Supporting Information

New Insights into Hexacoordinated Silicon Complexes with 8-Oxyquinolinato Ligands: 1,3-Shift of Si-Bound Hydrocarbyl Substituents and the Influence of Si-Bound Halides on the 8-Oxyquinolinate Coordination Features

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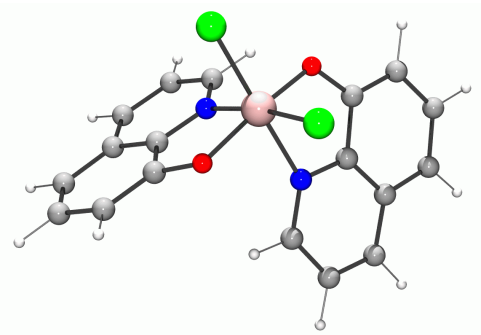

Fig. SI1. Molecular structure of *O,O-trans* (oxinate)$_2$SiCl$_2$ optimized at the MPW1PW91/6-311G(d,p) level.

Table SI1. Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structures of *O,O-trans* (oxinate)$_2$SiCl$_2$ (37 atoms), E = -2163,28298879 a.u.

C	1.72694000	-1.75988800	2.56517700
C	2.85269400	-2.07893300	1.84413300
C	-4.21382800	-1.64390500	0.23769100
C	-4.30898300	-0.91831400	1.40286000
C	0.82215500	-0.80557400	2.07213200
C	-2.85269300	-2.07893300	-1.84413400
C	-3.10055900	-1.44364900	-0.60806800
C	3.10056000	-1.44364900	0.60806700
C	-3.33883300	0.02550400	1.79908100
C	4.21382900	-1.64390400	-0.23769200
C	-1.72693900	-1.75988800	-2.56517700
C	-2.13223600	-0.50704400	-0.19879600
C	-2.23795100	0.23859800	0.99845900
C	2.13223700	-0.50704400	0.19879600
C	4.30898300	-0.91831300	-1.40286000
C	-0.82215400	-0.80557400	-2.07213200
C	2.23795100	0.23859900	-0.99845800
C	3.33883300	0.02550500	-1.79908100
H	1.52576300	-2.22723600	3.51976700
H	3.55827200	-2.80994400	2.22245900
H	-4.98171300	-2.35464200	-0.04024800
H	-5.16812500	-1.06733100	2.04645100
H	-3.55827000	-2.80994400	-2.22246000
H	4.98171400	-2.35464100	0.04024700
H	-0.06077400	-0.50574000	2.61990300
H	-3.45454400	0.59085100	2.71441400
H	-1.52576200	-2.22723600	-3.51976700
H	5.16812500	-1.06732900	-2.04645200
H	0.06077500	-0.50573900	-2.61990300
H	3.45454400	0.59085300	-2.71441400
N	1.02594900	-0.21393500	0.91275800
N	-1.02594900	-0.21393500	-0.91275800
O	-1.24504900	1.07459600	1.24420000
O	1.24504900	1.07459800	-1.24419900
Si	0.00000000	1.28791300	0.00000000
Cl	1.08368200	2.68344900	1.19295000
Cl	-1.08368400	2.68344900	-1.19295000

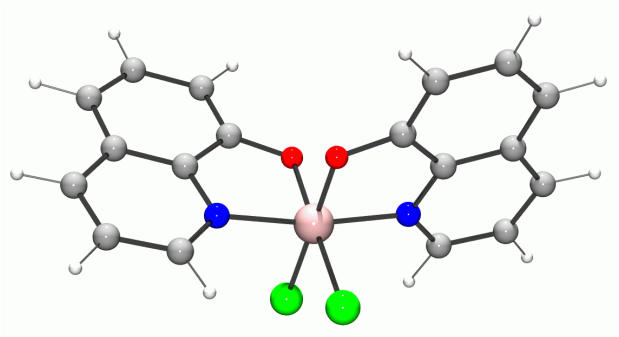

Fig. SI2. Molecular structure of *N,N-trans* (oxinate)$_2$SiCl$_2$ optimized at the MPW1PW91/6-311G(d,p) level.

Table SI2. Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structures of *N,N-trans* (oxinate)$_2$SiCl$_2$ (37 atoms), E = -2163,28589560 a.u.

