
<i>u130</i>	Si(5)...H(23)	249.3(8)	14.4(tied to <i>u160</i> )	—	-0.3	12.8
<i>u144</i>	Si(2)...H(36)	249.3(8)	14.3(tied to <i>u160</i> )	—	-0.3	12.7
<i>u135</i>	Si(5)...H(22)	249.3(8)	14.2(tied to <i>u160</i> )	—	-0.3	12.7
<i>u126</i>	Si(3)...H(28)	249.4(8)	14.6(tied to <i>u160</i> )	—	-0.4	13.0
<i>u114</i>	Si(3)...H(27)	249.4(8)	14.6(tied to <i>u160</i> )	—	-0.4	13.0
<i>u145</i>	Si(3)...H(29)	249.5(8)	14.2(tied to <i>u160</i> )	—	-0.3	12.7
<i>u116</i>	Si(45)...H(75)	249.5(8)	14.6(tied to <i>u160</i> )	—	-0.3	13.0
<i>u132</i>	Si(45)...H(74)	249.5(8)	14.7(tied to <i>u160</i> )	—	-0.3	13.0
<i>u147</i>	Si(45)...H(76)	249.6(8)	14.4(tied to <i>u160</i> )	—	-0.3	12.8
<i>u120</i>	Si(45)...H(71)	249.6(8)	14.6(tied to <i>u160</i> )	—	-0.3	13.0
<i>u138</i>	Si(45)...H(72)	249.6(8)	14.7(tied to <i>u160</i> )	—	-0.3	13.1

<i>u117</i>	Si(2)...H(41)	249.6(8)	14.6(tied to <i>u160</i> )	—	-0.3	13.0
<i>u139</i>	Si(45)...H(73)	249.6(8)	14.5(tied to <i>u160</i> )	—	-0.3	12.9
<i>u133</i>	Si(4)...H(33)	249.6(8)	14.8(tied to <i>u160</i> )	—	-0.3	13.2
<i>u119</i>	Si(4)...H(34)	249.6(8)	14.7(tied to <i>u160</i> )	—	-0.3	13.1
<i>u128</i>	Si(2)...H(39)	249.6(8)	14.6(tied to <i>u160</i> )	—	-0.3	12.9
<i>u118</i>	Si(4)...H(30)	249.6(8)	14.7(tied to <i>u160</i> )	—	-0.3	13.1
<i>u140</i>	Si(4)...H(31)	249.7(8)	14.7(tied to <i>u160</i> )	—	-0.3	13.1
<i>u146</i>	Si(2)...H(40)	249.7(8)	14.3(tied to <i>u160</i> )	—	-0.3	12.7
<i>u148</i>	Si(4)...H(35)	249.7(8)	14.5(tied to <i>u160</i> )	—	-0.3	12.9
<i>u141</i>	Si(4)...H(32)	249.7(8)	14.5(tied to <i>u160</i> )	—	-0.3	12.9
<i>u112</i>	Si(3)...H(25)	249.7(8)	14.6(tied to <i>u160</i> )	—	-0.3	13.0
<i>u129</i>	Si(3)...H(24)	249.7(8)	14.5(tied to <i>u160</i> )	—	-0.3	12.9
<i>u149</i>	Si(3)...H(26)	249.7(8)	14.3(tied to <i>u160</i> )	—	-0.3	12.7
<i>u113</i>	Si(5)...H(19)	249.8(8)	14.6(tied to <i>u160</i> )	—	-0.4	13.0
<i>u110</i>	Si(43)...H(82)	249.8(8)	14.5(tied to <i>u160</i> )	—	-0.4	12.9
<i>u127</i>	Si(43)...H(80)	249.8(8)	14.5(tied to <i>u160</i> )	—	-0.3	12.9
<i>u134</i>	Si(5)...H(20)	249.8(8)	14.4(tied to <i>u160</i> )	—	-0.3	12.8
<i>u143</i>	Si(5)...H(18)	249.8(8)	14.3(tied to <i>u160</i> )	—	-0.3	12.7
<i>u137</i>	Si(43)...H(81)	249.8(8)	14.1(tied to <i>u160</i> )	—	-0.3	12.6
<i>u136</i>	H(18)...H(40)	251.1(94)	48.5(fixed)	—	11.2	48.5
<i>u153</i>	Cl(55)...H(70)	252.3(41)	28.6(fixed)	—	9.1	28.6
<i>u124</i>	H(20)...H(29)	254.6(123)	44.4(fixed)	—	10.1	44.4
<i>u123</i>	H(64)...H(65)	255.5(86)	49.2(fixed)	—	17.2	49.2
<i>u107</i>	H(59)...H(81)	257.6(96)	47.8(fixed)	—	19.8	47.8
<i>u171</i>	Cl(15)...H(22)	258.3(88)	32.8(fixed)	—	6.8	32.8
<i>u122</i>	H(24)...H(33)	259.4(105)	50.7(fixed)	—	19.8	50.7
<i>u162</i>	Cl(56)...H(65)	264.5(42)	33.0(tied to <i>u160</i> )	—	9.4	29.4
<i>u151</i>	C(7)...H(32)	269.6(85)	32.4(fixed)	—	16.8	32.4
<i>u170</i>	Cl(16)...H(20)	274.1(43)	33.7(tied to <i>u160</i> )	—	6.8	30.0
<i>u160</i>	Cl(17)...H(37)	275.5(46)	33.8(27)	3.0	13.5	30.1
<i>u158</i>	C(49)...H(64)	276.9(42)	36.7(tied to <i>u160</i> )	—	14.2	32.7
<i>u152</i>	C(50)...H(73)	281.3(44)	33.8(fixed)	—	17.5	33.8
<i>u157</i>	C(9)...H(40)	281.9(55)	33.6(tied to <i>u160</i> )	—	10.0	29.9
<i>u163</i>	Cl(14)...H(24)	282.6(37)	29.2(fixed)	—	9.6	29.2
<i>u168</i>	Cl(17)...H(39)	285.2(57)	30.3(fixed)	—	8.2	30.3
<i>u192</i>	Cl(55)...H(72)	286.4(64)	56.4(tied to <i>u160</i> )	—	7.8	50.2
<i>u172</i>	Cl(14)...H(28)	288.0(41)	33.0(fixed)	—	7.1	33.0
<i>u215</i>	C(48)...H(67)	288.0(65)	41.4(tied to <i>u160</i> )	—	4.2	36.8
<i>u188</i>	Cl(56)...H(63)	288.3(56)	51.5(tied to <i>u160</i> )	—	6.8	45.7
<i>u159</i>	C(6)...H(29)	289.9(83)	33.5(tied to <i>u160</i> )	—	8.8	29.8
<i>u167</i>	C(13)...H(18)	290.7(57)	35.3(tied to <i>u160</i> )	—	7.8	31.4
<i>u169</i>	Cl(16)...H(23)	291.6(48)	30.5(fixed)	—	7.9	30.5
<i>u154</i>	C(8)...H(33)	294.3(63)	34.4(fixed)	—	17.1	34.4
<i>u231</i>	C(10)...H(22)	295.7(104)	40.1(tied to <i>u160</i> )	—	3.4	35.6

<i>u184</i>	C(10)...H(26)	296.8(40)	30.6(fixed)	—	8.0	30.6
<i>u156</i>	H(25)...H(27)	297.4(60)	35.5(fixed)	—	6.5	35.5
<i>u178</i>	C(11)...H(36)	297.6(74)	34.8(tied to <i>u160</i> )	—	12.2	31.0
<i>u230</i>	C(47)...H(80)	300.2(68)	40.1(tied to <i>u160</i> )	—	3.7	35.6
<i>u177</i>	C(12)...H(35)	300.3(78)	37.9(tied to <i>u160</i> )	—	15.3	33.7
<i>u278</i>	Si(4)...H(22)	300.3(80)	32.7(tied to <i>u160</i> )	—	3.5	29.1
<i>u155</i>	H(66)...H(68)	301.2(60)	35.5(fixed)	—	6.9	35.5
<i>u166</i>	H(38)...H(41)	302.7(59)	37.4(fixed)	—	9.7	37.4
<i>u187</i>	C(8)...H(31)	303.5(40)	32.8(fixed)	—	14.1	32.8
<i>u164</i>	H(19)...H(21)	303.6(59)	34.6(fixed)	—	6.1	34.6
<i>u264</i>	C(10)...H(23)	303.8(92)	43.7(tied to <i>u160</i> )	—	3.1	38.9
<i>u176</i>	C(10)...C(11)	304.0(42)	12.9(tied to <i>u403</i> )	—	-0.1	11.6
<i>u175</i>	C(8)...C(9)	304.0(40)	12.9(tied to <i>u403</i> )	—	-0.1	11.7
<i>u173</i>	C(49)...C(50)	305.0(40)	12.8(tied to <i>u403</i> )	—	-0.1	11.6
<i>u180</i>	C(12)...C(13)	305.1(39)	13.0(tied to <i>u403</i> )	—	-0.1	11.7
<i>u233</i>	Si(4)...Si(5)	306.4(49)	10.5(tied to <i>u403</i> )	—	0.0	9.5
<i>u323</i>	Cl(16)...H(32)	306.4(74)	59.7(fixed)	—	2.7	59.7
<i>u179</i>	C(47)...C(48)	306.5(40)	12.9(tied to <i>u403</i> )	—	-0.1	11.6
<i>u315</i>	Cl(57)...H(59)	307.3(64)	60.5(fixed)	—	3.2	60.5
<i>u182</i>	C(6)...C(7)	307.8(39)	13.1(tied to <i>u403</i> )	—	-0.1	11.8
<i>u198</i>	Cl(15)...H(36)	307.9(66)	46.3(fixed)	—	5.5	46.3
<i>u191</i>	Cl(16)...H(31)	308.7(61)	47.5(fixed)	—	8.0	47.5
<i>u229</i>	Si(45)...H(77)	308.8(36)	30.1(fixed)	—	4.5	30.1
<i>u165</i>	H(71)...H(75)	309.2(60)	40.7(fixed)	—	12.8	40.7
<i>u161</i>	H(30)...H(34)	309.4(62)	41.2(fixed)	—	13.8	41.2
<i>u174</i>	C(47)...H(67)	309.7(35)	29.9(fixed)	—	8.0	29.9
<i>u195</i>	Si(43)...Si(45)	310.1(7)	10.8(tied to <i>u403</i> )	—	0.0	9.8
<i>u254</i>	H(31)...H(33)	310.4(95)	50.0(fixed)	—	9.5	50.0
<i>u190</i>	Cl(14)...H(35)	310.8(68)	49.0(fixed)	—	8.1	49.0
<i>u209</i>	C(7)...Cl(17)	312.3(16)	13.0(tied to <i>u403</i> )	—	-0.1	11.7
<i>u222</i>	C(11)...H(26)	312.3(72)	36.6(fixed)	—	4.3	36.6
<i>u197</i>	Si(3)...Si(4)	313.3(7)	10.8(tied to <i>u403</i> )	—	0.0	9.8
<i>u212</i>	Si(2)...Si(5)	313.6(7)	10.6(tied to <i>u403</i> )	—	0.1	9.6
<i>u252</i>	Si(43)...Si(44)	313.7(9)	10.3(tied to <i>u403</i> )	—	0.1	9.3
<i>u228</i>	H(24)...H(28)	313.8(93)	40.0(fixed)	—	3.0	40.0
<i>u225</i>	C(50)...Cl(57)	314.6(16)	13.2(tied to <i>u403</i> )	—	-0.2	11.9
<i>u218</i>	Si(2)...Si(3)	314.6(7)	10.6(tied to <i>u403</i> )	—	0.0	9.5
<i>u221</i>	Si(43)...Si(46)	314.6(9)	10.5(tied to <i>u403</i> )	—	0.1	9.5
<i>u207</i>	C(8)...Cl(16)	314.9(16)	12.9(tied to <i>u403</i> )	—	-0.1	11.7
<i>u200</i>	H(65)...H(69)	315.2(92)	39.3(fixed)	—	4.4	39.3
<i>u214</i>	Si(3)...Si(5)	315.3(7)	10.7(tied to <i>u403</i> )	—	0.0	9.6
<i>u203</i>	C(49)...Cl(57)	315.4(16)	12.9(tied to <i>u403</i> )	—	-0.2	11.6
<i>u227</i>	Si(45)...Si(46)	315.4(9)	10.6(tied to <i>u403</i> )	—	0.0	9.6
<i>u224</i>	Si(2)...Si(4)	315.5(7)	10.7(tied to <i>u403</i> )	—	0.0	9.6



<i>u238</i>	H(37)...H(39)	315.5(92)	44.0(fixed)	—	4.5	44.0
<i>u237</i>	C(13)...H(28)	315.5(78)	37.4(fixed)	—	3.7	37.4
<i>u185</i>	C(48)...H(76)	315.7(82)	33.0(fixed)	—	12.7	33.0
<i>u265</i>	H(61)...H(64)	316.2(93)	49.5(fixed)	—	7.2	49.5
<i>u266</i>	Cl(15)...H(37)	316.4(60)	53.3(fixed)	—	3.7	53.3
<i>u213</i>	C(48)...Cl(58)	316.4(16)	13.0(tied to u403)	—	-0.1	11.8
<i>u208</i>	C(47)...Cl(58)	316.9(16)	13.0(tied to u403)	—	-0.1	11.7
<i>u199</i>	C(6)...Cl(17)	317.1(16)	12.9(tied to u403)	—	-0.2	11.6
<i>u219</i>	C(11)...Cl(15)	317.2(16)	12.9(tied to u403)	—	-0.1	11.7
<i>u217</i>	C(12)...Cl(14)	317.5(16)	13.0(tied to u403)	—	-0.1	11.7
<i>u253</i>	C(42)...C(49)	317.6(8)	12.0(tied to u403)	—	-0.1	10.9
<i>u210</i>	C(13)...Cl(14)	317.8(16)	13.1(tied to u403)	—	-0.2	11.8
<i>u240</i>	C(1)...C(11)	318.0(8)	11.9(tied to u403)	—	0.0	10.7
<i>u239</i>	C(1)...C(10)	318.0(8)	11.9(tied to u403)	—	0.0	10.7
<i>u211</i>	C(10)...Cl(15)	318.2(15)	12.9(tied to u403)	—	-0.1	11.7
<i>u205</i>	C(8)...H(27)	318.3(49)	25.4(fixed)	—	0.8	25.4
<i>u242</i>	C(1)...C(6)	318.3(8)	11.9(tied to u403)	—	0.0	10.8
<i>u250</i>	Si(4)...H(26)	318.6(39)	30.1(fixed)	—	4.6	30.1
<i>u241</i>	C(42)...C(47)	319.0(8)	11.8(tied to u403)	—	0.0	10.7
<i>u244</i>	C(1)...C(13)	319.1(8)	11.9(tied to u403)	—	0.0	10.7
<i>u223</i>	C(9)...Cl(16)	319.1(16)	13.2(tied to u403)	—	-0.2	11.9
<i>u261</i>	H(20)...H(23)	319.2(91)	38.5(fixed)	—	2.2	38.5
<i>u189</i>	C(9)...H(25)	319.3(43)	24.7(fixed)	—	1.3	24.7
<i>u245</i>	C(42)...C(48)	319.8(8)	11.8(tied to u403)	—	0.0	10.6
<i>u183</i>	C(49)...H(61)	319.9(34)	33.1(fixed)	—	15.0	33.1
<i>u251</i>	C(1)...C(9)	320.1(8)	11.9(tied to u403)	—	0.0	10.7
<i>u267</i>	C(6)...H(39)	320.1(73)	40.7(fixed)	—	3.8	40.7
<i>u220</i>	C(12)...H(41)	320.1(49)	26.1(fixed)	—	0.9	26.1
<i>u308</i>	Cl(56)...H(64)	320.1(56)	56.0(fixed)	—	3.2	56.0
<i>u275</i>	Si(3)...H(20)	320.4(45)	29.3(fixed)	—	3.4	29.3
<i>u186</i>	C(50)...H(66)	320.5(44)	24.8(fixed)	—	1.2	24.8
<i>u256</i>	C(42)...C(50)	321.0(8)	11.9(tied to u403)	—	0.0	10.8
<i>u201</i>	C(49)...H(68)	321.1(49)	25.3(fixed)	—	0.7	25.3
<i>u257</i>	C(1)...C(12)	321.5(8)	11.9(tied to u403)	—	0.0	10.8
<i>u193</i>	C(13)...H(38)	321.7(43)	26.8(fixed)	—	2.3	26.8
<i>u274</i>	Si(4)...H(36)	321.9(33)	32.8(fixed)	—	7.1	32.8
<i>u259</i>	C(1)...C(7)	322.0(8)	12.0(tied to u403)	—	0.0	10.8
<i>u260</i>	C(1)...C(8)	322.1(8)	12.0(tied to u403)	—	0.0	10.8
<i>u206</i>	C(10)...H(34)	322.4(45)	28.9(fixed)	—	2.6	28.9
<i>u280</i>	C(1)...Cl(16)	322.6(9)	12.4(tied to u403)	—	-0.2	11.2
<i>u279</i>	C(1)...Cl(14)	322.7(9)	12.4(tied to u403)	—	-0.2	11.2
<i>u270</i>	Si(45)...H(63)	322.7(32)	32.7(fixed)	—	7.9	32.7
<i>u194</i>	C(11)...H(30)	322.7(51)	28.8(fixed)	—	2.5	28.8
<i>u216</i>	C(7)...H(19)	322.9(49)	24.9(fixed)	—	0.7	24.9

<i>u</i> 269	Si(2)...H(35)	323.1(36)	34.3(fixed)	—	9.8	34.3
<i>u</i> 236	C(9)...H(20)	323.2(89)	37.7(fixed)	—	3.2	37.7
<i>u</i> 299	C(11)...H(31)	323.2(64)	33.4(fixed)	—	0.6	33.4
<i>u</i> 276	C(10)...H(33)	323.4(66)	34.3(fixed)	—	0.6	34.3
<i>u</i> 204	C(47)...H(62)	323.8(44)	27.2(fixed)	—	2.2	27.2
<i>u</i> 196	C(6)...H(21)	324.0(42)	24.0(fixed)	—	1.0	24.0
<i>u</i> 202	C(48)...H(60)	324.1(50)	29.1(fixed)	—	2.7	29.1
<i>u</i> 255	Cl(17)...H(21)	324.4(27)	26.5(fixed)	—	0.6	26.5
<i>u</i> 288	C(42)...Cl(55)	324.4(9)	12.4(tied to <i>u</i> 403)	—	-0.1	11.2
<i>u</i> 282	C(1)...Cl(15)	324.5(9)	12.4(tied to <i>u</i> 403)	—	-0.1	11.2
<i>u</i> 301	Si(5)...H(39)	324.7(44)	30.5(fixed)	—	4.1	30.5
<i>u</i> 291	C(1)...Cl(17)	325.3(9)	12.5(tied to <i>u</i> 403)	—	-0.2	11.3
<i>u</i> 285	C(42)...Cl(56)	325.4(9)	12.4(tied to <i>u</i> 403)	—	-0.1	11.2
<i>u</i> 305	Si(2)...H(28)	325.4(42)	30.0(fixed)	—	3.7	30.0
<i>u</i> 181	Cl(56)...H(69)	325.5(49)	34.6(fixed)	—	6.9	34.6
<i>u</i> 296	C(13)...H(29)	325.9(63)	41.0(fixed)	—	2.9	41.0
<i>u</i> 283	Si(43)...H(72)	326.0(41)	35.6(fixed)	—	9.0	35.6
<i>u</i> 234	Cl(57)...H(68)	326.2(33)	25.3(fixed)	—	0.3	25.3
<i>u</i> 281	Si(3)...H(31)	326.8(42)	33.7(fixed)	—	8.9	33.7
<i>u</i> 289	C(9)...H(24)	327.0(63)	27.4(fixed)	—	-0.1	27.4
<i>u</i> 300	C(13)...H(37)	327.3(64)	31.5(fixed)	—	0.0	31.5
<i>u</i> 268	C(8)...H(28)	327.4(61)	26.8(fixed)	—	0.1	26.8
<i>u</i> 258	C(49)...H(69)	327.5(62)	26.4(fixed)	—	0.2	26.4
<i>u</i> 271	C(50)...H(65)	328.0(63)	27.0(fixed)	—	0.0	27.0
<i>u</i> 246	Cl(55)...H(79)	328.1(26)	27.3(fixed)	—	0.8	27.3
<i>u</i> 303	C(48)...H(61)	328.1(62)	34.0(fixed)	—	0.7	34.0
<i>u</i> 277	C(9)...H(18)	328.1(86)	38.3(fixed)	—	2.9	38.3
<i>u</i> 294	C(47)...H(64)	328.2(64)	32.0(fixed)	—	0.3	32.0
<i>u</i> 249	Cl(16)...H(25)	328.4(27)	27.7(fixed)	—	0.8	27.7
<i>u</i> 284	Cl(17)...H(22)	328.7(38)	27.0(fixed)	—	0.4	27.0
<i>u</i> 272	C(12)...H(39)	328.8(61)	27.5(fixed)	—	0.2	27.5
<i>u</i> 247	Cl(56)...H(75)	328.9(27)	30.3(fixed)	—	1.0	30.3
<i>u</i> 243	Cl(56)...H(71)	329.2(33)	32.3(fixed)	—	1.4	32.3
<i>u</i> 226	Cl(17)...H(19)	329.6(33)	25.3(fixed)	—	0.1	25.3
<i>u</i> 317	Cl(14)...H(33)	329.9(79)	61.0(fixed)	—	3.1	61.0
<i>u</i> 262	Cl(15)...H(30)	330.0(33)	31.5(fixed)	—	1.0	31.5
<i>u</i> 248	Cl(15)...H(34)	330.1(26)	31.8(fixed)	—	1.7	31.8
<i>u</i> 292	C(48)...H(65)	330.6(57)	43.2(fixed)	—	2.7	43.2
<i>u</i> 286	Cl(16)...H(26)	330.8(38)	28.3(fixed)	—	0.6	28.3
<i>u</i> 263	Cl(14)...H(38)	331.1(27)	30.9(fixed)	—	1.5	30.9
<i>u</i> 304	C(6)...H(23)	331.2(63)	26.0(fixed)	—	-0.2	26.0
<i>u</i> 232	Cl(14)...H(41)	331.7(34)	26.4(fixed)	—	0.5	26.4
<i>u</i> 306	Si(46)...H(80)	332.2(42)	29.9(fixed)	—	3.6	29.9
<i>u</i> 235	Cl(16)...H(27)	332.3(33)	25.7(fixed)	—	0.3	25.7

<i>u287</i>	C(7)...H(20)	332.4(60)	26.0(fixed)	—	0.1	26.0
<i>u316</i>	Cl(55)...H(81)	332.4(39)	27.9(fixed)	—	0.0	27.9
<i>u273</i>	C(47)...H(81)	333.3(64)	40.8(fixed)	—	2.9	40.8
<i>u293</i>	Cl(55)...H(77)	333.3(38)	28.2(fixed)	—	0.6	28.2
<i>u368</i>	C(50)...Cl(55)	333.5(31)	22.6(tied to <i>u403</i> )	—	1.0	20.4
<i>u307</i>	Cl(56)...H(76)	333.6(38)	33.6(fixed)	—	1.0	33.6
<i>u309</i>	Cl(14)...H(40)	333.7(39)	29.3(fixed)	—	0.3	29.3
<i>u297</i>	Cl(56)...H(73)	334.1(39)	36.0(fixed)	—	1.3	36.0
<i>u302</i>	Cl(14)...H(36)	334.3(38)	32.6(fixed)	—	1.3	32.6
<i>u298</i>	Cl(17)...H(18)	334.6(38)	27.4(fixed)	—	0.2	27.4
<i>u311</i>	Cl(15)...H(35)	335.3(37)	36.0(fixed)	—	1.2	36.0
<i>u290</i>	C(11)...H(24)	335.8(80)	43.7(fixed)	—	2.7	43.7
<i>u429</i>	H(22)...H(30)	336.2(131)	52.4(fixed)	—	-0.3	52.4
<i>u409</i>	C(7)...Cl(15)	336.4(85)	27.1(tied to <i>u403</i> )	—	0.3	24.5
<i>u295</i>	Cl(15)...H(32)	336.7(38)	35.1(fixed)	—	0.5	35.1
<i>u313</i>	Cl(16)...H(29)	336.7(38)	28.2(fixed)	—	0.1	28.2
<i>u319</i>	C(1)...H(18)	336.9(27)	23.0(fixed)	—	0.8	23.0
<i>u343</i>	C(42)...H(67)	337.1(23)	22.3(fixed)	—	0.9	22.3
<i>u356</i>	C(7)...C(10)	337.6(81)	22.9(tied to <i>u403</i> )	—	1.1	20.6
<i>u329</i>	C(1)...H(32)	337.7(27)	26.7(fixed)	—	2.1	26.7
<i>u372</i>	C(47)...Cl(57)	337.9(25)	27.9(tied to <i>u403</i> )	—	0.7	25.2
<i>u312</i>	C(6)...H(40)	338.3(72)	43.7(fixed)	—	2.9	43.7
<i>u403</i>	Cl(15)...Cl(17)	338.3(102)	27.8(11)	—	0.9	25.1
<i>u320</i>	C(1)...H(40)	338.3(27)	23.9(fixed)	—	1.1	23.9
<i>u327</i>	C(1)...H(35)	338.4(23)	25.8(fixed)	—	2.5	25.8
<i>u325</i>	C(42)...H(59)	338.9(27)	26.9(fixed)	—	2.5	26.9
<i>u321</i>	C(1)...H(29)	339.6(26)	23.2(fixed)	—	0.9	23.2
<i>u374</i>	Si(4)...C(7)	339.7(64)	17.5(tied to <i>u403</i> )	—	0.3	15.8
<i>u328</i>	C(42)...H(63)	340.1(23)	24.6(fixed)	—	1.9	24.6
<i>u324</i>	C(42)...H(70)	340.7(26)	22.9(fixed)	—	0.8	22.9
<i>u338</i>	C(1)...H(22)	342.0(22)	21.6(fixed)	—	0.6	21.6
<i>u331</i>	C(42)...H(65)	342.0(23)	23.6(fixed)	—	0.6	23.6
<i>u375</i>	C(49)...Cl(56)	342.1(34)	23.0(tied to <i>u403</i> )	—	1.0	20.8
<i>u333</i>	Si(2)...Cl(17)	342.2(21)	18.8(tied to <i>u403</i> )	—	0.1	17.0
<i>u340</i>	C(1)...H(36)	342.4(22)	24.2(fixed)	—	1.8	24.2
<i>u347</i>	C(1)...H(26)	342.5(22)	22.2(fixed)	—	0.9	22.2
<i>u398</i>	Si(5)...Cl(15)	342.5(72)	19.5(tied to <i>u403</i> )	—	0.1	17.6
<i>u326</i>	H(30)...H(33)	342.7(81)	56.9(fixed)	—	-2.9	56.9
<i>u345</i>	C(1)...H(20)	342.7(29)	21.7(fixed)	—	0.4	21.7
<i>u335</i>	C(1)...H(33)	342.7(23)	27.8(fixed)	—	1.8	27.8
<i>u357</i>	H(31)...H(34)	343.0(72)	55.1(fixed)	—	-2.2	55.1
<i>u330</i>	C(1)...H(31)	343.5(29)	26.2(fixed)	—	1.9	26.2
<i>u349</i>	C(1)...H(39)	343.8(28)	22.5(fixed)	—	0.5	22.5
<i>u362</i>	C(48)...Cl(56)	344.1(21)	26.9(tied to <i>u403</i> )	—	0.9	24.3

<i>u339</i>	C(42)...H(61)	344.3(29)	27.1(fixed)	—	1.8	27.1
<i>u344</i>	Si(5)...Cl(16)	344.3(15)	18.8(tied to <i>u403</i> )	—	0.0	17.0
<i>u337</i>	C(42)...H(64)	344.7(23)	26.0(fixed)	—	1.4	26.0
<i>u371</i>	H(23)...H(31)	344.8(98)	65.6(fixed)	—	-0.4	65.6
<i>u367</i>	C(12)...Cl(17)	344.8(33)	22.6(tied to <i>u403</i> )	—	1.0	20.4
<i>u351</i>	C(1)...H(28)	345.1(28)	22.1(fixed)	—	0.4	22.1
<i>u346</i>	Si(3)...Cl(14)	345.4(20)	19.0(tied to <i>u403</i> )	—	0.0	17.2
<i>u355</i>	C(42)...H(69)	346.3(28)	21.9(fixed)	—	0.4	21.9
<i>u363</i>	H(37)...H(41)	346.4(79)	47.5(fixed)	—	-2.6	47.5
<i>u359</i>	C(48)...C(49)	346.6(33)	23.9(tied to <i>u403</i> )	—	0.9	21.6
<i>u332</i>	C(1)...H(37)	346.9(23)	26.1(fixed)	—	1.3	26.1
<i>u336</i>	C(1)...H(23)	346.9(23)	23.1(fixed)	—	0.5	23.1
<i>u342</i>	H(60)...H(64)	346.9(79)	53.6(fixed)	—	-2.9	53.6
<i>u376</i>	C(10)...Cl(16)	347.1(24)	27.5(tied to <i>u403</i> )	—	0.7	24.8
<i>u341</i>	C(1)...H(24)	347.2(23)	23.7(fixed)	—	0.6	23.7
<i>u354</i>	H(24)...H(27)	347.3(78)	41.7(fixed)	—	-1.9	41.7
<i>u350</i>	H(61)...H(62)	347.6(70)	53.6(fixed)	—	-2.0	53.6
<i>u310</i>	H(66)...H(69)	347.6(70)	41.2(fixed)	—	-1.9	41.2
<i>u314</i>	H(25)...H(28)	347.8(69)	41.3(fixed)	—	-2.0	41.3
<i>u384</i>	C(6)...Cl(16)	348.5(31)	24.4(tied to <i>u403</i> )	—	0.4	22.0
<i>u382</i>	H(34)...H(36)	348.9(76)	50.5(fixed)	—	7.4	50.5
<i>u318</i>	H(38)...H(39)	348.9(68)	45.8(fixed)	—	-1.9	45.8
<i>u402</i>	H(63)...H(65)	349.0(45)	65.1(fixed)	—	0.9	65.1
<i>u383</i>	H(70)...H(72)	349.1(47)	68.9(fixed)	—	0.4	68.9
<i>u414</i>	H(75)...H(77)	349.2(39)	51.7(fixed)	—	1.6	51.7
<i>u334</i>	Si(45)...C(53)	350.2(23)	17.9(tied to <i>u403</i> )	—	0.2	16.2
<i>u352</i>	C(12)...Cl(15)	350.7(36)	26.6(tied to <i>u403</i> )	—	0.9	24.0
<i>u348</i>	H(78)...H(82)	350.8(77)	41.2(fixed)	—	-1.8	41.2
<i>u360</i>	C(50)...C(51)	352.5(33)	23.4(tied to <i>u403</i> )	—	1.0	21.1
<i>u361</i>	H(19)...H(23)	352.6(78)	39.1(fixed)	—	-1.6	39.1
<i>u370</i>	C(8)...Cl(14)	352.9(29)	22.6(tied to <i>u403</i> )	—	1.0	20.4
<i>u364</i>	Si(3)...C(6)	353.5(23)	17.0(tied to <i>u403</i> )	—	0.3	15.4
<i>u322</i>	H(20)...H(21)	354.3(67)	39.0(fixed)	—	-2.2	39.0
<i>u380</i>	C(13)...Cl(17)	354.6(45)	24.6(tied to <i>u403</i> )	—	0.3	22.2
<i>u422</i>	H(69)...H(71)	354.6(40)	54.7(fixed)	—	-0.1	54.7
<i>u366</i>	Si(43)...Cl(58)	355.4(16)	19.4(tied to <i>u403</i> )	—	0.1	17.5
<i>u389</i>	Si(43)...Cl(57)	355.5(16)	18.7(tied to <i>u403</i> )	—	0.2	16.9
<i>u393</i>	H(26)...H(30)	355.9(58)	48.9(fixed)	—	3.5	48.9
<i>u392</i>	Si(3)...C(10)	356.3(21)	18.2(tied to <i>u403</i> )	—	0.2	16.5
<i>u353</i>	Si(4)...C(8)	356.4(29)	18.1(tied to <i>u403</i> )	—	0.2	16.3
<i>u396</i>	Si(5)...H(32)	356.4(52)	30.4(fixed)	—	8.5	30.4
<i>u385</i>	Si(43)...C(51)	356.7(19)	18.0(tied to <i>u403</i> )	—	0.2	16.2
<i>u369</i>	C(9)...C(13)	357.0(40)	23.5(tied to <i>u403</i> )	—	0.9	21.2
<i>u377</i>	Si(4)...C(12)	357.1(16)	17.8(tied to <i>u403</i> )	—	0.2	16.1

<i>u381</i>	Si(2)...C(9)	357.7(17)	17.7(tied to u403)	—	0.3	16.0
<i>u406</i>	C(9)...Cl(14)	358.2(30)	26.9(tied to u403)	—	0.2	24.3
<i>u461</i>	H(63)...H(67)	358.3(102)	45.0(fixed)	—	-3.6	45.0
<i>u400</i>	H(35)...H(38)	358.4(78)	47.7(fixed)	—	11.7	47.7
<i>u378</i>	Si(5)...C(13)	358.4(23)	17.5(tied to u403)	—	0.3	15.8
<i>u430</i>	Si(4)...H(23)	358.8(62)	32.6(fixed)	—	0.2	32.6
<i>u394</i>	H(24)...H(35)	359.0(72)	70.4(fixed)	—	0.5	70.4
<i>u386</i>	Si(2)...C(11)	359.0(24)	18.0(tied to u403)	—	0.2	16.2
<i>u373</i>	C(11)...Cl(14)	359.2(50)	27.6(tied to u403)	—	0.7	24.9
<i>u358</i>	C(8)...C(11)	359.6(51)	23.6(tied to u403)	—	0.9	21.3
<i>u387</i>	Si(45)...C(48)	359.9(18)	17.9(tied to u403)	—	0.2	16.2
<i>u391</i>	C(7)...Cl(16)	360.5(36)	24.4(tied to u403)	—	0.9	22.0
<i>u447</i>	H(26)...H(32)	361.5(57)	43.0(fixed)	—	0.2	43.0
<i>u408</i>	H(25)...H(31)	361.7(52)	43.6(fixed)	—	12.2	43.6
<i>u441</i>	Si(43)...H(70)	362.0(32)	26.4(fixed)	—	3.6	26.4
<i>u419</i>	H(29)...H(39)	362.4(51)	53.0(fixed)	—	2.2	53.0
<i>u365</i>	C(6)...C(9)	362.5(63)	23.6(tied to u403)	—	0.8	21.3
<i>u388</i>	H(71)...H(77)	363.8(55)	49.2(fixed)	—	3.0	49.2
<i>u395</i>	Si(43)...H(59)	364.1(34)	29.9(fixed)	—	9.3	29.9
<i>u416</i>	H(21)...H(32)	364.6(91)	34.2(fixed)	—	13.2	34.2
<i>u379</i>	Si(45)...C(50)	365.2(21)	17.9(tied to u403)	—	0.3	16.2
<i>u390</i>	C(6)...C(13)	365.3(43)	25.4(tied to u403)	—	0.7	23.0
<i>u417</i>	Si(3)...H(18)	366.2(55)	32.0(fixed)	—	0.2	32.0
<i>u418</i>	C(11)...C(12)	366.9(60)	23.5(tied to u403)	—	0.3	21.3
<i>u397</i>	H(62)...H(76)	367.0(81)	48.2(fixed)	—	9.0	48.2
<i>u411</i>	H(28)...H(41)	367.5(53)	48.6(fixed)	—	2.5	48.6
<i>u443</i>	H(33)...H(36)	367.6(95)	45.0(fixed)	—	3.1	45.0
<i>u399</i>	Si(3)...H(40)	367.7(36)	27.5(fixed)	—	4.7	27.5
<i>u423</i>	H(26)...H(34)	367.7(52)	54.4(fixed)	—	0.6	54.4
<i>u462</i>	H(61)...H(80)	367.8(109)	46.7(fixed)	—	-5.4	46.7
<i>u424</i>	C(8)...C(10)	367.8(31)	24.2(tied to u403)	—	0.3	21.9
<i>u436</i>	H(35)...H(37)	369.1(98)	45.2(fixed)	—	7.4	45.2
<i>u432</i>	H(64)...H(66)	369.2(46)	35.1(fixed)	—	10.2	35.1
<i>u410</i>	Si(43)...H(74)	369.6(32)	29.4(fixed)	—	7.1	29.4
<i>u457</i>	Si(3)...H(32)	370.3(58)	43.9(fixed)	—	-0.9	43.9
<i>u448</i>	Si(45)...H(65)	371.6(35)	27.1(fixed)	—	3.7	27.1
<i>u426</i>	H(18)...H(28)	371.7(86)	48.7(fixed)	—	2.1	48.7
<i>u401</i>	H(61)...H(66)	371.8(50)	43.9(fixed)	—	13.1	43.9
<i>u428</i>	H(19)...H(39)	372.1(50)	48.9(fixed)	—	3.3	48.9
<i>u437</i>	Si(2)...H(29)	372.2(50)	33.9(fixed)	—	0.3	33.9
<i>u405</i>	H(20)...H(27)	373.3(68)	47.7(fixed)	—	2.4	47.7
<i>u413</i>	Si(2)...H(18)	373.7(37)	27.6(fixed)	—	3.5	27.6
<i>u499</i>	H(23)...H(30)	374.2(106)	43.1(fixed)	—	-5.4	43.1
<i>u452</i>	Si(43)...H(73)	374.6(51)	44.7(fixed)	—	-0.6	44.7

<i>u444</i>	H(24)...H(31)	374.8(52)	39.3(fixed)	—	8.1	39.3
<i>u404</i>	Si(3)...H(33)	375.0(40)	31.4(fixed)	—	8.7	31.4
<i>u438</i>	Si(5)...H(40)	376.1(54)	35.4(fixed)	—	0.2	35.4
<i>u407</i>	Si(5)...H(29)	376.1(50)	27.1(fixed)	—	4.1	27.1
<i>u445</i>	Si(4)...H(37)	376.2(45)	41.7(fixed)	—	-0.4	41.7
<i>u420</i>	H(59)...H(82)	376.4(46)	35.5(fixed)	—	13.9	35.5
<i>u415</i>	Si(45)...H(78)	377.0(49)	34.2(fixed)	—	-0.3	34.2
<i>u435</i>	H(27)...H(40)	377.4(57)	32.3(fixed)	—	5.7	32.3
<i>u412</i>	C(47)...C(49)	377.5(27)	23.5(tied to <i>u403</i> )	—	0.4	21.3
<i>u427</i>	Si(4)...H(24)	379.1(58)	34.9(fixed)	—	-0.3	34.9
<i>u463</i>	H(22)...H(31)	379.8(95)	47.2(fixed)	—	-5.2	47.2
<i>u442</i>	H(20)...H(40)	380.4(56)	51.6(fixed)	—	2.8	51.6
<i>u439</i>	H(59)...H(67)	380.9(49)	43.6(fixed)	—	-0.3	43.6
<i>u446</i>	Si(5)...H(37)	382.1(34)	28.2(fixed)	—	6.2	28.2
<i>u455</i>	Si(2)...H(33)	382.2(51)	45.6(fixed)	—	-1.2	45.6
<i>u456</i>	H(26)...H(35)	382.5(104)	47.0(fixed)	—	-4.7	47.0
<i>u421</i>	Cl(55)...Cl(57)	382.9(39)	35.1(tied to <i>u483</i> )	—	0.4	27.1
<i>u546</i>	Cl(55)...H(69)	383.3(64)	32.4(fixed)	—	-2.2	32.4
<i>u453</i>	Si(45)...H(64)	384.2(46)	42.2(fixed)	—	-0.8	42.2
<i>u434</i>	Si(45)...H(70)	385.0(51)	33.2(fixed)	—	0.2	33.2
<i>u433</i>	H(19)...H(29)	385.1(87)	32.3(fixed)	—	4.8	32.3
<i>u450</i>	H(18)...H(41)	386.1(60)	34.1(fixed)	—	2.8	34.1
<i>u459</i>	Si(5)...C(10)	387.2(46)	17.0(tied to <i>u403</i> )	—	-0.1	15.3
<i>u425</i>	C(54)...Cl(58)	388.2(36)	33.2(tied to <i>u483</i> )	—	0.3	25.7
<i>u542</i>	Cl(56)...H(67)	388.5(63)	34.3(fixed)	—	-2.3	34.3
<i>u451</i>	Si(2)...H(24)	389.1(29)	27.2(fixed)	—	3.8	27.2
<i>u431</i>	H(25)...H(33)	389.5(66)	36.5(fixed)	—	13.1	36.5
<i>u449</i>	H(63)...H(74)	389.8(101)	44.7(fixed)	—	4.7	44.7
<i>u525</i>	C(49)...H(63)	392.1(64)	43.6(fixed)	—	-3.9	43.6
<i>u482</i>	Si(45)...Cl(55)	392.4(18)	22.4(tied to <i>u483</i> )	—	-0.4	17.3
<i>u460</i>	Si(43)...C(47)	393.6(19)	19.9(tied to <i>u483</i> )	—	-0.2	15.4
<i>u454</i>	Si(3)...H(23)	393.9(35)	27.2(fixed)	—	3.1	27.2
<i>u467</i>	Si(43)...C(52)	395.1(21)	20.0(tied to <i>u483</i> )	—	-0.1	15.4
<i>u484</i>	H(28)...H(39)	395.2(109)	42.5(fixed)	—	-2.0	42.5
<i>u473</i>	C(10)...H(35)	395.4(34)	14.7(fixed)	—	-6.1	14.7
<i>u509</i>	Si(43)...C(50)	395.6(17)	19.0(tied to <i>u483</i> )	—	-0.1	14.7
<i>u469</i>	C(11)...H(32)	395.7(34)	14.4(fixed)	—	-5.9	14.4
<i>u518</i>	C(50)...H(72)	396.3(66)	48.9(fixed)	—	-4.9	48.9
<i>u481</i>	Si(45)...Cl(58)	396.8(16)	22.2(tied to <i>u483</i> )	—	-0.3	17.1
<i>u472</i>	C(48)...H(59)	397.2(32)	14.6(fixed)	—	-6.2	14.6
<i>u476</i>	C(13)...H(36)	397.3(31)	14.0(fixed)	—	-5.0	14.0
<i>u468</i>	C(9)...H(26)	397.8(32)	13.6(fixed)	—	-3.7	13.6
<i>u470</i>	C(8)...H(29)	398.0(32)	13.3(fixed)	—	-3.5	13.3
<i>u475</i>	Si(2)...Cl(15)	398.1(23)	22.1(tied to <i>u483</i> )	—	-0.3	17.1

<i>u477</i>	C(47)...H(63)	398.2(32)	14.3(fixed)	—	-5.2	14.3
<i>u440</i>	H(61)...H(65)	398.2(44)	38.9(fixed)	—	8.9	38.9
<i>u483</i>	Si(4)...Cl(16)	398.4(15)	22.2(11)	1.7	-0.4	17.2
<i>u478</i>	C(12)...H(40)	398.5(32)	13.3(fixed)	—	-3.8	13.3
<i>u466</i>	C(50)...H(67)	398.7(32)	13.5(fixed)	—	-3.6	13.5
<i>u465</i>	C(49)...H(70)	398.9(32)	13.1(fixed)	—	-3.3	13.1
<i>u458</i>	Si(3)...C(11)	398.9(28)	19.9(tied to <i>u483</i> )	—	-0.1	15.4
<i>u489</i>	C(7)...H(31)	399.2(79)	47.7(fixed)	—	-4.5	47.7
<i>u464</i>	Si(3)...C(13)	399.4(21)	20.0(tied to <i>u483</i> )	—	-0.2	15.5
<i>u545</i>	Cl(17)...H(36)	399.9(64)	39.0(fixed)	—	-4.2	39.0
<i>u510</i>	Si(45)...C(49)	400.0(26)	18.9(tied to <i>u483</i> )	—	-0.2	14.6
<i>u563</i>	C(7)...H(30)	400.3(103)	35.1(fixed)	—	-5.8	35.1
<i>u556</i>	Cl(15)...H(23)	400.4(75)	34.6(fixed)	—	-2.5	34.6
<i>u479</i>	C(7)...H(18)	401.1(31)	13.3(fixed)	—	-3.3	13.3
<i>u471</i>	C(6)...H(22)	401.4(31)	13.4(fixed)	—	-3.1	13.4
<i>u516</i>	H(20)...H(39)	402.3(103)	44.7(fixed)	—	-1.2	44.7
<i>u540</i>	Si(4)...Cl(17)	403.3(57)	21.3(tied to <i>u483</i> )	—	-0.3	16.5
<i>u480</i>	Si(2)...C(6)	404.5(22)	20.7(tied to <i>u483</i> )	—	-0.2	16.0
<i>u485</i>	Si(4)...Cl(14)	405.5(29)	22.3(tied to <i>u483</i> )	—	-0.3	17.3
<i>u534</i>	H(29)...H(41)	405.8(91)	45.6(fixed)	—	-2.5	45.6
<i>u513</i>	Si(5)...C(12)	405.9(24)	18.9(tied to <i>u483</i> )	—	-0.1	14.6
<i>u474</i>	Si(5)...C(9)	406.3(33)	20.0(tied to <i>u483</i> )	—	-0.2	15.5
<i>u496</i>	H(18)...H(27)	406.4(108)	43.3(fixed)	—	-1.8	43.3
<i>u595</i>	Cl(15)...H(21)	406.5(108)	33.1(fixed)	—	-2.9	33.1
<i>u508</i>	C(8)...H(35)	406.6(73)	48.1(fixed)	—	-4.6	48.1
<i>u486</i>	H(20)...H(28)	406.7(115)	41.8(fixed)	—	-1.9	41.8
<i>u548</i>	Cl(16)...H(18)	407.0(56)	32.9(fixed)	—	-2.5	32.9
<i>u492</i>	C(1)...H(34)	407.3(10)	14.0(fixed)	—	-5.5	14.0
<i>u493</i>	C(1)...H(30)	407.6(9)	13.6(fixed)	—	-5.2	13.6
<i>u495</i>	C(42)...H(60)	408.3(9)	13.8(fixed)	—	-5.5	13.8
<i>u506</i>	C(42)...H(66)	409.1(9)	13.2(fixed)	—	-3.3	13.2
<i>u524</i>	Cl(17)...H(23)	409.3(14)	13.0(fixed)	—	-3.4	13.0
<i>u530</i>	Cl(15)...H(33)	409.4(13)	14.9(fixed)	—	-6.8	14.9
<i>u526</i>	Cl(56)...H(72)	409.5(14)	14.7(fixed)	—	-6.8	14.7
<i>u543</i>	Cl(14)...H(26)	409.6(52)	33.8(fixed)	—	-2.5	33.8
<i>u501</i>	C(42)...H(62)	409.7(9)	13.6(fixed)	—	-4.6	13.6
<i>u529</i>	Cl(56)...H(74)	410.2(13)	14.3(fixed)	—	-5.8	14.3
<i>u497</i>	C(1)...H(41)	410.2(9)	13.2(fixed)	—	-3.4	13.2
<i>u494</i>	C(1)...H(19)	410.3(9)	13.1(fixed)	—	-3.0	13.1
<i>u532</i>	Cl(15)...H(31)	410.6(13)	14.0(fixed)	—	-6.4	14.0
<i>u555</i>	Cl(55)...H(68)	410.6(43)	32.1(fixed)	—	-2.4	32.1
<i>u533</i>	Cl(55)...H(80)	410.8(14)	13.4(fixed)	—	-3.6	13.4
<i>u515</i>	C(1)...H(38)	410.9(9)	13.3(fixed)	—	-4.5	13.3
<i>u522</i>	Cl(16)...H(24)	411.1(14)	13.3(fixed)	—	-3.9	13.3

<i>u521</i>	Cl(55)...H(78)	411.2(13)	13.2(fixed)	—	-3.8	13.2
<i>u505</i>	C(1)...H(27)	411.2(9)	13.1(fixed)	—	-3.1	13.1
<i>u527</i>	Cl(14)...H(37)	411.7(13)	13.5(fixed)	—	-5.4	13.5
<i>u512</i>	C(42)...H(68)	411.9(9)	13.2(fixed)	—	-3.1	13.2
<i>u517</i>	C(1)...H(25)	412.5(9)	13.2(fixed)	—	-3.3	13.2
<i>u531</i>	Si(2)...C(8)	412.9(19)	18.8(tied to <i>u483</i> )	—	-0.1	14.5
<i>u520</i>	C(1)...H(21)	413.1(9)	13.0(fixed)	—	-2.9	13.0
<i>u514</i>	Cl(17)...H(20)	413.2(14)	13.1(fixed)	—	-3.4	13.1
<i>u523</i>	Cl(14)...H(39)	413.5(14)	13.4(fixed)	—	-3.9	13.4
<i>u528</i>	Cl(16)...H(28)	414.7(14)	13.4(fixed)	—	-3.6	13.4
<i>u535</i>	H(60)...H(81)	414.9(88)	44.5(fixed)	—	-6.0	44.5
<i>u541</i>	C(9)...H(39)	415.1(67)	34.8(fixed)	—	-2.5	34.8
<i>u502</i>	H(30)...H(35)	415.3(44)	29.6(fixed)	—	-7.0	29.6
<i>u491</i>	H(26)...H(27)	415.5(42)	26.5(fixed)	—	-3.4	26.5
<i>u519</i>	H(36)...H(41)	415.5(42)	27.9(fixed)	—	-5.0	27.9
<i>u537</i>	H(75)...H(78)	415.7(78)	46.5(fixed)	—	-4.7	46.5
<i>u488</i>	H(25)...H(29)	416.2(40)	25.4(fixed)	—	-3.0	25.4
<i>u538</i>	H(24)...H(34)	416.3(100)	46.9(fixed)	—	-6.2	46.9
<i>u547</i>	Cl(17)...H(40)	416.7(64)	36.0(fixed)	—	-3.1	36.0
<i>u536</i>	Si(3)...C(7)	417.0(24)	19.4(tied to <i>u483</i> )	—	-0.1	15.0
<i>u552</i>	Cl(17)...H(38)	417.1(35)	37.0(fixed)	—	-4.3	37.0
<i>u507</i>	H(59)...H(62)	417.4(40)	29.1(fixed)	—	-5.6	29.1
<i>u498</i>	H(32)...H(34)	417.5(42)	29.8(fixed)	—	-4.8	29.8
<i>u539</i>	H(19)...H(40)	418.0(100)	48.3(fixed)	—	-1.7	48.3
<i>u504</i>	H(38)...H(40)	418.0(40)	26.7(fixed)	—	-2.5	26.7
<i>u490</i>	H(67)...H(68)	418.0(42)	26.5(fixed)	—	-3.4	26.5
<i>u487</i>	H(66)...H(70)	418.1(40)	25.3(fixed)	—	-2.9	25.3
<i>u561</i>	Cl(14)...H(29)	418.3(54)	35.5(fixed)	—	-2.8	35.5
<i>u572</i>	H(31)...H(35)	418.9(61)	32.5(fixed)	—	-7.4	32.5
<i>u559</i>	H(32)...H(33)	419.1(61)	32.6(fixed)	—	-7.4	32.6
<i>u511</i>	H(71)...H(76)	419.1(42)	29.4(fixed)	—	-3.9	29.4
<i>u588</i>	C(8)...H(32)	419.2(57)	41.2(fixed)	—	-5.5	41.2
<i>u500</i>	H(18)...H(21)	420.4(39)	24.9(fixed)	—	-3.0	24.9
<i>u503</i>	H(19)...H(22)	420.5(41)	25.7(fixed)	—	-2.8	25.7
<i>u568</i>	H(59)...H(64)	421.6(59)	31.1(fixed)	—	-9.7	31.1
<i>u557</i>	Cl(16)...H(22)	422.1(59)	31.7(fixed)	—	-2.1	31.7
<i>u573</i>	Cl(56)...H(66)	422.4(38)	32.0(fixed)	—	-2.9	32.0
<i>u574</i>	C(11)...H(37)	422.8(79)	40.3(fixed)	—	-4.2	40.3
<i>u558</i>	H(36)...H(39)	423.5(58)	27.2(fixed)	—	-8.4	27.2
<i>u553</i>	H(26)...H(28)	424.3(58)	26.4(fixed)	—	-6.6	26.4
<i>u583</i>	Cl(16)...H(19)	424.3(45)	30.8(fixed)	—	-2.8	30.8
<i>u562</i>	H(24)...H(29)	424.4(59)	26.8(fixed)	—	-6.4	26.8
<i>u576</i>	H(61)...H(63)	424.8(58)	32.5(fixed)	—	-6.3	32.5
<i>u566</i>	C(49)...H(62)	424.8(39)	34.4(fixed)	—	-4.9	34.4



