Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical Study on Anion-π Interactions withTetraoxacalix[2]arene[2]triazine as Electron-Acceptor: Generality, Binding Strength, and Structure

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1. Table 1S

Table 1S. Comparing the calculated and experimental parameters of the complex $SCN^-\cdots$**1** (bond length: Å).

		d_1(SCN-C2)	d_2(NCS-C2′)	d_3(H1-H1′)	sum(*abs*)*
Exp		3.37731	4.00767	4.21976	
Methods	Base sets				
B3LYP	6-31+G(d,p)	3.76425	4.17133	3.74648	1.02388
M062X	6-31+G(d,p)	3.31852	3.62332	3.69999	0.96291
M06L	6-31+G(d,p)	3.4516	3.66886	3.42779	1.20507
M06	6-31+G(d,p)	3.42472	3.80923	3.6852	0.78041
M052X	6-31+G(d,p)	3.36769	3.7646	3.81786	0.65459
M05	6-31+G(d,p)	3.67218	3.99724	3.66926	0.8558
B3LYP-D3	6-31+G(d,p)	3.4952	3.7703	3.801	0.77402
MP2	6-31+G(d,p)	3.33894	3.64748	3.99894	0.61938
B3LYP	6-31++G(d,p)	3.76408	4.17127	3.74631	1.02382
M062X	6-31++G(d,p)	3.31852	3.62332	3.6999	0.96300
M06L	6-31++G(d,p)	3.4546	3.66886	3.42779	1.20807
M06	6-31++G(d,p)	3.44839	3.82258	3.69397	0.78196
M052X	6-31++G(d,p)	3.36728	3.76481	3.82086	0.65179
M05	6-31++G(d,p)	3.67049	3.9963	3.66498	0.85933
B3LYP-D3	6-31++G(d,p)	3.49481	3.77077	3.80018	0.77398
B3LYP	6-311+G(d,p)	3.77691	4.16885	3.77785	1.00269
M062X	6-311+G(d,p)	3.2984	3.61493	3.74266	0.94875
M06L	6-311+G(d,p)	3.44138	3.64642	3.4269	1.21818
M06	6-311+G(d,p)	3.4512	3.80506	3.67209	0.82417
M052X	6-311+G(d,p)	3.37375	3.70551	3.8329	0.69258
M05	6-311+G(d,p)	3.70979	4.06198	3.70539	0.90116
B3LYP-D3	6-311+G(d,p)	3.5081	3.75862	3.8384	0.7612
B3LYP	6-311++G(d,p)	3.7724	4.1611	3.77627	0.99201
M062X	6-311++G(d,p)	3.29449	3.61383	3.74348	0.95294
M06L	6-311++G(d,p)	3.44165	3.64587	3.4269	1.219
M06	6-311++G(d,p)	3.45034	3.80349	3.67168	0.82529
M052X	6-311++G(d,p)	3.37192	3.70333	3.83707	0.69242
M05	6-311++G(d,p)	3.70385	4.05748	3.70449	0.89162
B3LYP-D3	6-311++G(d,p)	3.5089	3.7568	3.8432	0.75902
B3LYP	aug-cc-pVDZ	3.83884	4.20115	3.73037	1.1444
M062X	aug-cc-pVDZ	3.35618	3.61642	3.6883	0.94384
M06L	aug-cc-pVDZ	3.48521	3.66586	3.38952	1.27995
M06	aug-cc-pVDZ	3.48844	3.80608	3.66266	0.86982
M052X	aug-cc-pVDZ	3.4086	3.73522	3.78242	0.74108
M05	aug-cc-pVDZ	3.72439	4.02414	3.69218	0.89113
B3LYP-D3	aug-cc-pVDZ	3.539	3.7612	3.7688	0.85912

* $\text{sum}(abs)=\sum_{n=1}^{3} abs(d_n^{cal}-d_n^{exp})$

2. Table 2S

Table 2S. The key parameters of anion-π and selected orbital interactions between the subfragments ($E^{(2)}_{ij}$: kcal/mol, bond length: Å)

	SCN^-···1	PF_6^-···1	BF_4^-···1	NO_3^-···1
d(Cl-Cl)	11.731	11.767	11.570	11.615
d(Y-C2*)	3.367	3.785	3.592	3.667
d(Y'-C2'*)	3.765	2.850	3.691	2.864
d(H1-H1′)	3.821	3.766	3.758	4.007
d(H2-H2′)	6.145	6.272	6.315	5.808
N···triazine(1) centroid	2.891	3.125	2.985	3.051
S···triazine(2) centroid	3.426	3.165	3.176	3.182
anion-π	LP(N)→σ*(N1-C1), 0.13	LP(F1)→σ*(C1-N2), 0.15	LP(F1)→σ*(C1-N2), 0.27	LP(O1)→σ*(N1-C2), 0.27
	LP(N)→σ*(N2-C2), 0.09	LP(F1)→σ*(N1-C3), 0.06	LP(F1)→σ*(N1-C3), 0.10	LP(O1)→σ*(N3-C3), 0.51
	LP(N)→σ*(N3-C3), 0.69	LP(F2)→σ*(N1'-C3'), 0.94	LP(F2)→σ*(N1'-C3'), 1.19	LP(O2)→σ*(N3'-C3'), 3.10
	LP(S)→σ*(N1'-C1'), 1.25	LP(F3)→σ*(C1'-N2'), 1.12	LP(F3)→σ*(C1'-N2'), 1.30	LP(O3)→σ*(N1'-C1'), 2.07
	LP(S)→σ*(N2'-C2'), 0.14	-	-	-
	LP(S)→σ*(N3'-C3'), 0.30	-	-	-
anion-H	LP(N)→σ*(C4-H), 0.67	LP(F1)→σ*(C4,4'-H), 1.46, 1.46	LP(F1)→σ*(C4,4'-H), 1.08, 0.99	LP(O1)→σ*(C4,4'-H), 1.41, 1.41
	LP(S)→σ*(C4'-H), 2.72	LP(F2,3)→σ*(C4,4'-H), 3.95, 3.93	LP(F2,3)→σ*(C4,4'-H), 4.37, 4.47	LP(O2,3)→σ*(C4,4'-H), 5.44, 5.44

*for SCN^-···1, PF_6^-···1, BF_4^-···1 and NO_3^-···1, the Y and Y' denote N, F1, F1, O1 and S, F2, F2, O2 respectively.

3. Figure 1S.

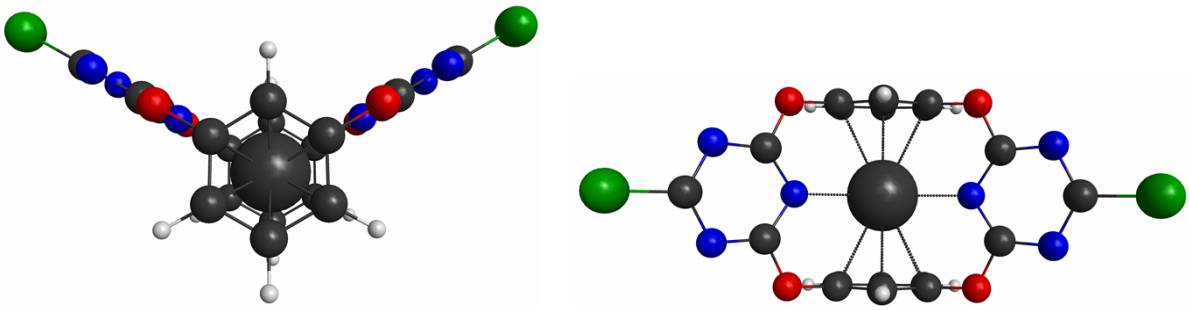

Figure 1S. Side view (a) and face view (b) of cation-π interaction complexes.

4. Table 3S

Table 3S. The key parameters of cation-π complexes and the key orbital interactions between the subfragments of cation-π ($E_{ij}^{(2)}$: kcal/mol, bond length: Å, angle: °)

	1···Na^+	**1**···K^+	**1**···Mg^{2+}	**1**···Ca^{2+}
dCl-Cl	12.095	11.760	12.010	12.046
dN1-$M^{+,2+}$	2.598	3.078	2.305	2.596
dN1′-$M^{+,2+}$	2.614	3.077	2.301	2.597
∠N1$M^{+,2+}$N1′	121.2	95.2	139.8	119.7
dCl-Cl in parent host molecule	12.180	12.180	12.180	12.180
σ(C4-C5)→LP*(M)	13.60	6.05	16.99	20.71
σ(C5-C6)→LP*(M)	9.20	4.76	26.17	9.85
σ(C6-C7)→LP*(M)	11.30	3.60	11.06	16.29
σ(C7-C8)→LP*(M)	7.57	6.04	24.60	7.19
σ(C8-C9)→LP*(M)	12.23	4.74	15.60	18.53
σ(C9-C4)→LP*(M)	11.04	7.27	33.77	10.50
σ(C4′-C5′)→LP*(M)	10.97	7.27	32.38	20.70
σ(C5′-C6′)→LP*(M)	12.11	4.76	15.62	9.84
σ(C6′-C7′)→LP*(M)	7.53	6.05	24.7	7.16
σ(C7′-C8′)→LP*(M)	11.42	3.62	11.05	16.29
σ(C8′-C9′)→LP*(M)	9.30	4.76	26.32	9.80
σ(C9′-C4′)→LP*(M)	13.64	6.05	16.71	10.46
LP(N1)→LP*(M)	29.06	14.97	55.15	43.88
LP(N1′)→LP*(M)	29.10	14.98	55.13	43.88

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5. Figure 2S

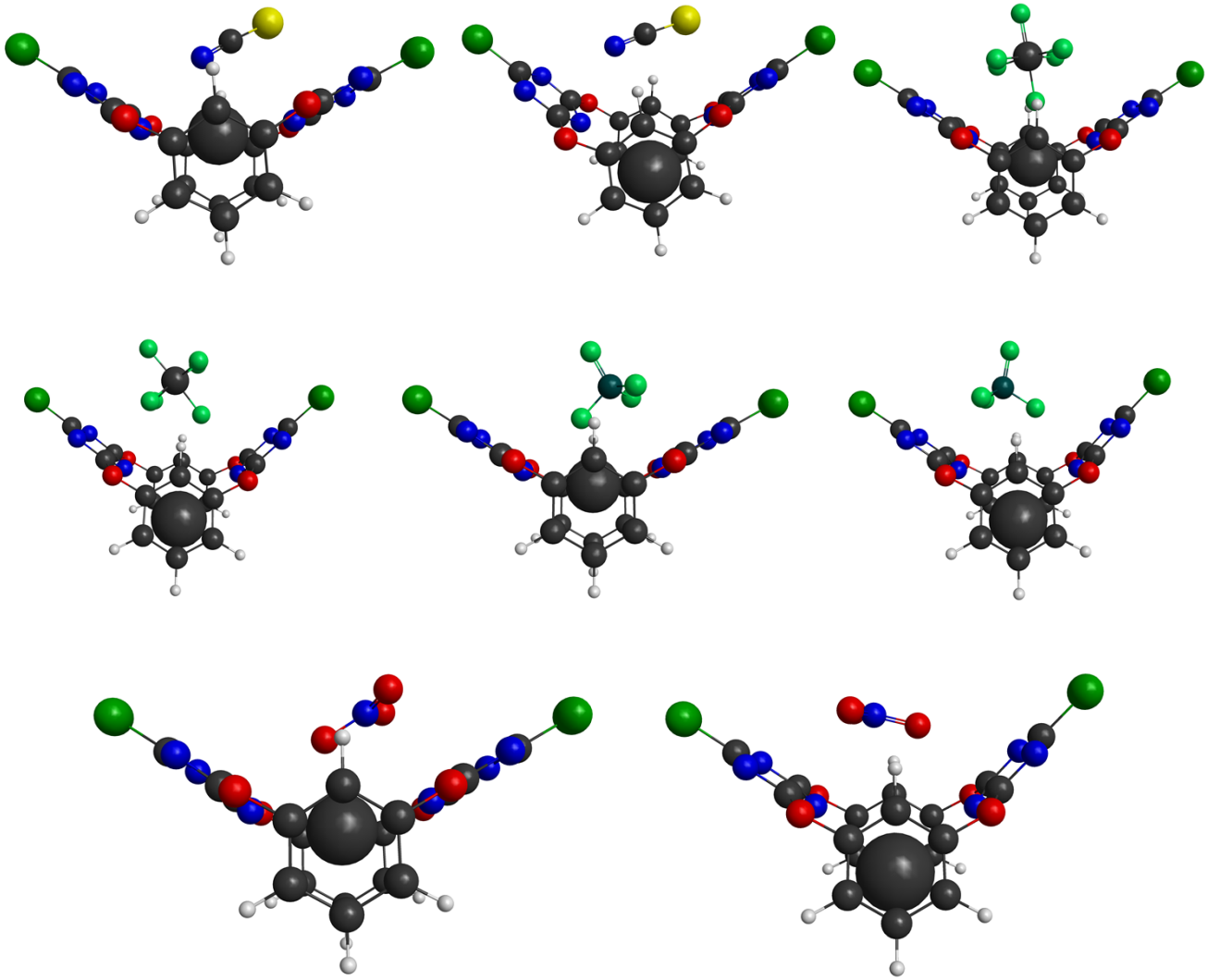

Figure 2S. The calculated geometries of anion-π-cation complexes

6. Table 4S

Table 4S. The key parameters of complexes ainon-π-cation and the key orbital interactions between the subfragments of ainon-π-cation ($E_{ij}^{(2)}$, kcal/mol)

		$SCN^-\cdots\mathbf{1}\cdots Na^+$	$SCN^-\cdots\mathbf{1}\cdots K^+$		$PF_6^-\cdots\mathbf{1}\cdots Na^+$	$PF_6^-\cdots\mathbf{1}\cdots K^+$
	dCl-Cl	12.10646	11.4075	dCl-Cl	11.84653	11.17328
	dN1-NCS	2.37457	2.96702	dN1-F	2.67284	2.76037
	dN1′-SCN	2.37469	2.98358	dN1′-F	2.80195	3.11414
	∠N1MN1′	165.011	100.852	∠N1MN1′	141.800	98.940
	N···triazine(1) centroid	3.113	3.277	N···triazine(1) centroid	3.386	2.830
	S···triazine(2) centroid	3.319	3.408	S···triazine(2) centroid	3.605	3.081
cation-π	BD(C4-C5)→LP*(M)	17.55	8.65	BD(C4-C5)→LP*(M)	14.55	8.02
	BD(C5-C6)→LP*(M)	16.64	9.09	BD(C5-C6)→LP*(M)	17.67	8.61
	BD(C6-C7)→LP*(M)	6.57	5.18	BD(C6-C7)→LP*(M)	8.74	4.97
	BD(C7-C8)→LP*(M)	11.43	8.33	BD(C7-C8)→LP*(M)	14.50	8.29
	BD(C8-C9)→LP*(M)	13.72	6.45	BD(C8-C9)→LP*(M)	13.40	6.41
	BD(C9-C4)→LP*(M)	19.67	9.01	BD(C9-C4)→LP*(M)	18.25	9.29
	BD(C4′-C5′)→LP*(M)	20.35	9.18	BD(C4′-C5′)→LP*(M)	14.55	9.42
	BD(C5′-C6′)→LP*(M)	13.95	6.64	BD(C5′-C6′)→LP*(M)	17.68	6.38
	BD(C6′-C7′)→LP*(M)	11.27	8.49	BD(C6′-C7′)→LP*(M)	8.74	8.29
	BD(C7′-C8′)→LP*(M)	6.12	5.31	BD(C7′-C8′)→LP*(M)	14.49	4.96
	BD(C8′-C9′)→LP*(M)	16.98	9.18	BD(C8′-C9′)→LP*(M)	13.40	8.71
	BD(C9′-C4′)→LP*(M)	16.48	8.58	BD(C9′-C4′)→LP*(M)	18.25	7.87
cation-l.p.	LP(N1)→LP*(M)	33.09	16.88	LP(N1)→LP*(M)	32.76	16.95
	LP(N1′)→LP*(M)	35.32	16.85	LP(N1′)→LP*(M)	33.20	16.92
anion-π	LP(N)→ BD*(C1-N2)	-	0.42	LP(F)→BD*(N1-C1)	-	0.49
	LP(S)→BD*(N1′-C1′)	3.76	-	LP(F)→BD*(N3-C3)	0.30	0.41
	LP(S)→BD*(C1′-N2′)	-	2.27	LP(F)→BD*(N3′-C3′)	0.25	1.63
anion-H	LP(N)→BD*(C4-H)	-	2.61	LP(F)→BD*(C4-H)	1.33	5.33
	LP(S)→BD*(C4′-H)	0.56	3.50	LP(F)→BD*(C4′-H)	1.20	5.47

Table 4S. continued

		BF_4^-···**1**···Na^+	BF_4^-···**1**···K^+		NO_3^-···**1**···Na^+	NO_3^-···**1**···K^+
	dCl-Cl	12.07376	11.13728	dCl-Cl	11.98759	11.19015
	dN1-F	2.654	2.76849	dN1-O	2.66466	2.80435
	dN1′-F	2.98294	3.07389	dN1′-O	3.05923	3.05718
	∠N1MN1′	154.019	99.312	∠N1MN1′	150.982	100.406
	N···triazine(1) centroid	3.224	2.849	N···triazine(1) centroid	3.177	2.864
	S···triazine(2) centroid	3.068	3.053	S···triazine(2) centroid	3.200	3.086
cation-π	BD(C4-C5)→LP*(M)	19.08	8.06	BD(C4-C5)→LP*(M)	15.76	8.35
	BD(C5-C6)→LP*(M)	13.38	8.67	BD(C5-C6)→LP*(M)	18.16	9.22
	BD(C6-C7)→LP*(M)	12.23	4.99	BD(C6-C7)→LP*(M)	7.94	5.49
	BD(C7-C8)→LP*(M)	7.21	8.35	BD(C7-C8)→LP*(M)	13.06	9.00
	BD(C8-C9)→LP*(M)	17.16	6.46	BD(C8-C9)→LP*(M)	13.32	7.02
	BD(C9-C4)→LP*(M)	15.66	9.35	BD(C9-C4)→LP*(M)	19.51	9.86
	BD(C4′-C5′)→LP*(M)	15.52	8.05	BD(C4′-C5′)→LP*(M)	15.75	8.33
	BD(C5′-C6′)→LP*(M)	17.51	8.68	BD(C5′-C6′)→LP*(M)	18.15	9.22
	BD(C6′-C7′)→LP*(M)	7.35	4.99	BD(C6′-C7′)→LP*(M)	7.95	5.47
	BD(C7′-C8′)→LP*(M)	12.09	8.34	BD(C7′-C8′)→LP*(M)	13.06	8.98
	BD(C8′-C9′)→LP*(M)	13.05	4.46	BD(C8′-C9′)→LP*(M)	13.33	7.02
	BD(C9′-C4′)→LP*(M)	19.24	9.32	BD(C9′-C4′)→LP*(M)	19.5	9.81
cation-l.p.	LP(N1)→LP*(M)	32.27	17.17	LP(N1)→LP*(M)	32.3	17.75
	LP(N1′)→LP*(M)	34.04	17.18	LP(N1′)→LP*(M)	35.22	18.05
anion-π	LP(F)→BD*(C1-N2)	0.19	0.52	LP(O)→BD*(N1-C1)	0.78	0.57
	LP(F)→BD*(N1-C3)	0.32	0.29	LP(O)→BD*(N3-C3)	0.49	0.89
	LP(F)→BD*(N1′-C3′)	2.51	2.12	LP(O)→BD*(N1′-C3′)	2.93	1.09
anion-H	LP(F)→BD*(C4-H)	1.89	1.67	LP(O)→BD*(C4-H)	3.58	2.25
	LP(F)→BD*(C4′-H)	0.77	1.63	LP(O)→BD*(C4′-H)	3.57	1.97

7. Table 5S

Table 5S. The interaction energies (ΔG^{CP}, kcal/mol) of $X_{1\text{-}4}^-\cdots$**1** ($X_{1\text{-}4}^-$ = SCN^-, PF_6^-, BF_4^-, NO_3^- respectively) complexes at different calculated levels.

	Gas				Solvent(SMD, opt)[d]				Solventt(PCM, opt)[e]				Solvent(SMD, sp)[f]				solvent(PCM, sp)[g]			
	SCN^-	PF_6^-	BF_4^-	NO_3^-	SCN^-	PF_6^-	BF_4^-	NO_3^-	SCN^-	PF_6^-	BF_4^-	NO_3^-	SCN^-	PF_6^-	BF_4^-	NO_3^-	SCN^-	PF_6^-	BF_4^-	NO_3^-
M05-2X/BS2[a]	-24.4	-19.2	-24.4	-29.0	-3.1	-1.4	-1.6	-5.0	-6.2	-4.5	-5.3	-6.7	-2.2	0.3	0.2	-4.3	-5.5	-3.5	-4.4	-5.8
	80.6[c]				5.3[c]				6.3[c]				10.4[c]				2.8[c]			
M05-2X/BS2[b]	-21.2	-7.4	-10.8	-15.0	6.9	11.0	9.5	7.9	3.4	8.7	7.7	5.5	7.3	12.1	13.7	9.7	4.0	8.3	9.2	8.1
	38.0[c]				51.7[c]				41.7[c]				59.2[c]				46.0[c]			
M05-2X/BS4[a]	-25.0	-19.5	-24.9	-29.3	-3.3	-1.1	-1.5	-5.1	-6.3	-4.3	-5.3	-6.6	-2.2	0.5	0.2	-4.3	-5.6	-3.4	-4.4	-5.8
	82.3[c]				5.4[c]				6.1[c]				10.6[c]				3.0[c]			
M05-2X/BS4[b]	-13.6	-6.1	-11.9	-15.7	7.2	9.1	8.5	7.6	4.3	10.1	7.3	6.4	9.2	13.9	13.2	9.3	5.7	10.0	8.7	7.8
	30.9[c]				48.8[c]				44.5[c]				62.0[c]				48.6[c]			
M06-2X/BS2[a]	-27.0	-21.2	-26.5	-31.9	-5.3	-2.5	-2.6	-7.3	-8.5	-5.6	-6.6	-8.9	-4.2	-0.8	-1.2	-6.7	-7.6	-4.7	-5.9	-8.2
	90.2[c]				5.7[c]				13.2[c]				7.1[c]				10.0[c]			
M06-2X/BS2[b]	-16.7	-9.5	-14.4	-20.0	4.9	10.3	9.1	4.4	2.3	6.5	5.6	3.4	5.3	11.0	12.3	7.3	0.8	3.0	3.3	2.5
	44.2[c]				45.1[c]				34.2[c]				52.3[c]				26.0[c]			
M06-2X/BS4[a]	-27.4	-21.4	-27.0	-32.0	-5.4	-2.4	-2.7	-7.3	-8.6	-5.6	-6.8	-8.8	-18.6	-15.0	-15.4	-20.8	-7.9	-4.8	-6.0	-8.1
	91.4[c]				5.8[c]				13.4[c]				53.4[c]				10.4[c]			
M06-2X/BS4[b]	-16.2	-9.1	-13.8	-17.9	3.2	11.0	9.8	4.7	0.0	8.9	6.3	5.0	-3.2	-1.2	-1.0	-2.9	-3.4	-2.0	-2.6	-3.4
	40.6[c]				45.1[c]				36.6[c]				8.1[c]				5.2[c]			

Table 5S. continued

	Gas				Solvent(SMD, opt)[d]				Solventt(PCM, opt)[e]				Solvent(SMD, sp)[f]				solvent(PCM, sp)[g]			
B3LYP-D3/BS2[a]	-26.3	-21.8	-24.9	-29.0	-4.2	-3.4	-2.0	-4.6	-7.4	-6.6	-5.5	-6.5	-3.1	-1.9	-0.2	-3.9	-6.6	-5.8	-4.7	-5.6
	85.6[c]				4.0[c]				9.6[c]				7.3[c]				6.7[c]			
B3LYP-D3/BS2[b]	-17.2	-9.0	-12.0	-15.5	4.6	7.3	8.5	6.9	-0.3	2.5	5.2	3.8	-1.3	-0.8	-0.1	-1.7	-2.8	-2.5	-2.0	-2.4
	37.3[c]				43.7[c]				27.6[c]				12.5[c]				6.7[c]			
B3LYP-D3/BS4[a]	-26.8	-22.2	-25.3	-29.4	-4.2	-3.2	-1.6	-4.7	-7.5	-6.5	-5.4	-6.6	-3.1	-1.9	-0.1	-4.0	-6.6	-5.7	-4.5	-5.7
	87.3[c]				4.5[c]				9.6[c]				7.3[c]				6.3[c]			
B3LYP-D3/BS4[b]	-17.3	-9.3	-12.2	-15.7	6.6	8.4	10.6	7.0	1.0	5.4	5.3	4.4	2.7	4.7	5.5	4.1	-2.8	-2.4	-1.9	-2.4
	38.1[c]				49.0[c]				32.5[c]				33.4[c]				6.9[c]			
MP2/BS1[a]	-24.0	-17.8	-21.9	-27.7									23.4	18.2	15.9	18.1	-4.2	-1.7	-1.5	-5.5
	75.1[c]												16.2[c]				5.2[c]			
ΔG_{exp}	-3.3	-3.4	-3.9	-5.8	-3.3	-3.4	-3.9	-5.8	-3.3	-3.4	-3.9	-5.8	-3.3	-3.4	-3.9	-5.8	-3.3	-3.4	-3.9	-5.8

[a,b]Denotes the ΔG^{CP} values are without and with corrected by the thermodynamic corrections.

[c] $sum(abs)=\sum_{n=1}^{4} abs(\Delta G^{CP,\,cal}_{X_n^-\cdots 1} - \Delta G^{exp}_{X_n^-\cdots 1})$

[d,e]The ΔG^{CP} is obtained based on the optimized geometries using SMD and PCM solvent models respectively;

[f,g]denote the single-point ΔG^{CP} energies using SMD and PCM solvent models respectively based on the gas optimized geometries at the same calculated level.