C	3.60430500	-2.32504900	-1.70429300
C	2.25557800	-1.97396300	-1.90732000
C	4.38970800	-1.74491900	-0.73441900
C	1.67569600	-1.00941800	-1.10948200
C	3.82965900	-0.75276400	0.09910300
C	2.47975200	-0.40984900	-0.10899000
C	4.49001100	-0.05436400	1.13225400
C	-2.25557700	-1.97396300	1.90732000
C	3.81457300	0.89277400	1.86330600
C	-3.60430400	-2.32504900	1.70429400
C	-1.67569500	-1.00941800	1.10948200
C	2.46824400	1.16945800	1.58479200
C	-4.38970800	-1.74491900	0.73442000
C	-2.47975200	-0.40984900	0.10898900
C	-3.82965900	-0.75276400	-0.09910200
C	-2.46824500	1.16945700	-1.58479200
C	-4.49001100	-0.05436500	-1.13225300
C	-3.81457300	0.89277300	-1.86330600
H	4.03588600	-3.08511800	-2.34521900
H	1.66875200	-2.44860900	-2.68247600
H	5.42436400	-2.03579000	-0.60538800
H	5.53165100	-0.26973500	1.34225000
H	-1.66875000	-2.44860800	2.68247600
H	-4.03588500	-3.08511800	2.34522100
H	4.30434700	1.43919800	2.65775700
H	-5.42436400	-2.03579100	0.60539000
H	-5.53165200	-0.26973600	-1.34224900
H	-4.30434800	1.43919700	-2.65775700
N	1.83316000	0.52824700	0.62301700
N	-1.83316000	0.52824600	-0.62301700
O	0.43621900	-0.57648900	-1.18052300
O	-0.43621900	-0.57648900	1.18052200
Si	0.00000000	0.69546800	-0.00000100
Cl	0.54950200	2.22274500	-1.46303200
Cl	-0.54950300	2.22274500	1.46303200
H	-1.89793300	1.90786500	-2.13151500
H	1.89793200	1.90786600	2.13151400

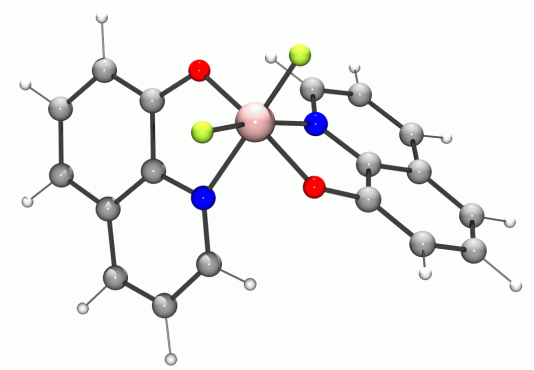

Fig. SI3. Molecular structure of *O,O-trans* (oxinate)$_2$SiF$_2$ optimized at the MPW1PW91/6-311G(d,p) level.

Table SI3. Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structures of *O,O-trans* (oxinate)$_2$SiF$_2$ (37 atoms), E = -1442,55103852 a.u.

C	-4.24726300	0.09453700	-1.35694000
C	-2.83516100	-1.95458900	-1.77736200
C	-4.36464900	1.26792600	-0.64767900
C	-3.10941400	-0.71751100	-1.15530700
C	2.83530500	1.95485100	-1.77702500
C	-1.68756200	-2.64146900	-1.46126300
C	1.68778200	2.64177200	-1.46075600
C	4.24730000	-0.09443200	-1.35690100
C	3.10950100	0.71765300	-1.15517500
C	-3.39641900	1.70373700	0.27992900
C	-2.14221500	-0.26949700	-0.23483100
C	0.78487600	2.10888600	-0.52567600
C	-0.78467400	-2.10866200	-0.52613100
C	4.36463900	-1.26790000	-0.64775600
C	-2.27072500	0.93659900	0.49868800
C	2.14229100	0.26959800	-0.23471700
C	3.39642100	-1.70374300	0.27983400
C	2.27075400	-0.93657000	0.49868300
H	-3.53805700	-2.36062600	-2.49613800
H	3.53818000	2.36093900	-2.49579800
H	1.46635000	3.59704900	-1.91755800
H	-1.46604500	-3.59665200	-1.91821500
H	5.01441400	0.21418500	-2.05572600
H	-0.11941200	2.62418700	-0.23189900
H	5.24137000	-1.88723400	-0.79824900
H	0.11965200	-2.62395200	-0.23248000
H	3.53158500	-2.62508300	0.83116200
N	-1.01111000	-0.94632900	0.05017800
N	1.01124100	0.94644800	0.05043100
O	-1.28105700	1.21694600	1.31794900
O	1.28119000	-1.21690700	1.31804500
Si	-0.00013000	-0.00022400	1.53352400
F	-0.81623300	-0.93424300	2.59075500
F	0.81562200	0.93355400	2.59127100
H	-5.01438500	-0.21406300	-2.05578400
H	-5.24141700	1.88725400	-0.79810000
H	-3.53161300	2.62507100	0.83130100

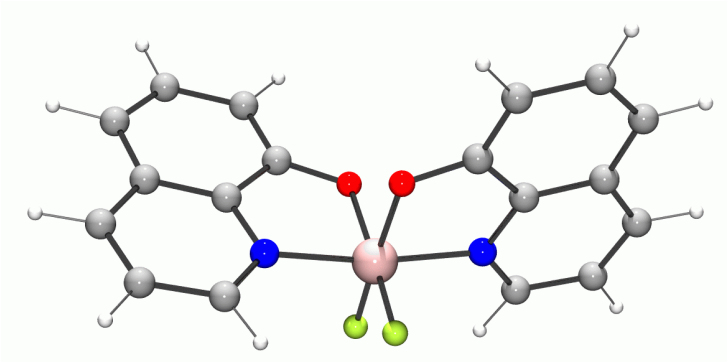

Fig. SI4. Molecular structure of *N,N-trans* (oxinate)$_2$SiF$_2$ optimized at the MPW1PW91/6-311G(d,p) level.