<i>u544</i>	C(6)...H(28)	425.4(84)	32.6(fixed)	—	-2.3	32.6
<i>u586</i>	C(12)...H(33)	425.6(80)	42.9(fixed)	—	-6.0	42.9
<i>u565</i>	C(50)...H(71)	426.1(45)	36.6(fixed)	—	-6.2	36.6
<i>u569</i>	H(37)...H(40)	426.4(59)	29.8(fixed)	—	-4.7	29.8
<i>u549</i>	H(67)...H(69)	426.5(58)	26.3(fixed)	—	-4.4	26.3
<i>u582</i>	Cl(17)...H(41)	426.6(56)	32.0(fixed)	—	-3.5	32.0
<i>u554</i>	H(65)...H(70)	427.0(59)	26.5(fixed)	—	-4.0	26.5
<i>u551</i>	C(13)...H(20)	427.4(65)	32.9(fixed)	—	-2.0	32.9
<i>u564</i>	Cl(14)...H(25)	428.6(37)	32.3(fixed)	—	-2.9	32.3
<i>u579</i>	C(10)...H(24)	429.0(50)	33.6(fixed)	—	-2.8	33.6
<i>u567</i>	H(20)...H(22)	429.1(57)	25.3(fixed)	—	-6.1	25.3
<i>u560</i>	C(9)...H(41)	429.9(51)	32.8(fixed)	—	-3.0	32.8
<i>u575</i>	H(18)...H(23)	430.5(58)	25.5(fixed)	—	-4.1	25.5
<i>u618</i>	Cl(55)...H(71)	432.5(28)	29.7(fixed)	—	-8.9	29.7
<i>u592</i>	C(12)...H(34)	432.8(60)	40.4(fixed)	—	-6.1	40.4
<i>u589</i>	Si(43)...H(76)	433.1(42)	35.1(fixed)	—	-1.9	35.1
<i>u593</i>	Cl(14)...H(27)	433.2(45)	32.8(fixed)	—	-3.2	32.8
<i>u585</i>	Si(5)...H(31)	433.3(52)	39.0(fixed)	—	-2.3	39.0
<i>u550</i>	C(6)...H(27)	433.8(69)	32.4(fixed)	—	-2.5	32.4
<i>u581</i>	C(49)...H(59)	434.1(49)	42.1(fixed)	—	-5.5	42.1
<i>u571</i>	C(8)...H(34)	434.2(57)	35.9(fixed)	—	-6.2	35.9
<i>u577</i>	Cl(16)...H(21)	434.9(39)	32.2(fixed)	—	-2.2	32.2
<i>u584</i>	Si(3)...H(35)	435.5(47)	38.5(fixed)	—	-2.1	38.5
<i>u590</i>	Si(43)...H(61)	435.5(45)	39.3(fixed)	—	-2.9	39.3
<i>u578</i>	C(13)...H(19)	437.6(56)	32.7(fixed)	—	-2.5	32.7
<i>u619</i>	Si(45)...H(67)	438.6(45)	27.1(fixed)	—	-1.4	27.1
<i>u599</i>	C(11)...H(38)	438.8(62)	35.6(fixed)	—	-5.1	35.6
<i>u607</i>	C(10)...H(21)	438.8(86)	23.5(fixed)	—	-3.3	23.5
<i>u608</i>	Cl(56)...H(62)	439.8(25)	28.2(fixed)	—	-7.2	28.2
<i>u601</i>	C(10)...H(25)	440.3(42)	32.8(fixed)	—	-3.5	32.8
<i>u627</i>	Si(43)...H(69)	441.0(44)	26.1(fixed)	—	-1.6	26.1
<i>u620</i>	Si(4)...H(21)	441.1(69)	18.3(fixed)	—	-3.7	18.3
<i>u587</i>	C(48)...H(74)	441.3(81)	40.9(fixed)	—	-4.9	40.9
<i>u594</i>	C(8)...H(30)	441.8(48)	39.5(fixed)	—	-5.7	39.5
<i>u625</i>	Cl(16)...H(30)	443.2(27)	28.6(fixed)	—	-8.4	28.6
<i>u661</i>	H(70)...H(81)	443.2(91)	37.6(fixed)	—	2.6	37.6
<i>u570</i>	C(47)...H(65)	443.8(44)	32.7(fixed)	—	-2.7	32.7
<i>u609</i>	C(48)...H(66)	445.3(38)	24.5(fixed)	—	-4.1	24.5
<i>u615</i>	Si(5)...H(36)	445.4(46)	32.0(fixed)	—	-1.9	32.0
<i>u600</i>	Si(3)...H(39)	445.7(44)	28.4(fixed)	—	-1.9	28.4
<i>u596</i>	C(47)...H(66)	446.3(41)	32.3(fixed)	—	-3.3	32.3
<i>u598</i>	C(48)...H(75)	447.2(64)	37.6(fixed)	—	-5.2	37.6
<i>u591</i>	C(49)...H(60)	448.2(45)	39.6(fixed)	—	-6.0	39.6
<i>u597</i>	Si(45)...H(79)	448.3(24)	19.5(fixed)	—	-4.4	19.5

<i>u605</i>	Cl(15)...H(38)	448.7(39)	27.4(fixed)	—	-6.7	27.4
<i>u580</i>	Cl(56)...H(70)	453.2(56)	35.1(fixed)	—	-2.6	35.1
<i>u622</i>	Si(43)...H(71)	453.2(23)	22.7(fixed)	—	-7.7	22.7
<i>u614</i>	Si(2)...H(34)	453.4(24)	23.5(fixed)	—	-7.7	23.5
<i>u611</i>	C(47)...H(82)	453.5(38)	24.0(fixed)	—	-3.7	24.0
<i>u606</i>	Si(2)...H(20)	453.5(43)	26.4(fixed)	—	-1.7	26.4
<i>u604</i>	Si(5)...H(28)	454.4(51)	26.8(fixed)	—	-1.8	26.8
<i>u623</i>	Si(3)...H(30)	454.5(23)	22.4(fixed)	—	-7.3	22.4
<i>u628</i>	Si(2)...H(26)	454.5(39)	26.9(fixed)	—	-1.3	26.9
<i>u616</i>	Cl(14)...H(34)	454.6(53)	29.5(fixed)	—	-8.9	29.5
<i>u617</i>	Si(4)...H(38)	455.1(19)	20.4(fixed)	—	-6.3	20.4
<i>u621</i>	Si(45)...H(62)	455.5(21)	21.8(fixed)	—	-6.5	21.8
<i>u603</i>	Si(4)...H(25)	455.7(27)	19.5(fixed)	—	-4.4	19.5
<i>u612</i>	Si(3)...H(19)	456.6(25)	18.1(fixed)	—	-3.8	18.1
<i>u624</i>	C(13)...H(27)	458.5(43)	24.3(fixed)	—	-4.0	24.3
<i>u626</i>	Si(5)...H(41)	459.2(26)	18.6(fixed)	—	-4.6	18.6
<i>u631</i>	Si(3)...H(22)	459.6(44)	25.0(fixed)	—	-1.3	25.0
<i>u630</i>	Si(2)...H(27)	460.0(21)	18.4(fixed)	—	-4.1	18.4
<i>u610</i>	C(11)...H(25)	460.6(54)	24.2(fixed)	—	-4.2	24.2
<i>u602</i>	Cl(56)...H(68)	461.9(49)	34.3(fixed)	—	-3.1	34.3
<i>u635</i>	H(59)...H(78)	462.5(41)	40.3(fixed)	—	9.3	40.3
<i>u613</i>	C(9)...H(19)	464.2(67)	24.4(fixed)	—	-3.7	24.4
<i>u629</i>	Si(45)...H(68)	466.1(25)	18.4(fixed)	—	-4.0	18.4
<i>u632</i>	C(6)...H(41)	466.3(46)	26.1(fixed)	—	-4.8	26.1
<i>u677</i>	H(20)...H(32)	470.8(83)	49.0(fixed)	—	8.9	49.0
<i>u655</i>	Si(5)...H(30)	471.4(58)	23.9(fixed)	—	-6.7	23.9
<i>u691</i>	C(50)...H(81)	471.8(65)	28.6(fixed)	—	2.2	28.6
<i>u641</i>	Si(4)...C(6)	474.5(38)	11.2(fixed)	—	-0.7	11.2
<i>u648</i>	Si(5)...C(11)	476.7(38)	11.0(fixed)	—	-0.7	11.0
<i>u633</i>	Si(2)...C(7)	478.4(9)	13.9(tied to <i>u662</i> )	—	-0.7	11.4
<i>u664</i>	H(34)...H(37)	478.6(69)	57.6(fixed)	—	-9.1	57.6
<i>u654</i>	H(32)...H(35)	479.6(25)	18.2(fixed)	—	-10.1	18.2
<i>u644</i>	Si(43)...H(60)	480.0(27)	25.4(fixed)	—	-6.8	25.4
<i>u718</i>	H(25)...H(32)	480.3(74)	53.7(fixed)	—	-8.7	53.7
<i>u653</i>	H(59)...H(63)	480.9(23)	18.3(fixed)	—	-9.7	18.3
<i>u647</i>	Si(43)...C(49)	481.2(8)	13.8(tied to <i>u662</i> )	—	-0.7	11.4
<i>u657</i>	H(36)...H(40)	482.1(23)	17.0(fixed)	—	-7.6	17.0
<i>u638</i>	Si(5)...C(8)	482.2(7)	13.8(tied to <i>u662</i> )	—	-0.7	11.4
<i>u637</i>	Si(3)...C(12)	482.3(8)	13.7(tied to <i>u662</i> )	—	-0.7	11.3
<i>u636</i>	Si(4)...C(9)	482.6(10)	13.7(tied to <i>u662</i> )	—	-0.7	11.3
<i>u634</i>	Si(45)...C(54)	482.7(9)	13.8(tied to <i>u662</i> )	—	-0.7	11.4
<i>u639</i>	Si(43)...C(48)	482.8(8)	13.7(tied to <i>u662</i> )	—	-0.7	11.3
<i>u642</i>	Si(4)...C(13)	483.0(10)	13.4(tied to <i>u662</i> )	—	-0.7	11.0
<i>u656</i>	H(26)...H(29)	483.0(23)	16.4(fixed)	—	-6.4	16.4

<i>u710</i>	C(11)...H(22)	483.2(88)	29.9(fixed)	—	2.5	29.9
<i>u660</i>	H(22)...H(37)	483.4(65)	46.8(fixed)	—	8.7	46.8
<i>u651</i>	H(67)...H(70)	483.6(23)	16.1(fixed)	—	-6.2	16.1
<i>u643</i>	Si(2)...C(10)	484.0(9)	13.4(tied to <i>u662</i> )	—	-0.7	11.1
<i>u683</i>	C(47)...H(78)	484.9(33)	28.8(fixed)	—	2.4	28.8
<i>u645</i>	Si(45)...C(47)	484.9(12)	13.4(tied to <i>u662</i> )	—	-0.7	11.0
<i>u670</i>	Si(43)...H(68)	485.1(26)	21.4(fixed)	—	-3.6	21.4
<i>u650</i>	H(18)...H(22)	485.3(22)	16.4(fixed)	—	-5.7	16.4
<i>u658</i>	Si(43)...H(75)	485.4(23)	22.9(fixed)	—	-5.7	22.9
<i>u663</i>	C(49)...H(73)	485.5(29)	30.6(fixed)	—	7.6	30.6
<i>u696</i>	C(6)...H(32)	487.5(66)	38.4(fixed)	—	7.3	38.4
<i>u640</i>	Si(3)...H(41)	487.6(30)	22.7(fixed)	—	-4.1	22.7
<i>u706</i>	H(33)...H(38)	487.7(75)	56.8(fixed)	—	-10.4	56.8
<i>u652</i>	Si(3)...H(34)	488.1(28)	24.0(fixed)	—	-7.0	24.0
<i>u666</i>	Si(2)...Cl(16)	491.0(8)	13.9(tied to <i>u662</i> )	—	-0.8	11.4
<i>u662</i>	Si(3)...Cl(17)	491.4(12)	14.1(8)	—	-0.8	11.6
<i>u674</i>	Si(2)...H(22)	491.6(21)	21.7(fixed)	—	0.1	21.7
<i>u671</i>	Si(43)...Cl(56)	491.7(8)	13.8(tied to <i>u662</i> )	—	-0.8	11.3
<i>u649</i>	Si(2)...H(19)	491.7(30)	22.0(fixed)	—	-3.5	22.0
<i>u665</i>	Si(5)...Cl(14)	491.7(11)	14.0(tied to <i>u662</i> )	—	-0.8	11.5
<i>u668</i>	Si(3)...Cl(15)	492.3(7)	13.6(tied to <i>u662</i> )	—	-0.8	11.2
<i>u735</i>	H(63)...H(66)	492.5(66)	47.5(fixed)	—	-9.9	47.5
<i>u675</i>	Si(45)...H(66)	492.5(26)	20.8(fixed)	—	-3.9	20.8
<i>u773</i>	H(21)...H(30)	492.6(116)	39.9(fixed)	—	-10.5	39.9
<i>u646</i>	Si(5)...H(27)	493.6(36)	22.3(fixed)	—	-3.7	22.3
<i>u733</i>	H(24)...H(32)	493.7(58)	41.7(fixed)	—	-9.7	41.7
<i>u659</i>	H(24)...H(40)	493.7(32)	37.5(fixed)	—	5.4	37.5
<i>u673</i>	H(24)...H(30)	493.8(70)	51.4(fixed)	—	-7.3	51.4
<i>u690</i>	H(59)...H(66)	494.0(64)	54.0(fixed)	—	-8.7	54.0
<i>u697</i>	Si(4)...H(20)	494.1(38)	21.2(fixed)	—	0.0	21.2
<i>u667</i>	Si(45)...Cl(57)	494.1(8)	14.0(tied to <i>u662</i> )	—	-0.8	11.5
<i>u728</i>	H(33)...H(37)	494.6(93)	47.9(fixed)	—	-11.8	47.9
<i>u676</i>	Si(5)...H(38)	495.3(23)	23.0(fixed)	—	-5.3	23.0
<i>u707</i>	Cl(55)...H(74)	496.2(43)	30.1(fixed)	—	5.1	30.1
<i>u730</i>	H(61)...H(82)	497.4(66)	53.1(fixed)	—	-10.4	53.1
<i>u669</i>	H(18)...H(37)	497.8(40)	37.1(fixed)	—	6.0	37.1
<i>u686</i>	Si(5)...H(26)	497.9(19)	21.3(fixed)	—	0.5	21.3
<i>u716</i>	Si(5)...H(35)	498.5(35)	21.5(fixed)	—	1.7	21.5
<i>u693</i>	H(23)...H(26)	499.9(60)	41.3(fixed)	—	6.5	41.3
<i>u692</i>	H(62)...H(74)	500.0(74)	56.5(fixed)	—	-9.2	56.5
<i>u724</i>	H(21)...H(31)	500.4(83)	51.8(fixed)	—	-9.6	51.8
<i>u703</i>	Si(43)...H(67)	500.9(18)	21.5(fixed)	—	0.6	21.5
<i>u685</i>	Si(3)...H(36)	501.0(19)	21.4(fixed)	—	1.5	21.4
<i>u751</i>	H(34)...H(38)	501.3(78)	50.8(fixed)	—	-12.9	50.8

<i>u678</i>	Si(2)...H(25)	502.9(22)	20.9(fixed)	—	-3.9	20.9
<i>u699</i>	C(8)...H(20)	503.1(44)	29.8(fixed)	—	2.5	29.8
<i>u689</i>	Si(43)...H(63)	503.4(18)	21.4(fixed)	—	1.4	21.4
<i>u679</i>	H(67)...H(81)	503.7(63)	41.2(fixed)	—	6.5	41.2
<i>u723</i>	Si(4)...H(39)	504.1(28)	20.8(fixed)	—	-0.1	20.8
<i>u704</i>	C(7)...H(37)	504.8(35)	36.3(fixed)	—	5.8	36.3
<i>u767</i>	C(50)...C(54)	504.8(47)	22.6(tied to <i>u662</i> )	—	-1.0	18.6
<i>u695</i>	Si(4)...H(28)	505.4(25)	21.2(fixed)	—	-0.1	21.2
<i>u680</i>	C(8)...H(40)	506.0(26)	28.9(fixed)	—	3.4	28.9
<i>u682</i>	Si(3)...H(21)	506.9(23)	20.5(fixed)	—	-3.4	20.5
<i>u672</i>	H(60)...H(65)	506.9(62)	50.7(fixed)	—	-7.6	50.7
<i>u720</i>	C(49)...H(81)	507.0(47)	31.7(fixed)	—	3.2	31.7
<i>u719</i>	C(7)...H(39)	507.6(45)	30.7(fixed)	—	3.2	30.7
<i>u709</i>	Cl(17)...H(32)	507.7(55)	30.3(fixed)	—	6.8	30.3
<i>u687</i>	H(28)...H(33)	507.8(62)	49.8(fixed)	—	9.7	49.8
<i>u711</i>	C(10)...H(36)	508.0(32)	34.1(fixed)	—	5.9	34.1
<i>u731</i>	H(25)...H(35)	508.1(74)	52.3(fixed)	—	-10.9	52.3
<i>u705</i>	C(47)...H(76)	508.4(32)	34.0(fixed)	—	6.6	34.0
<i>u725</i>	Si(2)...H(31)	508.7(25)	21.5(fixed)	—	1.0	21.5
<i>u698</i>	H(24)...H(36)	508.9(61)	43.9(fixed)	—	8.7	43.9
<i>u688</i>	Si(45)...H(80)	509.1(23)	21.3(fixed)	—	-0.1	21.3
<i>u727</i>	C(12)...H(28)	509.2(41)	30.7(fixed)	—	2.7	30.7
<i>u701</i>	C(13)...H(35)	509.5(36)	35.5(fixed)	—	8.4	35.5
<i>u712</i>	H(63)...H(78)	510.0(62)	43.9(fixed)	—	8.2	43.9
<i>u717</i>	H(59)...H(65)	510.0(51)	42.3(fixed)	—	-9.7	42.3
<i>u702</i>	C(12)...H(18)	510.4(24)	28.6(fixed)	—	2.3	28.6
<i>u694</i>	Cl(16)...H(33)	511.0(45)	30.5(fixed)	—	6.8	30.5
<i>u714</i>	C(50)...H(61)	511.0(42)	36.5(fixed)	—	7.9	36.5
<i>u729</i>	Si(45)...H(61)	511.3(26)	21.8(fixed)	—	1.0	21.8
<i>u757</i>	H(25)...H(30)	511.4(56)	47.3(fixed)	—	-10.6	47.3
<i>u754</i>	H(62)...H(75)	511.4(81)	48.9(fixed)	—	-12.0	48.9
<i>u746</i>	C(47)...C(53)	512.4(23)	18.9(fixed)	—	-0.9	18.9
<i>u713</i>	C(9)...H(31)	512.4(43)	34.8(fixed)	—	7.6	34.8
<i>u681</i>	H(23)...H(29)	512.6(33)	36.6(fixed)	—	4.1	36.6
<i>u737</i>	H(64)...H(74)	513.0(94)	46.2(fixed)	—	-11.4	46.2
<i>u783</i>	H(22)...H(34)	513.7(106)	35.3(fixed)	—	4.7	35.3
<i>u748</i>	H(60)...H(66)	513.7(57)	47.9(fixed)	—	-10.9	47.9
<i>u715</i>	C(6)...H(37)	514.0(33)	28.1(fixed)	—	4.4	28.1
<i>u750</i>	Si(4)...H(18)	514.2(32)	21.0(fixed)	—	-1.0	21.0
<i>u700</i>	C(13)...H(24)	514.4(23)	28.4(fixed)	—	2.4	28.4
<i>u772</i>	H(75)...H(79)	514.6(39)	39.9(fixed)	—	-10.2	39.9
<i>u738</i>	C(48)...H(78)	514.8(36)	32.5(fixed)	—	3.1	32.5
<i>u749</i>	Cl(56)...H(77)	514.8(37)	30.8(fixed)	—	3.4	30.8
<i>u739</i>	Cl(16)...H(40)	515.4(42)	33.4(fixed)	—	4.0	33.4

<i>u756</i>	H(27)...H(39)	515.7(65)	38.2(fixed)	—	-7.8	38.2
<i>u726</i>	Cl(17)...H(29)	516.4(63)	33.2(fixed)	—	3.5	33.2
<i>u768</i>	C(48)...Cl(57)	517.3(28)	19.9(fixed)	—	-1.1	19.9
<i>u684</i>	H(64)...H(69)	517.8(53)	46.5(fixed)	—	8.8	46.5
<i>u721</i>	C(9)...H(33)	517.8(53)	39.1(fixed)	—	7.7	39.1
<i>u800</i>	H(22)...H(36)	518.2(56)	48.9(fixed)	—	3.6	48.9
<i>u764</i>	Si(5)...H(33)	518.6(31)	22.8(fixed)	—	-1.0	22.8
<i>u752</i>	Si(2)...H(32)	518.8(21)	22.0(fixed)	—	-0.5	22.0
<i>u732</i>	C(48)...H(80)	518.9(43)	30.8(fixed)	—	2.6	30.8
<i>u742</i>	Si(45)...H(81)	518.9(19)	20.4(fixed)	—	-1.2	20.4
<i>u825</i>	H(68)...H(81)	518.9(75)	36.5(fixed)	—	0.1	36.5
<i>u774</i>	H(60)...H(82)	519.0(43)	41.9(fixed)	—	-11.3	41.9
<i>u747</i>	Si(45)...H(59)	519.3(20)	22.3(fixed)	—	-0.2	22.3
<i>u744</i>	Si(4)...H(29)	519.4(20)	20.7(fixed)	—	-1.1	20.7
<i>u745</i>	Si(4)...H(40)	519.6(21)	21.2(fixed)	—	-0.8	21.2
<i>u722</i>	C(54)...H(74)	520.4(43)	36.4(fixed)	—	6.4	36.4
<i>u740</i>	C(8)...H(23)	520.4(40)	32.3(fixed)	—	2.8	32.3
<i>u791</i>	C(10)...H(20)	520.7(49)	27.6(fixed)	—	1.5	27.6
<i>u766</i>	Si(43)...H(65)	521.1(19)	21.2(fixed)	—	-1.3	21.2
<i>u743</i>	Cl(14)...H(18)	521.3(53)	32.9(fixed)	—	2.9	32.9
<i>u708</i>	C(7)...H(29)	521.3(34)	28.4(fixed)	—	2.7	28.4
<i>u736</i>	C(12)...H(24)	522.2(35)	33.1(fixed)	—	3.3	33.1
<i>u762</i>	Si(43)...H(64)	522.9(19)	21.9(fixed)	—	-1.4	21.9
<i>u761</i>	Cl(15)...H(26)	523.2(40)	30.9(fixed)	—	3.5	30.9
<i>u778</i>	C(12)...H(22)	523.3(33)	29.0(fixed)	—	1.9	29.0
<i>u741</i>	Cl(55)...H(59)	523.5(40)	38.7(fixed)	—	7.9	38.7
<i>u769</i>	H(27)...H(41)	524.3(52)	37.6(fixed)	—	-8.0	37.6
<i>u755</i>	Si(2)...H(23)	524.5(19)	20.5(fixed)	—	-1.5	20.5
<i>u781</i>	Cl(56)...Cl(58)	524.6(32)	21.1(fixed)	—	-1.1	21.1
<i>u753</i>	Si(3)...H(37)	525.1(18)	22.2(fixed)	—	-1.5	22.2
<i>u788</i>	H(20)...H(31)	525.4(71)	52.5(fixed)	—	4.4	52.5
<i>u759</i>	H(19)...H(28)	526.3(86)	35.8(fixed)	—	-7.2	35.8
<i>u760</i>	Si(5)...H(24)	526.6(18)	20.8(fixed)	—	-1.5	20.8
<i>u777</i>	H(25)...H(34)	527.7(57)	41.6(fixed)	—	-11.7	41.6
<i>u787</i>	C(10)...Cl(17)	527.9(53)	19.8(fixed)	—	-1.0	19.8
<i>u765</i>	C(11)...Cl(16)	528.0(28)	19.7(fixed)	—	-1.0	19.7
<i>u734</i>	C(9)...H(23)	528.2(24)	28.5(fixed)	—	1.7	28.5
<i>u801</i>	C(7)...C(11)	528.5(65)	16.5(fixed)	—	-0.8	16.5
<i>u775</i>	H(20)...H(41)	528.5(65)	36.2(fixed)	—	-8.0	36.2
<i>u758</i>	H(19)...H(27)	528.6(73)	37.2(fixed)	—	-7.1	37.2
<i>u780</i>	H(19)...H(41)	531.2(56)	37.6(fixed)	—	-8.1	37.6
<i>u827</i>	C(6)...Cl(15)	531.5(73)	18.1(fixed)	—	-1.0	18.1
<i>u804</i>	Cl(15)...H(39)	531.6(44)	28.9(fixed)	—	1.9	28.9
<i>u799</i>	C(6)...C(10)	531.9(45)	18.2(fixed)	—	-0.7	18.2

<i>u878</i>	H(22)...H(35)	532.4(73)	34.2(fixed)	—	1.2	34.2
<i>u763</i>	C(8)...C(13)	533.0(17)	18.6(fixed)	—	-0.9	18.6
<i>u771</i>	C(6)...C(12)	533.5(18)	18.4(fixed)	—	-0.9	18.4
<i>u829</i>	H(60)...H(78)	534.2(50)	41.6(fixed)	—	0.7	41.6
<i>u770</i>	H(20)...H(25)	534.8(49)	35.1(fixed)	—	3.7	35.1
<i>u852</i>	Cl(17)...H(35)	537.4(59)	29.5(fixed)	—	5.5	29.5
<i>u798</i>	H(28)...H(35)	537.8(76)	53.7(fixed)	—	4.6	53.7
<i>u784</i>	Cl(14)...Cl(15)	538.7(41)	23.4(13)	—	-1.2	20.8
<i>u863</i>	H(63)...H(77)	539.7(54)	41.5(fixed)	—	6.8	41.5
<i>u789</i>	H(21)...H(39)	540.0(51)	35.9(fixed)	—	4.2	35.9
<i>u819</i>	C(7)...H(26)	540.9(39)	28.1(fixed)	—	2.6	28.1
<i>u817</i>	C(7)...C(12)	541.4(19)	18.7(fixed)	—	-0.8	18.7
<i>u793</i>	H(59)...H(79)	541.6(41)	38.6(fixed)	—	7.9	38.6
<i>u843</i>	H(19)...H(32)	542.0(68)	41.5(fixed)	—	7.6	41.5
<i>u794</i>	C(6)...C(8)	542.0(23)	16.1(fixed)	—	-0.8	16.1
<i>u792</i>	H(28)...H(38)	542.2(45)	36.1(fixed)	—	4.4	36.1
<i>u875</i>	H(22)...H(26)	542.3(70)	39.3(fixed)	—	3.9	39.3
<i>u818</i>	C(49)...Cl(55)	542.4(16)	19.8(tied to <i>u784</i> )	—	-0.9	17.6
<i>u823</i>	C(13)...Cl(15)	542.8(27)	22.3(tied to <i>u784</i> )	—	-0.9	19.8
<i>u846</i>	C(11)...H(23)	543.0(64)	33.8(fixed)	—	-0.6	33.8
<i>u905</i>	H(22)...H(33)	543.4(92)	34.0(fixed)	—	-1.2	34.0
<i>u796</i>	C(11)...H(28)	543.7(49)	28.3(fixed)	—	1.6	28.3
<i>u811</i>	C(47)...C(50)	543.9(17)	16.9(fixed)	—	-0.9	16.9
<i>u785</i>	H(61)...H(68)	544.2(43)	41.2(fixed)	—	9.9	41.2
<i>u807</i>	C(50)...H(77)	544.4(41)	27.7(fixed)	—	2.4	27.7
<i>u776</i>	C(7)...C(9)	544.4(18)	18.6(fixed)	—	-0.9	18.6
<i>u813</i>	C(9)...C(10)	544.4(21)	17.1(fixed)	—	-0.9	17.1
<i>u786</i>	H(30)...H(36)	544.4(35)	39.0(fixed)	—	8.6	39.0
<i>u834</i>	Cl(14)...H(31)	544.6(38)	29.2(fixed)	—	4.3	29.2
<i>u782</i>	H(60)...H(76)	545.2(34)	38.9(fixed)	—	9.5	38.9
<i>u859</i>	H(67)...H(80)	545.4(70)	39.5(fixed)	—	3.8	39.5
<i>u821</i>	C(49)...H(76)	545.6(33)	28.5(fixed)	—	4.2	28.5
<i>u802</i>	C(10)...C(12)	545.6(16)	16.8(fixed)	—	-0.8	16.8
<i>u808</i>	C(9)...C(12)	546.0(18)	16.7(fixed)	—	-0.8	16.7
<i>u779</i>	H(35)...H(41)	546.1(41)	40.4(fixed)	—	10.5	40.4
<i>u803</i>	C(7)...C(13)	546.1(24)	16.4(fixed)	—	-0.9	16.4
<i>u882</i>	C(11)...Cl(17)	546.6(56)	19.0(fixed)	—	-0.9	19.0
<i>u806</i>	C(47)...C(52)	546.9(18)	16.8(fixed)	—	-0.8	16.8
<i>u790</i>	H(27)...H(31)	547.1(46)	39.5(fixed)	—	9.5	39.5
<i>u816</i>	C(8)...H(36)	547.3(32)	28.1(fixed)	—	4.4	28.1
<i>u809</i>	C(11)...C(13)	547.4(24)	16.9(fixed)	—	-0.8	16.9
<i>u857</i>	H(26)...H(36)	547.4(53)	40.9(fixed)	—	6.7	40.9
<i>u856</i>	H(20)...H(26)	547.7(40)	32.5(fixed)	—	1.7	32.5
<i>u831</i>	C(49)...C(54)	548.4(28)	17.9(fixed)	—	-0.7	17.9

<i>u850</i>	Si(5)...H(34)	548.6(49)	16.6(fixed)	—	-4.5	16.6
<i>u805</i>	H(63)...H(69)	549.1(71)	50.8(fixed)	—	4.0	50.8
<i>u833</i>	Cl(56)...H(61)	549.2(34)	29.0(fixed)	—	4.6	29.0
<i>u851</i>	Si(4)...H(19)	550.0(49)	15.6(fixed)	—	-3.2	15.6
<i>u812</i>	C(9)...C(11)	550.1(38)	20.8(tied to <i>u784</i> )	—	-0.7	18.5
<i>u855</i>	Cl(14)...Cl(17)	550.1(20)	19.3(tied to <i>u784</i> )	—	-1.0	17.2
<i>u837</i>	C(48)...C(53)	550.4(20)	17.7(fixed)	—	-0.8	17.7
<i>u839</i>	C(47)...Cl(56)	550.5(20)	22.0(tied to <i>u784</i> )	—	-0.9	19.6
<i>u865</i>	Cl(16)...Cl(17)	551.3(15)	19.4(tied to <i>u784</i> )	—	-1.1	17.2
<i>u903</i>	C(9)...H(32)	551.3(56)	46.0(fixed)	—	-1.1	46.0
<i>u892</i>	C(50)...H(59)	551.6(51)	46.8(fixed)	—	-0.9	46.8
<i>u848</i>	C(10)...Cl(14)	552.1(27)	22.2(tied to <i>u784</i> )	—	-0.9	19.7
<i>u858</i>	H(22)...H(39)	552.5(46)	32.8(fixed)	—	2.4	32.8
<i>u868</i>	Cl(14)...Cl(16)	552.5(20)	19.5(tied to <i>u784</i> )	—	-1.1	17.3
<i>u820</i>	Si(2)...H(21)	552.6(14)	16.5(fixed)	—	-3.2	16.5
<i>u871</i>	H(66)...H(81)	552.7(50)	37.7(fixed)	—	2.2	37.7
<i>u840</i>	C(8)...H(18)	552.7(58)	33.2(fixed)	—	-0.6	33.2
<i>u893</i>	Cl(15)...Cl(16)	552.9(31)	23.0(tied to <i>u784</i> )	—	-1.1	20.4
<i>u797</i>	C(48)...H(69)	553.1(42)	28.5(fixed)	—	1.7	28.5
<i>u810</i>	C(48)...C(54)	553.1(23)	16.8(fixed)	—	-0.8	16.8
<i>u874</i>	C(6)...H(31)	553.7(58)	45.4(fixed)	—	-0.5	45.4
<i>u815</i>	C(48)...C(50)	553.7(31)	18.6(fixed)	—	-0.7	18.6
<i>u907</i>	C(7)...H(36)	554.2(47)	40.3(fixed)	—	-0.9	40.3
<i>u949</i>	H(69)...H(81)	554.2(62)	30.3(fixed)	—	-3.9	30.3
<i>u889</i>	Cl(55)...Cl(56)	554.4(24)	23.4(tied to <i>u784</i> )	—	-1.1	20.8
<i>u876</i>	H(59)...H(76)	554.9(40)	40.3(fixed)	—	3.3	40.3
<i>u867</i>	C(13)...Cl(16)	555.1(18)	20.9(tied to <i>u784</i> )	—	-0.9	18.6
<i>u795</i>	H(62)...H(80)	555.4(47)	36.0(fixed)	—	4.5	36.0
<i>u826</i>	Si(3)...H(38)	555.5(12)	16.8(fixed)	—	-4.0	16.8
<i>u864</i>	H(21)...H(37)	555.6(23)	40.5(fixed)	—	5.4	40.5
<i>u853</i>	C(49)...Cl(58)	555.8(20)	18.6(tied to <i>u784</i> )	—	-0.9	16.5
<i>u824</i>	Si(5)...H(25)	556.2(11)	16.6(fixed)	—	-3.3	16.6
<i>u854</i>	Si(43)...H(66)	556.2(12)	16.1(fixed)	—	-3.4	16.1
<i>u847</i>	C(7)...C(8)	556.5(28)	18.3(fixed)	—	-0.7	18.3
<i>u822</i>	Si(45)...H(82)	556.5(12)	15.9(fixed)	—	-3.1	15.9
<i>u869</i>	C(12)...H(29)	556.6(53)	34.9(fixed)	—	-0.6	34.9
<i>u830</i>	Si(43)...H(62)	557.0(11)	16.8(fixed)	—	-4.0	16.8
<i>u836</i>	C(8)...C(12)	557.1(18)	17.8(fixed)	—	-0.7	17.8
<i>u838</i>	C(9)...Cl(17)	557.2(42)	21.6(tied to <i>u784</i> )	—	-0.9	19.1
<i>u883</i>	H(28)...H(36)	557.2(38)	34.1(fixed)	—	1.8	34.1
<i>u895</i>	H(61)...H(70)	558.0(58)	42.2(fixed)	—	4.4	42.2
<i>u828</i>	Si(4)...H(27)	558.1(13)	15.9(fixed)	—	-3.2	15.9
<i>u900</i>	H(31)...H(36)	558.4(32)	34.8(fixed)	—	3.8	34.8
<i>u861</i>	C(10)...H(37)	558.5(48)	43.6(fixed)	—	-0.6	43.6

<i>u842</i>	Si(2)...H(30)	559.4(12)	15.9(fixed)	—	-4.3	15.9
<i>u844</i>	Si(4)...H(41)	559.5(12)	15.6(fixed)	—	-3.4	15.6
<i>u862</i>	C(47)...Cl(55)	559.5(17)	21.3(tied to <i>u784</i> )	—	-0.8	18.9
<i>u845</i>	Si(45)...H(60)	559.6(14)	15.9(fixed)	—	-4.6	15.9
<i>u881</i>	Cl(55)...Cl(58)	559.6(16)	19.8(tied to <i>u784</i> )	—	-1.1	17.6
<i>u814</i>	H(25)...H(40)	560.0(41)	36.6(fixed)	—	3.0	36.6
<i>u922</i>	H(61)...H(78)	561.2(38)	36.1(fixed)	—	-7.1	36.1
<i>u866</i>	C(8)...Cl(15)	561.3(27)	18.7(tied to <i>u784</i> )	—	-0.9	16.6
<i>u872</i>	C(6)...Cl(14)	561.3(31)	21.8(tied to <i>u784</i> )	—	-0.9	19.3
<i>u879</i>	H(35)...H(40)	561.4(47)	41.2(fixed)	—	5.0	41.2
<i>u884</i>	H(32)...H(36)	561.6(42)	40.4(fixed)	—	2.4	40.4
<i>u886</i>	C(47)...H(74)	561.7(49)	44.4(fixed)	—	-0.9	44.4
<i>u887</i>	C(9)...H(35)	561.8(63)	45.7(fixed)	—	-0.4	45.7
<i>u885</i>	H(35)...H(39)	562.0(34)	35.1(fixed)	—	6.8	35.1
<i>u890</i>	H(62)...H(78)	562.5(27)	40.1(fixed)	—	2.2	40.1
<i>u918</i>	C(48)...H(77)	562.7(44)	32.9(fixed)	—	-0.8	32.9
<i>u877</i>	C(7)...H(40)	562.8(55)	36.4(fixed)	—	-0.8	36.4
<i>u913</i>	H(67)...H(73)	563.3(33)	31.9(fixed)	—	2.7	31.9
<i>u849</i>	H(19)...H(37)	564.7(49)	36.2(fixed)	—	4.5	36.2
<i>u860</i>	C(52)...H(70)	565.0(55)	34.4(fixed)	—	-0.6	34.4
<i>u898</i>	C(13)...H(33)	565.0(56)	47.9(fixed)	—	-1.2	47.9
<i>u901</i>	H(61)...H(76)	565.2(34)	34.7(fixed)	—	4.0	34.7
<i>u891</i>	H(29)...H(31)	565.2(52)	40.6(fixed)	—	4.4	40.6
<i>u894</i>	H(28)...H(31)	565.2(46)	34.7(fixed)	—	6.0	34.7
<i>u930</i>	H(18)...H(32)	565.6(70)	39.6(fixed)	—	2.8	39.6
<i>u904</i>	H(20)...H(24)	566.1(51)	33.6(fixed)	—	-0.4	33.6
<i>u841</i>	H(18)...H(38)	566.2(37)	38.6(fixed)	—	1.2	38.6
<i>u832</i>	H(24)...H(41)	567.1(42)	37.5(fixed)	—	1.9	37.5
<i>u909</i>	H(28)...H(37)	567.9(49)	34.5(fixed)	—	-0.8	34.5
<i>u899</i>	C(50)...H(63)	568.0(58)	42.5(fixed)	—	-0.7	42.5
<i>u910</i>	H(64)...H(80)	568.5(52)	34.5(fixed)	—	-0.7	34.5
<i>u915</i>	C(49)...H(80)	568.8(58)	31.6(fixed)	—	-1.1	31.6
<i>u911</i>	H(23)...H(39)	569.8(48)	34.6(fixed)	—	0.4	34.6
<i>u959</i>	C(50)...H(82)	570.4(57)	27.5(fixed)	—	-3.3	27.5
<i>u888</i>	H(61)...H(69)	570.8(42)	35.7(fixed)	—	6.6	35.7
<i>u920</i>	Cl(16)...H(39)	570.9(51)	35.4(fixed)	—	-1.2	35.4
<i>u873</i>	H(64)...H(68)	571.3(55)	40.4(fixed)	—	6.3	40.4
<i>u970</i>	H(59)...H(70)	571.8(51)	49.6(fixed)	—	1.7	49.6
<i>u896</i>	H(63)...H(80)	572.7(38)	34.5(fixed)	—	1.3	34.5
<i>u870</i>	H(27)...H(33)	572.7(66)	42.4(fixed)	—	8.0	42.4
<i>u897</i>	H(24)...H(38)	572.9(25)	40.9(fixed)	—	2.1	40.9
<i>u906</i>	Cl(56)...H(78)	572.9(47)	35.9(fixed)	—	-0.9	35.9
<i>u917</i>	C(12)...H(26)	573.8(42)	32.6(fixed)	—	-0.7	32.6
<i>u902</i>	H(23)...H(25)	573.9(37)	38.8(fixed)	—	1.6	38.8



<i>u</i> 921	C(8)...H(22)	573.9(55)	30.8(fixed)	—	-1.0	30.8
<i>u</i> 912	Cl(57)...H(72)	574.1(52)	47.7(fixed)	—	-0.8	47.7
<i>u</i> 927	C(7)...H(34)	574.1(79)	23.0(fixed)	—	-1.3	23.0
<i>u</i> 969	C(7)...H(35)	575.0(55)	22.0(fixed)	—	-1.9	22.0
<i>u</i> 914	Cl(17)...H(28)	575.6(69)	34.0(fixed)	—	-1.2	34.0
<i>u</i> 835	H(21)...H(29)	576.3(53)	35.5(fixed)	—	2.3	35.5
<i>u</i> 931	H(23)...H(33)	576.3(63)	39.2(fixed)	—	1.1	39.2
<i>u</i> 1005	C(50)...H(80)	576.4(51)	24.4(fixed)	—	-3.5	24.4
<i>u</i> 977	C(47)...H(77)	576.7(34)	25.0(fixed)	—	-3.5	25.0
<i>u</i> 953	C(7)...H(33)	577.0(61)	22.3(fixed)	—	-1.8	22.3
<i>u</i> 976	Cl(15)...H(18)	577.0(61)	23.4(fixed)	—	-1.6	23.4
<i>u</i> 965	Cl(15)...H(19)	577.0(92)	24.3(fixed)	—	-1.8	24.3
<i>u</i> 945	C(49)...H(71)	577.2(39)	32.6(fixed)	—	-5.4	32.6
<i>u</i> 986	H(29)...H(32)	577.3(52)	49.0(fixed)	—	1.5	49.0
<i>u</i> 962	C(49)...H(72)	577.6(37)	34.2(fixed)	—	-5.9	34.2
<i>u</i> 908	Cl(15)...H(24)	578.0(58)	36.5(fixed)	—	-0.9	36.5
<i>u</i> 948	C(47)...H(70)	580.3(24)	22.6(fixed)	—	-1.5	22.6
<i>u</i> 979	Cl(55)...H(65)	580.8(21)	22.5(fixed)	—	-1.9	22.5
<i>u</i> 928	Cl(14)...H(20)	581.1(57)	33.4(fixed)	—	-1.2	33.4
<i>u</i> 880	H(23)...H(27)	581.2(42)	36.9(fixed)	—	1.1	36.9
<i>u</i> 1009	Cl(15)...H(20)	581.2(65)	22.7(fixed)	—	-2.1	22.7
<i>u</i> 996	Cl(55)...H(76)	582.1(36)	29.6(fixed)	—	-5.1	29.6
<i>u</i> 923	H(26)...H(40)	582.3(30)	30.8(fixed)	—	-0.7	30.8
<i>u</i> 925	C(47)...H(79)	583.1(31)	27.6(fixed)	—	-3.4	27.6
<i>u</i> 933	H(59)...H(74)	583.2(55)	48.5(fixed)	—	3.2	48.5
<i>u</i> 947	H(23)...H(37)	583.5(50)	38.9(fixed)	—	-1.1	38.9
<i>u</i> 926	C(48)...H(73)	583.5(25)	23.3(fixed)	—	-0.7	23.3
<i>u</i> 946	H(18)...H(36)	583.8(30)	32.1(fixed)	—	-2.9	32.1
<i>u</i> 974	Cl(55)...H(75)	583.8(35)	31.3(fixed)	—	-4.5	31.3
<i>u</i> 941	C(6)...H(26)	583.9(20)	21.7(fixed)	—	-1.5	21.7
<i>u</i> 954	C(10)...H(29)	585.4(20)	22.7(fixed)	—	-1.4	22.7
<i>u</i> 937	C(13)...H(22)	586.2(27)	22.2(fixed)	—	-1.6	22.2
<i>u</i> 961	H(65)...H(81)	586.3(46)	34.4(fixed)	—	-1.0	34.4
<i>u</i> 919	H(32)...H(37)	586.8(56)	47.8(fixed)	—	2.9	47.8
<i>u</i> 985	H(23)...H(34)	587.2(79)	39.3(fixed)	—	-1.2	39.3
<i>u</i> 924	C(12)...H(32)	587.6(27)	23.3(fixed)	—	-1.0	23.3
<i>u</i> 940	H(64)...H(81)	587.6(60)	39.2(fixed)	—	1.0	39.2
<i>u</i> 942	H(18)...H(24)	588.1(61)	37.5(fixed)	—	0.2	37.5
<i>u</i> 960	H(29)...H(37)	588.3(55)	39.0(fixed)	—	0.7	39.0
<i>u</i> 1003	H(64)...H(78)	588.8(45)	36.8(fixed)	—	-5.5	36.8
<i>u</i> 936	C(11)...H(40)	588.9(34)	22.9(fixed)	—	-1.3	22.9
<i>u</i> 988	Cl(16)...H(35)	589.2(36)	32.0(fixed)	—	-5.7	32.0
<i>u</i> 916	C(6)...H(25)	589.6(29)	22.6(fixed)	—	-1.6	22.6
<i>u</i> 1011	Cl(17)...H(30)	590.1(73)	32.1(fixed)	—	-5.3	32.1

<i>u972</i>	C(9)...H(36)	590.5(18)	22.2(fixed)	—	-1.5	22.2
<i>u963</i>	H(24)...H(39)	590.6(33)	30.8(fixed)	—	-4.6	30.8
<i>u975</i>	H(20)...H(37)	591.3(37)	29.7(fixed)	—	-2.3	29.7
<i>u934</i>	Cl(55)...H(66)	591.7(22)	23.8(fixed)	—	-1.6	23.8
<i>u968</i>	H(33)...H(40)	592.0(66)	50.9(fixed)	—	1.8	50.9
<i>u938</i>	C(47)...H(68)	592.3(22)	23.2(fixed)	—	-1.7	23.2
<i>u964</i>	C(50)...H(74)	592.4(30)	22.2(fixed)	—	-1.9	22.2
<i>u958</i>	H(29)...H(33)	592.4(50)	40.6(fixed)	—	2.9	40.6
<i>u955</i>	C(6)...H(24)	592.5(27)	21.7(fixed)	—	-1.9	21.7
<i>u967</i>	C(9)...H(37)	592.9(23)	22.0(fixed)	—	-2.0	22.0
<i>u992</i>	C(12)...H(31)	593.6(18)	21.4(fixed)	—	-2.5	21.4
<i>u952</i>	C(10)...H(27)	593.8(25)	23.4(fixed)	—	-1.8	23.4
<i>u1000</i>	C(6)...H(36)	593.9(33)	27.8(fixed)	—	-4.4	27.8
<i>u989</i>	C(10)...H(28)	594.0(30)	21.9(fixed)	—	-2.0	21.9
<i>u935</i>	C(9)...H(38)	594.4(22)	23.2(fixed)	—	-1.6	23.2
<i>u990</i>	C(11)...H(39)	594.7(20)	21.5(fixed)	—	-2.1	21.5
<i>u929</i>	C(13)...H(21)	594.7(31)	22.9(fixed)	—	-1.8	22.9
<i>u994</i>	Cl(55)...H(67)	594.9(18)	22.8(fixed)	—	-1.8	22.8
<i>u1010</i>	Cl(17)...H(31)	595.0(48)	33.6(fixed)	—	-5.5	33.6
<i>u973</i>	Cl(16)...H(34)	595.3(32)	32.5(fixed)	—	-5.3	32.5
<i>u957</i>	H(74)...H(81)	595.5(42)	38.1(fixed)	—	1.9	38.1
<i>u932</i>	C(12)...H(30)	595.6(18)	23.4(fixed)	—	-1.4	23.4
<i>u956</i>	H(22)...H(29)	595.7(35)	29.7(fixed)	—	-0.8	29.7
<i>u999</i>	H(23)...H(24)	595.8(52)	35.2(fixed)	—	-4.1	35.2
<i>u991</i>	C(13)...H(26)	596.4(28)	24.8(fixed)	—	-3.4	24.8
<i>u993</i>	H(24)...H(37)	596.5(48)	37.4(fixed)	—	-5.0	37.4
<i>u1016</i>	C(10)...H(18)	596.6(42)	23.7(fixed)	—	-2.8	23.7
<i>u982</i>	C(13)...H(23)	597.0(24)	21.8(fixed)	—	-1.9	21.8
<i>u944</i>	C(52)...H(60)	597.6(20)	23.5(fixed)	—	-1.5	23.5
<i>u1013</i>	C(10)...H(19)	598.0(59)	25.0(fixed)	—	-3.0	25.0
<i>u1024</i>	H(27)...H(32)	598.2(75)	52.8(fixed)	—	-2.8	52.8
<i>u984</i>	C(47)...H(69)	598.3(26)	21.8(fixed)	—	-1.9	21.8
<i>u943</i>	C(11)...H(41)	598.4(29)	23.3(fixed)	—	-1.7	23.3
<i>u987</i>	H(23)...H(40)	598.4(56)	40.0(fixed)	—	0.2	40.0
<i>u1004</i>	C(48)...H(72)	598.7(21)	21.4(fixed)	—	-2.7	21.4
<i>u995</i>	C(8)...H(39)	598.9(34)	25.7(fixed)	—	-3.8	25.7
<i>u1015</i>	H(59)...H(68)	599.0(71)	53.7(fixed)	—	-2.6	53.7
<i>u971</i>	H(18)...H(25)	599.2(66)	38.4(fixed)	—	-1.5	38.4
<i>u966</i>	C(12)...H(19)	599.7(34)	27.0(fixed)	—	-3.2	27.0
<i>u980</i>	C(50)...H(76)	600.8(20)	22.3(fixed)	—	-1.8	22.3
<i>u951</i>	C(8)...H(41)	601.2(33)	28.5(fixed)	—	-3.5	28.5
<i>u1008</i>	C(12)...H(20)	601.4(33)	23.9(fixed)	—	-3.3	23.9
<i>u950</i>	C(13)...H(25)	602.0(28)	27.3(fixed)	—	-3.4	27.3
<i>u997</i>	H(23)...H(28)	602.9(32)	30.3(fixed)	—	-5.0	30.3

