Electronic Supplementary Information (ESI): Tracking the Absence of Anion-π Interactions in Modified [2_3](1,3,5)cyclophanes: Insights from computation

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Table S1: Atom charges of cyclophanes **1**–**3c** from Natural Population Analysis (NPA), in a.u. Net NPA charge of $[Cr(CO)_3]^0$ group before coordenation with cyclophanes. Atoms are labeled as shown in Fig. 1 - Paper, and α atom in parenthesis.

	1	**1c**	**2**	**2c**	**3**	**3c**
H	0.212	0.216	-	-	-	-
α	-0.202 (C)	-0.209 (C)	-0.481 (N)	-0.480 (N)	0.754 (P)	0.764 (P)
C	-0.027	-0.017	0.441	0.449	-0.776	-0.768
$\mathbf{H}_b$	0.223	0.228	0.238	0.243	0.235	0.239
$\mathbf{C}_b$	-0.429	-0.429	-0.460	-0.459	-0.460	-0.459
$\mathbf{C'}_b$	-0.429	-0.427	-0.414	-0.411	-0.431	-0.433
$\mathbf{H'}_b$	0.223	0.232	0.228	0.236	0.230	0.237
C'	-0.027	-0.016	-0.044	-0.037	-0.023	0.025
$\mathbf{C'}_\alpha$	-0.202	-0.181	-0.196	-0.174	-0.221	-0.245
H'	0.212	0.247	0.220	0.254	0.229	0.263
Cr		-1.055		-1.061		-1.061
C		0.711		0.713		0.713
O		-0.463		-0.460		-0.457
$[Cr(CO)_3]$		-0.311		-0.302		-0.293

Table S2: Interactions between host-guest complexes (hydrogen bonds (*hb*) and σ-complexes (σ)), with involved atoms in parenthesis. Hydrogen bonds were classified as *weak* (*w*), *moderate* (***m***) and *strong* (***s***),[1] more detailed criteria and data are reported in Tbl. S3 and S4.

	BF_4^-	NO_3^-	Br^-	Cl^-	SO_4^{2-}	PO_4^{3-}
1	*8 hb w* (C–H···F)	*8 hb w* (C–H···O)	*4 hb w* (C–H···Br)	*4 hb w* (C–H···Cl)	*3 hb w* (C–H···O) *5 hb* ***m*** (C–H···O)	1 σ (O→C) *1 hb w* (C–H···O) *2 hb* ***m*** (C–H···O)
1c	*8 hb w* (C–H···F)	-	*4 hb w* (C–H···Br)	*4 hb w* (C–H···Cl)	*3 hb w* (C–H···O) *5 hb* ***m*** (C–H···O)	-
2	*1* σ (F→C)	*1* σ (O→C) *1 hb* ***m*** (C–H···O)	*1* σ (Br→C)	*1* σ (Cl→C)	*1* σ (O→C) *2 hb w* (C–H···O)	*1* σ (O→C) *1 hb w* (C–H···O) *1 hb* ***m*** (C–H···O)
2c	*1* σ (F→C) *2 hb w* (C–H···F)	*1* σ (O→C) *1 hb* ***m*** (C–H···O)	*1* σ (Br→C)	*1* σ (Cl→C)	*1* σ (O→C) *2 hb w* (C–H···O)	*1* σ (O→C) *1 hb w* (C–H···O) *1 hb* ***m*** (C–H···O)
3	*3 hb w* (C–H···F) *2 hb* ***m*** (C–H···F)	*1* σ (O→P)	*1* σ (Br→P)	*1* σ (Cl→P)	*1* σ (O→P)	*1* σ (O→P) *1 hb* ***m*** (C–H···O)
3c	*1* σ (F→P) *1 hb w* (C–H···F)	*1* σ (O→P) *1 hb w* (C–H···O)	*1* σ (Br→P)	*1* σ (Cl→P)	*1* σ (O→P)	-

Table S3: Criteria for hydrogen bond (*hb*) force classification.[1] Angle between proton donor and acceptor (**a(D–H···A)**), distances between proton and acceptor (**d(H···A)**), and proton donor and acceptor (**d(D–A)**). All distances are in Å, and angles in degrees.

hb force	**a(D–H···A)**	**d(H···A)**	**d(D–A)**
weak	90–150	3.2-2.2	4.0-3.2
moderate	130-180	2.2-1.5	3.2-2.5
strong	165-180	1.5-1.2	2.5-2.2

Table S4: Geometrical parameters for hydrogen bonds formed in host-guest complexes **1**·BF_4^-–**3**·PO_4^{3-}. Angle between proton donor (C atom) and acceptor (**a(C–H$\cdots$A)**), distances between proton and acceptor (**d(H$\cdots$A)**), and proton donor and acceptor (**d(C–A)**). Interaction force classification followed Table S3 criteria, and named by weak (*w*), moderate (***m***), or strong (***s***). Contacts far from those defined as weak were labeled as dispersive (d). All distances are in Å, and angles in degrees.

	a(C–H$\cdots$A)	**d(H$\cdots$A)**	**d(C–A)**	
1·BF_4^-	144.23	2.454	3.405	*w*
	145.30	2.444	3.404	*w*
	151.19	2.372	3.370	*w*
	151.49	2.362	3.362	*w*
	146.11	2.435	3.396	*w*
	145.64	2.448	3.406	*w*
	123.03	2.713	3.436	*w*
	123.31	2.709	3.436	*w*
1c·BF_4^-	142.55	2.368	3.306	*w*
	142.99	2.430	3.372	*w*
	144.22	2.368	3.316	*w*
	122.54	2.596	3.317	*w*
	137.75	2.445	3.334	*w*
	121.30	2.628	3.331	*w*
	151.72	2.289	3.292	*w*
	151.10	2.226	3.224	*w*
1·NO_3^-	123.19	2.768	3.491	*w*
	122.74	2.778	3.496	*w*
	145.97	2.426	3.387	*w*
	145.93	2.429	3.390	*w*
	144.49	2.476	3.429	*w*
	144.86	2.473	3.430	*w*
	151.34	2.411	3.410	*w*
	151.31	2.415	3.414	*w*
1·Br^-	118.47	3.884	4.511	d
	117.33	3.913	4.523	d
	126.23	3.155	3.906	*w*
	127.47	3.127	3.894	*w*
	157.34	2.626	3.665	*w*
	157.09	2.629	3.666	*w*
1c·Br^-	115.07	3.803	4.382	d
	120.46	3.651	4.312	d
	156.43	2.546	3.581	*w*
	152.39	2.509	3.521	*w*
	124.90	3.145	3.880	*w*
	123.89	3.156	3.877	*w*
1·Cl^-	114.68	3.827	4.399	d
	115.38	3.807	4.391	d
	124.84	2.953	3.692	*w*
	125.22	2.945	3.690	*w*
	155.25	2.441	3.471	*w*
	154.91	2.449	3.477	*w*
1c·Cl^-	115.81	3.597	4.192	d
	114.74	3.642	4.220	d
	120.32	3.054	3.731	*w*
	123.93	2.949	3.676	*w*
	154.50	2.375	3.402	*w*
	151.22	2.317	3.326	*w*
1·SO_4^{2-}	120.39	2.476	3.176	*w*
	122.69	2.430	3.161	*w*
	145.36	2.290	3.254	*w*
	142.37	2.187	3.130	***m***
	149.28	2.198	3.197	***m***
	151.78	2.152	3.169	***m***
	140.42	2.229	3.154	***m***
	147.21	2.241	3.220	***m***
1c·SO_4^{2-}	122.76	2.298	3.035	*w*
	129.18	2.299	3.115	*w*
	118.13	2.401	3.075	*w*
	152.26	2.125	3.147	***m***
	150.04	2.038	3.043	***m***
	145.62	2.234	3.201	***m***
	144.57	2.146	3.111	***m***
	140.83	2.130	3.060	***m***
1·PO_4^{3-}	103.07	3.554	3.953	d
	116.84	2.967	3.600	*w*
	141.35	2.185	3.128	***m***
	148.38	2.255	3.250	***m***
2c·BF_4^-	126.79	2.396	3.175	*w*
	128.47	2.372	3.171	*w*
2·NO_3^-	137.91	2.235	3.137	***m***
2c·NO_3^-	133.39	2.243	3.101	***m***
2·SO_4^{2-}	131.02	2.288	3.120	*w*
	112.22	2.517	3.102	*w*
2c·SO_4^{2-}	128.17	2.338	3.136	*w*
	112.05	2.476	3.061	*w*
2·PO_4^{3-}	110.05	2.649	3.197	*w*
	142.24	2.090	3.042	*w*
2c·PO_4^{3-}	126.20	2.306	3.086	*w*
	128.77	2.261	3.072	*w*
3·BF_4^-	131.41	3.008	3.823	*w*
	144.81	2.310	3.270	*w*
	134.33	2.618	3.472	*w*
	156.80	2.250	3.288	***m***
	168.14	2.172	3.250	***m***
3c·BF_4^-	126.20	2.509	3.280	*w*
3c·NO_3^-	127.70	2.990	3.543	*w*
3·PO_4^{3-}	150.84	2.191	3.204	***m***

Table S5: Sigma complex distances, in Å, their respective Wiberg Bonder Order in parenthesis and interacting atoms in brackets (donor and acceptor, respectively).

	1	**2**	**2c**	**3**	**3c**
$\mathbf{BF_4^-}$		2.748 (0.018) [F→C]	2.676 (0.024) [F→C]		2.376 (0.124) [F→P]
$\mathbf{NO_3^-}$		2.495 (0.094) [O→C]	2.304 (0.163) [O→C]	1.910 (0.469) [O→P]	1.872 (0.504) [O→P]
$\mathbf{Br^-}$		2.838 (0.203) [Br→C]	2.666 (0.299) [Br→C]	2.536 (0.550) [Br→P]	2.480 (0.604) [Br→P]
$\mathbf{Cl^-}$		2.547 (0.265) [Cl→C]	2.352 (0.393) [Cl→C]	2.293 (0.608) [Cl→P]	2.254 (0.651) [Cl→P]
$\mathbf{SO_4^{2-}}$		1.494 (0.820) [O→C]	1.470 (0.849) [O→C]	1.704 (0.679) [O→P]	1.690 (0.702) [O→P]
$\mathbf{PO_4^{3-}}$	1.453 (0.895) [O→C]	1.398 (0.984) [O→C]	1.399 (0.977) [O→C]	1.621 (0.821) [O→P]	

Table S6: ETS-NOCV analysis (kcal mol^{-1}) for $\mathbf{1}\cdot BF_4^-$–$\mathbf{3}\cdot PO_4^{3-}$.

	ΔE_{oi}	$\Delta E_{\text{oi},1}$	$\Delta E_{\text{oi},2}$	$\Delta E_{\text{oi},3}$	$\Delta E_{\text{oi},4}$	$\Delta E_{\text{oi},5}$	$\Delta E_{\text{oi},res}$
$\mathbf{1}\cdot BF_4^-$	-11.1	-2.0	-1.4	-1.1	-0.8	-0.6	-5.1
$\mathbf{1}\cdot NO_3^-$	-13.5	-2.2	-2.2	-1.6	-0.9	-0.7	-5.9
$\mathbf{1}\cdot Br^-$	-16.1	-5.0	-1.8	-2.0	-0.9	-0.9	-5.6
$\mathbf{1}\cdot Cl^-$	-19.3	-6.0	-2.5	-2.9	-1.1	-1.0	-5.7
$\mathbf{1}\cdot SO_4^{2-}$	-48.1	-6.7	-7.5	-5.6	-3.8	-3.1	-21.4
$\mathbf{1}\cdot PO_4^{3-}$	-386.1	-282.9	-19.0	-26.5	-6.9	-6.9	-44.0
$\mathbf{2}\cdot BF_4^-$	-7.3	-2.1	-0.7	-0.7	-0.5	-	-3.3
$\mathbf{2}\cdot NO_3^-$	-17.6	-8.8	-2.8	-1.1	-0.7	-0.6	-3.6
$\mathbf{2}\cdot Br^-$	-23.0	-14.0	-1.8	-1.3	-1.0	-0.5	-4.4
$\mathbf{2}\cdot Cl^-$	-33.7	-22.7	-2.5	-1.8	-1.6	-0.6	-4.5
$\mathbf{2}\cdot SO_4^{2-}$	-255.2	-195.0	-11.2	-17.7	-6.3	-3.2	-21.8
$\mathbf{2}\cdot PO_4^{3-}$	-415.9	-293.2	-25.8	-15.9	-19.3	-16.5	-45.3
$\mathbf{3}\cdot BF_4^-$	-11.9	-2.3	-1.7	-1.6	-0.9	-0.8	-4.7
$\mathbf{3}\cdot NO_3^-$	-111.2	-84.3	-5.2	-8.2	-2.9	-1.8	-8.8
$\mathbf{3}\cdot Br^-$	-72.9	-54.1	-4.4	-4.9	-2.0	-1.1	-6.4
$\mathbf{3}\cdot Cl^-$	-98.0	-72.6	-6.0	-7.9	-3.3	-1.5	-6.8
$\mathbf{3}\cdot SO_4^{2-}$	-245.0	-170.5	-19.5	-17.0	-10.9	-4.5	-22.6
$\mathbf{3}\cdot PO_4^{3-}$	-396.3	-252.4	-38.3	-19.9	-29.1	-11.9	-44.6

Table S7: ETS-NOCV analysis (kcal mol^{-1}) for **1c**·BF_4^-–**3c**·SO_4^{2-}.