Table 6S. The LMO-EDA results at M05-2X/**BS2** level for the complexes(kcal/mol)

Complexes	E_{ES}	E_{EX}	E_{REP}	E_{POL}	E_{DISP}	E_{TOT}
PF_6^-···**1**	-18.8	-8.3	37.3	-12.9	-18.1	-20.7
NO_3^-···**1**	-32.2	-19.6	65.9	-19.1	-25.5	-30.5
SCN^-···**1**	-27.1	-17.8	55.5	-14.9	-21.5	-25.8
BF_4^-···**1**	-24.2	-11.3	45.2	-16.2	-19.8	-26.2
PF_6^-···**1**-Na^+	-98.6	-20.2	77.46	-20.0	-30.8	-92.1
PF_6^-···**1**-K^+	-84.3	-13.6	54.2	-17.2	-23.0	-84.0
NO_3^-···**1**-Na^+	-116.9	-30.1	96.6	-25.4	-32.6	-108.4
NO_3^-···**1**-K^+	-103.1	-27.7	85.6	-22.5	-26.4	-94.2
SCN^-···**1**-Na^+	-110.1	-27.5	84.0	-23.0	-28.3	-105.0
SCN^-···**1**-K^+	-96.3	-26.1	77.7	-20.3	-26.4	-91.3
BF_4^-···**1**-Na^+	-107.5	-21.4	77.3	-22.0	-28.7	-102.2
BF_4^-···**1**-K^+	-93.2	-17.0	63.0	-20.1	-24.5	-91.9
1···Na^+	-25.9	-5.1	31.2	-27.1	-20.5	-47.3
1···K^+	-19.8	-6.4	36.6	-22.9	-19.0	-31.4
1···Mg^{2+}	-63.9	-9.3	51.4	-170.2	-32.5	-224.6
1···Ca^{2+}	-61.0	-17.5	92.5	-125.2	-39.8	-151.1
SCN^--**1**···K^+	-83.1	-9.4	46.1	-20.4	-25.9	-92.7
SCN^--**1**···Na^+	-114.3	-12.6	63.1	-32.1	-27.6	-123.6
PF_6^--**1**···Na^+	-102.8	-8.3	46.6	-30.1	-25.7	-120.2
PF_6^--**1**···K^+	-79.8	-8.5	43.7	-20.4	-25.0	-90.0
BF_4^--**1**···Na^+	-110.3	-10.8	54.1	-30.1	-26.2	-123.3
BF_4^--**1**···K^+	-82.8	-8.5	44.4	-20.3	-25.0	-92.2
NO_3^--**1**···Na^+	-112.1	-10.8	54.8	-30.8	-26.2	-125.13
NO_3^--**1**···K^+	-86.0	-9.7	48.4	-20.9	-26.5	-94.7

8. Table 6S

9. Table 7S

Table 7S. Comparing the interaction energies of binary complexes with and without BSSE corrrection(kcal/mol)

Phase		SCN^-···**1**	PF_6^-···**1**	BF_4^-···**1**	NO_3^-···**1**	**1**···M^+
gas	*E*	-25.7	-21.4	-25.9	-31.4	-63.3[a], -47.5[b], -30.0[c]
	E^{CP}	-24.4	-19.2	-24.4	-29.0	-62.1[a], -45.4[b], -29.0[c]
CH_3CN	*E*	-6.8	-5.7	-5.9	-8.2	12.2[a],7.2[b],1.9[c]
	E^{CP}	-5.5	-3.5	-4.4	-5.8	13.4[a], 9.3[b], 3.0[c]
C_6H_6	*E*	-13.6	-11.4	-13.2	-16.6	-17.3[a], -13.7[b],-9.6[c]
	E^{CP}	-12.3	-9.1	-11.6	-14.2	-16.2[a], -11.5[b], -8.5[c]

Superscript *a*, *b*, *c* denote M^+=Li^+, Na^+ and K^+ respectively.

10. Table 8S

Table 8S. Comparing the interaction energies of trimer complexes with and without BSSE correction in different phases(kcal/mol)

		X^-=SCN^-		X^-=PF_6^-		X^-=BF_4^-		X^-=NO_3^-	
	Gas	X^-···1-M^+	X^--1···M^+	X^-···1-M^+	X^--1···M^+	X^-···1-M^+	X^--1···M^+	X^-···1-M^+	X^--1···M^+
M^+=Li^+	*E*	-90.9	-128.5	-98.8	-140.7	-107.7	-145.0	-115.9	-147.8
	E^{CP}	-89.3	-127.3	-94.5	-138.7	-105.4	-143.2	-113.0	-146.1
M^+=Na^+	*E*	-95.9	-117.8	-89.6	-115.7	-96.1	-117.7	-104.5	-120.6
	E^{CP}	-94.2	-115.0	-86.2	-113.2	-93.8	-115.1	-101.4	-117.9
M^+=K^+	*E*	-88.6	-92.9	-81.6	-90.2	-89.0	-93.1	-96.8	-95.4
	E^{CP}	-87.0	-91.7	-79.0	-89.0	-87.2	-91.9	-94.1	-94.2
	CH_3CN								
M^+=Li^+	*E*	-6.2	12.8	-11.4	6.5	-14.9	3.3	-19.1	1.4
	E^{CP}	-4.6	14.0	-7.0	8.5	-12.6	5.1	-16.1	3.1
M^+=Na^+	*E*	-4.9	9.1	-5.4	7.6	-6.2	6.9	-9.5	5.9
	E^{CP}	-3.2	11.8	-2.0	10.0	-4.0	9.5	-6.4	8.6
M^+=K^+	*E*	-7.7	1.1	-6.5	1.1	-7.5	0.3	-9.6	0.5
	E^{CP}	-6.1	2.2	-3.9	2.3	-5.7	1.5	-6.9	1.8
	C_6H_6								
M^+=Li^+	*E*	-41.6	-45.3	-49.9	-55.8	-55.6	-59.7	-61.4	-62.0
	E^{CP}	-39.9	-44.1	-45.6	-53.9	-53.3	-57.9	-58.4	-60.3
M^+=Na^+	*E*	-44.6	-44.6	-41.4	-43.7	-45.1	-45.5	-50.5	-47.5
	E^{CP}	-42.9	-41.9	-38.0	-41.3	-42.8	-42.9	-47.4	-44.8
M^+=K^+	*E*	-40.6	-36.5	-37.1	-35.2	-40.8	-37.2	-45.3	-38.3
	E^{CP}	-39.0	-35.4	-34.4	-34.0	-38.9	-36.0	-42.6	-37.0

11. Cartesian coordinates of monomers and 1·SCN$^-$

monomer 1

Cl	6.0898	0.0000	-2.0924
Cl	-6.0897	-0.0000	-2.0925
O	-2.3957	2.2909	0.0271
O	2.3957	2.2909	0.0271
O	2.3956	-2.2909	0.0271
O	-2.3957	-2.2909	0.0271
N	-4.0888	1.1871	-0.9472
N	-2.3089	0.0000	0.0760
N	-4.0888	-1.1871	-0.9472
N	4.0888	1.1871	-0.9472
N	4.0888	-1.1871	-0.9473
N	2.3089	-0.0000	0.0759
C	-4.5940	-0.0000	-1.2365
C	-2.9375	1.1104	-0.2856
C	-2.9374	-1.1104	-0.2856
C	-1.1833	2.2988	0.7239
C	-1.2094	2.4383	2.1027
H	-2.1600	2.4961	2.6155
C	0.0000	2.5087	2.7892
H	0.0000	2.6239	3.8652
C	1.2094	2.4383	2.1026
H	2.1600	2.4961	2.6155
C	1.1833	2.2988	0.7238
C	-0.0000	2.2368	0.0059
H	-0.0000	2.1388	-1.0712
C	2.9374	1.1104	-0.2857
C	4.5940	-0.0000	-1.2365
C	2.9374	-1.1104	-0.2857
C	1.1833	-2.2988	0.7238
C	1.2094	-2.4383	2.1026
H	2.1600	-2.4961	2.6155
C	0.0000	-2.5087	2.7892
H	0.0000	-2.6239	3.8652
C	-1.2094	-2.4383	2.1027
H	-2.1600	-2.4961	2.6156
C	-1.1833	-2.2988	0.7239
C	-0.0000	-2.2368	0.0059
H	-0.0000	-2.1388	-1.0712

1·SCN$^-$ (B3LYP/BS1)

Cl	6.0315	-0.5939	-1.5898
Cl	-5.9915	-0.9152	-1.7746
O	-2.6185	2.3178	-0.4269
O	2.1998	2.2841	-0.7785
O	2.4928	-1.6813	1.5632
O	-2.3131	-1.9802	1.2227
N	-4.1450	0.7808	-1.0257
N	-2.3893	0.2040	0.4748
N	-3.9713	-1.4432	-0.1972
N	3.9268	0.8949	-1.1457
N	4.0988	-1.1334	0.0884
N	2.2465	0.3219	0.4411
C	-4.5329	-0.4771	-0.9039
C	-3.0374	1.0458	-0.3243
C	-2.8875	-1.0276	0.4698
C	-1.3523	2.6906	0.0356
C	-1.2999	3.6762	1.0181
H	-2.2227	4.0538	1.4454
C	-0.0531	4.1596	1.4219
H	0.0061	4.9298	2.1852
C	1.1165	3.6616	0.8452
H	2.0947	4.0302	1.1351
C	1.0156	2.6753	-0.1346
C	-0.2069	2.1740	-0.5677
H	-0.2836	1.4016	-1.3320
C	2.7874	1.1163	-0.4776
C	4.5090	-0.2405	-0.7965
C	2.9342	-0.7973	0.6553
C	1.2129	-1.5453	2.1144
C	1.1295	-1.3096	3.4841
H	2.0387	-1.1676	4.0583
C	-0.1311	-1.2683	4.0845
H	-0.2152	-1.0878	5.1520
C	-1.2829	-1.4580	3.3192
H	-2.2716	-1.4323	3.7647
C	-1.1516	-1.6904	1.9513
C	0.0868	-1.7539	1.3215
H	0.1845	-1.9584	0.2575
S	1.1653	-2.2205	-2.3128
C	-0.1379	-1.1898	-2.3624
N	-1.0597	-0.4470	-2.3550

1·SCN$^-$ (B3LYP/BS2**)**

Cl	6.031597	-0.594993	-1.589303
Cl	-5.991498	-0.916362	-1.774015
O	-2.618671	2.317646	-0.428155
O	2.199584	2.283447	-0.780332
O	2.492929	-1.680125	1.564561
O	-2.312994	-1.979560	1.223688
N	-4.145001	0.780175	-1.026178
N	-2.389173	0.204315	0.474625
N	-3.971181	-1.443461	-0.196486
N	3.926689	0.894051	-1.146487
N	4.098870	-1.133234	0.089328
N	2.246242	0.322020	0.440636
C	-4.532840	-0.477774	-0.903760
C	-3.037371	1.045577	-0.324945
C	-2.887329	-1.027429	0.470284
C	-1.352363	2.690530	0.034190
C	-1.299833	3.676210	1.016536
H	-2.222471	4.053899	1.443975
C	-0.052921	4.159659	1.420134
H	0.006548	4.929950	2.183245
C	1.116613	3.661590	0.843204
H	2.094861	4.030064	1.132983
C	1.015543	2.675109	-0.136538
C	-0.207088	2.173572	-0.569145
H	-0.283937	1.400834	-1.333026
C	2.787148	1.115802	-0.478667
C	4.509041	-0.241060	-0.796338
C	2.934204	-0.796853	0.655928
C	1.212985	-1.543794	2.115581
C	1.129357	-1.306872	3.485045
H	2.038517	-1.164288	4.059199
C	-0.131341	-1.265247	4.085281
H	-0.215602	-1.083898	5.152603
C	-1.283069	-1.455749	3.319960
H	-2.271804	-1.429704	3.765356
C	-1.151583	-1.689210	1.952289
C	0.087016	-1.752770	1.322624
H	0.184701	-1.957960	0.258746
S	1.165329	-2.221670	-2.311693
C	-0.137983	-1.191120	-2.361991
N	-1.059828	-0.448359	-2.354828

1·SCN$^-$ (B3LYP/BS3**)**

Cl	6.019609	-0.658671	-1.568121
Cl	-5.978073	-0.995274	-1.746729
O	-2.615513	2.292877	-0.533270
O	2.195196	2.249403	-0.871686
O	2.485680	-1.606842	1.626593
O	-2.313198	-1.916978	1.304856
N	-4.137513	0.731929	-1.065377
N	-2.391647	0.226362	0.461402
N	-3.964532	-1.446791	-0.141102
N	3.917817	0.846317	-1.182580
N	4.089944	-1.122266	0.132692
N	2.241894	0.341484	0.421688
C	-4.522895	-0.516129	-0.889262
C	-3.035434	1.029745	-0.374712
C	-2.886301	-1.002496	0.509860
C	-1.352255	2.683128	-0.078234
C	-1.301352	3.690755	0.876439
H	-2.223055	4.078649	1.291992
C	-0.058425	4.183289	1.268928
H	-0.000628	4.971981	2.010285
C	1.109422	3.671721	0.709226
H	2.085154	4.047386	0.991414
C	1.011245	2.662954	-0.242519
C	-0.207989	2.153284	-0.663373
H	-0.283479	1.361565	-1.405628
C	2.781681	1.096632	-0.525842
C	4.497955	-0.270276	-0.786807
C	2.927885	-0.764869	0.683856
C	1.207726	-1.441373	2.172931
C	1.124443	-1.133416	3.524553
H	2.032277	-0.962356	4.089543
C	-0.132755	-1.058841	4.120592
H	-0.216201	-0.821813	5.175008
C	-1.282114	-1.287216	3.368748
H	-2.268735	-1.236920	3.812380
C	-1.152552	-1.592061	2.018736
C	0.083216	-1.690070	1.395871
H	0.180907	-1.953072	0.346413
S	1.167336	-2.341264	-2.200062
C	-0.117814	-1.295321	-2.288289
N	-1.022987	-0.544527	-2.308739

1·SCN$^-$ (B3LYP/BS4**)**

Cl	6.018677	-0.658533	-1.568730
Cl	-5.976282	-0.996786	-1.749592
O	-2.617256	2.293307	-0.531149
O	2.193243	2.248648	-0.873492
O	2.486147	-1.605185	1.628093
O	-2.312498	-1.917801	1.303568
N	-4.138044	0.731724	-1.065019
N	-2.392518	0.226331	0.462265
N	-3.963057	-1.447973	-0.143377
N	3.916276	0.845920	-1.183930
N	4.089782	-1.121285	0.133260
N	2.241108	0.341870	0.421397
C	-4.521996	-0.517003	-0.890598
C	-3.036568	1.029870	-0.373454
C	-2.885817	-1.003170	0.508975
C	-1.353568	2.683326	-0.076944
C	-1.301683	3.691476	0.877053
H	-2.222869	4.080045	1.293109
C	-0.058227	4.183715	1.268313
H	0.000424	4.973051	2.008963
C	1.108990	3.671873	0.707602
H	2.084953	4.047869	0.988556
C	1.009837	2.662545	-0.243481
C	-0.209889	2.152756	-0.662761
H	-0.286353	1.360371	-1.404165
C	2.780253	1.096370	-0.526978
C	4.496992	-0.269959	-0.787153
C	2.927669	-0.763920	0.684436
C	1.207764	-1.440445	2.173785
C	1.123619	-1.132813	3.525399
H	2.030984	-0.961534	4.091077
C	-0.134027	-1.058718	4.120596
H	-0.218244	-0.822012	5.175049
C	-1.282834	-1.287928	3.368171
H	-2.269659	-1.238392	3.811436
C	-1.152362	-1.592403	2.018142
C	0.083801	-1.689397	1.395918
H	0.182615	-1.952494	0.346599
S	1.172960	-2.337585	-2.197989
C	-0.116676	-1.296991	-2.284893
N	-1.024786	-0.549728	-2.304630

1·SCN$^-$ (B3LYP/BS5**)**

Cl	6.037901	-0.624625	-1.573907
Cl	-6.002939	-0.954469	-1.753819
O	-2.618953	2.304543	-0.488546
O	2.204485	2.272414	-0.821595
O	2.490596	-1.648691	1.595936
O	-2.320034	-1.953079	1.266269
N	-4.148564	0.756470	-1.049023
N	-2.388033	0.211431	0.461674
N	-3.981222	-1.447780	-0.162444
N	3.932081	0.876181	-1.159134
N	4.099497	-1.131302	0.112664
N	2.244711	0.332208	0.434094
C	-4.539211	-0.496867	-0.892827
C	-3.037841	1.035098	-0.355504
C	-2.893210	-1.017672	0.490591
C	-1.353858	2.684658	-0.022786
C	-1.306911	3.693435	0.937223
H	-2.234088	4.084905	1.352252
C	-0.061531	4.188279	1.334653
H	-0.006066	4.980026	2.081913
C	1.111933	3.679417	0.773224
H	2.090644	4.061691	1.058163
C	1.016756	2.669811	-0.184363
C	-0.204333	2.155163	-0.608665
H	-0.279204	1.361116	-1.357530
C	2.790399	1.109443	-0.497100
C	4.510893	-0.253824	-0.787037
C	2.933441	-0.782346	0.670743
C	1.210104	-1.489863	2.143518
C	1.126892	-1.218498	3.507430
H	2.038676	-1.064469	4.081863
C	-0.134157	-1.160879	4.107530
H	-0.217796	-0.952594	5.174238
C	-1.287393	-1.370074	3.347888
H	-2.278282	-1.334526	3.797316
C	-1.157166	-1.637985	1.985711
C	0.081921	-1.717138	1.356935
H	0.179222	-1.951839	0.294683
S	1.157894	-2.320550	-2.248432
C	-0.105686	-1.235165	-2.343237
N	-0.996866	-0.457547	-2.371647

1·SCN$^-$ (M062X/BS1**)**

Cl	5.851546	-0.933464	-1.612406
Cl	-5.750331	-1.280807	-1.858852
O	-2.638191	2.232583	-0.674386
O	2.138674	2.122233	-1.095175
O	2.463504	-1.414739	1.808564
O	-2.302252	-1.792205	1.497556
N	-4.049897	0.571973	-1.195178
N	-2.418892	0.274691	0.503901
N	-3.866520	-1.514512	-0.080800
N	3.822106	0.664654	-1.311701
N	4.010457	-1.147705	0.210169
N	2.209069	0.387616	0.409240
C	-4.397953	-0.674901	-0.944450
C	-3.024574	0.969289	-0.445848
C	-2.858760	-0.970907	0.601097
C	-1.375106	2.643840	-0.269286
C	-1.300614	3.737129	0.583209
H	-2.216795	4.168309	0.971174
C	-0.047942	4.255350	0.904564
H	0.027657	5.111127	1.567710
C	1.105369	3.688066	0.370006
H	2.091959	4.082502	0.587534
C	0.982315	2.593757	-0.478327
C	-0.244981	2.042371	-0.812299
H	-0.329803	1.174611	-1.464646
C	2.720752	1.007467	-0.642965
C	4.392129	-0.415844	-0.817971
C	2.883349	-0.698860	0.760029
C	1.192558	-1.183499	2.323507
C	1.099603	-0.719860	3.628696
H	2.006506	-0.480723	4.172929
C	-0.162284	-0.584048	4.204825
H	-0.253724	-0.223091	5.224209
C	-1.305175	-0.911082	3.480532
H	-2.298385	-0.820159	3.906553
C	-1.162582	-1.370879	2.176726
C	0.074886	-1.517240	1.568964
H	0.176853	-1.886772	0.550588
S	1.373119	-2.086049	-1.924512
C	-0.155040	-1.429096	-1.933539
N	-1.232667	-0.958958	-1.899883

1·SCN$^-$ (M062X/BS2**)**

Cl	5.851546	-0.933464	-1.612406
Cl	-5.750331	-1.280807	-1.858852
O	-2.638191	2.232583	-0.674386
O	2.138674	2.122233	-1.095175
O	2.463504	-1.414739	1.808564
O	-2.302252	-1.792205	1.497556
N	-4.049897	0.571973	-1.195178
N	-2.418892	0.274691	0.503901
N	-3.866520	-1.514512	-0.080800
N	3.822106	0.664654	-1.311701
N	4.010457	-1.147705	0.210169
N	2.209069	0.387616	0.409240
C	-4.397953	-0.674901	-0.944450
C	-3.024574	0.969289	-0.445848
C	-2.858760	-0.970907	0.601097
C	-1.375106	2.643840	-0.269286
C	-1.300614	3.737129	0.583209
H	-2.216795	4.168309	0.971174
C	-0.047942	4.255350	0.904564
H	0.027657	5.111127	1.567710
C	1.105369	3.688066	0.370006
H	2.091959	4.082502	0.587534
C	0.982315	2.593757	-0.478327
C	-0.244981	2.042371	-0.812299
H	-0.329803	1.174611	-1.464646
C	2.720752	1.007467	-0.642965
C	4.392129	-0.415844	-0.817971
C	2.883349	-0.698860	0.760029
C	1.192558	-1.183499	2.323507
C	1.099603	-0.719860	3.628696
H	2.006506	-0.480723	4.172929
C	-0.162284	-0.584048	4.204825
H	-0.253724	-0.223091	5.224209
C	-1.305175	-0.911082	3.480532
H	-2.298385	-0.820159	3.906553
C	-1.162582	-1.370879	2.176726
C	0.074886	-1.517240	1.568964
H	0.176853	-1.886772	0.550588
S	1.373119	-2.086049	-1.924512
C	-0.155040	-1.429096	-1.933539
N	-1.232667	-0.958958	-1.899883

1·SCN$^-$ (M062X/BS3**)**

Cl	5.861165	-1.056214	-1.529728
Cl	-5.762813	-1.385829	-1.761781
O	-2.594807	2.160315	-0.889579
O	2.182798	2.060532	-1.200184
O	2.430809	-1.333412	1.861570
O	-2.341201	-1.642218	1.642682
N	-4.040119	0.490577	-1.255599
N	-2.424450	0.324275	0.468705
N	-3.895909	-1.483528	0.043719
N	3.852735	0.577590	-1.327059
N	3.994820	-1.162585	0.274056
N	2.218883	0.403051	0.380660
C	-4.408357	-0.719082	-0.893621
C	-3.011665	0.936795	-0.544523
C	-2.883154	-0.897568	0.675914
C	-1.345172	2.593508	-0.465812
C	-1.291902	3.697664	0.369517
H	-2.215615	4.130133	0.732370
C	-0.050702	4.224445	0.708768
H	0.007568	5.088624	1.359367
C	1.113506	3.654698	0.208394
H	2.091928	4.054773	0.442244
C	1.013388	2.548921	-0.622866
C	-0.203139	1.989759	-0.972211
H	-0.269583	1.113320	-1.610598
C	2.749837	0.964411	-0.692273
C	4.399007	-0.485367	-0.777837
C	2.870840	-0.672925	0.789546
C	1.171778	-1.041129	2.373410
C	1.106218	-0.493992	3.644554
H	2.024140	-0.242475	4.160162
C	-0.141350	-0.296824	4.226401
H	-0.211848	0.126590	5.220983
C	-1.297737	-0.648452	3.541364
H	-2.281090	-0.517231	3.975144
C	-1.184463	-1.193079	2.270876
C	0.039717	-1.398234	1.657520
H	0.120802	-1.832244	0.665089
S	1.364074	-2.130611	-1.850246
C	-0.184409	-1.531618	-1.849454
N	-1.271350	-1.102278	-1.811210

1·SCN$^-$ (M062X/BS4**)**

Cl	5.86336900	-1.06439200	-1.519552
Cl	-5.76407000	-1.39789000	-1.753170
O	-2.59443400	2.15304400	-0.906908
O	2.18360700	2.05314300	-1.212645
O	2.42870100	-1.32318900	1.868707
O	-2.34374600	-1.62997300	1.654402
N	-4.04041300	0.48123700	-1.260869
N	-2.42642600	0.32796500	0.466198
N	-3.89835400	-1.48252400	0.054262
N	3.85421500	0.56995900	-1.328904
N	3.99476600	-1.16087800	0.282398
N	2.21836300	0.40497300	0.377860
C	-4.40983200	-0.72519500	-0.889346
C	-3.01237000	0.93264100	-0.552393
C	-2.88557100	-0.89215900	0.682367
C	-1.34529200	2.58922800	-0.484473
C	-1.29316300	3.69901700	0.343420
H	-2.21731300	4.13373200	0.702458
C	-0.05242300	4.22809100	0.680696
H	0.00492300	5.09683700	1.325360
C	1.11237400	3.65595700	0.184480
H	2.09038100	4.05825100	0.416268
C	1.01344600	2.54455900	-0.639390
C	-0.20260500	1.98233800	-0.985672
H	-0.26830000	1.10105900	-1.617392
C	2.75046700	0.96017600	-0.697710
C	4.40006700	-0.48974100	-0.772913
C	2.86999400	-0.66856100	0.793667
C	1.17004400	-1.02587800	2.378738
C	1.10546500	-0.46736600	3.644941
H	2.02375800	-0.21204700	4.158020
C	-0.14173200	-0.26295900	4.225013
H	-0.21154900	0.16925800	5.215900
C	-1.29863100	-0.62028500	3.543862
H	-2.28171100	-0.48415400	3.976747
C	-1.18632100	-1.17654300	2.278362
C	0.03744600	-1.38841500	1.666400
H	0.11761800	-1.83101600	0.677741
S	1.36909000	-2.14490300	-1.837534
C	-0.17984100	-1.54733200	-1.835839
N	-1.26693500	-1.11849400	-1.795519

1·SCN$^-$ (M062X/BS5**)**

Cl	5.86661000	-0.95911100	-1.584154
Cl	-5.78175600	-1.30255900	-1.820600
O	-2.63520100	2.21530900	-0.731382
O	2.14713200	2.10454300	-1.132642
O	2.46139700	-1.38537600	1.831353
O	-2.30833600	-1.76797200	1.520709
N	-4.06183900	0.55381300	-1.208911
N	-2.41695900	0.28047300	0.486389
N	-3.88476200	-1.51270400	-0.049491
N	3.83444500	0.64500900	-1.317922
N	4.01676800	-1.14395300	0.237295
N	2.21195000	0.39743000	0.403954
C	-4.41563200	-0.68528100	-0.926425
C	-3.02707800	0.95826100	-0.473755
C	-2.86661200	-0.95985400	0.612097
C	-1.37268600	2.62722400	-0.318160
C	-1.30195500	3.72776000	0.526432
H	-2.22155200	4.16590700	0.907584
C	-0.05013600	4.24916900	0.848892
H	0.02230000	5.11326900	1.507350
C	1.10626700	3.67896300	0.322511
H	2.09361000	4.08020700	0.540448
C	0.98763400	2.57762800	-0.518465
C	-0.23891200	2.02127600	-0.850489
H	-0.32099100	1.14556300	-1.497407
C	2.72965500	0.99780000	-0.657718
C	4.40134800	-0.42727100	-0.801141
C	2.88589100	-0.68378900	0.773598
C	1.18806400	-1.13596200	2.336465
C	1.09323700	-0.64927300	3.633873
H	2.00107400	-0.40310400	4.179812
C	-0.16988900	-0.50283200	4.206220
H	-0.26262700	-0.12405600	5.222725
C	-1.31262900	-0.84293700	3.486548
H	-2.30820100	-0.74664900	3.914068
C	-1.16867000	-1.32593100	2.190513
C	0.07007500	-1.48089800	1.585643
H	0.17211500	-1.86838400	0.570577
S	1.39532300	-2.11743400	-1.890016
C	-0.14099500	-1.46405500	-1.919614
N	-1.22034900	-0.99827300	-1.904250