Table SI4. Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structures of *N,N-trans* (oxinate)$_2$SiF$_2$ (37 atoms), E = -1442,55531828 a.u.

C	3.63611500	-2.09428300	-1.71512400
C	2.27563000	-1.78239200	-1.90826100
C	4.42481200	-1.47718400	-0.76974300
C	1.67867700	-0.81355100	-1.12451900
C	3.85171400	-0.48257900	0.05228500
C	2.49225600	-0.17798300	-0.14879600
C	4.49811800	0.25277000	1.06927500
C	-2.27563000	-1.78239100	1.90826200
C	3.80298400	1.19421700	1.79243600
C	-3.63611600	-2.09428200	1.71512500
C	-1.67867700	-0.81355000	1.12452000
C	2.44647700	1.42689100	1.52113500
C	-4.42481300	-1.47718400	0.76974400
C	-2.49225600	-0.17798200	0.14879600
C	-3.85171400	-0.48257900	-0.05228400
C	-2.44647600	1.42689100	-1.52113600
C	-4.49811800	0.25276900	-1.06927500
C	-3.80298300	1.19421600	-1.79243700
H	4.07655000	-2.85802300	-2.34600800
H	1.69299700	-2.29223600	-2.66417400
H	5.46721800	-1.74380200	-0.65105000
H	5.54659900	0.06957400	1.27646700
H	-1.69299700	-2.29223500	2.66417500
H	-4.07655000	-2.85802200	2.34601000
H	4.28668200	1.76380700	2.57445300
H	-5.46721800	-1.74380200	0.65105100
H	-5.54659900	0.06957300	-1.27646800
H	-4.28668200	1.76380600	-2.57445400
N	1.83024800	0.74969500	0.57318500
N	-1.83024700	0.74969500	-0.57318500
O	0.43563300	-0.40604800	-1.18038300
O	-0.43563300	-0.40604700	1.18038400
Si	0.00000000	0.89205100	0.00000000
F	0.32396200	2.04337700	-1.14684000
F	-0.32396200	2.04337800	1.14683900
H	-1.84705400	2.15100000	-2.05579300
H	1.84705400	2.15100100	2.05579300

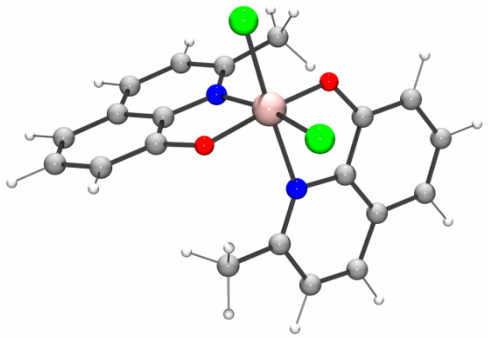

Fig. SI5. Molecular structure of *O,O-trans* (8-oxyquinaldinate)$_2$SiCl$_2$ optimized at the MPW1PW91/6-311G(d,p) level.

Table SI5. Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structures of *O,O-trans* (8-oxyquinaldinate)$_2$SiCl$_2$ (43 atoms), E = -2241,91335089 a.u.

C	-1.92462000	3.49257600	-2.40761800
C	-2.05874600	2.16197300	-1.97478600
C	-0.92293700	4.31008700	-1.94246800
C	-1.17036400	1.64491100	-1.05608500
C	0.00000000	3.80550900	-1.00170200
C	-0.13393900	2.47345800	-0.56427400
C	1.07397000	4.52915700	-0.44795800
C	2.05874600	-2.16197300	-1.97478600
C	1.90722200	3.91841100	0.44593900
C	1.92462000	-3.49257600	-2.40761800
C	1.17036400	-1.64491100	-1.05608500
C	1.71485800	2.57394500	0.84309500
C	0.92293700	-4.31008700	-1.94246800
C	0.13393900	-2.47345800	-0.56427400
C	0.00000000	-3.80550900	-1.00170200
C	-2.67113900	-1.97389100	1.81663000
C	-1.71485800	-2.57394500	0.84309500
C	-1.07397000	-4.52915700	-0.44795800
C	-1.90722200	-3.91841100	0.44593900
C	2.67113900	1.97389100	1.81663000
H	-2.63537300	3.87679900	-3.12979000
H	-2.85169200	1.52961300	-2.35189800
H	-0.82961300	5.33316300	-2.28444300
H	1.23497600	5.56151100	-0.73755000
H	2.85169200	-1.52961300	-2.35189800
H	2.63537300	-3.87679900	-3.12979000
H	2.74193900	4.45581600	0.87561600
H	-3.10751900	-1.05718200	1.42171400
H	0.82961300	-5.33316300	-2.28444300
H	-3.46597700	-2.68582400	2.03447300
H	3.10751900	1.05718200	1.42171400
H	-1.23497600	-5.56151100	-0.73755000
H	3.46597700	2.68582400	2.03447300
H	-2.74193900	-4.45581600	0.87561600
H	-2.16770100	-1.70889000	2.74698400
H	2.16770100	1.70889000	2.74698400
N	0.69759200	1.88106600	0.34240300
N	-0.69759200	-1.88106600	0.34240300
O	-1.20405000	0.41043000	-0.59358300
O	1.20405000	-0.41043000	-0.59358300
Si	0.00000000	0.00000000	0.62805100