	ΔE_{oi}	$\Delta E_{\text{oi,1}}$	$\Delta E_{\text{oi,2}}$	$\Delta E_{\text{oi,3}}$	$\Delta E_{\text{oi,4}}$	$\Delta E_{\text{oi,5}}$	$\Delta E_{\text{oi,}res}$
1c·BF_4^-	-13.8	-2.5	-1.8	-1.3	-0.8	-0.7	-6.7
1c·Br^-	-20.3	-6.5	-2.7	-2.1	-1.1	-0.9	-7.0
1c·Cl^-	-23.8	-7.7	-3.8	-2.7	-1.3	-1.1	-7.2
1c·SO_4^{2-}	-58.5	-7.8	-8.8	-6.8	-4.4	-3.2	-27.4
2c·BF_4^-	-10.1	-2.8	-1.7	-1.1	-0.7	-	-3.7
2c·NO_3^-	-26.6	-15.7	-2.8	-1.3	-1.0	-0.7	-5.2
2c·Br^-	-34.8	-23.1	-2.2	-1.7	-1.4	-0.7	-5.7
2c·Cl^-	-53.5	-38.6	-3.0	-2.2	-2.6	-0.9	-6.2
2c·SO_4^{2-}	-281.0	-209.7	-13.4	-18.7	-8.2	-4.2	-26.7
2c·PO_4^{3-}	-430.8	-290.9	-18.3	-23.9	-15.5	-25.9	-56.4
3c·BF_4^-	-26.7	-16.6	-2.1	-1.7	-1.2	-0.7	-4.4
3c·NO_3^-	-125.9	-93.7	-6.5	-9.3	-3.4	-2.5	-10.6
3c·Br^-	-85.5	-62.6	-5.5	-5.7	-2.7	-1.5	-7.4
3c·Cl^-	-110.1	-80.3	-7.0	-8.7	-4.1	-2.1	-7.9
3c·SO_4^{2-}	-260.9	-177.1	-21.7	-15.1	-14.8	-6.1	-26.1

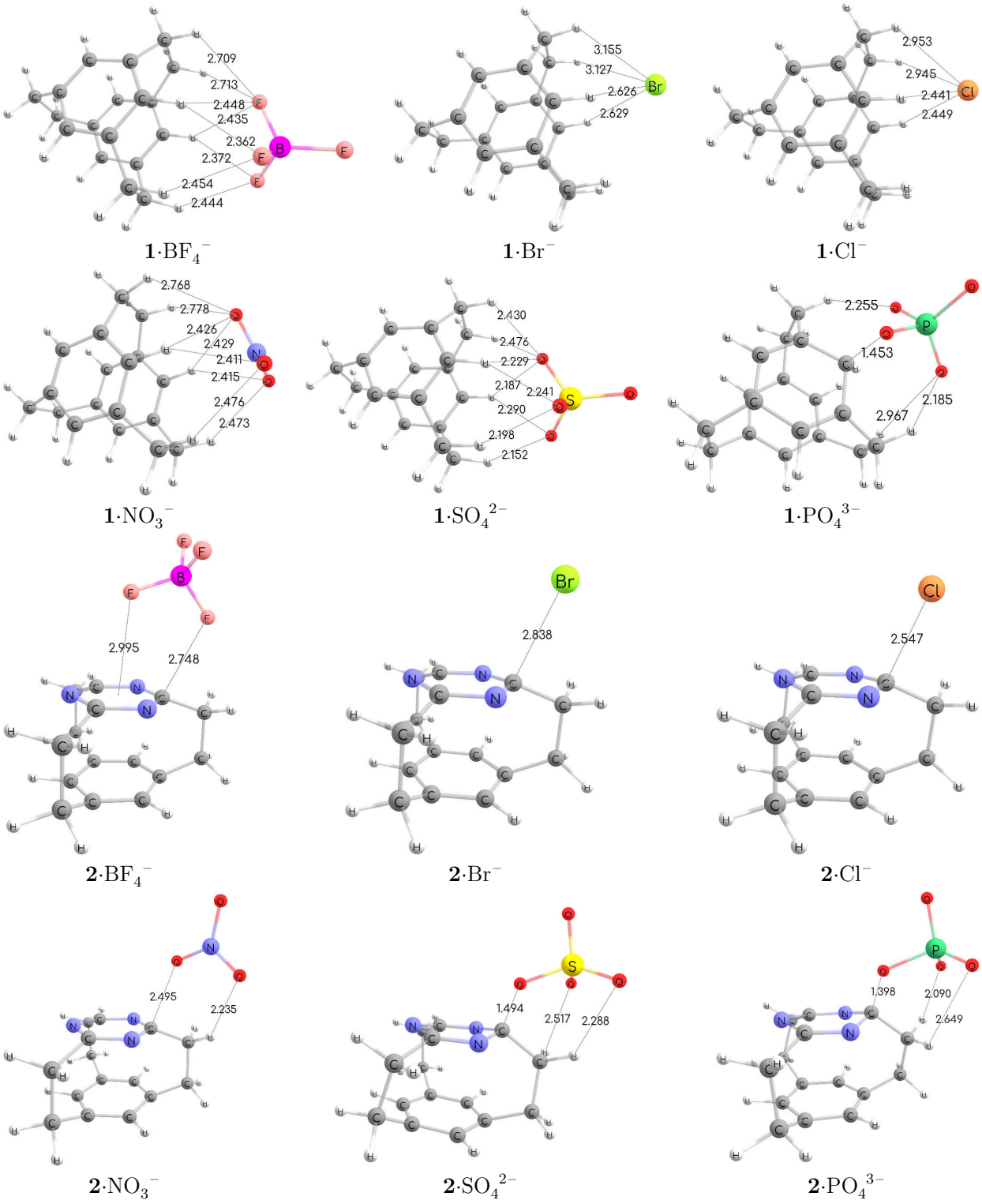
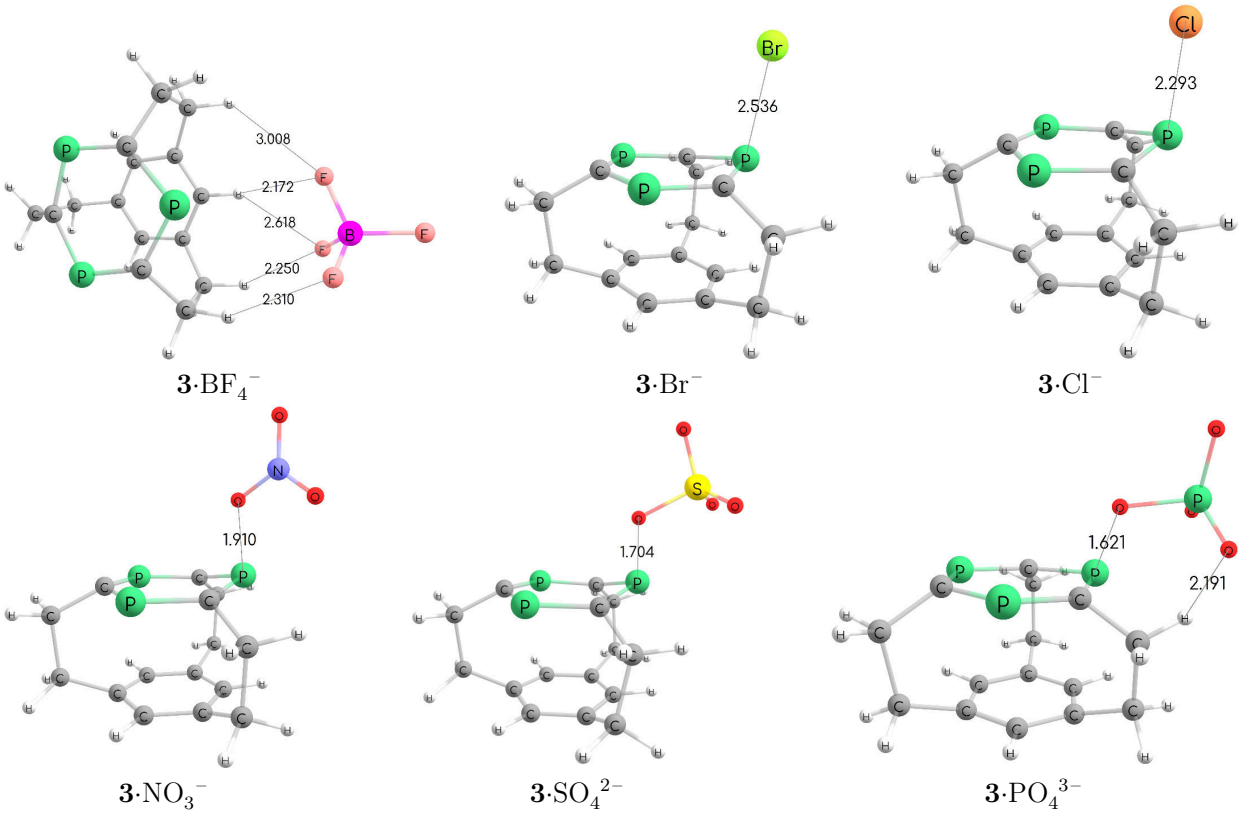


Figure S1: Optimized geometries of host-guest complexes $\mathbf{1}\cdot BF_4^-$–$\mathbf{3}\cdot PO_4^{3-}$.



3·BF_4^- **3**·Br^- **3**·Cl^-

3·NO_3^- **3**·SO_4^{2-} **3**·PO_4^{3-}

Figure S2: Optimized geometries of host-guest complexes **1**·BF_4^-–**3**·PO_4^{3-}.