1·SCN$^-$ (M06L/BS1**)**

Cl	5.86551200	-0.39576200	-1.75142700
Cl	-5.75827900	-0.70147000	-2.12420400
O	-2.69269000	2.34094600	0.05961400
O	2.07795500	2.34967100	-0.53764500
O	2.49363800	-1.78953300	1.41717200
O	-2.26786500	-2.15954000	0.88337800
N	-4.08178500	0.89575700	-0.93879500
N	-2.40194700	0.11591500	0.56704500
N	-3.84686100	-1.43987300	-0.52527900
N	3.78462900	1.02337600	-1.10885100
N	4.03162100	-1.09939600	-0.05072400
N	2.16853600	0.29341500	0.49101600
C	-4.40273100	-0.37894700	-1.07706300
C	-3.04347500	1.05569600	-0.11568600
C	-2.83271700	-1.10745100	0.27972900
C	-1.41112700	2.64986500	0.50310400
C	-1.30799100	3.55444700	1.55284700
H	-2.20913300	3.89783700	2.05024100
C	-0.04500000	4.00413000	1.92936200
H	0.05388800	4.71086200	2.74838100
C	1.09000900	3.56340200	1.25523400
H	2.08265500	3.91546200	1.51672200
C	0.93753500	2.65826800	0.21040100
C	-0.29966600	2.17558500	-0.18609400
H	-0.40861900	1.45309500	-0.99715500
C	2.67465400	1.16340200	-0.37624500
C	4.38532300	-0.12886300	-0.87395300
C	2.88109800	-0.82523300	0.57103000
C	1.20370800	-1.78115400	1.93913800
C	1.08723500	-1.87925600	3.32034900
H	1.98237800	-1.85861500	3.93271200
C	-0.18083800	-2.01775600	3.87866800
H	-0.28943600	-2.09608800	4.95656400
C	-1.30843100	-2.06525100	3.06411700
H	-2.30495900	-2.18782300	3.47531600
C	-1.14347500	-1.96528900	1.68723200
C	0.10118800	-1.81678900	1.09388300
H	0.21944200	-1.76171800	0.01292100
S	1.40169100	-1.59995000	-2.42132100
C	-0.05893500	-0.85773300	-2.28000200
N	-1.11458400	-0.32628900	-2.13516600

1·SCN$^-$ (M06L/BS2**)**

Cl	5.86551200	-0.39576200	-1.751427
Cl	-5.75827900	-0.70147000	-2.124204
O	-2.69269000	2.34094600	0.059614
O	2.07795500	2.34967100	-0.537645
O	2.49363800	-1.78953300	1.417172
O	-2.26786500	-2.15954000	0.883378
N	-4.08178500	0.89575700	-0.938795
N	-2.40194700	0.11591500	0.567045
N	-3.84686100	-1.43987300	-0.525279
N	3.78462900	1.02337600	-1.108851
N	4.03162100	-1.09939600	-0.050724
N	2.16853600	0.29341500	0.491016
C	-4.40273100	-0.37894700	-1.077063
C	-3.04347500	1.05569600	-0.115686
C	-2.83271700	-1.10745100	0.279729
C	-1.41112700	2.64986500	0.503104
C	-1.30799100	3.55444700	1.552847
H	-2.20913300	3.89783700	2.050241
C	-0.04500000	4.00413000	1.929362
H	0.05388800	4.71086200	2.748381
C	1.09000900	3.56340200	1.255234
H	2.08265500	3.91546200	1.516722
C	0.93753500	2.65826800	0.210401
C	-0.29966600	2.17558500	-0.186094
H	-0.40861900	1.45309500	-0.997155
C	2.67465400	1.16340200	-0.376245
C	4.38532300	-0.12886300	-0.873953
C	2.88109800	-0.82523300	0.571030
C	1.20370800	-1.78115400	1.939138
C	1.08723500	-1.87925600	3.320349
H	1.98237800	-1.85861500	3.932712
C	-0.18083800	-2.01775600	3.878668
H	-0.28943600	-2.09608800	4.956564
C	-1.30843100	-2.06525100	3.064117
H	-2.30495900	-2.18782300	3.475316
C	-1.14347500	-1.96528900	1.687232
C	0.10118800	-1.81678900	1.093883
H	0.21944200	-1.76171800	0.012921
S	1.40169100	-1.59995000	-2.421321
C	-0.05893500	-0.85773300	-2.280002
N	-1.11458400	-0.32628900	-2.135166

1·SCN$^-$ (M06L/BS3**)**

Cl	5.83084600	-0.43375400	-1.77592500
Cl	-5.72498900	-0.74579500	-2.13774700
O	-2.68803300	2.33659700	0.01890000
O	2.07923000	2.34973500	-0.55507500
O	2.49013300	-1.75819900	1.44787900
O	-2.26549000	-2.14045400	0.92731100
N	-4.06473400	0.87295500	-0.96332000
N	-2.39630100	0.12445500	0.56405400
N	-3.82795100	-1.45032500	-0.50925700
N	3.76758700	1.00592300	-1.12825700
N	4.01610400	-1.09700400	-0.04143500
N	2.16324100	0.30598900	0.49053900
C	-4.38026700	-0.40235500	-1.08284000
C	-3.03459900	1.04963000	-0.13755300
C	-2.82374600	-1.10259400	0.29772700
C	-1.41129300	2.65687000	0.46416800
C	-1.31497300	3.57621400	1.49876100
H	-2.21807600	3.92545800	1.98603000
C	-0.05722500	4.03380100	1.87376600
H	0.03583300	4.75260200	2.68139200
C	1.08016900	3.58654000	1.21308900
H	2.06928500	3.94605000	1.47314700
C	0.93581700	2.66671800	0.18329400
C	-0.29654200	2.17523500	-0.20941900
H	-0.40174000	1.44398700	-1.01114800
C	2.66713300	1.16203300	-0.38879000
C	4.36428500	-0.14334600	-0.88251900
C	2.87328100	-0.81089300	0.58373900
C	1.20270300	-1.74347800	1.97258400
C	1.08806500	-1.82391700	3.35277800
H	1.98290700	-1.79450000	3.96335300
C	-0.17671600	-1.95699500	3.91363500
H	-0.28351600	-2.02231900	4.99150200
C	-1.30340600	-2.01606800	3.10270700
H	-2.29778400	-2.13602300	3.51686600
C	-1.14149100	-1.93404700	1.72671400
C	0.10038000	-1.79112400	1.13157500
H	0.21933800	-1.75433700	0.05122200
S	1.39683000	-1.64454100	-2.37817500
C	-0.05375400	-0.88550900	-2.25210800
N	-1.09919900	-0.34451400	-2.11933800

1·SCN$^-$ (M06L/BS4**)**

Cl	5.83083200	-0.43337800	-1.775976
Cl	-5.72500000	-0.74538500	-2.138000
O	-2.68807900	2.33655400	0.019343
O	2.07919200	2.34983500	-0.554571
O	2.49008400	-1.75853100	1.447501
O	-2.26553200	-2.14069100	0.926799
N	-4.06476400	0.87311800	-0.963206
N	-2.39634500	0.12429600	0.564025
N	-3.82797900	-1.45025900	-0.509639
N	3.76756100	1.00615200	-1.128023
N	4.01607000	-1.09701000	-0.041653
N	2.16319700	0.30586300	0.490603
C	-4.38029200	-0.40216700	-1.083004
C	-3.03463800	1.04961900	-0.137390
C	-2.82378400	-1.10269800	0.297430
C	-1.41134400	2.65673500	0.464696
C	-1.31504100	3.57585500	1.499489
H	-2.21815200	3.92499000	1.986823
C	-0.05729900	4.03336500	1.874609
H	0.03574700	4.75199100	2.682393
C	1.08010500	3.58625200	1.213850
H	2.06921600	3.94570800	1.473998
C	0.93576900	2.66665300	0.183852
C	-0.29658400	2.17525100	-0.208983
H	-0.40176800	1.44417700	-1.010872
C	2.66709700	1.16209900	-0.388535
C	4.36425800	-0.14316900	-0.882527
C	2.87323800	-0.81103800	0.583570
C	1.20264800	-1.74392700	1.972195
C	1.08799500	-1.82466000	3.352370
H	1.98282900	-1.79537100	3.962962
C	-0.17679200	-1.95786200	3.913185
H	-0.28360500	-2.02341600	4.991037
C	-1.30347400	-2.01676600	3.102232
H	-2.29785600	-2.13681200	3.516354
C	-1.14154300	-1.93445100	1.726259
C	0.10033500	-1.79139700	1.131163
H	0.21930400	-1.75437800	0.050819
S	1.39720800	-1.64370000	-2.378312
C	-0.05361400	-0.88514300	-2.252131
N	-1.09884600	-0.34378100	-2.119176

1·SCN$^-$ (M06L/BS5**)**

Cl	5.86774400	-0.40650900	-1.74442600
Cl	-5.76719300	-0.72508200	-2.12151700
O	-2.70127100	2.34080100	0.03906600
O	2.07579500	2.34962200	-0.55433100
O	2.49555100	-1.77252100	1.44271500
O	-2.26850400	-2.15622300	0.89548800
N	-4.08672400	0.88557700	-0.95031400
N	-2.39984300	0.11819100	0.55920200
N	-3.84724300	-1.44927700	-0.52016000
N	3.78336200	1.01869700	-1.11271900
N	4.03333500	-1.09476400	-0.03181900
N	2.16198200	0.29972900	0.49137300
C	-4.40370400	-0.39131500	-1.07683700
C	-3.04608500	1.05152200	-0.12879800
C	-2.83218100	-1.10768800	0.28224700
C	-1.41816400	2.65349500	0.48304600
C	-1.31849100	3.58196500	1.51337200
H	-2.22305100	3.93976800	2.00159700
C	-0.05617300	4.04188200	1.88244400
H	0.04048500	4.76993600	2.68770300
C	1.08135900	3.58948000	1.21870700
H	2.07476500	3.95452300	1.47312300
C	0.93245800	2.66102700	0.19295200
C	-0.30382000	2.16482400	-0.19311300
H	-0.41164500	1.42529900	-0.99306300
C	2.67132000	1.16276100	-0.38186600
C	4.38338000	-0.13088100	-0.86423800
C	2.87984800	-0.81525100	0.58455400
C	1.20163900	-1.75737500	1.96045500
C	1.08130900	-1.85300100	3.34235100
H	1.97670300	-1.83281800	3.96031800
C	-0.18860800	-1.99249300	3.89811000
H	-0.29991700	-2.06963300	4.97942200
C	-1.31477600	-2.04483700	3.08051100
H	-2.31414200	-2.17232700	3.49213800
C	-1.14612600	-1.94749000	1.70318200
C	0.10021900	-1.79604300	1.11237500
H	0.21919900	-1.74437300	0.02871700
S	1.42698600	-1.64265700	-2.41756700
C	-0.03109700	-0.88466800	-2.27220300
N	-1.08057700	-0.34383000	-2.12625700

1·SCN$^-$ (M06/BS1**)**

Cl	5.92364500	-0.81460600	-1.598453
Cl	-5.84563800	-1.14537500	-1.824216
O	-2.60359700	2.24260200	-0.634753
O	2.17996900	2.18452200	-0.975066
O	2.45103100	-1.52827100	1.693191
O	-2.31928900	-1.84016700	1.417545
N	-4.07765200	0.64190200	-1.154335
N	-2.41191500	0.25541000	0.492221
N	-3.91589600	-1.48120500	-0.108624
N	3.87443000	0.74980300	-1.249931
N	4.03497400	-1.15535400	0.157604
N	2.22018000	0.35626000	0.407293
C	-4.44886800	-0.60108700	-0.928705
C	-3.01949100	0.98988200	-0.425644
C	-2.87883700	-0.98112600	0.562801
C	-1.35128500	2.64380700	-0.191583
C	-1.29997900	3.70871100	0.696288
H	-2.22795700	4.12238600	1.081586
C	-0.05841400	4.22277700	1.058593
H	0.00008300	5.05699500	1.753432
C	1.10692400	3.68258300	0.524969
H	2.08848100	4.07735300	0.773256
C	1.00720100	2.61814300	-0.361324
C	-0.20898600	2.06897000	-0.733318
H	-0.28353100	1.21323800	-1.408371
C	2.75669400	1.04683900	-0.586733
C	4.43646800	-0.35805100	-0.809663
C	2.89021200	-0.74759000	0.706028
C	1.18754100	-1.30582200	2.229955
C	1.11308800	-0.88411700	3.549002
H	2.02989900	-0.67122500	4.092010
C	-0.14032100	-0.75046200	4.140048
H	-0.21851300	-0.41877100	5.172578
C	-1.29216200	-1.03979100	3.416180
H	-2.28280800	-0.94663200	3.853437
C	-1.16781400	-1.46060000	2.098841
C	0.06154800	-1.60493600	1.477160
H	0.15621600	-1.94254900	0.443209
S	1.30215500	-2.16656500	-1.999455
C	-0.15686400	-1.38379000	-2.013717
N	-1.19659100	-0.81847300	-1.979497

1·SCN$^-$ (M06/BS2**)**

Cl	5.95183500	-0.73565100	-1.60814800
Cl	-5.89083500	-1.03122100	-1.83392500
O	-2.58675300	2.26234500	-0.55655800
O	2.20019400	2.22691200	-0.86557200
O	2.44294900	-1.62362600	1.60117700
O	-2.33171800	-1.90288100	1.32805400
N	-4.08921700	0.70368400	-1.11792500
N	-2.40792000	0.22981800	0.48944700
N	-3.93791900	-1.46364600	-0.16619700
N	3.89963900	0.80946900	-1.19756800
N	4.04158300	-1.17134000	0.10349000
N	2.23056900	0.33169500	0.42249600
C	-4.47239900	-0.54292600	-0.93968000
C	-3.01646900	1.00849600	-0.39071500
C	-2.88908800	-1.00288000	0.51503300
C	-1.33731400	2.63949200	-0.08454500
C	-1.29313900	3.65039700	0.86508100
H	-2.22429400	4.04035400	1.26703800
C	-0.05483500	4.14260100	1.26650100
H	-0.00151700	4.93447100	2.00962000
C	1.11460700	3.63446400	0.71099800
H	2.09419700	4.01288300	0.99048800
C	1.02219600	2.62482400	-0.23783700
C	-0.19089300	2.09840000	-0.65142900
H	-0.26129100	1.28638400	-1.37852300
C	2.77548300	1.07182200	-0.53048900
C	4.45556100	-0.32192500	-0.81289000
C	2.89340200	-0.79007200	0.66421300
C	1.18112800	-1.42232700	2.14961500
C	1.11234500	-1.06793000	3.48893800
H	2.03228900	-0.88749800	4.03830800
C	-0.13798300	-0.95995900	4.09104600
H	-0.21134800	-0.68140900	5.13941400
C	-1.29302100	-1.20916100	3.35754800
H	-2.28217800	-1.13621700	3.80177900
C	-1.17479100	-1.56245800	2.02008700
C	0.05154500	-1.67787300	1.38593600
H	0.13976600	-1.96133000	0.33521900
S	1.29634200	-2.04042600	-2.10833900
C	-0.16845200	-1.26753900	-2.09933100
N	-1.21227400	-0.71092000	-2.05088100

1·SCN$^-$ (M06/BS3**)**

Cl	5.90615500	-0.79047600	-1.62023900
Cl	-5.85150900	-1.09612700	-1.82974300
O	-2.58841200	2.24419800	-0.60226600
O	2.18720800	2.20801700	-0.91876200
O	2.44653300	-1.55205400	1.66168700
O	-2.31407000	-1.86660900	1.36917000
N	-4.07193900	0.66538200	-1.13665300
N	-2.39937600	0.23949500	0.48240300
N	-3.90931600	-1.47342000	-0.14201600
N	3.86925000	0.77371500	-1.22918500
N	4.02650100	-1.15266600	0.13641700
N	2.22119600	0.35343200	0.41745700
C	-4.44436200	-0.57632800	-0.93516300
C	-3.00807000	0.99350800	-0.41383800
C	-2.87081900	-0.99246700	0.53367200
C	-1.34180800	2.63853800	-0.14375900
C	-1.29665100	3.67582800	0.77073100
H	-2.22563800	4.07727100	1.16154200
C	-0.06246100	4.18134400	1.15257300
H	-0.00998600	4.99559200	1.86861300
C	1.10348300	3.66056900	0.61243600
H	2.08055700	4.05157400	0.87640900
C	1.01260200	2.62415600	-0.30101100
C	-0.19739400	2.08428800	-0.69137200
H	-0.26779900	1.25022100	-1.39080200
C	2.75748100	1.06177300	-0.55963900
C	4.42632800	-0.34084000	-0.81356300
C	2.88628600	-0.75536500	0.69256600
C	1.18359500	-1.34538400	2.19995800
C	1.10418800	-0.96771300	3.52801400
H	2.01770700	-0.77290700	4.07984700
C	-0.14642800	-0.85772100	4.11920100
H	-0.22740000	-0.56231100	5.16063600
C	-1.29217900	-1.12735700	3.38670100
H	-2.28177800	-1.05621900	3.82603900
C	-1.16600100	-1.50383300	2.06046300
C	0.06176600	-1.62101900	1.43920800
H	0.15924300	-1.92832000	0.39770200
S	1.29254100	-2.12456400	-2.02853700
C	-0.14996900	-1.31812900	-2.05026700
N	-1.17376600	-0.74038600	-2.02468000

1·SCN$^-$ (M06/BS5**)**

Cl	5.95461100	-0.76377600	-1.58960300
Cl	-5.90068500	-1.06860600	-1.81956600
O	-2.58380700	2.24409200	-0.61777400
O	2.20640300	2.21824000	-0.89298000
O	2.43355300	-1.59872100	1.62452600
O	-2.34471100	-1.87370800	1.36765100
N	-4.09004300	0.67785600	-1.14489400
N	-2.40845900	0.23631500	0.47463400
N	-3.95017900	-1.46629700	-0.13608200
N	3.90408000	0.79374400	-1.20250700
N	4.03907700	-1.17041200	0.12725400
N	2.22745000	0.34051900	0.41982400
C	-4.47678600	-0.56146900	-0.93262000
C	-3.01530100	0.99505900	-0.42432300
C	-2.89756300	-0.99213400	0.53147600
C	-1.33886200	2.62776900	-0.13490400
C	-1.30381700	3.65498700	0.79804600
H	-2.24066500	4.05483700	1.18688900
C	-0.06888700	4.15651500	1.19986100
H	-0.02250400	4.96488000	1.93140500
C	1.10609200	3.64314200	0.65995400
H	2.08475700	4.03470200	0.93865400
C	1.02338900	2.61714100	-0.27269200
C	-0.18641800	2.07888600	-0.68232600
H	-0.25256200	1.25003300	-1.39543100
C	2.77825300	1.06612100	-0.54116600
C	4.45404800	-0.33322600	-0.79883300
C	2.88887500	-0.77856100	0.67772000
C	1.17281200	-1.37450500	2.16928500
C	1.10719000	-0.99873400	3.50347300
H	2.03084800	-0.81465900	4.05262800
C	-0.14179000	-0.87964900	4.10713200
H	-0.21227300	-0.58589700	5.15568100
C	-1.29969500	-1.13964300	3.38115900
H	-2.28958600	-1.06394900	3.83210600
C	-1.18586500	-1.51312900	2.04838700
C	0.03946800	-1.63748300	1.41272500
H	0.12232200	-1.94040200	0.36402800
S	1.32625600	-2.08745500	-2.07390400
C	-0.13635300	-1.30064100	-2.07904900
N	-1.17356000	-0.73339400	-2.04092000

1·SCN$^-$ (M052X/BS1**)**

Cl	5.90316900	-1.12885500	-1.4384590
Cl	-5.82372300	-1.47473300	-1.5840360
O	-2.60217500	2.09108300	-1.0388020
O	2.18177500	1.95449100	-1.3638230
O	2.46078000	-1.19035100	1.9586760
O	-2.31450000	-1.53763800	1.7442650
N	-4.07445100	0.41449400	-1.2522720
N	-2.40822700	0.34401300	0.4341870
N	-3.90732100	-1.47563700	0.1700850
N	3.87027100	0.48301000	-1.3732020
N	4.02842100	-1.13040800	0.3589440
N	2.23702200	0.42602600	0.3466600
C	-4.44238300	-0.76827400	-0.8032060
C	-3.01893200	0.89500400	-0.6018830
C	-2.87451500	-0.85626100	0.7379220
C	-1.34473600	2.55223900	-0.6562400
C	-1.28738400	3.71614300	0.0956620
H	-2.20813300	4.17595200	0.4289810
C	-0.04092800	4.26244400	0.3921810
H	0.02331100	5.17101800	0.9775940
C	1.12124900	3.65144800	-0.0686250
H	2.10195100	4.06093400	0.1342730
C	1.01195700	2.48767200	-0.8180140
C	-0.20775100	1.90943200	-1.1285090
H	-0.28346700	0.98982400	-1.6994930
C	2.76209200	0.90756000	-0.7683210
C	4.43054100	-0.52941200	-0.7425950
C	2.89891400	-0.61170600	0.8364850
C	1.19422200	-0.85607700	2.4384780
C	1.12083700	-0.16526200	3.6384610
H	2.03410700	0.15177100	4.1240380
C	-0.13379600	0.09464500	4.1851120
H	-0.21224400	0.63262400	5.1214070
C	-1.28611100	-0.33776000	3.5358160
H	-2.27294300	-0.15464700	3.9398780
C	-1.15950500	-1.02595400	2.3367800
C	0.06937100	-1.30409000	1.7609890
H	0.16104000	-1.84162600	0.8226800
S	1.28757100	-2.39940900	-1.6353750
C	-0.21459800	-1.70483400	-1.7858130
N	-1.27337800	-1.20103100	-1.8574820

1·SCN$^-$ (M052X/BS2**)**

Cl	5.90239200	-1.13594600	-1.43372300
Cl	-5.82250100	-1.48332400	-1.57739700
O	-2.60413800	2.08762300	-1.04587300
O	2.17916300	1.94560700	-1.37626100
O	2.46238800	-1.17771400	1.96613900
O	-2.31218600	-1.53088300	1.74994300
N	-4.07466900	0.40860100	-1.25327200
N	-2.40766400	0.34564400	0.43270800
N	-3.90597800	-1.47578800	0.17649600
N	3.86889100	0.47550700	-1.37704100
N	4.02871100	-1.12729700	0.36472300
N	2.23655900	0.42816400	0.34399100
C	-4.44166800	-0.77269500	-0.79948500
C	-3.01942800	0.89240000	-0.60495300
C	-2.87312000	-0.85371600	0.74132000
C	-1.34587800	2.54967400	-0.66722300
C	-1.28669100	3.71670200	0.07966300
H	-2.20663000	4.17863600	0.41217400
C	-0.03945700	4.26324000	0.37244500
H	0.02614800	5.17431300	0.95374500
C	1.12171200	3.64950000	-0.08722600
H	2.10290700	4.05912100	0.11284700
C	1.01056700	2.48265500	-0.83154800
C	-0.20991200	1.90401100	-1.13812200
H	-0.28664000	0.98217200	-1.70526500
C	2.76070100	0.90306900	-0.77430200
C	4.42997300	-0.53282500	-0.74066900
C	2.89940400	-0.60603600	0.83987900
C	1.19522100	-0.84219900	2.44341500
C	1.12023100	-0.14446900	3.63926400
H	2.03276900	0.17629800	4.12370400
C	-0.13509900	0.11744500	4.18337200
H	-0.21480600	0.66064200	5.11650500
C	-1.28645700	-0.31992500	3.53573400
H	-2.27375000	-0.13533900	3.93792200
C	-1.15820300	-1.01497100	2.34081300
C	0.07134400	-1.29511600	1.76753400
H	0.16442400	-1.83824400	0.83259400
S	1.28698500	-2.40887000	-1.62150100
C	-0.21450600	-1.71385800	-1.77621700
N	-1.27279000	-1.20947300	-1.85116600

1·SCN$^-$ (M052X/BS3**)**

Cl	5.87525000	-1.24136100	-1.36033100
Cl	-5.79919200	-1.61131600	-1.49072400
O	-2.59938600	1.99753700	-1.20648200
O	2.17743000	1.85990400	-1.49439500
O	2.44862300	-1.03380500	2.03604700
O	-2.32071200	-1.39044600	1.85063300
N	-4.06125400	0.30526700	-1.29830100
N	-2.41518200	0.37793900	0.39962500
N	-3.89979900	-1.45954500	0.26787900
N	3.85498400	0.38354300	-1.40418500
N	4.01516600	-1.09136700	0.43919600
N	2.22884300	0.45643300	0.31348600
C	-4.42774600	-0.83607600	-0.76023300
C	-3.01649500	0.84079900	-0.68053200
C	-2.87624700	-0.79527300	0.79222600
C	-1.34824000	2.48890500	-0.84424600
C	-1.29846800	3.68885800	-0.15749000
H	-2.22100400	4.16271600	0.14430800
C	-0.05853500	4.25293300	0.11582000
H	-0.00035200	5.19079000	0.65015400
C	1.10549900	3.62320000	-0.30300900
H	2.08205300	4.04653000	-0.11742100
C	1.00544300	2.42325400	-0.98737900
C	-0.20857100	1.82799600	-1.27174600
H	-0.27785500	0.88086100	-1.79303100
C	2.75323700	0.85526200	-0.83073300
C	4.41258700	-0.57863300	-0.70356700
C	2.88814600	-0.54129500	0.87686800
C	1.18401300	-0.66195900	2.49015300
C	1.11041000	0.11145800	3.63447600
H	2.02258300	0.45965500	4.09672200
C	-0.14059600	0.41101200	4.15990400
H	-0.21735000	1.01321900	5.05436100
C	-1.29077600	-0.06526100	3.54580100
H	-2.27550500	0.14513800	3.93710700
C	-1.16638300	-0.83600300	2.40211600
C	0.05978400	-1.15293900	1.84896200
H	0.14895200	-1.75757500	0.95425500
S	1.33036100	-2.49651300	-1.44680500
C	-0.17432800	-1.82401500	-1.62654500
N	-1.23194800	-1.33805800	-1.71786300