Cl	-1.29409800	0.83548000	2.18327900
Cl	1.29409800	-0.83548000	2.18327900

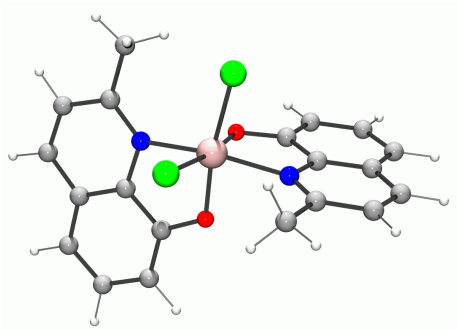

Fig. SI6. Molecular structure of *N,N-trans* (8-oxyquinaldinate)$_2$SiCl$_2$ optimized at the MPW1PW91/6-311G(d,p) level.

Table SI6. Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structures of *N,N-trans* (8-oxyquinaldinate)$_2$SiCl$_2$ (43 atoms), E = -2241,91011815 a.u.

C	-1.92462000	3.49257600	-2.40761800
C	-2.05874600	2.16197300	-1.97478600
C	-0.92293700	4.31008700	-1.94246800
C	-1.17036400	1.64491100	-1.05608500
C	0.00000000	3.80550900	-1.00170200
C	-0.13393900	2.47345800	-0.56427400
C	1.07397000	4.52915700	-0.44795800
C	2.05874600	-2.16197300	-1.97478600
C	1.90722200	3.91841100	0.44593900
C	1.92462000	-3.49257600	-2.40761800
C	1.17036400	-1.64491100	-1.05608500
C	1.71485800	2.57394500	0.84309500
C	0.92293700	-4.31008700	-1.94246800
C	0.13393900	-2.47345800	-0.56427400
C	0.00000000	-3.80550900	-1.00170200
C	-2.67113900	-1.97389100	1.81663000
C	-1.71485800	-2.57394500	0.84309500
C	-1.07397000	-4.52915700	-0.44795800
C	-1.90722200	-3.91841100	0.44593900
C	2.67113900	1.97389100	1.81663000
H	-2.63537300	3.87679900	-3.12979000
H	-2.85169200	1.52961300	-2.35189800
H	-0.82961300	5.33316300	-2.28444300
H	1.23497600	5.56151100	-0.73755000
H	2.85169200	-1.52961300	-2.35189800
H	2.63537300	-3.87679900	-3.12979000
H	2.74193900	4.45581600	0.87561600
H	-3.10751900	-1.05718200	1.42171400
H	0.82961300	-5.33316300	-2.28444300
H	-3.46597700	-2.68582400	2.03447300
H	3.10751900	1.05718200	1.42171400
H	-1.23497600	-5.56151100	-0.73755000
H	3.46597700	2.68582400	2.03447300
H	-2.74193900	-4.45581600	0.87561600
H	-2.16770100	-1.70889000	2.74698400
H	2.16770100	1.70889000	2.74698400
N	0.69759200	1.88106600	0.34240300
N	-0.69759200	-1.88106600	0.34240300
O	-1.20405000	0.41043000	-0.59358300
O	1.20405000	-0.41043000	-0.59358300
Si	0.00000000	0.00000000	0.62805100
Cl	-1.29409800	0.83548000	2.18327900

Cl	1.29409800	-0.83548000	2.18327900

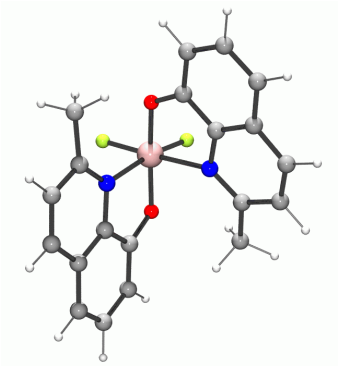

Fig. SI7. Molecular structure of *O,O-trans* (8-oxyquinaldinate)$_2$SiF$_2$ optimized at the MPW1PW91/6-311G(d,p) level.

Table SI7. Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structures of *O,O-trans* (8-oxyquinaldinate)2SiF2 (43 atoms), E = -1521,18085065 a.u.