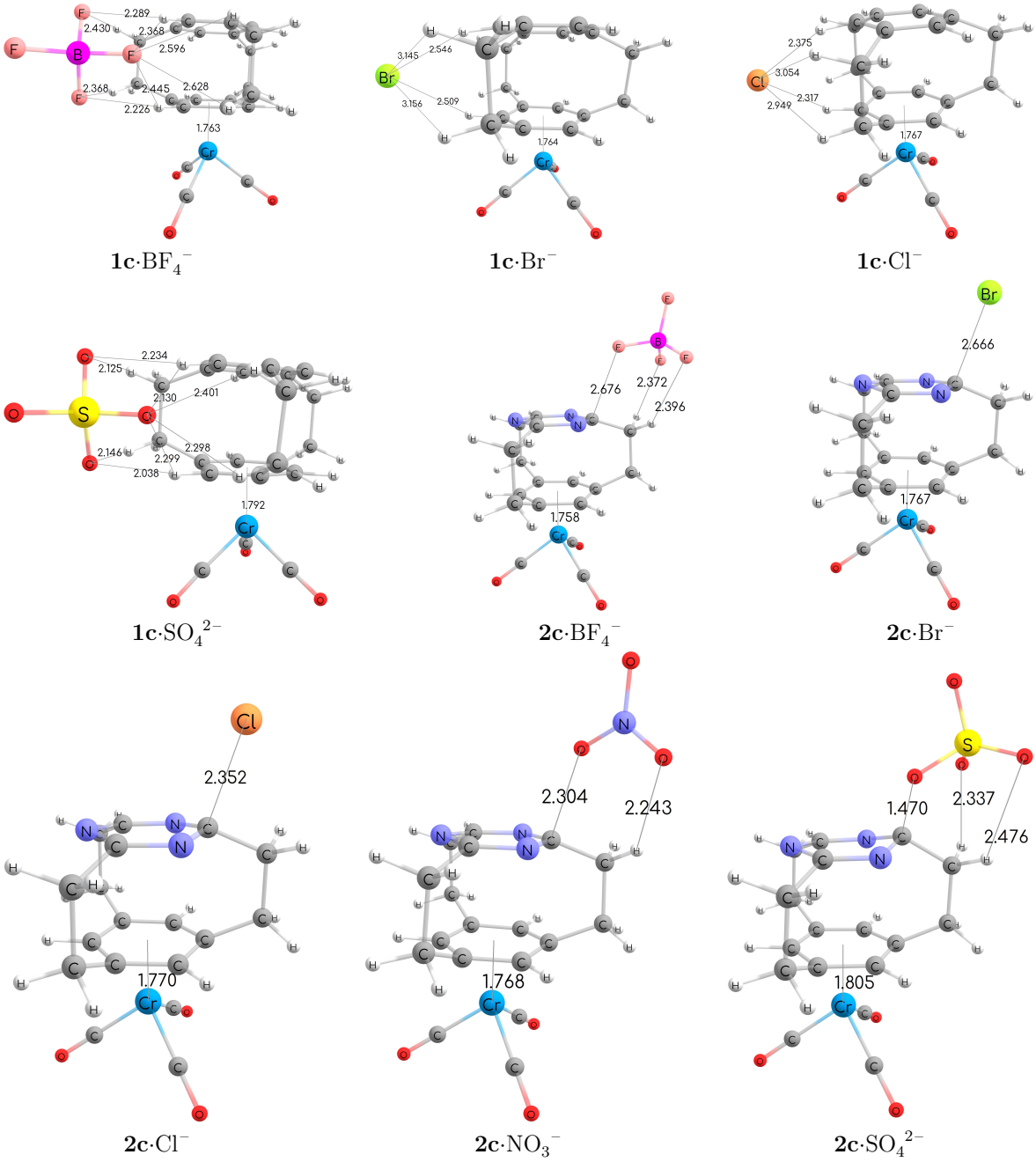
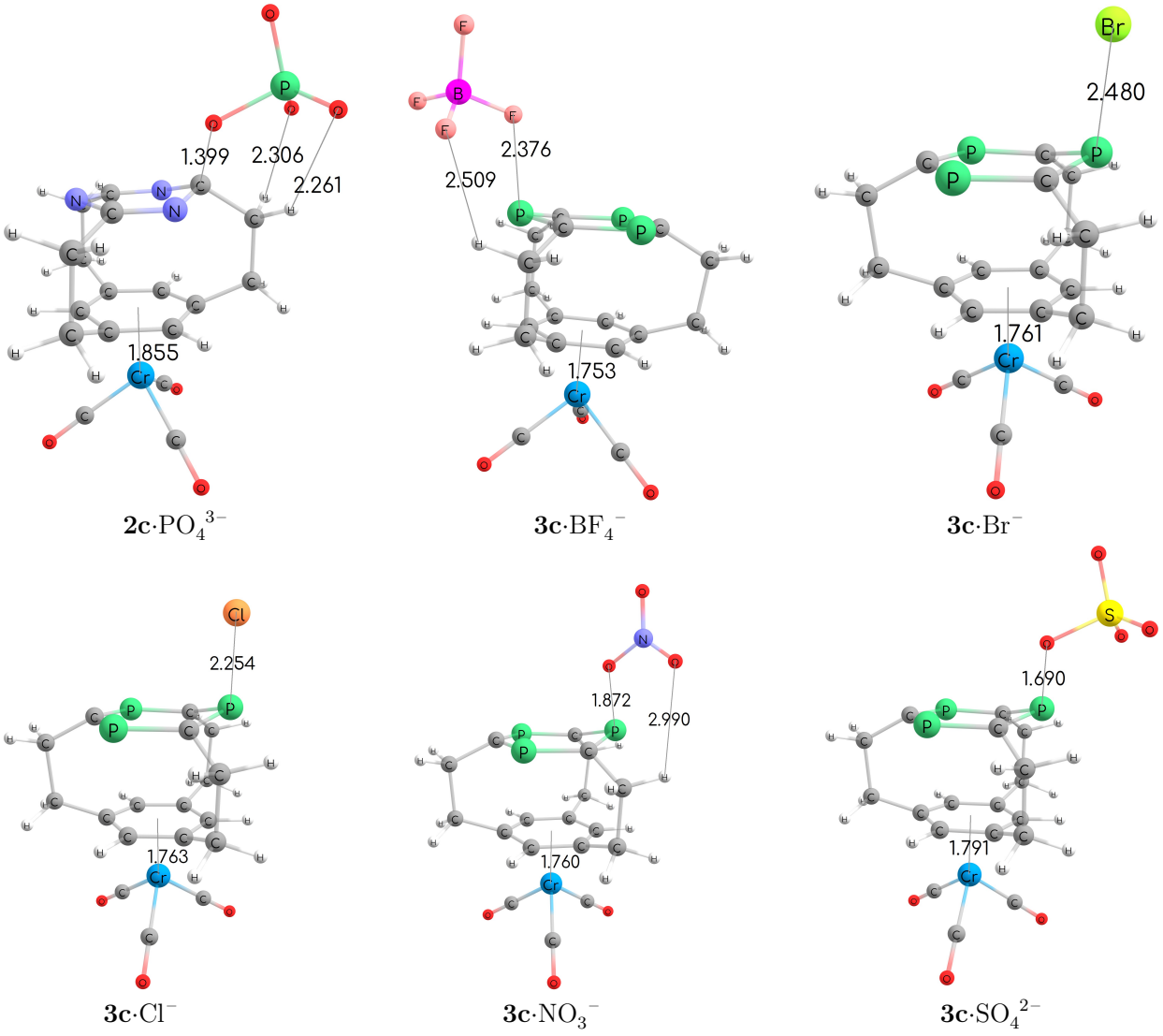


Figure S3: Optimized geometries of host-guest complexes **1c**·BF_4^-–**3c**·SO_4^{2-}.



2c·PO_4^{3-} **3c**·BF_4^- **3c**·Br^-

3c·Cl^- **3c**·NO_3^- **3c**·SO_4^{2-}

Figure S4: Optimized geometries of host-guest complexes **1c**·BF_4^-–**3c**·SO_4^{2-}.

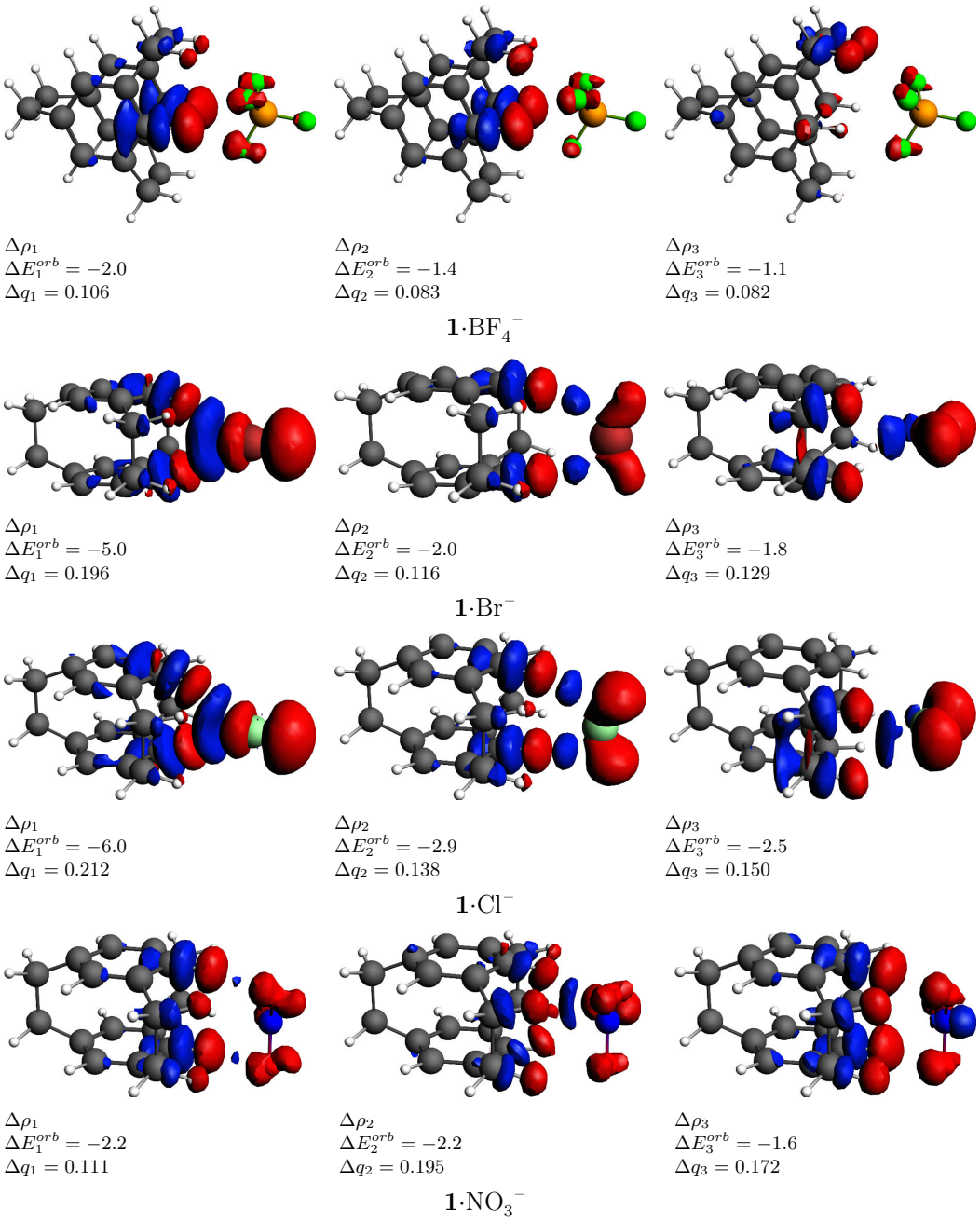


Figure S5: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and cyclophanes **1**–**3** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

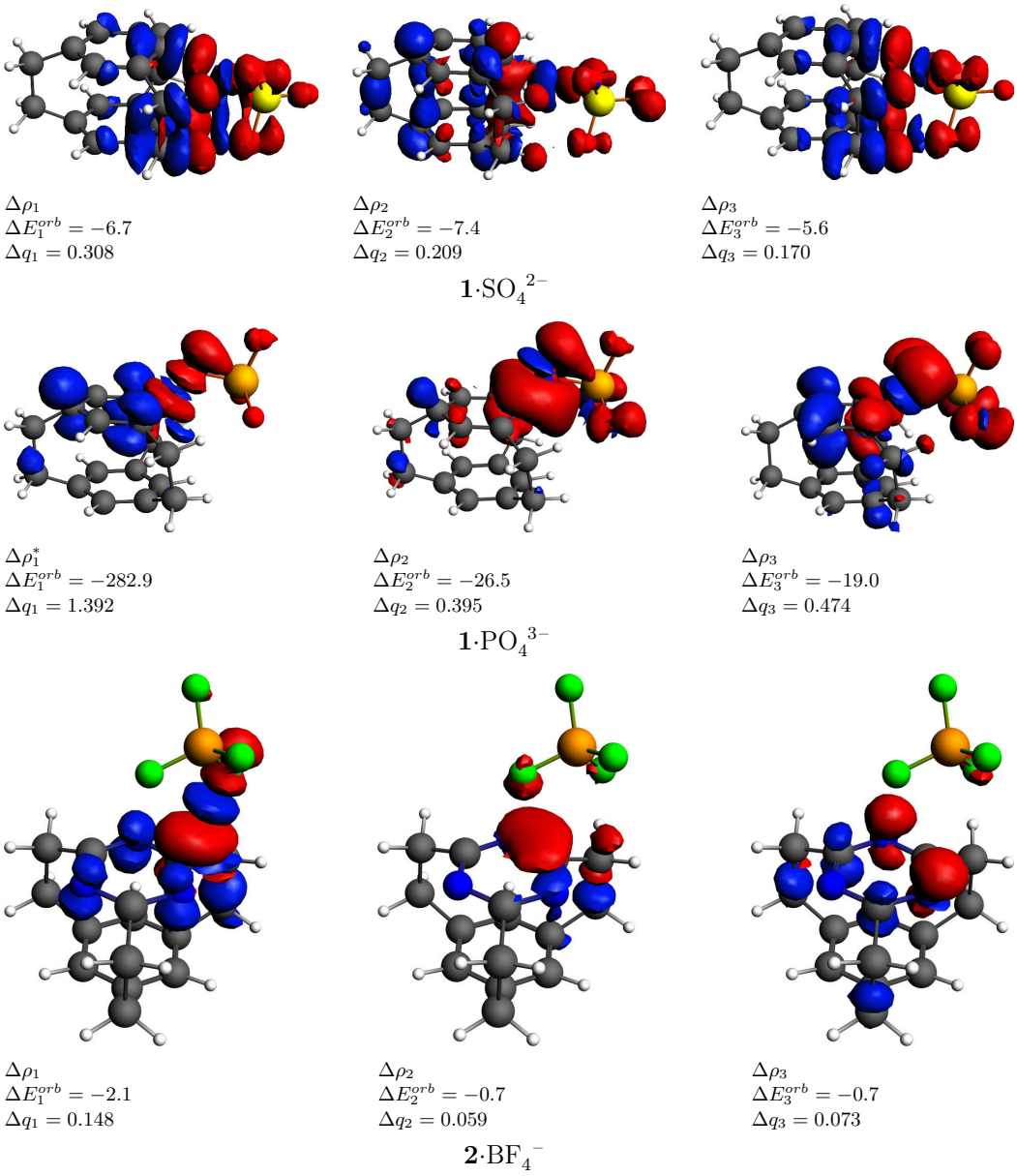


Figure S6: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and cyclophanes **1**–**3** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