1·SCN$^-$ (M052X/BS4**)**

Cl	5.87357400	-1.25652300	-1.3487290
Cl	-5.79518500	-1.63066400	-1.4768710
O	-2.60101000	1.98624900	-1.2262130
O	2.17530400	1.84296500	-1.5165610
O	2.44897600	-1.00944100	2.0470990
O	-2.32025600	-1.37008800	1.8652850
N	-4.06062400	0.29108400	-1.3022540
N	-2.41587500	0.38300300	0.3960360
N	-3.89804200	-1.45755000	0.2819720
N	3.85269400	0.36728200	-1.4108070
N	4.01490300	-1.08522900	0.4501760
N	2.22790600	0.46020100	0.3071160
C	-4.42588100	-0.84531100	-0.7529030
C	-3.01707700	0.83423200	-0.6890790
C	-2.87573700	-0.78671100	0.8003350
C	-1.34936500	2.48059500	-0.8695580
C	-1.29837100	3.68630300	-0.1931220
H	-2.22032000	4.16324900	0.1055380
C	-0.05781300	4.25164400	0.0747120
H	0.00143900	5.19407700	0.6008450
C	1.10551000	3.61786200	-0.3399680
H	2.08239500	4.04224000	-0.1585160
C	1.00417500	2.41221500	-1.0140170
C	-0.21045700	1.81542500	-1.2924360
H	-0.28064100	0.86369500	-1.8051300
C	2.75146700	0.84575100	-0.8419880
C	4.41113600	-0.58619700	-0.6990350
C	2.88779000	-0.53064600	0.8818840
C	1.18416700	-0.63296200	2.4969590
C	1.11011800	0.15351400	3.6322810
H	2.02201700	0.50752000	4.0906440
C	-0.14112500	0.45898600	4.1538100
H	-0.21816300	1.07133700	5.0413520
C	-1.29107000	-0.02517400	3.5454940
H	-2.27586700	0.18943400	3.9342920
C	-1.16620300	-0.80889800	2.4107050
C	0.06011700	-1.13165100	1.8612990
H	0.14964200	-1.74687200	0.9738790
S	1.33109100	-2.51371400	-1.4150280
C	-0.17304800	-1.84204800	-1.6023760
N	-1.23019900	-1.35623500	-1.6996840

1·SCN$^-$ (M052X/BS5**)**

Cl	5.90941900	-1.11719600	-1.4342970
Cl	-5.83326500	-1.47408400	-1.5942220
O	-2.60700000	2.08838500	-1.0410300
O	2.17977200	1.95893900	-1.3620360
O	2.45526600	-1.19156700	1.9555590
O	-2.32275600	-1.54375400	1.7382130
N	-4.08013000	0.41350900	-1.2576310
N	-2.40973000	0.33820000	0.4283090
N	-3.91723500	-1.47867900	0.1659270
N	3.87025900	0.48995500	-1.3707020
N	4.02900000	-1.12512900	0.3624370
N	2.23084400	0.42833000	0.3469370
C	-4.44948000	-0.76869000	-0.8073050
C	-3.02281500	0.89108800	-0.6059150
C	-2.88131600	-0.86052000	0.7324260
C	-1.35036900	2.54728200	-0.6497790
C	-1.29490500	3.71378300	0.0996730
H	-2.21871600	4.17805500	0.4301230
C	-0.04892900	4.26257700	0.3958490
H	0.01352600	5.17654200	0.9801100
C	1.11523400	3.65279900	-0.0632040
H	2.09730900	4.06949500	0.1377140
C	1.00919900	2.48653600	-0.8104680
C	-0.21055900	1.90452200	-1.1174540
H	-0.28464700	0.98020800	-1.6881740
C	2.75995700	0.91155200	-0.7660230
C	4.43068800	-0.52136500	-0.7377880
C	2.89510200	-0.60894900	0.8357340
C	1.18761800	-0.85283800	2.4314720
C	1.11228000	-0.16785100	3.6355770
H	2.02709600	0.14667800	4.1278820
C	-0.14321300	0.08761500	4.1835830
H	-0.22247900	0.62146400	5.1265550
C	-1.29570000	-0.34351400	3.5325990
H	-2.28498200	-0.16595100	3.9427900
C	-1.16856000	-1.02560300	2.3293680
C	0.06164500	-1.29636200	1.7510080
H	0.15321300	-1.82958400	0.8058320
S	1.32744900	-2.40423800	-1.6190240
C	-0.18042500	-1.70776600	-1.7819290
N	-1.23859300	-1.20606100	-1.8643950

1·SCN$^-$ (M05/BS1**)**

Cl	6.00490100	-0.49224800	-1.58316100
Cl	-5.96450600	-0.79207000	-1.84609900
O	-2.60148800	2.31309900	-0.29767800
O	2.19551000	2.31360600	-0.59706600
O	2.45248700	-1.79602600	1.42118400
O	-2.33191500	-2.04840000	1.08671700
N	-4.12919200	0.83841400	-0.99468100
N	-2.40587700	0.16967500	0.50081900
N	-3.97205100	-1.43023300	-0.30139300
N	3.91990900	0.96629700	-1.05202600
N	4.07572600	-1.14698900	0.02823800
N	2.22804300	0.28333700	0.47464400
C	-4.51835400	-0.41975600	-0.94787700
C	-3.03375400	1.05055700	-0.26434200
C	-2.90058000	-1.05463300	0.39989600
C	-1.35239700	2.66046000	0.19761100
C	-1.31270100	3.58671000	1.23418400
H	-2.24093300	3.93859500	1.67086900
C	-0.07432800	4.04699300	1.67702400
H	-0.02519000	4.77110900	2.48432500
C	1.10067800	3.58880200	1.08587400
H	2.07447900	3.94286700	1.40622700
C	1.01325000	2.66243200	0.05071200
C	-0.20092200	2.18131300	-0.41937100
H	-0.26829600	1.44922400	-1.22254900
C	2.77897700	1.13488300	-0.37883000
C	4.48942300	-0.19193900	-0.78097300
C	2.90975400	-0.84716100	0.60314200
C	1.18673900	-1.69952300	1.98525400
C	1.11062800	-1.57530000	3.36799100
H	2.02349200	-1.48694500	3.94655800
C	-0.14408100	-1.57756400	3.97442900
H	-0.22169900	-1.48396800	5.05313100
C	-1.29852500	-1.70079900	3.20521600
H	-2.28448300	-1.70897900	3.65644600
C	-1.17603400	-1.82306300	1.82470300
C	0.05712500	-1.83517500	1.18587000
H	0.14423200	-1.94508500	0.10860700
S	1.30051600	-1.88012600	-2.50109400
C	-0.09522700	-1.01027000	-2.39437400
N	-1.09532100	-0.37785000	-2.27429000

1·SCN$^-$ (M05/BS2**)**

Cl	6.00494000	-0.48926200	-1.583059
Cl	-5.96380600	-0.78841700	-1.848866
O	-2.60132300	2.31377000	-0.293491
O	2.19575300	2.31504100	-0.591937
O	2.45158200	-1.79913400	1.417326
O	-2.33305300	-2.05013800	1.083740
N	-4.12888900	0.84047700	-0.993516
N	-2.40618800	0.16898500	0.501550
N	-3.97219400	-1.42936400	-0.304209
N	3.92017600	0.96858000	-1.049078
N	4.07511800	-1.14725100	0.026212
N	2.22725700	0.28217700	0.474925
C	-4.51815600	-0.41773300	-0.949150
C	-3.03370500	1.05122800	-0.262382
C	-2.90105500	-1.05506600	0.398266
C	-1.35230200	2.66016900	0.202782
C	-1.31286400	3.58480400	1.240803
H	-2.24122100	3.93602500	1.677721
C	-0.07464300	4.04462600	1.684480
H	-0.02569800	4.76766300	2.492746
C	1.10045400	3.58747600	1.092734
H	2.07417000	3.94130600	1.413588
C	1.01330700	2.66262000	0.056201
C	-0.20071200	2.18174700	-0.414554
H	-0.26780200	1.45055700	-1.218546
C	2.77886700	1.13569400	-0.376175
C	4.48935200	-0.19041000	-0.780606
C	2.90901000	-0.84852900	0.601380
C	1.18597800	-1.70391400	1.981893
C	1.11030900	-1.58422800	3.365059
H	2.02340700	-1.49807300	3.943577
C	-0.14413700	-1.58851700	3.971992
H	-0.22133400	-1.49874400	5.051040
C	-1.29882500	-1.70921800	3.202790
H	-2.28463500	-1.71915600	3.654283
C	-1.17686600	-1.82681900	1.821821
C	0.05603800	-1.83633200	1.182410
H	0.14251500	-1.94246200	0.104772
S	1.30248800	-1.87308600	-2.507708
C	-0.09421200	-1.00541400	-2.396492
N	-1.09487700	-0.37454900	-2.272706

1·SCN$^-$ (M05/BS3**)**

Cl	5.97680900	-0.58652400	-1.5868500
Cl	-5.94230200	-0.91602200	-1.7934080
O	-2.60351800	2.29246900	-0.4339750
O	2.18222500	2.27434000	-0.7543750
O	2.46783100	-1.67074900	1.5443300
O	-2.30471000	-1.96892300	1.2003550
N	-4.11822700	0.77135000	-1.0416570
N	-2.39319400	0.20399600	0.4826820
N	-3.94405300	-1.44638300	-0.2217350
N	3.89336900	0.89625800	-1.1404330
N	4.07134800	-1.12382700	0.0903760
N	2.22570500	0.32329900	0.4459230
C	-4.49634200	-0.48092100	-0.9214250
C	-3.02616200	1.03335700	-0.3288670
C	-2.87837500	-1.02485500	0.4558670
C	-1.35436000	2.67212100	0.0335570
C	-1.30901000	3.65012500	1.0159730
H	-2.23417600	4.02431800	1.4383530
C	-0.07190900	4.13199900	1.4260070
H	-0.01910500	4.89845700	2.1917120
C	1.09707400	3.64283100	0.8575490
H	2.07159900	4.01286100	1.1537810
C	1.00522000	2.66459300	-0.1228870
C	-0.20825300	2.16196300	-0.5588860
H	-0.27961600	1.38806900	-1.3209470
C	2.76455300	1.11323700	-0.4672570
C	4.46869400	-0.23304100	-0.7907400
C	2.91251500	-0.78896000	0.6523390
C	1.19967600	-1.54295200	2.0953920
C	1.11353000	-1.31242000	3.4598610
H	2.02101700	-1.17342800	4.0352700
C	-0.14194700	-1.27286900	4.0543640
H	-0.22748000	-1.09577700	5.1210900
C	-1.28736500	-1.45952800	3.2916430
H	-2.27551400	-1.43557400	3.7356820
C	-1.15600700	-1.68798300	1.9292870
C	0.07853200	-1.74504900	1.3046940
H	0.17729300	-1.94096700	0.2406710
S	1.22683000	-2.16639300	-2.2914550
C	-0.09154900	-1.18223500	-2.2937860
N	-1.03432200	-0.47125700	-2.2544040

1·SCN$^-$ (M05/BS4**)**

Cl	5.976672	-0.5842276	-1.588306
Cl	-5.941303	-0.9117527	-1.796295
O	-2.604458	2.2937488	-0.425082
O	2.181043	2.2742020	-0.751512
O	2.468654	-1.6737933	1.542098
O	-2.303612	-1.9732013	1.194454
N	-4.118523	0.7740133	-1.038016
N	-2.393047	0.2021459	0.484137
N	-3.943127	-1.4465124	-0.225945
N	3.893095	0.8975902	-1.139119
N	4.071709	-1.1242996	0.088610
N	2.225932	0.3219731	0.446820
C	-4.495874	-0.4789411	-0.922311
C	-3.026550	1.0340062	-0.324437
C	-2.877681	-1.0268379	0.453137
C	-1.354527	2.6718263	0.041616
C	-1.307534	3.6480316	1.025750
H	-2.232015	4.0219499	1.449878
C	-0.069714	4.1285262	1.435270
H	-0.015676	4.8936975	2.202231
C	1.098366	3.6400953	0.864338
H	2.073376	4.0093942	1.159938
C	1.004928	2.6637436	-0.117826
C	-0.209294	2.1623311	-0.553218
H	-0.281727	1.3899292	-1.316635
C	2.764246	1.1132386	-0.465557
C	4.468707	-0.2320854	-0.791241
C	2.913005	-0.7904213	0.651435
C	1.200099	-1.5479580	2.092690
C	1.113038	-1.3210894	3.457724
H	2.020120	-1.1833079	4.034078
C	-0.142815	-1.2835322	4.051606
H	-0.229042	-1.1094266	5.118803
C	-1.287717	-1.4690301	3.287814
H	-2.276111	-1.4468832	3.731423
C	-1.155465	-1.6937495	1.924911
C	0.079446	-1.7484419	1.300808
H	0.178667	-1.9416781	0.236321
S	1.227712	-2.1527092	-2.298004
C	-0.094921	-1.1743071	-2.297487
N	-1.040549	-0.4673739	-2.256144

1·SCN$^-$ (M05/BS5**)**

Cl	6.00572000	-0.58336000	-1.558243
Cl	-5.97499800	-0.90785200	-1.787030
O	-2.60868100	2.28950400	-0.440099
O	2.19015400	2.27295700	-0.747896
O	2.46318200	-1.69316300	1.538251
O	-2.32197200	-1.98402800	1.194823
N	-4.13494400	0.77358200	-1.046412
N	-2.40059500	0.19565000	0.479095
N	-3.97002300	-1.45364000	-0.221462
N	3.91524800	0.90183700	-1.122502
N	4.08183200	-1.13663700	0.098475
N	2.22733600	0.31587600	0.453398
C	-4.51928600	-0.48063700	-0.921139
C	-3.03555300	1.02793100	-0.333577
C	-2.89580700	-1.03303600	0.451878
C	-1.35700300	2.66006800	0.039870
C	-1.31544700	3.63802800	1.027863
H	-2.24496400	4.01660200	1.448991
C	-0.07581300	4.11963400	1.444136
H	-0.02448600	4.88721300	2.215734
C	1.09820600	3.63127500	0.875639
H	2.07516500	4.00421900	1.176968
C	1.00853100	2.65352700	-0.110985
C	-0.20656500	2.14831400	-0.552282
H	-0.27739700	1.37218000	-1.318362
C	2.77601800	1.11022200	-0.455531
C	4.48668300	-0.23440800	-0.773546
C	2.91559600	-0.80044500	0.654412
C	1.19171500	-1.55198600	2.087321
C	1.10622500	-1.31459100	3.454665
H	2.01712800	-1.17645500	4.033395
C	-0.15266000	-1.27035200	4.050998
H	-0.23767600	-1.08784600	5.121802
C	-1.30211700	-1.45898700	3.287532
H	-2.29358400	-1.43247600	3.734963
C	-1.17017900	-1.69385900	1.922463
C	0.06702400	-1.75452600	1.294602
H	0.16204800	-1.95228700	0.226637
S	1.28485000	-2.10091900	-2.341391
C	-0.07538500	-1.15945500	-2.321268
N	-1.04780600	-0.47785400	-2.270184

1·SCN$^-$ (B3LYP-D3/BS1**)**

Cl,0,-0.1821895941,0.1582434931,0.1637361558
Cl,0,-0.1106680419,0.1338045479,11.9241855493
O,0,3.4345817862,-0.1449192947,8.599807034
O,0,3.0091105572,0.343754477,3.8294448784
O,0,0.2674591238,-3.343051012,3.5131506933
O,0,-0.0679205558,-3.1189646683,8.3063605504
N,0,1.7694128938,-0.0562278245,10.1147764723
N,0,1.7482624031,-1.7019590234,8.3962648953
N,0,-0.056350597,-1.5729260092,9.9424936594
N,0,1.4889695135,0.2270633547,2.1740832918
N,0,0.1003477019,-1.6974259992,1.9847350999
N,0,1.6875575638,-1.5434687559,3.7524933259
C,0,0.6135199871,-0.5763297679,10.4959915835
C,0,2.2667202823,-0.6537951568,9.027682759
C,0,0.5713169467,-2.0879018459,8.8784221811
C,0,3.86830412,-0.4271055696,7.3016640899
C,0,5.1016127993,-1.052955399,7.1557377582
H,0,5.6434055871,-1.3765167216,8.0374694298
C,0,5.6115987454,-1.2428744255,5.869030977
H,0,6.5726597173,-1.7298288747,5.7359913891
C,0,4.8945944378,-0.8054891464,4.754668565
H,0,5.2743875333,-0.9332993552,3.7470842137
C,0,3.6631653519,-0.1851682298,4.9514887819
C,0,3.1224538648,0.0188804471,6.213288512
H,0,2.1488344705,0.4810187924,6.3589518228
C,0,2.021785329,-0.3570803245,3.2546062335
C,0,0.5478281981,-0.510261371,1.6073316984
C,0,0.6982673376,-2.1434907944,3.0950684615
C,0,0.6373301983,-3.7945395914,4.7846098315
C,0,1.404926162,-4.9514391897,4.8616672852
H,0,1.7534100239,-5.4230499534,3.9496067543
C,0,1.7033210499,-5.4770254598,6.1213621845
H,0,2.3013703086,-6.3794098507,6.2016372281
C,0,1.237798216,-4.8473101968,7.2762941113
H,0,1.4567085442,-5.2365596209,8.264375962
C,0,0.4735338565,-3.6903985509,7.1477947453
C,0,0.1514673779,-3.1425544999,5.9137665972
H,0,-0.4484282429,-2.2413368336,5.8195601971
S,0,-1.3431235284,0.0470105744,4.821206625
C,0,-0.5245905677,0.3616216211,6.2313179244
N,0,0.079142853,0.5507751423,7.2310045343

1·SCN$^-$ (B3LYP-D3/BS2**)**

Cl,0,-0.1825406509,0.1581882388,0.1641306896
Cl,0,-0.1107289385,0.1340374902,11.9238065403
O,0,3.4349624039,-0.1452308637,8.6000314633
O,0,3.0086686091,0.3446052457,3.8298568505
O,0,0.268781523,-3.3434418771,3.5128826931
O,0,-0.0678742106,-3.118792237,8.3061223321
N,0,1.7694471263,-0.0561735122,10.1145551318
N,0,1.7483365252,-1.7018439549,8.3959301198
N,0,-0.0562412596,-1.5729155046,9.9423115856
N,0,1.4890480163,0.2271689405,2.1741323851
N,0,0.1006761442,-1.6974564863,1.9850169513
N,0,1.6876494999,-1.5430075507,3.752971054
C,0,0.6135335783,-0.576266303,10.4957748595
C,0,2.2668759154,-0.6538449278,9.0276094558
C,0,0.5714157407,-2.0878067238,8.8781629673
C,0,3.8684310115,-0.4270120022,7.3017159168
C,0,5.1015279926,-1.0531767241,7.1554260142
H,0,5.6432710436,-1.3771813147,8.0369893672
C,0,5.6112464751,-1.2429615467,5.8686194955
H,0,6.5722228409,-1.7299469143,5.735297936
C,0,4.8942516963,-0.804937691,4.7545453418
H,0,5.2737474722,-0.9327320417,3.7468736831
C,0,3.6630014529,-0.1843662216,4.9517072619
C,0,3.1222884973,0.0191913677,6.2135854979
H,0,2.1487548647,0.4813415855,6.3594151567
C,0,2.0217347966,-0.3566274466,3.2548904188
C,0,0.5478741721,-0.5102214499,1.6075366025
C,0,0.6988599408,-2.1434634583,3.0952132459
C,0,0.6379449766,-3.7947856062,4.7845617517
C,0,1.4049845483,-4.9520437638,4.8619714267
H,0,1.7534496291,-5.4238727496,3.9500504319
C,0,1.7028702199,-5.4776606042,6.1217462526
H,0,2.3003773998,-6.3803507834,6.2022455365
C,0,1.2373331398,-4.8476317779,7.2764524517
H,0,1.4558966489,-5.2367235396,8.2646473688
C,0,0.4736086303,-3.6903603366,7.1476588998
C,0,0.152474075,-3.1421299683,5.9135438863
H,0,-0.4472552472,-2.2408459755,5.8192428958
S,0,-1.3433010661,0.0473682907,4.82093736
C,0,-0.5247272639,0.36135085,6.2311317593
N,0,0.0790157442,0.5500689816,7.2309130037

1·SCN$^-$ (B3LYP-D3/BS3**)**

Cl,0,-0.1952304587,0.1740943463,0.1849342513
Cl,0,-0.1212605865,0.1415248893,11.9107311186
O,0,3.4246744702,-0.1355800089,8.594461393
O,0,3.0138540249,0.3367950622,3.8294257771
O,0,0.2628797395,-3.3304057411,3.5212884955
O,0,-0.0558401693,-3.1196675147,8.3084900259
N,0,1.7609254693,-0.0501864229,10.1067075851
N,0,1.7492576604,-1.6973154646,8.3987897587
N,0,-0.0531278832,-1.5709792578,9.9374349114
N,0,1.4857142288,0.2300253513,2.1846949036
N,0,0.0969921297,-1.6862974953,1.9961946335
N,0,1.6854353856,-1.5390523882,3.7546570043
C,0,0.6102646623,-0.5727531481,10.486571588
C,0,2.2621645552,-0.6471676789,9.0249605761
C,0,0.5760593818,-2.0867083764,8.878651031
C,0,3.859799486,-0.4300295069,7.2999271739
C,0,5.0774887605,-1.0790261165,7.1576018334
H,0,5.6114551769,-1.4092185082,8.0393763131
C,0,5.5832939845,-1.2840332947,5.8753664198
H,0,6.5328331516,-1.7896442089,5.7453812405
C,0,4.8774746329,-0.8391541428,4.7612574997
H,0,5.2545435295,-0.9798925115,3.7563552552
C,0,3.6612770503,-0.1957983695,4.952934266
C,0,3.1265323957,0.0236079117,6.2107754318
H,0,2.1633757911,0.5041210697,6.3540374085
C,0,2.0222068187,-0.3560397976,3.2583235418
C,0,0.5434808889,-0.5023018239,1.6219540228
C,0,0.6943418053,-2.1348913224,3.1019426269
C,0,0.6426423631,-3.7824657366,4.7890493223
C,0,1.4260128284,-4.9246392485,4.8616510161
H,0,1.7778333474,-5.3884220219,3.9490714104
C,0,1.7365089393,-5.4462676014,6.1160710888
H,0,2.3472749104,-6.3380095852,6.1926491033
C,0,1.2672044623,-4.8267474186,7.270651778
H,0,1.4956739243,-5.2136496641,8.255480036
C,0,0.4871767176,-3.6841509655,7.1480527701
C,0,0.1537303986,-3.1413768559,5.9187171844
H,0,-0.458113283,-2.2496078023,5.826765895
S,0,-1.3620264371,0.0257929284,4.8184181892
C,0,-0.523425877,0.3420384804,6.2130158092
N,0,0.090535338,0.530989094,7.1973943529

1·SCN$^-$ (B3LYP-D3/BS4**)**

Cl,0,-0.1966483767,0.1761201913,0.1860441113
Cl,0,-0.1224281501,0.1418354734,11.9105696348
O,0,3.4226673577,-0.1340054183,8.5933045367
O,0,3.0161305521,0.3344643554,3.8275779477
O,0,0.2596085103,-3.328743073,3.5224124574
O,0,-0.0552365648,-3.1212556643,8.3098839124
N,0,1.7594217915,-0.0492994034,10.1061340853
N,0,1.7484453934,-1.697113884,8.3988775763
N,0,-0.0535496091,-1.5715629327,9.938047243
N,0,1.4864206407,0.2296809892,2.1841164086
N,0,0.0944807218,-1.6844847957,1.9972583237
N,0,1.684801721,-1.5393993776,3.7542243842
C,0,0.6092751119,-0.572547733,10.4865029744
C,0,2.2607546114,-0.6462719403,9.0243929333
C,0,0.5758063501,-2.0873557194,8.8794045929
C,0,3.8584911337,-0.4305062342,7.2993821722
C,0,5.0752610309,-1.0815243546,7.1585638363
H,0,5.6082008254,-1.4116320948,8.040984986
C,0,5.5815042231,-1.2886922095,5.8768387178
H,0,6.5304205439,-1.7957950722,5.7479587342
C,0,4.8772881828,-0.8435088552,4.761836671
H,0,5.254901898,-0.985785124,3.7573589149
C,0,3.6620059814,-0.1980230323,4.9520407795
C,0,3.1266816167,0.0233079134,6.2093146236
H,0,2.1640519424,0.5051004896,6.3515707652
C,0,2.0229544141,-0.3569974742,3.2573727985
C,0,0.5424583022,-0.5012667829,1.6224479419
C,0,0.6921696344,-2.133831927,3.1025323492
C,0,0.641491007,-3.7810771183,4.7895374125
C,0,1.4282764896,-4.9209507768,4.8608900935
H,0,1.7807618441,-5.3833190667,3.9478520645
C,0,1.7418462393,-5.4419061462,6.1148382106
H,0,2.3555135979,-6.3317554137,6.190488489
C,0,1.2714056455,-4.8245847938,7.2701272492
H,0,1.5021720919,-5.2111142326,8.2545603546
C,0,0.4878589854,-3.6842829359,7.1487030053
C,0,0.1517851316,-3.1418410414,5.9199376955
H,0,-0.4623786844,-2.2515455376,5.8288799521
S,0,-1.3614066055,0.0245549685,4.8181669674
C,0,-0.5228463254,0.3420761505,6.2125640593
N,0,0.0910745069,0.5323487678,7.1967140766