C	-4.17814400	0.14033200	-1.45913500
C	-2.83500100	-1.93717000	-1.87985900
C	-4.31930200	1.27626100	-0.69921900
C	-3.06972300	-0.70543000	-1.23625600
C	2.83510300	1.93724000	-1.87974000
C	-1.77178500	-2.70288100	-1.49136100
C	1.77188000	2.70295900	-1.49125500
C	4.17817500	-0.14031900	-1.45909900
C	3.06976700	0.70546100	-1.23620500
C	-3.38628500	1.63118200	0.29322700
C	-2.11864400	-0.33654900	-0.26502600
C	0.87377800	2.27063100	-0.48352200
C	-0.87374100	-2.27059400	-0.48354500
C	4.31928600	-1.27627300	-0.69921200
C	-2.27955000	0.83621800	0.51035100
C	2.11865400	0.33656000	-0.26500800
C	3.38625200	-1.63120400	0.29321100
C	2.27951700	-0.83623400	0.51035800
H	-3.51510800	-2.28397500	-2.64988500
H	3.51525600	2.28407500	-2.64971200
H	1.60193200	3.67354600	-1.93905300
H	-1.60178800	-3.67344400	-1.93919500
H	4.91345500	0.12751100	-2.20759000
C	-0.20177600	3.21114800	-0.04548400
H	5.17888100	-1.91788400	-0.85372200
C	0.20176800	-3.21114800	-0.04548200
H	3.53158600	-2.51283000	0.90392100
N	-1.02671200	-1.07212000	0.06649000
N	1.02673000	1.07213500	0.06648700
O	-1.34610300	1.08307900	1.40362800
O	1.34608600	-1.08307700	1.40361600
Si	-0.00005200	0.00001900	1.62388400
F	-0.73114900	-1.01266000	2.67173300
F	0.73105700	1.01247800	2.67189100
H	-4.91341000	-0.12749700	-2.20764700
H	-5.17891200	1.91785700	-0.85372400
H	-3.53163000	2.51279400	0.90395800
H	-0.07274900	-4.22761600	-0.32746000
H	0.35341700	-3.15280500	1.02913800
H	1.15405500	-2.97503500	-0.52647500

H	0.07244500	4.22756500	-0.32792700
H	-0.35304800	3.15319700	1.02921800
H	-1.15418300	2.97466700	-0.52603900

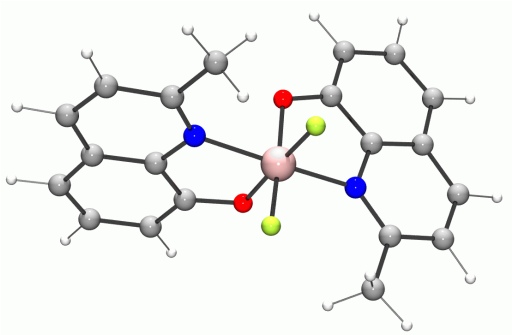

Fig. SI8. Molecular structure of *N,N-trans* (8-oxyquinaldinate)$_2$SiF$_2$ optimized at the MPW1PW91/6-311G(d,p) level.

Table SI8. Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structures of *N,N-trans* (8-oxyquinaldinate)$_2$SiF$_2$ (43 atoms), E = -1521,19147477 a.u.

C	-3.49329700	2.05961500	2.21458600
C	-2.13116600	2.12573800	1.87010600
C	-4.34879300	1.13754200	1.65887500
C	-1.61074400	1.24639600	0.94072900
C	-3.84758900	0.22243800	0.70798300
C	-2.48604400	0.29286400	0.35858000
C	-4.59105400	-0.78414500	0.06006200
C	2.13041500	-2.12831000	1.86738000
C	-3.97439100	-1.61643100	-0.83442600
C	3.49263200	-2.06331400	2.21173700
C	1.61023600	-1.24738300	0.93936300
C	-2.59902500	-1.48931700	-1.13690600
C	4.34846800	-1.14082700	1.65723800
C	2.48590000	-0.29340100	0.35848500
C	3.84752200	-0.22410100	0.70777600
C	1.97074400	2.43454100	-2.10544300
C	2.59943400	1.49107000	-1.13424600
C	4.59134200	0.78312800	0.06126800
C	3.97490500	1.61710800	-0.83179500
C	-1.97010000	-2.43090000	-2.10977500
H	-3.87415400	2.76292500	2.94620400
H	-1.47747700	2.85821300	2.32539700
H	-5.39383500	1.10086200	1.93960500
H	-5.64734000	-0.89747100	0.27784700
H	1.47647100	-2.86114600	2.32172400
H	3.87327500	-2.76786600	2.94227100
H	-4.53333700	-2.39746600	-1.33256300
H	1.12826300	2.95228600	-1.64796900
H	5.39357000	-1.10503200	1.93786200
H	2.70849400	3.16132800	-2.44278700
H	-1.12779400	-2.94959100	-1.65303600
H	5.64771600	0.89562800	0.27905400
H	-2.70777200	-3.15699600	-2.44878000
H	4.53410100	2.39870000	-1.32878100
H	1.56771100	1.89826000	-2.96415200
H	-1.56673300	-1.89295900	-2.96727600
N	-1.89064700	-0.53645700	-0.54135700
N	1.89074500	0.53755500	-0.54012400
O	-0.36141500	1.20731900	0.54271300
O	0.36086700	-1.20710700	0.54162000
Si	0.00005900	0.00084900	-0.72201300

