Supporting Information

Valence Bond Structures for N_3^-, $N_3^{\cdot}$ and $N_6^{\cdot-}$

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Un-normalised coefficients and equations used to calculate the *k* and *l* polarity parameters for Tables 3 and 4.

N_3^- Anion

Lewis VB structure	C_i **A1**	C_i **A1 ↔ A2**	C_i **A3**	C_i **A3 ↔ A4**
1	0.159968	0.094024		
2		0.094024		
3			0.359157	0.206174
4				0.206174
5	–0.339876	–0.239007	–0.262335	–0.199148
6	–0.339876	–0.239007		–0.199148
7		–0.239007	–0.262335	–0.199148
8		–0.239007		–0.199148
9	0.223009	0.164529	0.146090	0.126743

k and *l* equations:
A1: $k + l + 2d_5 = 0.\ kl = d_9.\ d_i = C_i/C_1$
A1 ↔ **A2**: $k + l + 2d_5 = 0.\ 2kl = d_9.\ d_i = C_i/C_1$
A3: $k + l + 2d_5 = 0.\ kl = d_9.\ d_i = C_i/C_3$
A3 ↔ **A4**: $k + l + 2d_5 = 0.\ 2kl = d_9.\ d_i = C_i/C_3$

$N_3^{\cdot}$ Radical

Lewis VB structure	C_i **R1**	C_i **R1 ↔ R2**	C_i **R3**	C_i **R3 ↔ R4**
1	0.299774	0.203241		
2		–0.203241		
3				0.221367
4			0.319797	–0.221367
5	–0.384592	–0.191007		0.221354
6		0.191007	–0.460025	–0.221354
7		–0.118387	0.119697	0.128824
8	0.135225	0.118387		–0.128824
9		0.248072		
10	–0.360013	–0.248072		
11			–0.108046	–0.104306
12				0.104306

k and *l* equations:
R1: $k + l + d_5 + d_{10} = 0.\ kl = d_8.\ d_i = C_i/C_1$
R1 ↔ **R2**: $k + l + d_5 + d_{10} = 0.\ kl = d_8.\ d_i = C_i/C_1$
R3: $k + l + d_6 + d_{11} = 0.\ kl = d_7.\ d_i = C_i/C_4$
R3 ↔ **R4**: $k + l + d_6 + d_{11} = 0.\ kl = d_7.\ d_i = C_i/C_3$