1·SCN$^-$ (B3LYP-D3/BS5**)**

Cl,0,-0.1819575235,0.1607086625,0.1586087724
Cl,0,-0.1025741043,0.1270871095,11.940666387
O,0,3.4365045204,-0.1470184616,8.6046875141
O,0,3.0055905221,0.3483956366,3.8317011731
O,0,0.2676484271,-3.3413684078,3.5119338016
O,0,-0.0716575215,-3.1147699984,8.3089020963
N,0,1.7747670456,-0.0595296137,10.1234496337
N,0,1.7462688584,-1.6996640433,8.3961972832
N,0,-0.0542322999,-1.5754406069,9.9514393627
N,0,1.4881819324,0.2306296692,2.1735134907
N,0,0.1012075515,-1.6969698694,1.981951632
N,0,1.6854244104,-1.5400939088,3.755574649
C,0,0.6196553766,-0.5813871868,10.5049583811
C,0,2.267639153,-0.655108479,9.0318275605
C,0,0.570807493,-2.0864040884,8.8825418876
C,0,3.8664769819,-0.434015654,7.3046507437
C,0,5.1029793352,-1.0547980417,7.1564400096
H,0,5.6523619838,-1.376082914,8.0391054177
C,0,5.6124589452,-1.2409366608,5.8680811392
H,0,6.5795657848,-1.7245644962,5.7329160909
C,0,4.8928857023,-0.8037170431,4.7542777374
H,0,5.2770375222,-0.926881568,3.7436091596
C,0,3.6583217695,-0.1883666143,4.9526896209
C,0,3.1171109026,0.0090172089,6.2163265195
H,0,2.1375184462,0.4676556385,6.3649821562
C,0,2.0193978189,-0.3539755617,3.2556266103
C,0,0.5491666364,-0.5093764333,1.6065992417
C,0,0.6980667559,-2.1405976026,3.0949281507
C,0,0.6420442275,-3.78882094,4.7848203939
C,0,1.4051634326,-4.9495726944,4.8634854745
H,0,1.751564723,-5.4282309745,3.949684661
C,0,1.7003753928,-5.4764461376,6.1242879845
H,0,2.2956817548,-6.3855174278,6.2054359668
C,0,1.2360609628,-4.8446841267,7.2795256332
H,0,1.4515260944,-5.2395048051,8.2704035621
C,0,0.4764007728,-3.6838782226,7.1503679068
C,0,0.1596646849,-3.1338280519,5.9150439998
H,0,-0.4399255935,-2.2275400116,5.8201711378
S,0,-1.3633308788,0.032647504,4.7995334706
C,0,-0.5268269996,0.3573270858,6.2039645692
N,0,0.0868727141,0.5531312641,7.1953030597

12. Cartesian coordinates of monomers and 1·PF_6^-

1·PF_6^- (M052X/BS2)

Cl,0,1.4324985283,5.952683152,-0.01165836
O,0,-1.0365277632,2.493490092,2.291009127
N,0,0.1131128544,4.0601587108,1.179709948
N,0,-1.1059318666,2.4013361114,-0.0010327
C,0,0.4433722861,4.5283448125,-0.00748742
C,0,-0.6617961032,2.9786687257,1.10471200
C,0,-1.6906340746,1.2604584065,2.34823815
C,0,-3.0322668249,1.2542970115,2.69946230
H,0,-3.5495661706,2.1940638858,2.83934542
C,0,-3.6702448505,0.0285414189,2.87164958
H,0,-4.7166697787,0.0000941633,3.14811588
C,0,-0.9564787958,0.09995612,2.1630867848
H,0,0.0880779398,0.1213120302,1.880294682
Cl,0,1.4776344894,-5.8143559173,-0.002392
O,0,-0.9152488651,-2.2982555563,2.2949936
N,0,0.2051189566,-3.8879236392,1.18620246
N,0,-0.9606760604,-2.1940831636,0.0024399
C,0,0.5263063499,-4.3627858758,-0.0005524
C,0,-0.5371336709,-2.7853544248,1.1090128
C,0,-1.625399457,-1.1000546983,2.34845829
C,0,-2.9664647558,-1.1605553315,2.7002268
H,0,-3.4329541341,-2.1262764126,2.8419185
O,0,-1.0495980241,2.4891296208,-2.2936091
N,0,0.1063448452,4.0578974227,-1.19187365
C,0,-0.6681237969,2.9765514574,-1.1104043
C,0,-1.7047180117,1.2563599967,-2.3447378
C,0,-3.0484663622,1.2503258889,-2.6877961
H,0,-3.5661098463,2.1901285948,-2.8261637
C,0,-3.688120867,0.0246212517,-2.85398572
H,0,-4.7362176324,-0.003743735,-3.1240515
C,0,-0.9700581858,0.0957984291,-2.1620637
H,0,0.0761981218,0.1171926337,-1.88566197
O,0,-0.9309415399,-2.3027028567,-2.290176
N,0,0.1967558831,-3.8903835406,-1.1859988
C,0,-0.5448007074,-2.7875615718,-1.105860
C,0,-1.6407234525,-1.104184565,-2.3412863
C,0,-2.983932496,-1.1645583264,-2.6847921
H,0,-3.4517769892,-2.130270451,-2.8220021
P,0,2.5846050936,-0.2678302518,-0.0108306
F,0,1.7598154343,-1.0985302361,1.14403539
F,0,3.7385063995,-1.4013873228,-0.0129469
F,0,3.3587009338,0.5674331417,1.141661367
F,0,1.7515838254,-1.1026857382,-1.1568048
F,0,1.3781103329,0.8610066396,-0.00854879
F,0,3.3503878088,0.5632618969,-1.17185364

1·PF_6^- (B3LYP-D3/BS2)

Cl,0,1.5266340902,5.9151383856,-0.012387
O,0,-1.025475298,2.4821536428,2.30139854
N,0,0.1568238145,4.0357667378,1.18353318
N,0,-1.1109611395,2.4051910538,-0.001101
C,0,0.4983454682,4.5012603745,-0.0079490
C,0,-0.6468609991,2.9677559726,1.1112598
C,0,-1.6921660405,1.2513048251,2.3592057
C,0,-3.0387203353,1.2542569639,2.7081149
H,0,-3.5542652187,2.1984568027,2.8429775
C,0,-3.6891459631,0.0308154374,2.8809514
H,0,-4.7395579316,0.0115904254,3.1538307
C,0,-0.9681986808,0.0792977789,2.1775765
H,0,0.0771035267,0.0898022257,1.89413751
Cl,0,1.5272217512,-5.8225071192,-0.00252
O,0,-0.9441964885,-2.327115541,2.3051082
N,0,0.2056913381,-3.9072347491,1.1903292
N,0,-0.9876385135,-2.2244332894,0.002371
C,0,0.5379234889,-4.3804897676,-0.000622
C,0,-0.5571199214,-2.8108628912,1.116138
C,0,-1.6477181204,-1.1195269735,2.360879
C,0,-2.9939185959,-1.1680177458,2.710307
H,0,-3.47482912,-2.1299975183,2.84780028
O,0,-1.0401430961,2.4783642391,-2.304222
N,0,0.1492497032,4.0338053779,-1.1964667
C,0,-0.6539545527,2.9659220501,-1.117318
C,0,-1.7071034127,1.2473843491,-2.355763
C,0,-3.0558359901,1.2496837245,-2.696159
H,0,-3.5722808711,2.1936310634,-2.829336
C,0,-3.7072667739,0.025922483,-2.8628393
H,0,-4.759381427,0.0061896736,-3.1290411
C,0,-0.9819312137,0.075717444,-2.1767586
H,0,0.0651413836,0.0867373783,-1.8999499
O,0,-0.9585779896,-2.3308983395,-2.30041
N,0,0.1982635093,-3.9091862342,-1.190250
C,0,-0.5640814554,-2.8126925471,-1.11309
C,0,-1.6625228977,-1.1234444707,-2.35376
C,0,-3.0109021005,-1.1725892257,-2.69459
H,0,-3.4926138183,-2.1348213416,-2.82743
P,0,2.6006450948,-0.1953149717,-0.010634
F,0,1.7748853575,-1.0377501496,1.1535160
F,0,3.7687665969,-1.3332368476,-0.013413
F,0,3.377211781,0.6489413386,1.152485274
F,0,1.7676093768,-1.0395400587,-1.168284
F,0,1.3814929575,0.9370592813,-0.0076893
F,0,3.3699077269,0.647138752,-1.17989877

1·PF_6^- (MP2/BS1)

Cl	-5.57204900	-2.02168000	-0.00033200
O	-2.50918300	0.96692400	-2.30615800
N	-3.90541600	-0.42174100	-1.19770500
N	-2.43778200	1.03834200	-0.00022700
C	-4.32410900	-0.82669700	-0.00029000
C	-2.94718600	0.50797600	-1.11226500
C	-1.29644100	1.67907700	-2.27293600
C	-1.32400200	3.06636800	-2.39599300
H	-2.27460000	3.58226200	-2.43890800
C	-0.10694500	3.75463300	-2.44938400
H	-0.10387700	4.83385800	-2.54411100
C	-0.11272800	0.95026400	-2.21645700
H	-0.10790400	-0.12647400	-2.11390500
Cl	5.76120000	-1.53390100	0.00012200
O	2.29110400	0.96743500	-2.30437000
N	3.87498600	-0.20051900	-1.19808200
N	2.17329100	0.97858800	0.00035200
C	4.34431700	-0.54222100	0.00023200
C	2.77708900	0.55991000	-1.11188500
C	1.07571900	1.67216500	-2.26694000
C	1.10617300	3.06010900	-2.39238900
H	2.05894500	3.57234700	-2.43543100
O	-2.51142900	0.96937400	2.30559500
N	-3.90650600	-0.42069600	1.19719800
C	-2.94829800	0.50904800	1.11180400
C	-1.29758100	1.67966300	2.27279400
C	-1.32361500	3.06700500	2.39609400
H	-2.27373600	3.58379400	2.43886700
C	-0.10604800	3.75417000	2.45009100
H	-0.10202200	4.83336500	2.54516300
C	-0.11460300	0.94955100	2.21597800
H	-0.11121400	-0.12718300	2.11293100
O	2.28904200	0.96418900	2.30510000
N	3.87392100	-0.20225100	1.19858600
C	2.77604900	0.55826300	1.11253900
C	1.07444100	1.67045100	2.26737900
C	1.10636000	3.05828800	2.39318000
H	2.05973500	3.56932100	2.43686900
P	0.19212900	-2.54817400	-0.00013800
F	1.03278100	-1.71147500	-1.15822700
F	1.33845600	-3.70963900	0.00041600
F	-0.64398600	-3.32751300	-1.16858300
F	1.03056700	-1.71245000	1.16022800
F	-0.95366800	-1.33999200	-0.00063700
F	-0.64616100	-3.32863900	1.16598800

13. Cartesian coordinates of monomers and $1{\cdot}BF_4^-$

$1{\cdot}BF_4^-$ (M052X/BS2)

F	-0.87617400	-1.76294200	-0.017997
F	1.09422800	-2.06986700	-1.166130
F	1.09199400	-2.08806400	1.130474
F	0.13591500	-3.83783200	-0.032440
B	0.36154700	-2.46838700	-0.021728
Cl	-5.73136700	-2.16866200	-0.020062
Cl	5.83132000	-1.75098600	-0.016385
O	2.29212900	0.63303300	-2.286277
O	-2.49830700	0.62364400	-2.284812
O	-2.49397100	0.57349100	2.299790
O	2.29564000	0.59545900	2.298474
N	3.89021400	-0.48786700	-1.190434
N	2.17939800	0.63925300	0.006407
N	3.89184800	-0.50767500	1.181890
N	-3.96056300	-0.67168100	-1.190574
N	-3.95829700	-0.69782100	1.180224
N	-2.41692800	0.67422400	0.008276
C	4.36705000	-0.81652100	-0.007291
C	2.77656700	0.23788000	-1.105129
C	2.77835600	0.21958200	1.110210
C	1.07592500	1.31184400	-2.336680
C	1.10132400	2.65532700	-2.683954
H	2.05427000	3.14837100	-2.822555
C	-0.10658100	3.32706300	-2.854375
H	-0.10629800	4.37505500	-3.126718
C	-1.31495300	2.65572400	-2.684898
H	-2.26824300	3.14817600	-2.822665
C	-1.28492100	1.31336900	-2.337635
C	-0.10524200	0.60976400	-2.154718
H	-0.09456400	-0.43714200	-1.876217
C	-2.94952700	0.19215500	-1.103396
C	-4.39768100	-1.05662800	-0.008799
C	-2.94748700	0.16799800	1.110128
C	-1.28279800	1.26638200	2.363048
C	-1.31612900	2.60435100	2.726511
H	-2.27051800	3.09299300	2.870191
C	-0.10928900	3.27654600	2.903464
H	-0.11147500	4.32121500	3.188322
C	1.10029800	2.61012100	2.723883
H	2.05200100	3.10422800	2.867154
C	1.07806500	1.27094800	2.360401
C	-0.10151600	0.56795400	2.171846
H	-0.08818700	-0.47580900	1.881953

$1{\cdot}BF_4^-$ (B3LYP-D3/BS2)

F,0,3.3913278788,9.5299032154,14.59310563
F,0,5.5007621453,8.8079720883,14.00135441
F,0,3.7631714013,7.300095448,14.134112830
F,0,3.8123995993,8.8534495498,12.42061689
B,0,4.1126205389,8.6255066158,13.76109427
Cl,0,0.2367976674,13.1846146607,15.058918
Cl,0,7.8017826506,4.3858032432,13.6928601
O,0,7.590446558,8.3815767216,16.458996048
O,0,4.487622342,11.9983131984,17.10430751
O,0,1.0217495974,8.976323841,17.368601759
O,0,4.1254763682,5.3601021235,16.72570728
N,0,7.6254652144,6.5332377412,15.17607151
N,0,5.7904540047,6.9519042589,16.63360033
N,0,5.8339087182,4.9712556533,15.31372943
N,0,2.5079632535,12.4891454827,16.1549130
N,0,0.7173691782,10.9277900867,16.2913435
N,0,2.8115527202,10.4283850111,17.3082940
C,0,6.9918740045,5.4171182988,14.85421740
C,0,6.9550132095,7.2662110143,16.07302628
C,0,5.2771892391,5.8031741717,16.20212477
C,0,6.9347903688,9.2906297258,17.29594584
C,0,7.3838751256,9.406226761,18.608109261
H,0,8.1632629811,8.7427156896,18.96586666
C,0,6.8172555434,10.382820566,19.42986145
H,0,7.1551046544,10.4874535335,20.4561424
C,0,5.8211030292,11.2281628783,18.9368863
H,0,5.3699816129,11.9979504671,19.5529353
C,0,5.406091229,11.0731741722,17.61811244
C,0,5.9449835238,10.1132075796,16.7705283
H,0,5.6085560773,9.9917115868,15.74667255
C,0,3.234592029,11.6002630662,16.84402125
C,0,1.2719273262,12.0736345617,15.9301485
C,0,1.5582957147,10.13864572,16.971843148
C,0,1.8579650551,7.9798640103,17.88948390
C,0,1.7646140044,7.6925719827,19.24749333
H,0,1.1179442055,8.2922968614,19.87816669
C,0,2.5101316501,6.6290777055,19.76045054
H,0,2.4512789855,6.3886020742,20.81735658
C,0,3.3278946151,5.8708189246,18.91996926
H,0,3.9109045716,5.03636164,19.2934158338
C,0,3.3874191101,6.1977609662,17.56854999
C,0,2.6606723242,7.24930305,17.0221825903
H,0,2.7364099733,7.4859640535,15.96646195

14. Cartesian coordinates of monomers and 1·NO_3^-

1·NO_3^- (M052X/BS2)

Cl	2.29605600	-5.74694500	0.000000
Cl	1.90352900	5.86113500	0.000000
O	-0.42733900	2.29590900	2.292370
O	-0.45430100	-2.49256500	2.292218
N	0.82163600	-3.96651000	1.186043
N	-0.53512400	-2.42352800	0.000000
N	-0.44098100	2.18041800	0.000000
N	0.66881600	3.90895000	1.187020
C	-1.11966900	1.08523800	2.327810
C	-2.48415400	1.12205600	2.579841
H	-2.98051400	2.07880200	2.674307
C	-3.17518400	-0.08050900	2.706886
H	-4.23985700	-0.07140400	2.903777
C	-2.50421000	-1.29480200	2.582930
H	-3.01543800	-2.24359300	2.677072
C	-1.14058000	-1.27503900	2.330695
C	-0.41494400	-0.10180200	2.205325
H	0.65138000	-0.09865700	2.003564
C	-0.04000500	-2.95187100	1.107643
C	1.18936600	-4.40587100	0.000000
C	-0.04081300	2.78417200	1.108991
C	0.98340000	4.38494500	0.000000
O	-0.42733900	2.29590900	-2.292370
O	-0.45430100	-2.49256500	-2.292218
N	0.82163600	-3.96651000	-1.186043
N	0.66881600	3.90895000	-1.187020
C	-1.11966900	1.08523800	-2.327810
C	-2.48415400	1.12205600	-2.579841
H	-2.98051400	2.07880200	-2.674307
C	-3.17518400	-0.08050900	-2.706886
H	-4.23985700	-0.07140400	-2.903777
C	-2.50421000	-1.29480200	-2.582930
H	-3.01543800	-2.24359300	-2.677072
C	-1.14058000	-1.27503900	-2.330695
C	-0.41494400	-0.10180200	-2.205325
H	0.65138000	-0.09865700	-2.003564
C	-0.04000500	-2.95187100	-1.107643
C	-0.04081300	2.78417200	-1.108991
N	2.13264500	0.42053100	0.000000
O	2.22878900	1.03690300	-1.080161
O	1.90719500	-0.80941900	0.000000
O	2.22878900	1.03690300	1.080161

1·NO_3^- (B3LYP-D3/BS2)

Cl,0,-0.0000000045,-10.3367081172,7.8305
Cl,0,0.0000000045,1.3920533356,7.8399964
O,0,-2.3024181833,-2.1074925932,5.360784
O,0,-2.302615026,-6.9133803688,5.2480191
N,0,-1.1902591916,-8.4630390789,6.444865
N,0,-0.0000000019,-6.8495260199,5.161825
N,0,0.0000000017,-2.2175890449,5.3413409
N,0,-1.1910117356,-0.5271436799,6.519813
C,0,-2.3394866405,-3.3099680548,4.644190
C,0,-2.587762562,-3.2501593926,3.2760981
H,0,-2.6775138468,-2.2846825237,2.790678
C,0,-2.7131233018,-4.4441031679,2.562479
H,0,-2.9056163354,-4.4171477282,1.494443
C,0,-2.5888754017,-5.6725580392,3.215047
H,0,-2.677991102,-6.6125998106,2.6820088
C,0,-2.340572592,-5.6786610376,4.5838213
C,0,-2.2191670696,-4.5131407747,5.329500
H,0,-2.0151261178,-4.5240417197,6.397382
C,0,-1.1145246919,-7.4002955534,5.632464
C,0,-0.0000000034,-8.9250584575,6.790846
C,0,-1.1160066027,-1.6297297595,5.764345
C,0,0.0000000034,-0.0582232972,6.8535909
O,0,2.3024181869,-2.1074925968,5.3607849
O,0,2.3026150222,-6.9133803723,5.2480191
N,0,1.1902591855,-8.4630390807,6.4448654
N,0,1.1910117417,-0.5271436817,6.5198134
C,0,2.3394866423,-3.3099680584,4.6441908
C,0,2.5877625638,-3.2501593966,3.2760981
H,0,2.67751385,-2.2846825279,2.790678681
C,0,2.7131233018,-4.4441031721,2.5624796
H,0,2.9056163354,-4.4171477326,1.4944439
C,0,2.5888753998,-5.6725580432,3.2150472
H,0,2.6779910986,-6.6125998147,2.6820088
C,0,2.3405725901,-5.6786610412,4.5838213
C,0,2.2191670695,-4.5131407781,5.3295006
H,0,2.0151261177,-4.5240417228,6.3973821
C,0,1.1145246873,-7.4002955551,5.6324647
C,0,1.1160066071,-1.6297297613,5.7643457
N,0,0.0000000002,-4.1732982537,7.9420564
O,0,1.0932722839,-3.5491615527,8.0385423
O,0,-0.0000000007,-5.4157404712,7.714311
O,0,-1.0932722824,-3.549161551,8.0385423

1·NO_3^- (MP2/BS1**)**

Cl	2.45212000	-5.61216900	0.000000
Cl	2.04748000	5.78122400	0.000000
O	-0.44119900	2.29881400	2.304241
O	-0.49202700	-2.50275900	2.305100
N	0.87705400	-3.92013000	1.197853
N	-0.56033300	-2.43073400	0.000000
N	-0.44492100	2.17947800	0.000000
N	0.72632000	3.88572500	1.198870
C	-1.15674000	1.08984800	2.260731
C	-2.54718300	1.13553300	2.358352
H	-3.05018500	2.09390600	2.386566
C	-3.25591100	-0.06992600	2.404486
H	-4.33684400	-0.05514500	2.477775
C	-2.57988200	-1.29430700	2.365974
H	-3.10742900	-2.23916700	2.395614
C	-1.19061800	-1.28059600	2.267330
C	-0.44588000	-0.10608500	2.229995
H	0.63516200	-0.10885500	2.138858
C	-0.03838500	-2.94587900	1.112368
C	1.27190100	-4.34397000	0.000000
C	-0.02483000	2.78102600	1.113132
C	1.06211600	4.35418200	0.000000
O	-0.44119900	2.29881400	-2.304241
O	-0.49202700	-2.50275900	-2.305100
N	0.87705400	-3.92013000	-1.197853
N	0.72632000	3.88572500	-1.198870
C	-1.15674000	1.08984800	-2.260731
C	-2.54718300	1.13553300	-2.358352
H	-3.05018500	2.09390600	-2.386566
C	-3.25591100	-0.06992600	-2.404486
H	-4.33684400	-0.05514500	-2.477775
C	-2.57988200	-1.29430700	-2.365974
H	-3.10742900	-2.23916700	-2.395614
C	-1.19061800	-1.28059600	-2.267330
C	-0.44588000	-0.10608500	-2.229995
H	0.63516200	-0.10885500	-2.138858
C	-0.03838500	-2.94587900	-1.112368
C	-0.02483000	2.78102600	-1.113132
N	2.06071300	0.36846800	0.000000
O	2.15377600	0.99936500	-1.100346
O	1.84127300	-0.88720200	0.000000
O	2.15377600	0.99936500	1.100346

15. Cartesian coordinates of monomers and M^+·1

Li^+·1(M05-2X/BS2)

Cl,0,-6.1025999206,0.0049019456,-2.060412
Cl,0,6.1028155644,-0.0094014394,-2.058100
O,0,2.3789411292,-2.3040495383,-0.0320246
O,0,-2.3818967601,-2.298160327,-0.0379377
O,0,-2.3798433858,2.3045851566,-0.0377559
O,0,2.3809335866,2.2987557617,-0.04376032
N,0,4.0827363661,-1.1899784127,-0.9542106
N,0,2.2282821152,-0.0026202282,-0.0607407
N,0,4.0837484654,1.178527993,-0.960332773
N,0,-4.0841638621,-1.18024865,-0.95835381
N,0,-4.0831156775,1.1882466595,-0.9582998
N,0,-2.2286840005,0.00315341,-0.061683605
C,0,4.6072955525,-0.0067173348,-1.2483561
C,0,2.9099724421,-1.1187393478,-0.3589642
C,0,2.9109884147,1.1113617724,-0.36466505
C,0,1.184942873,-2.3018409096,0.669835465
C,0,1.2082676854,-2.2620060928,2.05880487
H,0,2.1576830831,-2.2492942103,2.57790303
C,0,-0.0049145722,-2.2516382868,2.7476782
H,0,-0.006206289,-2.2371620545,3.82972356
C,0,-1.2164017862,-2.2590183566,2.0558978
H,0,-2.1669277125,-2.244147722,2.57289890
C,0,-1.189829552,-2.2987315567,0.66699493
C,0,-0.0016456922,-2.3412593635,-0.053497
H,0,-0.0006354679,-2.4000431818,-1.135133
C,0,-2.9115198888,-1.1114236696,-0.362504
C,0,-4.6074962899,0.0042292148,-1.2497526
C,0,-2.9105227819,1.1183755415,-0.3625011
C,0,-1.1859234198,2.3037218477,0.66406875
C,0,-1.2092774881,2.2666321706,2.05304751
H,0,-2.1586592484,2.2554976889,2.57223420
C,0,0.0039057811,2.2573053876,2.741966163
H,0,0.0052310909,2.2446226499,3.824032605
C,0,1.21529346,2.2634381341,2.0500569625
H,0,2.1659536935,2.2494162216,2.566850795
C,0,1.1886271819,2.3008823897,0.661015667
C,0,0.0004921553,2.3417106601,-0.05956070
H,0,-0.000814477,2.3979442306,-1.14134358
Li,0,0.0060956324,0.0006978466,0.62417646

Li^+·1(B3LYP-D3/BS2)

Cl,0,6.0994679276,-0.0005226975,-2.046908
Cl,0,-6.0995517568,-0.0016768882,-2.04714
O,0,-2.39144812,2.3222758897,0.0096485976
O,0,2.3915624356,2.3226606363,0.011079192
O,0,2.3914534116,-2.3220867279,0.01272338
O,0,-2.3915680922,-2.3224709964,0.0134006
N,0,-4.0748272556,1.1855631326,-0.9180014
N,0,-2.1968416274,-0.0001328776,-0.035537
N,0,-4.074885145,-1.187171063,-0.91606522
N,0,4.0748329155,1.1862814362,-0.91714036
N,0,4.0747727855,-1.1864470337,-0.9163253
N,0,2.1967888802,0.0002686888,-0.03521822
C,0,-4.6006963899,-0.0010364379,-1.216785
C,0,-2.8945020074,1.1237034638,-0.3237210
C,0,-2.8945625482,-1.1244052174,-0.321871
C,0,-1.1935888047,2.3916024229,0.70991932
C,0,-1.2165682126,2.5467652002,2.09335269
H,0,-2.16646094,2.6047637304,2.612442172
C,0,-0.000779356,2.6382057591,2.778065165
H,0,-0.0011044549,2.7744841904,3.85399294
C,0,1.215429682,2.5470076491,2.0940541434
H,0,2.1650104878,2.6051669134,2.613695224
C,0,1.1932935342,2.3918293831,0.710618257
C,0,0.000064632,2.337721485,-0.0098991262
H,0,0.0003786793,2.2797330521,-1.09382909
C,0,2.8945136837,1.1241883773,-0.32285693
C,0,4.6006359624,-0.0001990854,-1.2164973
C,0,2.8944552517,-1.1238821648,-0.3220884
C,0,1.1935007833,-2.3906528277,0.71287648
C,0,1.2162507307,-2.5443275304,2.09647576
H,0,2.1660596287,-2.601782849,2.615778736
C,0,0.0003520622,-2.634985114,2.781099451
H,0,0.0005055565,-2.7700996943,3.85717403
C,0,-1.2157474912,-2.5444904508,2.0968025
H,0,-2.1654126158,-2.60207933,2.616353267
C,0,-1.193382584,-2.3908235109,0.71319841
C,0,-0.000037627,-2.3375205206,-0.0071879
H,0,-0.0001790306,-2.2807158854,-1.091180
Li,0,-0.0006549711,0.0003694926,0.4221820