<i>u1037</i>	H(23)...H(35)	603.4(55)	34.4(fixed)	—	-4.2	34.4
<i>u978</i>	C(6)...H(38)	603.8(25)	29.6(fixed)	—	-4.3	29.6
<i>u1002</i>	H(29)...H(38)	604.4(59)	40.5(fixed)	—	-1.5	40.5
<i>u1001</i>	H(30)...H(37)	605.0(55)	50.3(fixed)	—	-1.8	50.3
<i>u939</i>	C(50)...H(75)	605.3(27)	23.2(fixed)	—	-1.4	23.2
<i>u1020</i>	C(12)...H(21)	605.7(28)	26.1(fixed)	—	-3.2	26.1
<i>u1007</i>	C(9)...H(22)	606.3(27)	23.2(fixed)	—	-3.1	23.2
<i>u1030</i>	Cl(15)...H(40)	606.4(32)	25.5(fixed)	—	-3.4	25.5
<i>u1045</i>	Cl(17)...H(34)	607.7(73)	30.4(fixed)	—	-4.5	30.4
<i>u1025</i>	C(50)...H(79)	608.9(32)	25.8(fixed)	—	-3.2	25.8
<i>u1022</i>	Cl(15)...H(41)	609.4(37)	27.2(fixed)	—	-3.3	27.2
<i>u1012</i>	C(7)...H(28)	609.5(34)	24.6(fixed)	—	-3.5	24.6
<i>u1027</i>	C(12)...H(23)	609.6(28)	24.4(fixed)	—	-3.0	24.4
<i>u1032</i>	H(18)...H(26)	609.6(52)	33.7(fixed)	—	-3.0	33.7
<i>u1044</i>	Cl(14)...H(32)	611.0(32)	27.5(fixed)	—	-4.7	27.5
<i>u1014</i>	H(60)...H(74)	611.1(57)	51.5(fixed)	—	-2.4	51.5
<i>u1021</i>	C(11)...H(29)	611.3(38)	24.2(fixed)	—	-2.9	24.2
<i>u1006</i>	H(21)...H(40)	611.4(63)	42.0(fixed)	—	-2.0	42.0
<i>u1039</i>	Cl(56)...H(59)	611.7(26)	27.7(fixed)	—	-4.7	27.7
<i>u1050</i>	Cl(17)...H(33)	612.0(46)	29.1(fixed)	—	-5.3	29.1
<i>u1029</i>	C(49)...H(75)	612.4(28)	27.5(fixed)	—	-3.9	27.5
<i>u983</i>	C(7)...H(27)	612.8(31)	27.8(fixed)	—	-3.3	27.8
<i>u1043</i>	H(18)...H(31)	613.7(32)	46.3(fixed)	—	-1.6	46.3
<i>u1026</i>	Cl(58)...H(71)	614.2(31)	29.4(fixed)	—	-4.1	29.4
<i>u1040</i>	C(49)...H(74)	614.3(26)	26.9(fixed)	—	-4.5	26.9
<i>u1019</i>	H(33)...H(41)	614.3(66)	54.7(fixed)	—	-2.8	54.7
<i>u981</i>	C(9)...H(21)	614.4(32)	26.4(fixed)	—	-3.1	26.4
<i>u1042</i>	H(29)...H(36)	614.7(48)	35.2(fixed)	—	-3.4	35.2
<i>u1055</i>	H(28)...H(32)	614.8(48)	43.6(fixed)	—	-4.2	43.6
<i>u1033</i>	C(50)...H(78)	614.9(30)	24.2(fixed)	—	-3.2	24.2
<i>u1023</i>	C(48)...H(70)	615.4(32)	23.9(fixed)	—	-2.8	23.9
<i>u1036</i>	H(22)...H(40)	617.1(51)	36.2(fixed)	—	-3.1	36.2
<i>u1053</i>	H(23)...H(36)	617.2(30)	43.1(fixed)	—	-2.0	43.1
<i>u1066</i>	H(20)...H(30)	617.3(58)	31.3(fixed)	—	-7.9	31.3
<i>u1017</i>	C(11)...H(27)	617.4(50)	25.2(fixed)	—	-3.1	25.2
<i>u1018</i>	C(48)...H(68)	617.7(41)	25.5(fixed)	—	-3.1	25.5
<i>u1049</i>	H(59)...H(69)	618.3(41)	44.4(fixed)	—	-3.9	44.4
<i>u998</i>	H(62)...H(81)	618.3(62)	39.8(fixed)	—	-1.4	39.8
<i>u1047</i>	H(29)...H(35)	619.7(62)	47.0(fixed)	—	-1.4	47.0
<i>u1046</i>	H(31)...H(37)	619.9(43)	42.5(fixed)	—	-4.8	42.5
<i>u1028</i>	Cl(14)...H(30)	620.3(40)	29.2(fixed)	—	-4.0	29.2
<i>u1041</i>	C(7)...H(24)	620.9(33)	24.8(fixed)	—	-3.2	24.8
<i>u1035</i>	C(8)...H(37)	620.9(27)	27.2(fixed)	—	-4.1	27.2
<i>u1031</i>	C(8)...H(38)	621.0(26)	27.6(fixed)	—	-4.0	27.6

<i>u1034</i>	C(7)...H(25)	622.9(36)	26.3(fixed)	—	-3.3	26.3
<i>u1059</i>	H(22)...H(38)	623.9(36)	33.0(fixed)	—	-6.1	33.0
<i>u1038</i>	H(63)...H(81)	624.1(49)	34.7(fixed)	—	-3.7	34.7
<i>u1070</i>	H(64)...H(77)	624.1(29)	41.0(fixed)	—	-4.0	41.0
<i>u1067</i>	C(6)...H(30)	624.9(56)	24.1(fixed)	—	-9.0	24.1
<i>u1051</i>	H(61)...H(74)	624.9(45)	43.1(fixed)	—	-5.4	43.1
<i>u1054</i>	H(33)...H(39)	625.3(47)	45.5(fixed)	—	-4.6	45.5
<i>u1084</i>	H(21)...H(36)	626.5(71)	44.9(fixed)	—	-5.2	44.9
<i>u1048</i>	H(63)...H(70)	627.9(58)	44.0(fixed)	—	-1.8	44.0
<i>u1052</i>	H(19)...H(31)	627.9(83)	50.4(fixed)	—	-4.8	50.4
<i>u1072</i>	C(11)...H(21)	628.5(71)	19.1(fixed)	—	-5.2	19.1
<i>u1100</i>	H(62)...H(77)	631.2(66)	40.5(fixed)	—	-6.0	40.5
<i>u1068</i>	H(22)...H(24)	631.5(39)	36.8(fixed)	—	-2.8	36.8
<i>u1063</i>	H(26)...H(37)	632.4(28)	41.1(fixed)	—	-3.4	41.1
<i>u1056</i>	C(6)...C(11)	632.7(21)	13.4(fixed)	—	-1.3	13.4
<i>u1099</i>	H(68)...H(82)	633.3(89)	37.4(fixed)	—	-6.0	37.4
<i>u1060</i>	C(49)...C(53)	633.7(15)	13.4(fixed)	—	-1.3	13.4
<i>u1065</i>	H(65)...H(80)	634.0(59)	36.9(fixed)	—	-2.9	36.9
<i>u1057</i>	C(10)...C(13)	635.6(16)	13.4(fixed)	—	-1.3	13.4
<i>u1104</i>	H(66)...H(80)	636.0(63)	37.2(fixed)	—	-5.0	37.2
<i>u1061</i>	H(27)...H(35)	636.4(74)	50.4(fixed)	—	-5.1	50.4
<i>u1123</i>	H(67)...H(72)	636.7(42)	35.7(fixed)	—	-6.9	35.7
<i>u1058</i>	C(47)...C(51)	636.7(16)	13.3(fixed)	—	-1.4	13.3
<i>u1071</i>	C(7)...H(38)	639.1(22)	24.7(fixed)	—	-7.7	24.7
<i>u1148</i>	H(69)...H(80)	639.6(63)	28.8(fixed)	—	-7.9	28.8
<i>u1062</i>	H(63)...H(68)	639.7(67)	47.1(fixed)	—	-5.1	47.1
<i>u1146</i>	H(68)...H(80)	640.0(48)	31.3(fixed)	—	-8.9	31.3
<i>u1075</i>	C(50)...H(60)	640.9(22)	23.3(fixed)	—	-9.6	23.3
<i>u1069</i>	C(13)...H(34)	641.1(23)	24.0(fixed)	—	-9.6	24.0
<i>u1077</i>	C(9)...H(30)	642.2(24)	23.0(fixed)	—	-9.1	23.0
<i>u1086</i>	H(28)...H(34)	642.8(48)	32.3(fixed)	—	-8.3	32.3
<i>u1081</i>	C(7)...Cl(14)	643.0(7)	14.3(13)	1.4	-1.5	13.7
<i>u1073</i>	C(10)...H(38)	643.0(19)	20.9(fixed)	—	-8.0	20.9
<i>u1082</i>	C(12)...Cl(16)	643.1(7)	14.3(tied to <i>u1081</i> )	—	-1.5	13.7
<i>u1076</i>	C(47)...H(75)	643.2(21)	22.2(fixed)	—	-8.3	22.2
<i>u1134</i>	H(60)...H(77)	643.2(48)	35.3(fixed)	—	-8.3	35.3
<i>u1064</i>	C(8)...H(19)	643.3(25)	19.1(fixed)	—	-5.2	19.1
<i>u1080</i>	C(48)...Cl(55)	643.4(7)	14.3(tied to <i>u1081</i> )	—	-1.5	13.7
<i>u1078</i>	C(9)...Cl(15)	643.5(7)	14.4(tied to <i>u1081</i> )	—	-1.5	13.8
<i>u1094</i>	H(21)...H(26)	644.0(40)	30.8(fixed)	—	-2.5	30.8
<i>u1074</i>	C(7)...H(41)	644.6(28)	19.7(fixed)	—	-6.1	19.7
<i>u1087</i>	C(50)...Cl(58)	645.0(7)	14.3(tied to <i>u1081</i> )	—	-1.5	13.7
<i>u1105</i>	H(26)...H(38)	645.4(63)	39.8(fixed)	—	-6.0	39.8
<i>u1102</i>	H(60)...H(79)	645.9(49)	42.1(fixed)	—	-8.8	42.1

<i>u1091</i>	C(8)...Cl(17)	646.0(7)	14.2(tied to <i>u1081</i> )	—	-1.5	13.6
<i>u1092</i>	C(49)...H(82)	646.4(31)	22.9(fixed)	—	-5.2	22.9
<i>u1083</i>	C(9)...H(34)	646.4(37)	24.6(fixed)	—	-9.4	24.6
<i>u1088</i>	C(12)...H(27)	646.9(22)	19.4(fixed)	—	-5.6	19.4
<i>u1125</i>	C(49)...H(77)	647.0(27)	24.2(fixed)	—	-0.3	24.2
<i>u1089</i>	H(67)...H(82)	647.1(41)	30.9(fixed)	—	-2.9	30.9
<i>u1111</i>	H(61)...H(79)	648.4(46)	42.2(fixed)	—	-9.2	42.2
<i>u1097</i>	H(63)...H(79)	649.1(35)	31.2(fixed)	—	-1.9	31.2
<i>u1109</i>	C(11)...H(20)	649.1(35)	24.1(fixed)	—	-0.7	24.1
<i>u1112</i>	C(13)...H(32)	649.2(32)	27.8(fixed)	—	0.6	27.8
<i>u1124</i>	H(22)...H(25)	649.3(75)	36.3(fixed)	—	-5.0	36.3
<i>u1093</i>	H(25)...H(36)	649.7(35)	31.2(fixed)	—	-1.7	31.2
<i>u1085</i>	C(50)...H(62)	650.5(30)	23.8(fixed)	—	-7.9	23.8
<i>u1096</i>	C(48)...H(79)	650.7(22)	22.1(fixed)	—	-5.6	22.1
<i>u1110</i>	C(6)...H(35)	650.8(28)	27.1(fixed)	—	1.0	27.1
<i>u1149</i>	H(65)...H(77)	651.1(29)	34.1(fixed)	—	1.9	34.1
<i>u1120</i>	C(10)...H(39)	651.5(34)	24.6(fixed)	—	-0.7	24.6
<i>u1106</i>	C(10)...H(40)	651.5(32)	26.1(fixed)	—	-0.3	26.1
<i>u1107</i>	C(47)...H(73)	651.7(31)	28.3(fixed)	—	1.0	28.3
<i>u1131</i>	H(32)...H(39)	651.8(35)	35.5(fixed)	—	4.1	35.5
<i>u1133</i>	Cl(14)...H(22)	652.1(22)	24.5(fixed)	—	-0.8	24.5
<i>u1108</i>	C(11)...H(18)	652.2(31)	25.5(fixed)	—	-0.7	25.5
<i>u1079</i>	H(62)...H(69)	653.6(41)	31.8(fixed)	—	-6.6	31.8
<i>u1090</i>	C(48)...H(82)	653.7(25)	19.3(fixed)	—	-5.5	19.3
<i>u1139</i>	H(20)...H(36)	653.8(40)	31.0(fixed)	—	-5.3	31.0
<i>u1127</i>	C(49)...H(78)	653.8(28)	25.5(fixed)	—	-0.8	25.5
<i>u1113</i>	Cl(16)...H(41)	654.0(24)	23.0(fixed)	—	-6.0	23.0
<i>u1115</i>	Cl(56)...H(79)	654.3(22)	19.8(fixed)	—	-6.1	19.8
<i>u1135</i>	H(26)...H(39)	654.5(39)	29.8(fixed)	—	-5.2	29.8
<i>u1121</i>	Cl(55)...H(60)	654.6(22)	25.1(fixed)	—	-9.6	25.1
<i>u1116</i>	C(6)...H(33)	655.3(29)	28.6(fixed)	—	0.5	28.6
<i>u1101</i>	C(8)...H(21)	655.7(27)	22.2(fixed)	—	-4.9	22.2
<i>u1098</i>	Cl(17)...H(27)	655.8(43)	23.5(fixed)	—	-5.5	23.5
<i>u1119</i>	C(47)...H(72)	655.8(32)	28.1(fixed)	—	0.5	28.1
<i>u1095</i>	C(12)...H(25)	655.8(22)	22.5(fixed)	—	-5.7	22.5
<i>u1141</i>	Cl(55)...H(63)	655.9(23)	26.6(fixed)	—	0.4	26.6
<i>u1136</i>	Cl(15)...H(29)	656.0(28)	26.1(fixed)	—	-0.6	26.1
<i>u1128</i>	H(18)...H(35)	656.5(46)	37.5(fixed)	—	4.1	37.5
<i>u1117</i>	C(13)...H(31)	656.7(32)	27.3(fixed)	—	0.5	27.3
<i>u1130</i>	H(59)...H(72)	657.4(30)	39.4(fixed)	—	6.6	39.4
<i>u1140</i>	Cl(56)...H(81)	657.7(27)	25.5(fixed)	—	-0.8	25.5
<i>u1144</i>	Cl(16)...H(36)	657.7(22)	26.3(fixed)	—	0.5	26.3
<i>u1132</i>	H(20)...H(33)	658.3(51)	35.5(fixed)	—	3.7	35.5
<i>u1129</i>	H(31)...H(40)	659.3(32)	37.6(fixed)	—	4.2	37.6

<i>u</i> 1158	H(32)...H(40)	659.4(69)	41.1(fixed)	—	1.5	41.1
<i>u</i> 1118	Cl(14)...H(19)	659.9(35)	22.9(fixed)	—	-5.3	22.9
<i>u</i> 1126	Cl(15)...H(25)	659.9(25)	19.7(fixed)	—	-6.2	19.7
<i>u</i> 1157	Cl(17)...H(26)	660.0(23)	24.4(fixed)	—	-0.5	24.4
<i>u</i> 1150	Cl(55)...H(64)	661.6(23)	28.0(fixed)	—	-0.1	28.0
<i>u</i> 1147	Cl(15)...H(28)	661.9(30)	25.0(fixed)	—	-0.9	25.0
<i>u</i> 1143	Cl(16)...H(37)	662.1(23)	28.3(fixed)	—	-0.3	28.3
<i>u</i> 1145	H(22)...H(28)	662.2(39)	28.4(fixed)	—	-4.6	28.4
<i>u</i> 1142	H(19)...H(36)	662.4(46)	35.0(fixed)	—	-7.5	35.0
<i>u</i> 1159	H(59)...H(73)	662.9(68)	44.4(fixed)	—	2.8	44.4
<i>u</i> 1151	Cl(56)...H(80)	665.3(28)	24.8(fixed)	—	-0.9	24.8
<i>u</i> 1152	Cl(14)...H(23)	665.3(23)	25.7(fixed)	—	-1.2	25.7
<i>u</i> 1153	Cl(17)...H(24)	666.3(23)	25.9(fixed)	—	-0.9	25.9
<i>u</i> 1137	H(26)...H(41)	667.3(40)	32.5(fixed)	—	-6.6	32.5
<i>u</i> 1114	H(19)...H(38)	667.9(43)	39.6(fixed)	—	-7.2	39.6
<i>u</i> 1103	H(25)...H(41)	668.5(46)	38.2(fixed)	—	-6.5	38.2
<i>u</i> 1138	H(25)...H(39)	669.2(43)	32.6(fixed)	—	-6.8	32.6
<i>u</i> 1176	H(21)...H(35)	669.5(62)	25.7(fixed)	—	-5.6	25.7
<i>u</i> 1160	H(18)...H(33)	669.8(52)	41.2(fixed)	—	1.3	41.2
<i>u</i> 1188	H(67)...H(77)	670.4(52)	31.2(fixed)	—	-1.1	31.2
<i>u</i> 1168	H(21)...H(34)	671.3(91)	26.3(fixed)	—	-5.9	26.3
<i>u</i> 1161	H(65)...H(78)	672.1(57)	37.2(fixed)	—	-0.1	37.2
<i>u</i> 1155	H(20)...H(38)	674.0(40)	32.1(fixed)	—	-7.1	32.1
<i>u</i> 1156	H(22)...H(27)	678.0(39)	30.3(fixed)	—	-6.1	30.3
<i>u</i> 1163	H(22)...H(41)	678.3(35)	26.4(fixed)	—	-6.1	26.4
<i>u</i> 1172	H(20)...H(35)	678.4(42)	35.0(fixed)	—	-1.0	35.0
<i>u</i> 1164	H(19)...H(26)	679.5(27)	25.5(fixed)	—	-5.3	25.5
<i>u</i> 1186	H(71)...H(81)	680.3(25)	25.6(fixed)	—	-11.0	25.6
<i>u</i> 1192	H(21)...H(33)	680.6(63)	23.3(fixed)	—	-7.1	23.3
<i>u</i> 1122	H(21)...H(27)	681.2(45)	36.8(fixed)	—	-5.9	36.8
<i>u</i> 1154	H(21)...H(28)	681.5(47)	30.8(fixed)	—	-6.2	30.8
<i>u</i> 1182	H(34)...H(39)	682.7(27)	29.5(fixed)	—	-9.6	29.5
<i>u</i> 1177	H(62)...H(73)	683.5(25)	25.5(fixed)	—	-9.3	25.5
<i>u</i> 1181	H(61)...H(72)	683.5(64)	41.0(fixed)	—	-0.9	41.0
<i>u</i> 1185	H(31)...H(39)	683.7(63)	36.2(fixed)	—	-1.3	36.2
<i>u</i> 1196	H(19)...H(30)	684.6(68)	32.5(fixed)	—	-11.1	32.5
<i>u</i> 1189	H(31)...H(38)	685.5(26)	26.4(fixed)	—	-8.6	26.4
<i>u</i> 1187	H(29)...H(30)	685.6(21)	25.2(fixed)	—	-10.4	25.2
<i>u</i> 1175	H(27)...H(36)	686.0(27)	25.9(fixed)	—	-5.4	25.9
<i>u</i> 1166	H(60)...H(68)	686.7(27)	30.7(fixed)	—	-11.1	30.7
<i>u</i> 1184	H(34)...H(40)	686.8(32)	26.1(fixed)	—	-10.9	26.1
<i>u</i> 1178	H(28)...H(30)	687.1(37)	28.8(fixed)	—	-9.0	28.8
<i>u</i> 1180	H(32)...H(38)	687.9(26)	24.7(fixed)	—	-9.1	24.7
<i>u</i> 1162	H(19)...H(25)	688.8(33)	26.4(fixed)	—	-6.3	26.4

<i>u1165</i>	H(34)...H(41)	689.4(30)	31.2(fixed)	—	-11.1	31.2
<i>u1171</i>	H(27)...H(30)	689.6(29)	30.4(fixed)	—	-10.5	30.4
<i>u1190</i>	H(61)...H(75)	690.3(28)	27.4(fixed)	—	-8.9	27.4
<i>u1167</i>	H(21)...H(41)	691.0(37)	26.9(fixed)	—	-7.4	26.9
<i>u1169</i>	H(30)...H(38)	691.2(23)	28.2(fixed)	—	-9.1	28.2
<i>u1173</i>	H(60)...H(69)	691.3(34)	29.1(fixed)	—	-9.4	29.1
<i>u1170</i>	H(60)...H(75)	691.3(25)	29.4(fixed)	—	-9.4	29.4
<i>u1202</i>	H(18)...H(30)	691.6(53)	26.5(fixed)	—	-10.9	26.5
<i>u1174</i>	H(27)...H(38)	693.5(29)	26.7(fixed)	—	-6.7	26.7
<i>u1193</i>	H(64)...H(82)	696.1(30)	23.2(fixed)	—	-7.2	23.2
<i>u1183</i>	H(63)...H(82)	696.2(26)	25.7(fixed)	—	-5.8	25.7
<i>u1194</i>	H(27)...H(37)	696.6(24)	23.1(fixed)	—	-7.4	23.1
<i>u1191</i>	H(19)...H(24)	696.7(28)	22.9(fixed)	—	-6.8	22.9
<i>u1197</i>	H(21)...H(38)	698.9(19)	33.8(fixed)	—	-9.7	33.8
<i>u1195</i>	H(23)...H(41)	699.2(26)	23.1(fixed)	—	-7.6	23.1
<i>u1199</i>	H(66)...H(82)	702.3(39)	31.5(fixed)	—	-7.3	31.5
<i>u1179</i>	H(62)...H(82)	704.1(32)	26.4(fixed)	—	-6.3	26.4
<i>u1205</i>	H(29)...H(34)	707.6(35)	27.0(fixed)	—	-11.3	27.0
<i>u1207</i>	H(23)...H(38)	708.2(33)	26.8(fixed)	—	-9.9	26.8
<i>u1200</i>	H(27)...H(34)	709.3(49)	33.0(fixed)	—	-11.5	33.0
<i>u1201</i>	H(62)...H(79)	709.4(22)	32.0(fixed)	—	-8.2	32.0
<i>u1198</i>	H(62)...H(68)	710.3(41)	32.0(fixed)	—	-10.0	32.0
<i>u1206</i>	H(62)...H(70)	711.8(30)	26.2(fixed)	—	-9.9	26.2
<i>u1208</i>	H(65)...H(82)	712.4(30)	26.0(fixed)	—	-7.6	26.0
<i>u1209</i>	C(6)...H(34)	713.6(30)	16.8(fixed)	—	-7.0	16.8
<i>u1217</i>	H(64)...H(79)	714.1(30)	27.6(fixed)	—	-9.2	27.6
<i>u1203</i>	H(25)...H(38)	715.8(20)	32.7(fixed)	—	-8.4	32.7
<i>u1213</i>	C(11)...H(19)	717.2(30)	15.9(fixed)	—	-4.6	15.9
<i>u1204</i>	H(21)...H(25)	717.8(25)	31.1(fixed)	—	-7.1	31.1
<i>u1215</i>	C(53)...H(66)	719.3(14)	16.3(fixed)	—	-4.9	16.3
<i>u1210</i>	C(13)...H(30)	719.6(15)	16.4(fixed)	—	-6.7	16.4
<i>u1212</i>	H(25)...H(37)	719.9(31)	27.9(fixed)	—	-9.0	27.9
<i>u1216</i>	H(21)...H(24)	720.8(35)	25.9(fixed)	—	-7.5	25.9
<i>u1214</i>	C(47)...H(71)	720.9(15)	16.7(fixed)	—	-7.1	16.7
<i>u1211</i>	C(10)...H(41)	721.9(14)	16.0(fixed)	—	-5.1	16.0
<i>u1220</i>	Cl(16)...H(38)	727.8(10)	16.4(fixed)	—	-6.4	16.4
<i>u1218</i>	Cl(14)...H(21)	729.2(10)	16.2(fixed)	—	-4.9	16.2
<i>u1222</i>	Cl(55)...H(62)	729.4(9)	16.7(fixed)	—	-6.4	16.7
<i>u1224</i>	H(20)...H(34)	730.0(39)	26.3(fixed)	—	-6.4	26.3
<i>u1221</i>	Cl(15)...H(27)	730.1(9)	16.2(fixed)	—	-5.1	16.2
<i>u1223</i>	Cl(56)...H(82)	730.7(10)	16.2(fixed)	—	-5.0	16.2
<i>u1219</i>	Cl(17)...H(25)	730.9(11)	16.4(fixed)	—	-5.1	16.4
<i>u1228</i>	H(30)...H(39)	734.1(28)	26.4(fixed)	—	-6.2	26.4
<i>u1226</i>	H(66)...H(77)	734.6(23)	25.7(fixed)	—	-3.8	25.7

<i>u</i> 1225	H(19)...H(35)	735.4(33)	26.9(fixed)	—	-2.2	26.9
<i>u</i> 1229	H(60)...H(72)	740.1(25)	28.6(fixed)	—	-5.4	28.6
<i>u</i> 1232	H(18)...H(34)	740.3(30)	26.6(fixed)	—	-8.1	26.6
<i>u</i> 1231	H(59)...H(71)	742.0(28)	28.5(fixed)	—	-6.9	28.5
<i>u</i> 1227	H(31)...H(41)	742.4(26)	27.2(fixed)	—	-3.3	27.2
<i>u</i> 1233	H(32)...H(41)	742.5(28)	27.3(fixed)	—	-4.8	27.3
<i>u</i> 1230	H(30)...H(40)	742.7(30)	26.5(fixed)	—	-7.4	26.5
<i>u</i> 1235	H(65)...H(79)	745.7(24)	25.8(fixed)	—	-5.6	25.8
<i>u</i> 1234	H(19)...H(33)	747.0(29)	28.0(fixed)	—	-4.5	28.0
<i>u</i> 1238	H(19)...H(34)	792.6(46)	20.2(fixed)	—	-9.3	20.2
<i>u</i> 1236	H(66)...H(79)	799.0(18)	20.0(fixed)	—	-7.9	20.0
<i>u</i> 1239	H(60)...H(71)	800.7(19)	20.1(fixed)	—	-11.3	20.1
<i>u</i> 1237	H(30)...H(41)	801.5(18)	19.8(fixed)	—	-9.4	19.8

<sup>a</sup> Distances in pm. Values in parentheses are the standard deviations on the last digits. See Figure 1 for atom numbering.

**Table S12** Refined and calculated [B3LYP/6-31G(d)] amplitudes of vibration ( $u_{h1}$ ), associated  $r_a$  distances and corresponding correction values ( $k_{h1}$ ) for the refinement of C(SiBrMe<sub>2</sub>)<sub>4</sub> (**4**).<sup>a</sup>

	Atom pair	$r_a$	$u_{GED}$	Restraint	$k_{h1}$	$u_{calc.}$
<i>u</i> 14	C(10)-H(31)	108.9(5)	9.6(4)	0.8	0.4	7.7
<i>u</i> 23	C(10)-H(30)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 831	C(51)-H(71)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 1	C(10)-H(32)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 12	C(11)-H(33)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 825	C(48)-H(64)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 826	C(47)-H(61)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 24	C(12)-H(38)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 10	C(8)-H(24)	108.9(5)	9.5(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 11	C(7)-H(23)	108.9(5)	9.5(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 4	C(12)-H(36)	108.9(5)	9.5(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 8	C(12)-H(37)	108.9(5)	9.5(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 17	C(6)-H(19)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 18	C(9)-H(27)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 19	C(13)-H(41)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 20	C(11)-H(34)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 21	C(7)-H(21)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 22	C(8)-H(25)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 829	C(50)-H(68)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 830	C(47)-H(60)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 832	C(49)-H(66)	108.9(5)	9.6(tied to <i>u</i> 14)	—	0.4	7.7
<i>u</i> 2	C(11)-H(35)	108.9(5)	9.5(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 5	C(13)-H(40)	108.9(5)	9.5(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 6	C(8)-H(26)	108.9(5)	9.5(tied to <i>u</i> 14)	—	0.4	7.6
<i>u</i> 7	C(7)-H(22)	108.9(5)	9.5(tied to <i>u</i> 14)	—	0.4	7.6



<i>u822</i>	C(47)-H(59)	108.9(5)	9.5(tied to u14)	—	0.4	7.6
<i>u823</i>	C(48)-H(63)	108.9(5)	9.5(tied to u14)	—	0.4	7.6
<i>u824</i>	C(49)-H(67)	108.9(5)	9.5(tied to u14)	—	0.4	7.6
<i>u9</i>	C(6)-H(18)	108.9(5)	9.5(tied to u14)	—	0.4	7.6
<i>u3</i>	C(9)-H(29)	108.9(5)	9.5(tied to u14)	—	0.4	7.6
<i>u16</i>	C(9)-H(28)	108.9(5)	9.6(tied to u14)	—	0.4	7.6
<i>u828</i>	C(50)-H(69)	108.9(5)	9.6(tied to u14)	—	0.4	7.6
<i>u821</i>	C(50)-H(70)	108.9(5)	9.5(tied to u14)	—	0.4	7.6
<i>u13</i>	C(6)-H(20)	108.9(5)	9.6(tied to u14)	—	0.4	7.6
<i>u15</i>	C(13)-H(39)	108.9(5)	9.6(tied to u14)	—	0.4	7.6
<i>u827</i>	C(49)-H(65)	108.9(5)	9.6(tied to u14)	—	0.4	7.6
<i>u34</i>	H(36)...H(38)	176.2(9)	12.5(fixed)	—	-0.3	12.5
<i>u40</i>	H(30)...H(31)	176.2(9)	12.6(fixed)	—	-0.2	12.6
<i>u35</i>	H(36)...H(37)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u27</i>	H(33)...H(35)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u39</i>	H(33)...H(34)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u836</i>	H(59)...H(60)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u28</i>	H(31)...H(32)	176.2(9)	12.6(fixed)	—	-0.2	12.6
<i>u32</i>	H(30)...H(32)	176.2(9)	12.6(fixed)	—	-0.2	12.6
<i>u842</i>	H(60)...H(61)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u33</i>	H(34)...H(35)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u834</i>	H(59)...H(61)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u43</i>	H(37)...H(38)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u837</i>	H(62)...H(63)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u835</i>	H(63)...H(64)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u841</i>	H(62)...H(64)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u37</i>	H(39)...H(41)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u25</i>	H(25)...H(26)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u26</i>	H(18)...H(19)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u833</i>	H(66)...H(67)	176.2(9)	12.5(fixed)	—	-0.2	12.5
<i>u29</i>	H(40)...H(41)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u30</i>	H(27)...H(29)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u839</i>	H(68)...H(69)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u31</i>	H(21)...H(22)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u36</i>	H(19)...H(20)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u38</i>	H(27)...H(28)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u42</i>	H(24)...H(25)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u840</i>	H(65)...H(66)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u41</i>	H(21)...H(23)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u843</i>	H(65)...H(67)	176.3(9)	12.5(fixed)	—	-0.2	12.5
<i>u838</i>	H(68)...H(70)	176.3(9)	12.5(fixed)	—	-0.1	12.5
<i>u44</i>	H(24)...H(26)	176.3(9)	12.5(fixed)	—	-0.1	12.5
<i>u45</i>	H(39)...H(40)	176.3(9)	12.5(fixed)	—	-0.1	12.5
<i>u46</i>	H(28)...H(29)	176.3(9)	12.5(fixed)	—	-0.1	12.5

<i>u47</i>	H(18)...H(20)	176.3(9)	12.5(fixed)	—	-0.1	12.5
<i>u48</i>	H(22)...H(23)	176.3(9)	12.5(fixed)	—	-0.1	12.5
<i>u844</i>	H(69)...H(70)	176.3(9)	12.5(fixed)	—	-0.1	12.5
<i>u50</i>	Si(5)-C(7)	185.6(3)	5.4(3)	0.6	0.2	5.8
<i>u845</i>	Si(43)-C(54)	185.6(3)	5.4(tied to <i>u50</i> )	—	0.2	5.8
<i>u55</i>	Si(3)-C(8)	185.7(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u52</i>	Si(2)-C(13)	185.8(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u53</i>	Si(4)-C(11)	185.8(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u54</i>	Si(4)-C(10)	185.8(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u846</i>	Si(45)-C(51)	185.9(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u847</i>	Si(45)-C(52)	185.9(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u51</i>	Si(3)-C(9)	186.0(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u56</i>	Si(5)-C(6)	186.2(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u49</i>	Si(2)-C(12)	186.2(3)	5.4(tied to <i>u50</i> )	—	0.2	5.8
<i>u848</i>	Si(43)-C(53)	186.5(3)	5.4(tied to <i>u50</i> )	—	0.2	5.9
<i>u849</i>	C(42)-Si(45)	190.6(5)	6.2(tied to <i>u60</i> )	—	0.3	6.8
<i>u60</i>	C(1)-Si(5)	190.6(5)	6.4(6)	0.7	0.3	6.6
<i>u58</i>	C(1)-Si(3)	191.1(5)	6.3(tied to <i>u60</i> )	—	0.3	6.7
<i>u59</i>	C(1)-Si(2)	191.2(5)	6.3(tied to <i>u60</i> )	—	0.3	6.7
<i>u57</i>	C(1)-Si(4)	191.5(5)	6.2(tied to <i>u60</i> )	—	0.3	6.6
<i>u850</i>	C(42)-Si(43)	191.7(5)	6.4(tied to <i>u60</i> )	—	0.3	6.8
<i>u61</i>	H(35)...H(36)	219.8(60)	41.2(fixed)	—	29.2	41.2
<i>u67</i>	H(23)...H(32)	221.9(70)	45.1(fixed)	—	18.7	45.1
<i>u853</i>	H(63)...H(76)	223.6(68)	41.5(fixed)	—	17.1	45.4
<i>u855</i>	H(59)...H(80)	224.9(1)	44.8(fixed)	—	0.3	6.6
<i>u71</i>	H(28)...H(40)	225.6(1)	43.8(fixed)	—	0.3	6.7
<i>u80</i>	H(22)...H(32)	226.6(1)	45.4(fixed)	—	0.3	6.8
<i>u63</i>	Si(4)-Br(15)	226.6(1)	7.3(tied to <i>u64</i> )	—	0.3	6.8
<i>u852</i>	Si(43)-Br(55)	227.2(1)	7.4(tied to <i>u64</i> )	—	0.3	6.8
<i>u64</i>	Si(5)-Br(17)	227.6(1)	7.6(2)	—	0.3	6.9
<i>u854</i>	Si(45)-Br(56)	227.7(78)	7.6(tied to <i>u64</i> )	—	18.8	44.8
<i>u65</i>	Si(3)-Br(16)	232.6(87)	7.6(tied to <i>u64</i> )	—	12.5	43.8
<i>u66</i>	Si(2)-Br(14)	235.1(58)	7.7(tied to <i>u64</i> )	—	24.8	39.7
<i>u851</i>	H(61)...H(67)	242.1(73)	39.7(fixed)	—	25.5	41.5
<i>u83</i>	H(18)...H(39)	243.8(99)	46.6(fixed)	—	10.6	46.6
<i>u82</i>	H(20)...H(29)	245.0(7)	44.8(fixed)	—	-0.4	13.0
<i>u72</i>	Si(5)...H(21)	245.0(7)	13.0(fixed)	—	-0.4	13.0
<i>u864</i>	Si(43)...H(80)	245.0(7)	13.0(fixed)	—	-0.4	13.0
<i>u861</i>	Si(43)...H(82)	245.1(7)	13.0(fixed)	—	-0.3	12.9
<i>u87</i>	Si(5)...H(23)	245.1(7)	12.9(fixed)	—	-0.4	12.7
<i>u90</i>	Si(5)...H(22)	245.1(7)	12.7(fixed)	—	-0.3	12.6
<i>u868</i>	Si(43)...H(81)	245.1(7)	12.6(fixed)	—	-0.3	13.0
<i>u73</i>	Si(3)...H(25)	245.1(7)	13.0(fixed)	—	-0.3	12.9
<i>u88</i>	Si(3)...H(24)	245.2(7)	12.9(fixed)	—	-0.3	12.7

<i>u</i> 100	Si(3)...H(26)	245.2(7)	12.7(fixed)	—	-0.4	13.1
<i>u</i> 76	Si(2)...H(41)	245.2(7)	13.1(fixed)	—	-0.3	13.0
<i>u</i> 86	Si(2)...H(39)	245.3(7)	13.0(fixed)	—	-0.3	13.1
<i>u</i> 78	Si(4)...H(30)	245.3(7)	13.1(fixed)	—	-0.3	13.2
<i>u</i> 89	Si(4)...H(33)	245.3(7)	13.2(fixed)	—	-0.3	13.1
<i>u</i> 79	Si(4)...H(34)	245.3(7)	13.1(fixed)	—	-0.3	12.8
<i>u</i> 98	Si(2)...H(40)	245.3(7)	12.8(fixed)	—	-0.3	12.9
<i>u</i> 92	Si(4)...H(32)	245.3(7)	12.9(fixed)	—	-0.3	13.0
<i>u</i> 862	Si(45)...H(75)	245.3(7)	13.0(fixed)	—	-0.2	13.1
<i>u</i> 94	Si(4)...H(31)	245.3(7)	13.1(fixed)	—	-0.3	13.0
<i>u</i> 866	Si(45)...H(74)	245.4(7)	13.0(fixed)	—	-0.2	12.9
<i>u</i> 99	Si(4)...H(35)	245.4(7)	12.9(fixed)	—	-0.3	13.1
<i>u</i> 863	Si(45)...H(71)	245.4(7)	13.1(fixed)	—	-0.4	13.0
<i>u</i> 77	Si(3)...H(27)	245.4(7)	13.0(fixed)	—	-0.3	12.8
<i>u</i> 870	Si(45)...H(76)	245.4(7)	12.8(fixed)	—	-0.4	13.0
<i>u</i> 85	Si(3)...H(28)	245.4(7)	13.0(fixed)	—	-0.3	12.9
<i>u</i> 867	Si(45)...H(73)	245.4(7)	12.9(fixed)	—	-0.2	13.1
<i>u</i> 869	Si(45)...H(72)	245.4(7)	13.1(fixed)	—	-0.3	12.7
<i>u</i> 97	Si(3)...H(29)	245.6(7)	12.7(fixed)	—	-0.4	13.0
<i>u</i> 75	Si(5)...H(19)	245.6(7)	13.0(fixed)	—	-0.3	12.9
<i>u</i> 91	Si(5)...H(20)	245.6(7)	12.9(fixed)	—	-0.3	12.7
<i>u</i> 96	Si(5)...H(18)	245.7(7)	12.7(fixed)	—	-0.2	13.0
<i>u</i> 74	Si(2)...H(38)	245.7(7)	13.0(fixed)	—	-0.2	13.0
<i>u</i> 84	Si(2)...H(37)	245.7(7)	13.0(fixed)	—	-0.2	12.7
<i>u</i> 95	Si(2)...H(36)	245.9(7)	12.7(fixed)	—	-0.3	13.1
<i>u</i> 860	Si(43)...H(79)	245.9(7)	13.1(fixed)	—	-0.3	13.0
<i>u</i> 865	Si(43)...H(78)	245.9(7)	13.0(fixed)	—	-0.3	12.7
<i>u</i> 871	Si(43)...H(77)	246.8(70)	12.7(fixed)	—	14.7	44.3
<i>u</i> 856	H(74)...H(78)	250.1(96)	47.2(fixed)	—	10.7	44.8
<i>u</i> 857	H(64)...H(65)	252.6(63)	47.1(fixed)	—	16.4	47.2
<i>u</i> 115	Br(15)...H(22)	252.6(63)	32.6(fixed)	—	16.4	47.1
<i>u</i> 101	C(7)...H(32)	256.1(54)	31.9(fixed)	—	23.7	39.0
<i>u</i> 876	Br(55)...H(70)	259.4(105)	29.2(fixed)	—	13.2	47.4
<i>u</i> 62	H(26)...H(31)	261.5(116)	39.0(fixed)	—	12.6	44.5
<i>u</i> 81	H(29)...H(40)	263.3(34)	47.4(fixed)	—	9.6	29.2
<i>u</i> 69	H(18)...H(29)	263.4(50)	44.5(fixed)	—	15.5	31.9
<i>u</i> 859	H(59)...H(81)	264.3(75)	48.6(fixed)	—	17.8	45.3
<i>u</i> 858	H(64)...H(67)	267.8(110)	44.3(fixed)	—	18.7	48.6
<i>u</i> 93	H(18)...H(40)	269.6(116)	49.9(fixed)	—	11.4	49.9
<i>u</i> 103	H(25)...H(27)	272.8(72)	36.0(fixed)	—	7.4	32.6
<i>u</i> 121	C(11)...H(36)	275.5(77)	31.0(fixed)	—	18.9	47.9
<i>u</i> 70	H(24)...H(33)	279.2(47)	47.9(fixed)	—	7.4	36.0
<i>u</i> 120	C(12)...H(35)	281.5(30)	32.9(fixed)	—	9.6	28.6
<i>u</i> 104	C(9)...H(40)	283.8(47)	30.4(fixed)	—	7.0	36.1

<i>u872</i>	C(50)...H(73)	284.0(47)	32.7(fixed)	—	9.6	37.3
<i>u874</i>	H(66)...H(68)	284.7(47)	36.1(fixed)	—	6.7	35.3
<i>u107</i>	H(38)...H(41)	287.0(48)	37.3(fixed)	—	10.3	30.4
<i>u108</i>	H(19)...H(21)	287.4(31)	35.3(fixed)	—	12.5	29.1
<i>u148</i>	C(10)...H(22)	288.2(41)	37.6(fixed)	—	16.4	32.7
<i>u110</i>	Br(14)...H(24)	289.1(51)	28.6(fixed)	—	7.3	29.5
<i>u68</i>	H(26)...H(33)	291.2(47)	45.3(fixed)	—	12.5	39.7
<i>u150</i>	C(10)...H(23)	291.7(51)	39.6(fixed)	—	3.1	37.6
<i>u875</i>	H(60)...H(62)	291.9(50)	39.7(fixed)	—	13.0	31.2
<i>u111</i>	Br(17)...H(37)	294.1(38)	29.1(fixed)	—	9.3	29.2
<i>u105</i>	C(6)...H(29)	294.8(47)	30.0(fixed)	—	13.3	40.4
<i>u109</i>	C(13)...H(18)	297.2(20)	31.2(fixed)	—	-0.1	11.9
<i>u878</i>	C(47)...H(67)	297.7(59)	29.7(fixed)	—	9.2	30.0
<i>u106</i>	H(30)...H(34)	297.8(46)	40.4(fixed)	—	11.1	31.0
<i>u884</i>	C(48)...H(76)	297.8(59)	33.2(fixed)	—	8.7	29.8
<i>u114</i>	Br(16)...H(20)	298.3(64)	29.5(fixed)	—	8.2	31.2
<i>u118</i>	C(8)...C(9)	298.7(20)	11.7(tied to u137)	—	-0.1	11.9
<i>u895</i>	C(47)...H(80)	299.1(42)	36.3(fixed)	—	7.6	31.8
<i>u122</i>	C(12)...C(13)	299.6(19)	11.8(tied to u137)	—	-0.1	11.8
<i>u142</i>	C(13)...H(28)	299.7(48)	37.6(fixed)	—	14.2	32.9
<i>u879</i>	C(49)...C(50)	299.9(19)	11.7(tied to u137)	—	-0.2	12.0
<i>u123</i>	C(6)...C(7)	300.8(19)	11.8(tied to u137)	—	-0.1	11.8
<i>u881</i>	C(47)...C(48)	301.6(46)	11.6(tied to u137)	—	7.9	29.7
<i>u145</i>	Si(4)...Si(5)	301.9(19)	13.4(tied to u137)	—	-0.1	11.7
<i>u184</i>	Si(4)...H(22)	303.6(46)	30.4(fixed)	—	6.2	44.2
<i>u117</i>	C(10)...C(11)	304.5(57)	11.6(tied to u137)	—	3.3	39.6
<i>u873</i>	C(49)...H(64)	305.0(25)	31.2(fixed)	—	0.1	9.7
<i>u131</i>	C(8)...H(27)	305.1(47)	25.7(fixed)	—	8.6	29.6
<i>u113</i>	Br(17)...H(39)	305.3(37)	29.8(fixed)	—	0.8	25.7
<i>u894</i>	Si(45)...H(77)	306.5(63)	30.4(fixed)	—	3.7	36.3
<i>u877</i>	Br(56)...H(65)	306.8(27)	29.2(fixed)	—	1.4	24.9
<i>u125</i>	C(9)...H(25)	307.2(37)	24.9(fixed)	—	1.0	26.3
<i>u893</i>	Br(56)...H(63)	307.6(32)	44.2(fixed)	—	3.5	30.4
<i>u885</i>	Si(43)...Si(45)	307.7(8)	9.8(tied to u137)	—	0.0	9.9
<i>u116</i>	Br(14)...H(28)	309.0(37)	31.8(fixed)	—	0.8	25.9
<i>u136</i>	C(12)...H(41)	309.2(37)	26.3(fixed)	—	0.8	25.2
<i>u915</i>	C(50)...Br(57)	309.4(8)	12.5(tied to u137)	—	0.0	9.8
<i>u137</i>	Si(2)...Si(3)	309.7(27)	13.6(5)	1.0	2.2	26.4
<i>u162</i>	C(7)...Br(17)	309.7(29)	12.3(tied to u137)	—	4.3	30.4
<i>u887</i>	C(49)...H(68)	309.7(27)	25.9(fixed)	—	1.2	24.9
<i>u880</i>	C(49)...H(61)	310.1(67)	32.3(fixed)	—	3.8	37.6
<i>u126</i>	C(13)...H(38)	310.9(65)	26.4(fixed)	—	15.8	32.6
<i>u882</i>	C(50)...H(66)	311.0(27)	24.9(fixed)	—	1.2	24.5
<i>u167</i>	C(10)...Br(15)	311.0(8)	12.1(tied to u137)	—	0.0	9.8

<i>u</i> 135	C(7)...H(19)	312.2(37)	25.2(fixed)	—	2.7	28.3
<i>u</i> 173	C(11)...Br(15)	312.2(53)	12.2(tied to <i>u</i> 137)	—	3.9	37.4
<i>u</i> 133	Si(2)...Si(5)	312.3(27)	13.6(tied to <i>u</i> 137)	—	1.9	26.8
<i>u</i> 128	C(6)...H(21)	312.7(9)	24.5(fixed)	—	0.0	9.7
<i>u</i> 903	C(49)...Br(57)	313.5(70)	12.2(tied to <i>u</i> 137)	—	8.0	47.5
<i>u</i> 905	C(52)...Br(56)	313.6(9)	12.2(tied to <i>u</i> 137)	—	0.0	9.8
<i>u</i> 112	Br(16)...H(23)	313.9(8)	29.6(fixed)	—	0.0	9.9
<i>u</i> 161	C(8)...Br(16)	313.9(36)	12.2(tied to <i>u</i> 137)	—	2.4	28.4
<i>u</i> 904	C(47)...Br(58)	314.2(27)	12.3(tied to <i>u</i> 137)	—	2.3	28.6
<i>u</i> 896	Si(45)...Si(46)	314.3(46)	13.5(tied to <i>u</i> 137)	—	14.1	32.3
<i>u</i> 160	C(6)...Br(17)	314.6(9)	12.1(tied to <i>u</i> 137)	—	0.1	9.5
<i>u</i> 888	C(47)...H(62)	314.6(8)	26.8(fixed)	—	0.0	9.9
<i>u</i> 166	C(12)...Br(14)	314.8(8)	12.3(tied to <i>u</i> 137)	—	0.1	9.8
<i>u</i> 886	C(48)...H(60)	315.3(55)	28.3(fixed)	—	11.4	33.2
<i>u</i> 892	Si(43)...Si(46)	318.5(9)	13.5(tied to <i>u</i> 137)	—	0.0	11.0
<i>u</i> 175	C(9)...Br(16)	318.8(8)	12.5(tied to <i>u</i> 137)	—	-0.2	12.7
<i>u</i> 155	C(6)...H(39)	319.3(9)	40.3(fixed)	—	0.0	10.8
<i>u</i> 129	Si(3)...Si(4)	319.4(9)	13.8(tied to <i>u</i> 137)	—	0.0	10.9
<i>u</i> 923	Br(56)...H(64)	319.5(8)	53.6(fixed)	—	-0.2	12.4
<i>u</i> 170	Br(15)...H(37)	319.7(9)	49.5(fixed)	—	0.0	10.9
<i>u</i> 902	Si(43)...Si(44)	320.0(9)	13.2(tied to <i>u</i> 137)	—	0.0	10.9
<i>u</i> 164	C(13)...Br(14)	320.0(8)	12.4(tied to <i>u</i> 137)	—	-0.1	12.3
<i>u</i> 134	Si(3)...Si(5)	320.1(43)	13.7(tied to <i>u</i> 137)	—	4.1	49.5
<i>u</i> 130	C(10)...H(34)	320.1(8)	28.6(fixed)	—	-0.1	12.4
<i>u</i> 139	Si(2)...Si(4)	320.2(9)	13.5(tied to <i>u</i> 137)	—	0.0	10.8
<i>u</i> 127	C(11)...H(30)	320.6(75)	28.4(fixed)	—	4.0	40.3
<i>u</i> 140	C(9)...H(20)	320.8(9)	38.1(fixed)	—	-0.1	11.0
<i>u</i> 938	Br(55)...H(81)	320.9(61)	29.8(fixed)	—	7.8	45.3
<i>u</i> 147	C(1)...C(6)	321.0(8)	10.8(tied to <i>u</i> 137)	—	-0.2	12.3
<i>u</i> 198	Br(17)...H(22)	321.1(51)	28.5(fixed)	—	4.2	40.4
<i>u</i> 215	Br(15)...H(35)	321.2(8)	36.6(fixed)	—	-0.1	12.4
<i>u</i> 897	C(42)...C(47)	321.4(9)	10.7(tied to <i>u</i> 137)	—	0.0	10.9
<i>u</i> 143	C(1)...C(11)	321.6(8)	10.7(tied to <i>u</i> 137)	—	-0.1	12.3
<i>u</i> 144	C(1)...C(10)	321.8(8)	10.8(tied to <i>u</i> 137)	—	-0.1	12.4
<i>u</i> 201	Br(15)...H(32)	322.0(9)	35.5(fixed)	—	0.0	11.1
<i>u</i> 149	C(1)...C(13)	322.2(51)	10.8(tied to <i>u</i> 137)	—	5.1	43.9
<i>u</i> 132	Br(16)...H(31)	322.5(8)	45.3(fixed)	—	-0.2	12.2
<i>u</i> 898	C(42)...C(48)	322.5(9)	10.7(tied to <i>u</i> 137)	—	0.0	11.0
<i>u</i> 924	Br(56)...H(76)	322.6(8)	33.9(fixed)	—	-0.1	12.4
<i>u</i> 197	Br(16)...H(26)	322.7(50)	29.4(fixed)	—	3.6	39.4
<i>u</i> 922	Br(56)...H(73)	323.0(8)	36.8(fixed)	—	-0.2	12.6
<i>u</i> 899	C(42)...C(49)	323.1(50)	10.9(tied to <i>u</i> 137)	—	4.4	40.2
<i>u</i> 921	Br(55)...H(77)	323.2(9)	29.4(fixed)	—	0.0	11.1
<i>u</i> 199	Br(14)...H(36)	323.2(55)	33.1(fixed)	—	4.5	47.0