F	-0.39827400	1.10919500	-1.88565600
F	0.39886800	-1.10639600	-1.88658900

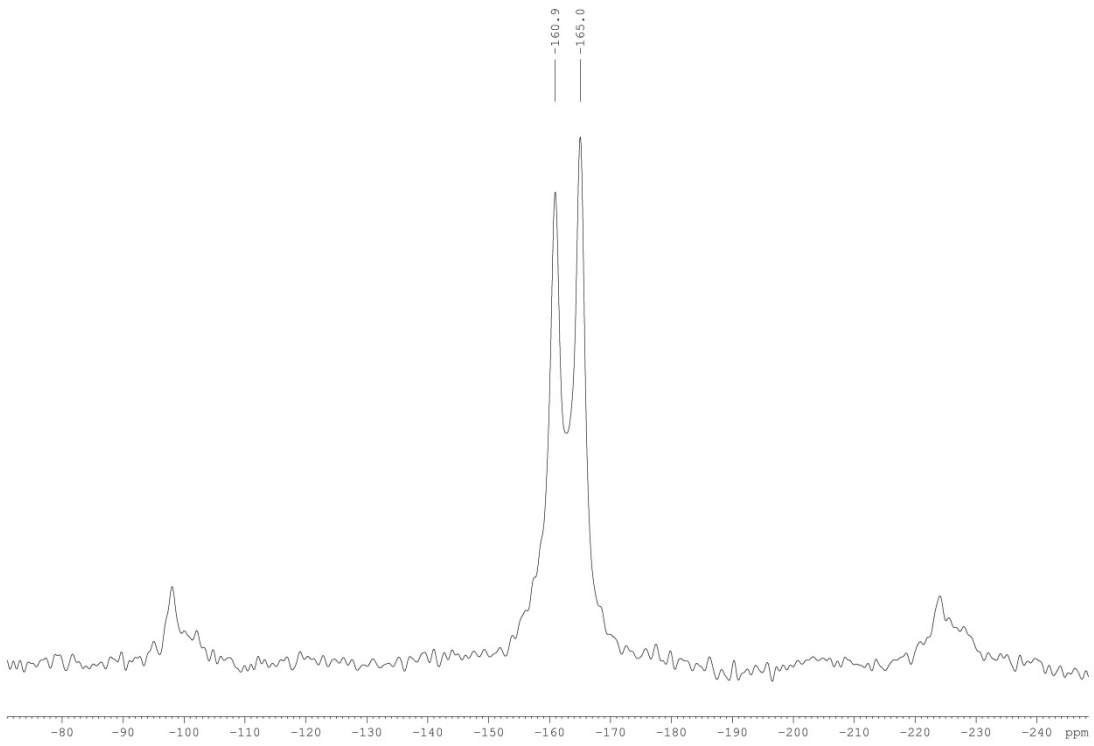

Fig. SI8. ^{29}Si CP/MAS NMR spectrum (79,5 MHz, ν_{spin} = 5 kHz) of the chloroform solvate of (oxinate)$_2$SiF$_2$.