Na^+·1(M05-2X/BS2)

Cl	-6.04805900	0.00271100	-2.15003800
Cl	6.04661700	-0.00609300	-2.15137300
O	2.37137000	-2.31201600	-0.06407800
O	-2.40594900	-2.30807800	-0.01015800
O	-2.37201800	2.31132000	-0.06743800
O	2.40569000	2.30773500	-0.01237700
N	4.04347800	-1.18752500	-1.01744200
N	2.27057700	-0.00208200	0.03139200
N	4.06177000	1.17998400	-0.98994200
N	-4.06247200	-1.18167900	-0.98806300
N	-4.04433600	1.18561600	-1.01851600
N	-2.27014000	0.00165700	0.03030500
C	4.57143300	-0.00437200	-1.30221400
C	2.90528900	-1.11650200	-0.35586900
C	2.92184000	1.11115800	-0.33123400
C	1.17924700	-2.37173800	0.63628800
C	1.21798000	-2.52677800	2.01879900
H	2.17410500	-2.59761000	2.52091600
C	0.01302500	-2.61379400	2.71856300
H	0.02471000	-2.75992500	3.79089300
C	-1.20733400	-2.52462900	2.04546200
H	-2.15246000	-2.59391600	2.56811200
C	-1.19866000	-2.36941800	0.66290000
C	-0.01736000	-2.31622900	-0.06957900
H	-0.02887500	-2.22385200	-1.14831600
C	-2.92199200	-1.11182200	-0.33030700
C	-4.57236000	0.00215700	-1.30165200
C	-2.90563600	1.11529200	-0.35766100
C	-1.18041000	2.37195500	0.63333100
C	-1.21981200	2.53074000	2.01489100
H	-2.17604400	2.60381200	2.51644800
C	-0.01473100	2.61987000	2.71468000
H	-0.02665800	2.76930400	3.78655000
C	1.20591600	2.52921100	2.04229500
H	2.15081800	2.60054400	2.56510000
C	1.19791300	2.37041800	0.66009200
C	0.01670800	2.31491000	-0.07222800
H	0.02819900	2.21968400	-1.15071600
Na	0.00904700	0.00121600	1.31035800

Na^+·1(B3LYP-D3/BS2)

Cl,0,-6.0392774463,0.0017128559,-2.189926
Cl,0,6.0390768111,-0.0051959969,-2.189470
O,0,2.397532208,-2.3295630672,-0.01894630
O,0,-2.4029476888,-2.3265533947,-0.014789
O,0,-2.3980150944,2.3297660744,-0.0228391
O,0,2.4024074027,2.3267488271,-0.01888573
N,0,4.0437898532,-1.190207436,-1.00586775
N,0,2.2619205455,-0.0012655651,0.04865360
N,0,4.0462914196,1.1839674104,-1.00581112
N,0,-4.0467382303,-1.1854500054,-1.003860
N,0,-4.0441860554,1.1887410166,-1.0080293
N,0,-2.262531172,0.0015803856,0.048797591
C,0,4.5643517469,-0.0036644215,-1.3134393
C,0,2.9058151231,-1.1242874312,-0.3315404
C,0,2.9080608251,1.1204119534,-0.33170174
C,0,1.1922151474,-2.4377031741,0.66052459
C,0,1.2151711228,-2.7226700124,2.02643509
H,0,2.1664623438,-2.8352300707,2.53428010
C,0,-0.000718597,-2.8743773504,2.70325668
H,0,0.000018248,-3.115277942,3.7609049271
C,0,-1.2175794099,-2.7212342127,2.0284612
H,0,-2.1681683982,-2.8326592174,2.5378683
C,0,-1.1965414828,-2.4362530613,0.6625376
C,0,-0.0026766685,-2.3216414638,-0.050779
H,0,-0.0034283337,-2.1358093637,-1.118707
C,0,-2.9086473169,-1.1207734798,-0.329632
C,0,-4.5647676099,0.0016678385,-1.3135448
C,0,-2.9062546497,1.1239887779,-0.3335277
C,0,-1.1926570747,2.4391019144,0.65645022
C,0,-1.2155815077,2.7263746321,2.02187664
H,0,-2.166850849,2.8398537021,2.529557965
C,0,0.0003588945,2.8790821954,2.698403084
H,0,-0.000314385,3.1217311531,3.755651842
C,0,1.2171733432,2.724707526,2.023815029
H,0,2.1677855099,2.8368924346,2.533012019
C,0,1.1960938202,2.4375217333,0.658348855
C,0,0.0021955281,2.3218058069,-0.05471616
H,0,0.0028758961,2.1342156458,-1.12233726
Na,0,-0.0012878187,0.0011807825,1.2676924

K^+·1(M05-2X/BS2)

Cl	5.87985400	-0.00034900	-2.433971
Cl	-5.88011700	0.00011400	-2.433624
O	-2.39790500	2.31161100	-0.056134
O	2.39718900	2.31208000	-0.058003
O	2.39809900	-2.31170500	-0.055633
O	-2.39692800	-2.31219300	-0.058317
N	-3.96957800	1.18243800	-1.147928
N	-2.27263100	-0.00030900	0.026497
N	-3.96909200	-1.18264700	-1.149052
N	3.96904900	1.18249100	-1.149143
N	3.96955500	-1.18259700	-1.147845
N	2.27280400	0.00023000	0.026779
C	-4.46725700	-0.00004900	-1.480301
C	-2.88183200	1.11086500	-0.403086
C	-2.88140500	-1.11131700	-0.404114
C	-1.18929100	2.44633100	0.600419
C	-1.21144400	2.94550900	1.899183
H	-2.16282300	3.16392200	2.366542
C	0.00054800	3.20157300	2.541856
H	0.00086600	3.62342500	3.538750
C	1.21212100	2.94580500	1.898280
H	2.16379900	3.16448000	2.364906
C	1.18907800	2.44660600	0.599546
C	-0.00032400	2.20291300	-0.078514
H	-0.00064100	1.85775600	-1.104336
C	2.88151000	1.11121300	-0.403970
C	4.46716700	-0.00011900	-1.480394
C	2.88194100	-1.11096800	-0.402836
C	1.18941400	-2.44624600	0.600785
C	1.21134400	-2.94460300	1.899878
H	2.16264800	-3.16264100	2.367569
C	-0.00075600	-3.20030500	2.542509
H	-0.00122500	-3.62152600	3.539670
C	-1.21223500	-2.94494700	1.898578
H	-2.16398500	-3.16336800	2.365182
C	-1.18897500	-2.44653900	0.599534
C	0.00054300	-2.20329600	-0.078490
H	0.00099200	-1.85879100	-1.104535
K	-0.00002200	-0.00049500	2.101671

K^+·1(B3LYP-D3/BS2)

Cl,0,5.803584009,-0.0002817912,-2.530819
Cl,0,-5.8036041111,-0.0001358694,-2.5308
O,0,-2.4113062874,2.328196836,-0.0010073
O,0,2.4111011747,2.3280546597,-0.0012482
O,0,2.411326165,-2.3280785259,-0.0004226
O,0,-2.4110790206,-2.3279375807,-0.00085
N,0,-3.9286786464,1.1862196619,-1.163512
N,0,-2.2651640506,0.000145286,0.07393769
N,0,-3.9285476764,-1.1861920895,-1.16343
N,0,3.9286307979,1.1860633108,-1.1635111
N,0,3.9287619096,-1.1863476706,-1.163087
N,0,2.2651872524,-0.0000114268,0.0740297
C,0,-4.4174594537,-0.0000278321,-1.51673
C,0,-2.863101105,1.1190401316,-0.3758083
C,0,-2.8629800248,-1.1188476857,-0.37571
C,0,-1.1945015233,2.5207369705,0.6317773
C,0,-1.215399525,3.1751503826,1.86540543
H,0,-2.1674865798,3.4449267684,2.3084840
C,0,0.0000516383,3.5058038525,2.47474412
H,0,0.0001153567,4.0389415975,3.41962822
C,0,1.2154233115,3.1750265507,1.86531446
H,0,2.167571807,3.4446810693,2.308335448
C,0,1.194371241,2.5206334625,0.631675056
C,0,-0.0001037721,2.1977123221,-0.013153
H,0,-0.0001624595,1.7334698623,-0.991586
C,0,2.8630144264,1.1188862893,-0.3758489
C,0,4.4176254577,-0.0001753353,-1.516452
C,0,2.8631369314,-1.1190013165,-0.375462
C,0,1.1944983497,-2.5204773647,0.6323596
C,0,1.2153492331,-3.1746005971,1.8661429
H,0,2.1674196536,-3.4442658563,2.3093249
C,0,-0.0001262234,-3.5051141658,2.475511
H,0,-0.0002271584,-4.0380291195,3.420520
C,0,-1.2154736237,-3.1744813193,1.865955
H,0,-2.1676390628,-3.4440346688,2.309001
C,0,-1.1943741351,-2.5203760642,0.632164
C,0,0.0001259373,-2.1976077617,-0.012694
H,0,0.00022239,-1.7336005211,-0.99123930

16. Cartesian coordinates of monomers and M^{2+}·1

Mg^{2+}·1(M05-2X/BS2)

Cl,0,-6.0028832426,-0.0139275238,-2.1598
Cl,0,6.0065594154,-0.0487005974,-2.14830
O,0,2.362966411,-2.3074640045,0.03999488
O,0,-2.3654749747,-2.2998702606,0.010636
O,0,-2.3605713264,2.3149296237,-0.044102
O,0,2.3674939712,2.3052026739,-0.0550420
N,0,4.0307582095,-1.2047510239,-0.949978
N,0,2.1624528724,-0.0028212357,-0.094846
N,0,4.0321702683,1.1593805217,-0.9999092
N,0,-4.0293063117,-1.1847097491,-0.97213
N,0,-4.0272263699,1.1799348393,-0.998884
N,0,-2.1617228001,0.0061573383,-0.099655
C,0,4.5579425899,-0.0298094629,-1.298613
C,0,2.8728544136,-1.1289027658,-0.354492
C,0,2.8748058037,1.1104613219,-0.4005988
C,0,1.1861004178,-2.2754895716,0.7454922
C,0,1.2032851937,-2.0486868838,2.1220508
H,0,2.1511512655,-1.9651009842,2.6399490
C,0,-0.0177695983,-1.9545045256,2.800854
H,0,-0.0255700781,-1.8052629831,3.873586
C,0,-1.2291021614,-2.051040131,2.1073270
H,0,-2.182635136,-1.969657862,2.61518861
C,0,-1.1969689734,-2.274049072,0.7297943
C,0,-0.0013404634,-2.4087006633,0.026562
H,0,0.00567087,-2.6001255665,-1.04110377
C,0,-2.8731993094,-1.1163509553,-0.37245
C,0,-4.5548137202,-0.005481686,-1.309325
C,0,-2.8705418768,1.1235066275,-0.398917
C,0,-1.1858822777,2.3062060304,0.6659275
C,0,-1.2080927071,2.1173172453,2.0486461
H,0,-2.1581638246,2.0514268575,2.5651434
C,0,0.009200732,2.0378705833,2.735440998
H,0,0.0115116354,1.917733721,3.811833183
C,0,1.2232995015,2.1129328719,2.04318107
H,0,2.1753110666,2.0417061431,2.55533613
C,0,1.1960266234,2.3018967592,0.66005769
C,0,0.0036872281,2.4184256217,-0.0526535
H,0,0.0021762303,2.5809286855,-1.1255162
Mg,0,-0.0026235676,0.0097910425,0.694997

Ca^{2+}·1(M05-2X/BS2)

Cl,0,-6.0197879321,-0.0151748042,-2.1465
Cl,0,6.0260929972,-0.0466756737,-2.12963
O,0,2.37624287,-2.3292134703,0.001435232
O,0,-2.3914238758,-2.3166540178,0.000820
O,0,-2.3755526532,2.33223356,-0.07728940
O,0,2.3921164919,2.3199169983,-0.0640494
N,0,4.028413857,-1.2058094226,-0.9712951
N,0,2.245882155,-0.00298654,0.0530712383
N,0,4.036417992,1.1582992342,-1.00474386
N,0,-4.0332084575,-1.1847246683,-0.97956
N,0,-4.0251248756,1.1792597656,-1.019279
N,0,-2.2453761655,0.0087487025,0.0465855
C,0,4.5660515511,-0.0298909414,-1.293558
C,0,2.8998319672,-1.1299857554,-0.317088
C,0,2.9073889507,1.1086481355,-0.3488181
C,0,1.1871382295,-2.4045353256,0.6830384
C,0,1.2083696438,-2.519340926,2.07550492
H,0,2.1591982349,-2.5887315521,2.5907831
C,0,-0.008765913,-2.5955659752,2.7647848
H,0,-0.0093043161,-2.7318039153,3.839624
C,0,-1.2252647332,-2.5128056624,2.075067
H,0,-2.1766581522,-2.5770967957,2.589959
C,0,-1.202904509,-2.3981771816,0.6826389
C,0,-0.007670877,-2.3766079972,-0.038189
H,0,-0.0073074611,-2.3279157429,-1.12160
C,0,-2.905911301,-1.1147628386,-0.322507
C,0,-4.5619836271,-0.0060582704,-1.30644
C,0,-2.8983168482,1.1237083362,-0.359983
C,0,-1.1884019315,2.4285608199,0.6050137
C,0,-1.2135895846,2.5862694632,1.9932067
H,0,-2.1658739366,2.6713892121,2.5034098
C,0,0.0015871949,2.6839344933,2.68322299
H,0,-0.0008859593,2.8532654057,3.7533460
C,0,1.2200329566,2.5801371564,1.99980666
H,0,2.1699680189,2.6603769987,2.51515503
C,0,1.2016273319,2.4224893238,0.61153176
C,0,0.008426094,2.3785036096,-0.11164457
H,0,0.0111053975,2.296190916,-1.19302467
Ca,0,-0.0010428245,0.0229863459,1.352833

17. Cartesian coordinates of monomers and $M^+ \cdot 1 \cdot SCN^-$

$Li^+ \cdot 1 \cdot SCN^-$(M05-2X/BS2)

Cl	5.85877	-1.21819	-1.21168
Cl	-5.75757	-1.92251	-1.30645
O	-2.83647	1.93521	-1.27241
O	1.83445	1.32265	-2.00263
O	2.53922	-0.41548	2.19989
O	-2.11248	-1.38676	1.81385
N	-4.16771	0.12552	-1.2488
N	-2.43021	0.35884	0.34854
N	-3.78003	-1.59402	0.33619
N	3.65651	0.09138	-1.59409
N	4.07172	-0.71755	0.59368
N	2.08077	0.4962	0.13457
C	-4.42717	-1.04027	-0.6717
C	-3.14342	0.75337	-0.70215
C	-2.783	-0.8505	0.78614
C	-1.5332	2.37636	-1.12226
C	-1.29783	3.55762	-0.43162
H	-2.13149	4.10985	-0.01609
C	0.01858	4.00629	-0.30849
H	0.22168	4.9332	0.20803
C	1.06951	3.26495	-0.84295
H	2.09806	3.58762	-0.7434
C	0.78637	2.07839	-1.50507
C	-0.50703	1.62329	-1.69029
H	-0.69782	0.6796	-2.18791
C	2.53865	0.60467	-1.11624
C	4.37085	-0.54934	-0.68253
C	2.89332	-0.22024	0.91847
C	1.22662	-0.14598	2.53966
C	0.96144	0.95358	3.34594
H	1.78201	1.55881	3.70947
C	-0.36885	1.243	3.66853
H	-0.59715	2.08935	4.30179
C	-1.39835	0.45199	3.16618
H	-2.43685	0.67772	3.37284
C	-1.08367	-0.63462	2.3466
C	0.22184	-0.97655	2.03909
H	0.469	-1.8043	1.37925
S	1.62243	-2.91124	-0.62949
C	0.29237	-2.0059	-0.98625
N	-0.65386	-1.32926	-1.16292
Li	-0.08233	1.17889	0.8633

$Na^+ \cdot 1 \cdot SCN^-$(M05-2X/BS2)

Cl,0,6.0769626681,-0.9206569913,-1.1911193359
Cl,0,-6.0094881051,-1.5504205469,-1.4870424772
O,0,-2.6338073864,1.8990346299,-1.3866271375
O,0,2.1470219497,1.8617305567,-1.5552515702
O,0,2.368290104,-1.2253079001,1.8843818504
O,0,-2.4207843676,-1.4970872625,1.7418787733
N,0,-4.1722895667,0.2723867764,-1.3850340078
N,0,-2.5314627603,0.3310046146,0.3184175104
N,0,-4.062390624,-1.4708085874,0.2208436797
N,0,3.9320336934,0.5207111091,-1.3532647805
N,0,4.0815440479,-1.0090768317,0.4562996308
N,0,2.1760872071,0.379331434,0.2269048519
C,0,-4.5995322348,-0.8405052695,-0.8108828092
C,0,-3.112924932,0.7926617166,-0.7879615669
C,0,-3.011302197,-0.8442958891,0.7237540741
C,0,-1.4126838953,2.4217208303,-0.9706502364
C,0,-1.3900700031,3.3495275526,0.0634689465
H,0,-2.3216409437,3.6749733817,0.507072279
C,0,-0.1579351762,3.817980168,0.5201580156
H,0,-0.1233724248,4.5437202869,1.3220337308
C,0,1.0293217916,3.3331607753,-0.0247324572
H,0,1.9945261362,3.648071403,0.3498553233
C,0,0.9661308278,2.4035495784,-1.0584914867
C,0,-0.2467268573,1.9829731073,-1.5983807168
H,0,-0.2828004809,1.2337548455,-2.377367335
C,0,2.7612111837,0.8812308144,-0.8619099528
C,0,4.5312109405,-0.4209467403,-0.6370862383
C,0,2.8733363382,-0.6009368872,0.8074985498
C,0,1.1189600243,-0.8444129914,2.3601674982
C,0,1.0558421614,0.181157608,3.2972033184
H,0,1.9738207902,0.6330998707,3.6491342567
C,0,-0.1913142139,0.6088164705,3.7486018521
H,0,-0.2553799478,1.4004605871,4.4835291529
C,0,-1.3577003035,0.0430447826,3.2377569324
H,0,-2.3367373545,0.3913789502,3.5387862864
C,0,-1.2560469795,-0.977587366,2.2990286139
C,0,-0.024412382,-1.4880095895,1.8867869099
H,0,0.0495929163,-2.2813985567,1.1514986093
S,0,1.6535248105,-2.7389836955,-1.3732456562
C,0,0.3694130739,-1.7228503336,-1.3737092115
N,0,-0.540324113,-0.9729686492,-1.3018161586
Na,0,-0.1760304154,0.5837692382,0.4816444

Na^+·1·SCN^-(B3LYP-D3/BS2)

Cl,0,6.0769626681,-0.9206569913,-1.1911193359
Cl,0,-6.0094881051,-1.5504205469,-1.4870424772
O,0,-2.6338073864,1.8990346299,-1.3866271375
O,0,2.1470219497,1.8617305567,-1.5552515702
O,0,2.368290104,-1.2253079001,1.8843818504
O,0,-2.4207843676,-1.4970872625,1.7418787733
N,0,-4.1722895667,0.2723867764,-1.3850340078
N,0,-2.5314627603,0.3310046146,0.3184175104
N,0,-4.062390624,-1.4708085874,0.2208436797
N,0,3.9320336934,0.5207111091,-1.3532647805
N,0,4.0815440479,-1.0090768317,0.4562996308
N,0,2.1760872071,0.379331434,0.2269048519
C,0,-4.5995322348,-0.8405052695,-0.8108828092
C,0,-3.112924932,0.7926617166,-0.7879615669
C,0,-3.011302197,-0.8442958891,0.7237540741
C,0,-1.4126838953,2.4217208303,-0.9706502364
C,0,-1.3900700031,3.3495275526,0.0634689465
H,0,-2.3216409437,3.6749733817,0.507072279
C,0,-0.1579351762,3.817980168,0.5201580156
H,0,-0.1233724248,4.5437202869,1.3220337308
C,0,1.0293217916,3.3331607753,-0.0247324572
H,0,1.9945261362,3.648071403,0.3498553233
C,0,0.9661308278,2.4035495784,-1.0584914867
C,0,-0.2467268573,1.9829731073,-1.5983807168
H,0,-0.2828004809,1.2337548455,-2.377367335
C,0,2.7612111837,0.8812308144,-0.8619099528
C,0,4.5312109405,-0.4209467403,-0.6370862383
C,0,2.8733363382,-0.6009368872,0.8074985498
C,0,1.1189600243,-0.8444129914,2.3601674982
C,0,1.0558421614,0.181157608,3.2972033184
H,0,1.9738207902,0.6330998707,3.6491342567
C,0,-0.1913142139,0.6088164705,3.7486018521
H,0,-0.2553799478,1.4004605871,4.4835291529
C,0,-1.3577003035,0.0430447826,3.2377569324
H,0,-2.3367373545,0.3913789502,3.5387862864
C,0,-1.2560469795,-0.977587366,2.2990286139
C,0,-0.024412382,-1.4880095895,1.8867869099
H,0,0.0495929163,-2.2813985567,1.1514986093
S,0,1.6535248105,-2.7389836955,-1.3732456562
C,0,0.3694130739,-1.7228503336,-1.3737092115
N,0,-0.540324113,-0.9729686492,-1.3018161586
Na,0,-0.1760304154,0.5837692382,0.481644489

K^+·1·SCN^-(M05-2X/BS2)

Cl,0,5.7749244094,-1.1749195125,-1.479412
Cl,0,-5.6245800066,-1.5294833867,-1.71723
O,0,-2.6745194053,2.2058649832,-0.9530488
O,0,2.0879980254,1.9128707579,-1.45089158
O,0,2.4740297819,-1.1139455728,2.02429327
O,0,-2.3000863377,-1.5182442544,1.7590356
N,0,-3.9994362906,0.4381214391,-1.2673831
N,0,-2.4127592136,0.426338977,0.501650882
N,0,-3.801535505,-1.4643386863,0.12197294
N,0,3.7398159643,0.4261403479,-1.42524968
N,0,3.9703915111,-1.0873574529,0.37760823
N,0,2.1716164254,0.46900401,0.3607301251
C,0,-4.3388949064,-0.7756736574,-0.865221
C,0,-3.0170853377,0.9607757955,-0.5608077
C,0,-2.83108172,-0.8167178243,0.745432224
C,0,-1.400961682,2.6807205601,-0.72359579
C,0,-1.2861867828,3.9175206193,-0.0949828
H,0,-2.1838170754,4.4399444468,0.20875277
C,0,-0.0147182601,4.4600225341,0.09806480
H,0,0.0907894159,5.432015617,0.5629067218
C,0,1.1190779722,3.7653282073,-0.32167643
H,0,2.1151129623,4.1704615746,-0.20028176
C,0,0.9564845374,2.5331801958,-0.95188984
C,0,-0.2927713495,1.9733181881,-1.1857746
H,0,-0.409528737,1.0051552287,-1.66867989
C,0,2.6658885207,0.8872019495,-0.80670111
C,0,4.3419821897,-0.5497133883,-0.7701199
C,0,2.8572734606,-0.5644035576,0.85956249
C,0,1.2072874832,-0.9042760748,2.52950596
C,0,1.120294103,-0.3725388519,3.813405023
H,0,2.030408251,-0.1240319189,4.343419678
C,0,-0.1393033827,-0.2103627168,4.3921181
H,0,-0.222983015,0.1760997129,5.399819713
C,0,-1.2891680137,-0.5585238615,3.6843180
H,0,-2.2775243694,-0.4549940986,4.1124763
C,0,-1.1550009579,-1.0895967017,2.4031064
C,0,0.0835565881,-1.2968887422,1.80724033
H,0,0.1864867128,-1.7451255182,0.82290126
S,0,1.3598709283,-2.4532254502,-1.4155022
C,0,-0.0783443366,-1.6539283053,-1.581972
N,0,-1.0969269439,-1.0681318233,-1.635961
K,0,-0.1003498037,1.7299416622,1.82700551

K^+·1·SCN^-(B3LYP-D3/BS2)

Cl,0,5.720546282,-1.2402596525,-1.512951
Cl,0,-5.5801693124,-1.5184567038,-1.7789
O,0,-2.6986203029,2.2689811285,-0.851566
O,0,2.0741204357,1.9285661957,-1.4672529
O,0,2.4965439826,-1.0451839897,2.0912267
O,0,-2.2865217357,-1.5579221914,1.759939
N,0,-3.9852117652,0.4755992354,-1.238677
N,0,-2.4010988639,0.4295557097,0.5425562
N,0,-3.7638668296,-1.4744341664,0.092669
N,0,3.6953876675,0.4021201705,-1.4420234
N,0,3.9539176719,-1.0717507858,0.3984217
N,0,2.1580777769,0.5014160743,0.37942607
C,0,-4.3090112723,-0.7626895066,-0.88049
C,0,-3.0127725229,0.9976918423,-0.507589
C,0,-2.8057637207,-0.832163071,0.7537212
C,0,-1.4120716443,2.7583439786,-0.719522
C,0,-1.2849735124,4.0667350655,-0.244373
H,0,-2.1752140016,4.6217267355,0.0300199
C,0,-0.0089009686,4.6350413222,-0.162432
H,0,0.1034567969,5.6569751933,0.18487840
C,0,1.1210456876,3.8986425934,-0.5335160
H,0,2.1183134422,4.3215296194,-0.4878597
C,0,0.9465538311,2.593654419,-1.00285930
C,0,-0.3092826534,2.0062344632,-1.132571
H,0,-0.4343757783,0.9867988383,-1.507488
C,0,2.6358668037,0.8987941551,-0.8111763
C,0,4.3070837865,-0.5677396943,-0.776854
C,0,2.8495461197,-0.5303163999,0.8950730
C,0,1.2168472126,-0.9243825492,2.6015196
C,0,1.1112156094,-0.5331349123,3.9391934
H,0,2.012297013,-0.3099144881,4.49958116
C,0,-0.1565262534,-0.4726020605,4.528681
H,0,-0.252010985,-0.1926068973,5.5727237
C,0,-1.3000013042,-0.7756121199,3.782093
H,0,-2.292202697,-0.7392197359,4.2175686
C,0,-1.1491941526,-1.1617468566,2.447560
C,0,0.1000752374,-1.2734134021,1.8401537
H,0,0.2164427973,-1.6343973661,0.8215906
S,0,1.3277016889,-2.5315782057,-1.310505
C,0,-0.0341381576,-1.6306153047,-1.55678
N,0,-1.0044251476,-0.9594683136,-1.66374
K,0,-0.1029604515,1.774807084,1.88955190