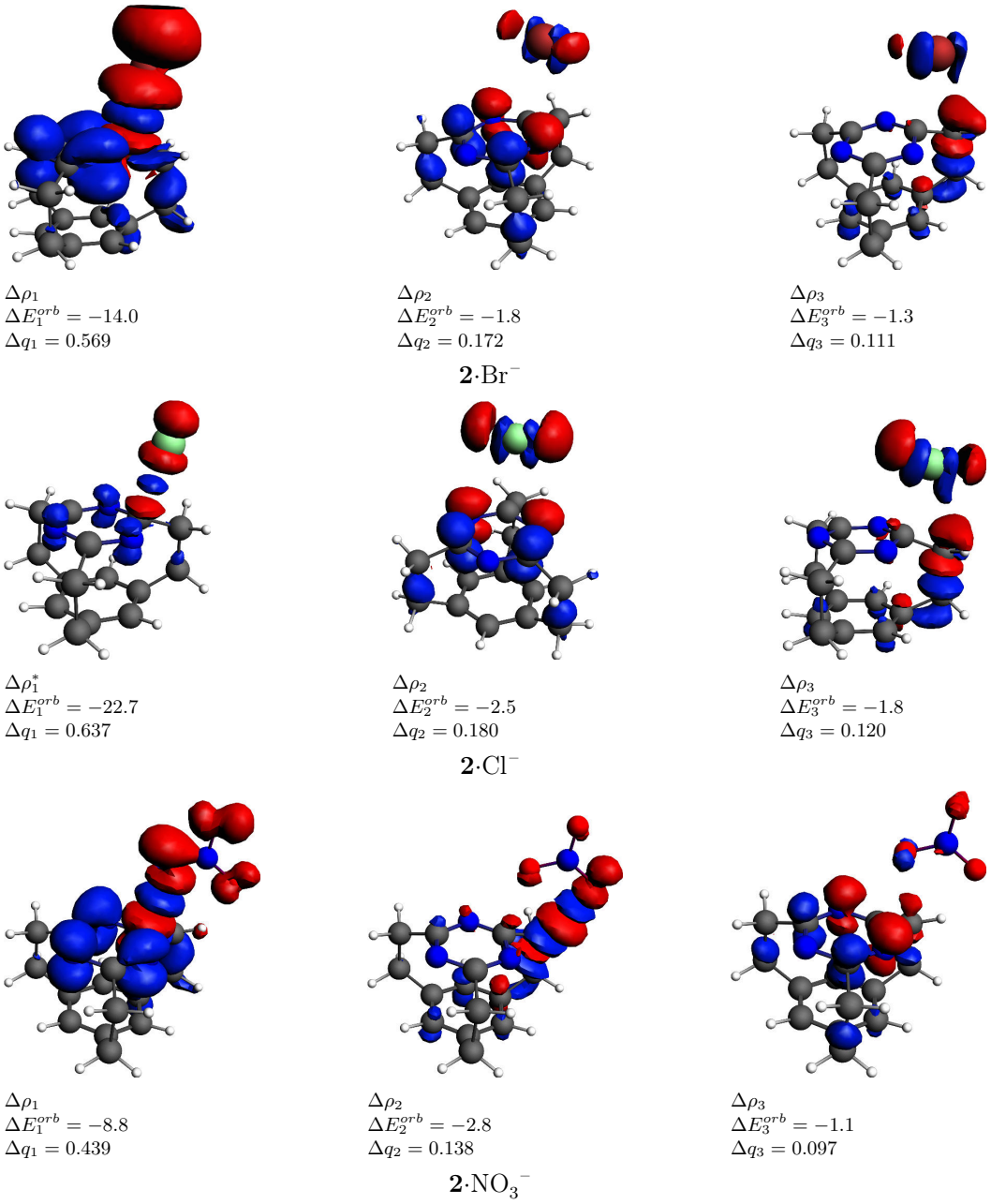
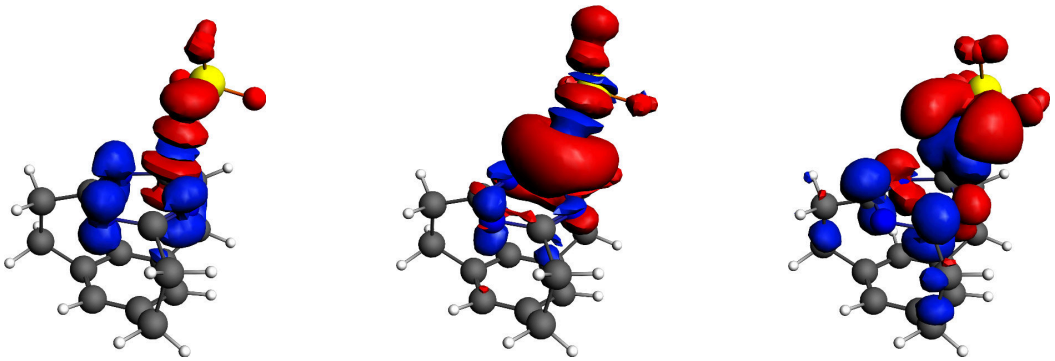


Figure S7: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and cyclophanes **1**–**3** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

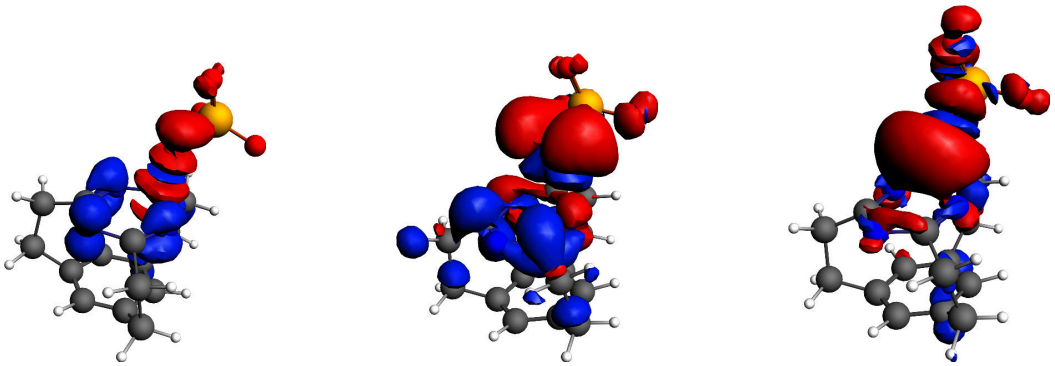


$\Delta\rho_1^*$
$\Delta E_1^{orb} = -195.0$
$\Delta q_1 = 1.164$

$\Delta\rho_2$
$\Delta E_2^{orb} = -17.7$
$\Delta q_2 = 0.288$

$\Delta\rho_3$
$\Delta E_3^{orb} = -11.2$
$\Delta q_3 = 0.300$

2·SO_4^{2-}

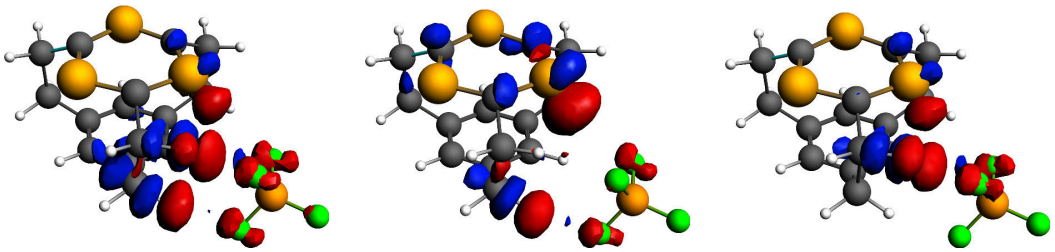


$\Delta\rho_1^*$
$\Delta E_1^{orb} = -293.2$
$\Delta q_1 = 1.295$

$\Delta\rho_2$
$\Delta E_2^{orb} = -25.7$
$\Delta q_2 = 0.480$

$\Delta\rho_3$
$\Delta E_3^{orb} = -19.3$
$\Delta q_3 = 0.372$

2·PO_4^{3-}



$\Delta\rho_1$
$\Delta E_1^{orb} = -2.3$
$\Delta q_1 = 0.118$

$\Delta\rho_2$
$\Delta E_2^{orb} = -1.7$
$\Delta q_2 = 0.108$

$\Delta\rho_3$
$\Delta E_3^{orb} = -1.6$
$\Delta q_3 = 0.093$

3·BF_4^-

Figure S8: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and cyclophanes **1**–**3** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

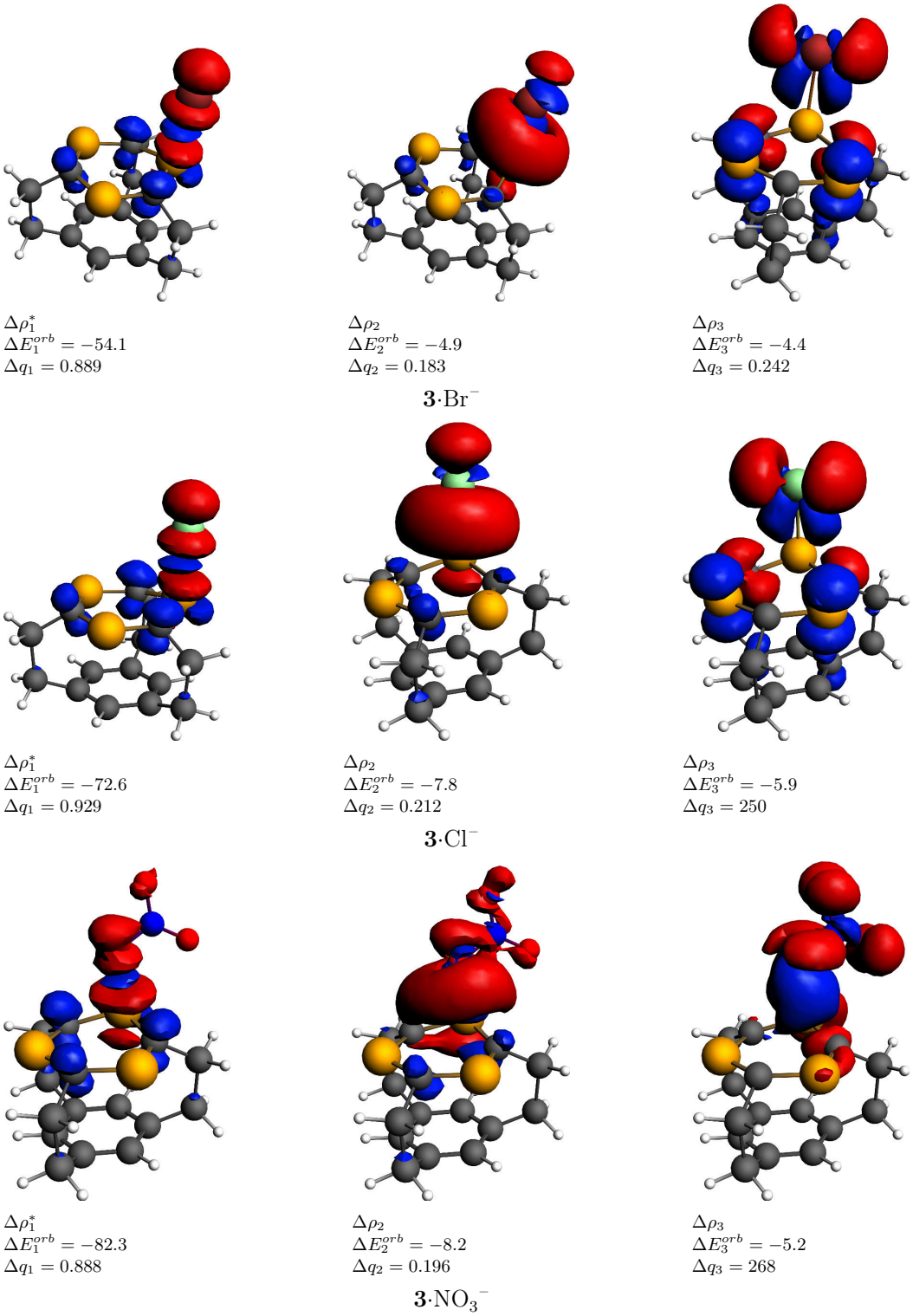
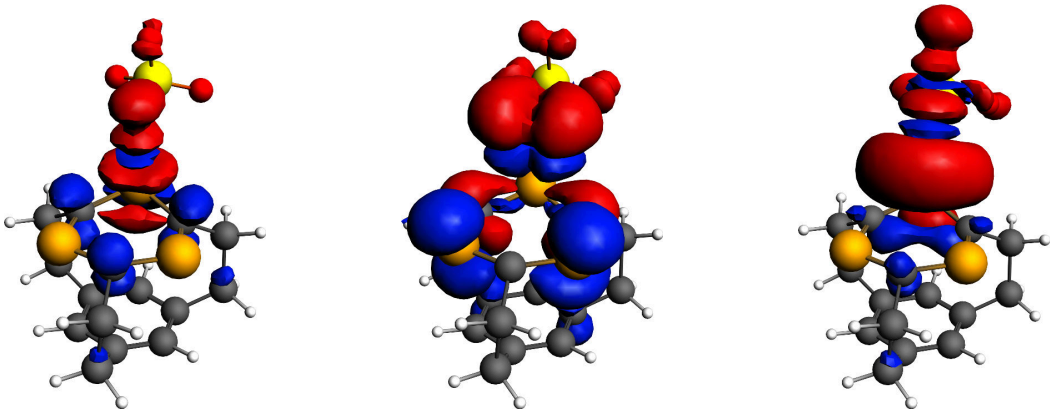