<i>u221</i>	Br(16)...H(29)	323.6(9)	30.0(fixed)	—	0.0	11.0
<i>u152</i>	C(1)...C(9)	323.8(74)	10.8(tied to <i>u137</i> )	—	3.4	38.1
<i>u182</i>	Br(17)...H(21)	324.1(43)	28.2(fixed)	—	8.0	30.7
<i>u891</i>	Br(55)...H(72)	324.2(28)	47.5(fixed)	—	3.3	53.6
<i>u910</i>	Br(55)...H(82)	324.3(8)	26.3(fixed)	—	-0.2	12.5
<i>u202</i>	Br(17)...H(18)	324.5(50)	29.0(fixed)	—	7.4	49.0
<i>u154</i>	C(1)...C(7)	325.3(27)	11.0(tied to <i>u137</i> )	—	-0.2	27.3
<i>u207</i>	Br(14)...H(40)	325.9(27)	31.2(fixed)	—	-0.2	30.6
<i>u900</i>	C(42)...C(50)	326.3(50)	10.9(tied to <i>u137</i> )	—	8.5	48.9
<i>u234</i>	H(23)...H(31)	326.7(15)	65.6(fixed)	—	0.8	28.2
<i>u189</i>	Br(15)...H(30)	326.8(38)	32.1(fixed)	—	0.1	27.2
<i>u157</i>	C(1)...C(8)	326.9(42)	11.0(tied to <i>u137</i> )	—	3.9	30.3
<i>u153</i>	C(1)...C(12)	327.2(30)	10.9(tied to <i>u137</i> )	—	4.3	30.9
<i>u181</i>	Br(15)...H(34)	327.4(27)	31.9(fixed)	—	-0.2	26.4
<i>u911</i>	Br(55)...H(79)	327.4(46)	28.2(fixed)	—	3.6	29.5
<i>u913</i>	Br(56)...H(75)	327.9(35)	30.4(fixed)	—	1.5	26.3
<i>u916</i>	Br(56)...H(71)	327.9(22)	33.1(fixed)	—	7.0	32.4
<i>u178</i>	Br(16)...H(25)	328.0(38)	29.0(fixed)	—	0.1	28.0
<i>u119</i>	C(10)...H(26)	328.0(27)	30.7(fixed)	—	0.1	31.0
<i>u158</i>	Br(17)...H(19)	328.1(38)	26.4(fixed)	—	0.2	27.2
<i>u187</i>	Br(14)...H(38)	328.1(27)	31.8(fixed)	—	-0.1	27.3
<i>u914</i>	Si(45)...H(63)	328.6(38)	32.4(fixed)	—	0.4	33.6
<i>u102</i>	C(8)...H(33)	328.7(27)	32.6(fixed)	—	6.1	33.4
<i>u151</i>	Si(4)...H(26)	329.0(38)	30.9(fixed)	—	0.0	29.8
<i>u171</i>	Br(16)...H(27)	329.0(27)	26.8(fixed)	—	0.5	33.4
<i>u174</i>	Si(2)...H(35)	329.2(29)	33.8(fixed)	—	8.9	33.8
<i>u232</i>	C(7)...C(10)	329.3(35)	15.9(tied to <i>u298</i> )	—	2.1	32.1
<i>u185</i>	Si(4)...H(36)	329.3(38)	33.4(fixed)	—	0.0	26.5
<i>u165</i>	Br(14)...H(41)	329.3(15)	27.6(fixed)	—	2.5	31.9
<i>u883</i>	Br(56)...H(69)	329.3(15)	33.6(fixed)	—	0.9	28.2
<i>u192</i>	Si(2)...H(28)	329.6(38)	30.3(fixed)	—	0.4	32.5
<i>u172</i>	Si(3)...H(20)	329.8(15)	29.5(fixed)	—	1.8	30.4
<i>u907</i>	C(48)...H(65)	329.9(45)	41.9(fixed)	—	4.4	30.6
<i>u159</i>	Br(15)...H(36)	329.9(59)	47.0(fixed)	—	3.9	37.5
<i>u890</i>	C(48)...H(67)	330.2(48)	37.4(fixed)	—	7.6	33.6
<i>u283</i>	H(35)...H(37)	330.4(15)	44.8(fixed)	—	0.9	29.0
<i>u220</i>	Br(14)...H(33)	330.6(52)	59.6(fixed)	—	2.9	41.9
<i>u191</i>	C(9)...H(24)	330.6(38)	27.3(fixed)	—	1.3	35.5
<i>u216</i>	C(1)...Br(14)	330.8(20)	8.9(tied to <i>u298</i> )	—	0.5	28.5
<i>u217</i>	C(1)...Br(16)	331.0(20)	9.0(tied to <i>u298</i> )	—	1.1	36.6
<i>u294</i>	H(33)...H(36)	331.2(35)	44.3(fixed)	—	2.3	33.1
<i>u288</i>	H(22)...H(30)	331.3(55)	52.8(fixed)	—	7.4	47.8
<i>u194</i>	C(13)...H(37)	331.6(15)	30.6(fixed)	—	1.4	31.8
<i>u176</i>	C(8)...H(28)	331.6(38)	27.2(fixed)	—	1.3	36.8

<i>u</i> 124	C(8)...H(31)	331.9(20)	31.9(fixed)	—	1.0	33.9
<i>u</i> 186	Si(5)...H(39)	331.9(20)	30.6(fixed)	—	0.7	29.4
<i>u</i> 183	C(12)...H(39)	332.0(40)	28.0(fixed)	—	8.8	34.1
<i>u</i> 195	C(6)...H(23)	332.1(35)	26.4(fixed)	—	1.2	26.4
<i>u</i> 931	C(42)...Br(56)	332.2(37)	8.9(tied to <i>u</i> 298)	—	0.2	30.0
<i>u</i> 901	C(49)...H(69)	332.6(20)	27.2(fixed)	—	0.6	29.4
<i>u</i> 213	C(1)...Br(15)	332.8(20)	8.9(tied to <i>u</i> 298)	—	1.4	33.1
<i>u</i> 224	C(1)...Br(17)	332.9(37)	9.0(tied to <i>u</i> 298)	—	0.2	29.0
<i>u</i> 291	C(7)...Br(15)	332.9(81)	18.3(tied to <i>u</i> 298)	—	1.3	65.6
<i>u</i> 919	C(48)...H(61)	333.2(44)	33.6(fixed)	—	13.1	31.9
<i>u</i> 954	C(50)...Br(55)	333.3(37)	15.7(tied to <i>u</i> 298)	—	0.4	31.2
<i>u</i> 933	C(42)...Br(55)	333.8(35)	8.9(tied to <i>u</i> 298)	—	1.4	26.8
<i>u</i> 146	H(24)...H(28)	334.6(43)	40.4(fixed)	—	0.9	21.2
<i>u</i> 912	C(50)...H(65)	335.7(35)	27.3(fixed)	—	1.6	27.6
<i>u</i> 917	C(47)...H(64)	335.8(40)	31.0(fixed)	—	3.8	30.1
<i>u</i> 204	C(1)...H(18)	338.0(5)	23.4(fixed)	—	-0.2	11.9
<i>u</i> 190	C(7)...H(20)	338.1(5)	26.5(fixed)	—	-0.2	11.9
<i>u</i> 909	Si(43)...H(72)	338.2(73)	34.1(fixed)	—	2.7	59.5
<i>u</i> 918	Si(45)...H(69)	338.3(52)	30.1(fixed)	—	-2.5	46.2
<i>u</i> 193	C(11)...H(31)	338.6(67)	32.5(fixed)	—	-0.3	52.8
<i>u</i> 179	C(10)...H(33)	338.7(52)	33.4(fixed)	—	-1.9	41.8
<i>u</i> 298	Br(15)...Br(17)	338.8(29)	19.1(14)	—	0.8	23.4
<i>u</i> 163	H(37)...H(39)	339.7(52)	43.9(fixed)	—	3.2	59.6
<i>u</i> 141	Br(14)...H(35)	339.8(72)	47.8(fixed)	—	3.0	42.5
<i>u</i> 169	H(20)...H(23)	339.9(74)	39.4(fixed)	—	2.8	42.2
<i>u</i> 906	C(47)...H(81)	340.1(5)	42.5(fixed)	—	-0.1	11.8
<i>u</i> 889	H(65)...H(69)	340.2(5)	40.2(fixed)	—	-0.1	11.9
<i>u</i> 212	C(1)...H(32)	340.3(5)	26.7(fixed)	—	-0.2	11.9
<i>u</i> 205	C(1)...H(40)	340.4(16)	24.3(fixed)	—	2.2	25.8
<i>u</i> 926	C(42)...H(59)	340.6(5)	26.4(fixed)	—	-0.1	11.8
<i>u</i> 209	C(1)...H(35)	340.6(29)	25.8(fixed)	—	1.8	26.7
<i>u</i> 242	Si(4)...C(7)	340.8(29)	12.1(tied to <i>u</i> 298)	—	1.1	24.3
<i>u</i> 935	C(42)...H(67)	340.8(29)	22.3(fixed)	—	2.2	26.4
<i>u</i> 927	C(42)...H(63)	341.1(16)	24.5(fixed)	—	0.8	22.3
<i>u</i> 908	H(61)...H(64)	341.3(16)	49.0(fixed)	—	1.6	24.5
<i>u</i> 208	C(1)...H(29)	341.5(88)	23.7(fixed)	—	2.8	39.5
<i>u</i> 226	C(1)...H(20)	341.9(52)	22.0(fixed)	—	-1.4	50.8
<i>u</i> 223	C(1)...H(22)	342.2(29)	22.2(fixed)	—	0.5	22.0
<i>u</i> 925	C(42)...H(70)	342.2(51)	23.6(fixed)	—	-1.7	39.8
<i>u</i> 156	H(31)...H(33)	342.4(39)	48.9(fixed)	—	8.4	32.6
<i>u</i> 251	H(34)...H(36)	342.4(51)	49.1(fixed)	—	-1.8	54.7
<i>u</i> 218	C(1)...H(33)	342.5(65)	27.0(fixed)	—	2.4	59.1
<i>u</i> 930	C(42)...H(61)	342.6(28)	26.7(fixed)	—	1.0	23.7
<i>u</i> 227	C(1)...H(39)	342.7(51)	22.7(fixed)	—	-0.8	41.8

<i>u</i> 256	Si(5)...H(32)	343.0(16)	30.5(fixed)	—	0.6	22.2
<i>u</i> 230	C(1)...H(26)	343.2(51)	22.4(fixed)	—	-2.0	51.5
<i>u</i> 928	Si(45)...C(53)	343.4(30)	12.3(tied to <i>u</i> 298)	—	0.2	16.1
<i>u</i> 211	C(1)...H(31)	343.5(51)	25.9(fixed)	—	-1.8	41.7
<i>u</i> 188	C(13)...H(29)	343.7(28)	42.2(fixed)	—	0.8	23.6
<i>u</i> 929	C(42)...H(65)	343.8(24)	23.6(fixed)	—	0.9	20.9
<i>u</i> 932	C(42)...H(64)	343.9(29)	25.4(fixed)	—	1.8	26.7
<i>u</i> 225	C(1)...H(36)	343.9(29)	24.4(fixed)	—	0.6	22.7
<i>u</i> 944	H(61)...H(81)	344.0(51)	69.2(fixed)	—	-2.1	52.8
<i>u</i> 255	Si(3)...Br(14)	344.0(17)	13.4(tied to <i>u</i> 298)	—	1.6	27.0
<i>u</i> 229	C(1)...H(28)	344.1(51)	22.4(fixed)	—	-0.8	41.7
<i>u</i> 233	Br(16)...H(32)	344.2(29)	59.1(fixed)	—	1.8	25.9
<i>u</i> 180	C(9)...H(18)	344.4(51)	39.5(fixed)	—	-0.5	45.5
<i>u</i> 219	C(1)...H(23)	344.5(16)	23.8(fixed)	—	0.8	22.4
<i>u</i> 241	H(37)...H(41)	345.0(16)	46.2(fixed)	—	0.6	23.6
<i>u</i> 250	Si(2)...Br(17)	345.1(16)	13.2(tied to <i>u</i> 298)	—	1.3	25.4
<i>u</i> 235	H(24)...H(27)	345.2(16)	41.8(fixed)	—	1.4	24.4
<i>u</i> 940	C(42)...H(69)	345.7(28)	22.2(fixed)	—	0.5	22.4
<i>u</i> 177	Si(3)...H(31)	346.4(68)	32.6(fixed)	—	0.9	25.4
<i>u</i> 138	C(11)...H(26)	346.7(21)	37.5(fixed)	—	0.2	16.4
<i>u</i> 222	C(1)...H(24)	346.9(28)	24.2(fixed)	—	0.5	22.2
<i>u</i> 214	C(1)...H(37)	347.0(16)	25.7(fixed)	—	0.6	23.8
<i>u</i> 275	H(21)...H(32)	347.5(50)	33.9(fixed)	—	-0.7	40.1
<i>u</i> 200	H(25)...H(28)	348.2(16)	41.8(fixed)	—	0.6	24.2
<i>u</i> 941	H(61)...H(62)	348.2(12)	51.5(fixed)	—	0.0	17.8
<i>u</i> 937	Br(55)...H(73)	349.0(16)	59.5(fixed)	—	1.3	25.7
<i>u</i> 293	Si(5)...Br(15)	349.2(66)	13.6(tied to <i>u</i> 298)	—	2.9	42.5
<i>u</i> 934	H(60)...H(64)	350.0(35)	50.8(fixed)	—	7.8	30.5
<i>u</i> 203	H(38)...H(39)	350.3(14)	45.5(fixed)	—	0.0	17.6
<i>u</i> 236	H(31)...H(34)	351.1(63)	52.8(fixed)	—	0.3	24.3
<i>u</i> 920	H(66)...H(69)	351.4(88)	41.7(fixed)	—	2.8	44.9
<i>u</i> 239	H(19)...H(23)	351.6(44)	39.8(fixed)	—	1.0	69.2
<i>u</i> 265	H(35)...H(38)	353.5(22)	45.5(fixed)	—	0.9	20.2
<i>u</i> 206	H(30)...H(33)	353.6(47)	54.7(fixed)	—	6.6	49.1
<i>u</i> 943	H(60)...H(67)	353.9(23)	49.4(fixed)	—	0.9	23.8
<i>u</i> 973	Br(55)...Br(57)	354.2(62)	20.4(tied to <i>u</i> 298)	—	3.4	49.4
<i>u</i> 936	H(78)...H(82)	355.3(10)	41.7(fixed)	—	0.0	17.6
<i>u</i> 254	Si(5)...Br(16)	355.7(41)	13.2(tied to <i>u</i> 298)	—	0.1	18.0
<i>u</i> 948	C(48)...Br(56)	356.4(23)	17.9(tied to <i>u</i> 298)	—	0.9	20.6
<i>u</i> 280	Si(4)...H(23)	356.7(52)	33.8(fixed)	—	11.7	33.9
<i>u</i> 210	H(20)...H(21)	357.7(30)	40.1(fixed)	—	0.9	21.5
<i>u</i> 965	Si(43)...Br(57)	357.7(41)	13.1(tied to <i>u</i> 298)	—	0.9	21.3
<i>u</i> 279	C(11)...C(12)	358.4(61)	16.4(tied to <i>u</i> 298)	—	7.1	44.8
<i>u</i> 942	C(47)...C(54)	359.1(59)	16.2(tied to <i>u</i> 298)	—	3.0	44.3



<i>u168</i>	C(11)...H(24)	360.0(38)	42.5(fixed)	—	0.8	21.4
<i>u953</i>	H(62)...H(76)	360.0(26)	46.9(fixed)	—	0.2	15.6
<i>u956</i>	Si(45)...H(78)	360.0(21)	33.9(fixed)	—	0.3	16.0
<i>u976</i>	H(61)...H(80)	360.5(39)	47.4(fixed)	—	0.3	33.8
<i>u196</i>	C(6)...H(40)	360.5(17)	44.9(fixed)	—	0.2	17.4
<i>u950</i>	Si(43)...H(59)	361.0(37)	29.7(fixed)	—	0.8	23.5
<i>u240</i>	C(9)...C(13)	361.2(16)	16.1(tied to u298)	—	0.2	16.3
<i>u257</i>	C(8)...Br(14)	361.7(23)	15.2(tied to u298)	—	0.2	16.6
<i>u971</i>	H(63)...H(74)	362.5(37)	44.1(fixed)	—	0.4	21.9
<i>u258</i>	Si(3)...H(40)	362.5(13)	28.0(fixed)	—	0.2	16.5
<i>u259</i>	C(12)...Br(17)	362.7(52)	15.5(tied to u298)	—	1.2	61.7
<i>u246</i>	Si(4)...C(12)	362.7(50)	12.3(tied to u298)	—	10.6	45.5
<i>u963</i>	H(60)...H(80)	362.9(22)	53.4(fixed)	—	0.2	16.2
<i>u947</i>	Si(45)...C(48)	363.0(21)	12.4(tied to u298)	—	0.2	16.5
<i>u228</i>	Si(4)...C(8)	363.1(27)	12.5(tied to u298)	—	0.3	15.9
<i>u253</i>	Si(2)...C(11)	363.3(30)	12.4(tied to u298)	—	8.6	29.7
<i>u959</i>	Si(43)...Br(58)	364.1(32)	13.5(tied to u298)	—	0.1	53.4
<i>u268</i>	H(28)...H(41)	365.1(32)	49.1(fixed)	—	4.9	28.0
<i>u247</i>	C(12)...Br(15)	365.4(37)	17.7(tied to u298)	—	0.7	24.5
<i>u968</i>	H(59)...H(67)	365.9(47)	41.4(fixed)	—	1.7	51.5
<i>u272</i>	H(29)...H(39)	366.1(43)	54.8(fixed)	—	2.4	49.1
<i>u238</i>	Si(3)...C(6)	366.2(34)	11.7(tied to u298)	—	-0.2	33.9
<i>u245</i>	Si(2)...C(9)	366.3(44)	12.1(tied to u298)	—	0.3	21.8
<i>u310</i>	H(22)...H(31)	366.4(14)	48.0(fixed)	—	0.1	18.0
<i>u323</i>	H(23)...H(30)	367.3(32)	42.3(fixed)	—	0.3	23.7
<i>u967</i>	C(48)...C(52)	367.3(38)	17.4(tied to u298)	—	0.3	21.8
<i>u237</i>	C(6)...C(9)	367.5(66)	16.0(tied to u298)	—	-5.0	48.0
<i>u269</i>	C(6)...Br(16)	367.5(17)	16.5(tied to u298)	—	0.3	16.3
<i>u271</i>	Si(2)...H(18)	367.7(108)	27.9(fixed)	—	-5.0	47.4
<i>u946</i>	Si(43)...C(51)	368.2(29)	12.2(tied to u298)	—	0.9	20.9
<i>u939</i>	C(48)...C(49)	368.6(48)	16.1(tied to u298)	—	0.7	21.3
<i>u243</i>	Si(5)...C(13)	368.8(48)	11.9(tied to u298)	—	2.2	54.8
<i>u319</i>	H(28)...H(39)	370.6(19)	42.8(fixed)	—	0.7	24.8
<i>u945</i>	Si(45)...C(50)	370.8(52)	12.2(tied to u298)	—	0.7	22.7
<i>u957</i>	C(47)...C(49)	371.0(69)	15.9(tied to u298)	—	0.5	27.1
<i>u248</i>	C(6)...C(13)	371.0(52)	17.1(tied to u298)	—	8.0	46.9
<i>u263</i>	C(10)...Br(16)	371.8(61)	18.7(tied to u298)	—	-0.1	41.4
<i>u277</i>	H(18)...H(28)	372.0(19)	50.2(fixed)	—	0.2	16.5
<i>u970</i>	Si(43)...H(70)	372.4(39)	27.4(fixed)	—	3.8	27.9
<i>u264</i>	Si(5)...H(29)	373.1(38)	27.6(fixed)	—	0.4	21.1
<i>u267</i>	C(13)...Br(17)	373.2(29)	16.4(tied to u298)	—	6.4	28.7
<i>u295</i>	Si(4)...H(37)	373.2(49)	40.0(fixed)	—	12.3	42.9
<i>u966</i>	H(61)...H(65)	373.2(32)	38.6(fixed)	—	3.8	27.4
<i>u952</i>	C(47)...Br(57)	373.3(35)	18.5(tied to u298)	—	0.9	21.4

<i>u285</i>	C(9)...Br(14)	374.0(53)	17.8(tied to <i>u298</i> )	—	0.9	21.2
<i>u949</i>	H(61)...H(66)	374.9(63)	42.9(fixed)	—	2.0	50.2
<i>u262</i>	C(11)...Br(14)	375.0(73)	18.7(tied to <i>u298</i> )	—	0.8	68.3
<i>u286</i>	H(27)...H(40)	375.1(63)	32.8(fixed)	—	0.1	33.0
<i>u951</i>	H(63)...H(65)	375.2(40)	61.7(fixed)	—	0.7	24.8
<i>u276</i>	H(19)...H(39)	376.3(37)	48.8(fixed)	—	4.3	27.6
<i>u961</i>	H(59)...H(82)	377.4(54)	35.4(fixed)	—	3.3	48.8
<i>u252</i>	Si(3)...C(10)	377.9(27)	12.4(tied to <i>u298</i> )	—	-0.1	40.0
<i>u304</i>	Si(5)...C(10)	379.5(37)	13.8(tied to <i>u298</i> )	—	8.0	30.3
<i>u261</i>	H(20)...H(27)	379.6(69)	48.3(fixed)	—	-4.8	42.3
<i>u273</i>	Si(4)...H(24)	379.9(55)	34.9(fixed)	—	0.2	34.5
<i>u955</i>	C(49)...Br(56)	380.3(51)	15.7(tied to <i>u298</i> )	—	2.4	48.3
<i>u270</i>	C(7)...Br(16)	380.6(49)	18.9(tied to <i>u298</i> )	—	5.9	32.8
<i>u302</i>	Si(2)...H(33)	380.7(60)	44.2(fixed)	—	3.8	48.7
<i>u974</i>	Si(45)...H(64)	380.9(43)	40.6(fixed)	—	0.2	23.2
<i>u322</i>	C(7)...H(31)	381.0(26)	47.4(fixed)	—	-0.2	15.6
<i>u958</i>	Si(43)...H(74)	381.5(35)	28.7(fixed)	—	-0.2	34.9
<i>u278</i>	Si(3)...H(18)	381.8(39)	33.0(fixed)	—	12.5	35.4
<i>u960</i>	H(62)...H(67)	383.1(53)	51.5(fixed)	—	8.2	38.6
<i>u244</i>	H(26)...H(30)	383.2(103)	48.7(fixed)	—	-2.0	42.8
<i>u324</i>	H(20)...H(39)	383.7(60)	44.7(fixed)	—	0.1	36.3
<i>u292</i>	H(20)...H(40)	383.8(67)	53.3(fixed)	—	4.3	44.1
<i>u231</i>	C(8)...C(11)	384.5(33)	15.9(tied to <i>u298</i> )	—	-1.0	44.2
<i>u287</i>	Si(2)...H(29)	385.2(54)	34.5(fixed)	—	8.9	33.7
<i>u320</i>	H(20)...H(28)	385.6(27)	42.5(fixed)	—	-0.6	40.6
<i>u284</i>	H(19)...H(29)	385.7(55)	32.5(fixed)	—	0.6	54.4
<i>u260</i>	Si(3)...H(33)	385.8(72)	30.3(fixed)	—	2.8	53.3
<i>u964</i>	Si(45)...H(70)	386.3(55)	34.4(fixed)	—	-0.8	43.1
<i>u296</i>	H(18)...H(41)	386.5(66)	33.9(fixed)	—	-4.1	47.4
<i>u986</i>	C(50)...H(72)	386.7(54)	48.7(fixed)	—	0.2	34.4
<i>u977</i>	Si(43)...C(47)	387.4(64)	13.8(tied to <i>u298</i> )	—	-3.5	44.3
<i>u311</i>	C(8)...H(29)	388.8(18)	13.5(fixed)	—	-3.7	13.5
<i>u309</i>	C(9)...H(26)	388.9(16)	13.8(fixed)	—	-3.7	13.8
<i>u315</i>	C(13)...H(36)	389.2(16)	14.1(fixed)	—	-4.7	14.1
<i>u982</i>	C(48)...H(59)	389.5(17)	14.8(fixed)	—	-5.9	14.8
<i>u316</i>	C(12)...H(40)	389.7(17)	13.6(fixed)	—	-4.0	13.6
<i>u297</i>	H(26)...H(32)	390.7(16)	41.6(fixed)	—	-4.9	14.0
<i>u289</i>	Si(5)...H(40)	390.7(16)	36.3(fixed)	—	-5.7	14.3
<i>u249</i>	H(24)...H(35)	390.8(26)	68.3(fixed)	—	3.8	27.6
<i>u1011</i>	Br(55)...H(69)	390.8(17)	32.9(fixed)	—	-5.6	14.3
<i>u983</i>	C(47)...H(63)	390.9(24)	14.0(fixed)	—	5.7	27.9
<i>u313</i>	C(10)...H(35)	390.9(16)	14.3(fixed)	—	-3.6	13.7
<i>u981</i>	C(50)...H(67)	391.1(28)	13.7(fixed)	—	3.6	27.4
<i>u308</i>	C(11)...H(32)	391.1(17)	14.3(fixed)	—	-3.6	13.3

<i>u980</i>	C(49)...H(70)	391.2(17)	13.3(fixed)	—	-3.4	13.5
<i>u317</i>	C(7)...H(18)	391.3(61)	13.5(fixed)	—	0.6	41.6
<i>u307</i>	Si(3)...C(13)	391.4(63)	13.9(tied to <i>u298</i> )	—	5.0	32.5
<i>u312</i>	C(6)...H(22)	391.6(36)	13.6(fixed)	—	0.3	21.8
<i>u975</i>	Si(43)...H(73)	391.7(16)	43.1(fixed)	—	-3.3	13.6
<i>u274</i>	C(8)...C(10)	391.8(67)	19.3(tied to <i>u298</i> )	—	3.0	33.9
<i>u369</i>	C(7)...H(30)	392.1(14)	33.8(fixed)	—	-0.2	15.6
<i>u387</i>	Br(15)...H(23)	394.1(53)	35.2(fixed)	—	-1.0	42.8
<i>u969</i>	C(50)...Br(56)	395.0(48)	22.2(tied to <i>u298</i> )	—	11.0	42.7
<i>u299</i>	Si(5)...H(37)	395.2(17)	27.9(fixed)	—	-0.2	15.7
<i>u367</i>	C(11)...H(37)	395.3(35)	39.9(fixed)	—	0.4	25.1
<i>u290</i>	H(24)...H(31)	395.7(111)	39.0(fixed)	—	-1.2	44.7
<i>u300</i>	Si(2)...H(24)	396.4(62)	27.6(fixed)	—	-4.5	48.7
<i>u306</i>	Si(3)...H(32)	396.7(66)	42.8(fixed)	—	-2.6	32.9
<i>u325</i>	H(26)...H(27)	397.8(21)	27.0(fixed)	—	-0.1	15.4
<i>u321</i>	H(25)...H(29)	399.1(69)	25.7(fixed)	—	-4.6	46.4
<i>u318</i>	Si(2)...C(6)	399.1(108)	14.2(tied to <i>u298</i> )	—	-2.0	42.5
<i>u281</i>	H(26)...H(34)	399.3(49)	54.4(fixed)	—	7.3	39.0
<i>u266</i>	H(25)...H(31)	399.6(32)	42.7(fixed)	—	-3.3	27.0
<i>u336</i>	H(36)...H(41)	399.8(33)	28.1(fixed)	—	-3.1	25.7
<i>u962</i>	H(64)...H(66)	400.4(32)	33.7(fixed)	—	-4.3	28.1
<i>u388</i>	C(12)...H(33)	401.8(25)	42.1(fixed)	—	-0.2	16.1
<i>u326</i>	H(38)...H(40)	402.2(33)	26.8(fixed)	—	-2.8	26.8
<i>u972</i>	Si(45)...H(65)	402.6(30)	27.4(fixed)	—	3.4	27.5
<i>u998</i>	Si(45)...Br(58)	402.7(27)	21.9(tied to <i>u346</i> )	—	-0.1	15.4
<i>u987</i>	H(59)...H(62)	402.7(32)	29.2(fixed)	—	-5.2	29.2
<i>u985</i>	H(67)...H(68)	402.8(57)	27.0(fixed)	—	-5.6	33.8
<i>u314</i>	Si(5)...C(9)	402.9(32)	13.8(tied to <i>u298</i> )	—	-3.3	27.0
<i>u996</i>	Si(43)...C(50)	403.1(17)	13.3(tied to <i>u298</i> )	—	-0.2	15.1
<i>u984</i>	H(66)...H(70)	403.6(32)	25.6(fixed)	—	-3.2	25.6
<i>u348</i>	C(9)...H(39)	404.1(32)	35.5(fixed)	—	-3.0	25.4
<i>u328</i>	H(18)...H(21)	404.2(32)	25.4(fixed)	—	-3.0	26.2
<i>u979</i>	Si(43)...C(52)	404.7(32)	13.6(tied to <i>u298</i> )	—	-3.3	28.7
<i>u331</i>	H(19)...H(22)	404.9(22)	26.2(fixed)	—	-0.2	15.7
<i>u988</i>	H(60)...H(63)	405.0(32)	28.7(fixed)	—	-4.9	29.1
<i>u405</i>	Br(15)...H(21)	405.3(15)	34.0(fixed)	—	-0.2	17.4
<i>u346</i>	Si(2)...Br(15)	405.4(32)	22.0(10)	—	-4.4	29.7
<i>u329</i>	H(30)...H(35)	406.3(9)	29.1(fixed)	—	-5.2	13.9
<i>u327</i>	H(32)...H(34)	406.5(69)	29.7(fixed)	—	11.8	34.9
<i>u989</i>	C(42)...H(60)	406.7(18)	13.9(fixed)	—	-0.3	17.5
<i>u330</i>	C(1)...H(34)	406.7(9)	13.8(fixed)	—	-5.1	13.8
<i>u332</i>	C(1)...H(30)	407.1(9)	13.6(fixed)	—	-5.0	13.6
<i>u993</i>	H(62)...H(65)	407.9(9)	45.3(fixed)	—	-4.3	13.5
<i>u1013</i>	Br(55)...H(68)	407.9(9)	34.1(fixed)	—	-3.1	13.2

<i>u360</i>	Br(15)...H(33)	408.6(9)	18.8(tied to <i>u346</i> )	—	-3.6	13.4
<i>u990</i>	C(42)...H(62)	409.7(9)	13.5(fixed)	—	-3.3	13.4
<i>u334</i>	C(1)...H(19)	410.0(9)	13.2(fixed)	—	-3.3	13.3
<i>u361</i>	Br(15)...H(31)	410.2(60)	14.3(fixed)	—	-3.9	45.3
<i>u335</i>	C(1)...H(41)	410.2(9)	13.4(fixed)	—	-3.2	13.3
<i>u1002</i>	Br(56)...H(72)	410.5(50)	14.7(fixed)	—	-3.6	41.4
<i>u1004</i>	Br(55)...H(80)	410.6(9)	14.0(fixed)	—	-4.2	13.3
<i>u991</i>	C(42)...H(66)	410.9(9)	13.4(fixed)	—	-3.2	13.4
<i>u1001</i>	Br(56)...H(74)	411.0(9)	14.5(fixed)	—	-3.4	13.4
<i>u337</i>	C(1)...H(27)	411.2(19)	13.3(fixed)	—	-0.4	17.5
<i>u303</i>	Si(3)...C(11)	411.7(17)	13.6(tied to <i>u298</i> )	—	-0.1	14.9
<i>u341</i>	C(1)...H(21)	411.9(61)	13.3(fixed)	—	-2.6	35.5
<i>u301</i>	Si(3)...H(23)	412.7(19)	27.5(fixed)	—	-0.1	14.8
<i>u356</i>	Br(17)...H(23)	413.3(31)	13.7(fixed)	—	-2.7	32.5
<i>u339</i>	C(1)...H(38)	413.3(68)	13.3(fixed)	—	-2.7	35.2
<i>u992</i>	C(42)...H(68)	413.4(14)	13.4(fixed)	—	-0.4	17.6
<i>u340</i>	C(1)...H(25)	414.0(20)	13.4(fixed)	—	-0.2	14.9
<i>u350</i>	Si(4)...Br(16)	414.1(9)	22.3(tied to <i>u346</i> )	—	-6.5	14.9
<i>u1000</i>	Br(55)...H(78)	414.6(9)	13.7(fixed)	—	-6.2	14.3
<i>u357</i>	Br(14)...H(37)	414.8(36)	13.8(fixed)	—	-4.2	36.1
<i>u354</i>	Br(16)...H(24)	415.1(40)	13.8(fixed)	—	-2.6	34.1
<i>u978</i>	H(63)...H(67)	415.9(9)	44.3(fixed)	—	-6.7	14.7
<i>u353</i>	Br(17)...H(20)	416.1(34)	13.7(fixed)	—	-0.3	16.8
<i>u359</i>	Br(16)...H(28)	416.1(8)	14.0(fixed)	—	-3.9	14.0
<i>u386</i>	Si(4)...Br(17)	416.3(47)	21.2(tied to <i>u346</i> )	—	-3.6	39.9
<i>u999</i>	Si(45)...Br(55)	416.6(8)	22.1(tied to <i>u346</i> )	—	-5.5	14.5
<i>u355</i>	Br(14)...H(39)	417.0(8)	14.0(fixed)	—	-3.8	13.7
<i>u352</i>	Si(4)...Br(14)	417.5(67)	22.2(tied to <i>u346</i> )	—	-3.3	34.0
<i>u351</i>	C(6)...H(28)	418.0(8)	33.2(fixed)	—	-3.9	13.7
<i>u342</i>	Si(5)...C(12)	418.2(16)	18.8(tied to <i>u346</i> )	—	-0.3	17.6
<i>u383</i>	Si(5)...H(31)	418.4(8)	38.4(fixed)	—	-5.2	13.8
<i>u344</i>	Si(2)...C(8)	418.6(8)	18.7(tied to <i>u346</i> )	—	-4.1	13.8
<i>u1007</i>	C(47)...H(65)	419.7(9)	32.7(fixed)	—	-3.6	13.7
<i>u1018</i>	C(48)...H(74)	420.0(8)	40.1(fixed)	—	-3.9	14.0
<i>u358</i>	C(13)...H(20)	420.6(49)	33.5(fixed)	—	-5.3	42.1
<i>u305</i>	H(26)...H(35)	420.7(9)	46.4(fixed)	—	-4.2	14.0
<i>u373</i>	Br(14)...H(26)	420.8(63)	32.5(fixed)	—	-4.4	46.7
<i>u382</i>	Br(17)...H(36)	421.3(44)	36.1(fixed)	—	-2.5	33.5
<i>u995</i>	Si(45)...C(49)	422.1(50)	18.8(tied to <i>u346</i> )	—	-2.1	38.4
<i>u282</i>	H(25)...H(33)	422.2(102)	34.9(fixed)	—	-2.8	46.6
<i>u997</i>	H(60)...H(81)	422.5(21)	45.3(fixed)	—	-0.1	15.1
<i>u372</i>	Br(17)...H(38)	422.6(67)	38.8(fixed)	—	-2.4	33.2
<i>u395</i>	C(12)...H(34)	422.7(27)	39.2(fixed)	—	-2.9	34.1
<i>u381</i>	Br(14)...H(25)	423.1(97)	34.1(fixed)	—	-5.5	45.3

<i>u1017</i>	Si(43)...H(61)	423.1(25)	39.0(fixed)	—	-7.5	30.3
<i>u404</i>	C(10)...H(21)	423.4(25)	24.3(fixed)	—	-3.8	38.8
<i>u994</i>	C(49)...H(63)	423.6(67)	41.4(fixed)	—	-2.8	33.1
<i>u347</i>	Si(3)...C(7)	423.7(115)	19.0(tied to <i>u346</i> )	—	-2.2	44.5
<i>u1014</i>	C(49)...H(59)	424.1(26)	39.8(fixed)	—	-4.6	26.7
<i>u345</i>	H(29)...H(41)	424.2(25)	46.6(fixed)	—	-7.0	31.8
<i>u378</i>	Br(16)...H(18)	424.3(25)	33.1(fixed)	—	-5.1	29.2
<i>u338</i>	H(18)...H(27)	424.3(33)	44.5(fixed)	—	-6.1	27.4
<i>u1009</i>	H(59)...H(64)	424.5(33)	30.3(fixed)	—	-6.9	31.6
<i>u370</i>	H(36)...H(39)	424.8(34)	27.4(fixed)	—	-4.7	26.7
<i>u1008</i>	C(50)...H(71)	424.9(33)	35.0(fixed)	—	-6.0	31.9
<i>u371</i>	H(24)...H(29)	425.9(74)	26.7(fixed)	—	-2.1	33.5
<i>u401</i>	C(11)...H(38)	426.0(25)	34.5(fixed)	—	-4.4	25.8
<i>u365</i>	H(32)...H(33)	426.1(33)	31.8(fixed)	—	-4.4	26.9
<i>u376</i>	H(31)...H(35)	426.5(25)	31.6(fixed)	—	-4.4	26.9
<i>u379</i>	H(37)...H(40)	427.2(33)	29.2(fixed)	—	-4.3	25.7
<i>u363</i>	H(26)...H(28)	429.0(46)	26.7(fixed)	—	-2.5	32.7
<i>u1012</i>	H(61)...H(63)	429.4(71)	31.9(fixed)	—	-5.3	45.0
<i>u343</i>	H(24)...H(34)	430.3(43)	45.0(fixed)	—	-4.3	33.8
<i>u1003</i>	H(67)...H(69)	430.6(46)	26.9(fixed)	—	-2.6	39.0
<i>u380</i>	H(18)...H(23)	430.7(56)	25.8(fixed)	—	-3.6	33.5
<i>u1005</i>	H(65)...H(70)	431.8(49)	26.9(fixed)	—	-2.9	32.1
<i>u374</i>	H(20)...H(22)	431.8(67)	25.7(fixed)	—	-3.5	35.7
<i>u364</i>	C(9)...H(41)	432.0(58)	33.3(fixed)	—	-5.4	39.8
<i>u396</i>	Si(3)...H(39)	432.4(50)	28.9(fixed)	—	-3.3	33.9
<i>u392</i>	Br(17)...H(41)	433.3(46)	33.5(fixed)	—	-5.9	35.0
<i>u394</i>	Br(16)...H(19)	433.6(45)	32.1(fixed)	—	-3.8	24.3
<i>u1010</i>	Br(56)...H(67)	433.8(114)	33.5(fixed)	—	-2.0	49.5
<i>u1016</i>	C(49)...H(60)	434.0(54)	39.9(fixed)	—	-3.1	35.0
<i>u1006</i>	C(49)...H(62)	434.3(54)	33.8(fixed)	—	-3.3	33.3
<i>u333</i>	C(8)...H(35)	435.7(38)	46.7(fixed)	—	-5.7	39.2
<i>u397</i>	Br(14)...H(27)	436.5(48)	33.9(fixed)	—	-2.5	31.1
<i>u1023</i>	C(48)...H(75)	437.7(28)	36.8(fixed)	—	-1.9	34.0
<i>u377</i>	Br(17)...H(40)	437.9(53)	35.7(fixed)	—	-4.3	40.1
<i>u411</i>	Si(4)...H(21)	439.1(35)	18.6(fixed)	—	-2.1	37.9
<i>u390</i>	Br(14)...H(29)	439.6(52)	35.0(fixed)	—	-5.5	39.9
<i>u349</i>	H(19)...H(40)	439.9(44)	49.5(fixed)	—	-1.9	28.9
<i>u1022</i>	Si(45)...H(79)	441.8(29)	19.5(fixed)	—	-2.8	33.3
<i>u368</i>	C(10)...H(24)	442.2(40)	33.7(fixed)	—	-4.9	34.5
<i>u389</i>	Br(16)...H(22)	442.4(32)	31.1(fixed)	—	-2.4	34.3
<i>u362</i>	C(6)...H(27)	443.1(30)	32.8(fixed)	—	-4.2	18.6
<i>u1019</i>	Si(44)...H(63)	443.4(63)	34.0(fixed)	—	-2.8	32.8
<i>u402</i>	Si(2)...H(20)	445.1(64)	27.0(fixed)	—	-2.7	32.8
<i>u385</i>	Br(16)...H(21)	445.4(21)	34.3(fixed)	—	-4.3	19.5

<i>u</i> 400	Si(5)...H(28)	446.4(42)	27.3(fixed)	—	-2.7	33.7
<i>u</i> 1032	Br(56)...H(62)	446.7(40)	27.5(fixed)	—	-3.3	31.8
<i>u</i> 375	C(13)...H(19)	447.2(46)	32.8(fixed)	—	-1.6	26.5
<i>u</i> 1031	Si(43)...H(69)	447.7(54)	26.5(fixed)	—	-5.7	34.9
<i>u</i> 384	Si(3)...H(35)	448.0(58)	37.9(fixed)	—	-5.2	39.6
<i>u</i> 1021	C(47)...H(66)	448.1(49)	31.8(fixed)	—	-1.7	27.0
<i>u</i> 1015	Br(56)...H(66)	448.3(27)	33.3(fixed)	—	-6.4	27.5
<i>u</i> 391	C(8)...H(32)	448.9(45)	39.6(fixed)	—	-1.8	27.3
<i>u</i> 1025	C(47)...H(82)	450.3(41)	24.5(fixed)	—	-4.8	36.8
<i>u</i> 1045	H(70)...H(81)	453.4(24)	37.4(fixed)	—	-1.9	30.9
<i>u</i> 410	Si(2)...H(34)	456.0(28)	22.9(fixed)	—	-1.5	26.8
<i>u</i> 408	C(13)...H(27)	456.0(26)	24.5(fixed)	—	-7.2	22.6
<i>u</i> 442	H(34)...H(37)	456.7(20)	55.4(fixed)	—	-7.2	22.9
<i>u</i> 1028	Si(45)...H(62)	456.8(33)	21.3(fixed)	—	-4.0	24.5
<i>u</i> 366	C(8)...H(34)	456.8(44)	34.9(fixed)	—	-4.1	24.4
<i>u</i> 413	Si(4)...H(38)	456.9(25)	20.0(fixed)	—	-1.4	26.5
<i>u</i> 415	Br(15)...H(38)	457.4(40)	27.0(fixed)	—	-6.1	27.0
<i>u</i> 416	Si(5)...H(36)	457.5(14)	30.9(fixed)	—	-6.0	21.3
<i>u</i> 1020	Br(56)...H(70)	458.3(42)	35.3(fixed)	—	-8.4	28.5
<i>u</i> 399	Si(4)...H(25)	458.5(24)	19.6(fixed)	—	-4.3	18.7
<i>u</i> 1027	Si(43)...H(71)	458.7(18)	22.6(fixed)	—	-5.9	20.0
<i>u</i> 414	Si(2)...H(27)	459.1(41)	18.7(fixed)	—	-4.3	24.5
<i>u</i> 439	Si(5)...H(30)	460.0(59)	23.3(fixed)	—	-2.8	35.3
<i>u</i> 393	C(8)...H(30)	460.0(22)	39.1(fixed)	—	-4.5	19.6
<i>u</i> 1026	Br(56)...H(68)	460.0(83)	35.1(fixed)	—	4.4	37.4
<i>u</i> 470	H(33)...H(37)	460.2(27)	47.4(fixed)	—	-4.0	18.4
<i>u</i> 418	Si(2)...H(26)	460.6(28)	26.5(fixed)	—	-4.8	18.9
<i>u</i> 406	Si(3)...H(19)	461.7(50)	18.4(fixed)	—	-5.2	39.1
<i>u</i> 420	Br(16)...H(30)	463.7(50)	28.4(fixed)	—	-3.2	35.1
<i>u</i> 412	Si(5)...H(41)	464.7(23)	18.9(fixed)	—	-7.9	28.4
<i>u</i> 1030	Si(45)...H(67)	466.0(24)	26.8(fixed)	—	-6.8	22.3
<i>u</i> 407	C(9)...H(19)	466.1(28)	24.4(fixed)	—	-1.5	25.4
<i>u</i> 1033	Br(55)...H(71)	466.2(21)	28.5(fixed)	—	-4.2	18.6
<i>u</i> 469	H(33)...H(38)	466.9(33)	54.3(fixed)	—	-6.5	23.3
<i>u</i> 1040	H(59)...H(63)	467.1(39)	18.4(fixed)	—	-3.6	32.6
<i>u</i> 1029	Si(45)...H(68)	468.4(51)	18.6(fixed)	—	-4.0	24.4
<i>u</i> 417	C(6)...H(41)	469.4(45)	25.9(fixed)	—	-8.2	29.0
<i>u</i> 1024	C(52)...H(79)	469.5(55)	24.4(fixed)	—	-5.1	25.9
<i>u</i> 434	H(32)...H(35)	471.0(16)	17.9(fixed)	—	-9.2	18.4
<i>u</i> 437	H(36)...H(40)	471.3(16)	17.4(fixed)	—	-9.6	17.9
<i>u</i> 436	H(26)...H(29)	471.5(17)	16.8(fixed)	—	-7.5	17.4
<i>u</i> 421	Br(14)...H(34)	471.6(17)	29.0(fixed)	—	-6.5	16.8
<i>u</i> 409	Si(3)...H(30)	473.3(17)	22.3(fixed)	—	-6.4	16.4
<i>u</i> 1041	H(67)...H(70)	473.7(18)	16.4(fixed)	—	-0.7	11.4