18. Cartesian coordinates of monomers and $M^+ \cdot 1 \cdot PF_6^-$

$Li^+ \cdot 1 \cdot PF_6^-$(M05-2X/BS2)

Cl,0,6.2173081193,1.410189032,-0.003866698
O,0,2.5537584655,-0.7206932598,-2.3066594118
N,0,4.2296486336,0.2470659112,-1.188537717
N,0,2.4349988123,-0.7568143946,-0.0031785352
C,0,4.7347125783,0.548999733,-0.0035850817
C,0,3.07902233,-0.4023167527,-1.1180550671
C,0,1.3793427778,-1.4652787866,-2.3308936711
C,0,1.4633749302,-2.8496561576,-2.369737786
H,0,2.4350743213,-3.3250492157,-2.3766888321
C,0,0.2834942736,-3.589289219,-2.3991132788
H,0,0.3289899082,-4.6697819328,-2.4384315132
C,0,0.1651508583,-0.7882920332,-2.3524655782
H,0,0.1130799718,0.2950309347,-2.3581195489
Cl,0,-6.0950539017,0.7857205311,-0.0017745858
O,0,-2.2219840817,-0.9281950197,-2.3058091668
N,0,-3.99063611,-0.1480146034,-1.1869646006
N,0,-2.0756741733,-0.8995444127,-0.0022558805
C,0,-4.5229502206,0.1004459181,-0.0019634784
C,0,-2.7683567634,-0.6439846777,-1.1176883353
C,0,-0.9886722781,-1.5639798731,-2.3283766401
C,0,-0.9536049976,-2.9514827612,-2.3659021032
H,0,-1.8823523317,-3.5062366521,-2.3706847711
O,0,2.5538552158,-0.7193580086,2.3002651544
N,0,4.2296500534,0.2478171374,1.1815504678
C,0,3.0790212521,-0.401620613,1.1114977157
C,0,1.3797452914,-1.4644053362,2.3251972916
C,0,1.4644105305,-2.8487450232,2.364652312
H,0,2.4363201351,-3.3237129667,2.3714293383
C,0,0.2848971511,-3.5888956439,2.3949498773
H,0,0.3309126897,-4.6693461591,2.4348131735
C,0,0.1652976018,-0.7879126618,2.3469346582
H,0,0.1127504765,0.2953595077,2.3517757073
O,0,-2.2217953424,-0.9289328528,2.301346472
N,0,-3.9903961731,-0.148138746,1.1828897846
C,0,-2.7681736573,-0.6442389355,1.1133733828
C,0,-0.9881836039,-1.5642172855,2.3237562537
C,0,-0.9525192961,-2.9516557601,2.3620031994
H,0,-1.881022229,-3.506808797,2.367540132
P,0,-0.5546557253,2.5219932611,-0.0019420405
F,0,-1.4077636998,1.7125468622,-1.1459438134
F,0,-1.5945699451,3.72907225,-0.0020303298
F,0,0.3557900347,3.1758310946,-1.1528269328
F,0,-1.4080403985,1.7124911721,1.1418183888
F,0,0.5162300153,1.1784272153,-0.0018777034
F,0,0.3555350496,3.175742964,1.1491755016
Li,0,0.1158702814,-0.6025447433,-0.003229

$Li^+ \cdot 1 \cdot PF_6^-$(M05-2X/BS2)

Cl,0,6.219505943,1.4376914285,-0.0035053946
O,0,2.5469663905,-0.7303568791,-2.3178672917
N,0,4.2262576134,0.2481599276,-1.1925771518
N,0,2.4193522074,-0.7490620086,-0.0028007055
C,0,4.7324544927,0.5570248708,-0.0032300297
C,0,3.0701770873,-0.4038532159,-1.1246666892
C,0,1.3742470526,-1.4864400268,-2.3482366267
C,0,1.4634806415,-2.874157408,-2.3845725568
H,0,2.4376059081,-3.3495743874,-2.3838328925
C,0,0.2845831271,-3.6222474015,-2.4147207514
H,0,0.3367701776,-4.7052232786,-2.4479369063
C,0,0.1501192375,-0.8195478989,-2.3687336032
H,0,0.0900606294,0.2642566931,-2.3795825475
Cl,0,-6.1281080601,0.7912122107,-0.0012414792
O,0,-2.2455236759,-0.9645728447,-2.3165086754
N,0,-4.0179531837,-0.1743089287,-1.1904794889
N,0,-2.0839677397,-0.8985447552,-0.0019788768
C,0,-4.5527310084,0.0822692695,-0.0015286138
C,0,-2.7875595646,-0.6662468818,-1.1251807216
C,0,-1.0052523932,-1.6002879799,-2.3478133478
C,0,-0.960413755,-2.9907097183,-2.3824727181
H,0,-1.8848281848,-3.5567634808,-2.3805409678
O,0,2.5478228005,-0.7303527287,2.3122185051
N,0,4.2266918017,0.2481713439,1.1863051387
C,0,3.0705842284,-0.4038384256,1.1188232432
C,0,1.3751115589,-1.4864287857,2.3430297077
C,0,1.464355106,-2.8741445734,2.3794079172
H,0,2.4384782288,-3.3495657324,2.3783537022
C,0,0.285465769,-3.6222286054,2.4100166968
H,0,0.3376616287,-4.7052028094,2.4432763166
C,0,0.1509928415,-0.8195306505,2.3639157148
H,0,0.0909328736,0.2642718753,2.3747430453
O,0,-2.2446682926,-0.9645485646,2.3126116377
N,0,-4.0175049755,-0.1742770666,1.1872285665
C,0,-2.7871332665,-0.6662113049,1.1214821343
C,0,-1.004389198,-1.6002683262,2.3434693108
C,0,-0.9595410566,-2.9906890762,2.3781885938
H,0,-1.8839574893,-3.5567410155,2.3766344184
P,0,-0.495476566,2.613728923,-0.0030032752
F,0,-1.2964912671,1.7302696221,-1.1550926033
F,0,-1.6338306294,3.7429097076,-0.003253316
F,0,0.3685226133,3.3327445787,-1.1626408651
F,0,-1.2968780209,1.7304211173,1.1489468957
F,0,0.6709815126,1.3285097571,-0.0027431786
F,0,0.3681511145,3.3328858339,1.156827421
Li,0,0.0707125716,-0.3910121601,-0.0023714013

Na^+·1·PF_6^-(M05-2X/BS2)

Cl,0,5.8122538858,2.0107245066,0.0010969974
O,0,2.4953021114,-0.6160343022,-2.315813356
N,0,4.0027744553,0.5882992784,-1.1861126369
N,0,2.4576897492,-0.7633515772,-0.0021850252
C,0,4.4633594025,0.9516011759,-0.0001939525
C,0,2.9861321635,-0.2537162477,-1.1169076871
C,0,1.3427387409,-1.3888582164,-2.3723252227
C,0,1.4585266118,-2.7754283658,-2.3627042024
H,0,2.441543364,-3.2267609732,-2.3355997531
C,0,0.2965412516,-3.5478234655,-2.3762940852
H,0,0.3688412776,-4.6275823916,-2.3797041989
C,0,0.1083303435,-0.7475474186,-2.4398811839
H,0,0.0344811384,0.3321193384,-2.4408844832
Cl,0,-5.9973111349,1.0755719029,-0.0020214614
O,0,-2.2765414097,-0.9406961857,-2.3175064846
N,0,-3.9691533541,-0.0140076733,-1.1881959904
N,0,-2.1954705322,-1.0463305881,-0.002892021
C,0,-4.4838351162,0.2658383733,-0.002367117
C,0,-2.8148218941,-0.6529224366,-1.1183794824
C,0,-1.0300166187,-1.5468717588,-2.3725797519
C,0,-0.9576918792,-2.9370973302,-2.363263246
H,0,-1.8717442022,-3.5156320564,-2.3374536862
O,0,2.4942632493,-0.6201142082,2.3117640176
N,0,4.0020175747,0.5864157745,1.1848746664
C,0,2.9855202556,-0.2555830667,1.1137171124
C,0,1.3416766189,-1.3929911193,2.3667536776
C,0,1.4573607958,-2.7795596661,2.3547869785
H,0,2.4403275963,-3.2309593881,2.3270285468
C,0,0.2952845325,-3.5518509478,2.366953002
H,0,0.3674786876,-4.6316220762,2.368568571
C,0,0.1073020502,-0.7517262172,2.4351861643
H,0,0.033701076,0.3279463289,2.4379791277
O,0,-2.277510765,-0.9443680863,2.3118253086
N,0,-3.9691628316,-0.0149995983,1.1832598594
C,0,-2.8151438733,-0.6543684809,1.1129417548
C,0,-1.0311202505,-1.5507750085,2.3663384704
C,0,-0.9588888868,-2.9409941961,2.3547579324
H,0,-1.8729833285,-3.5194117158,2.3277958409
P,0,-0.2788353861,2.163273556,-0.0003576247
F,0,-1.3892542913,1.8228312872,-1.1490827784
F,0,-0.6647636722,3.7106082383,0.0000599522
F,0,0.8455726756,2.3697978812,-1.1541852731
F,0,-1.3883497867,1.8224641443,1.1490847898
F,0,0.1196897962,0.5319483901,-0.0009311303
F,0,0.8465733172,2.3692714194,1.1525645443
Na,0,0.1691533221,-1.7111365922,-0.00314919

Na^+·1·PF_6^-(B3LYP-D3/BS2)

Cl,0,5.7408451412,2.1097217713,0.0002361935
O,0,2.4693369316,-0.60003952,-2.333907066
N,0,3.9504927561,0.6339893666,-1.1903293735
N,0,2.40602492,-0.7309973999,-0.0026553578
C,0,4.4064006506,1.0105516208,-0.0008805599
C,0,2.9387894571,-0.2225854107,-1.1265307097
C,0,1.3256124243,-1.3894414004,-2.4305624164
C,0,1.4642151676,-2.7752454127,-2.5255564253
H,0,2.4551473791,-3.2149146592,-2.5323972826
C,0,0.3113508068,-3.5654459024,-2.5921785299
H,0,0.402483891,-4.6433637358,-2.6735828011
C,0,0.0748251244,-0.7683800587,-2.4547736726
H,0,-0.0161487137,0.3080847375,-2.3906072929
Cl,0,-5.9921475684,1.1203932836,0.0004755407
O,0,-2.3138631941,-1.0044873146,-2.3337946821
N,0,-3.9802974348,-0.0352605223,-1.1901518008
N,0,-2.2293333192,-1.1229390303,-0.0025684546
C,0,-4.4927504687,0.2597271994,-0.0006997858
C,0,-2.8396479773,-0.7106760305,-1.1263623098
C,0,-1.0539223464,-1.5906236552,-2.4303790941
C,0,-0.9577928618,-2.9800430191,-2.5252857028
H,0,-1.860820943,-3.5798772299,-2.5319262534
O,0,2.4698567465,-0.6054001945,2.3288691834
N,0,3.9507212327,0.6313018785,1.1878046214
C,0,2.9390297443,-0.2251535158,1.1222586295
C,0,1.3261777285,-1.3950456259,2.4239589043
C,0,1.4648221785,-2.7810686294,2.515666947
H,0,2.4557618377,-3.2207386552,2.5212273956
C,0,0.3119857514,-3.571439058,2.5807209281
H,0,0.4031531861,-4.6495447096,2.6595594527
C,0,0.0753870794,-0.7740661356,2.4499129494
H,0,-0.0156114161,0.3025446204,2.3882563467
O,0,-2.3133342185,-1.0099311539,2.3289547997
N,0,-3.9799960278,-0.0379833052,1.187946489
C,0,-2.8393840577,-0.7132803636,1.122317403
C,0,-1.0533622851,-1.5962636775,2.4238807065
C,0,-0.9571833311,-2.985899396,2.5155117977
H,0,-1.8602002256,-3.5857622492,2.520969031
P,0,-0.1767928759,2.2166181647,0.0009829763
F,0,-1.3259104745,2.0507946582,-1.1586469384
F,0,-0.3110954789,3.8166337766,0.0028231898
F,0,0.9839640523,2.2447080176,-1.1585714683
F,0,-1.3257020254,2.048158063,1.1603921145
F,0,-0.0350775815,0.5282664887,-0.0009506432
F,0,0.9841337951,2.2420508922,1.1603984294
Na,0,0.1516936732,-1.6600573275,-0.003459118

$K^+ \cdot 1 \cdot PF_6^-$(M05-2X/BS2)

Cl,0,5.4155943188,2.2626967817,-0.0089853305
O,0,2.5672053406,-0.8635603812,-2.3133343728
N,0,3.8394110894,0.5773830997,-1.1881354523
N,0,2.4581985984,-0.9508670527,-0.002932344
C,0,4.2393655592,1.0154015573,-0.0065491972
C,0,2.9430404346,-0.3897290414,-1.1127754871
C,0,1.3759967894,-1.5470847031,-2.4611330771
C,0,1.4372992603,-2.851267288,-2.9444142768
H,0,2.4030029497,-3.2961645071,-3.145020517
C,0,0.2447524356,-3.5319954983,-3.1918429865
H,0,0.2721891049,-4.5363625108,-3.5947279888
C,0,0.1710120878,-0.8924540548,-2.2278758044
H,0,0.1322538158,0.1291029469,-1.8679429418
Cl,0,-5.7207368526,1.3547939175,0.000908836
O,0,-2.2263125852,-1.0021994985,-2.3161552262
N,0,-3.7956017859,0.0908000931,-1.183945923
N,0,-2.0959940871,-1.0803868142,-0.0039685875
C,0,-4.2870093478,0.4138478888,-0.0009405507
C,0,-2.6973251373,-0.6399102374,-1.1123404321
C,0,-0.9967630184,-1.6120647575,-2.4581348306
C,0,-0.9830198294,-2.9185001079,-2.9415038658
H,0,-1.9225001768,-3.4164804448,-3.1422142028
O,0,2.55418898,-0.8417939252,2.3073970103
N,0,3.8333758536,0.5873912849,1.1762855788
C,0,2.9367441342,-0.3800761073,1.1048579755
C,0,1.3700538868,-1.5381012067,2.4543368601
C,0,1.4439860644,-2.8414605064,2.9380986273
H,0,2.4138443295,-3.277166612,3.1388688023
C,0,0.2579092272,-3.5332328251,3.1859139888
H,0,0.2948548827,-4.5371213363,3.5892356609
C,0,0.1590373346,-0.895106364,2.220559614
H,0,0.1119216181,0.1252876143,1.858467365
O,0,-2.2376558629,-1.0286965456,2.3083285017
N,0,-3.8022905909,0.0760964178,1.1809546809
C,0,-2.7032647805,-0.6527737586,1.1062669197
C,0,-1.0019674217,-1.6255124912,2.4512962435
C,0,-0.9756520265,-2.9314182106,2.9355166809
H,0,-1.9103123866,-3.4381671826,3.1367481184
P,0,-0.3203104904,2.4952442926,0.0029382702
F,0,-1.1419041758,1.6520382357,-1.1535115869
F,0,-1.4490151661,3.6356117084,-0.0029442577
F,0,0.5318415196,3.2379146826,-1.1453722562
F,0,-1.1606661506,1.645829249,1.141660711
F,0,0.8043064894,1.2591399707,0.0085669169
F,0,0.5130110037,3.2313675058,1.1690429152
K,0,0.2357415943,-2.9627030374,-0.0031824

$K^+ \cdot 1 \cdot PF_6^-$(B3LYP-D3/BS2)

Cl,0,5.4275238012,2.2541583923,-0.0022599996
O,0,2.5624541127,-0.8737520272,-2.3290358939
N,0,3.8366048712,0.5612619695,-1.1884908879
N,0,2.4524326533,-0.9779416487,-0.0031960819
C,0,4.2445379764,0.9962610829,-0.0026193879
C,0,2.9349182439,-0.4101306289,-1.1200992411
C,0,1.3691405661,-1.5473562062,-2.5295229571
C,0,1.4422969408,-2.791618721,-3.1611066073
H,0,2.4129152379,-3.2044160966,-3.4119011351
C,0,0.2533857523,-3.4551908979,-3.4821166958
H,0,0.2912051625,-4.4121176176,-3.9923994982
C,0,0.1527837088,-0.9371393518,-2.2212581004
H,0,0.1054176812,0.0418828655,-1.7580638396
Cl,0,-5.6970550822,1.3987062952,0.0002243947
O,0,-2.2575171356,-1.0727767785,-2.3294293593
N,0,-3.7933835953,0.0684324354,-1.1868314603
N,0,-2.105983497,-1.1325737519,-0.0020557569
C,0,-4.2780054234,0.4122440891,-0.0006682608
C,0,-2.7046738172,-0.6871178148,-1.1193445763
C,0,-1.0123236294,-1.641290777,-2.5278205579
C,0,-0.9839734452,-2.8880156477,-3.159918794
H,0,-1.9187430414,-3.3767235843,-3.4106054517
O,0,2.5637497277,-0.8763002854,2.322691892
N,0,3.8372291168,0.5600001204,1.1830075935
C,0,2.9355290898,-0.4113343296,1.1140547099
C,0,1.3705148035,-1.5500509138,2.5231169715
C,0,1.4439604024,-2.7949914017,3.1533343562
H,0,2.4146975853,-3.2080901467,3.403171294
C,0,0.2552008747,-3.4588599613,3.4742836789
H,0,0.2932617701,-4.4163108623,3.9835643787
C,0,0.1540121176,-0.9394595181,2.2161684126
H,0,0.1064226857,0.0401025075,1.7541376294
O,0,-2.2562277622,-1.0751253112,2.325465366
N,0,-3.7927623855,0.0671783015,1.1848735695
C,0,-2.7040635,-0.6882687629,1.1160201664
C,0,-1.010954055,-1.6439084626,2.5225886009
C,0,-0.9823138099,-2.8913066365,3.1533418861
H,0,-1.9169633476,-3.3802413253,3.4040333131
P,0,-0.3111195438,2.4947977233,-0.0007046528
F,0,-1.1465698941,1.6426394448,-1.1590355641
F,0,-1.4493815357,3.6420883648,0.0001823509
F,0,0.5389158256,3.2402609078,-1.1659331254
F,0,-1.1460562844,1.6413152113,1.1570148678
F,0,0.8205674578,1.2473065998,-0.0017244431
F,0,0.5395060778,3.2389678943,1.1649328477
K,0,0.2407233719,-3.0276044977,-0.0036996

19. Cartesian coordinates of monomers and $M^+ \cdot 1 \cdot BF_4^-$

$Li^+ \cdot 1 \cdot BF_4^-$(M05-2X/BS2)

F,0,-0.4521810587,-1.5421674417,-0.1231868437
F,0,1.431237554,-2.0505705282,-1.3145118165
F,0,1.4268216419,-2.2329995462,0.9800145906
F,0,0.2322863295,-3.7451554691,-0.2969872224
B,0,0.6993406612,-2.4676618521,-0.1945262689
Cl,0,-6.185543001,-1.7426498873,-0.1509361023
Cl,0,6.0946792041,-1.3049585378,-0.0914922543
O,0,2.275605656,0.6959657394,-2.2506640415
O,0,-2.5016909268,0.5364626442,-2.2730675661
O,0,-2.510643699,0.1713979888,2.3189183121
O,0,2.2665352923,0.331626162,2.3412808932
N,0,4.0163556122,-0.2256469607,-1.1983979276
N,0,2.1159135388,0.4729584052,0.0417676259
N,0,4.0118082399,-0.4128638794,1.1636891713
N,0,-4.1860805249,-0.5059843128,-1.2376063884
N,0,-4.1908173995,-0.6936132877,1.125257877
N,0,-2.3923041222,0.3972688118,0.026600409
C,0,4.5383624944,-0.5808481248,-0.0370881651
C,0,2.8056153626,0.2916268235,-1.0899615711
C,0,2.8012410937,0.1152247373,1.1334179909
C,0,1.0502362646,1.3442823784,-2.2248010266
C,0,1.028520015,2.7308463791,-2.1563288033
H,0,1.9625000178,3.2752454812,-2.116980657
C,0,-0.2025064709,3.3813017778,-2.1413613742
H,0,-0.2377088106,4.4619792703,-2.0968881444
C,0,-1.3894252599,2.6531883862,-2.1707427222
H,0,-2.3564338517,3.1372854338,-2.1423853624
C,0,-1.3184638502,1.2689239689,-2.2379418635
C,0,-0.1109513174,0.5839749287,-2.309005114
H,0,-0.0625982563,-0.4967081354,-2.3872762081
C,0,-3.0326225711,0.1315990991,-1.1144880729
C,0,-4.695365137,-0.8957942325,-0.0806895276
C,0,-3.0369800769,-0.04514905,1.1088724028
C,0,-1.3277128971,0.9001321811,2.4045041328
C,0,-1.3990306137,2.2777020657,2.5561837104
H,0,-2.366103624,2.7604538967,2.6006904751
C,0,-0.2123218397,3.0010739579,2.6468477121
H,0,-0.2478146775,4.075242047,2.7732894806
C,0,1.0189373869,2.3561584598,2.5641202135
H,0,1.9527901147,2.8998210368,2.6149749418
C,0,1.0410346664,0.9761300182,2.413098253
C,0,-0.1201827706,0.2123565788,2.3715506193
H,0,-0.0717631298,-0.8671576436,2.2786145336
Li,0,-0.1135872596,0.2290262313,0.0178516

$Li^+ \cdot 1 \cdot BF_4^-$(B3LYP-D3/BS2)

F,0,-0.478073103,-1.6304568,-0.1304848046
F,0,1.4137820604,-2.1397686758,-1.324177323
F,0,1.4091984854,-2.3223584941,0.9753627762
F,0,0.2156290727,-3.8399946225,-0.3045444523
B,0,0.6848627922,-2.5613681513,-0.2020820494
Cl,0,-6.204148978,-1.7532319801,-0.1518023819
Cl,0,6.1178071223,-1.3133147867,-0.0920349614
O,0,2.2903175443,0.7214583191,-2.261711933
O,0,-2.5045358507,0.5442335405,-2.2865125698
O,0,-2.5138621272,0.1774745097,2.3334795645
O,0,2.2809963337,0.35482321,2.3561634367
N,0,4.0319353503,-0.2079162862,-1.2004065201
N,0,2.114456696,0.4726880436,0.0416837926
N,0,4.027155663,-0.3959912629,1.1684999944
N,0,-4.1925859423,-0.5004842174,-1.2410866956
N,0,-4.1973694866,-0.6886809161,1.1295524016
N,0,-2.3780437899,0.3832322085,0.0255244973
C,0,4.5574283372,-0.570207803,-0.036185587
C,0,2.8138668769,0.3071176208,-1.0962238399
C,0,2.8093490169,0.1294129861,1.1420064135
C,0,1.0596955434,1.3708240347,-2.2541522402
C,0,1.0302000209,2.7615061258,-2.2021734325
H,0,1.9612061023,3.3152019673,-2.1621411734
C,0,-0.2072078303,3.4086763286,-2.1974022358
H,0,-0.2468762432,4.492121932,-2.1623650915
C,0,-1.3947495886,2.6738833597,-2.2171619508
H,0,-2.3634531139,3.1594835268,-2.1890434064
C,0,-1.3209638836,1.285355813,-2.2677308302
C,0,-0.1047075483,0.6062728133,-2.3274263128
H,0,-0.0530530112,-0.4760971459,-2.3956949575
C,0,-3.0295794343,0.1323575364,-1.1220017573
C,0,-4.7049940901,-0.8951561731,-0.080657817
C,0,-3.0340955658,-0.0453487277,1.1164729625
C,0,-1.3304535155,0.9118896313,2.4366107248
C,0,-1.4044655831,2.2910283096,2.6054559942
H,0,-2.3731990873,2.7752988726,2.6504237374
C,0,-0.2170816306,3.0193477005,2.7066343931
H,0,-0.2569443377,4.0947640409,2.8428187889
C,0,1.0204968594,2.3791256948,2.6141951392
H,0,1.9514848757,2.9318978749,2.6657531797
C,0,1.0502137889,0.9976510906,2.4462251652
C,0,-0.1142366133,0.2314953667,2.3932895064
H,0,-0.0625234811,-0.8481056027,2.2901380947
Li,0,-0.1038907065,0.1191851872,0.0091437648

Na^+·1·BF_4^-(M05-2X/BS2)