Figure S9: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and cyclophanes **1**–**3** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

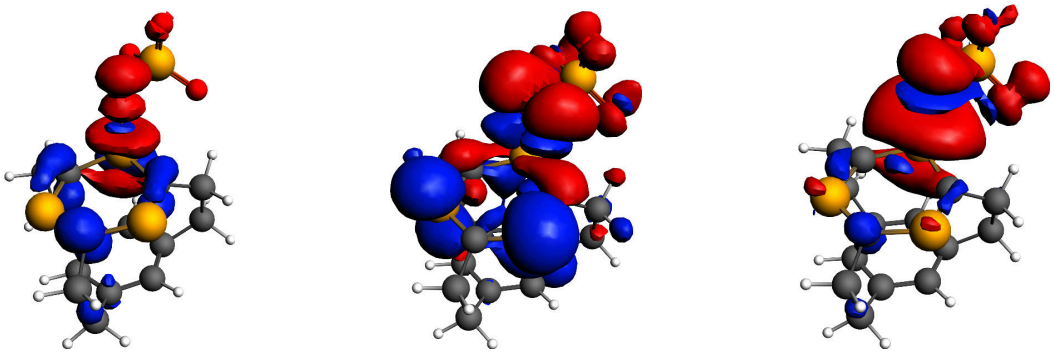


$\Delta\rho_1^*$
$\Delta E_1^{orb} = -170.5$
$\Delta q_1 = 1.135$

$\Delta\rho_2$
$\Delta E_2^{orb} = -19.5$
$\Delta q_2 = 0.399$

$\Delta\rho_3$
$\Delta E_3^{orb} = -17.0$
$\Delta q_3 = 0.312$

3·SO_4^{2-}



$\Delta\rho_1^*$
$\Delta E_1^{orb} = -252.4$
$\Delta q_1 = 1.343$

$\Delta\rho_2$
$\Delta E_2^{orb} = -39.3$
$\Delta q_2 = 0.441$

$\Delta\rho_3$
$\Delta E_3^{orb} = -29.1$
$\Delta q_3 = 0.603$

3·PO_4^{3-}

Figure S10: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and cyclophanes **1**–**3** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

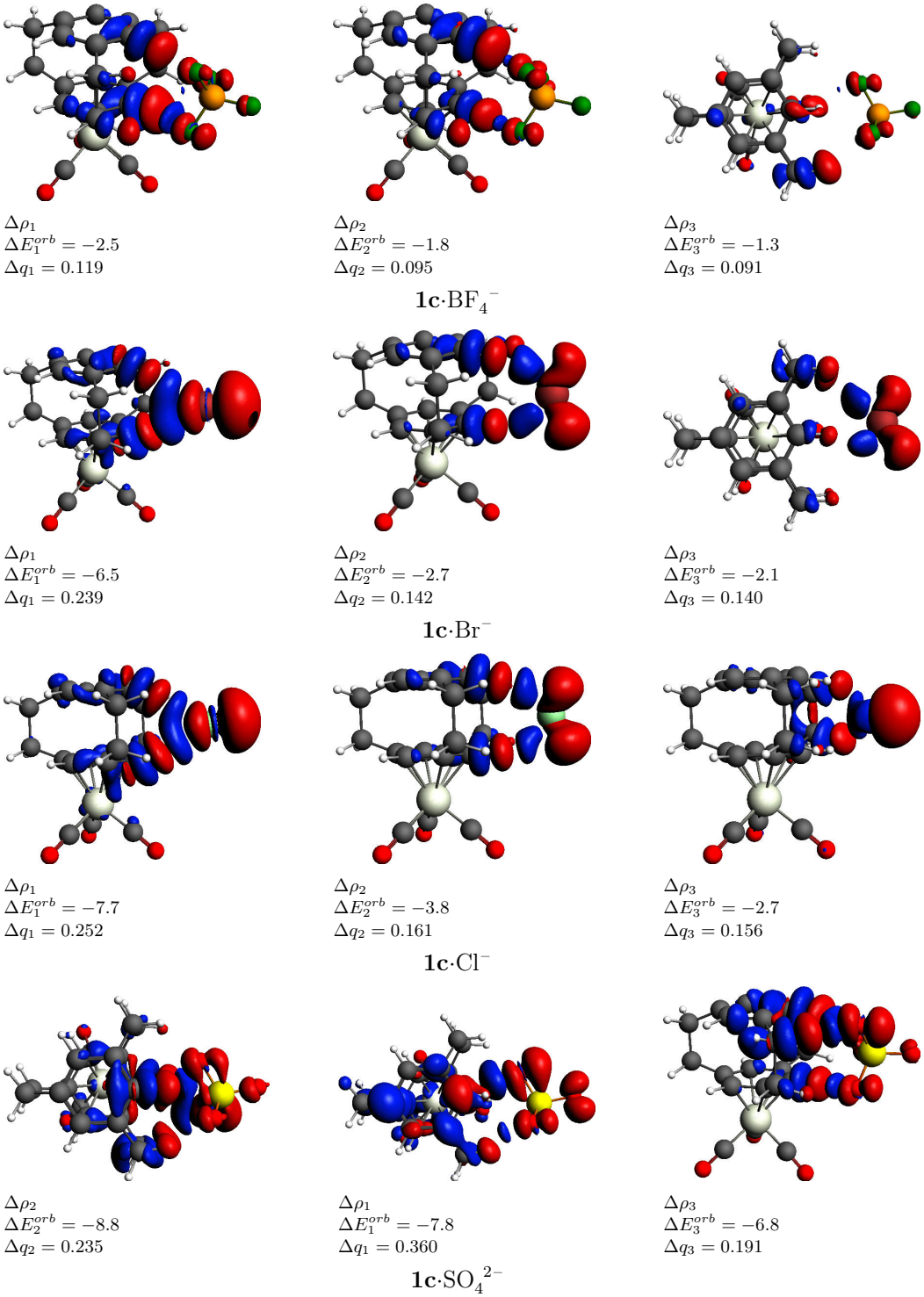
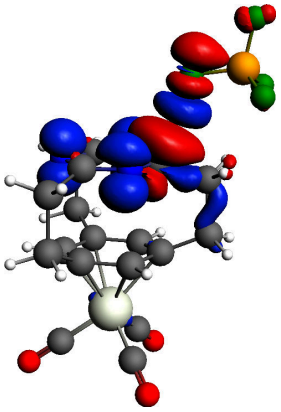
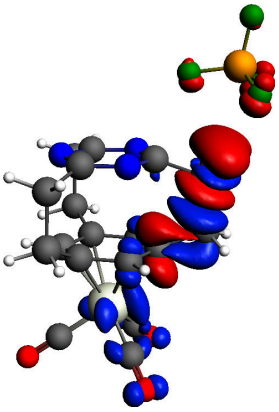


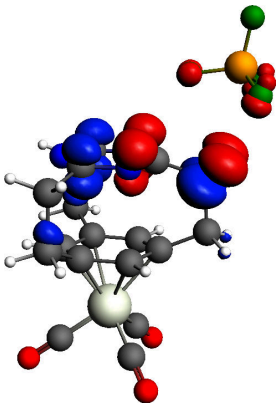
Figure S11: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and the cyclophanes **1c**–**3c** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.



$\Delta\rho_1$
$\Delta E_1^{orb} = -2.8$
$\Delta q_1 = 0.183$

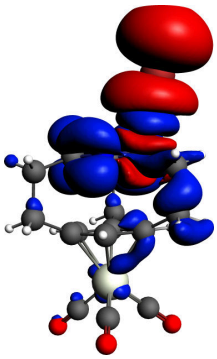


$\Delta\rho_2$
$\Delta E_2^{orb} = -1.7$
$\Delta q_2 = 0.111$

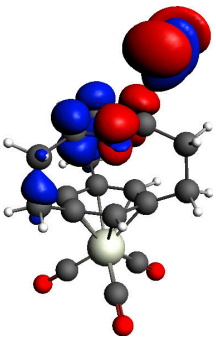


$\Delta\rho_3$
$\Delta E_3^{orb} = -1.1$
$\Delta q_3 = 0.089$

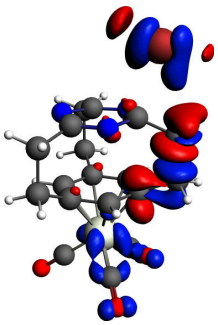
2c·BF_4^-



$\Delta\rho_1$
$\Delta E_1^{orb} = -23.1$
$\Delta q_1 = 0.687$

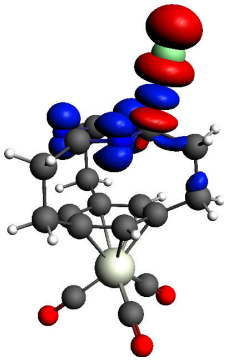


$\Delta\rho_2$
$\Delta E_2^{orb} = -2.2$
$\Delta q_2 = 0.190$

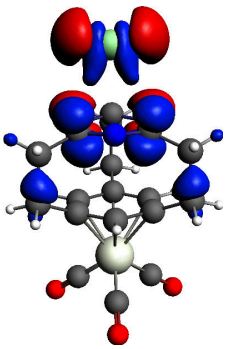


$\Delta\rho_3$
$\Delta E_3^{orb} = -1.7$
$\Delta q_3 = 0.134$

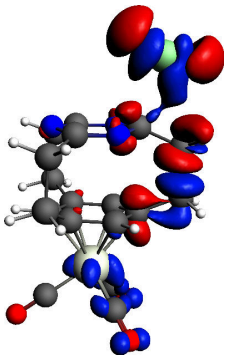
2c·Br^-



$\Delta\rho_1^*$
$\Delta E_1^{orb} = -38.6$
$\Delta q_1 = 0.765$



$\Delta\rho_2$
$\Delta E_2^{orb} = -3.0$
$\Delta q_2 = 0.191$



$\Delta\rho_4$
$\Delta E_4^{orb} = -2.6$
$\Delta q_4 = 0.117$

2c·Cl^-

Figure S12: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and the cyclophanes **1c**–**3c** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

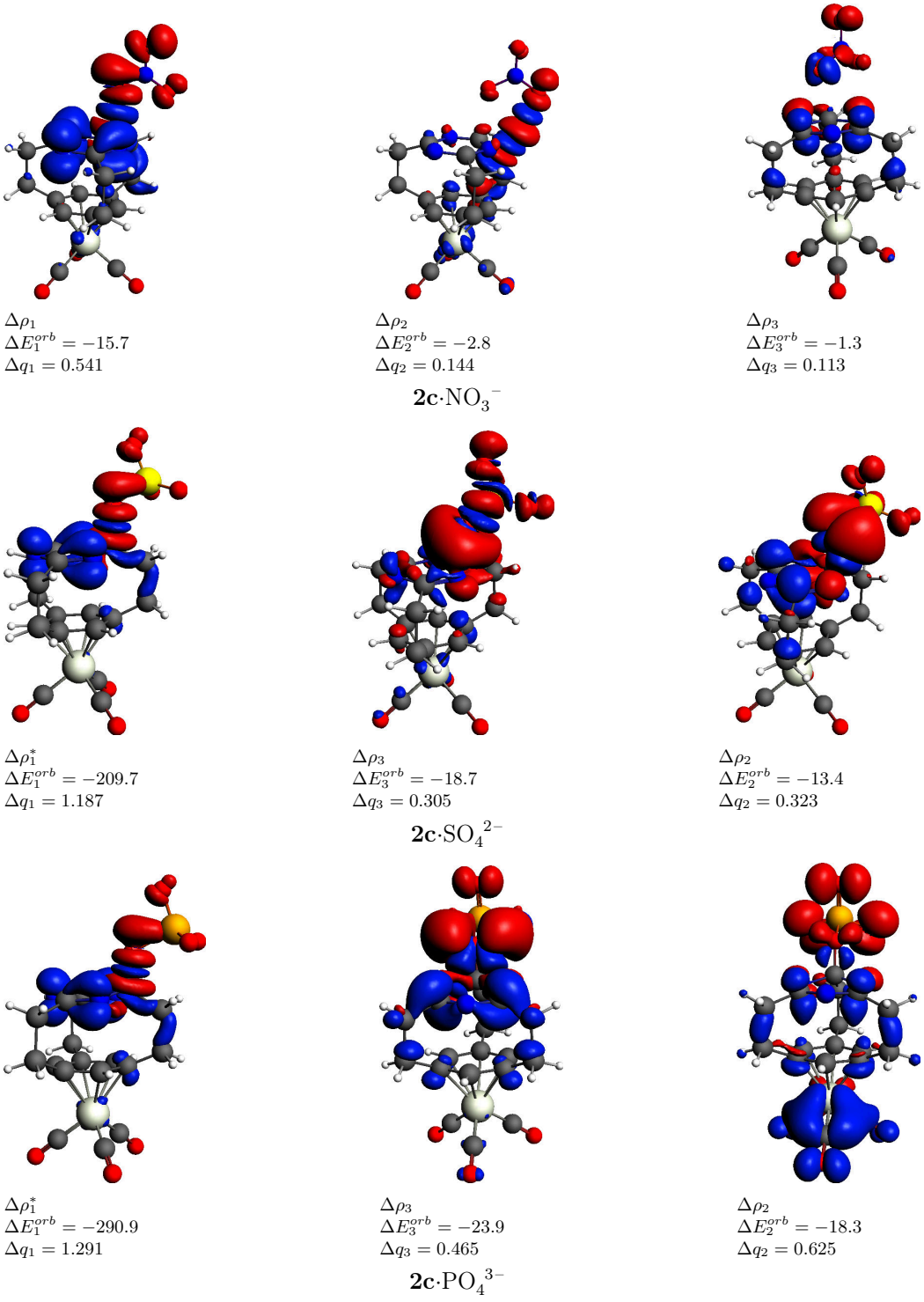


Figure S13: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and the cyclophanes **1c**–**3c** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