<i>u431</i>	H(18)...H(22)	473.7(43)	16.8(fixed)	—	-8.0	55.4
<i>u398</i>	C(10)...H(25)	473.8(17)	32.6(fixed)	—	-6.0	16.8
<i>u435</i>	Si(5)...C(11)	473.9(16)	10.1(tied to <i>u422</i> )	—	-0.7	11.2
<i>u419</i>	Si(3)...H(22)	474.2(56)	25.4(fixed)	—	-4.3	24.2
<i>u1043</i>	H(71)...H(78)	475.3(10)	50.5(fixed)	—	-0.7	11.7
<i>u422</i>	Si(2)...C(7)	475.7(46)	10.5(9)	—	8.8	39.9
<i>u427</i>	Si(4)...C(6)	477.3(9)	10.2(tied to <i>u422</i> )	—	-0.7	11.6
<i>u1037</i>	Si(43)...H(60)	478.3(10)	24.4(fixed)	—	-0.7	11.6
<i>u1049</i>	H(70)...H(77)	478.7(24)	42.4(fixed)	—	-6.6	24.4
<i>u424</i>	Si(3)...C(12)	479.9(7)	10.4(tied to <i>u422</i> )	—	-0.7	11.6
<i>u471</i>	C(11)...H(22)	480.2(7)	31.2(fixed)	—	-0.7	11.7
<i>u1039</i>	Si(43)...C(49)	481.3(7)	10.4(tied to <i>u422</i> )	—	-0.7	11.5
<i>u465</i>	H(21)...H(31)	481.7(28)	52.0(fixed)	—	-4.3	23.0
<i>u426</i>	Si(3)...H(41)	482.4(9)	23.0(fixed)	—	-0.7	11.2
<i>u425</i>	Si(5)...C(8)	482.6(7)	10.4(tied to <i>u422</i> )	—	-0.7	11.2
<i>u1034</i>	Si(45)...C(54)	483.5(11)	10.4(tied to <i>u422</i> )	—	-0.7	11.5
<i>u1053</i>	H(62)...H(74)	484.1(10)	54.2(fixed)	—	-0.7	11.3
<i>u1036</i>	Si(43)...C(48)	484.4(41)	10.3(tied to <i>u422</i> )	—	2.6	31.2
<i>u1061</i>	C(50)...H(81)	484.7(77)	28.6(fixed)	—	8.2	48.7
<i>u1035</i>	H(59)...H(78)	485.0(20)	39.9(fixed)	—	-5.3	22.6
<i>u438</i>	H(22)...H(37)	485.3(49)	45.0(fixed)	—	-9.6	54.3
<i>u1038</i>	Si(45)...C(47)	485.5(69)	10.0(tied to <i>u422</i> )	—	-9.5	52.0
<i>u429</i>	Si(4)...C(13)	485.6(56)	10.0(tied to <i>u422</i> )	—	-10.4	47.4
<i>u423</i>	Si(4)...C(9)	485.7(58)	10.3(tied to <i>u422</i> )	—	2.3	28.6
<i>u430</i>	Si(2)...C(10)	485.8(62)	10.1(tied to <i>u422</i> )	—	-6.9	50.5
<i>u443</i>	Si(2)...H(22)	487.8(38)	22.0(fixed)	—	5.6	37.1
<i>u432</i>	Si(2)...H(19)	488.1(31)	22.2(fixed)	—	-3.7	22.2
<i>u440</i>	H(24)...H(40)	489.6(20)	37.1(fixed)	—	0.2	22.0
<i>u510</i>	H(21)...H(30)	490.0(24)	38.5(fixed)	—	-6.5	23.5
<i>u403</i>	C(11)...H(25)	490.1(50)	24.2(fixed)	—	6.5	38.2
<i>u1069</i>	H(64)...H(74)	490.4(55)	45.1(fixed)	—	8.8	45.0
<i>u1062</i>	H(61)...H(82)	490.4(26)	53.2(fixed)	—	-3.8	22.0
<i>u1042</i>	Si(43)...H(75)	492.0(31)	22.6(fixed)	—	7.1	30.0
<i>u460</i>	C(6)...H(32)	492.0(30)	38.2(fixed)	—	-3.9	22.7
<i>u1055</i>	Si(43)...H(67)	494.2(63)	21.7(fixed)	—	-10.7	38.5
<i>u1048</i>	Si(43)...H(68)	494.4(59)	22.0(fixed)	—	6.8	42.4
<i>u428</i>	Si(5)...H(27)	495.4(26)	22.7(fixed)	—	0.1	21.3
<i>u449</i>	H(20)...H(32)	496.1(17)	48.7(fixed)	—	1.5	21.7
<i>u1059</i>	H(59)...H(65)	496.1(16)	40.8(fixed)	—	1.2	21.8
<i>u472</i>	Si(5)...H(35)	496.1(16)	21.7(fixed)	—	0.5	21.7
<i>u1044</i>	C(49)...H(73)	496.2(61)	30.0(fixed)	—	-10.3	53.2
<i>u455</i>	Si(5)...H(26)	496.6(13)	21.6(fixed)	—	0.5	21.6
<i>u452</i>	Si(3)...H(36)	497.0(49)	21.8(fixed)	—	5.7	36.7
<i>u1063</i>	C(49)...H(81)	497.3(65)	33.1(fixed)	—	-8.6	51.2

<i>u433</i>	Si(3)...H(34)	497.7(17)	23.5(fixed)	—	-4.9	23.5
<i>u448</i>	C(8)...H(40)	498.0(50)	28.7(fixed)	—	-8.3	54.2
<i>u444</i>	H(18)...H(37)	498.7(18)	36.7(fixed)	—	-3.9	21.6
<i>u493</i>	Br(17)...H(32)	499.5(29)	30.4(fixed)	—	3.6	28.7
<i>u1054</i>	H(59)...H(66)	500.1(56)	51.2(fixed)	—	-9.3	40.8
<i>u458</i>	Si(4)...H(20)	501.7(36)	21.3(fixed)	—	2.2	29.0
<i>u454</i>	H(24)...H(36)	501.7(18)	43.2(fixed)	—	-3.9	21.2
<i>u1052</i>	Si(43)...H(63)	502.1(14)	21.7(fixed)	—	1.1	21.7
<i>u451</i>	H(23)...H(26)	503.5(21)	41.9(fixed)	—	0.1	21.5
<i>u501</i>	H(34)...H(38)	504.4(47)	49.1(fixed)	—	8.6	43.2
<i>u445</i>	Si(5)...H(38)	504.5(6)	23.5(fixed)	—	-0.8	12.0
<i>u446</i>	Si(2)...H(25)	505.0(20)	21.6(fixed)	—	0.0	20.9
<i>u441</i>	H(24)...H(30)	505.2(43)	50.9(fixed)	—	2.8	29.9
<i>u491</i>	H(27)...H(39)	505.9(40)	39.1(fixed)	—	3.0	30.8
<i>u483</i>	Si(2)...Br(16)	505.9(48)	12.2(tied to <i>u474</i> )	—	6.4	30.4
<i>u521</i>	H(22)...H(34)	506.1(40)	36.4(fixed)	—	3.4	33.1
<i>u459</i>	C(12)...H(18)	506.5(6)	28.5(fixed)	—	-0.8	12.1
<i>u1060</i>	C(47)...H(76)	506.7(58)	33.7(fixed)	—	-6.8	50.9
<i>u1050</i>	Si(45)...H(80)	506.9(36)	21.5(fixed)	—	7.0	41.9
<i>u1065</i>	Si(45)...Br(57)	507.2(8)	12.3(tied to <i>u474</i> )	—	-0.8	12.1
<i>u482</i>	Si(5)...Br(14)	507.5(59)	12.3(tied to <i>u474</i> )	—	-10.0	45.1
<i>u474</i>	Si(3)...Br(17)	507.8(8)	12.4(5)	—	-0.8	12.0
<i>u1067</i>	Si(43)...Br(56)	508.0(5)	12.1(tied to <i>u474</i> )	—	-0.8	11.9
<i>u1047</i>	Si(45)...H(66)	508.1(23)	21.2(fixed)	—	0.0	21.3
<i>u462</i>	C(13)...H(35)	508.2(40)	35.1(fixed)	—	2.5	28.5
<i>u1077</i>	H(62)...H(75)	508.3(43)	47.5(fixed)	—	3.5	30.7
<i>u457</i>	C(8)...H(20)	508.6(20)	29.9(fixed)	—	5.7	33.7
<i>u477</i>	Si(4)...H(39)	508.7(19)	20.9(fixed)	—	-3.6	21.4
<i>u476</i>	C(10)...H(36)	508.8(48)	34.7(fixed)	—	-12.1	49.1
<i>u450</i>	H(23)...H(29)	509.0(50)	36.3(fixed)	—	4.4	36.3
<i>u461</i>	C(7)...H(37)	510.2(25)	35.2(fixed)	—	5.0	34.7
<i>u481</i>	Si(3)...Br(15)	510.4(52)	12.0(tied to <i>u474</i> )	—	-9.5	45.3
<i>u1051</i>	C(47)...H(78)	510.5(28)	29.0(fixed)	—	2.4	28.1
<i>u473</i>	C(12)...H(28)	510.9(28)	30.8(fixed)	—	7.5	35.1
<i>u1070</i>	H(60)...H(66)	510.9(6)	48.1(fixed)	—	-0.8	11.8
<i>u456</i>	Si(4)...H(28)	511.4(57)	21.3(fixed)	—	-10.3	48.1
<i>u480</i>	H(24)...H(32)	511.5(20)	40.8(fixed)	—	0.9	21.9
<i>u466</i>	C(13)...H(24)	511.8(36)	28.1(fixed)	—	5.4	35.2
<i>u1082</i>	C(50)...C(54)	512.0(61)	18.9(tied to <i>u474</i> )	—	-8.2	39.1
<i>u447</i>	Si(3)...H(21)	512.3(41)	21.4(fixed)	—	7.7	35.1
<i>u1058</i>	H(63)...H(78)	512.5(54)	43.0(fixed)	—	4.6	36.4
<i>u468</i>	C(7)...H(39)	512.9(22)	30.7(fixed)	—	0.9	21.6
<i>u495</i>	Si(4)...H(18)	514.2(51)	21.3(fixed)	—	8.5	45.3
<i>u1066</i>	Si(45)...H(61)	514.2(66)	21.9(fixed)	—	-8.6	51.5



<i>u</i> 463	C(7)...H(29)	514.3(20)	28.4(fixed)	—	-1.1	21.3
<i>u</i> 498	H(19)...H(28)	514.7(55)	36.5(fixed)	—	-9.2	40.8
<i>u</i> 1074	Si(45)...H(59)	515.8(42)	22.1(fixed)	—	-1.0	18.5
<i>u</i> 484	Si(2)...H(31)	516.7(32)	21.6(fixed)	—	3.9	27.9
<i>u</i> 503	Si(5)...H(33)	516.7(13)	22.6(fixed)	—	-0.9	22.6
<i>u</i> 572	H(22)...H(35)	516.8(20)	34.7(fixed)	—	-0.4	22.1
<i>u</i> 496	Si(2)...H(32)	517.4(21)	22.2(fixed)	—	-1.3	20.9
<i>u</i> 1057	C(50)...H(61)	517.5(38)	35.1(fixed)	—	2.9	28.4
<i>u</i> 1072	Si(46)...H(70)	517.6(42)	20.9(fixed)	—	7.9	43.0
<i>u</i> 475	H(25)...H(32)	517.6(39)	51.5(fixed)	—	2.9	30.9
<i>u</i> 478	C(6)...H(37)	517.6(21)	27.9(fixed)	—	-0.5	22.2
<i>u</i> 1064	C(48)...H(80)	518.1(37)	30.9(fixed)	—	5.8	35.2
<i>u</i> 486	C(12)...H(24)	518.4(47)	33.4(fixed)	—	-11.0	47.5
<i>u</i> 507	H(20)...H(41)	519.3(33)	36.9(fixed)	—	3.4	33.4
<i>u</i> 1046	H(64)...H(69)	520.1(23)	45.3(fixed)	—	-0.8	21.5
<i>u</i> 490	Si(4)...H(40)	520.6(21)	21.5(fixed)	—	-1.1	21.0
<i>u</i> 489	Si(4)...H(29)	521.4(24)	21.0(fixed)	—	-0.9	18.9
<i>u</i> 530	C(7)...C(11)	521.4(65)	16.8(fixed)	—	-10.6	51.1
<i>u</i> 497	Si(2)...H(23)	522.0(14)	21.2(fixed)	—	-1.5	21.2
<i>u</i> 1092	C(50)...H(77)	522.7(13)	28.0(fixed)	—	-1.3	21.7
<i>u</i> 1080	H(60)...H(82)	522.7(47)	40.3(fixed)	—	-9.5	39.1
<i>u</i> 1079	Si(43)...H(65)	522.7(67)	21.4(fixed)	—	-7.6	36.5
<i>u</i> 494	Si(3)...H(37)	522.8(14)	22.2(fixed)	—	-1.4	22.2
<i>u</i> 546	C(10)...Br(17)	523.1(57)	20.7(tied to <i>u</i> 579)	—	9.2	48.3
<i>u</i> 1076	Si(43)...H(64)	523.3(13)	21.7(fixed)	—	-1.3	21.4
<i>u</i> 1075	C(47)...C(53)	524.2(39)	18.9(fixed)	—	7.1	33.7
<i>u</i> 1106	H(67)...H(80)	524.3(39)	40.0(fixed)	—	4.5	30.0
<i>u</i> 1056	C(50)...H(64)	524.8(14)	35.2(fixed)	—	-1.4	21.2
<i>u</i> 500	Si(5)...H(24)	525.6(41)	21.2(fixed)	—	-11.3	40.3
<i>u</i> 515	C(12)...H(22)	526.0(75)	28.8(fixed)	—	-8.3	36.9
<i>u</i> 506	H(27)...H(41)	526.8(51)	38.1(fixed)	—	-8.5	38.1
<i>u</i> 590	Br(17)...H(35)	526.8(46)	29.6(fixed)	—	7.1	37.6
<i>u</i> 487	C(8)...H(23)	527.5(28)	33.0(fixed)	—	3.2	33.0
<i>u</i> 1068	H(63)...H(66)	527.7(22)	45.3(fixed)	—	-0.9	18.4
<i>u</i> 504	C(8)...C(13)	527.8(30)	18.4(fixed)	—	3.1	32.5
<i>u</i> 464	C(9)...H(31)	527.8(31)	33.7(fixed)	—	-0.8	16.8
<i>u</i> 1083	Br(55)...H(59)	528.1(75)	38.7(fixed)	—	4.7	50.9
<i>u</i> 513	Br(16)...H(40)	528.2(44)	34.6(fixed)	—	1.7	27.4
<i>u</i> 1102	H(68)...H(81)	528.4(38)	36.5(fixed)	—	6.1	30.6
<i>u</i> 1071	C(48)...H(78)	529.4(40)	32.5(fixed)	—	2.0	28.1
<i>u</i> 1078	H(62)...H(66)	530.7(44)	39.1(fixed)	—	1.5	34.7
<i>u</i> 540	H(22)...H(36)	530.9(42)	47.8(fixed)	—	2.1	28.8
<i>u</i> 578	C(6)...Br(15)	531.4(40)	19.1(tied to <i>u</i> 579)	—	-1.0	20.2
<i>u</i> 1086	Br(56)...H(77)	531.9(31)	31.3(fixed)	—	-0.7	18.2

<i>u529</i>	C(6)...C(10)	532.0(45)	18.2(fixed)	—	4.2	34.6
<i>u485</i>	C(9)...H(23)	533.0(51)	28.1(fixed)	—	3.3	47.8
<i>u502</i>	Br(17)...H(29)	533.5(26)	34.2(fixed)	—	-0.9	18.4
<i>u509</i>	C(6)...C(12)	533.5(31)	18.4(fixed)	—	3.3	31.3
<i>u553</i>	H(19)...H(32)	534.7(46)	41.6(fixed)	—	7.3	38.7
<i>u522</i>	C(10)...H(20)	534.7(41)	27.4(fixed)	—	4.5	36.2
<i>u514</i>	H(20)...H(31)	535.1(45)	50.9(fixed)	—	3.8	35.3
<i>u549</i>	C(11)...H(23)	535.3(67)	35.0(fixed)	—	1.7	36.5
<i>u453</i>	H(28)...H(33)	535.6(58)	48.3(fixed)	—	3.7	34.2
<i>u1110</i>	C(49)...Br(55)	535.9(46)	18.6(tied to <i>u579</i> )	—	6.7	41.6
<i>u488</i>	Br(16)...H(33)	535.9(55)	30.6(fixed)	—	-10.2	47.1
<i>u499</i>	H(19)...H(27)	536.6(32)	37.7(fixed)	—	2.4	28.0
<i>u1073</i>	Br(55)...H(74)	537.4(63)	30.0(fixed)	—	-7.6	37.7
<i>u467</i>	C(9)...H(33)	537.4(62)	37.6(fixed)	—	-8.6	37.7
<i>u1099</i>	C(49)...C(54)	538.3(44)	18.3(fixed)	—	4.5	36.0
<i>u511</i>	H(19)...H(41)	538.8(63)	37.7(fixed)	—	3.8	40.0
<i>u516</i>	Br(14)...H(18)	539.6(44)	33.7(fixed)	—	-1.0	18.7
<i>u479</i>	H(25)...H(35)	540.1(55)	51.1(fixed)	—	3.2	33.7
<i>u1084</i>	H(60)...H(76)	541.4(27)	38.4(fixed)	—	2.1	29.2
<i>u492</i>	H(25)...H(30)	541.7(44)	47.1(fixed)	—	5.1	29.6
<i>u505</i>	H(20)...H(25)	541.7(29)	35.3(fixed)	—	-1.1	20.2
<i>u520</i>	H(28)...H(38)	542.1(57)	36.2(fixed)	—	-11.2	40.4
<i>u1088</i>	H(59)...H(79)	542.3(39)	38.5(fixed)	—	-0.5	35.0
<i>u561</i>	Si(5)...H(34)	542.4(21)	16.4(fixed)	—	8.3	38.4
<i>u1095</i>	C(47)...C(52)	542.8(34)	17.0(fixed)	—	7.3	38.5
<i>u519</i>	H(35)...H(41)	543.3(29)	39.7(fixed)	—	-0.9	18.3
<i>u523</i>	H(30)...H(36)	543.3(26)	39.4(fixed)	—	7.4	39.4
<i>u1113</i>	Br(56)...Br(58)	543.4(25)	22.5(tied to <i>u579</i> )	—	-4.3	16.4
<i>u536</i>	H(25)...H(40)	543.8(39)	37.0(fixed)	—	9.7	39.7
<i>u1111</i>	H(66)...H(81)	544.0(26)	38.7(fixed)	—	-0.8	16.3
<i>u532</i>	C(10)...C(12)	544.2(23)	16.9(fixed)	—	-1.1	20.2
<i>u600</i>	C(11)...Br(17)	544.6(29)	19.9(tied to <i>u579</i> )	—	9.5	39.7
<i>u535</i>	C(8)...H(36)	544.9(20)	28.0(fixed)	—	-0.8	16.8
<i>u512</i>	C(7)...C(9)	545.0(17)	18.3(fixed)	—	-0.8	16.9
<i>u539</i>	C(7)...H(26)	545.2(13)	28.3(fixed)	—	-0.9	17.0
<i>u537</i>	C(11)...C(13)	545.5(26)	17.1(fixed)	—	-3.2	15.7
<i>u517</i>	H(21)...H(39)	545.6(19)	36.0(fixed)	—	-0.9	18.1
<i>u593</i>	H(22)...H(33)	545.8(35)	35.2(fixed)	—	4.0	28.0
<i>u542</i>	Si(2)...H(21)	545.9(36)	16.7(fixed)	—	-1.1	22.0
<i>u560</i>	Si(4)...H(19)	546.3(11)	15.7(fixed)	—	-3.4	16.7
<i>u563</i>	Br(15)...H(39)	546.4(21)	29.2(fixed)	—	-0.8	16.8
<i>u541</i>	C(7)...C(12)	546.6(18)	18.7(fixed)	—	-0.8	18.3
<i>u544</i>	Si(3)...H(38)	546.6(10)	16.8(fixed)	—	-4.0	16.8
<i>u558</i>	C(10)...H(37)	546.7(26)	41.6(fixed)	—	-0.8	16.5

<i>u524</i>	C(6)...C(8)	546.8(36)	16.3(fixed)	—	-1.0	35.2
<i>u528</i>	C(11)...Br(16)	547.2(27)	20.7(tied to <i>u579</i> )	—	-0.8	18.7
<i>u533</i>	C(9)...C(12)	547.5(21)	16.8(fixed)	—	-0.9	17.1
<i>u551</i>	H(20)...H(26)	547.7(26)	32.5(fixed)	—	2.6	28.3
<i>u1096</i>	Si(45)...H(82)	548.5(42)	16.2(fixed)	—	2.0	32.5
<i>u527</i>	Br(15)...H(26)	548.6(34)	31.8(fixed)	—	3.2	37.0
<i>u1109</i>	H(59)...H(76)	548.7(11)	39.9(fixed)	—	-3.3	16.2
<i>u1081</i>	H(61)...H(68)	550.2(62)	39.7(fixed)	—	-0.3	44.2
<i>u1093</i>	C(48)...Br(57)	550.4(40)	20.2(fixed)	—	4.6	36.0
<i>u1107</i>	Si(43)...H(66)	550.5(32)	16.2(fixed)	—	3.3	31.8
<i>u1115</i>	C(47)...H(74)	551.0(20)	42.5(fixed)	—	-0.9	20.1
<i>u1094</i>	C(47)...C(50)	551.4(9)	16.8(fixed)	—	-3.4	16.7
<i>u531</i>	C(7)...C(13)	551.4(40)	16.5(fixed)	—	2.0	28.2
<i>u543</i>	Si(5)...H(25)	552.2(10)	16.7(fixed)	—	-3.4	16.2
<i>u565</i>	C(6)...H(31)	552.3(17)	44.2(fixed)	—	-0.8	16.9
<i>u1087</i>	H(62)...H(80)	552.4(29)	36.0(fixed)	—	-0.7	18.5
<i>u1098</i>	Si(43)...H(62)	552.5(9)	16.7(fixed)	—	-3.8	16.7
<i>u508</i>	H(25)...H(34)	552.5(43)	40.4(fixed)	—	2.8	32.7
<i>u574</i>	C(13)...Br(15)	552.8(52)	20.6(tied to <i>u579</i> )	—	4.1	49.0
<i>u1090</i>	C(48)...C(54)	552.8(45)	17.4(tied to <i>u579</i> )	—	5.8	40.9
<i>u564</i>	H(26)...H(36)	552.9(36)	40.9(fixed)	—	2.4	38.7
<i>u1097</i>	C(49)...H(76)	553.4(37)	28.4(fixed)	—	2.3	33.7
<i>u1103</i>	Si(45)...H(60)	553.4(29)	16.0(fixed)	—	2.7	39.9
<i>u548</i>	H(18)...H(38)	553.6(30)	38.6(fixed)	—	-0.3	41.6
<i>u552</i>	H(22)...H(39)	553.6(38)	32.7(fixed)	—	-0.9	19.5
<i>u571</i>	H(22)...H(26)	553.9(10)	40.1(fixed)	—	-4.4	16.0
<i>u569</i>	H(28)...H(36)	554.5(62)	33.7(fixed)	—	4.6	52.2
<i>u550</i>	C(8)...C(12)	554.8(40)	18.1(fixed)	—	3.7	40.1
<i>u584</i>	C(13)...H(33)	555.1(32)	46.3(fixed)	—	3.8	28.4
<i>u557</i>	Si(4)...H(41)	555.3(25)	15.7(fixed)	—	-0.7	18.1
<i>u545</i>	Si(4)...H(27)	555.3(11)	16.1(fixed)	—	-3.5	15.7
<i>u556</i>	Si(2)...H(30)	555.4(53)	16.0(fixed)	—	0.4	40.5
<i>u538</i>	C(9)...C(10)	555.5(18)	17.5(tied to <i>u579</i> )	—	-0.8	17.1
<i>u1126</i>	C(49)...H(80)	555.5(11)	32.1(fixed)	—	-3.3	16.1
<i>u1085</i>	C(48)...H(69)	556.0(10)	28.2(fixed)	—	-4.2	16.0
<i>u1091</i>	C(48)...C(50)	556.8(47)	18.9(tied to <i>u579</i> )	—	1.8	27.8
<i>u582</i>	H(32)...H(36)	557.8(36)	40.5(fixed)	—	-0.7	18.1
<i>u573</i>	H(35)...H(40)	558.1(27)	40.9(fixed)	—	-0.8	42.5
<i>u581</i>	H(35)...H(39)	558.5(64)	34.9(fixed)	—	-0.7	34.2
<i>u1121</i>	C(47)...Br(56)	558.7(46)	20.3(tied to <i>u579</i> )	—	5.9	41.4
<i>u579</i>	Br(14)...Br(15)	558.8(38)	22.1(6)	—	9.0	38.2
<i>u1116</i>	H(61)...H(70)	559.4(58)	40.9(fixed)	—	4.3	40.9
<i>u554</i>	C(7)...C(8)	559.7(47)	19.0(tied to <i>u579</i> )	—	1.7	38.6
<i>u635</i>	C(7)...H(35)	560.8(34)	22.0(fixed)	—	1.6	40.5

<i>u1108</i>	H(63)...H(77)	561.0(8)	41.4(fixed)	—	-0.9	19.8
<i>u1124</i>	C(47)...Br(55)	561.2(23)	19.8(tied to <i>u579</i> )	—	-0.8	18.1
<i>u1089</i>	H(63)...H(69)	561.5(20)	49.0(fixed)	—	-0.7	18.5
<i>u518</i>	H(27)...H(31)	562.1(57)	38.2(fixed)	—	-1.2	45.1
<i>u1147</i>	H(69)...H(81)	562.2(33)	30.7(fixed)	—	4.6	40.0
<i>u589</i>	H(31)...H(36)	562.8(18)	35.2(fixed)	—	4.3	29.4
<i>u568</i>	H(21)...H(37)	562.9(46)	40.0(fixed)	—	1.7	37.1
<i>u609</i>	C(7)...H(34)	563.0(35)	23.0(fixed)	—	4.2	40.9
<i>u1100</i>	C(48)...C(53)	563.0(31)	18.5(tied to <i>u579</i> )	—	5.9	34.9
<i>u547</i>	H(21)...H(29)	563.1(56)	36.1(fixed)	—	-0.6	35.7
<i>u1122</i>	H(61)...H(76)	563.8(28)	34.6(fixed)	—	-1.2	21.6
<i>u555</i>	C(8)...H(18)	564.0(36)	34.2(fixed)	—	-1.1	46.3
<i>u1114</i>	H(63)...H(80)	564.1(29)	34.1(fixed)	—	3.0	35.2
<i>u1119</i>	Br(56)...H(61)	565.5(37)	29.4(fixed)	—	-1.2	39.0
<i>u599</i>	C(7)...H(36)	566.0(47)	39.0(fixed)	—	5.5	39.9
<i>u594</i>	C(13)...Br(16)	566.1(47)	19.6(tied to <i>u579</i> )	—	-0.3	34.6
<i>u1120</i>	C(50)...H(59)	566.6(55)	45.1(fixed)	—	-0.6	35.7
<i>u1101</i>	H(60)...H(78)	566.6(54)	40.5(fixed)	—	-1.0	32.1
<i>u575</i>	H(29)...H(31)	567.1(58)	39.6(fixed)	—	-1.6	30.7
<i>u559</i>	H(24)...H(41)	567.2(27)	37.1(fixed)	—	3.1	34.6
<i>u534</i>	C(9)...C(11)	567.4(32)	18.6(tied to <i>u579</i> )	—	4.0	29.4
<i>u613</i>	H(18)...H(32)	567.7(61)	39.5(fixed)	—	-0.8	37.3
<i>u1137</i>	Br(55)...H(61)	568.1(37)	47.4(fixed)	—	1.8	34.1
<i>u1123</i>	C(49)...Br(58)	568.2(31)	17.4(tied to <i>u579</i> )	—	1.9	40.7
<i>u1105</i>	C(48)...H(81)	568.4(41)	35.7(fixed)	—	2.5	36.1
<i>u525</i>	C(11)...H(28)	568.5(46)	27.8(fixed)	—	3.7	35.8
<i>u1132</i>	H(59)...H(74)	568.5(50)	46.8(fixed)	—	-0.2	33.9
<i>u567</i>	C(12)...H(29)	568.9(54)	35.7(fixed)	—	4.0	39.6
<i>u592</i>	C(9)...H(32)	568.9(52)	44.9(fixed)	—	-1.3	44.9
<i>u588</i>	C(9)...Br(17)	569.1(21)	20.0(tied to <i>u579</i> )	—	-0.8	19.3
<i>u591</i>	C(10)...Br(14)	569.2(57)	20.6(tied to <i>u579</i> )	—	2.0	39.5
<i>u620</i>	Br(14)...Br(16)	569.6(19)	18.5(tied to <i>u579</i> )	—	-0.9	19.2
<i>u667</i>	Br(15)...H(19)	569.8(22)	24.8(fixed)	—	-0.9	20.1
<i>u583</i>	Br(14)...H(31)	570.0(32)	29.4(fixed)	—	2.2	31.4
<i>u1127</i>	H(59)...H(77)	570.6(49)	31.4(fixed)	—	0.6	34.6
<i>u596</i>	H(28)...H(37)	570.7(43)	34.6(fixed)	—	-1.3	23.0
<i>u526</i>	H(28)...H(35)	571.0(40)	52.2(fixed)	—	-0.8	40.9
<i>u671</i>	Br(15)...H(18)	571.0(36)	23.9(fixed)	—	6.2	34.9
<i>u585</i>	H(24)...H(38)	571.5(46)	40.7(fixed)	—	-0.4	34.7
<i>u601</i>	H(32)...H(37)	571.7(20)	45.5(fixed)	—	-0.9	16.9
<i>u566</i>	H(19)...H(37)	572.5(32)	35.8(fixed)	—	-1.8	22.0
<i>u615</i>	Br(14)...Br(17)	572.6(32)	18.4(tied to <i>u579</i> )	—	-0.9	19.5
<i>u587</i>	H(20)...H(24)	572.6(50)	33.9(fixed)	—	-0.6	44.6
<i>u641</i>	H(23)...H(34)	574.3(12)	40.3(fixed)	—	-1.1	18.0

<i>u605</i>	H(26)...H(40)	575.8(42)	30.5(fixed)	—	-4.5	36.5
<i>u570</i>	C(7)...H(40)	576.8(13)	37.3(fixed)	—	-1.0	18.0
<i>u1125</i>	H(64)...H(80)	577.0(57)	34.7(fixed)	—	-0.4	47.4
<i>u598</i>	C(6)...Br(14)	577.0(31)	20.2(tied to <i>u579</i> )	—	-0.9	19.7
<i>u1144</i>	H(65)...H(81)	577.2(54)	35.8(fixed)	—	7.2	41.4
<i>u1104</i>	H(64)...H(68)	577.5(31)	39.9(fixed)	—	-0.6	30.5
<i>u1129</i>	C(48)...H(73)	577.7(34)	23.4(fixed)	—	-0.9	32.7
<i>u1154</i>	Br(55)...H(66)	577.9(35)	24.4(fixed)	—	3.0	46.8
<i>u597</i>	H(23)...H(39)	578.3(31)	34.6(fixed)	—	2.0	39.6
<i>u619</i>	Br(16)...Br(17)	578.6(41)	18.4(tied to <i>u579</i> )	—	3.0	45.5
<i>u1131</i>	Br(56)...H(78)	578.6(25)	35.8(fixed)	—	-1.8	22.7
<i>u1112</i>	H(61)...H(69)	579.1(36)	34.9(fixed)	—	1.3	40.1
<i>u1149</i>	C(54)...H(68)	579.6(58)	27.5(fixed)	—	-1.7	24.8
<i>u650</i>	Br(16)...H(39)	580.3(21)	36.3(fixed)	—	-0.7	23.4
<i>u628</i>	C(7)...H(33)	580.6(36)	22.7(fixed)	—	-1.0	32.8
<i>u1164</i>	Br(55)...H(67)	580.9(10)	23.3(fixed)	—	-1.1	18.0
<i>u1117</i>	C(50)...H(63)	581.1(52)	40.9(fixed)	—	-3.5	27.5
<i>u604</i>	H(23)...H(33)	581.4(31)	40.1(fixed)	—	1.9	39.1
<i>u646</i>	Br(15)...Br(16)	581.8(41)	21.8(tied to <i>u579</i> )	—	-5.5	34.3
<i>u626</i>	H(18)...H(36)	582.1(37)	31.4(fixed)	—	5.5	33.9
<i>u603</i>	C(12)...H(26)	582.3(41)	32.7(fixed)	—	-1.6	23.9
<i>u642</i>	Br(17)...H(28)	582.7(54)	34.8(fixed)	—	-1.1	36.3
<i>u607</i>	C(12)...H(32)	582.8(53)	23.3(fixed)	—	-1.0	40.3
<i>u1157</i>	C(50)...H(80)	583.1(37)	24.6(fixed)	—	-2.4	31.4
<i>u1130</i>	H(61)...H(78)	583.2(32)	36.5(fixed)	—	-1.1	31.6
<i>u595</i>	C(8)...Br(15)	583.7(33)	17.5(tied to <i>u579</i> )	—	-0.8	35.8
<i>u1141</i>	C(49)...H(72)	584.0(26)	34.3(fixed)	—	-1.0	23.3
<i>u1150</i>	Br(55)...Br(56)	584.1(50)	21.9(tied to <i>u579</i> )	—	-3.6	24.6
<i>u633</i>	H(33)...H(40)	584.2(22)	49.5(fixed)	—	-0.9	17.0
<i>u586</i>	H(23)...H(25)	584.5(54)	39.1(fixed)	—	1.3	36.4
<i>u649</i>	H(29)...H(32)	584.5(60)	48.3(fixed)	—	-1.1	34.8
<i>u686</i>	Br(17)...H(30)	584.5(26)	31.9(fixed)	—	-1.5	21.9
<i>u614</i>	C(6)...H(26)	584.8(57)	21.9(fixed)	—	1.2	48.3
<i>u1118</i>	H(62)...H(78)	584.9(27)	39.6(fixed)	—	-1.6	22.5
<i>u606</i>	C(8)...H(22)	585.6(42)	31.6(fixed)	—	-0.8	35.8
<i>u577</i>	C(9)...H(35)	585.9(29)	44.6(fixed)	—	-1.5	22.2
<i>u616</i>	C(11)...H(40)	586.2(20)	23.1(fixed)	—	-1.1	21.4
<i>u1146</i>	Br(55)...Br(58)	586.2(27)	18.7(tied to <i>u579</i> )	—	-1.5	24.4
<i>u1128</i>	C(48)...H(77)	586.3(26)	32.8(fixed)	—	-1.1	21.3
<i>u1139</i>	C(47)...H(70)	586.8(25)	22.5(fixed)	—	-3.4	27.9
<i>u612</i>	C(13)...H(22)	586.9(26)	22.2(fixed)	—	-3.5	24.6
<i>u1152</i>	H(59)...H(70)	588.0(23)	48.3(fixed)	—	-1.4	22.2
<i>u618</i>	H(23)...H(37)	588.2(36)	38.4(fixed)	—	-2.0	31.1
<i>u1133</i>	C(47)...H(79)	588.9(50)	27.9(fixed)	—	1.2	48.3

<i>u1140</i>	C(48)...H(71)	589.3(27)	23.6(fixed)	—	-1.7	22.7
<i>u580</i>	H(28)...H(31)	589.3(21)	33.9(fixed)	—	-1.6	23.1
<i>u623</i>	C(10)...H(29)	589.6(40)	22.9(fixed)	—	-5.4	31.2
<i>u681</i>	Br(15)...H(20)	589.6(29)	23.1(fixed)	—	-1.3	23.1
<i>u654</i>	H(30)...H(37)	590.0(13)	48.1(fixed)	—	-1.1	18.3
<i>u617</i>	C(12)...H(30)	590.7(45)	23.3(fixed)	—	-3.1	25.3
<i>u632</i>	C(9)...H(36)	590.9(40)	22.2(fixed)	—	1.0	38.4
<i>u638</i>	H(24)...H(39)	591.2(19)	31.1(fixed)	—	-1.4	22.9
<i>u668</i>	C(10)...H(19)	591.7(17)	25.3(fixed)	—	-1.5	23.3
<i>u657</i>	Br(14)...H(20)	591.9(45)	34.3(fixed)	—	1.8	49.5
<i>u622</i>	C(13)...H(25)	592.0(24)	27.7(fixed)	—	-3.4	27.7
<i>u576</i>	H(23)...H(27)	592.2(61)	36.4(fixed)	—	-1.1	34.3
<i>u562</i>	H(27)...H(33)	592.4(38)	41.4(fixed)	—	-3.8	26.1
<i>u658</i>	C(8)...H(39)	592.5(28)	26.1(fixed)	—	-1.8	22.9
<i>u1151</i>	C(47)...H(77)	592.6(54)	24.6(fixed)	—	-5.1	31.9
<i>u630</i>	H(22)...H(29)	592.9(22)	29.8(fixed)	—	-1.8	23.0
<i>u685</i>	Br(17)...H(31)	593.0(14)	33.7(fixed)	—	-1.6	23.6
<i>u682</i>	H(23)...H(35)	593.2(38)	35.5(fixed)	—	-0.8	29.8
<i>u624</i>	C(11)...H(41)	593.4(30)	23.3(fixed)	—	-1.8	23.3
<i>u1162</i>	Br(55)...H(65)	593.4(24)	23.1(fixed)	—	-3.5	24.2
<i>u656</i>	C(11)...H(39)	593.9(40)	21.7(fixed)	—	1.3	37.3
<i>u602</i>	C(6)...H(25)	594.1(38)	22.7(fixed)	—	-2.2	23.1
<i>u661</i>	C(13)...H(26)	594.4(11)	24.2(fixed)	—	-2.0	23.1
<i>u611</i>	Br(15)...H(24)	594.6(38)	36.7(fixed)	—	-0.2	30.0
<i>u610</i>	C(9)...H(38)	594.8(57)	23.1(fixed)	—	0.9	40.2
<i>u1143</i>	C(49)...H(71)	594.9(25)	31.2(fixed)	—	-1.9	22.1
<i>u1160</i>	H(60)...H(74)	595.0(21)	49.4(fixed)	—	-2.1	21.7
<i>u648</i>	H(24)...H(37)	595.2(38)	37.8(fixed)	—	-3.7	28.3
<i>u645</i>	H(20)...H(37)	595.5(22)	30.0(fixed)	—	-1.7	23.3
<i>u655</i>	C(12)...H(31)	595.6(30)	21.6(fixed)	—	-1.9	21.9
<i>u1145</i>	C(50)...H(76)	595.8(21)	22.3(fixed)	—	-1.8	22.4
<i>u631</i>	C(8)...H(41)	595.8(25)	28.3(fixed)	—	-4.2	26.7
<i>u663</i>	C(6)...H(36)	596.0(66)	26.7(fixed)	—	0.2	38.3
<i>u1156</i>	C(48)...H(72)	596.6(37)	21.7(fixed)	—	-1.8	37.8
<i>u639</i>	C(6)...H(38)	596.8(20)	29.8(fixed)	—	-2.4	21.6
<i>u608</i>	C(13)...H(21)	596.9(37)	22.9(fixed)	—	-0.7	36.7
<i>u1136</i>	C(47)...H(68)	596.9(35)	23.0(fixed)	—	-1.6	48.1
<i>u664</i>	C(12)...H(20)	598.0(20)	24.5(fixed)	—	-1.7	22.3
<i>u672</i>	C(10)...H(18)	598.4(59)	24.0(fixed)	—	0.6	39.7
<i>u1135</i>	H(64)...H(70)	598.5(32)	37.3(fixed)	—	-3.0	24.0
<i>u1142</i>	C(50)...H(74)	598.6(25)	22.4(fixed)	—	-1.8	22.0
<i>u1165</i>	C(50)...H(79)	598.6(46)	26.0(fixed)	—	-5.3	33.7
<i>u637</i>	C(9)...H(37)	598.8(30)	22.1(fixed)	—	-1.9	22.0
<i>u629</i>	C(6)...H(24)	599.0(19)	21.9(fixed)	—	-2.7	21.7

<i>u1138</i>	H(64)...H(81)	599.0(40)	40.2(fixed)	—	-3.3	24.5
<i>u651</i>	H(23)...H(24)	599.5(31)	36.3(fixed)	—	-4.0	29.8
<i>u643</i>	C(12)...H(19)	600.3(37)	27.0(fixed)	—	-3.3	27.0
<i>u674</i>	H(33)...H(41)	600.4(18)	53.0(fixed)	—	-1.4	23.2
<i>u1134</i>	C(50)...H(75)	600.5(47)	23.2(fixed)	—	2.2	39.3
<i>u704</i>	Br(17)...H(34)	601.1(38)	30.5(fixed)	—	-4.0	35.5
<i>u1148</i>	C(47)...H(69)	602.4(34)	22.0(fixed)	—	-2.4	36.6
<i>u1155</i>	H(64)...H(78)	602.4(71)	36.6(fixed)	—	-1.7	39.4
<i>u627</i>	H(18)...H(24)	603.2(32)	38.3(fixed)	—	-1.0	36.3
<i>u644</i>	C(13)...H(23)	604.3(32)	22.0(fixed)	—	-4.3	31.3
<i>u666</i>	C(7)...H(28)	604.4(44)	25.0(fixed)	—	-2.0	30.5
<i>u1168</i>	C(50)...H(78)	604.8(20)	24.7(fixed)	—	-1.8	23.3
<i>u634</i>	H(29)...H(37)	604.9(33)	39.7(fixed)	—	-2.4	49.4
<i>u660</i>	H(23)...H(28)	605.3(41)	30.5(fixed)	—	-3.5	25.0
<i>u665</i>	C(9)...H(22)	605.3(65)	23.3(fixed)	—	0.2	40.8
<i>u625</i>	C(10)...H(27)	606.5(29)	23.3(fixed)	—	-3.2	23.3
<i>u640</i>	C(9)...H(21)	606.7(25)	27.0(fixed)	—	-5.7	31.7
<i>u621</i>	H(29)...H(33)	606.8(24)	39.3(fixed)	—	-2.0	22.0
<i>u670</i>	Br(16)...H(34)	607.0(27)	32.8(fixed)	—	-5.0	29.0
<i>u676</i>	Br(16)...H(35)	607.1(18)	31.7(fixed)	—	-3.4	26.0
<i>u636</i>	H(18)...H(25)	607.4(61)	39.4(fixed)	—	-1.6	41.2
<i>u722</i>	Br(17)...H(33)	607.6(24)	28.8(fixed)	—	-4.9	32.8
<i>u675</i>	C(12)...H(21)	609.0(30)	26.3(fixed)	—	-3.2	27.0
<i>u653</i>	C(10)...H(28)	609.0(74)	22.0(fixed)	—	-3.0	51.8
<i>u677</i>	C(12)...H(23)	610.0(27)	25.2(fixed)	—	-3.4	26.3
<i>u691</i>	Br(15)...H(41)	610.5(41)	28.1(fixed)	—	-2.7	53.0
<i>u1159</i>	Br(55)...H(75)	610.7(36)	31.3(fixed)	—	-3.4	28.1
<i>u692</i>	H(31)...H(37)	612.0(48)	40.9(fixed)	—	-4.3	30.5
<i>u1166</i>	Br(55)...H(76)	612.9(35)	29.0(fixed)	—	-3.2	25.9
<i>u652</i>	H(23)...H(40)	613.0(41)	40.8(fixed)	—	-3.4	27.6
<i>u695</i>	H(19)...H(31)	613.4(22)	49.6(fixed)	—	-3.1	24.7
<i>u647</i>	C(7)...H(27)	613.5(67)	27.6(fixed)	—	-2.1	42.9
<i>u1163</i>	H(59)...H(68)	613.6(59)	51.8(fixed)	—	-3.1	34.5
<i>u659</i>	H(29)...H(38)	613.8(29)	41.2(fixed)	—	-3.0	25.2
<i>u680</i>	H(18)...H(26)	614.9(61)	34.5(fixed)	—	-1.4	41.1
<i>u1173</i>	H(61)...H(74)	615.3(35)	41.5(fixed)	—	-3.0	24.2
<i>u1153</i>	H(62)...H(81)	615.5(39)	41.1(fixed)	—	-1.7	45.6
<i>u689</i>	H(18)...H(31)	616.1(89)	45.6(fixed)	—	-4.7	49.6
<i>u1171</i>	Br(56)...H(60)	616.5(25)	29.9(fixed)	—	-4.0	27.3
<i>u696</i>	Br(15)...H(40)	617.8(27)	25.9(fixed)	—	-3.8	29.9
<i>u697</i>	H(33)...H(39)	617.9(28)	44.2(fixed)	—	-3.6	25.9
<i>u1161</i>	C(48)...H(70)	618.1(30)	24.2(fixed)	—	-4.3	40.9
<i>u679</i>	C(8)...H(38)	618.7(40)	27.3(fixed)	—	-3.0	24.2
<i>u684</i>	C(8)...H(37)	618.7(72)	27.2(fixed)	—	-3.1	51.4

<i>u717</i>	C(11)...H(21)	619.2(52)	19.4(fixed)	—	-3.4	35.7
<i>u1158</i>	C(48)...H(68)	620.1(27)	25.9(fixed)	—	-3.7	27.2
<i>u1179</i>	H(65)...H(80)	620.4(41)	37.5(fixed)	—	-3.1	25.4
<i>u678</i>	H(27)...H(32)	620.4(56)	51.4(fixed)	—	-3.2	36.9
<i>u1186</i>	H(68)...H(77)	620.8(30)	31.6(fixed)	—	-5.0	28.8
<i>u662</i>	H(21)...H(40)	622.7(30)	42.9(fixed)	—	-5.0	41.5
<i>u690</i>	H(29)...H(36)	622.9(25)	35.7(fixed)	—	-4.1	26.7
<i>u688</i>	C(7)...H(24)	624.0(25)	25.4(fixed)	—	-3.8	27.0
<i>u703</i>	H(22)...H(38)	624.2(22)	32.8(fixed)	—	-3.2	25.4
<i>u1177</i>	Br(56)...H(59)	624.3(34)	27.0(fixed)	—	-4.3	44.2
<i>u1170</i>	C(49)...H(74)	624.5(51)	26.7(fixed)	—	-3.6	35.8
<i>u699</i>	H(23)...H(36)	624.7(20)	43.2(fixed)	—	-4.8	27.0
<i>u687</i>	H(22)...H(40)	625.2(36)	36.9(fixed)	—	-8.6	23.4
<i>u1169</i>	H(63)...H(81)	625.3(45)	35.8(fixed)	—	-4.2	42.9
<i>u673</i>	C(11)...H(29)	625.5(48)	24.2(fixed)	—	-7.3	30.6
<i>u709</i>	C(6)...H(30)	626.0(32)	23.4(fixed)	—	-5.7	19.4
<i>u1191</i>	H(66)...H(80)	626.1(36)	37.3(fixed)	—	-2.3	43.2
<i>u683</i>	C(7)...H(25)	627.0(25)	26.3(fixed)	—	-3.5	26.3
<i>u705</i>	Br(14)...H(32)	629.4(43)	27.2(fixed)	—	-5.2	32.8
<i>u1167</i>	C(49)...H(75)	629.9(54)	27.0(fixed)	—	-2.7	37.5
<i>u1174</i>	H(59)...H(69)	630.4(29)	42.9(fixed)	—	-4.7	27.2
<i>u708</i>	H(20)...H(30)	631.2(41)	30.6(fixed)	—	-4.2	42.8
<i>u669</i>	C(11)...H(27)	631.4(50)	25.4(fixed)	—	-2.2	43.4
<i>u694</i>	Br(14)...H(30)	631.6(32)	30.0(fixed)	—	-3.8	30.0
<i>u698</i>	C(6)...C(11)	631.7(56)	13.6(fixed)	—	-1.8	46.3
<i>u701</i>	H(28)...H(32)	632.8(11)	42.8(fixed)	—	-1.3	13.6
<i>u1187</i>	C(49)...H(82)	634.8(57)	23.5(fixed)	—	-5.1	37.3
<i>u707</i>	H(26)...H(37)	636.4(16)	41.2(fixed)	—	-1.3	13.5
<i>u1176</i>	C(49)...C(53)	636.5(33)	13.7(fixed)	—	-3.0	41.2
<i>u1172</i>	H(63)...H(70)	636.8(16)	43.4(fixed)	—	-1.3	13.6
<i>u1175</i>	C(47)...C(51)	637.0(43)	13.5(fixed)	—	-5.7	43.3
<i>u711</i>	H(22)...H(24)	637.1(35)	37.9(fixed)	—	-3.2	31.6
<i>u700</i>	C(10)...C(13)	637.4(33)	13.6(fixed)	—	-3.6	40.5
<i>u1184</i>	C(47)...H(75)	637.6(15)	21.7(fixed)	—	-1.4	13.7
<i>u1183</i>	H(64)...H(77)	638.4(27)	40.5(fixed)	—	-2.8	37.9
<i>u715</i>	C(13)...H(34)	639.6(47)	23.2(fixed)	—	-5.2	45.8
<i>u713</i>	C(7)...H(38)	640.0(25)	24.9(fixed)	—	-9.0	23.7
<i>u725</i>	H(21)...H(36)	640.8(20)	43.3(fixed)	—	-8.9	23.2
<i>u1197</i>	H(68)...H(82)	641.3(13)	37.5(fixed)	—	-7.7	21.7
<i>u693</i>	H(29)...H(35)	641.6(25)	46.3(fixed)	—	-5.8	19.7
<i>u720</i>	H(25)...H(36)	641.8(28)	31.4(fixed)	—	-6.3	20.0
<i>u719</i>	C(10)...H(38)	641.9(27)	20.4(fixed)	—	-7.2	24.9
<i>u721</i>	H(21)...H(26)	642.2(40)	31.6(fixed)	—	-6.5	35.6
<i>u1196</i>	H(61)...H(77)	642.3(26)	35.6(fixed)	—	-5.5	19.4



<i>u1181</i>	C(50)...H(60)	642.5(56)	23.7(fixed)	—	-5.2	49.6
<i>u718</i>	C(12)...H(27)	642.8(25)	19.7(fixed)	—	-5.5	23.5
<i>u710</i>	C(7)...H(41)	642.8(18)	20.0(fixed)	—	-7.5	20.4
<i>u706</i>	C(8)...H(19)	645.0(35)	19.4(fixed)	—	-2.1	31.4
<i>u1190</i>	H(61)...H(79)	645.1(84)	42.4(fixed)	—	-6.4	37.5
<i>u1205</i>	H(69)...H(80)	646.4(47)	29.2(fixed)	—	-8.7	42.4
<i>u1206</i>	H(68)...H(80)	646.7(27)	31.5(fixed)	—	-7.3	23.4
<i>u730</i>	C(6)...H(35)	647.4(65)	27.3(fixed)	—	-5.0	29.2
<i>u1178</i>	H(63)...H(68)	647.5(26)	45.8(fixed)	—	-2.8	31.6
<i>u723</i>	C(12)...H(25)	647.6(40)	23.2(fixed)	—	-6.0	38.7
<i>u747</i>	H(26)...H(39)	649.8(44)	30.0(fixed)	—	-6.5	31.5
<i>u1185</i>	C(48)...H(82)	650.1(23)	19.5(fixed)	—	-8.5	22.9
<i>u1182</i>	C(50)...H(62)	650.1(40)	23.4(fixed)	—	-5.7	31.3
<i>u1198</i>	C(49)...H(77)	650.2(24)	24.4(fixed)	—	-5.7	23.2
<i>u731</i>	C(13)...H(32)	650.3(20)	28.0(fixed)	—	-5.8	19.5
<i>u712</i>	C(9)...H(30)	651.0(20)	22.9(fixed)	—	0.7	27.3
<i>u742</i>	H(32)...H(39)	651.1(31)	35.8(fixed)	—	-0.5	24.8
<i>u736</i>	H(26)...H(38)	651.2(38)	38.7(fixed)	—	-5.2	30.0
<i>u1188</i>	H(63)...H(79)	651.4(42)	31.1(fixed)	—	-5.9	39.5
<i>u729</i>	C(11)...H(18)	651.5(32)	26.0(fixed)	—	0.5	28.0
<i>u737</i>	C(10)...H(39)	651.6(34)	24.8(fixed)	—	3.9	35.8
<i>u744</i>	H(25)...H(39)	651.7(31)	33.4(fixed)	—	-0.6	24.3
<i>u783</i>	H(21)...H(35)	651.9(33)	25.6(fixed)	—	-8.8	23.9
<i>u748</i>	H(20)...H(36)	653.1(22)	30.8(fixed)	—	-0.4	24.4
<i>u740</i>	H(18)...H(35)	653.6(44)	37.7(fixed)	—	-8.7	41.0
<i>u1194</i>	C(47)...H(73)	654.2(38)	27.9(fixed)	—	-5.2	30.8
<i>u1180</i>	H(62)...H(69)	654.5(34)	31.3(fixed)	—	0.7	27.9
<i>u745</i>	C(7)...Br(14)	654.6(46)	15.4(14)	—	-7.4	31.4
<i>u728</i>	C(11)...H(20)	655.0(33)	24.3(fixed)	—	-0.6	26.0
<i>u724</i>	C(8)...H(21)	655.5(32)	23.2(fixed)	—	-2.2	31.1
<i>u1192</i>	H(60)...H(79)	656.3(32)	41.0(fixed)	—	0.6	27.9
<i>u702</i>	H(27)...H(35)	657.0(19)	49.6(fixed)	—	-5.3	23.2
<i>u1201</i>	C(48)...Br(55)	657.0(39)	15.4(tied to u745)	—	-8.3	33.9
<i>u726</i>	H(25)...H(41)	657.4(21)	38.7(fixed)	—	-5.6	22.4
<i>u746</i>	C(12)...Br(16)	657.4(44)	15.4(tied to u745)	—	-6.8	33.4
<i>u727</i>	C(10)...H(40)	657.6(35)	26.6(fixed)	—	-0.3	26.6
<i>u1195</i>	C(47)...H(72)	657.9(41)	27.9(fixed)	—	-5.4	36.5
<i>u743</i>	C(9)...Br(15)	658.2(45)	15.5(tied to u745)	—	-6.7	38.7
<i>u1208</i>	Br(55)...H(60)	658.2(6)	24.7(fixed)	—	-1.5	14.3
<i>u1189</i>	C(48)...H(79)	658.4(27)	22.4(fixed)	—	0.4	28.2
<i>u1202</i>	C(50)...Br(58)	659.2(6)	15.3(tied to u745)	—	-1.5	14.3
<i>u778</i>	H(21)...H(34)	659.7(42)	26.4(fixed)	—	3.8	37.7
<i>u714</i>	C(9)...H(34)	659.7(6)	23.9(fixed)	—	-1.5	14.3
<i>u749</i>	C(8)...Br(17)	660.4(33)	15.3(tied to u745)	—	6.2	38.8