F,0,3.7987503567,9.1076006316,15.2761172366
F,0,5.6833555168,8.6098327275,14.0772308169
F,0,3.9597409713,7.0871618817,14.2131210842
F,0,3.6951981725,9.0187673654,12.9746492343
B,0,4.2863143619,8.4481217674,14.0732095677
Cl,0,0.1124969528,13.3510162353,15.3963599811
Cl,0,7.9210044048,4.2637949958,13.904624967
O,0,7.5622229981,8.4150602907,16.3383543063
O,0,4.4668276276,12.0170150956,16.9908760416
O,0,0.9894964599,8.9856166355,17.2554162214
O,0,4.0795436332,5.3789683116,16.6033069313
N,0,7.6663451075,6.4795795845,15.2211505288
N,0,5.772810822,6.9600913724,16.5608280363
N,0,5.8813521022,4.9218809031,15.3586980858
N,0,2.4254421905,12.5819193328,16.272368186
N,0,0.6407152171,11.0258956079,16.4079680767
N,0,2.7638231497,10.475983379,17.3010039253
C,0,7.0620084288,5.3390087104,14.9335954027
C,0,6.9603121273,7.2539843884,16.0256664533
C,0,5.2790976629,5.7879455914,16.1540805203
C,0,6.9112322534,9.3092864434,17.1749231716
C,0,7.0929848062,9.1883363043,18.5494284586
H,0,7.7507095619,8.4183545025,18.9306698976
C,0,6.4103558395,10.0560095673,19.4004551591
H,0,6.5479197314,9.9783957257,20.4710103911
C,0,5.5332571913,11.0081930527,18.882501807
H,0,4.9648893733,11.6669540875,19.5257224437
C,0,5.3776110283,11.0976753567,17.5034104639
C,0,6.0999355011,10.2975188545,16.6197021661
H,0,5.956754138,10.3496725055,15.5479109089
C,0,3.1776980915,11.6627435961,16.8555425325
C,0,1.170234614,12.1993760561,16.1024010735
C,0,1.4987269842,10.1990048753,16.9832011254
C,0,1.8204215752,7.9966933948,17.7740232674
C,0,2.0071152701,7.9342934263,19.1507294311
H,0,1.4876017988,8.6356432606,19.790223082
C,0,2.8757650007,6.9747138205,19.6692838931
H,0,3.0266053243,6.9085987623,20.7388236523
C,0,3.5686196614,6.1160529997,18.8174145104
H,0,4.2747463769,5.3882548859,19.1949251196
C,0,3.3547196245,6.2089121905,17.4453234939
C,0,2.4383796739,7.1055729066,16.8981916828
H,0,2.3127582994,7.1743247225,15.8251632298
Na,0,4.3525996375,8.6671010445,17.46249299

Na^+·1·BF_4^-(B3LYP-D3/BS2)

F,0,1.0288767467,2.5298550425,-0.0107302772
F,0,-0.934147416,2.2983032226,-1.1490628196
F,0,-0.933691452,2.3034679896,1.1295411854
F,0,-0.5037591334,4.2949435323,-0.0139180851
B,0,-0.3466907654,2.9477604175,-0.011615386
Cl,0,6.2858989736,1.5213664471,-0.0057923242
Cl,0,-6.2542905236,1.1804055431,-0.00374133
O,0,-2.3462919964,-0.5612072602,-2.3122963946
O,0,2.456992439,-0.38894208,-2.3134610019
O,0,2.4573340543,-0.3729297024,2.3156268627
O,0,-2.3459301965,-0.5453774611,2.3160416939
N,0,-4.1392435756,0.2248916168,-1.1927793772
N,0,-2.2266802348,-0.5273895193,0.0017671922
N,0,-4.1390405932,0.2330559803,1.191453816
N,0,4.2166248951,0.4697914087,-1.1940556417
N,0,4.2168003037,0.4780544547,1.1900372121
N,0,2.3422898175,-0.3733862043,0.0010647599
C,0,-4.6739014643,0.47858926,-0.0014729797
C,0,-2.9123381635,-0.2801568995,-1.1240601805
C,0,-2.9121445031,-0.2724465422,1.1259914566
C,0,-1.1125911813,-1.2215846634,-2.3229870519
C,0,-1.0829446324,-2.6094354135,-2.2310899793
H,0,-2.0125307847,-3.1635204713,-2.1688934628
C,0,0.154344933,-3.2562339333,-2.2057191658
H,0,0.1930701509,-4.3382886287,-2.1398194256
C,0,1.3423090945,-2.523099042,-2.2332513801
H,0,2.3091508424,-3.0095720156,-2.1729525985
C,0,1.2714103243,-1.1367037793,-2.3255128977
C,0,0.0544081802,-0.4636865793,-2.4284455136
H,0,0.006917667,0.6168787706,-2.5296556205
C,0,3.0149191209,-0.0933762596,-1.1250319547
C,0,4.7401555104,0.7477181824,-0.0029999347
C,0,3.0150873929,-0.0855754157,1.1250931198
C,0,1.2717954611,-1.120656549,2.3329785825
C,0,1.342735168,-2.5076502731,2.2501780716
H,0,2.3095907797,-2.994488773,2.1931327452
C,0,0.1547949683,-3.2409937867,2.2276987692
H,0,0.193552355,-4.3234711433,2.1691713724
C,0,-1.0825183003,-2.5940767542,2.2486990273
H,0,-2.0120865732,-3.148604527,2.190299162
C,0,-1.1122110674,-1.2056339908,2.3311458322
C,0,0.0547760637,-0.4470085562,2.4314184776
H,0,0.0072523147,0.6342137506,2.525224162
Na,0,0.0222260005,0.4700256051,-0.0016207

$K^+ \cdot 1 \cdot BF_4^-$(M05-2X/BS2)

F,0,3.4930373364,9.4328673756,14.8885891411
F,0,5.5489454979,8.7532796688,14.12936661
F,0,3.8195309141,7.2501770078,14.2607408242
F,0,3.7773487296,8.9106249352,12.6558666178
B,0,4.1551201969,8.5877748781,13.9355707861
Cl,0,0.4257545712,12.9347640524,14.7361275075
Cl,0,7.655840267,4.5411073938,13.5909299907
O,0,7.561912365,8.4199599449,16.4344252098
O,0,4.4790681836,12.0185712459,17.1717706567
O,0,1.0013553366,8.9886460887,17.4376692882
O,0,4.0798024116,5.3876672859,16.6949866436
N,0,7.5250658521,6.6264566179,15.1219268283
N,0,5.7414443075,7.0021922697,16.6483791353
N,0,5.7440849643,5.0757489659,15.2550251865
N,0,2.5894263236,12.3686436026,16.046192485
N,0,0.8099902846,10.8182244884,16.1821264695
N,0,2.8197171602,10.4195075471,17.3861359817
C,0,6.8912356987,5.5209248562,14.7760393835
C,0,6.8890601508,7.3249422901,16.0458989965
C,0,5.2179962173,5.8697857486,16.1709363436
C,0,6.9840792874,9.3731296927,17.2470169373
C,0,7.5504058814,9.5674792045,18.5051379318
H,0,8.3807410633,8.9448311147,18.8114045492
C,0,7.0544767899,10.5870388254,19.3182437107
H,0,7.5022021408,10.7685256039,20.2869807571
C,0,5.9969092706,11.3859488079,18.8822054707
H,0,5.602530496,12.1933747217,19.4849021185
C,0,5.4621603636,11.1556685853,17.6176917224
C,0,5.9495262586,10.1694261539,16.7667915766
H,0,5.5376174455,10.0060095754,15.7767026609
C,0,3.2590537822,11.5580026717,16.8467473449
C,0,1.3746494783,11.9354797984,15.7595584165
C,0,1.5903998055,10.1042424734,16.9742786125
C,0,1.761204187,7.9305374987,17.8990404981
C,0,1.5734992287,7.5292302836,19.2187968666
H,0,0.8815733527,8.0764417599,19.8453087775
C,0,2.2598774168,6.4061843325,19.6819167515
H,0,2.1059242266,6.0618833565,20.6966142612
C,0,3.1295548456,5.7135124892,18.8390133195
H,0,3.6609555721,4.8298508941,19.1672002469
C,0,3.2864256424,6.1514382526,17.5256440439
C,0,2.5953398445,7.2477857893,17.0202360659
H,0,2.7245340856,7.5566523008,15.9884319974
K,0,4.5691223861,8.5463867004,18.923530836

$K^+ \cdot 1 \cdot BF_4^-$(B3LYP-D3/BS2)

F,0,3.4595058258,9.4643125078,14.8441966235
F,0,5.5312265377,8.7789083855,14.123154296
F,0,3.7988291602,7.2690264892,14.2549115942
F,0,3.7762881735,8.9066391497,12.6185904584
B,0,4.1372394008,8.6053375529,13.9114768156
Cl,0,0.3927950175,12.9788916526,14.800982231
Cl,0,7.6465778219,4.5490574235,13.5663703584
O,0,7.6032023614,8.4010743002,16.4877781
O,0,4.4960110275,12.0244290112,17.1797105213
O,0,0.9947627746,8.9726345268,17.4454426513
O,0,4.1001530055,5.3476596247,16.7537901678
N,0,7.5356662127,6.6218973181,15.1465233213
N,0,5.7626394736,6.9835624694,16.7016480461
N,0,5.7505002295,5.0658824331,15.2820730239
N,0,2.5850626678,12.3827032569,16.0839798269
N,0,0.8006160932,10.8273127746,16.2194144545
N,0,2.8320631369,10.4064300772,17.3967808281
C,0,6.8965226646,5.516176606,14.7901082364
C,0,6.9119278443,7.3160679812,16.0903894446
C,0,5.2291058617,5.8492525731,16.2181706428
C,0,7.049459201,9.4022648282,17.2646834019
C,0,7.7009676214,9.7005416343,18.4653417787
H,0,8.5616578177,9.1117918164,18.7622024506
C,0,7.2422627461,10.7743730874,19.2356037314
H,0,7.750966605,11.0318127468,20.1589239417
C,0,6.1377091484,11.5245450724,18.818136533
H,0,5.7699869815,12.3679641869,19.3916116291
C,0,5.5161008846,11.1923082622,17.6115422598
C,0,5.9669236578,10.1506889753,16.8005452972
H,0,5.5023390622,9.9190441702,15.847142073
C,0,3.2711914319,11.5587684832,16.8672449774
C,0,1.3603787087,11.9562270074,15.8048764207
C,0,1.5903859985,10.0937115485,16.9948165316
C,0,1.7179667766,7.8817603303,17.8998231132
C,0,1.4109837421,7.4046989333,19.1768606663
H,0,0.6763338659,7.9283315936,19.7781487512
C,0,2.0407785605,6.240753027,19.6303630746
H,0,1.7983033482,5.8435141187,20.6106598268
C,0,2.97393528,5.5804186186,18.8241348946
H,0,3.4663648157,4.6707165095,19.1489353241
C,0,3.2518860651,6.092195938,17.5529770108
C,0,2.6168710041,7.2306547189,17.0548613818
H,0,2.8254295928,7.5856749989,16.0503976806
K,0,4.5786214139,8.5409104307,18.986775167

20. Cartesian coordinates of monomers and $M^+ \cdot 1 \cdot NO_3^-$

$Li^+ \cdot 1 \cdot BF_4^-$(M05-2X/BS2)

Cl,0,0.0001703341,-10.6474885756,7.3272271847
Cl,0,-0.0019924283,1.5246119277,7.5268577767
O,0,-2.3040221069,-2.1488047458,5.4161761231
O,0,-2.3036633506,-6.9254477163,5.301441777
N,0,-1.1851468814,-8.6258838142,6.2241790862
N,0,0.0004714519,-6.8113799172,5.2595252915
N,0,-0.0002576006,-2.3176229406,5.464180757
N,0,-1.185791502,-0.4762326777,6.3848797672
C,0,-2.3306383607,-3.3345948835,4.6958532391
C,0,-2.3702044622,-3.2754165444,3.3090390337
H,0,-2.3738720518,-2.3116948332,2.8175940949
C,0,-2.4035524971,-4.4673217223,2.588994973
H,0,-2.4425521368,-4.4405063483,1.5079090017
C,0,-2.3723965281,-5.6938910164,3.2484403406
H,0,-2.3775085875,-6.6316467394,2.7090721468
C,0,-2.3325620558,-5.7019553891,4.6362347349
C,0,-2.3551357666,-4.5367051886,5.393636123
H,0,-2.3288876428,-4.5504727842,6.4784189181
C,0,-1.1160613365,-7.4579832631,5.6042679272
C,0,0.0000829676,-9.1387271532,6.5085206432
C,0,-1.1165815515,-1.6473413012,5.7764607067
C,0,-0.0013276333,0.027006772,6.6870102271
O,0,2.3035576693,-2.1488579941,5.4201478011
O,0,2.3045898177,-6.9249933585,5.3034016601
N,0,1.1855773034,-8.6257385245,6.225081719
N,0,1.183649306,-0.4759474512,6.3864613621
C,0,2.3305071979,-3.3342076882,4.6990116601
C,0,2.366505246,-3.2742896978,3.3121226524
H,0,2.3681915728,-2.3103627069,2.8210654853
C,0,2.3985192906,-4.4658325902,2.5915774767
H,0,2.4345446106,-4.4386719065,1.5104102706
C,0,2.3693377443,-5.6926222402,3.250719939
H,0,2.3728583433,-6.6301453056,2.710921919
C,0,2.3329693838,-5.7013366814,4.6386580432
C,0,2.3569845623,-4.5362237525,5.3965826783
H,0,2.3325268722,-4.5507112245,6.4813359296
C,0,1.1168203704,-7.4579620315,5.6051287417
C,0,1.115524938,-1.6470790988,5.7779888646
N,0,-0.001860875,-3.7960467355,7.9058368153
O,0,1.0778801172,-3.2769509593,8.1828765967
O,0,-0.000311972,-4.9023370723,7.2512733136
O,0,-1.0831870025,-3.2788062713,8.1805358202
Li,0,0.0014438509,-4.6296178147,5.413936978

$Li^+ \cdot 1 \cdot BF_4^-$(B3LYP-D3/BS2)

Cl,0,6.1491775833,0.0021866034,-1.9369609455
Cl,0,-6.0947689818,0.0082852508,-1.5113385056
O,0,-2.2913123222,2.323738035,0.400621376
O,0,2.5043216489,2.3229073873,0.2613511708
N,0,4.1632975638,1.1917071119,-0.7352096882
N,0,2.3689912444,0.0033895211,0.2877719206
N,0,-2.1118935404,0.0056927338,0.3276842961
N,0,-4.0191184017,1.1949490008,-0.4702233942
C,0,-1.0648288587,2.3754260107,1.0586218995
C,0,-1.0478233516,2.4501769653,2.4487490917
H,0,-1.9833879704,2.4613571658,2.996157364
C,0,0.1843815132,2.5027311692,3.1043185775
H,0,0.215354119,2.5657051958,4.1867509083
C,0,1.3776511514,2.4528130988,2.3798814405
H,0,2.3425447153,2.4656144079,2.8737191912
C,0,1.3145275436,2.3773385119,0.9915362804
C,0,0.1043253349,2.3795489985,0.298619523
H,0,0.0631371411,2.3271240534,-0.7855928032
C,0,3.0135869695,1.1270618188,-0.0700703569
C,0,4.6661622316,0.0026484809,-1.0459073154
C,0,-2.8073935591,1.1298964735,0.0673942729
C,0,-4.5440542573,0.0072679236,-0.7469061666
O,0,-2.2940039482,-2.3121686031,0.3998908684
O,0,2.5016099193,-2.3162579234,0.2592582138
N,0,4.1618828567,-1.1861038645,-0.7363263556
N,0,-4.0204858728,-1.1811037216,-0.4706125411
C,0,-1.0673761206,-2.3655540935,1.0574928778
C,0,-1.050069697,-2.4412531536,2.4475653247
H,0,-1.9854935738,-2.4517720259,2.9952352107
C,0,0.1822604426,-2.4955566759,3.1027541171
H,0,0.2134663359,-2.5592972499,4.1851387185
C,0,1.3753784008,-2.4464224206,2.3780167325
H,0,2.3403926788,-2.4605755668,2.8715838884
C,0,1.3119496972,-2.3699303274,0.9897361287
C,0,0.1015615589,-2.3704043655,0.2971473268
H,0,0.0600442065,-2.3172723946,-0.7870353347
C,0,3.0122655141,-1.1207219714,-0.0710961674
C,0,-2.8086821353,-1.1176349498,0.0670256066
N,0,-0.7687858787,0.0049572625,-2.3112496907
O,0,-1.2921204097,-1.0885943531,-2.5827206351
O,0,0.364323477,0.0054021486,-1.6663616116
O,0,-1.2924160761,1.0980187325,-2.5838683549
Li,0,0.1630711079,0.0045265988,0.14881354

Na^+·1·BF_4^-(M05-2X/BS2)

Cl,0,-0.0006377855,-10.5036638744,7.5794160319
Cl,0,0.0002657248,1.4838434964,7.6345775307
O,0,-2.315271089,-2.1413918432,5.4488669795
O,0,-2.3120222224,-6.9307858628,5.3055403646
N,0,-1.1863836247,-8.558609127,6.3461169917
N,0,-0.0006031326,-6.9107611213,5.1270558164
N,0,-0.0008866856,-2.2450892844,5.3895136349
N,0,-1.1872031714,-0.4940411087,6.4584226292
C,0,-2.3664877379,-3.3278917789,4.7284286201
C,0,-2.3515913637,-3.2630127207,3.3381215747
H,0,-2.3226086289,-2.2966232029,2.852155856
C,0,-2.3625018568,-4.4501922926,2.607328013
H,0,-2.359349002,-4.416247332,1.5257392657
C,0,-2.3544887836,-5.6820417876,3.2618815778
H,0,-2.3241674493,-6.6156368914,2.7157980259
C,0,-2.3678705169,-5.7029859234,4.6522065141
C,0,-2.4328032442,-4.5381389868,5.414838834
H,0,-2.4035340379,-4.5565758237,6.4979197694
C,0,-1.1161799397,-7.4680770629,5.5985980523
C,0,-0.0006073643,-9.054315065,6.6579092102
C,0,-1.1197475703,-1.6288987163,5.7842674274
C,0,-0.0001549292,0.0034976108,6.7625367993
O,0,2.313603051,-2.1397398282,5.4437717753
O,0,2.3106797594,-6.9293258091,5.3076785698
N,0,1.1851275638,-8.5578611775,6.3471962157
N,0,1.186586916,-0.4930547387,6.4554999299
C,0,2.3645877694,-3.3272510294,4.7249367825
C,0,2.349441249,-3.2644396905,3.3345487859
H,0,2.3204818294,-2.2988031066,2.8471014931
C,0,2.3605625108,-4.4528056053,2.6056126481
H,0,2.3573297758,-4.4205534638,1.5239754905
C,0,2.3528932322,-5.6836667312,3.2620341022
H,0,2.3229361868,-6.6180686682,2.7173040061
C,0,2.3663791233,-5.7025926961,4.6523960702
C,0,2.4312541182,-4.5365024468,5.4131494476
H,0,2.4018179125,-4.5532837475,6.4962469817
C,0,1.1149228657,-7.4673620315,5.5996096957
C,0,1.1184169131,-1.6280612312,5.7817231288
N,0,-0.0007790419,-3.9410452701,7.688020741
O,0,1.0787261052,-3.4251145727,7.997334237
O,0,-0.0003742761,-4.9999241753,6.9842920948
O,0,-1.0807094748,-3.427398099,7.9994588683
Na,0,-0.0006714676,-4.5494579125,4.65430276

Na^+·1·BF_4^-(B3LYP-D3/BS2)

Cl,0,-6.0461858997,-0.0000957939,-2.0871382176
Cl,0,6.0640657853,-0.0001882453,-1.7059541197
O,0,2.3223752928,-2.3296113547,0.3156208547
O,0,-2.4916867702,-2.3268718,0.2519894025
N,0,-4.1069623469,-1.1897535753,-0.8104777148
N,0,-2.4662160042,0.0000914241,0.4311231302
N,0,2.2081560154,0.0000127495,0.3694630815
N,0,4.0193561502,-1.1905000766,-0.6102394748
C,0,1.0995227006,-2.4150535136,0.9810655393
C,0,1.1030814175,-2.490741586,2.3744412231
H,0,2.0471580161,-2.4913347192,2.9073991375
C,0,-0.1185687087,-2.5477822244,3.0510270496
H,0,-0.1319416824,-2.6119135129,4.1337860898
C,0,-1.3241434941,-2.4932998338,2.3447493042
H,0,-2.2805183985,-2.4936005938,2.8552143478
C,0,-1.286139704,-2.4156904073,0.9529134225
C,0,-0.0842240849,-2.4409712655,0.238659815
H,0,-0.0556947839,-2.3487257742,-0.8427094707
C,0,-3.0216327705,-1.1244632455,-0.0447341239
C,0,-4.6010868641,-0.0000246639,-1.1330258021
C,0,2.8470791485,-1.127566733,0.009549209
C,0,4.5354643112,-0.0001078819,-0.8943515219
O,0,2.3224317903,2.3296393907,0.3152601064
O,0,-2.491628541,2.3270065512,0.2515881482
N,0,-4.1069441168,1.1897516846,-0.810686072
N,0,4.0193874788,1.1903388033,-0.6104128135
C,0,1.0995714203,2.4152089073,0.980667608
C,0,1.1031344794,2.4910754419,2.3740328345
H,0,2.0472135504,2.4917159335,2.9069865009
C,0,-0.1185098206,2.5482206379,3.0506179623
H,0,-0.1318743762,2.6124882687,4.1333689045
C,0,-1.3240892684,2.4936717608,2.3443520163
H,0,-2.2804626162,2.494056461,2.8548197901
C,0,-1.2860910452,2.4158923773,0.952524854
C,0,-0.0841791357,2.4410514005,0.2382622147
H,0,-0.0556837801,2.3486825985,-0.8430951582
C,0,-3.0215415752,1.1245596176,-0.0450398949
C,0,2.8471648014,1.1275299196,0.0094920697
N,0,0.5776227992,-0.0002033382,-2.1072519041
O,0,1.1054641527,1.0928250061,-2.402190482
O,0,-0.5186394477,-0.0000321167,-1.4311587636
O,0,1.1052505464,-1.0933897057,-2.4019981594
Na,0,-0.1293891349,0.000067024,0.87024852

$K^+ \cdot 1 \cdot BF_4^-$(M05-2X/BS2)

Cl	5.463169046636	-0.001657140535	-2.6739872
Cl	-5.715189415180	-0.002752457093	-2.1613070
O	-2.282840525728	2.317379604666	0.2840541
O	2.511535624280	2.316364831218	0.3457492
N	3.829476385955	1.183533653055	-1.0469652
N	2.410621220974	0.004124897665	0.4502305
N	-2.136893822458	0.001842494076	0.3408995
N	-3.821114770060	1.183362364735	-0.8516593
C	-1.079106547390	2.462611433780	0.9445988
C	-1.121527856689	2.908238318909	2.2644902
H	-2.081499961539	3.088498510921	2.7304330
C	0.078932569663	3.143024868936	2.9363003
H	0.062497647895	3.516601217805	3.9522422
C	1.300332063311	2.910803937954	2.3021362
H	2.245703862266	3.090346545699	2.7969772
C	1.293490048938	2.466306357078	0.9829022
C	0.119003309076	2.266505131920	0.2659289
H	0.124488470934	1.953058433880	-0.7747175
C	2.902898028216	1.112468950950	-0.1060969
C	4.245797500256	0.000517892914	-1.4606545
C	-2.732718188204	1.112936275320	-0.1050853
C	-4.296659845223	-0.000576707328	-1.1910945
O	-2.279215001099	-2.314007874871	0.2863434
O	2.515470413961	-2.308727496840	0.3582352
N	3.832018338465	-1.180953508846	-1.0402360
N	-3.818763942209	-1.183151456955	-0.8512041
C	-1.076577903911	-2.456412906122	0.9498617
C	-1.121678018910	-2.897293671605	2.2709862
H	-2.082627579589	-3.076368255307	2.7353317
C	0.077556087170	-3.129001778193	2.9460430
H	0.059149820407	-3.499146907427	3.9632181
C	1.300248565193	-2.898544738182	2.3135705
H	2.244672457338	-3.076000617472	2.8109287
C	1.295966478111	-2.458462582179	0.9930450
C	0.122780720175	-2.261739933585	0.2733259
H	0.130813848047	-1.950991930167	-0.7678196
C	2.904693994083	-1.106551188790	-0.1004720
C	-2.730485884514	-1.110763813498	-0.1044497
N	-0.416020411972	-0.019467103061	-2.1581368
O	-1.022125173481	-1.098277714917	-2.2846219
O	0.799134876628	-0.021631303928	-1.8447817
O	-1.018164849907	1.061337839846	-2.2860198
K	0.090042319992	0.004889525634	2.2897571

$K^+ \cdot 1 \cdot BF_4^-$(B3LYP-D3/BS2)

Cl,0,5.5612697389,-0.0039233855,-2.5986024
Cl,0,-5.7341923372,-0.0059633265,-2.171765
O,0,-2.3181748977,2.3299246469,0.330477679
O,0,2.5023109576,2.3294070165,0.3367055233
N,0,3.8626826126,1.1847930241,-1.013544344
N,0,2.398927254,0.0015667279,0.4512761583
N,0,-2.1646244405,0.0004576247,0.389169779
N,0,-3.840111755,1.1840741239,-0.829660165
C,0,-1.0992723549,2.5139610942,0.961110213
C,0,-1.124999546,3.0599559167,2.2479304369
H,0,-2.0796177674,3.2730606338,2.715885674
C,0,0.0869575903,3.3452757029,2.8863949599
H,0,0.0836062586,3.7911178424,3.875739585
C,0,1.3033393058,3.0610127635,2.2556735384
H,0,2.2551612796,3.2735505241,2.7294803177
C,0,1.2826386258,2.5155873071,0.9695538503
C,0,0.094607506,2.2676646665,0.2830903279
H,0,0.0836304189,1.8925555126,-0.738479223
C,0,2.9044536672,1.1182522307,-0.095417812
C,0,4.2958771322,-0.0018074316,-1.41648146
C,0,-2.7559181538,1.1191726435,-0.06598813
C,0,-4.3178352611,-0.0034576895,-1.1745036
O,0,-2.317023936,-2.3293134228,0.340555488
O,0,2.5034136473,-2.3266506261,0.346274528
N,0,3.8632683561,-1.1869533485,-1.00866870
N,0,-3.8395442045,-1.1892481578,-0.8245031
C,0,-1.0979874043,-2.5099890981,0.97192223
C,0,-1.1233460516,-3.0501781463,2.26119105
H,0,-2.0778228769,-3.2615271031,2.73023107
C,0,0.0888031265,-3.3321450907,2.900789617
H,0,0.0857426484,-3.7735295991,3.892131907
C,0,1.3049874319,-3.0502243458,2.268645804
H,0,2.2569576586,-3.2601878254,2.743302804
C,0,1.2839045761,-2.5105776929,0.980100798
C,0,0.0957021643,-2.2662376265,0.292656847
H,0,0.0844589912,-1.8959194466,-0.73065985
C,0,2.9050044111,-1.1171064449,-0.09083003
C,0,-2.7553750797,-1.1205166282,-0.0611246
N,0,-0.3794338912,-0.0047724097,-2.1917054
O,0,-0.9917007447,-1.0983340667,-2.3082968
O,0,0.8517515609,-0.0037667096,-1.88899155
O,0,-0.9923348827,1.0879576921,-2.31282428
K,0,0.0971426652,0.0052539281,2.3400371332

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