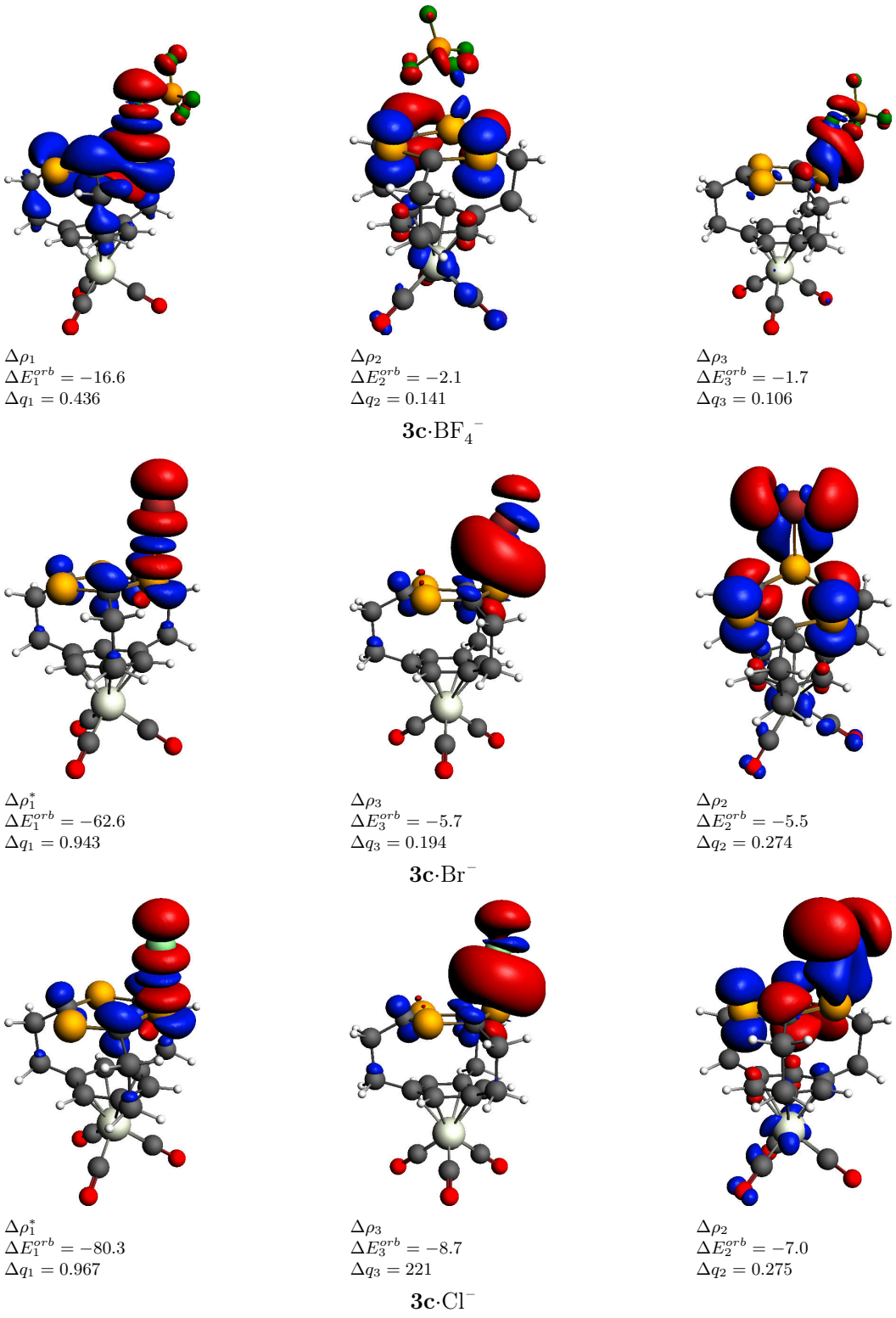


Figure S14: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and the cyclophanes **1c**–**3c** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

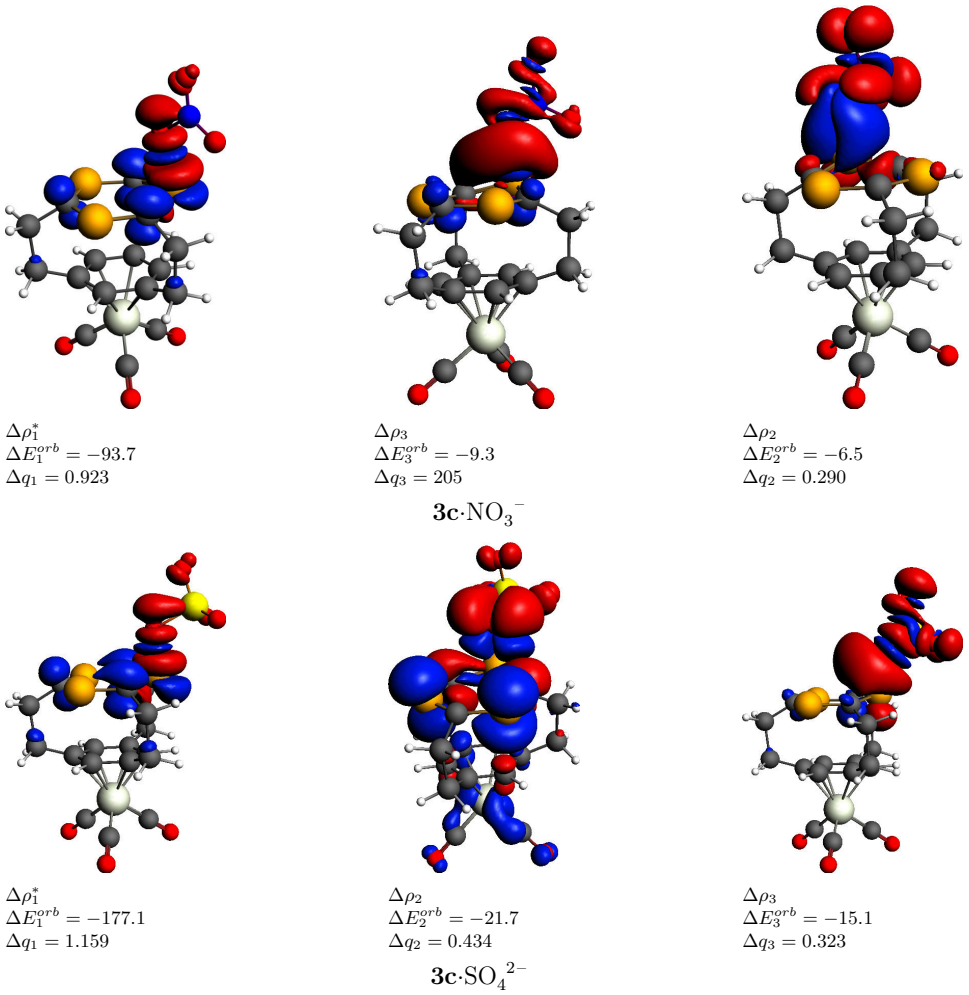


Figure S15: Surface plots of the density deformation channels, $\Delta\rho_i$, their relative energy, ΔE_i^{orb}, in kcal·mol^{-1}, and the charge transferred, Δq_i, in a.u., between the anions and the cyclophanes **1c**–**3c** fragments. Red and blue regions indicates the decrease and the increase of electronic density, respectively. The contour value is 0.0003, except for channels indicated by * and **, where the cutoff is 0.003 and 0.008, respectively.

Cartesian coordinates of optimized structures

1·BF_4^- (-1121.7799 a. u.)

C	-0.620621000	-2.462530000	-1.065120000
C	0.319416000	-1.430422000	-1.203901000
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C	0.643419000	-1.446489000	1.218836000
C	-0.302211000	-2.477659000	1.320926000
C	-0.980917000	-2.964610000	0.194143000
C	-1.027743000	1.004223000	0.227669000
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C	-2.633904000	-0.482430000	-0.785280000
C	-2.952588000	-1.029022000	0.466650000
C	-2.318885000	-0.501236000	1.601196000
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H	-1.592545000	0.522169000	-3.084332000
C	0.249236000	-0.518886000	-2.398122000
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H	0.028499000	-1.089980000	-3.312060000
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H	-4.018347000	-2.600722000	1.486757000

C	-2.350704000	-3.561134000	0.373813000
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H	1.641100000	-0.103119000	-0.142313000
F	2.137552000	2.148236000	0.681754000
B	2.395974000	2.594852000	-0.652950000
F	1.185798000	3.103388000	-1.205294000
F	3.384909000	3.594374000	-0.641285000
F	2.828073000	1.482027000	-1.430051000

1·Br^- (-3271.5726 a. u.)

C	-0.691463000	-1.644392000	-1.170462000
C	0.681089000	-1.440103000	-1.378006000
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C	-0.320709000	-2.019061000	1.184039000
C	-1.213178000	-1.882686000	0.109974000
C	1.272313000	1.201758000	0.211656000
C	0.409241000	1.282843000	-0.891361000
C	-0.968372000	1.139436000	-0.667755000
C	-1.477521000	0.819745000	0.600017000

C	-0.586973000	0.745553000	1.681801000
C	0.795334000	0.885515000	1.492707000
H	-1.637595000	1.090747000	-1.532445000
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H	-1.383834000	-1.427744000	-1.990006000
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H	1.943348000	1.460928000	-2.395605000
H	0.291099000	1.402768000	-3.039106000
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H	2.179785000	-0.787641000	-2.781845000
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H	-3.529612000	0.496605000	0.012148000
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H	1.325874000	0.330465000	3.498431000
H	2.722095000	0.661565000	2.438431000
C	1.862723000	-1.376039000	2.200041000
H	1.518209000	-1.892817000	3.104923000
H	2.931357000	-1.595610000	2.056974000
H	2.352379000	1.200915000	0.034347000
H	2.600567000	-1.317888000	-0.408759000
Br	-2.134827000	-1.314736000	4.289273000

1·Cl^- (-1157.3872 a. u.)

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C	1.651349000	-1.978328000	-0.227178000
C	1.048862000	-1.722893000	1.014210000
C	-0.341364000	-1.547727000	1.068085000
C	-1.112694000	-1.530242000	-0.104472000
C	2.048619000	0.820556000	-0.522690000
C	1.294983000	0.772484000	-1.705017000
C	-0.085432000	1.009417000	-1.621260000
C	-0.726764000	1.186580000	-0.385868000
C	0.055223000	1.227643000	0.779023000
C	1.437668000	0.998117000	0.728046000
H	-0.697472000	0.864977000	-2.517270000
H	-0.464721000	1.221661000	1.748900000
H	-0.813273000	-1.201839000	2.000290000
H	-1.053308000	-1.669248000	-2.254825000
C	1.828144000	-0.011021000	-2.874268000
H	2.906856000	0.163823000	-3.000603000
H	1.331877000	0.296997000	-3.806350000
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H	2.593809000	-2.094955000	-2.754136000
H	1.023835000	-1.963235000	-3.569708000
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H	-2.758927000	1.171216000	-1.114888000
H	-2.590959000	1.283655000	0.672569000
C	-2.408987000	-0.767617000	-0.079529000

H	-3.077169000	-1.100179000	-0.888480000
H	-2.906519000	-0.899352000	0.890864000
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H	1.701562000	0.934706000	2.857769000
H	3.194668000	0.635119000	1.928533000
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H	1.370506000	-1.295378000	3.092564000
H	2.865787000	-1.626780000	2.177555000
H	3.102898000	0.528390000	-0.560039000
H	2.743937000	-2.001191000	-0.290652000
Cl	-2.040695000	0.362995000	3.415619000

1·NO_3^- (-977.5825 a. u.)