<i>u1193</i>	H(62)...H(77)	660.5(6)	39.5(fixed)	—	-1.5	14.4
<i>u750</i>	H(22)...H(28)	660.5(33)	29.0(fixed)	—	0.4	27.2
<i>u1200</i>	H(59)...H(72)	660.6(40)	38.8(fixed)	—	-4.7	29.0
<i>u733</i>	C(6)...H(33)	661.0(6)	28.2(fixed)	—	-1.5	14.2
<i>u734</i>	C(13)...H(31)	661.8(6)	27.2(fixed)	—	-1.5	14.2
<i>u738</i>	H(22)...H(25)	662.2(25)	36.5(fixed)	—	-0.9	25.7
<i>u754</i>	H(20)...H(38)	663.2(36)	32.6(fixed)	—	-6.8	31.8
<i>u1199</i>	C(49)...H(78)	664.3(48)	25.7(fixed)	—	3.7	35.2
<i>u1203</i>	H(60)...H(77)	664.4(32)	33.9(fixed)	—	1.7	34.2
<i>u732</i>	H(19)...H(38)	664.5(35)	39.9(fixed)	—	-7.5	33.6
<i>u757</i>	Br(16)...H(41)	664.8(25)	23.8(fixed)	—	-9.3	24.7
<i>u765</i>	Br(14)...H(22)	664.8(34)	25.3(fixed)	—	-6.0	25.6
<i>u751</i>	H(26)...H(41)	664.9(45)	31.8(fixed)	—	-7.0	39.9
<i>u716</i>	H(28)...H(34)	666.5(49)	31.4(fixed)	—	-6.9	32.6
<i>u755</i>	H(19)...H(36)	666.5(46)	33.6(fixed)	—	-6.5	26.4
<i>u1207</i>	Br(56)...H(79)	667.1(24)	20.1(fixed)	—	-6.3	23.8
<i>u739</i>	H(31)...H(40)	667.4(35)	37.6(fixed)	—	4.1	37.6
<i>u1204</i>	H(65)...H(77)	669.5(71)	34.2(fixed)	—	1.2	41.4
<i>u752</i>	Br(17)...H(27)	669.5(17)	24.1(fixed)	—	-0.7	25.3
<i>u762</i>	Br(15)...H(29)	670.0(20)	26.9(fixed)	—	-6.0	20.1
<i>u753</i>	H(21)...H(28)	671.0(35)	31.7(fixed)	—	-5.8	24.1
<i>u760</i>	H(32)...H(40)	671.5(73)	41.4(fixed)	—	2.1	43.3
<i>u769</i>	Br(16)...H(36)	671.8(46)	26.8(fixed)	—	-6.4	31.7
<i>u741</i>	H(20)...H(33)	674.0(27)	35.2(fixed)	—	-0.6	26.9
<i>u1209</i>	H(59)...H(73)	674.1(35)	43.3(fixed)	—	-6.2	26.8
<i>u763</i>	H(22)...H(41)	674.8(34)	26.8(fixed)	—	-5.5	23.4
<i>u759</i>	Br(14)...H(19)	675.8(16)	23.4(fixed)	—	0.1	26.8
<i>u1212</i>	Br(56)...H(81)	676.0(16)	26.5(fixed)	—	0.1	26.9
<i>u1211</i>	Br(55)...H(63)	676.3(16)	26.9(fixed)	—	-0.1	27.7
<i>u781</i>	Br(17)...H(26)	676.4(52)	24.9(fixed)	—	1.2	40.9
<i>u1213</i>	Br(55)...H(64)	676.6(30)	27.7(fixed)	—	-5.5	25.9
<i>u766</i>	H(19)...H(26)	676.9(27)	25.9(fixed)	—	-0.8	26.5
<i>u1221</i>	H(59)...H(75)	677.7(31)	25.2(fixed)	—	-0.8	25.4
<i>u794</i>	H(19)...H(30)	677.9(47)	31.9(fixed)	—	-6.1	37.5
<i>u758</i>	H(18)...H(33)	678.4(15)	40.9(fixed)	—	-0.6	24.9
<i>u772</i>	H(27)...H(36)	678.5(40)	26.2(fixed)	—	-10.8	31.9
<i>u768</i>	Br(15)...H(28)	678.6(30)	25.4(fixed)	—	-5.6	26.2
<i>u735</i>	H(21)...H(27)	678.7(39)	37.5(fixed)	—	-6.4	30.2
<i>u1215</i>	Br(56)...H(80)	679.6(28)	25.1(fixed)	—	-0.7	25.1
<i>u770</i>	Br(14)...H(23)	679.8(21)	26.7(fixed)	—	-8.5	25.2
<i>u789</i>	H(21)...H(33)	680.1(25)	23.6(fixed)	—	-7.3	23.6
<i>u767</i>	Br(16)...H(37)	680.4(38)	28.2(fixed)	—	-1.0	35.3
<i>u774</i>	Br(17)...H(24)	680.5(15)	26.6(fixed)	—	-1.0	26.7
<i>u1223</i>	H(67)...H(77)	680.9(32)	31.1(fixed)	—	-1.3	31.1

<i>u761</i>	Br(15)...H(25)	681.2(14)	20.0(fixed)	—	-0.3	28.2
<i>u777</i>	H(20)...H(35)	681.3(40)	35.3(fixed)	—	0.0	37.1
<i>u784</i>	H(32)...H(38)	681.3(16)	24.4(fixed)	—	-0.9	26.6
<i>u756</i>	H(22)...H(27)	682.0(20)	30.2(fixed)	—	-6.3	20.0
<i>u786</i>	H(34)...H(39)	682.5(27)	28.7(fixed)	—	-10.6	25.3
<i>u1210</i>	H(65)...H(78)	682.8(66)	37.1(fixed)	—	-0.5	40.8
<i>u1220</i>	H(60)...H(75)	682.8(22)	28.9(fixed)	—	-9.1	28.7
<i>u785</i>	H(34)...H(40)	683.6(29)	25.7(fixed)	—	-10.5	31.1
<i>u1222</i>	H(71)...H(81)	683.8(64)	25.3(fixed)	—	-1.1	36.3
<i>u776</i>	H(34)...H(41)	683.9(29)	30.4(fixed)	—	-7.0	26.9
<i>u1217</i>	H(61)...H(72)	684.1(26)	40.8(fixed)	—	-8.5	24.4
<i>u782</i>	H(31)...H(39)	685.4(33)	36.3(fixed)	—	-7.7	27.2
<i>u780</i>	H(30)...H(38)	685.8(31)	27.6(fixed)	—	-6.6	26.7
<i>u787</i>	H(29)...H(30)	686.4(22)	25.1(fixed)	—	-10.4	30.4
<i>u1219</i>	H(63)...H(82)	686.7(28)	25.8(fixed)	—	-10.2	25.7
<i>u775</i>	H(27)...H(38)	686.9(15)	26.9(fixed)	—	-8.8	28.9
<i>u1214</i>	H(60)...H(68)	687.3(32)	31.1(fixed)	—	-8.7	29.6
<i>u764</i>	H(19)...H(25)	688.0(18)	26.7(fixed)	—	-8.7	27.6
<i>u771</i>	H(21)...H(41)	689.4(21)	27.2(fixed)	—	-10.0	25.1
<i>u1224</i>	H(61)...H(75)	689.9(22)	26.8(fixed)	—	-8.1	25.8
<i>u790</i>	H(31)...H(38)	690.2(27)	25.8(fixed)	—	-6.0	25.8
<i>u1227</i>	H(66)...H(82)	690.7(21)	32.1(fixed)	—	-8.4	26.8
<i>u797</i>	H(18)...H(30)	692.4(39)	26.3(fixed)	—	-10.6	26.3
<i>u1216</i>	H(60)...H(69)	695.3(25)	29.6(fixed)	—	-7.5	23.3
<i>u1218</i>	H(62)...H(82)	696.7(31)	26.5(fixed)	—	-8.5	28.7
<i>u791</i>	H(27)...H(37)	696.8(26)	23.3(fixed)	—	-6.7	26.5
<i>u795</i>	H(21)...H(38)	696.9(21)	34.2(fixed)	—	-7.4	23.4
<i>u1225</i>	H(64)...H(82)	697.0(29)	23.4(fixed)	—	-7.1	23.1
<i>u773</i>	H(27)...H(30)	697.2(26)	30.1(fixed)	—	-10.0	30.1
<i>u788</i>	H(19)...H(24)	697.9(29)	23.1(fixed)	—	-7.8	23.4
<i>u792</i>	H(23)...H(41)	698.6(30)	23.4(fixed)	—	-7.7	32.1
<i>u779</i>	H(28)...H(30)	699.8(25)	28.7(fixed)	—	-9.4	34.2
<i>u1230</i>	H(65)...H(82)	702.6(34)	26.6(fixed)	—	-9.5	32.1
<i>u800</i>	H(23)...H(38)	706.5(22)	27.4(fixed)	—	-8.5	33.0
<i>u798</i>	H(25)...H(38)	709.4(32)	33.0(fixed)	—	-9.6	26.2
<i>u1226</i>	H(62)...H(68)	709.5(28)	32.1(fixed)	—	-9.5	27.4
<i>u802</i>	C(6)...H(34)	710.0(25)	16.7(fixed)	—	-7.9	26.6
<i>u806</i>	C(11)...H(19)	710.4(39)	16.1(fixed)	—	-10.9	32.6
<i>u1229</i>	H(62)...H(70)	710.4(13)	26.2(fixed)	—	-6.6	16.7
<i>u801</i>	H(25)...H(37)	712.3(36)	28.1(fixed)	—	-10.8	26.6
<i>u1232</i>	C(49)...H(79)	712.8(12)	16.4(fixed)	—	-4.8	16.1
<i>u799</i>	H(29)...H(34)	715.8(27)	26.6(fixed)	—	-8.8	28.1
<i>u1231</i>	C(47)...H(71)	716.1(21)	16.6(fixed)	—	-8.1	31.8
<i>u803</i>	C(13)...H(30)	717.2(12)	16.5(fixed)	—	-6.8	16.6

<i>u</i> 796	H(21)...H(25)	717.2(14)	32.1(fixed)	—	-6.5	16.5
<i>u</i> 793	H(27)...H(34)	717.7(21)	32.6(fixed)	—	-7.6	32.1
<i>u</i> 805	H(21)...H(24)	718.0(11)	26.7(fixed)	—	-5.0	16.4
<i>u</i> 1228	H(62)...H(79)	719.1(24)	31.8(fixed)	—	-8.8	27.4
<i>u</i> 1233	H(64)...H(79)	719.6(14)	27.4(fixed)	—	-5.2	16.2
<i>u</i> 804	C(10)...H(41)	720.6(23)	16.2(fixed)	—	-7.8	26.7
<i>u</i> 808	H(19)...H(35)	729.8(30)	27.1(fixed)	—	-6.0	26.3
<i>u</i> 1234	H(66)...H(77)	731.4(21)	26.0(fixed)	—	-2.7	27.1
<i>u</i> 807	H(20)...H(34)	731.8(22)	26.3(fixed)	—	-5.9	26.3
<i>u</i> 810	H(30)...H(39)	733.2(20)	26.3(fixed)	—	-3.8	26.0
<i>u</i> 813	H(18)...H(34)	738.9(23)	26.7(fixed)	—	-5.3	28.3
<i>u</i> 816	Br(16)...H(38)	739.9(26)	16.8(fixed)	—	-7.6	26.7
<i>u</i> 814	Br(14)...H(21)	740.6(26)	16.7(fixed)	—	-5.0	27.5
<i>u</i> 1237	Br(55)...H(62)	740.7(7)	17.0(fixed)	—	-6.2	16.8
<i>u</i> 817	H(32)...H(41)	740.9(27)	27.5(fixed)	—	-6.6	28.0
<i>u</i> 1236	H(59)...H(71)	741.5(7)	28.0(fixed)	—	-5.2	16.7
<i>u</i> 1235	H(60)...H(72)	742.2(8)	28.3(fixed)	—	-6.2	17.0
<i>u</i> 815	Br(17)...H(25)	743.8(8)	16.9(fixed)	—	-5.3	16.9
<i>u</i> 1238	Br(56)...H(82)	743.9(7)	16.7(fixed)	—	-5.2	16.7
<i>u</i> 812	Br(15)...H(27)	744.8(26)	16.6(fixed)	—	-3.6	27.2
<i>u</i> 811	H(30)...H(40)	744.9(31)	26.9(fixed)	—	-7.1	26.9
<i>u</i> 809	H(31)...H(41)	745.3(7)	27.2(fixed)	—	-5.2	16.6
<i>u</i> 818	H(19)...H(33)	745.9(22)	27.7(fixed)	—	-4.6	27.7
<i>u</i> 1239	H(65)...H(79)	750.4(21)	25.9(fixed)	—	-5.6	25.9
<i>u</i> 820	H(19)...H(34)	784.2(26)	20.0(fixed)	—	-9.2	20.0
<i>u</i> 1240	H(66)...H(79)	792.2(15)	20.1(fixed)	—	-7.9	20.1
<i>u</i> 1241	H(60)...H(71)	792.6(14)	20.2(fixed)	—	-10.8	20.2
<i>u</i> 819	H(30)...H(41)	794.6(15)	19.9(fixed)	—	-9.3	19.9

<sup>a</sup> Distances in pm. Values in parentheses are the standard deviations on the last digits. See Figure 1 for atom numbering.

**Table S13** Least-squares correlation matrix ( $\times 100$ ) for the GED refinement of  $C(\text{SiHMe}_2)_4$  (**1**).<sup>a</sup>

	$p_2$	$p_6$	$p_9$	$p_{10}$	$p_{11}$	$p_{12}$	$p_{13}$	$p_{15}$	$p_{19}$	$p_{25}$	$p_{26}$	$p_{27}$	$p_{28}$	$p_{30}$	$p_{31}$	$p_{32}$	$p_{33}$	$p_{35}$	$p_{38}$	$u_{1016}$	$u_{1082}$	$u_{1859}$	$u_{2037}$	$u_{3698}$	$k_2$	
$p_1$	64																									
$p_2$	100	54	-72	58																						
$p_4$																										-52
$p_6$		100	-74		-60				-55																	
$p_9$			100																		56					
$p_{11}$					100	-62	81	-79		-69	52				87	-56	75	-60								
$p_{12}$						100	-55		-75				84		-52		-56	52								
$p_{13}$							100	-72	80	-66		-52	-78		63	-53	66									
$p_{15}$								100	-78				57	50	-66		-59	54								
$p_{19}$									100	-76			-75	-60	74	-63	66	-64					-51			
$p_{25}$										100			59		-56		-53									
$p_{28}$													100		-67	59	-67	53	50							
$p_{30}$														100	-50											
$u_{362}$																										78
$u_{1016}$																					100	54				
$u_{1859}$																							100	52		

<sup>a</sup> Only absolute values  $\geq 50$  are shown.  $k_2$  is a scale factor.

**Table S14** Least-squares correlation matrix ( $\times 100$ ) for the GED refinement of  $C(\text{SiFMe}_2)_4$  (2).<sup>a</sup>

	$p_2$	$p_7$	$p_9$	$p_{10}$	$u_{151}$	$u_{325}$	$u_{838}$	$u_{1442}$	$u_{1874}$	$u_{2449}$	$k_2$
$p_1$	86			-67							
$p_2$	100			-64			51				
$p_3$					62	52					68
$p_6$		-82	-64								
$p_7$		100	61					70		59	
$p_9$			100							56	
$p_{10}$				100			-68				
$u_{47}$						54					56
$u_{151}$					100	70					83
$u_{325}$						100					90
$u_{646}$											53
$u_{838}$							100				50
$u_{1442}$								100	56		

<sup>a</sup> Only absolute values  $\geq 50$  are shown.  $k_2$  is a scale factor.

**Table S15** Least-squares correlation matrix ( $\times 100$ ) for the GED refinement of  $C(\text{SiClMe}_2)_4$  (3).<sup>a</sup>

	$p_2$	$p_9$	$u_{86}$	$u_{403}$	$u_{784}$	$k_2$
$p_1$	-50	-64				
$p_{10}$				-62	-52	
$u_{73}$			-64			
$u_{91}$						56

<sup>a</sup> Only absolute values  $\geq 50$  are shown.  $k_2$  is a scale factor.

**Table S16** Least-squares correlation matrix ( $\times 100$ ) for the GED refinement of  $C(\text{SiBrMe}_2)_4$  (4).<sup>a</sup>

	$p_8$	$p_9$	$p_{10}$	$u_{60}$	$u_{64}$	$u_{137}$	$u_{298}$	$u_{346}$	$u_{474}$	$k_2$
$p_1$				70						
$p_2$	57					-55				
$p_6$			76			-52	-77			
$p_7$										
$p_8$	100	69					71			
$p_9$		100	-55				61			
$p_{10}$			100				-75	52		
$u_{50}$					55					64
$u_{64}$					100					82
$u_{422}$									60	

<sup>a</sup> Only absolute values  $\geq 50$  are shown.  $k_2$  is a scale factor.

**Table S17** GED-determined coordinates (in Å) for C(SiHMe<sub>2</sub>)<sub>4</sub> (**1**).

Conformer	1			2			
	x	y	z	x	y	z	
C(1)	0.000	0.000	0.000	C(42)	0.000	0.000	0.000
Si(2)	-1.061	-1.568	0.000	Si(43)	-1.894	0.000	0.000
Si(3)	1.061	0.000	1.568	Si(44)	0.688	1.764	0.000
Si(4)	-1.053	1.574	0.000	Si(45)	0.642	-1.054	-1.436
Si(5)	1.053	0.000	-1.574	Si(46)	0.652	-1.052	1.433
C(6)	2.527	-1.184	-1.520	C(47)	2.459	-1.579	1.249
C(7)	1.728	1.700	-2.055	C(48)	-0.350	-2.623	1.759
C(8)	2.535	1.184	1.506	C(49)	2.519	1.882	0.459
C(9)	0.104	0.393	3.152	C(50)	0.470	2.681	-1.640
C(10)	-2.527	1.520	1.184	C(51)	0.591	-2.917	-1.113
C(11)	-1.728	2.055	-1.700	C(52)	2.406	-0.636	-1.976
C(12)	-2.535	-1.506	-1.184	C(53)	-2.669	-1.666	-0.451
C(13)	-0.104	-3.152	-0.393	C(54)	-2.669	0.544	1.638
H(14)	-1.623	-1.736	1.379	H(55)	-2.353	0.980	-1.037
H(15)	-0.180	2.704	0.452	H(56)	-0.248	-0.791	-2.612
H(16)	1.623	-1.379	1.736	H(57)	-0.063	2.550	1.032
H(17)	0.180	-0.452	-2.704	H(58)	0.568	-0.219	2.676
H(18)	2.198	-2.211	-1.327	H(59)	3.112	-0.705	1.140
H(19)	3.071	-1.176	-2.471	H(60)	2.794	-2.144	2.127
H(20)	3.229	-0.900	-0.727	H(61)	2.594	-2.214	0.366
H(21)	2.228	1.662	-3.029	H(62)	-0.002	-3.129	2.667
H(22)	0.920	2.439	-2.118	H(63)	-1.413	-2.389	1.890
H(23)	2.455	2.057	-1.316	H(64)	-0.259	-3.327	0.924
H(24)	2.199	2.227	1.480	H(65)	3.146	1.412	-0.307
H(25)	3.177	1.057	2.386	H(66)	2.832	2.928	0.557
H(26)	3.146	1.003	0.614	H(67)	2.717	1.379	1.413
H(27)	0.758	0.333	4.030	H(68)	0.844	3.709	-1.567
H(28)	-0.319	1.403	3.113	H(69)	1.019	2.178	-2.445
H(29)	-0.721	-0.314	3.296	H(70)	-0.587	2.725	-1.927
H(30)	-3.071	2.471	1.176	H(71)	0.930	-3.477	-1.993
H(31)	-3.229	0.727	0.900	H(72)	1.239	-3.187	-0.271
H(32)	-2.198	1.327	2.211	H(73)	-0.427	-3.246	-0.875
H(33)	-2.455	1.316	-2.057	H(74)	3.127	-0.890	-1.191
H(34)	-2.228	3.029	-1.662	H(75)	2.681	-1.191	-2.880
H(35)	-0.920	2.118	-2.439	H(76)	2.506	0.434	-2.194
H(36)	-3.146	-0.614	-1.003	H(77)	-2.272	-2.037	-1.403
H(37)	-2.199	-1.480	-2.227	H(78)	-2.459	-2.417	0.319
H(38)	-3.177	-2.386	-1.057	H(79)	-3.757	-1.577	-0.550
H(39)	0.319	-3.113	-1.403	H(80)	-2.400	-0.145	2.446
H(40)	0.721	-3.296	0.314	H(81)	-2.325	1.546	1.919
H(41)	-0.758	-4.030	-0.333	H(82)	-3.762	0.569	1.564

Conformer	3			4			
	x	y	z	x	y	z	
C(83)	0.000	0.000	0.000	C(124)	0.000	0.000	0.000
Si(84)	-1.894	0.000	0.000	Si(125)	-1.894	0.000	0.000
Si(85)	0.599	1.797	0.000	Si(126)	0.617	1.790	0.000
Si(86)	0.648	-1.053	-1.434	Si(127)	0.692	-1.043	-1.421
Si(87)	0.686	-1.045	1.423	Si(128)	0.710	-1.039	1.415
C(88)	2.526	-1.454	1.267	C(129)	-0.162	-2.698	1.672
C(89)	-0.223	-2.682	1.690	C(130)	0.727	-0.159	3.090
C(90)	2.412	2.009	0.493	C(131)	2.404	1.994	0.587
C(91)	0.367	2.690	-1.651	C(132)	0.485	2.655	-1.677
C(92)	-0.297	-0.819	-3.056	C(133)	0.623	-2.909	-1.117
C(93)	0.683	-2.910	-1.078	C(134)	2.475	-0.626	-1.892
C(94)	-2.669	-1.598	-0.652	C(135)	-2.669	-1.667	-0.445
C(95)	-2.669	0.339	1.692	C(136)	-2.669	0.550	1.636
H(96)	-2.335	1.104	-0.912	H(137)	-2.338	0.979	-1.044
H(97)	2.064	-0.632	-1.690	H(138)	-0.149	-0.772	-2.631
H(98)	-0.216	2.541	1.014	H(139)	-0.244	2.559	0.955
H(99)	0.527	-0.255	2.686	H(140)	2.136	-1.349	1.076
H(100)	3.125	-0.539	1.193	H(141)	-0.135	-3.300	0.757
H(101)	2.877	-2.018	2.139	H(142)	0.320	-3.274	2.471
H(102)	2.718	-2.058	0.373	H(143)	-1.212	-2.549	1.948
H(103)	0.137	-3.187	2.594	H(144)	1.252	-0.758	3.842
H(104)	-1.301	-2.518	1.802	H(145)	1.232	0.811	3.017
H(105)	-0.070	-3.358	0.841	H(146)	-0.293	0.017	3.450
H(106)	3.077	1.566	-0.258	H(147)	3.103	1.531	-0.119
H(107)	2.670	3.070	0.590	H(148)	2.668	3.054	0.678
H(108)	2.616	1.523	1.454	H(149)	2.550	1.524	1.566
H(109)	0.687	3.736	-1.578	H(150)	0.812	3.699	-1.606
H(110)	0.956	2.211	-2.442	H(151)	1.110	2.156	-2.426
H(111)	-0.685	2.679	-1.958	H(152)	-0.549	2.649	-2.041
H(112)	0.150	-1.416	-3.859	H(153)	0.992	-3.461	-1.989
H(113)	-1.343	-1.128	-2.948	H(154)	1.239	-3.188	-0.255
H(114)	-0.284	0.231	-3.369	H(155)	-0.404	-3.236	-0.920
H(115)	-0.333	-3.307	-0.969	H(156)	3.166	-0.889	-1.083
H(116)	1.174	-3.456	-1.893	H(157)	2.782	-1.174	-2.790
H(117)	1.230	-3.121	-0.152	H(158)	2.586	0.446	-2.096
H(118)	-2.272	-1.849	-1.642	H(159)	-2.272	-2.042	-1.396
H(119)	-2.459	-2.437	0.020	H(160)	-2.459	-2.415	0.328
H(120)	-3.757	-1.498	-0.739	H(161)	-3.757	-1.579	-0.544
H(121)	-2.400	-0.445	2.410	H(162)	-2.400	-0.137	2.447
H(122)	-2.325	1.299	2.095	H(163)	-2.325	1.553	1.914
H(123)	-3.762	0.373	1.622	H(164)	-3.762	0.575	1.562



Conformer	5			6			
	x	y	z	x	y	z	
C(165)	0.000	0.000	0.000	C(206)	0.000	0.000	0.000
Si(166)	-1.061	-1.568	0.000	Si(207)	-1.894	0.000	0.000
Si(167)	-1.061	1.568	0.000	Si(208)	0.753	1.738	0.000
Si(168)	1.061	0.000	1.568	Si(209)	0.661	-1.050	-1.431
Si(169)	1.061	0.000	-1.568	Si(210)	0.661	-1.050	1.431
C(170)	0.116	-0.449	-3.144	C(211)	2.454	-1.613	1.215
C(171)	2.568	-1.141	-1.485	C(212)	-0.364	-2.598	1.793
C(172)	-2.568	1.485	1.141	C(213)	0.781	2.570	-1.698
C(173)	-0.116	3.144	0.449	C(214)	-0.084	2.945	1.192
C(174)	0.116	0.449	3.144	C(215)	0.558	-2.915	-1.134
C(175)	2.568	1.141	1.485	C(216)	2.449	-0.665	-1.913
C(176)	-2.568	-1.485	-1.141	C(217)	-2.669	-1.613	-0.612
C(177)	-0.116	-3.144	-0.449	C(218)	-2.669	0.381	1.683
H(178)	-1.581	-1.756	1.393	H(219)	-2.355	1.076	-0.935
H(179)	1.581	-1.393	1.756	H(220)	-0.189	-0.750	-2.628
H(180)	-1.581	1.756	-1.393	H(221)	2.180	1.620	0.443
H(181)	1.581	1.393	-1.756	H(222)	0.616	-0.199	2.663
H(182)	-0.729	0.232	-3.301	H(223)	3.121	-0.753	1.083
H(183)	0.768	-0.387	-4.023	H(224)	2.796	-2.175	2.091
H(184)	-0.279	-1.470	-3.086	H(225)	2.558	-2.260	0.336
H(185)	3.205	-1.013	-2.367	H(226)	-0.006	-3.101	2.699
H(186)	3.173	-0.926	-0.596	H(227)	-1.419	-2.343	1.943
H(187)	2.261	-2.192	-1.439	H(228)	-0.303	-3.312	0.963
H(188)	-2.261	1.439	2.192	H(229)	-0.236	2.781	-2.048
H(189)	-3.205	2.367	1.013	H(230)	1.330	3.518	-1.661
H(190)	-3.173	0.596	0.926	H(231)	1.267	1.927	-2.441
H(191)	-0.768	4.023	0.387	H(232)	0.421	3.917	1.183
H(192)	0.279	3.086	1.470	H(233)	-1.132	3.106	0.914
H(193)	0.729	3.301	-0.232	H(234)	-0.061	2.561	2.218
H(194)	0.768	0.387	4.023	H(235)	0.910	-3.471	-2.011
H(195)	-0.279	1.470	3.086	H(236)	1.175	-3.210	-0.277
H(196)	-0.729	-0.232	3.301	H(237)	-0.474	-3.224	-0.931
H(197)	2.261	2.192	1.439	H(238)	3.140	-0.946	-1.110
H(198)	3.205	1.013	2.367	H(239)	2.738	-1.216	-2.816
H(199)	3.173	0.926	0.596	H(240)	2.579	0.405	-2.113
H(200)	-3.173	-0.596	-0.926	H(241)	-2.272	-1.890	-1.595
H(201)	-2.261	-1.439	-2.192	H(242)	-2.459	-2.436	0.081
H(202)	-3.205	-2.367	-1.013	H(243)	-3.757	-1.516	-0.701
H(203)	0.279	-3.086	-1.470	H(244)	-2.400	-0.384	2.420
H(204)	0.729	-3.301	0.232	H(245)	-2.325	1.351	2.062
H(205)	-0.768	-4.023	-0.387	H(246)	-3.762	0.413	1.612

Conformer	7			8			
	x	y	z	x	y	z	
C(247)	0.000	0.000	0.000	C(288)	0.000	0.000	0.000
Si(248)	-1.894	0.000	0.000	Si(289)	-1.053	-1.574	0.000
Si(249)	0.747	1.740	0.000	Si(290)	-1.105	1.538	0.000
Si(250)	0.759	-1.027	-1.399	Si(291)	1.105	0.000	-1.538
Si(251)	0.819	-1.010	1.377	Si(292)	1.053	0.000	1.574
C(252)	0.911	-0.119	3.042	C(293)	1.706	-1.705	2.070
C(253)	2.569	-1.600	0.968	C(294)	0.181	0.719	3.090
C(254)	0.809	2.557	-1.705	C(295)	-1.875	1.939	-1.680
C(255)	-0.119	2.955	1.163	C(296)	-2.519	1.476	1.255
C(256)	2.594	-0.685	-1.703	C(297)	2.519	-1.255	-1.476
C(257)	-0.121	-0.839	-3.063	C(298)	1.875	1.680	-1.939
C(258)	-2.669	-1.631	-0.562	C(299)	-0.181	-3.090	-0.719
C(259)	-2.669	0.432	1.671	C(300)	-1.706	-2.070	1.705
H(260)	-2.348	1.049	-0.969	H(301)	-2.248	-1.308	-0.864
H(261)	0.636	-2.463	-0.991	H(302)	0.250	-0.372	-2.711
H(262)	2.160	1.600	0.477	H(303)	-0.250	2.711	0.372
H(263)	-0.025	-2.233	1.575	H(304)	2.248	0.864	1.308
H(264)	-0.087	0.179	3.383	H(305)	2.298	-2.148	1.260
H(265)	1.351	-0.767	3.809	H(306)	2.344	-1.637	2.958
H(266)	1.527	0.785	2.969	H(307)	0.880	-2.389	2.298
H(267)	2.947	-2.274	1.746	H(308)	0.871	0.802	3.937
H(268)	2.588	-2.140	0.015	H(309)	-0.214	1.719	2.877
H(269)	3.260	-0.753	0.891	H(310)	-0.657	0.083	3.398
H(270)	-0.201	2.762	-2.078	H(311)	-2.592	1.165	-1.977
H(271)	1.353	3.507	-1.665	H(312)	-2.405	2.898	-1.650
H(272)	1.312	1.909	-2.432	H(313)	-1.106	2.003	-2.459
H(273)	0.383	3.929	1.156	H(314)	-3.095	2.409	1.242
H(274)	-1.162	3.110	0.861	H(315)	-3.206	0.652	1.030
H(275)	-0.117	2.581	2.193	H(316)	-2.135	1.330	2.271
H(276)	2.989	-1.339	-2.489	H(317)	3.095	-1.242	-2.409
H(277)	2.753	0.354	-2.015	H(318)	3.206	-1.030	-0.652
H(278)	3.181	-0.858	-0.793	H(319)	2.135	-2.271	-1.330
H(279)	0.001	0.176	-3.458	H(320)	2.592	1.977	-1.165
H(280)	0.285	-1.540	-3.801	H(321)	2.405	1.650	-2.898
H(281)	-1.194	-1.037	-2.963	H(322)	1.106	2.459	-2.003
H(282)	-2.272	-1.938	-1.537	H(323)	0.214	-2.877	-1.719
H(283)	-2.459	-2.433	0.155	H(324)	0.657	-3.398	-0.083
H(284)	-3.757	-1.537	-0.655	H(325)	-0.871	-3.937	-0.802
H(285)	-2.400	-0.310	2.431	H(326)	-0.880	-2.298	2.389
H(286)	-2.325	1.413	2.019	H(327)	-2.298	-1.260	2.148
H(287)	-3.762	0.462	1.599	H(328)	-2.344	-2.958	1.637

Conformer	9		
	x	y	z
C(329)	0.000	0.000	0.000
Si(330)	-1.061	-1.568	0.000
Si(331)	1.061	0.000	1.568
Si(332)	-1.064	1.567	0.000
Si(333)	1.064	0.000	-1.567
C(334)	1.783	1.691	-2.015
C(335)	0.177	-0.648	-3.106
C(336)	2.569	1.140	1.484
C(337)	0.116	0.450	3.144
C(338)	-1.783	2.015	-1.691
C(339)	-0.177	3.106	0.648
C(340)	-2.569	-1.484	-1.140
C(341)	-0.116	-3.144	-0.450
H(342)	-1.576	-1.750	1.395
H(343)	-2.225	1.317	0.914
H(344)	1.576	-1.395	1.750
H(345)	2.225	-0.914	-1.317
H(346)	2.385	2.091	-1.191
H(347)	2.426	1.621	-2.900
H(348)	0.986	2.411	-2.231
H(349)	0.870	-0.735	-3.950
H(350)	-0.257	-1.637	-2.921
H(351)	-0.635	0.027	-3.403
H(352)	2.262	2.191	1.438
H(353)	3.206	1.012	2.366
H(354)	3.173	0.924	0.596
H(355)	0.768	0.389	4.023
H(356)	-0.278	1.472	3.086
H(357)	-0.729	-0.229	3.301
H(358)	-2.426	2.900	-1.621
H(359)	-0.986	2.231	-2.411
H(360)	-2.385	1.191	-2.091
H(361)	0.635	3.403	-0.027
H(362)	-0.870	3.950	0.735
H(363)	0.257	2.921	1.637
H(364)	-3.173	-0.596	-0.924
H(365)	-2.262	-1.438	-2.191
H(366)	-3.206	-2.366	-1.012
H(367)	0.278	-3.086	-1.472
H(368)	0.729	-3.301	0.229
H(369)	-0.768	-4.023	-0.389

**Table S18** GED-determined coordinates (in Å) for C(SiFMe<sub>2</sub>)<sub>4</sub> (2).

Conformer	1			2			
	x	y	z	x	y	z	
C(1)	0.000	0.000	0.000	C(42)	0.000	0.000	0.000
Si(2)	-1.893	0.000	0.000	Si(43)	-1.893	0.000	0.000
Si(3)	0.631	1.784	0.000	Si(44)	0.709	1.755	0.000
Si(4)	0.670	-0.936	-1.502	Si(45)	0.581	-0.952	-1.529
Si(5)	0.682	-0.933	1.499	Si(46)	0.664	-0.937	1.504
C(6)	2.403	-0.397	1.975	C(47)	-0.208	-0.489	3.091
C(7)	0.633	-2.794	1.391	C(48)	2.507	-0.843	1.776
C(8)	-0.098	2.907	-1.298	C(49)	0.631	2.666	1.625
C(9)	0.492	2.611	1.666	C(50)	2.450	1.842	-0.663
C(10)	0.937	0.159	-2.988	C(51)	0.451	0.039	-3.103
C(11)	-0.298	-2.442	-2.023	C(52)	-0.203	-2.623	-1.796
C(12)	-2.708	-1.591	0.530	C(53)	-2.708	-1.564	0.604
C(13)	-2.625	1.412	0.973	C(54)	-2.625	1.456	0.906
F(14)	-2.306	0.218	-1.537	F(55)	-2.316	0.145	-1.543
F(15)	2.112	-1.472	-1.041	F(56)	2.142	-1.233	-1.274
F(16)	2.198	1.699	-0.341	F(57)	-0.203	2.613	-1.006
F(17)	-0.304	-0.523	2.699	F(58)	0.363	-2.495	1.254
H(18)	2.414	0.679	2.167	H(59)	-1.281	-0.664	2.984
H(19)	2.718	-0.927	2.878	H(60)	0.177	-1.102	3.909
H(20)	3.099	-0.625	1.164	H(61)	-0.036	0.566	3.320
H(21)	0.956	-3.228	2.341	H(62)	2.791	-1.494	2.606
H(22)	-0.386	-3.125	1.174	H(63)	3.030	-1.164	0.871
H(23)	1.299	-3.136	0.595	H(64)	2.793	0.186	2.010
H(24)	-1.165	3.049	-1.107	H(65)	1.270	2.168	2.358
H(25)	0.404	3.877	-1.271	H(66)	0.974	3.695	1.488
H(26)	0.034	2.461	-2.288	H(67)	-0.398	2.676	1.994
H(27)	0.924	3.614	1.618	H(68)	2.781	2.883	-0.693
H(28)	-0.560	2.686	1.954	H(69)	3.120	1.270	-0.016
H(29)	1.029	2.024	2.415	H(70)	2.482	1.425	-1.672
H(30)	1.378	-0.424	-3.801	H(71)	0.854	-0.540	-3.938
H(31)	-0.019	0.571	-3.320	H(72)	-0.597	0.277	-3.303
H(32)	1.611	0.979	-2.726	H(73)	1.018	0.968	-3.002
H(33)	-1.289	-2.141	-2.373	H(74)	-1.269	-2.501	-2.002
H(34)	0.227	-2.957	-2.831	H(75)	0.273	-3.123	-2.644
H(35)	-0.407	-3.122	-1.175	H(76)	-0.078	-3.237	-0.900
H(36)	-2.332	-2.419	-0.077	H(77)	-2.332	-2.420	0.036
H(37)	-2.486	-1.787	1.582	H(78)	-2.486	-1.711	1.664
H(38)	-3.790	-1.512	0.399	H(79)	-3.790	-1.492	0.470
H(39)	-2.346	1.319	2.026	H(80)	-2.346	1.413	1.961
H(40)	-2.251	2.362	0.584	H(81)	-2.251	2.387	0.472
H(41)	-3.715	1.393	0.887	H(82)	-3.715	1.433	0.821

Conformer	3			4			
	x	y	z	x	y	z	
C(83)	0.000	0.000	0.000	C(124)	0.000	0.000	0.000
Si(84)	-1.082	-1.553	0.000	Si(125)	-1.082	-1.553	0.000
Si(85)	-1.088	1.549	0.000	Si(126)	-1.138	1.512	0.000
Si(86)	1.082	0.000	-1.553	Si(127)	1.082	0.000	1.553
Si(87)	1.088	0.000	1.549	Si(128)	1.138	0.000	-1.512
C(88)	1.762	1.687	1.971	C(129)	0.306	0.632	-3.056
C(89)	2.485	-1.235	1.564	C(130)	1.984	-1.617	-1.896
C(90)	-2.485	1.564	-1.235	C(131)	-1.984	1.896	1.617
C(91)	-1.762	1.971	1.687	C(132)	-0.306	3.056	-0.632
C(92)	2.596	1.077	-1.391	C(133)	2.700	-0.898	1.318
C(93)	0.214	0.408	-3.152	C(134)	0.268	-0.612	3.114
C(94)	-0.214	-3.152	0.408	C(135)	-0.268	-3.114	0.612
C(95)	-2.596	-1.391	1.077	C(136)	-2.700	-1.318	0.898
F(96)	-1.607	-1.724	-1.508	F(137)	-1.443	-1.830	-1.541
F(97)	1.607	-1.508	-1.724	F(138)	1.443	1.541	1.830
F(98)	-0.104	2.744	-0.430	F(139)	-2.313	1.153	-1.035
F(99)	0.104	-0.430	2.744	F(140)	2.313	1.035	-1.153
H(100)	0.938	2.394	2.092	H(141)	-0.083	1.638	-2.880
H(101)	2.330	1.634	2.903	H(142)	1.026	0.664	-3.877
H(102)	2.418	2.033	1.168	H(143)	-0.520	-0.030	-3.328
H(103)	2.983	-1.216	2.537	H(144)	2.687	-1.479	-2.722
H(104)	2.093	-2.238	1.380	H(145)	2.528	-1.967	-1.015
H(105)	3.209	-0.983	0.785	H(146)	1.239	-2.365	-2.179
H(106)	-3.209	0.785	-0.983	H(147)	-1.239	2.179	2.365
H(107)	-2.983	2.537	-1.216	H(148)	-2.687	2.722	1.479
H(108)	-2.093	1.380	-2.238	H(149)	-2.528	1.015	1.967
H(109)	-2.330	2.903	1.634	H(150)	-1.026	3.877	-0.664
H(110)	-2.418	1.168	2.033	H(151)	0.520	3.328	0.030
H(111)	-0.938	2.092	2.394	H(152)	0.083	2.880	-1.638
H(112)	3.209	0.990	-2.291	H(153)	3.304	-0.813	2.225
H(113)	2.295	2.120	-1.260	H(154)	2.509	-1.954	1.110
H(114)	3.183	0.761	-0.525	H(155)	3.247	-0.459	0.480
H(115)	-0.138	1.442	-3.127	H(156)	0.026	-1.673	3.013
H(116)	0.906	0.284	-3.989	H(157)	0.946	-0.478	3.961
H(117)	-0.640	-0.260	-3.289	H(158)	-0.651	-0.049	3.297
H(118)	0.640	-3.289	-0.260	H(159)	0.651	-3.297	0.049
H(119)	0.138	-3.127	1.442	H(160)	-0.026	-3.013	1.673
H(120)	-0.906	-3.989	0.284	H(161)	-0.946	-3.961	0.478
H(121)	-2.295	-1.260	2.120	H(162)	-2.509	-1.110	1.954
H(122)	-3.183	-0.525	0.761	H(163)	-3.247	-0.480	0.459
H(123)	-3.209	-2.291	0.990	H(164)	-3.304	-2.225	0.813

Conformer	5			6			
	x	y	z	x	y	z	
C(165)	0.000	0.000	0.000	C(206)	0.000	0.000	0.000
Si(166)	-1.082	-1.553	0.000	Si(207)	-1.893	0.000	0.000
Si(167)	-1.097	1.542	0.000	Si(208)	0.632	1.784	0.000
Si(168)	1.082	0.000	-1.553	Si(209)	0.689	-0.932	-1.496
Si(169)	1.097	0.000	1.542	Si(210)	0.640	-0.942	1.512
C(170)	2.541	-1.173	1.414	C(211)	2.329	-0.377	2.066
C(171)	0.224	-0.287	3.164	C(212)	0.635	-2.802	1.376
C(172)	-0.224	3.164	-0.287	C(213)	-0.022	2.881	-1.359
C(173)	-2.541	1.414	-1.173	C(214)	0.400	2.643	1.639
C(174)	2.600	1.071	-1.388	C(215)	-0.333	-2.419	-1.968
C(175)	0.216	0.416	-3.151	C(216)	2.481	-1.436	-1.388
C(176)	-0.216	-3.151	0.416	C(217)	-2.708	-1.595	0.519
C(177)	-2.600	-1.388	1.071	C(218)	-2.625	1.405	0.983
F(178)	-1.607	-1.738	-1.507	F(219)	-2.334	0.227	-1.527
F(179)	1.607	-1.507	-1.738	F(220)	0.624	0.064	-2.755
F(180)	-1.715	1.648	1.479	F(221)	2.215	1.681	-0.252
F(181)	1.715	1.479	1.648	F(222)	-0.386	-0.587	2.695
H(182)	3.137	-0.930	0.530	H(223)	2.309	0.696	2.273
H(183)	3.168	-1.085	2.305	H(224)	2.618	-0.914	2.973
H(184)	2.177	-2.200	1.330	H(225)	3.061	-0.579	1.280
H(185)	0.930	-0.169	3.990	H(226)	0.929	-3.242	2.333
H(186)	-0.587	0.437	3.280	H(227)	-0.367	-3.150	1.113
H(187)	-0.191	-1.298	3.187	H(228)	1.340	-3.117	0.603
H(188)	0.191	3.187	-1.298	H(229)	-1.098	3.026	-1.231
H(189)	-0.930	3.990	-0.169	H(230)	0.478	3.852	-1.323
H(190)	0.587	3.280	0.437	H(231)	0.164	2.416	-2.331
H(191)	-3.168	2.305	-1.085	H(232)	0.835	3.645	1.595
H(192)	-2.177	1.330	-2.200	H(233)	-0.666	2.724	1.866
H(193)	-3.137	0.530	-0.930	H(234)	0.894	2.071	2.428
H(194)	3.213	0.984	-2.289	H(235)	0.079	-2.879	-2.870
H(195)	2.303	2.114	-1.254	H(236)	-0.321	-3.148	-1.154
H(196)	3.186	0.750	-0.523	H(237)	-1.364	-2.111	-2.160
H(197)	-0.132	1.451	-3.123	H(238)	2.611	-2.171	-0.590
H(198)	0.907	0.291	-3.988	H(239)	2.799	-1.876	-2.337
H(199)	-0.641	-0.248	-3.290	H(240)	3.099	-0.560	-1.174
H(200)	0.641	-3.290	-0.248	H(241)	-2.332	-2.418	-0.094
H(201)	0.132	-3.123	1.451	H(242)	-2.486	-1.798	1.570
H(202)	-0.907	-3.988	0.291	H(243)	-3.790	-1.515	0.389
H(203)	-2.303	-1.254	2.114	H(244)	-2.346	1.305	2.034
H(204)	-3.186	-0.523	0.750	H(245)	-2.251	2.358	0.600
H(205)	-3.213	-2.289	0.984	H(246)	-3.715	1.387	0.897

Conformer	7		
	x	y	z
C(247)	0.000	0.000	0.000
Si(248)	-1.893	0.000	0.000
Si(249)	0.668	1.771	0.000
Si(250)	0.616	-0.946	-1.519
Si(251)	0.681	-0.934	1.499
C(252)	-0.185	-0.495	3.091
C(253)	2.524	-0.824	1.759
C(254)	-0.147	2.950	-1.193
C(255)	0.695	2.544	1.697
C(256)	0.738	0.118	-3.045
C(257)	-0.314	-2.507	-1.939
C(258)	-2.708	-1.604	0.489
C(259)	-2.625	1.387	1.009
F(260)	-2.319	0.257	-1.527
F(261)	2.110	-1.425	-1.178
F(262)	2.198	1.677	-0.481
F(263)	0.382	-2.488	1.227
H(264)	-1.258	-0.679	2.990
H(265)	0.210	-1.106	3.906
H(266)	-0.022	0.561	3.321
H(267)	2.820	-1.474	2.587
H(268)	3.045	-1.139	0.851
H(269)	2.803	0.207	1.994
H(270)	0.596	3.337	-1.895
H(271)	-0.931	2.429	-1.748
H(272)	-0.590	3.784	-0.642
H(273)	0.348	1.819	2.438
H(274)	1.713	2.853	1.945
H(275)	0.039	3.418	1.714
H(276)	1.153	-0.466	-3.871
H(277)	-0.255	0.479	-3.324
H(278)	1.389	0.974	-2.848
H(279)	-1.337	-2.260	-2.232
H(280)	0.183	-3.021	-2.767
H(281)	-0.338	-3.168	-1.069
H(282)	-2.332	-2.416	-0.139
H(283)	-2.486	-1.827	1.536
H(284)	-3.790	-1.522	0.361
H(285)	-2.346	1.267	2.059
H(286)	-2.251	2.346	0.644
H(287)	-3.715	1.370	0.923

**Table S19** GED-determined coordinates (in Å) for C(SiClMe<sub>2</sub>)<sub>4</sub> (**3**).

Conformer	1			2		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C(1)	0.000	0.000	0.000	C(42)	0.000	0.000
Si(2)	-1.920	0.000	0.000	Si(43)	-1.125	-1.548
Si(3)	0.665	1.799	0.000	Si(44)	1.125	0.000
Si(4)	0.680	-0.943	-1.524	Si(45)	-1.132	1.557
Si(5)	0.642	-0.955	1.543	Si(46)	1.132	0.000
C(6)	0.681	0.111	3.112	C(47)	2.525	-1.281
C(7)	2.321	-1.800	1.331	C(48)	1.896	1.687
C(8)	0.791	2.622	-1.704	C(49)	2.604	1.167
C(9)	-0.291	2.989	1.120	C(50)	0.241	0.385
C(10)	2.525	-0.634	-1.836	C(51)	-2.525	1.480
C(11)	-0.230	-0.523	-3.133	C(52)	-1.896	1.953
C(12)	-2.729	-1.581	-0.647	C(53)	-2.604	-1.407
C(13)	-2.683	0.391	1.690	C(54)	-0.241	-3.182
Cl(14)	-2.543	1.531	-1.280	Cl(55)	-1.927	-1.805
Cl(15)	0.448	-2.976	-1.228	Cl(56)	0.014	3.220
Cl(16)	2.627	1.746	0.709	Cl(57)	1.927	-1.895
Cl(17)	-0.659	-2.526	1.952	Cl(58)	-0.014	-0.503
H(18)	-0.323	0.533	3.319	H(59)	2.109	-2.296
H(19)	0.994	-0.496	3.985	H(60)	3.102	-1.283
H(20)	1.396	0.949	2.994	H(61)	3.218	-1.051
H(21)	2.584	-2.373	2.243	H(62)	2.486	1.635
H(22)	2.297	-2.500	0.472	H(63)	1.104	2.452
H(23)	3.114	-1.048	1.148	H(64)	2.568	2.011
H(24)	-0.213	2.722	-2.161	H(65)	2.261	2.217
H(25)	1.238	3.632	-1.614	H(66)	3.250	1.082
H(26)	1.426	2.016	-2.381	H(67)	3.209	0.919
H(27)	0.187	3.989	1.121	H(68)	0.946	0.301
H(28)	-1.336	3.099	0.767	H(69)	-0.170	1.415
H(29)	-0.312	2.609	2.161	H(70)	-0.595	-0.324
H(30)	2.882	-1.251	-2.684	H(71)	-3.102	2.426
H(31)	2.703	0.433	-2.077	H(72)	-3.218	0.646
H(32)	3.118	-0.895	-0.937	H(73)	-2.109	1.321
H(33)	-0.093	0.547	-3.387	H(74)	-2.568	1.133
H(34)	0.160	-1.136	-3.970	H(75)	-2.486	2.890
H(35)	-1.315	-0.723	-3.027	H(76)	-1.104	2.079
H(36)	-2.380	-1.803	-1.675	H(77)	-3.209	-0.513
H(37)	-2.474	-2.441	0.004	H(78)	-2.261	-1.320
H(38)	-3.832	-1.472	-0.667	H(79)	-3.250	-2.303
H(39)	-2.418	-0.395	2.426	H(80)	0.170	-3.167
H(40)	-2.312	1.365	2.067	H(81)	0.595	-3.347
H(41)	-3.788	0.441	1.614	H(82)	-0.946	-4.033