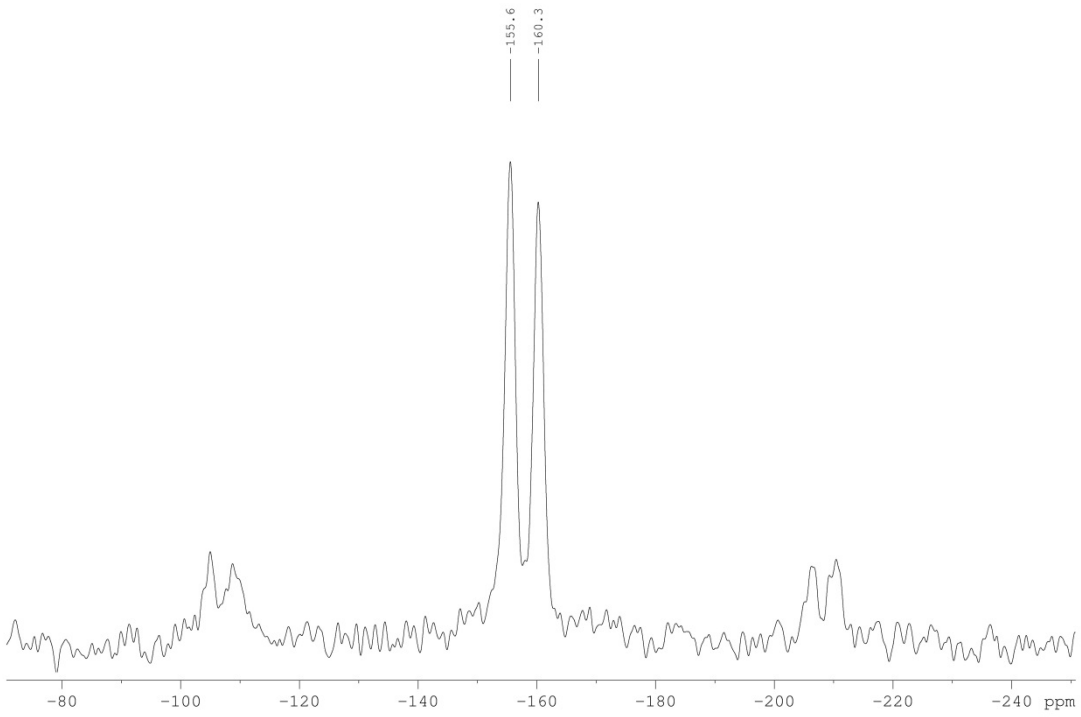

Fig. SI9. ^{29}Si CP/MAS NMR spectrum (79,5 MHz, ν_{spin} = 4 kHz) of (8-oxyquinolinate)$_2$SiF$_2$.

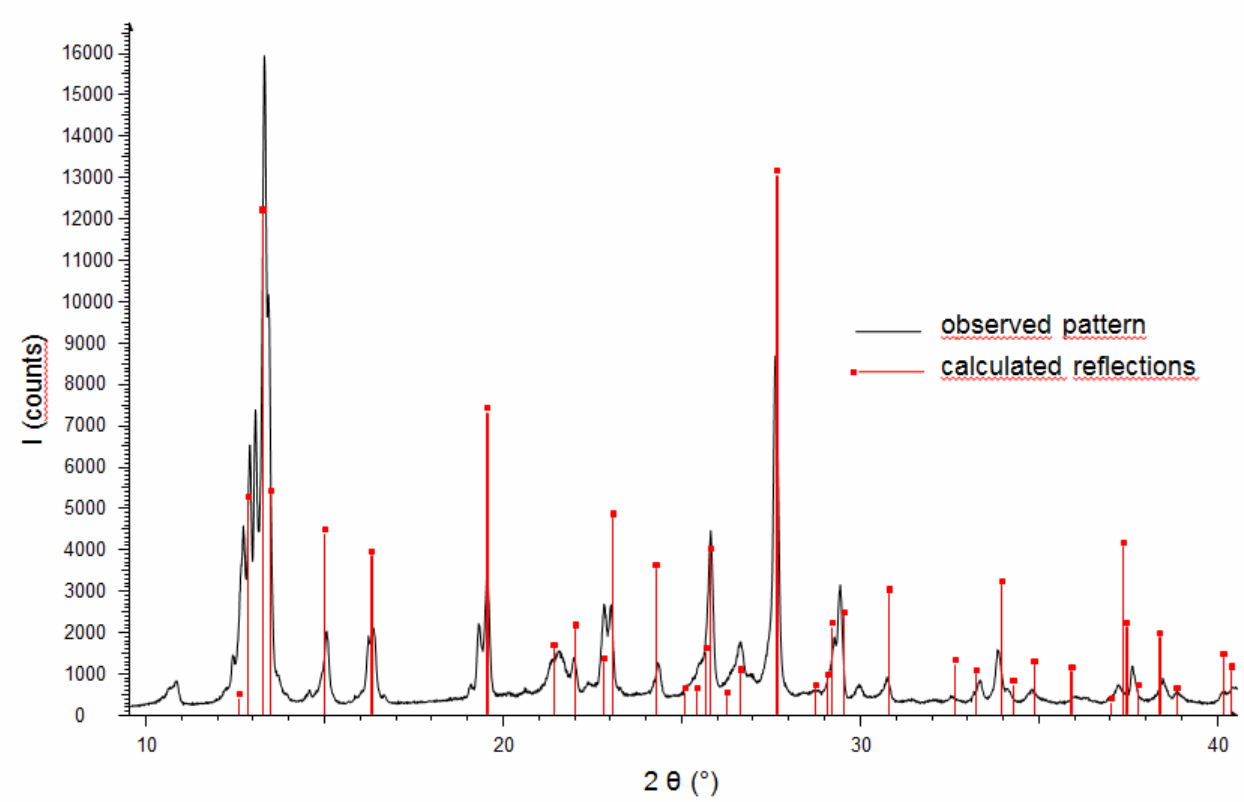

Fig. SI9. Powder X-ray diffractogram of a sample of (oxinate)$_2$SiCl$_2$ and superposition of the reflections calculated from the crystal structure of this compound.