C	-0.686339000	-2.508219000	-0.816592000
C	0.443619000	-1.709799000	-1.047791000
C	1.035068000	-1.050517000	0.040138000
C	0.448139000	-1.081492000	1.314620000
C	-0.681762000	-1.890479000	1.510139000
C	-1.290167000	-2.575205000	0.447786000
C	-0.602153000	1.211064000	-0.555595000
C	-1.141325000	0.481592000	-1.625741000
C	-2.309093000	-0.265049000	-1.409722000
C	-2.881079000	-0.378196000	-0.133844000
C	-2.306528000	0.351403000	0.917448000
C	-1.138075000	1.107301000	0.737386000
H	-2.675231000	-0.916484000	-2.209122000
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H	-1.204828000	-1.840885000	2.470003000

H	-1.212658000	-2.939895000	-1.673374000
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H	-4.340538000	-1.420693000	1.060746000
C	-2.758922000	-2.891423000	0.534120000
H	-3.026004000	-3.693550000	-0.169475000
H	-3.023520000	-3.235772000	1.544579000
C	-0.229061000	1.358533000	1.908717000
H	-0.812110000	1.593801000	2.811581000
H	0.452746000	2.192031000	1.694034000
C	0.707776000	0.069079000	2.247413000
H	0.511172000	-0.221150000	3.290272000
H	1.748730000	0.407231000	2.158743000
H	0.347348000	1.732634000	-0.697730000
H	1.868072000	-0.368334000	-0.145832000
N	2.784679000	1.952438000	-0.218529000
O	2.656531000	1.544711000	-1.417841000
O	2.203518000	3.016943000	0.150342000
O	3.468156000	1.275709000	0.607214000

$\mathbf{1}{\cdot}SO_4^{2-}$ (-1396.3732 a. u.)

C	-0.037753000	-1.921434000	-0.666949000

C	0.967886000	-0.960587000	-0.858359000
C	1.522094000	-0.324354000	0.263857000
C	1.003415000	-0.552865000	1.550245000
C	-0.000984000	-1.521604000	1.708569000
C	-0.567404000	-2.183892000	0.607419000
C	-0.397367000	1.744928000	-0.040540000
C	-0.892936000	1.057846000	-1.160067000
C	-1.952029000	0.152308000	-0.986093000
C	-2.454428000	-0.152455000	0.289792000
C	-1.926564000	0.540349000	1.391866000
C	-0.865351000	1.449596000	1.251329000
H	-2.259992000	-0.471727000	-1.832841000
H	-2.216593000	0.219535000	2.398933000
H	-0.487501000	-1.622277000	2.685531000
H	-0.552827000	-2.331406000	-1.543255000
C	0.015117000	0.937983000	-2.354419000
H	0.612130000	1.853719000	-2.456217000
H	-0.561583000	0.749884000	-3.275874000
C	1.096132000	-0.262850000	-2.185468000
H	2.079320000	0.219989000	-2.260203000
H	0.954235000	-0.972165000	-3.018497000
C	-3.084274000	-1.501863000	0.514638000
H	-3.719290000	-1.778040000	-0.342604000
H	-3.726028000	-1.489470000	1.410147000
C	-1.983681000	-2.684259000	0.714470000
H	-2.183733000	-3.457483000	-0.044857000
H	-2.159221000	-3.138273000	1.702928000

C	0.070796000	1.718333000	2.396620000
H	-0.480715000	1.804107000	3.347972000
H	0.648803000	2.636428000	2.190672000
C	1.181034000	0.540999000	2.565795000
H	1.100618000	0.145815000	3.592500000
H	2.157124000	1.033344000	2.405310000
H	0.495645000	2.375922000	-0.146663000
H	2.227727000	0.504671000	0.115346000
O	1.921571000	3.802362000	0.830491000
S	3.071737000	3.057969000	0.183201000
O	2.533729000	2.330925000	-1.047693000
O	4.154301000	4.005761000	-0.215988000
O	3.601103000	2.017476000	1.148641000

1·PO_4^{3-} (-1339.3824 a. u.)

C	-0.746634000	-1.134641000	-1.090842000
C	0.651224000	-1.175300000	-1.212888000
C	1.389682000	-1.698902000	-0.134474000
C	0.782905000	-2.078583000	1.071528000
C	-0.614810000	-2.000080000	1.158156000
C	-1.391174000	-1.477581000	0.107492000
C	1.750716000	0.832631000	1.100682000
C	1.114460000	1.293339000	-0.032751000
C	-0.363694000	1.610157000	-0.042508000
C	-1.057397000	1.045768000	1.174761000
C	-0.342936000	0.589681000	2.260601000
C	1.086902000	0.473610000	2.319436000
H	-0.806243000	1.139818000	-0.939538000

H	-0.913815000	0.139747000	3.093944000
H	-1.091001000	-2.157677000	2.131336000
H	-1.318191000	-0.595065000	-1.852294000
C	1.740850000	1.158976000	-1.385215000
H	2.846623000	1.162895000	-1.296611000
H	1.389978000	1.976330000	-2.046976000
C	1.312252000	-0.205872000	-2.157077000
H	2.221905000	-0.633509000	-2.620005000
H	0.610947000	0.091188000	-2.950946000
C	-2.502443000	0.674746000	0.980108000
H	-2.946839000	1.367261000	0.239591000
H	-3.062993000	0.739870000	1.935142000
C	-2.717583000	-0.829913000	0.418298000
H	-3.346153000	-0.773142000	-0.485996000
H	-3.263275000	-1.424489000	1.176712000
C	1.638407000	-0.688622000	3.094136000
H	1.050377000	-0.820364000	4.025639000
H	2.698378000	-0.538135000	3.409589000
C	1.618945000	-2.119977000	2.333128000
H	1.252474000	-2.898457000	3.037822000
H	2.658378000	-2.397920000	2.068897000
H	2.820830000	0.571083000	1.008791000
H	2.481464000	-1.619205000	-0.162542000
O	-0.443208000	2.862259000	-2.839149000
P	-1.432991000	3.363504000	-1.754137000
O	-2.728189000	2.513708000	-1.689660000
O	-0.625628000	3.026116000	-0.237325000

O	-1.628387000	4.882815000	-1.690474000

2·BF_4^- (-1169.9299 a. u.)

C	-0.760584000	-3.040822000	-1.032340000
C	0.622784000	-2.929931000	-1.234340000
C	1.450726000	-2.758894000	-0.115085000
C	0.916322000	-2.583505000	1.169806000
C	-0.471289000	-2.701909000	1.336664000
C	-1.327965000	-2.871738000	0.238979000
N	1.231685000	-0.022944000	-0.497469000
C	0.383575000	-0.237106000	-1.512841000
N	-0.957058000	-0.278776000	-1.405961000
C	-1.420888000	-0.184956000	-0.145768000
N	-0.663870000	0.025683000	0.939133000
C	0.661959000	0.081068000	0.717830000
H	-0.905738000	-2.429648000	2.301099000
H	-1.418936000	-3.032422000	-1.904184000
C	0.971536000	-0.854535000	-2.749692000
H	1.965243000	-0.430827000	-2.934466000
H	0.318569000	-0.654086000	-3.607040000
C	1.119639000	-2.457628000	-2.578420000
H	2.180183000	-2.711877000	-2.710768000
H	0.554961000	-2.934420000	-3.391569000
C	-2.794776000	-0.738659000	0.101607000
H	-3.435318000	-0.534629000	-0.764156000
H	-3.221461000	-0.270972000	0.996026000
C	-2.736665000	-2.339739000	0.334285000
H	-3.382421000	-2.811353000	-0.419359000

H	-3.164819000	-2.549964000	1.323902000
C	1.547384000	-0.177962000	1.896856000
H	1.115697000	0.303621000	2.779481000
H	2.535927000	0.248892000	1.701453000
C	1.695725000	-1.764723000	2.170203000
H	1.343872000	-1.964823000	3.191651000
H	2.764800000	-2.015046000	2.127545000
H	2.506785000	-2.531138000	-0.276379000
F	1.121773000	4.652132000	0.064947000
F	1.152377000	2.712402000	1.338752000
B	0.322828000	3.605192000	0.583915000
F	-0.277804000	2.883643000	-0.485268000
F	-0.682984000	4.131228000	1.429755000

2·Br^- (-3370.5486 a. u.)

C	-0.843008000	-1.705452000	-0.863231000
C	0.538910000	-1.589638000	-1.068258000
C	1.387252000	-1.679348000	0.044079000
C	0.876703000	-1.755072000	1.347817000
C	-0.510565000	-1.857193000	1.518860000
C	-1.386226000	-1.781230000	0.427431000
N	1.269609000	1.077827000	0.228797000
C	0.397816000	1.169990000	-0.814582000
N	-0.950022000	1.044329000	-0.652801000
C	-1.380083000	0.927568000	0.600399000
N	-0.602914000	0.962661000	1.708970000
C	0.722901000	0.955732000	1.436670000
H	-0.921487000	-1.766362000	2.527379000

H	-1.512986000	-1.500134000	-1.700919000
C	0.933501000	0.736913000	-2.153406000
H	1.928217000	1.171930000	-2.289112000
H	0.273130000	1.129722000	-2.932269000
C	1.031746000	-0.868064000	-2.297277000
H	2.081881000	-1.125578000	-2.496162000
H	0.444683000	-1.163820000	-3.178835000
C	-2.766018000	0.368227000	0.784225000
H	-3.431981000	0.782811000	0.018266000
H	-3.136704000	0.642054000	1.779962000
C	-2.775105000	-1.239923000	0.653698000
H	-3.435651000	-1.509936000	-0.182388000
H	-3.212123000	-1.654256000	1.573528000
C	1.617317000	0.419238000	2.523280000
H	1.223856000	0.720794000	3.502151000
H	2.627843000	0.823640000	2.393178000
C	1.700680000	-1.191538000	2.477405000
H	1.349669000	-1.580702000	3.443566000
H	2.757335000	-1.473043000	2.367998000
H	2.447774000	-1.453539000	-0.089911000
Br	0.615649000	3.903962000	-1.542247000

2·Cl^- (-1208.3432 a. u.)

C	-0.860484000	-1.720005000	-0.844026000
C	0.517133000	-1.600767000	-1.072180000
C	1.384580000	-1.685689000	0.025518000
C	0.895888000	-1.762502000	1.337385000
C	-0.488156000	-1.868244000	1.531462000

C	-1.382303000	-1.796158000	0.455294000
N	1.268182000	1.066497000	0.251116000
C	0.417899000	1.184150000	-0.815513000
N	-0.936545000	1.039924000	-0.677514000
C	-1.387494000	0.917881000	0.565986000
N	-0.635399000	0.953253000	1.692704000
C	0.697095000	0.943763000	1.443553000
H	-0.882732000	-1.777128000	2.546525000
H	-1.543720000	-1.515646000	-1.671187000
C	0.981097000	0.720682000	-2.137428000
H	2.007145000	1.093475000	-2.214205000
H	0.388326000	1.168640000	-2.940770000
C	0.981098000	-0.880147000	-2.313134000
H	2.001055000	-1.189396000	-2.585043000
H	0.323369000	-1.129061000	-3.158522000
C	-2.776923000	0.353638000	0.719249000
H	-3.397825000	0.705861000	-0.113246000
H	-3.211091000	0.693045000	1.668617000
C	-2.767625000	-1.258234000	0.708827000
H	-3.471965000	-1.596909000	-0.064662000
H	-3.142785000	-1.611740000	1.679773000
C	1.569221000	0.407964000	2.550514000
H	1.114474000	0.655633000	3.518154000
H	2.564298000	0.864480000	2.487740000
C	1.736589000	-1.191945000	2.451056000
H	1.454318000	-1.626057000	3.421178000
H	2.799489000	-1.414989000	2.282415000

H	2.441550000	-1.454103000	-0.125276000
Cl	0.652761000	3.645491000	-1.426232000

2·NO_3^- (-1026.5885 a. u.)

C	-0.822999000	-2.108408000	-0.626256000
C	1.441785000	-1.562522000	-0.001960000
C	1.045826000	-1.350871000	1.327198000
C	-0.293601000	-1.587394000	1.666487000
C	-1.250464000	-1.908857000	0.693298000
N	0.915143000	1.109842000	-0.580842000
C	-0.051201000	0.741152000	-1.425139000
N	-1.357782000	0.602351000	-1.111463000
C	-1.618898000	0.735283000	0.208781000
N	-0.731444000	1.081557000	1.143353000
C	0.541083000	1.267212000	0.714474000
H	-0.637072000	-1.293252000	2.660662000
H	-1.576470000	-2.213053000	-1.410711000
C	0.396559000	0.069790000	-2.694789000
H	1.272441000	0.588667000	-3.102341000
H	-0.420743000	0.093994000	-3.426442000
C	0.801611000	-1.470775000	-2.420279000
H	1.872741000	-1.581357000	-2.636749000
H	0.247309000	-2.093506000	-3.136250000
C	-2.886592000	0.090504000	0.700256000
H	-3.687526000	0.233998000	-0.035935000
H	-3.174069000	0.548239000	1.653610000
C	-2.681247000	-1.496290000	0.929364000
H	-3.354548000	-2.029427000	0.244351000

H	-2.994455000	-1.728110000	1.956837000
C	1.626520000	1.131679000	1.735474000
H	1.381370000	1.762099000	2.600155000
H	2.554010000	1.501728000	1.285620000
C	1.837969000	-0.397034000	2.188198000
H	1.525550000	-0.494180000	3.237422000
H	2.915168000	-0.612940000	2.138513000
H	2.443418000	-1.250248000	-0.306171000
C	0.510543000	-1.886293000	-0.999629000
N	0.655651000	4.454925000	1.880867000
O	0.449709000	5.692228000	1.805107000
O	0.851396000	3.896088000	2.999774000
O	0.670512000	3.757096000	0.805038000

2·SO_4^{2-} (-1444.5418 a. u.)