**Table S20** GED-determined coordinates (in Å) for C(SiBrMe<sub>2</sub>)<sub>4</sub> (**4**).

Conformer	1			2			
	x	y	z	x	y	z	
C(1)	0.000	0.000	0.000	C(42)	0.000	0.000	0.000
Si(2)	-1.911	0.000	0.000	Si(43)	-1.135	-1.544	0.000
Si(3)	0.602	1.813	0.000	Si(44)	1.135	0.000	1.544
Si(4)	0.685	-0.936	-1.523	Si(45)	-1.128	1.535	0.000
Si(5)	0.633	-0.941	1.531	Si(46)	1.128	0.000	-1.535
C(6)	0.629	0.020	3.126	C(47)	2.455	-1.301	-1.580
C(7)	2.261	-1.821	1.401	C(48)	1.889	1.626	-2.015
C(8)	0.779	2.684	-1.630	C(49)	2.735	0.945	1.394
C(9)	-0.267	2.997	1.140	C(50)	0.372	0.445	3.176
C(10)	2.521	-0.832	-1.786	C(51)	-2.455	1.580	1.301
C(11)	-0.176	-0.605	-3.135	C(52)	-1.889	2.015	-1.626
C(12)	-2.794	-1.481	-0.701	C(53)	-2.735	-1.394	-0.945
C(13)	-2.737	0.417	1.611	C(54)	-0.372	-3.176	-0.445
Br(14)	-2.599	1.672	-1.383	Br(55)	-1.857	-1.942	2.100
Br(15)	0.366	-3.145	-1.256	Br(56)	0.107	3.366	0.505
Br(16)	2.733	1.836	0.787	Br(57)	1.857	-2.100	1.942
Br(17)	-0.771	-2.659	1.988	Br(58)	-0.107	-0.505	-3.366
H(18)	-0.378	0.377	3.355	H(59)	2.015	-2.298	-1.505
H(19)	0.969	-0.609	3.952	H(60)	3.018	-1.240	-2.514
H(20)	1.293	0.885	3.053	H(61)	3.150	-1.166	-0.748
H(21)	2.481	-2.357	2.328	H(62)	2.474	1.519	-2.932
H(22)	2.241	-2.542	0.581	H(63)	1.113	2.376	-2.186
H(23)	3.068	-1.108	1.215	H(64)	2.551	1.987	-1.224
H(24)	-0.190	2.763	-2.128	H(65)	2.537	2.007	1.229
H(25)	1.176	3.691	-1.484	H(66)	3.327	0.842	2.307
H(26)	1.461	2.135	-2.284	H(67)	3.324	0.568	0.555
H(27)	0.189	3.988	1.081	H(68)	1.112	0.369	3.977
H(28)	-1.322	3.084	0.869	H(69)	-0.009	1.468	3.154
H(29)	-0.203	2.648	2.174	H(70)	-0.457	-0.229	3.407
H(30)	2.817	-1.428	-2.653	H(71)	-3.018	2.514	1.240
H(31)	2.825	0.203	-1.958	H(72)	-3.150	0.748	1.166
H(32)	3.054	-1.209	-0.910	H(73)	-2.015	1.505	2.298
H(33)	-0.072	0.447	-3.415	H(74)	-2.551	1.224	-1.987
H(34)	0.254	-1.218	-3.931	H(75)	-2.474	2.932	-1.519
H(35)	-1.240	-0.838	-3.055	H(76)	-1.113	2.186	-2.376
H(36)	-2.488	-1.655	-1.735	H(77)	-3.324	-0.555	-0.568
H(37)	-2.563	-2.376	-0.117	H(78)	-2.537	-1.229	-2.007
H(38)	-3.876	-1.326	-0.682	H(79)	-3.327	-2.307	-0.842
H(39)	-2.480	-0.321	2.374	H(80)	0.009	-3.154	-1.468
H(40)	-2.418	1.402	1.960	H(81)	0.457	-3.407	0.229
H(41)	-3.823	0.427	1.492	H(82)	-1.112	-3.977	-0.369

**Table S21** Calculated coordinates [MP2/aug-cc-pVDZ; in Å] for all nine conformers of C(SiHMe<sub>2</sub>)<sub>4</sub> (**1**).<sup>a</sup>

Conformer	1			2			
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>	
C(1)	0.000	0.000	-0.075	C(42)	0.135	-0.057	-0.007
Si(2)	1.088	-1.098	-1.201	Si(43)	1.638	-1.152	0.462
Si(3)	-1.090	1.103	-1.194	Si(44)	-0.740	0.508	1.590
Si(4)	1.111	1.089	1.036	Si(45)	-1.004	-1.098	-1.132
Si(5)	-1.109	-1.094	1.032	Si(46)	0.793	1.449	-0.985
C(6)	-2.589	-1.842	0.106	C(47)	1.471	2.820	0.141
C(7)	-1.813	-0.159	2.530	C(48)	-0.501	2.222	-2.138
C(8)	-2.531	1.921	-0.267	C(49)	-1.969	1.931	1.313
C(9)	-0.121	2.502	-2.032	C(50)	-1.684	-0.899	2.445
C(10)	2.588	1.843	0.111	C(51)	-2.763	-0.400	-1.303
C(11)	1.819	0.146	2.527	C(52)	-1.201	-2.891	-0.534
C(12)	2.531	-1.919	-0.280	C(53)	2.346	-2.076	-1.038
C(13)	0.117	-2.493	-2.044	C(54)	3.064	-0.170	1.234
H(14)	1.659	-0.223	-2.281	H(55)	1.178	-2.159	1.477
H(15)	0.268	2.222	1.553	H(56)	-0.382	-1.120	-2.499
H(16)	-1.664	0.233	-2.276	H(57)	0.312	0.994	2.545
H(17)	-0.267	-2.231	1.540	H(58)	1.928	0.968	-1.843
H(18)	-2.284	-2.504	-0.716	H(59)	2.247	2.451	0.827
H(19)	-3.189	-2.435	0.817	H(60)	1.919	3.609	-0.488
H(20)	-3.245	-1.062	-0.314	H(61)	0.680	3.288	0.747
H(21)	-2.316	-0.880	3.197	H(62)	-0.045	3.079	-2.662
H(22)	-1.050	0.371	3.120	H(63)	-0.856	1.513	-2.903
H(23)	-2.563	0.581	2.210	H(64)	-1.373	2.595	-1.577
H(24)	-2.164	2.499	0.598	H(65)	-2.789	1.628	0.643
H(25)	-3.039	2.622	-0.951	H(66)	-2.414	2.213	2.283
H(26)	-3.283	1.202	0.092	H(67)	-1.499	2.832	0.889
H(27)	-0.776	2.992	-2.772	H(68)	-2.046	-0.548	3.426
H(28)	0.185	3.268	-1.301	H(69)	-2.564	-1.210	1.859
H(29)	0.776	2.139	-2.558	H(70)	-1.049	-1.782	2.612
H(30)	3.191	2.430	0.825	H(71)	-3.306	-0.996	-2.056
H(31)	3.242	1.067	-0.317	H(72)	-3.319	-0.482	-0.355
H(32)	2.281	2.513	-0.704	H(73)	-2.780	0.651	-1.624
H(33)	2.575	-0.586	2.202	H(74)	-1.712	-2.924	0.441
H(34)	2.317	0.864	3.201	H(75)	-1.824	-3.442	-1.260
H(35)	1.060	-0.394	3.111	H(76)	-0.247	-3.430	-0.431
H(36)	3.284	-1.201	0.078	H(77)	1.615	-2.723	-1.545
H(37)	2.167	-2.500	0.583	H(78)	2.734	-1.360	-1.780
H(38)	3.037	-2.618	-0.968	H(79)	3.188	-2.709	-0.707
H(39)	-0.188	-3.261	-1.314	H(80)	3.534	0.503	0.498
H(40)	-0.780	-2.128	-2.567	H(81)	2.743	0.428	2.102
H(41)	0.772	-2.980	-2.786	H(82)	3.836	-0.879	1.577

Conformer	3			4			
	x	y	z	x	y	z	
C(83)	0.140	0.001	-0.136	C(124)	0.070	-0.021	0.123
Si(84)	1.907	0.041	-0.884	Si(125)	1.519	-1.220	0.488
Si(85)	-0.865	-1.218	-1.214	Si(126)	-1.201	-0.253	1.534
Si(86)	-0.585	1.763	-0.269	Si(127)	-0.668	-0.435	-1.586
Si(87)	0.211	-0.576	1.680	Si(128)	0.702	1.782	0.156
C(88)	0.481	-2.447	1.857	C(129)	-0.474	3.004	-0.696
C(89)	-1.361	-0.157	2.663	C(130)	2.384	2.006	-0.697
C(90)	-2.487	-1.794	-0.409	C(131)	-2.399	1.209	1.716
C(91)	-1.274	-0.492	-2.918	C(132)	-2.220	-1.844	1.359
C(92)	0.051	2.929	1.089	C(133)	-2.414	0.266	-1.852
C(93)	-2.484	1.817	-0.198	C(134)	-0.773	-2.303	-1.912
C(94)	2.901	1.588	-0.418	C(135)	2.685	-1.469	-0.993
C(95)	2.960	-1.462	-0.402	C(136)	2.560	-0.661	1.972
H(96)	1.757	0.028	-2.378	H(137)	-1.495	2.983	-0.287
H(97)	-0.161	2.322	-1.598	H(138)	-0.076	4.025	-0.565
H(98)	-0.013	-2.437	-1.431	H(139)	-0.528	2.807	-1.780
H(99)	1.368	0.123	2.339	H(140)	2.619	3.084	-0.733
H(100)	1.430	-2.783	1.417	H(141)	3.210	1.501	-0.176
H(101)	0.492	-2.706	2.930	H(142)	2.349	1.634	-1.735
H(102)	-0.332	-3.022	1.384	H(143)	-2.990	1.370	0.800
H(103)	-1.254	-0.547	3.689	H(144)	-3.102	0.992	2.538
H(104)	-1.555	0.924	2.736	H(145)	-1.875	2.146	1.963
H(105)	-2.248	-0.634	2.215	H(146)	-2.839	-1.973	2.263
H(106)	-3.152	-0.945	-0.184	H(147)	-2.901	-1.810	0.493
H(107)	-3.016	-2.459	-1.113	H(148)	-1.577	-2.733	1.260
H(108)	-2.325	-2.358	0.522	H(149)	-2.737	0.032	-2.881
H(109)	-1.786	-1.257	-3.527	H(150)	-3.143	-0.194	-1.166
H(110)	-1.943	0.381	-2.847	H(151)	-2.460	1.357	-1.723
H(111)	-0.366	-0.180	-3.455	H(152)	-1.489	-2.779	-1.223
H(112)	-0.333	3.945	0.895	H(153)	-1.136	-2.469	-2.941
H(113)	-0.303	2.625	2.086	H(154)	0.191	-2.823	-1.807
H(114)	1.149	2.982	1.123	H(155)	2.155	-1.654	-1.940
H(115)	-2.863	1.383	0.741	H(156)	3.335	-0.593	-1.138
H(116)	-2.808	2.872	-0.236	H(157)	3.334	-2.339	-0.793
H(117)	-2.964	1.292	-1.038	H(158)	3.032	0.319	1.800
H(118)	2.444	2.518	-0.791	H(159)	1.957	-0.591	2.890
H(119)	3.027	1.668	0.674	H(160)	3.365	-1.395	2.147
H(120)	3.905	1.503	-0.868	H(161)	0.919	-2.554	0.830
H(121)	3.201	-1.459	0.673	H(162)	0.228	0.177	-2.627
H(122)	2.470	-2.415	-0.652	H(163)	-0.432	-0.358	2.819
H(123)	3.912	-1.413	-0.958	H(164)	0.843	2.187	1.596

Conformer	5			6			
	x	y	z	x	y	z	
C(165)	0.000	0.000	0.000	C(206)	-0.011	0.011	-0.083
Si(166)	-1.074	1.115	1.121	Si(207)	0.693	-1.733	-0.431
Si(167)	1.074	-1.115	1.121	Si(208)	-0.030	0.380	1.787
Si(168)	1.073	1.116	-1.121	Si(209)	-1.789	0.084	-0.790
Si(169)	-1.073	-1.115	-1.121	Si(210)	1.069	1.283	-1.018
C(170)	-2.495	-0.182	-1.963	C(211)	2.639	1.771	-0.068
C(171)	-1.833	-2.592	-0.198	C(212)	0.167	2.899	-1.435
C(172)	1.834	-2.591	0.198	C(213)	-1.467	-0.463	2.700
C(173)	2.495	-0.181	1.963	C(214)	1.543	-0.188	2.686
C(174)	2.495	0.182	-1.963	C(215)	-2.786	1.574	-0.163
C(175)	1.833	2.592	-0.198	C(216)	-2.815	-1.467	-0.395
C(176)	-1.834	2.591	0.198	C(217)	0.243	-2.347	-2.170
C(177)	-2.495	0.181	1.963	C(218)	2.586	-1.819	-0.312
H(178)	-2.147	0.720	-2.490	H(219)	0.123	-2.677	0.590
H(179)	-2.971	-0.848	-2.703	H(220)	-1.669	0.201	-2.283
H(180)	-3.270	0.115	-1.238	H(221)	-0.163	1.868	1.963
H(181)	-2.338	-3.249	-0.927	H(222)	1.490	0.649	-2.313
H(182)	-1.091	-3.198	0.344	H(223)	3.285	0.910	0.163
H(183)	-2.587	-2.255	0.530	H(224)	3.221	2.475	-0.687
H(184)	2.589	-2.254	-0.530	H(225)	2.391	2.285	0.876
H(185)	2.339	-3.248	0.927	H(226)	0.876	3.573	-1.944
H(186)	1.093	-3.197	-0.345	H(227)	-0.693	2.748	-2.106
H(187)	2.971	-0.847	2.703	H(228)	-0.183	3.406	-0.521
H(188)	3.270	0.116	1.238	H(229)	-1.447	-1.552	2.530
H(189)	2.146	0.720	2.491	H(230)	-1.348	-0.289	3.783
H(190)	2.971	0.848	-2.703	H(231)	-2.458	-0.086	2.408
H(191)	3.270	-0.114	-1.238	H(232)	1.473	0.117	3.744
H(192)	2.147	-0.719	-2.490	H(233)	1.629	-1.287	2.663
H(193)	2.587	2.255	0.530	H(234)	2.464	0.243	2.269
H(194)	2.338	3.249	-0.927	H(235)	-3.808	1.515	-0.577
H(195)	1.091	3.198	0.344	H(236)	-2.873	1.575	0.935
H(196)	-1.093	3.197	-0.345	H(237)	-2.352	2.536	-0.468
H(197)	-2.589	2.254	-0.529	H(238)	-3.125	-1.473	0.661
H(198)	-2.339	3.248	0.927	H(239)	-3.730	-1.454	-1.012
H(199)	-3.270	-0.116	1.238	H(240)	-2.287	-2.411	-0.595
H(200)	-2.146	-0.721	2.490	H(241)	-0.839	-2.427	-2.349
H(201)	-2.971	0.847	2.703	H(242)	0.661	-1.667	-2.930
H(202)	-0.184	1.653	2.206	H(243)	0.688	-3.345	-2.329
H(203)	0.184	1.653	-2.206	H(244)	3.060	-1.206	-1.096
H(204)	0.184	-1.653	2.206	H(245)	2.974	-1.496	0.665
H(205)	-0.184	-1.653	-2.206	H(246)	2.902	-2.864	-0.473

Conformer	7			8			
	x	y	z	x	y	z	
C(247)	-0.004	0.132	-0.191	C(288)	0.000	0.156	0.000
Si(248)	0.018	-0.259	1.670	Si(289)	0.349	-0.892	1.554
Si(249)	1.167	1.596	-0.595	Si(290)	1.507	1.299	-0.302
Si(250)	-1.750	0.666	-0.768	Si(291)	-1.511	1.295	0.301
Si(251)	0.538	-1.342	-1.280	Si(292)	-0.346	-0.893	-1.554
C(252)	-0.172	-3.009	-0.708	C(293)	-1.453	-2.399	-1.210
C(253)	2.422	-1.549	-1.388	C(294)	1.228	-1.511	-2.414
C(254)	0.419	3.300	-0.227	C(295)	1.565	2.745	0.927
C(255)	2.812	1.536	0.352	C(296)	3.179	0.415	-0.137
C(256)	-2.638	1.780	0.489	C(297)	-3.180	0.406	0.137
C(257)	-2.905	-0.790	-1.153	C(298)	-1.572	2.741	-0.927
C(258)	-1.466	-1.303	2.235	C(299)	-1.224	-1.514	2.414
C(259)	1.574	-1.200	2.222	C(300)	1.459	-2.395	1.210
H(260)	-0.019	1.047	2.414	H(301)	1.078	-0.014	2.532
H(261)	-1.567	1.443	-2.040	H(302)	-1.404	1.835	1.699
H(262)	1.458	1.524	-2.066	H(303)	1.399	1.839	-1.700
H(263)	0.027	-1.069	-2.666	H(304)	-1.077	-0.017	-2.532
H(264)	-1.269	-2.999	-0.623	H(305)	-2.412	-2.117	-0.752
H(265)	0.104	-3.784	-1.444	H(306)	-1.670	-2.908	-2.165
H(266)	0.246	-3.316	0.265	H(307)	-0.960	-3.131	-0.550
H(267)	2.647	-2.424	-2.021	H(308)	0.944	-2.105	-3.299
H(268)	2.918	-0.675	-1.838	H(309)	1.868	-0.683	-2.757
H(269)	2.865	-1.730	-0.395	H(310)	1.823	-2.160	-1.750
H(270)	0.179	3.405	0.845	H(311)	1.669	2.363	1.956
H(271)	1.170	4.068	-0.478	H(312)	2.449	3.369	0.708
H(272)	-0.488	3.514	-0.813	H(313)	0.677	3.395	0.898
H(273)	3.446	2.370	0.004	H(314)	3.978	1.128	-0.402
H(274)	2.649	1.673	1.434	H(315)	3.355	0.094	0.903
H(275)	3.369	0.600	0.199	H(316)	3.276	-0.462	-0.794
H(276)	-3.564	2.168	0.030	H(317)	-3.981	1.117	0.402
H(277)	-2.927	1.224	1.395	H(318)	-3.355	0.085	-0.903
H(278)	-2.028	2.640	0.800	H(319)	-3.275	-0.471	0.794
H(279)	-3.065	-1.429	-0.270	H(320)	-1.675	2.358	-1.956
H(280)	-3.886	-0.389	-1.460	H(321)	-2.458	3.362	-0.709
H(281)	-2.530	-1.419	-1.976	H(322)	-0.687	3.393	-0.898
H(282)	-2.437	-0.819	2.049	H(323)	-1.866	-0.687	2.757
H(283)	-1.471	-2.283	1.731	H(324)	-1.817	-2.164	1.750
H(284)	-1.386	-1.485	3.320	H(325)	-0.939	-2.107	3.299
H(285)	1.619	-2.202	1.766	H(326)	0.968	-3.129	0.551
H(286)	2.504	-0.668	1.976	H(327)	2.418	-2.111	0.752
H(287)	1.540	-1.337	3.317	H(328)	1.678	-2.904	2.165

Conformer	9		
	x	y	z
C(329)	0.000	0.226	0.000
Si(330)	1.439	1.400	0.475
Si(331)	-1.440	1.400	-0.475
Si(332)	-0.484	-0.826	1.513
Si(333)	0.484	-0.826	-1.513
C(334)	-0.683	-2.295	-1.816
C(335)	2.237	-1.552	-1.397
C(336)	-2.761	0.583	-1.565
C(337)	-2.274	2.162	1.049
C(338)	0.683	-2.294	1.816
C(339)	-2.236	-1.552	1.397
C(340)	2.761	0.584	1.565
C(341)	2.273	2.162	-1.049
H(342)	0.847	2.527	1.272
H(343)	-0.426	0.068	2.720
H(344)	-0.848	2.526	-1.272
H(345)	0.426	0.068	-2.720
H(346)	-1.738	-1.994	-1.896
H(347)	-0.397	-2.788	-2.761
H(348)	-0.599	-3.046	-1.014
H(349)	2.436	-2.151	-2.302
H(350)	3.023	-0.786	-1.325
H(351)	2.330	-2.221	-0.526
H(352)	-3.227	-0.284	-1.071
H(353)	-3.555	1.321	-1.773
H(354)	-2.351	0.255	-2.534
H(355)	-3.026	2.899	0.719
H(356)	-2.790	1.411	1.669
H(357)	-1.543	2.684	1.687
H(358)	0.397	-2.787	2.761
H(359)	0.599	-3.046	1.014
H(360)	1.738	-1.993	1.896
H(361)	-2.330	-2.221	0.526
H(362)	-2.436	-2.151	2.302
H(363)	-3.023	-0.786	1.325
H(364)	2.351	0.255	2.534
H(365)	3.227	-0.284	1.071
H(366)	3.555	1.322	1.773
H(367)	2.789	1.412	-1.669
H(368)	1.543	2.684	-1.687
H(369)	3.026	2.899	-0.719

<sup>a</sup> Calculated sums of electronic and thermal free energies (ZPE corrected) using M06-2X/6-31G(d) = -1517.24701 (conformer 1), -1517.24543 (2), -1517.245059 (3), -1517.244945 (4), -1517.246681 (5), -1517.244397 (6), -1517.244397 (7), -1517.244735 (8), and -1517.24459 (9) Hartrees.

**Table S22** Calculated coordinates [MP2/*aug-cc-pVDZ*; in Å] for the seven lowest energy conformers of C(SiFMe<sub>2</sub>)<sub>4</sub> (**2**).<sup>a</sup>

Conformer	1			2			
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>	
C(1)	0.001	-0.002	0.002	C(42)	-0.008	-0.026	-0.008
Si(2)	-0.016	-0.334	1.868	Si(43)	1.452	-0.604	-1.084
Si(3)	-1.791	-0.023	-0.638	Si(44)	-1.645	-0.104	-0.970
Si(4)	1.032	-1.334	-0.886	Si(45)	0.327	1.801	0.465
Si(5)	0.778	1.696	-0.362	Si(46)	-0.133	-1.112	1.544
C(6)	0.254	2.446	-1.997	C(47)	0.066	-2.956	1.201
C(7)	2.649	1.758	-0.205	C(48)	-1.686	-0.838	2.562
C(8)	-2.762	-1.559	-0.120	C(49)	-2.339	-1.843	-1.177
C(9)	-2.778	1.532	-0.241	C(50)	-3.001	1.006	-0.291
C(10)	0.057	-2.828	-1.458	C(51)	-0.040	3.024	-0.910
C(11)	2.571	-1.869	0.053	C(52)	2.033	2.121	1.176
C(12)	1.526	0.195	2.800	C(53)	2.969	-1.111	-0.093
C(13)	-1.536	0.328	2.752	C(54)	1.032	-1.904	-2.371
F(14)	-0.092	-2.005	2.002	F(55)	1.935	0.757	-1.926
F(15)	1.605	-0.573	-2.263	F(56)	-0.755	2.127	1.701
F(16)	-1.677	-0.081	-2.303	F(57)	-1.303	0.430	-2.513
F(17)	0.189	2.681	0.866	F(58)	1.152	-0.696	2.523
H(18)	-0.835	2.550	-2.107	H(59)	0.940	-3.200	0.581
H(19)	0.711	3.445	-2.100	H(60)	0.184	-3.477	2.166
H(20)	0.618	1.806	-2.816	H(61)	-0.829	-3.365	0.706
H(21)	2.969	2.810	-0.295	H(62)	-1.588	-1.396	3.508
H(22)	3.013	1.376	0.759	H(63)	-1.830	0.228	2.792
H(23)	3.123	1.187	-1.019	H(64)	-2.583	-1.216	2.045
H(24)	-2.311	-2.072	0.743	H(65)	-2.767	-2.220	-0.234
H(25)	-3.796	-1.280	0.141	H(66)	-3.157	-1.798	-1.916
H(26)	-2.806	-2.275	-0.955	H(67)	-1.593	-2.566	-1.537
H(27)	-3.557	1.645	-1.014	H(68)	-3.858	0.979	-0.986
H(28)	-3.283	1.432	0.732	H(69)	-3.342	0.639	0.689
H(29)	-2.175	2.450	-0.215	H(70)	-2.689	2.051	-0.162
H(30)	0.743	-3.530	-1.959	H(71)	-0.105	4.035	-0.473
H(31)	-0.399	-3.347	-0.600	H(72)	0.786	3.008	-1.638
H(32)	-0.730	-2.547	-2.173	H(73)	-0.970	2.821	-1.459
H(33)	2.305	-2.404	0.978	H(74)	2.810	1.994	0.406
H(34)	3.148	-2.556	-0.587	H(75)	2.070	3.166	1.526
H(35)	3.222	-1.019	0.306	H(76)	2.250	1.459	2.027
H(36)	2.447	-0.234	2.380	H(77)	3.212	-0.379	0.690
H(37)	1.613	1.293	2.808	H(78)	2.848	-2.091	0.393
H(38)	1.434	-0.148	3.844	H(79)	3.823	-1.180	-0.787
H(39)	-1.591	1.423	2.645	H(80)	0.735	-2.857	-1.903
H(40)	-2.474	-0.114	2.381	H(81)	0.228	-1.567	-3.042
H(41)	-1.456	0.089	3.825	H(82)	1.931	-2.096	-2.980

Conformer	3			4			
	x	y	z	x	y	z	
C(83)	-0.003	-0.015	0.021	C(124)	0.000	0.021	0.000
Si(84)	-1.291	-0.771	-1.186	Si(125)	-0.629	1.095	-1.432
Si(85)	-0.892	0.486	1.639	Si(126)	1.446	-1.100	-0.551
Si(86)	0.805	1.539	-0.771	Si(127)	-1.446	-1.100	0.551
Si(87)	1.362	-1.302	0.398	Si(128)	0.629	1.095	1.432
C(88)	2.382	-0.980	1.946	C(129)	-0.665	1.610	2.688
C(89)	2.526	-1.685	-1.026	C(130)	1.630	2.592	0.872
C(90)	-2.487	1.455	1.418	C(131)	3.084	-0.208	-0.794
C(91)	-1.186	-0.903	2.872	C(132)	1.726	-2.594	0.548
C(92)	2.446	2.046	-0.004	C(133)	-1.726	-2.594	-0.548
C(93)	-0.296	3.048	-0.931	C(134)	-3.084	-0.208	0.794
C(94)	-0.603	-1.592	-2.725	C(135)	-1.630	2.592	-0.872
C(95)	-2.534	-1.929	-0.378	C(136)	0.665	1.611	-2.688
F(96)	-2.191	0.526	-1.734	F(137)	-1.739	0.146	-2.245
F(97)	1.178	1.089	-2.337	F(138)	-1.007	-1.656	2.064
F(98)	0.160	1.551	2.389	F(139)	1.007	-1.657	-2.064
F(99)	0.535	-2.730	0.680	F(140)	1.739	0.146	2.245
H(100)	1.804	-0.609	2.799	H(141)	-1.172	0.737	3.126
H(101)	2.865	-1.923	2.239	H(142)	-0.168	2.166	3.501
H(102)	3.176	-0.249	1.743	H(143)	-1.419	2.276	2.237
H(103)	3.216	-2.478	-0.707	H(144)	2.127	3.024	1.758
H(104)	1.997	-2.033	-1.920	H(145)	2.411	2.321	0.147
H(105)	3.125	-0.812	-1.317	H(146)	1.001	3.380	0.429
H(106)	-3.302	0.825	1.039	H(147)	3.500	0.114	0.174
H(107)	-2.792	1.842	2.401	H(148)	3.793	-0.921	-1.247
H(108)	-2.380	2.303	0.734	H(149)	3.011	0.663	-1.461
H(109)	-1.557	-0.461	3.808	H(150)	2.433	-3.275	0.046
H(110)	-1.949	-1.600	2.503	H(151)	2.173	-2.259	1.498
H(111)	-0.290	-1.489	3.105	H(152)	0.812	-3.153	0.788
H(112)	2.800	2.952	-0.517	H(153)	-2.433	-3.275	-0.046
H(113)	2.329	2.282	1.061	H(154)	-2.173	-2.259	-1.498
H(114)	3.228	1.284	-0.110	H(155)	-0.812	-3.153	-0.788
H(115)	-0.461	3.531	0.041	H(156)	-3.500	0.114	-0.174
H(116)	0.219	3.770	-1.580	H(157)	-3.793	-0.921	1.246
H(117)	-1.264	2.807	-1.384	H(158)	-3.011	0.663	1.461
H(118)	0.158	-0.978	-3.218	H(159)	-2.411	2.321	-0.147
H(119)	-0.181	-2.581	-2.499	H(160)	-1.001	3.380	-0.429
H(120)	-1.438	-1.741	-3.425	H(161)	-2.127	3.024	-1.758
H(121)	-2.027	-2.793	0.072	H(162)	1.419	2.276	-2.237
H(122)	-3.148	-1.445	0.391	H(163)	1.172	0.737	-3.126
H(123)	-3.216	-2.300	-1.157	H(164)	0.168	2.166	-3.501



Conformer	5			6			
	x	y	z	x	y	z	
C(165)	0.000	0.000	0.004	C(206)	-0.013	0.001	-0.008
Si(166)	-0.153	-1.554	-1.086	Si(207)	0.216	1.864	-0.321
Si(167)	-1.560	0.151	1.086	Si(208)	1.641	-0.887	-0.355
Si(168)	0.152	1.554	-1.086	Si(209)	-1.365	-0.710	-1.149
Si(169)	1.560	-0.151	1.085	Si(210)	-0.498	-0.265	1.806
C(170)	3.169	0.198	0.171	C(211)	-0.033	-1.943	2.507
C(171)	1.708	-1.777	2.012	C(212)	-2.301	0.112	2.198
C(172)	-1.707	1.777	2.012	C(213)	2.353	-0.544	-2.054
C(173)	-3.169	-0.199	0.172	C(214)	2.940	-0.614	0.989
C(174)	0.922	3.025	-0.204	C(215)	-2.806	0.457	-1.450
C(175)	-1.456	2.073	-1.905	C(216)	-1.966	-2.406	-0.601
C(176)	1.455	-2.073	-1.905	C(217)	-1.092	2.966	0.459
C(177)	-0.922	-3.025	-0.203	C(218)	1.920	2.512	0.136
F(178)	-1.198	-1.151	-2.325	F(219)	0.066	2.067	-1.972
F(179)	1.197	1.151	-2.326	F(220)	-0.667	-0.967	-2.638
F(180)	-1.419	-1.034	2.255	F(221)	1.285	-2.520	-0.308
F(181)	1.420	1.034	2.255	F(222)	0.379	0.879	2.662
H(182)	3.093	0.989	-0.588	H(223)	1.044	-2.150	2.437
H(183)	3.928	0.496	0.914	H(224)	-0.327	-1.981	3.570
H(184)	3.530	-0.713	-0.331	H(225)	-0.563	-2.746	1.971
H(185)	2.561	-1.706	2.707	H(226)	-2.435	0.061	3.292
H(186)	0.798	-1.997	2.590	H(227)	-2.602	1.116	1.866
H(187)	1.908	-2.617	1.327	H(228)	-2.984	-0.624	1.746
H(188)	-1.908	2.617	1.328	H(229)	2.395	0.535	-2.270
H(189)	-2.561	1.706	2.708	H(230)	3.377	-0.950	-2.112
H(190)	-0.798	1.998	2.590	H(231)	1.733	-1.016	-2.829
H(191)	-3.928	-0.496	0.915	H(232)	3.480	-1.564	1.140
H(192)	-3.530	0.712	-0.331	H(233)	3.675	0.140	0.666
H(193)	-3.093	-0.989	-0.587	H(234)	2.525	-0.290	1.954
H(194)	1.026	3.853	-0.925	H(235)	-3.513	-0.032	-2.141
H(195)	0.277	3.365	0.621	H(236)	-3.350	0.689	-0.521
H(196)	1.913	2.808	0.220	H(237)	-2.470	1.396	-1.915
H(197)	-2.155	2.518	-1.179	H(238)	-2.512	-2.380	0.355
H(198)	-1.227	2.844	-2.660	H(239)	-2.656	-2.796	-1.368
H(199)	-1.948	1.226	-2.405	H(240)	-1.120	-3.103	-0.508
H(200)	1.947	-1.226	-2.406	H(241)	-2.117	2.671	0.192
H(201)	2.155	-2.518	-1.180	H(242)	-0.994	2.972	1.556
H(202)	1.226	-2.844	-2.660	H(243)	-0.930	3.995	0.096
H(203)	-0.276	-3.365	0.621	H(244)	2.118	2.352	1.208
H(204)	-1.913	-2.809	0.220	H(245)	2.727	2.046	-0.448
H(205)	-1.027	-3.853	-0.924	H(246)	1.947	3.597	-0.063

Conformer	7		
	x	y	z
C(247)	0.001	0.026	0.008
Si(248)	0.426	-0.105	1.850
Si(249)	-1.872	-0.169	-0.239
Si(250)	0.893	-1.400	-0.917
Si(251)	0.585	1.696	-0.689
C(252)	0.216	3.153	0.451
C(253)	-0.023	2.055	-2.423
C(254)	-2.625	-1.583	0.761
C(255)	-2.880	1.398	0.031
C(256)	-0.071	-3.009	-0.939
C(257)	2.659	-1.686	-0.350
C(258)	2.124	0.542	2.324
C(259)	-0.880	0.621	2.996
F(260)	0.453	-1.748	2.177
F(261)	1.020	-0.912	-2.506
F(262)	-2.090	-0.545	-1.849
F(263)	2.251	1.606	-0.749
H(264)	0.644	3.034	1.458
H(265)	0.658	4.062	0.008
H(266)	-0.867	3.323	0.555
H(267)	0.385	3.022	-2.759
H(268)	0.302	1.265	-3.116
H(269)	-1.123	2.112	-2.466
H(270)	-3.348	-1.193	1.497
H(271)	-3.174	-2.249	0.075
H(272)	-1.874	-2.181	1.296
H(273)	-3.941	1.155	-0.148
H(274)	-2.789	1.767	1.065
H(275)	-2.604	2.211	-0.658
H(276)	0.492	-3.736	-1.547
H(277)	-0.177	-3.421	0.077
H(278)	-1.067	-2.890	-1.391
H(279)	2.703	-2.052	0.687
H(280)	3.105	-2.455	-1.003
H(281)	3.258	-0.767	-0.442
H(282)	2.910	0.198	1.638
H(283)	2.149	1.642	2.339
H(284)	2.360	0.183	3.340
H(285)	-0.993	1.705	2.835
H(286)	-1.864	0.144	2.872
H(287)	-0.562	0.465	4.040

<sup>a</sup> Calculated sums of electronic and thermal free energies (ZPE corrected) using M06-2X/6-31G(d) = -1914.428553 (conformer 1), -1914.428269 (2), -1914.427942 (3), -1914.427475 (4), -1914.427203 (5), -1914.427064 (6), and -1914.425975 (7) Hartrees.

**Table S23** Calculated coordinates [MP2/aug-cc-pVDZ; in Å] for the two lowest energy conformers of C(SiClMe<sub>2</sub>)<sub>4</sub> (**3**).<sup>a</sup>

Conformer	1			2			
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>	
C(1)	0.072	0.008	-0.027	C(42)	0.069	0.000	0.000
Si(2)	-0.332	1.734	-0.761	Si(43)	-0.997	-1.225	-1.036
Si(3)	1.956	-0.324	-0.163	Si(44)	-0.997	1.225	1.036
Si(4)	-0.838	-1.358	-1.018	Si(45)	1.157	0.986	-1.229
Si(5)	-0.439	-0.013	1.829	Si(46)	1.157	-0.986	1.229
C(6)	0.789	0.844	2.974	C(47)	0.216	-1.757	2.665
C(7)	-0.946	-1.677	2.538	C(48)	2.670	-0.067	1.868
C(8)	2.562	-1.084	-1.777	C(49)	-0.145	1.898	2.580
C(9)	3.069	1.123	0.290	C(50)	-1.726	2.681	0.098
C(10)	-0.319	-3.115	-0.578	C(51)	0.215	1.757	-2.665
C(11)	-0.759	-1.144	-2.888	C(52)	2.670	0.067	-1.868
C(12)	-2.080	1.982	-1.403	C(53)	-0.144	-1.898	-2.579
C(13)	0.180	3.191	0.317	C(54)	-1.726	-2.681	-0.098
Cl(14)	0.901	1.948	-2.502	Cl(55)	-2.657	-0.151	-1.817
Cl(15)	-2.899	-1.264	-0.530	Cl(56)	1.955	2.667	-0.183
Cl(16)	2.410	-1.834	1.282	Cl(57)	-2.657	0.151	1.817
Cl(17)	-2.193	1.184	2.032	Cl(58)	1.955	-2.667	0.183
H(18)	0.978	1.885	2.672	H(59)	-0.554	-2.461	2.319
H(19)	0.332	0.863	3.978	H(60)	0.946	-2.315	3.276
H(20)	1.743	0.300	3.037	H(61)	-0.275	-1.007	3.302
H(21)	-1.259	-1.496	3.580	H(62)	3.240	-0.773	2.497
H(22)	-1.802	-2.107	1.997	H(63)	3.329	0.289	1.065
H(23)	-0.106	-2.387	2.541	H(64)	2.385	0.800	2.483
H(24)	2.404	-0.402	-2.625	H(65)	0.725	2.518	2.315
H(25)	3.646	-1.253	-1.657	H(66)	-0.888	2.535	3.089
H(26)	2.099	-2.056	-1.998	H(67)	0.166	1.122	3.293
H(27)	4.107	0.748	0.295	H(68)	-2.395	3.208	0.799
H(28)	2.994	1.924	-0.462	H(69)	-0.934	3.380	-0.214
H(29)	2.851	1.533	1.286	H(70)	-2.314	2.366	-0.774
H(30)	-0.933	-3.799	-1.188	H(71)	0.945	2.315	-3.276
H(31)	0.742	-3.307	-0.800	H(72)	-0.275	1.007	-3.302
H(32)	-0.492	-3.347	0.481	H(73)	-0.554	2.461	-2.319
H(33)	0.263	-1.293	-3.265	H(74)	2.384	-0.800	-2.483
H(34)	-1.411	-1.915	-3.332	H(75)	3.239	0.773	-2.497
H(35)	-1.105	-0.159	-3.230	H(76)	3.329	-0.289	-1.065
H(36)	-2.366	1.252	-2.172	H(77)	0.166	-1.122	-3.293
H(37)	-2.807	1.924	-0.580	H(78)	0.725	-2.518	-2.315
H(38)	-2.119	2.989	-1.851	H(79)	-0.888	-2.535	-3.089
H(39)	-0.441	3.255	1.223	H(80)	-0.934	-3.380	0.214
H(40)	1.241	3.150	0.602	H(81)	-2.314	-2.366	0.774
H(41)	0.024	4.107	-0.277	H(82)	-2.395	-3.208	-0.800

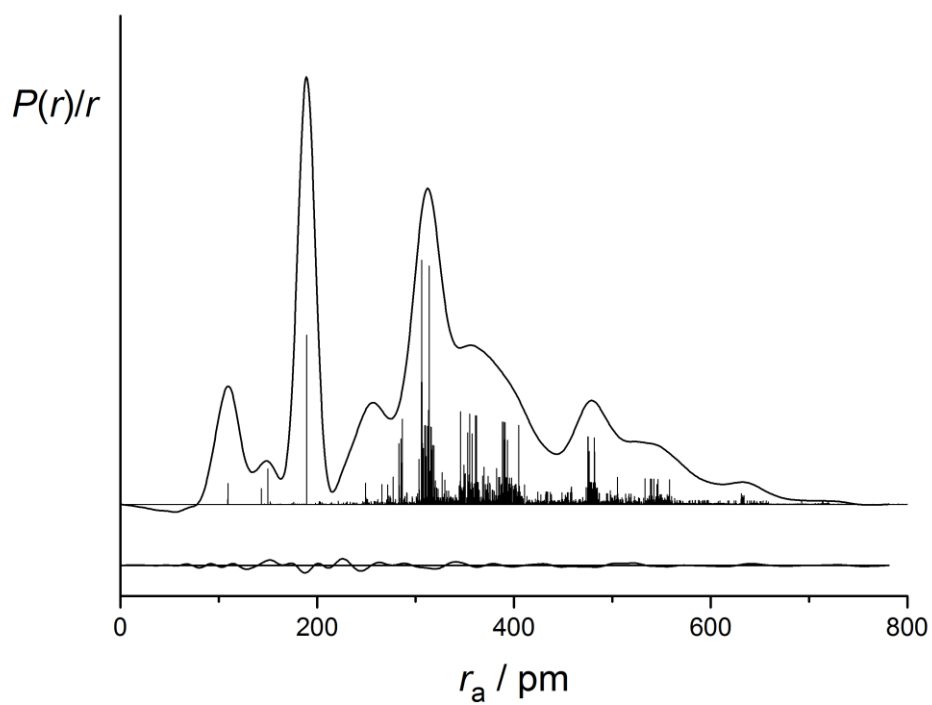
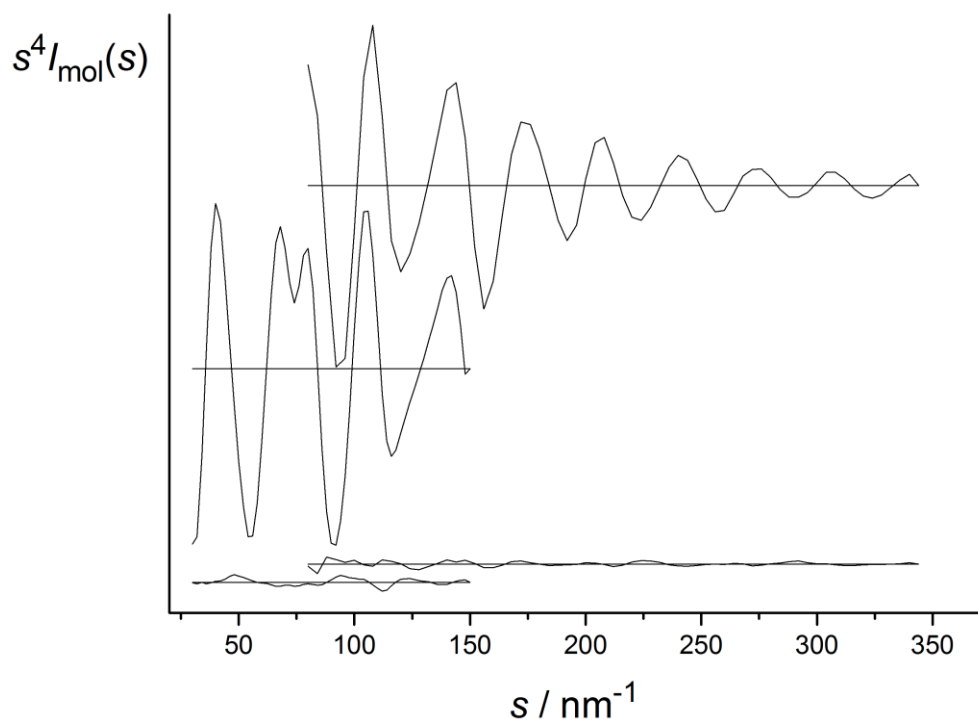
<sup>a</sup> Calculated sums of electronic and thermal free energies (ZPE corrected) using M06-2X/6-31G(d) = -3355.810002 (conformer 1) and -3355.810540 (2) Hartrees.

**Table S24** Calculated coordinates [MP2/aug-cc-pVDZ(-PP); in Å] for the two lowest energy conformers of C(SiBrMe<sub>2</sub>)<sub>4</sub> (**4**).<sup>a</sup>

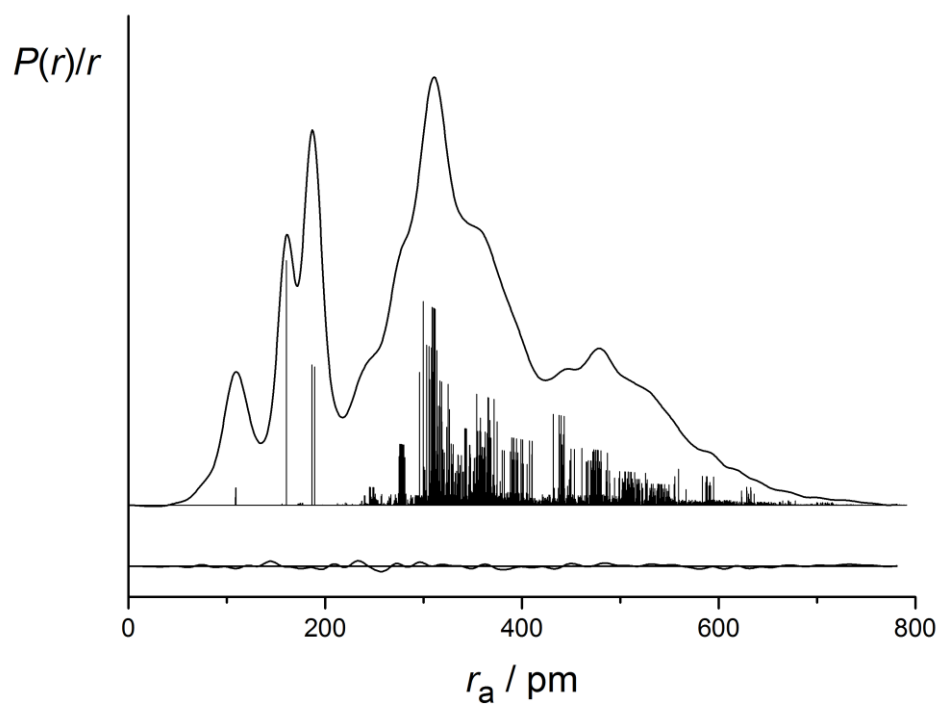
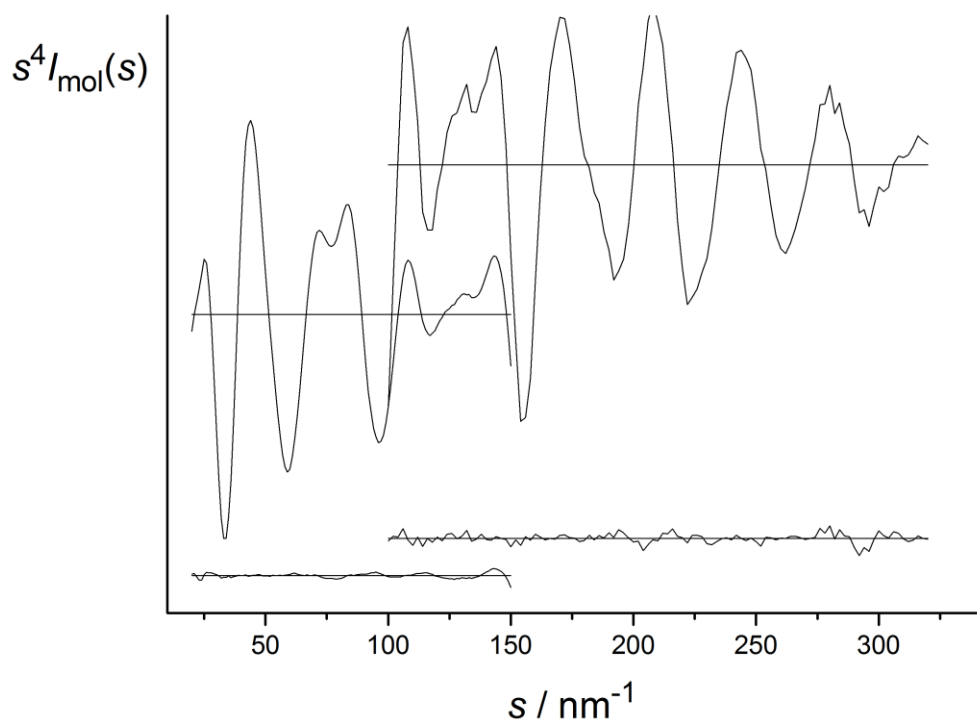
Conformer	1			2			
	x	y	z	x	y	z	
C(1)	-0.211	0.001	-0.020	C(42)	-0.164	0.000	0.000
Si(2)	0.144	1.702	-0.842	Si(43)	0.893	1.191	-1.088
Si(3)	-2.103	-0.343	-0.055	Si(44)	0.893	-1.192	1.089
Si(4)	0.336	0.021	1.820	Si(45)	-1.251	-1.027	-1.200
Si(5)	0.693	-1.374	-1.024	Si(46)	-1.251	1.027	1.200
C(6)	-0.182	-1.865	-2.621	C(47)	-0.307	1.859	2.602
C(7)	1.240	-2.894	-0.060	C(48)	-2.763	0.133	1.880
C(8)	-3.115	0.315	1.394	C(49)	0.041	-1.788	2.666
C(9)	-2.977	0.071	-1.670	C(50)	1.610	-2.696	0.217
C(10)	-0.188	-1.495	2.808	C(51)	-0.307	-1.859	-2.602
C(11)	-0.160	1.575	2.763	C(52)	-2.763	-0.133	-1.880
C(12)	1.707	2.596	-0.298	C(53)	0.040	1.788	-2.666
C(13)	-0.020	1.725	-2.719	C(54)	1.610	2.696	-0.217
Br(14)	-1.524	3.140	-0.179	Br(55)	2.690	0.052	-1.905
Br(15)	2.607	-0.008	1.923	Br(56)	-2.143	-2.797	-0.055
Br(16)	-2.391	-2.610	0.164	Br(57)	2.690	-0.052	1.905
Br(17)	2.673	-0.536	-1.814	Br(58)	-2.143	2.797	0.054
H(18)	-0.338	-1.000	-3.283	H(59)	0.466	2.543	2.224
H(19)	0.486	-2.571	-3.143	H(60)	-1.041	2.450	3.177
H(20)	-1.143	-2.367	-2.434	H(61)	0.177	1.139	3.277
H(21)	1.774	-3.542	-0.775	H(62)	-3.307	0.858	2.509
H(22)	1.939	-2.627	0.746	H(63)	-3.442	-0.215	1.089
H(23)	0.383	-3.448	0.349	H(64)	-2.484	-0.733	2.497
H(24)	-3.112	1.414	1.426	H(65)	-0.836	-2.413	2.439
H(25)	-4.148	-0.035	1.228	H(66)	0.787	-2.408	3.194
H(26)	-2.783	-0.083	2.364	H(67)	-0.253	-0.977	3.347
H(27)	-4.012	-0.299	-1.578	H(68)	2.253	-3.207	0.954
H(28)	-3.009	1.159	-1.833	H(69)	0.811	-3.391	-0.087
H(29)	-2.515	-0.420	-2.537	H(70)	2.223	-2.422	-0.652
H(30)	0.208	-1.361	3.830	H(71)	-1.041	-2.449	-3.177
H(31)	-1.281	-1.609	2.866	H(72)	0.177	-1.139	-3.277
H(32)	0.232	-2.423	2.397	H(73)	0.466	-2.543	-2.224
H(33)	-1.253	1.667	2.854	H(74)	-2.484	0.734	-2.497
H(34)	0.273	1.486	3.774	H(75)	-3.307	-0.858	-2.510
H(35)	0.221	2.499	2.305	H(76)	-3.442	0.215	-1.089
H(36)	1.730	2.793	0.783	H(77)	-0.253	0.977	-3.347
H(37)	2.606	2.027	-0.570	H(78)	-0.836	2.412	-2.439
H(38)	1.712	3.565	-0.826	H(79)	0.787	2.407	-3.194
H(39)	0.775	1.137	-3.202	H(80)	0.811	3.391	0.087
H(40)	-1.002	1.363	-3.054	H(81)	2.223	2.422	0.652
H(41)	0.080	2.777	-3.036	H(82)	2.253	3.207	-0.954

<sup>a</sup> Calculated sums of electronic and thermal free energies (ZPE corrected) using M06-2X/6-31G(d) with pseudopotential aug-cc-pVDZ-PP = -3183.183054 (conformer 1) and -3183.181908 (2) Hartrees.