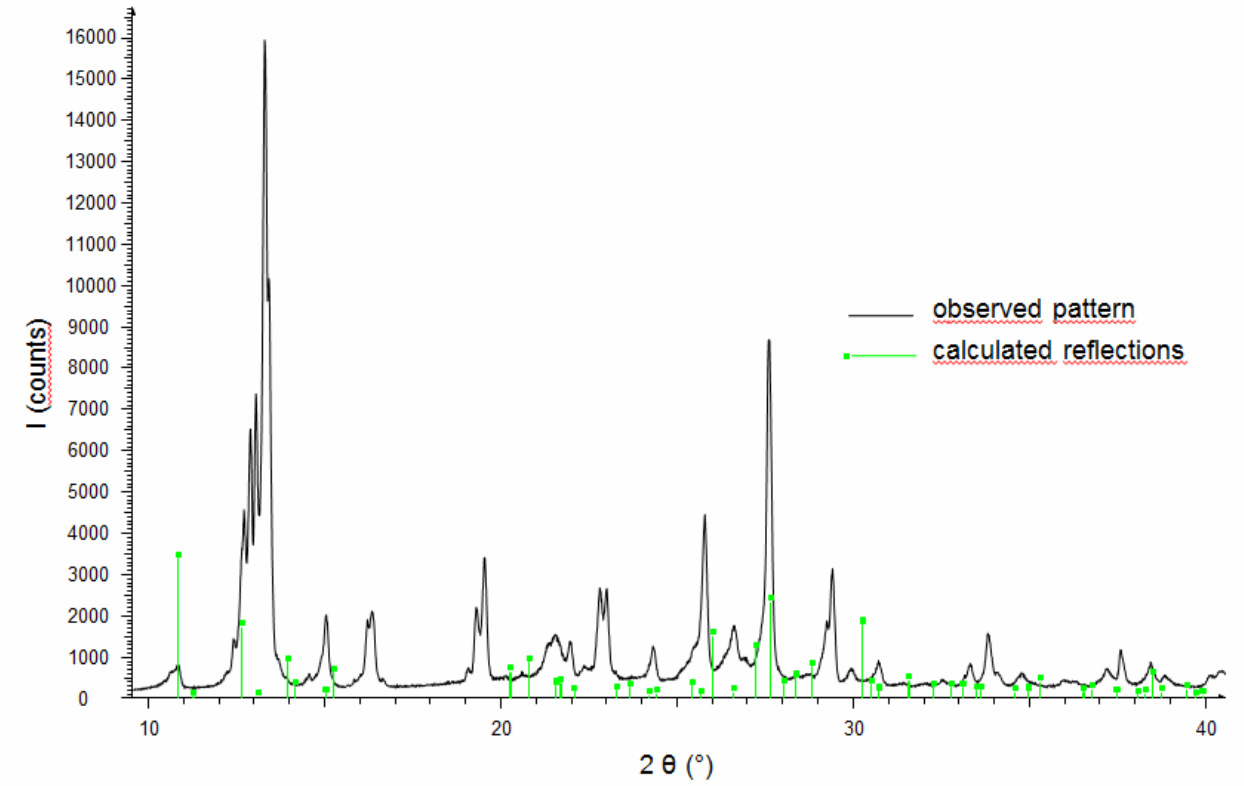

Fig. SI10. Powder X-ray diffractogram of a sample of (oxinate)$_2$SiCl$_2$ and superposition of the reflections calculated from the crystal structure of 8-hydroxyquinoline hydrochloride (G. B. Deacon, T. Dierkes, M. Hübner, P. C. Junk, Y. Lorenz, A. Urbatsch, *Eur. J. Inorg. Chem.* **2011**, 4338-4348.).

The powder X-ray diffraction data of $(oxinate)_2SiCl_2$ were collected at room temperature on a Bruker D5000 instrument (Bragg-Brentano configuration, flat sample, measured in reflexion mode) with CuKα radiation within 27 h (2Theta range for data collection: 5-70° in increments of 0.02°).
An offset of 0.183° for 2Theta was applied to this powder diffraction pattern (which was recorded at room temperature) in order to account for thermal expansion of the unit cell by about 2% (because the single-crystal X-ray diffraction data had been collected at 150 K).

The sample was covered with polyethylene foil (to protect the sample from moisture). This polyethylene and the sample carrier contribute to the diffraction to 21.5° and 29.5° 2Theta.

Reflections which cannot be assigned to the combination of sample carrier, polyethylene foil, $(oxinate)_2SiCl_2$ (according to single crystal structure) and 8-hydroxyquinoline hydrochloride (which might have formed in small amounts during synthesis and/or sample preparation) are found in the following 2Theta ranges:

2θ range (deg)	Refls. observed	expected for $(oxinate)_2SiCl_2$	expected for 8-hydroxyquinoline hydrochloride
10-11	≥ 2	0	1
12-14	≥ 5	3	1
16-17	≥ 2	1	0
19-20	≥ 3	1	0