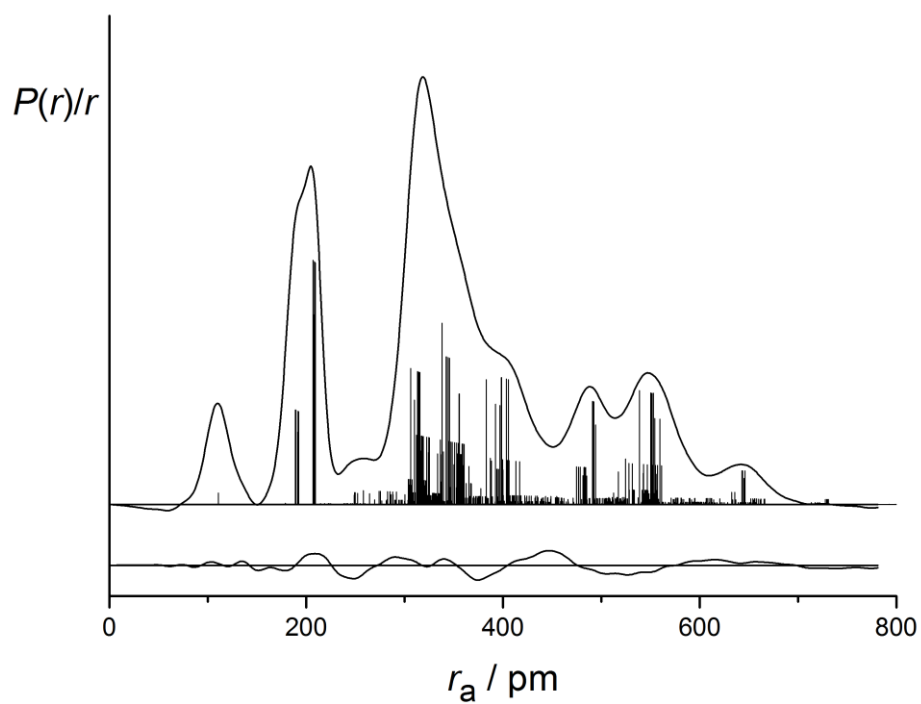
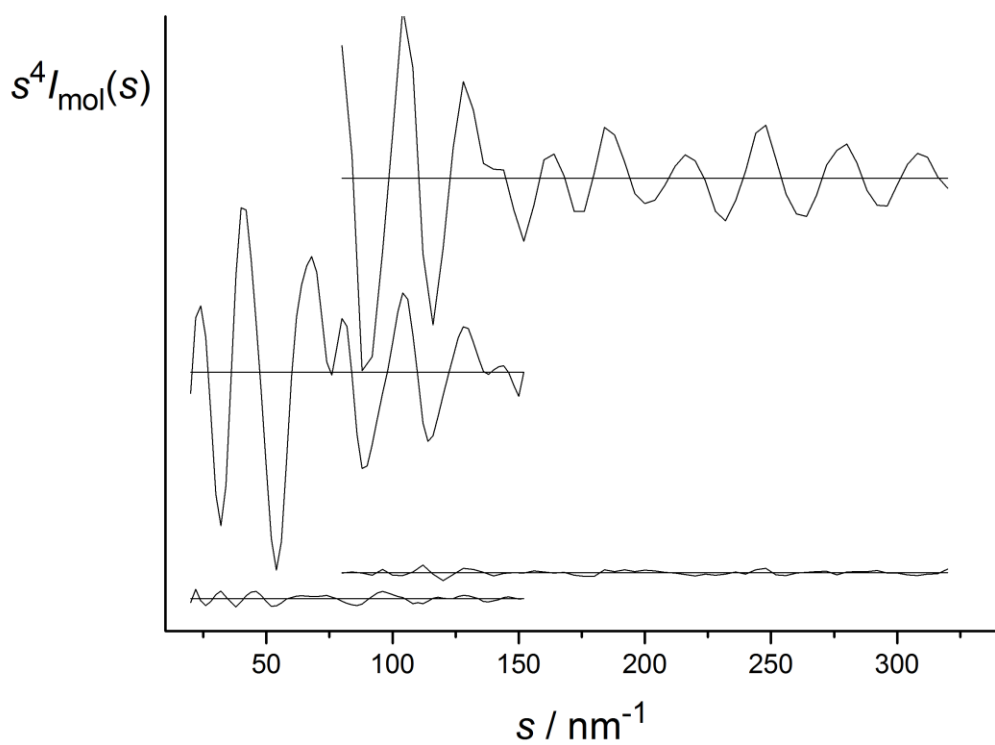
**Figure S1** Experimental and weighted difference (experimental – theoretical) molecular scattering intensities (top) for C(SiHMe<sub>2</sub>)<sub>4</sub> (**1**), and larger version of RDC shown in Fig. 3.



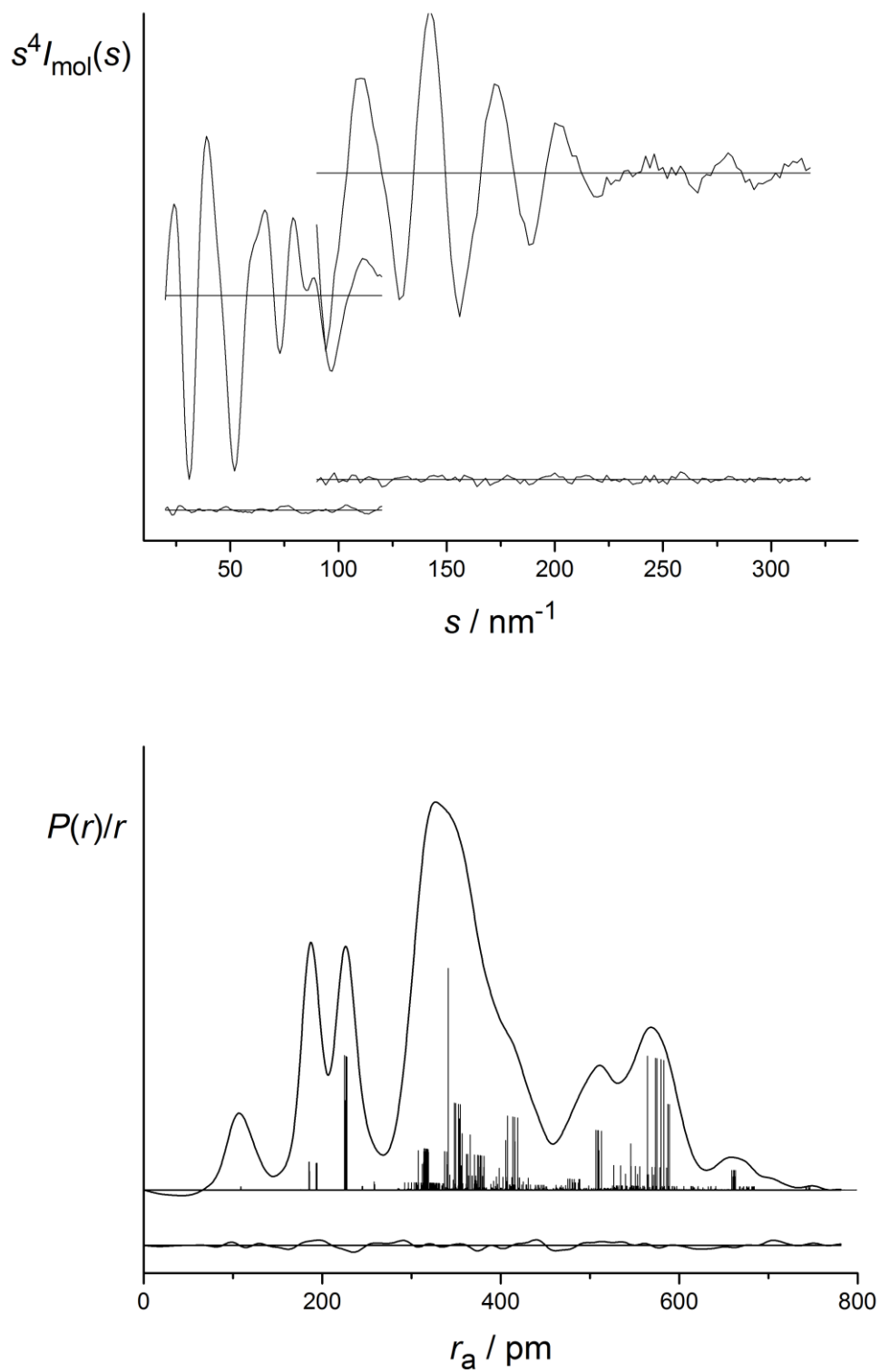
**Figure S2** Experimental and weighted difference (experimental – theoretical) molecular scattering intensities (top) for C(SiFMe<sub>2</sub>)<sub>4</sub> (**2**), and (bottom) larger version of RDC shown in Fig. 3.



**Figure S3** Experimental and weighted difference (experimental – theoretical) molecular scattering intensities (top) for  $C(SiClMe_2)_4$  (**3**), and (bottom) larger version of RDC shown in Fig. 3.



**Figure S4** Experimental and weighted difference (experimental – theoretical) molecular scattering intensities (top) for  $C(SiBrMe_2)_4$  (**4**), and (bottom) larger version of RDC shown in Fig. 3.





## NMR

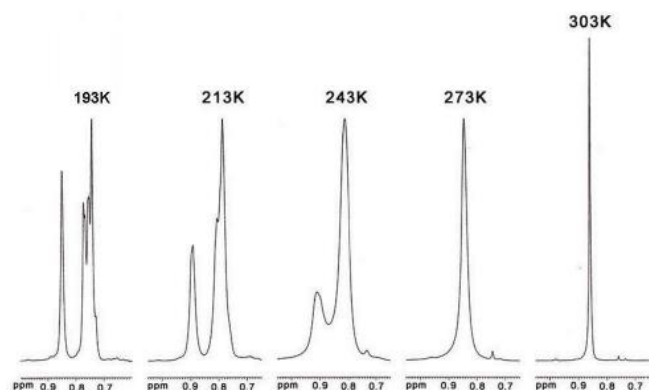
### **C(SiHMe<sub>2</sub>)<sub>4</sub>**

The room temperature <sup>1</sup>H NMR spectrum of C(SiHMe<sub>2</sub>)<sub>4</sub> shows a methyl doublet at 0.24 ppm (<sup>3</sup>J<sub>H-H</sub> = 3.4 Hz, <sup>1</sup>J<sub>C-H</sub> = 120 Hz, <sup>2</sup>J<sub>Si-H</sub> = 6.9 Hz) and a septet at 4.09 ppm (<sup>3</sup>J<sub>H-H</sub> = 3.4 Hz, <sup>1</sup>J<sub>Si-H</sub> = 185 Hz) and the <sup>29</sup>Si{H} spectrum shows a singlet at -15.79 ppm. Variable temperature 500 MHz <sup>1</sup>H NMR spectra of a CDCl<sub>3</sub> solution of C(SiHMe<sub>2</sub>)<sub>4</sub> recorded in the range of 333 to 213 K showed no significant changes in the appearance of the spectra. Similarly, no significant change was seen when the <sup>29</sup>Si{H} spectrum was recorded in CDCl<sub>3</sub>/CD<sub>2</sub>Cl<sub>2</sub> solution at 213 K. The only changes observed were slight chemical shift changes, which were attributed to the change in temperature.

### **C(SiClMe<sub>2</sub>)<sub>4</sub>**

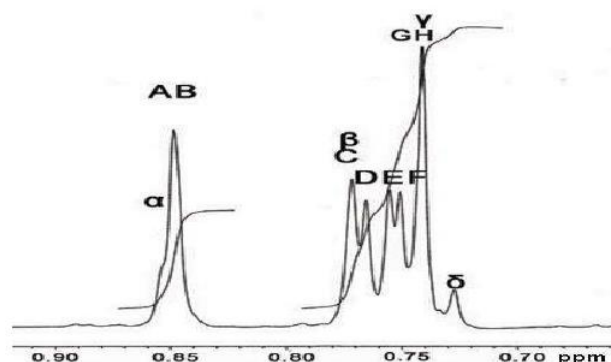
500 MHz <sup>1</sup>H NMR spectra of C(SiClMe<sub>2</sub>)<sub>4</sub> in CDCl<sub>3</sub>/CD<sub>2</sub>Cl<sub>2</sub> were recorded over a temperature range from 303 to 193 K and are shown in Figure S5.

**Figure S5** 500 MHz <sup>1</sup>H NMR variable temperature spectra of C(SiClMe<sub>2</sub>)<sub>4</sub> in CDCl<sub>3</sub>/CD<sub>2</sub>Cl<sub>2</sub>.



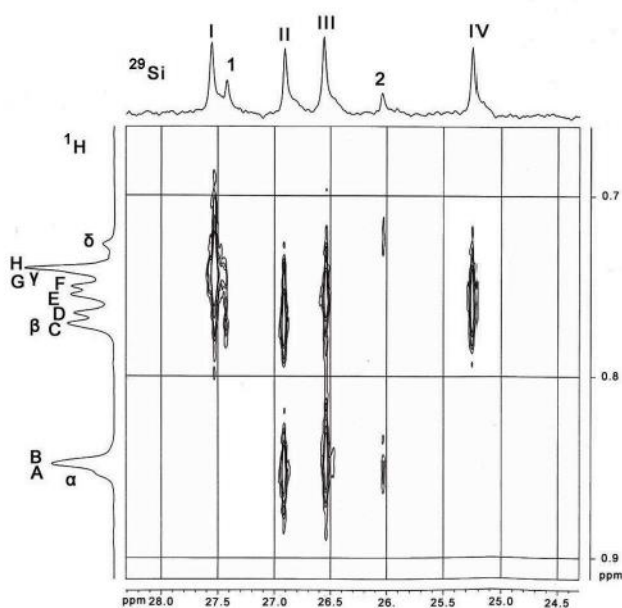
At 303 K a single, slightly broadened signal attributable to eight equivalent methyl groups was observed at 0.86 ppm. This broadened further and then split into several distinct signals on lowering the temperature. At 193 K at least seven peaks were observed (this is shown in more detail in the expansion in Figure S6). See below for an explanation of the labelling system used.

**Figure S6** Expansion of the 500 MHz  $^1\text{H}$  NMR spectrum of  $\text{C}(\text{SiClMe}_2)_4$  in  $\text{CDCl}_3/\text{CD}_2\text{Cl}_2$  at 193 K.



The overall appearance of the 193 K  $^1\text{H}$  NMR spectrum of  $\text{C}(\text{SiClMe}_2)_4$  is very similar to that of the analogous bromide  $\text{C}(\text{SiBrMe}_2)_4$  recorded at 213 K. The lower temperature required to freeze out the conformers is presumably due to the less sterically demanding nature of the chlorine atoms in  $\text{C}(\text{SiClMe}_2)_4$ , which lowers the energy barriers to rotation and the resolution of the signals in the  $^1\text{H}$  NMR spectrum of  $\text{C}(\text{SiClMe}_2)_4$  recorded at 193 K (Figure S6) is still poor compared to that of  $\text{C}(\text{SiBrMe}_2)_4$  at 213 K. It is thought that a major  $C_1$  conformer of  $\text{C}(\text{SiClMe}_2)_4$  giving rise to eight large proton resonances is present in the mixture, as well as a less abundant  $C_2$  conformer, which yields four proton signals of lower intensities. Integration of all signals revealed that the  $C_1$  conformer gives rise to *ca.* 85% of the conformer mixture, while the  $C_2$  conformer makes up the remaining 15% of the mixture. Assignments of  $^1\text{H}$  NMR signals in Figure S6 have been made with the help of a 2D  $^1\text{H}/^{29}\text{Si}$  NMR correlation spectrum (shown in Figure S7). A large, broad signal at 0.85 ppm is assumed to be due to coinciding signals A and B of the  $C_1$  conformer. The small signal labelled  $\alpha$  is assigned to the  $C_2$  conformer. Large resonances at 0.771, 0.765, 0.755, and 0.751 ppm are labelled C, D, E and F, respectively, and have been assigned to the  $C_1$  conformer. Signals G and H of the  $C_1$  conformer are assumed to give rise to the large signal at 0.74 ppm, and the small signal at 0.73 ppm (labelled  $\delta$ ) has been assigned to the  $C_2$  conformer. Signals  $\beta$  and  $\gamma$  belonging to the  $C_2$  conformer appear to be concealed by the large signals at 0.771 ppm (C) and 0.74 ppm (G/H), respectively.

**Figure S7** 2D  $^1\text{H}/^{29}\text{Si}$  NMR shift correlation spectrum of  $\text{C}(\text{SiClMe}_2)_4$  in  $\text{CDCl}_3/\text{CD}_2\text{Cl}_2$  at 201 K.



99 MHz  $^{29}\text{Si}\{^1\text{H}\}$  INEPT NMR spectra of  $\text{C}(\text{SiClMe}_2)_4$  in  $\text{CDCl}_3/\text{CD}_2\text{Cl}_2$  were recorded at 298 and 201 K. At 298 K just one broad  $^{29}\text{Si}$  NMR signal due to four equivalent silicon atoms was seen at 24.04 ppm. At 201 K four large resonances at 27.55, 26.91, 26.56, and 25.24 ppm of similar intensities labelled I, II, III and IV had emerged alongside two small resonances at 27.42 and 26.04 ppm labelled 1 and 2 (see Figure S7). This low-temperature spectrum is similar to that of  $\text{C}(\text{SiBrMe}_2)_4$  at 213 K. Again, the four large resonances (I to IV) and the two smaller signals (1 and 2) probably arise from a  $C_1$  conformer and a less abundant  $C_2$  conformer, respectively.

A 2D  $^1\text{H}/^{29}\text{Si}$  NMR shift correlation spectrum of  $\text{C}(\text{SiClMe}_2)_4$  in  $\text{CDCl}_3/\text{CD}_2\text{Cl}_2$  recorded at 201 K is shown in Figure S7. Analysis of this spectrum led to the following conclusions. A small  $^1\text{H}$  NMR signal labelled  $\alpha$ , which is hidden under a large peak at approximately 0.85 ppm, and a small  $^1\text{H}$  NMR signal labelled  $\delta$  at 0.73 ppm are both associated with the  $^{29}\text{Si}$  NMR resonance labelled 2 at 26.04 ppm. The  $^{29}\text{Si}$  NMR resonance labelled 1 at 27.42 ppm interacts with a small signal labelled  $\beta$  that appears to be hidden under the larger  $^1\text{H}$  NMR peak at 0.771 ppm.  $^{29}\text{Si}$  NMR resonance 1 also interacts with a small signal labelled  $\gamma$ , which is hidden by a larger  $^1\text{H}$  NMR signals at 0.74 ppm. These four small proton signals and two small silicon signals are thus assigned to the minor  $C_2$  conformer. The large  $^{29}\text{Si}$  NMR signals I, II, III and IV assigned to the major  $C_1$  conformer present in solution of  $\text{C}(\text{SiClMe}_2)_4$  are all observed to relate to the large  $^1\text{H}$  NMR resonances. Resonance IV at 25.24 ppm interacts with a proton signal at 0.765 ppm labelled D and a proton signal at

0.751 ppm labelled F.  $^{29}\text{Si}$  NMR signal III correlates with a  $^1\text{H}$  NMR resonance labelled B, which coincides with other signals at approximately 0.85 ppm. Signal III is also linked to a  $^1\text{H}$  NMR resonance labelled E at 0.755 ppm. Signal II at 26.91 ppm is associated with proton signal A overlapping with other signals at 0.85 ppm and signal C seen at 0.771 ppm. The remaining  $^{29}\text{Si}$  NMR signal I at 27.55 ppm interacts with proton signals G and H both located within the large  $^1\text{H}$  NMR signal at 0.74 ppm.

A summary of the interpretation of this 2D  $^1\text{H}/^{29}\text{Si}$  NMR correlation experiment is given in Table S25.

**Table S25** Signal assignments derived from the 2D  $^1\text{H}/^{29}\text{Si}$  NMR shift correlation spectrum of  $\text{C}(\text{SiClMe}_2)_4$  at 201 K.

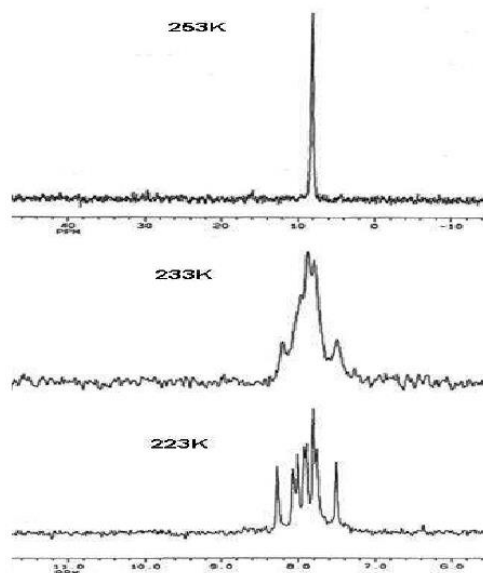
$C_1$ conformer		$C_2$ conformer	
$^1\text{H}$	$^{29}\text{Si}$	$^1\text{H}$	$^{29}\text{Si}$
I	G and H	1	$\beta$ and $\gamma$
II	A and C	2	$\alpha$ and $\delta$
III	B and E		
IV	D and F		

Although saturation transfer experiments were useful for  $\text{C}(\text{SiBrMe}_2)_4$  signal assignment (see below) no  $^1\text{H}$  NMR saturation transfer experiments could be carried out for  $\text{C}(\text{SiClMe}_2)_4$  due to the close proximity of resonances in the  $^1\text{H}$  NMR spectrum. The energy transfer processes occurring between conformers of  $\text{C}(\text{SiClMe}_2)_4$  in solution at low temperature were not, therefore, investigated. Given the similarities of the  $^1\text{H}$  NMR spectrum of  $\text{C}(\text{SiClMe}_2)_4$  in Figure S6 to that of the analogous bromide, it is likely that similar processes occur.

A series of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of  $\text{C}(\text{SiClMe}_2)_4$  in  $\text{CDCl}_3$  was recorded in the range of 298 to 223 K at 126 MHz (Figure S8). At 298 K a single sharp signal due to the carbon atoms of eight methyl groups was seen at 8.28 ppm. On reaching 223 K, this signal had split out into one large peak at 7.79 ppm and seven smaller peaks at 8.25, 8.06, 8.00, 7.91, 7.88, and 7.75 ppm. Another small peak at 15.40 ppm that may be due to a quaternary carbon (these carbons are usually very difficult to observe) was observed beyond the range of the spectra shown in Figure S8. However, this signal was not seen at higher temperatures. For a  $C_1$  conformer eight different  $^{13}\text{C}$  NMR signals for methyl groups would be expected. For a  $C_2$  conformer there should be four methyl signals. Eight methyl-carbon signals are seen in the  $^{13}\text{C}$  NMR spectrum and may belong to a  $C_1$  conformer of  $\text{C}(\text{SiClMe}_2)_4$ . Four carbon signals corresponding to a  $C_2$  conformer cannot be seen although

these may be hidden by the larger signals and similar to the  $^1\text{H}$  NMR spectrum. It has not been possible to assign any  $^{13}\text{C}$  NMR resonances in the absence of a  $^{13}\text{C}/^1\text{H}$  NMR or  $^{13}\text{C}/^{29}\text{Si}$  NMR shift correlation spectrum but this does not detract from the arguments based on the  $^1\text{H}$  and  $^{29}\text{Si}$  spectra above.

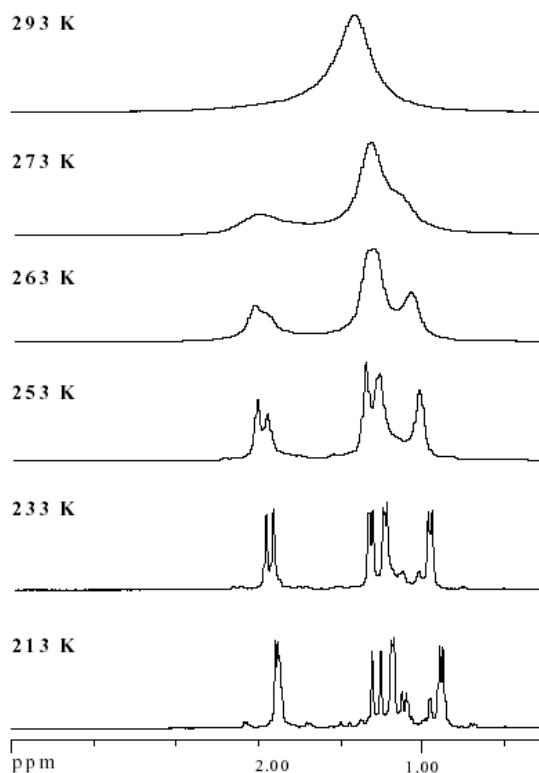
**Figure S8** 126 MHz  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of  $\text{C}(\text{SiClMe}_2)_4$  in the range 253 to 223 K.



#### $\text{C}(\text{SiBrMe}_2)_4$ and $\text{C}(\text{SiMe}_2)_4$

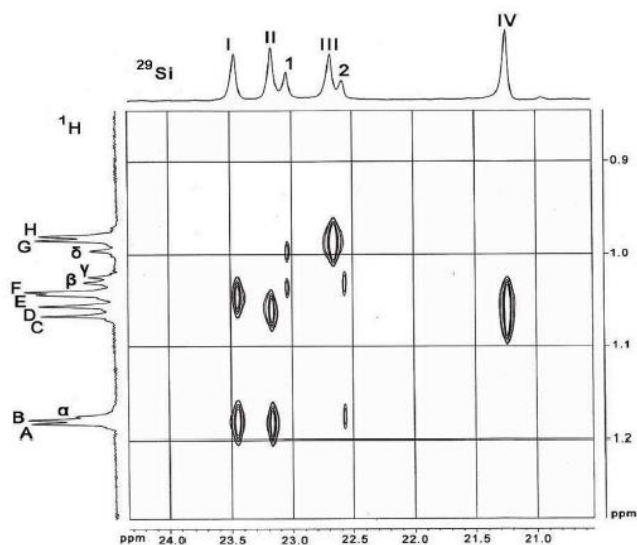
A series of 500 MHz  $^1\text{H}$  NMR spectra of  $\text{C}(\text{SiBrMe}_2)_4$  in  $\text{CDCl}_3$  was recorded in the temperature range 293 to 213 K and is shown in Figure S9. At 293 K a single broad signal is seen at 1.08 ppm which suggests that hindered rotation is occurring even at room temperature. This resonance broadens further and splits out into other signals between the temperatures of 293 and 273 K and more complicated splitting occurs on lowering the temperature to 213 K.

**Figure S9** 500 MHz  $^1\text{H}$  NMR spectra of  $\text{C}(\text{SiBrMe}_2)_4$  in  $\text{CDCl}_3$  in the temperature range from 293 to 213 K.



A better resolved 500 MHz  $^1\text{H}$  NMR spectrum of  $\text{C}(\text{SiBrMe}_2)_4$  in  $\text{CDCl}_3/\text{CD}_2\text{Cl}_2$  solution was obtained at 213 K (Figure S10). Eight large peaks were observed at 1.183, 1.179, 1.066, 1.055, 1.042, 1.040, 0.984, and 0.980 ppm and are labelled A, B, C, D, E, F, G, H, respectively. Four smaller signals were seen at 1.175, 1.029, 1.023, and 0.996 ppm and are labelled  $\alpha$ ,  $\beta$ ,  $\gamma$ , and  $\delta$ , respectively.

**Figure S10** 2D  $^1\text{H}/^{29}\text{Si}$  NMR correlation spectrum of  $\text{C}(\text{SiBrMe}_2)_4$  in  $\text{CDCl}_3/\text{CD}_2\text{Cl}_2$  at 213 K.



The  $^1\text{H}$  part of the spectrum shown in Figure S10 is consistent with the presence of two different conformers of  $\text{C}(\text{SiBrMe}_2)_4$  at low temperature. The four smaller peaks may be assigned to a  $C_2$  conformer and the eight larger peaks are consistent with the eight different methyl-group proton environments of a  $C_1$  conformer. Integration of all signals leads to the conclusion that the  $C_1$  conformer is the most abundant and makes up *ca.* 85% of the conformer mixture, while the  $C_2$  conformer gives rise to the remaining 15% of the conformer mixture.

A 119 MHz  $^{29}\text{Si}\{^1\text{H}\}$  inverse-gated NMR spectrum of a solution of  $\text{C}(\text{SiBrMe}_2)_4$  in  $\text{CDCl}_3$  was recorded at 300 K and shows a single broad resonance due to four equivalent silicon nuclei at 19.99 ppm. The 99 MHz  $^{29}\text{Si}\{^1\text{H}\}$  INEPT NMR spectrum in  $\text{CDCl}_3/\text{CD}_2\text{Cl}_2$  recorded at 213 K (Figure S10) is complicated, but may be related to the corresponding  $^1\text{H}$  NMR spectrum also shown in Figure S10. Four large resonances at 23.47, 23.17, 22.68, and 21.24 ppm labelled I, II, III and IV, respectively, and corresponding to a conformer of  $C_1$  symmetry are observed together with two smaller signals at 23.04 and 22.58 ppm labelled 1 and 2, respectively, which have been assigned to a less abundant  $C_2$  conformer. A 2D  $^1\text{H}/^{29}\text{Si}$  NMR shift correlation spectrum recorded at 213 K is shown in Figure S10. This correlation spectrum was used to assign the individual  $^1\text{H}$  NMR signals to the  $^{29}\text{Si}$  NMR resonances.

Table S26 gives a summary of the  $^1\text{H}/^{29}\text{Si}$  NMR signal pairings as assigned from the spectrum in Figure S10. Proton signals E and F have both been assigned to two different silicon atoms as they are so close together that it is impossible to see which one is

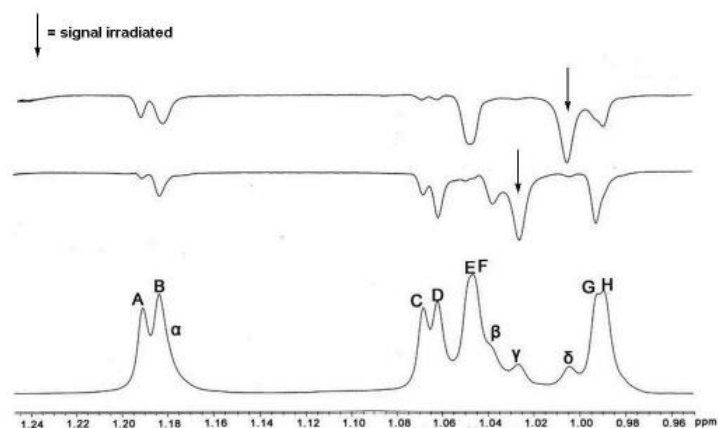
associated with a particular  $^{29}\text{Si}$  NMR signal. The 2D  $^1\text{H}/^{29}\text{Si}$  NMR correlation spectrum is thus consistent with the presence of a more abundant  $C_1$  isomer and a less abundant  $C_2$  isomer, as seen for  $\text{C}(\text{SiClMe}_2)_4$ .

**Table S26** Summary of the signal assignments from the 2D  $^1\text{H}/^{29}\text{Si}$  NMR correlation spectrum of  $\text{C}(\text{SiBrMe}_2)_4$  at 213 K.

$C_1$ conformer		$C_2$ conformer	
$^{29}\text{Si}$	$^1\text{H}$	$^{29}\text{Si}$	$^1\text{H}$
I	E/F and B	1	$\beta$ and $\delta$
II	A and D	2	$\alpha$ and $\gamma$
III	G and H		
IV	E/F and C		

Several saturation transfer  $^1\text{H}$  NMR experiments of  $\text{C}(\text{SiBrMe}_2)_4$  at 213 K were carried out in order to investigate the dynamic processes occurring at low temperature. This was done by selectively irradiating a signal of one conformer and observing the response of other signals across the spectrum. When the signal at 0.996 ppm labelled  $\delta$  in the original  $^1\text{H}$  NMR spectrum and assigned to the  $C_2$  conformer was selectively irradiated, the signals labelled A, E, F, and H belonging to the  $C_1$  conformer and  $\alpha$  belonging to the  $C_2$  conformer were increased (see Figure S11). Irradiation at the resonance of  $\gamma$  at 1.023 ppm gave rise to increased signals of B, C, D, and G of the  $C_1$  conformer and  $\beta$  of the  $C_2$  conformer (Figure S11).

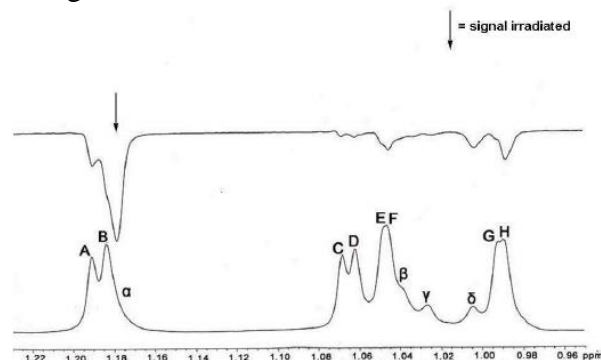
**Figure S11**  $^1\text{H}$  NMR saturation transfer experiments of  $\text{C}(\text{SiBrMe}_2)_4$  at 213 K. Irradiation of signal  $\delta$  (upper spectrum) and irradiation of signal  $\gamma$  (middle spectrum).





Irradiation of signal  $\alpha$  at 1.175 ppm led to an increase of resonances A, E, F, and H of the  $C_1$  conformer and  $\delta$  belonging to the  $C_2$  conformer (Figure 12). Signals E and F have been assigned tentatively and the increase in signal H could also be due to signal G.

**Figure S12**  $^1\text{H}$  NMR saturation transfer experiment of  $\text{C}(\text{SiBrMe}_2)_4$  at 213 K on irradiation of signal  $\alpha$ .



When signals labelled C at 1.066 ppm and A at 1.183 ppm of the  $C_1$  conformer were selectively irradiated in different saturation transfer experiments, no other signals appeared to be increased as a result. Table S27 summarises the results of the  $^1\text{H}$  NMR saturation transfer experiments.

**Table S27** Results of the  $^1\text{H}$  NMR saturation transfer experiments of  $\text{C}(\text{SiBrMe}_2)_4$  at 213 K.

$C_1$ conformer	$C_2$ conformer
$\alpha$	A, E, F, H, and $\delta$
$\gamma$	B, C, D, G, and $\beta$
$\delta$	A, E, F, H, and $\alpha$

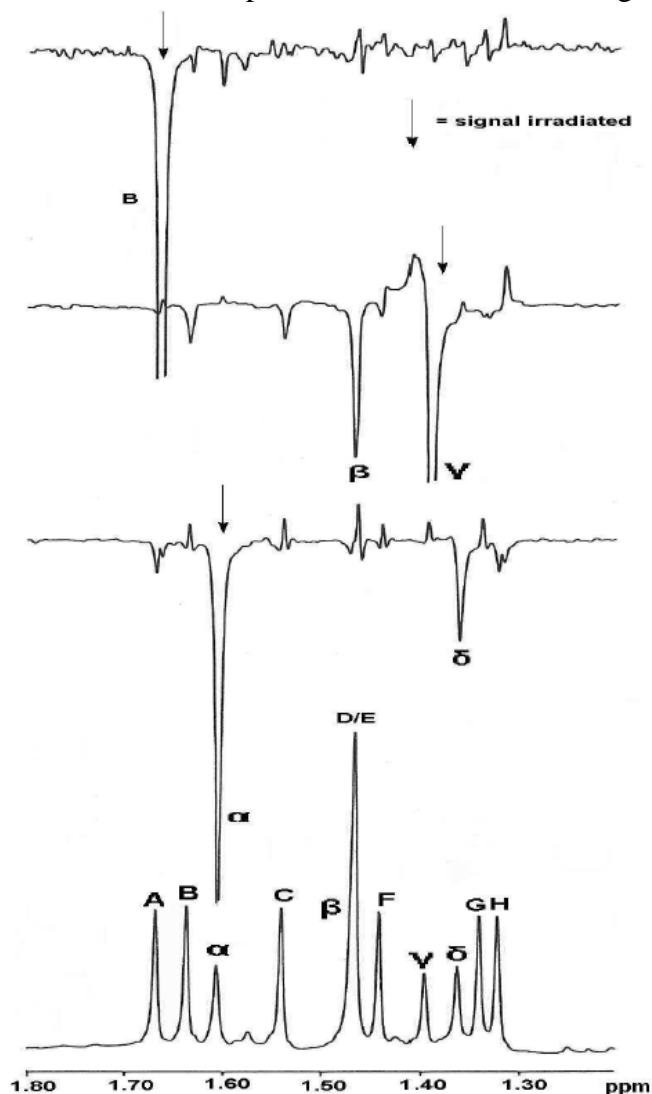
These observations lead to the conclusion that at 213 K two different processes occur within  $\text{C}(\text{SiBrMe}_2)_4$ . One process involves an energy transfer between the  $C_2$  and the  $C_1$  conformers. The other energy transfer process occurs within the  $C_2$  conformer. The latter process involves rotations of approximately  $120^\circ$  in the same direction (either clockwise or anticlockwise) of all four silyl groups of the  $C_2$  conformer of  $\text{C}(\text{SiBrMe}_2)_4$ , thus resulting in  $C_2$  symmetry again. The intramolecular rotations converting a  $C_2$  into a  $C_1$  conformer and *vice versa* in the former process have not been calculated for  $\text{C}(\text{SiBrMe}_2)_4$ . However, the dihedral angle  $\text{H}(14)\text{--Si}(2)\text{--C}(1)\text{--Si}(3)$  of the analogous compound  $\text{C}(\text{SiHMe}_2)_4$  was calculated to rotate by  $93.2^\circ$  on going from the  $C_2$  to the  $C_1$  conformer and *vice versa* (see

Figure 1 for atom numbering). The equivalent dihedral angles for  $C(\text{SiBrMe}_2)_4$  are expected to undergo rotations of similar magnitudes.

From the 2D  $^1\text{H}/^{29}\text{Si}$  NMR spectroscopy discussed above it is known that proton signals of the  $C_1$  conformer A, E, F, and H are associated with silicon signals II, either I or IV, either I or IV and III, respectively. All of these proton signals belonging to the  $C_1$  conformer exchange with both  $\alpha$  located on one silicon and  $\delta$  located on another silicon of the  $C_2$  conformer (Figure S10). Signals  $\alpha$  and  $\delta$  also exchange with each other (Figure S10). The signals of the  $C_1$  conformer labelled B, C, D, and G have been assigned to silicon signals I, IV, II and III and exchange with both signals  $\beta$  and  $\gamma$  of conformer  $C_2$  (Figure S10). No  $^1\text{H}$  NMR saturation transfer spectrum has been recorded in which signal  $\beta$  associated with silicon 1 was irradiated. However, it can be assumed that  $\beta$  also exchanges with protons B, C, D, and G of conformer  $C_1$ . It is known that proton signals  $\gamma$  on silicon 2 and  $\beta$  on silicon 1 exchange with each other.

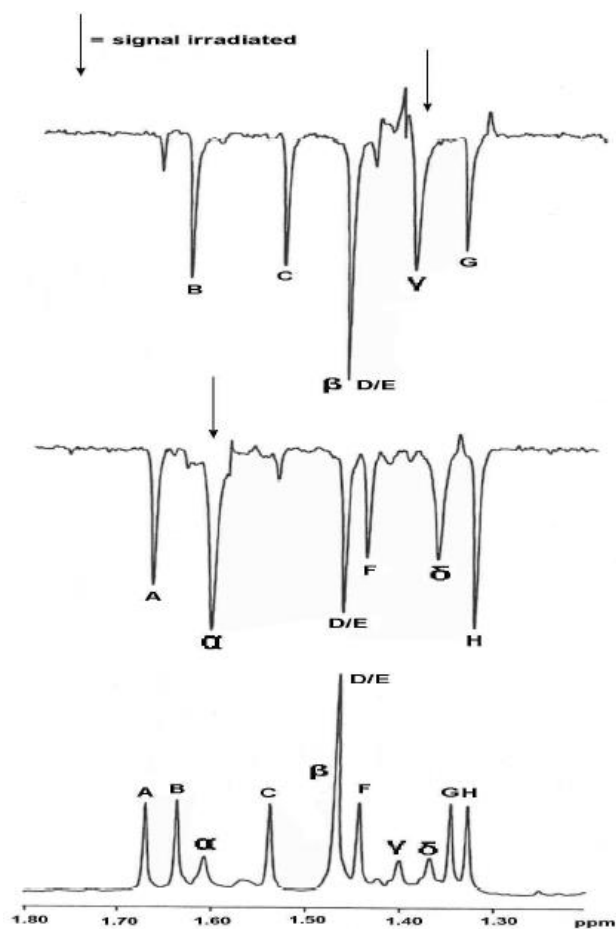
Similar exchange processes between  $C_1$  and  $C_2$  conformers as well as within a  $C_2$  conformer were observed when low-temperature 360 MHz  $^1\text{H}$  NMR saturation transfer spectra of the analogous compound  $C(\text{SiMe}_2)_4$  in  $\text{CD}_2\text{Cl}_2$  were recorded in previous work.<sup>54</sup> Rotations within  $C(\text{SiMe}_2)_4$  are more sterically hindered than  $C(\text{SiBrMe}_2)_4$  due to the bulkier iodine substituents and gives rise to low-temperature spectra that are better resolved than in the analogous bromide. The  $^1\text{H}$  NMR spectrum of  $C(\text{SiMe}_2)_4$  at 223 K is shown at the bottom of Figure S13. Eight large signals labelled A to H can be seen and are assumed to be due to a  $C_1$  conformer. Another four smaller signals labelled  $\alpha$  to  $\delta$  are observed and assigned to a less abundant  $C_2$  conformer. The largest signal seen appears to be due to two large signals D and E and a small signal  $\beta$ . The appearance of this spectrum resembles that of the analogous bromide. Figure S13 also shows three  $^1\text{H}$  NMR saturation experiments at 223 K. When signal  $\alpha$  belonging to the  $C_2$  conformer was irradiated, signal  $\delta$ , which is also due to the  $C_2$  conformer, was enlarged.

**Figure S13** 360 MHz  $^1\text{H}$  NMR spectrum of  $\text{C}(\text{SiMe}_2)_4$  at 223 K (bottom) and  $^1\text{H}$  NMR saturation transfer experiments on irradiation of signals  $\alpha$ ,  $\gamma$  and B.



Irradiation of signal  $\gamma$  of the  $C_2$  conformer led to the increase of signal  $\beta$  of the  $C_2$  conformer. When signal B belonging to the  $C_1$  conformer was irradiated no energy transfer occurred. Raising the temperature to 243 K did not change the appearance of the  $^1\text{H}$  NMR spectrum of  $\text{C}(\text{SiMe}_2)_4$  as can be seen at the bottom of Figure S14.  $^1\text{H}$  NMR saturation transfer experiments conducted at this temperature, however, yielded results different to those obtained at 223 K. Irradiation of signal  $\alpha$  resulted in an increase of signal  $\delta$  (Figure S14) as seen above at lower temperature. At the same time, signals A, D, E, F, and H due to the  $C_1$  conformer were also enhanced. When signal  $\gamma$  was irradiated, energy transfer occurred to signal  $\beta$  (Figure S14) as expected from the saturation transfer spectrum at 223 K. Increases in signals B, C, D, E and G due to the  $C_1$  conformer were also seen.

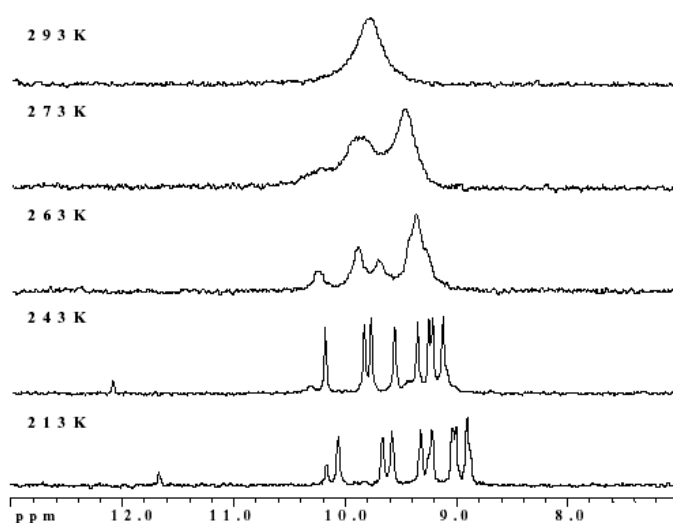
**Figure S14** 360 MHz  $^1\text{H}$  NMR spectrum of  $\text{C}(\text{SiMe}_2)_4$  at 243 K (bottom) and  $^1\text{H}$  NMR saturation transfer experiments on irradiation of signals  $\alpha$  and  $\gamma$ .



The energy exchange between signals of  $C_1$  and  $C_2$  conformers of  $\text{C}(\text{SiMe}_2)_4$ , which only occurs at higher temperatures, appears to be the higher temperature process. The lower temperature process still occurring at 223 K is the energy transfer between two signals of the  $C_2$  conformer. Intramolecular rotations converting a  $C_1$  into a  $C_2$  conformer are assumed to be energetically less favourable than the rotations within the  $C_2$  conformer. In the  $^1\text{H}$  NMR saturation transfer spectra of  $\text{C}(\text{SiBrMe}_2)_4$  both exchange processes are still seen at 213 K. This is attributed to the smaller bromine substituents, which permit both types of rotation at low temperature.

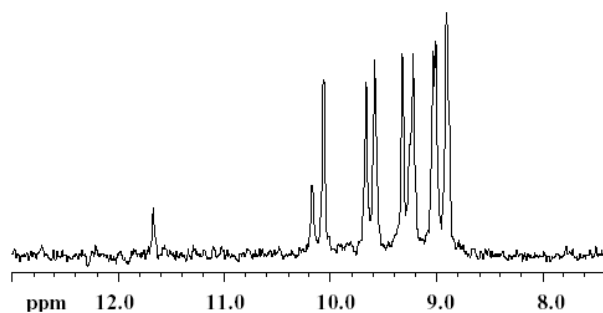
A series of variable temperature 126 MHz  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of  $\text{C}(\text{SiBrMe}_2)_4$  in  $\text{CDCl}_3$  were recorded in the temperature range of 293 to 213 K (Figure S15).

**Figure S15** 126 MHz  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of  $\text{C}(\text{SiBrMe}_2)_4$  in  $\text{CDCl}_3$  in the range from 293 to 213 K.



At 293 K a single broad peak, that corresponds to the carbon atoms of eight equivalent methyl groups, and is consistent with the broad signal seen in the  $^1\text{H}$  NMR spectrum at 293 K, was visible at 9.78 ppm. This signal broadened further and split into several other signals on lowering the temperature, Figure S16.

**Figure S16** Expansion of the  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of  $\text{C}(\text{SiBrMe}_2)_4$  at 213 K.



Eight large signals at 10.12, 9.74, 9.66, 9.42, 9.28, 9.13, 9.10 and 8.99 ppm, as well as two small signals at 11.83 and 10.24 ppm were observed. A  $C_1$  conformer of  $\text{C}(\text{SiBrMe}_2)_4$  is expected to give rise to eight different  $^{13}\text{C}$  NMR signals, whereas a  $C_2$  conformer will give rise to only four  $^{13}\text{C}$  NMR signals. The eight large  $^{13}\text{C}$  NMR signals seen are consistent with the more abundant  $C_1$  conformer seen in the  $^1\text{H}$  NMR and  $^{29}\text{Si}$  NMR spectra discussed above. Only two of the expected four small signals are observed for a less abundant  $C_2$  conformer. It is likely that another two small signals are hidden under the larger signals. It is also possible that the small signal at 11.83 ppm, which only became visible between 263 and 243 K, is due to a quaternary carbon, but these are usually very difficult to observe.