C	-0.944535000	-1.444049000	-0.836341000
C	1.357995000	-1.549967000	-0.149679000
C	0.980541000	-1.952219000	1.137769000
C	-0.382708000	-2.144268000	1.401254000
C	-1.360547000	-1.858637000	0.437164000
N	1.200232000	1.176704000	0.501121000
C	0.108342000	1.647936000	-0.334771000
N	-1.218154000	1.186117000	0.049153000
C	-1.350211000	0.731311000	1.265343000
N	-0.378676000	0.571858000	2.219447000
C	0.870649000	0.719480000	1.683754000
H	-0.696352000	-2.291699000	2.438240000
H	-1.696178000	-1.050158000	-1.523921000

C	0.359379000	1.261673000	-1.818484000
H	1.128619000	1.939724000	-2.209665000
H	-0.574654000	1.503252000	-2.338837000
C	0.796252000	-0.211715000	-2.172717000
H	1.891158000	-0.237964000	-2.288519000
H	0.364649000	-0.454572000	-3.159820000
C	-2.656780000	0.018378000	1.579443000
H	-3.506460000	0.609853000	1.209044000
H	-2.737232000	-0.085217000	2.671286000
C	-2.728690000	-1.430829000	0.909555000
H	-3.418146000	-1.390643000	0.052791000
H	-3.150219000	-2.140498000	1.642126000
C	1.965400000	-0.003519000	2.452917000
H	1.890754000	0.238566000	3.524673000
H	2.934631000	0.346984000	2.072538000
C	1.886638000	-1.591249000	2.290128000
H	1.494339000	-2.032861000	3.219372000
H	2.910329000	-1.977114000	2.146647000
H	2.391805000	-1.238222000	-0.317685000
C	0.408669000	-1.233702000	-1.130367000
O	-0.126141000	5.502185000	-0.558992000
S	0.035948000	4.281976000	-1.365866000
O	-1.125184000	3.955927000	-2.216711000
O	0.107233000	3.131725000	-0.157428000
O	1.326341000	4.215449000	-2.088613000

2·PO_4^{3-} (-1389.7906 a. u.)

C	-1.073395000	-1.431489000	-0.710742000

C	1.186571000	-2.097400000	-0.187971000
C	0.919956000	-1.981930000	1.184122000
C	-0.377982000	-1.631177000	1.582575000
C	-1.376692000	-1.299436000	0.651633000
N	1.946918000	0.634037000	-0.049388000
C	0.980280000	0.815177000	-1.016213000
N	-0.242804000	1.231408000	-0.878204000
C	-0.667620000	1.677975000	0.483162000
N	0.200416000	1.117852000	1.553660000
C	1.389807000	0.712067000	1.205387000
H	-0.549349000	-1.366089000	2.629286000
H	-1.767151000	-1.004663000	-1.439107000
C	1.324918000	0.158879000	-2.350578000
H	2.421578000	0.065224000	-2.416195000
H	0.966080000	0.783508000	-3.183954000
C	0.666926000	-1.287482000	-2.497031000
H	1.397993000	-1.971238000	-2.971537000
H	-0.200807000	-1.214788000	-3.172393000
C	-2.131095000	1.174431000	0.701951000
H	-2.653097000	1.441183000	-0.226671000
H	-2.549001000	1.833431000	1.487504000
C	-2.441182000	-0.319508000	1.087468000
H	-3.428421000	-0.579676000	0.657839000
H	-2.544360000	-0.393917000	2.184212000
C	2.179667000	-0.047383000	2.265984000
H	1.779763000	0.239972000	3.249383000
H	3.248145000	0.228986000	2.216485000

C	2.066756000	-1.631732000	2.102603000
H	1.944489000	-2.081575000	3.106204000
H	3.007016000	-2.025275000	1.679917000
H	2.228532000	-2.190445000	-0.509178000
C	0.208560000	-1.797524000	-1.151388000
P	-1.944209000	4.251534000	0.792135000
O	-2.861454000	4.074427000	-0.426984000
O	-2.578149000	3.820808000	2.133985000
O	-0.593244000	3.073051000	0.531448000
O	-1.137188000	5.551595000	0.843898000

3·BF_4^- (-2029.7927 a. u.)

C	-0.618944000	-0.062913000	-0.899180000
C	0.783894000	-0.119859000	-0.995276000
C	1.469241000	-1.078662000	-0.227762000
C	0.799415000	-1.923487000	0.674732000
C	-0.602382000	-1.840077000	0.743887000
C	-1.321515000	-0.894693000	-0.009948000
P	2.157239000	0.880782000	1.812600000
C	1.108469000	1.940601000	0.909328000
P	-0.623194000	2.179935000	0.962838000
C	-1.290052000	1.011598000	2.082111000
P	-0.540133000	-0.166658000	3.122222000
C	1.182511000	-0.131628000	2.847710000
H	-1.133518000	-2.451270000	1.477798000
H	-1.163577000	0.701541000	-1.460253000
C	1.667187000	2.295433000	-0.442712000
H	2.740092000	2.532695000	-0.385546000

H	1.125119000	3.140219000	-0.890071000
C	1.520447000	1.064884000	-1.530872000
H	2.541698000	0.783091000	-1.821781000
H	0.992579000	1.493778000	-2.392245000
C	-2.682673000	0.604504000	1.676883000
H	-3.264317000	1.470160000	1.328913000
H	-3.218162000	0.131665000	2.514280000
C	-2.689454000	-0.476259000	0.433910000
H	-3.219730000	0.010826000	-0.393212000
H	-3.274899000	-1.340313000	0.777529000
C	1.813802000	-1.480644000	3.071593000
H	1.408134000	-1.967681000	3.971339000
H	2.904522000	-1.390458000	3.188222000
C	1.557174000	-2.521930000	1.820519000
H	1.013143000	-3.381521000	2.235190000
H	2.548115000	-2.866981000	1.495028000
H	2.561729000	-1.093418000	-0.254130000
B	-1.512313000	2.943960000	-3.053848000
F	-2.442477000	2.302722000	-2.180001000
F	-0.759771000	1.939312000	-3.732056000
F	-2.198960000	3.746622000	-3.982599000
F	-0.617918000	3.740525000	-2.282551000

3·Br^- (-4234.2179 a. u.)

C	-0.830412000	-1.696887000	-0.851052000
C	0.554850000	-1.572991000	-1.056083000
C	1.389739000	-1.543527000	0.068830000
C	0.880427000	-1.606907000	1.372924000

C	-0.510429000	-1.729587000	1.536347000
C	-1.387915000	-1.725425000	0.438937000
P	1.633028000	1.568970000	0.075148000
C	0.426189000	1.266167000	-1.185975000
P	-1.298885000	1.173365000	-1.122340000
C	-1.834595000	1.109058000	0.533904000
P	-0.882384000	1.131568000	1.993394000
C	0.798828000	1.227460000	1.601306000
H	-0.928284000	-1.701647000	2.544881000
H	-1.498771000	-1.642709000	-1.712921000
C	0.977915000	0.612508000	-2.425869000
H	1.992046000	0.978643000	-2.646300000
H	0.338597000	0.844865000	-3.292263000
C	1.066318000	-1.020339000	-2.351602000
H	2.119379000	-1.299146000	-2.497332000
H	0.491086000	-1.418353000	-3.199885000
C	-3.090110000	0.281921000	0.689350000
H	-3.811969000	0.507181000	-0.111721000
H	-3.582825000	0.486333000	1.653480000
C	-2.827023000	-1.337996000	0.637044000
H	-3.443508000	-1.738478000	-0.180810000
H	-3.206244000	-1.757244000	1.580006000
C	1.658836000	0.545964000	2.632842000
H	1.278975000	0.759049000	3.644899000
H	2.697250000	0.905535000	2.579600000
C	1.714997000	-1.085131000	2.501596000
H	1.378005000	-1.503390000	3.460715000

H	2.768318000	-1.366550000	2.363286000
H	2.453500000	-1.333927000	-0.070664000
Br	1.759362000	4.101456000	0.100988000

3·Cl^- (-2072.0171 a. u.)

C	-0.849903000	-1.710881000	-0.847738000
C	0.534994000	-1.602765000	-1.065627000
C	1.380033000	-1.573842000	0.050985000
C	0.882810000	-1.634555000	1.358933000
C	-0.507945000	-1.742540000	1.536334000
C	-1.395732000	-1.729398000	0.447071000
P	1.649371000	1.595013000	0.055108000
C	0.439512000	1.244423000	-1.198991000
P	-1.284393000	1.156890000	-1.115602000
C	-1.808290000	1.112686000	0.546504000
P	-0.838172000	1.115193000	1.993950000
C	0.840040000	1.208451000	1.589810000
H	-0.914695000	-1.710885000	2.549180000
H	-1.524802000	-1.654448000	-1.704275000
C	0.981296000	0.573796000	-2.433987000
H	2.003576000	0.919163000	-2.651398000
H	0.350828000	0.819080000	-3.303410000
C	1.038886000	-1.060106000	-2.366738000
H	2.084470000	-1.358668000	-2.528359000
H	0.443866000	-1.445588000	-3.207259000
C	-3.071136000	0.297845000	0.712930000
H	-3.798425000	0.530476000	-0.080989000
H	-3.552471000	0.507094000	1.681444000

C	-2.828543000	-1.325418000	0.658111000
H	-3.456965000	-1.718896000	-0.154134000
H	-3.203647000	-1.740353000	1.604984000
C	1.704892000	0.506773000	2.603972000
H	1.345568000	0.726384000	3.621936000
H	2.748469000	0.849830000	2.534271000
C	1.734396000	-1.124512000	2.479714000
H	1.398145000	-1.534308000	3.443106000
H	2.781945000	-1.423752000	2.332686000
H	2.443454000	-1.370388000	-0.098779000
Cl	1.624517000	3.887594000	0.083045000

3·NO_3^- (-1890.2543 a. u.)

C	-0.917901000	-1.737204000	-0.750558000
C	0.461316000	-1.858195000	-0.991048000
C	1.329767000	-1.815011000	0.113228000
C	0.860924000	-1.556653000	1.413463000
C	-0.517603000	-1.395693000	1.599445000
C	-1.424377000	-1.474855000	0.535155000
P	2.012064000	0.967893000	-0.348645000
C	0.825513000	0.919291000	-1.622298000
P	-0.908824000	1.064901000	-1.504181000
C	-1.382456000	1.348677000	0.132966000
P	-0.404213000	1.791014000	1.545972000
C	1.249756000	1.267004000	1.175909000
H	-0.884623000	-1.080885000	2.580146000
H	-1.602989000	-1.723641000	-1.600991000
C	1.230966000	-0.026584000	-2.731123000

H	2.299731000	0.087188000	-2.971973000
H	0.657567000	0.170319000	-3.650413000
C	0.999739000	-1.611814000	-2.372604000
H	1.968354000	-2.116470000	-2.501558000
H	0.307410000	-2.016410000	-3.125005000
C	-2.739626000	0.775536000	0.440634000
H	-3.421531000	0.963179000	-0.403597000
H	-3.170847000	1.250207000	1.333551000
C	-2.770832000	-0.840688000	0.689694000
H	-3.491631000	-1.269597000	-0.020629000
H	-3.155659000	-1.007734000	1.705854000
C	1.989672000	0.612954000	2.314959000
H	1.684500000	1.046757000	3.278973000
H	3.072950000	0.778321000	2.201675000
C	1.797301000	-1.005996000	2.442302000
H	1.422124000	-1.212369000	3.455092000
H	2.790771000	-1.467313000	2.351164000
H	2.407186000	-1.863842000	-0.059193000
O	-0.774559000	5.688195000	1.360063000
O	-2.160635000	4.036741000	1.776543000
N	-1.060965000	4.494082000	1.450301000
O	-0.052261000	3.627395000	1.155360000

3·SO_4^{2-} (-2310.8644 a. u.)

C	-0.861493000	-1.883225000	-0.759217000
C	0.529781000	-1.972562000	-0.937452000
C	1.347880000	-1.819683000	0.194191000
C	0.818141000	-1.473794000	1.451482000

C	-0.571476000	-1.342768000	1.568156000
C	-1.430657000	-1.544573000	0.480894000
P	1.985265000	0.934584000	-0.597186000
C	0.758152000	0.775310000	-1.829077000
P	-0.975368000	0.906118000	-1.634674000
C	-1.381929000	1.277423000	-0.000251000
P	-0.370865000	1.924233000	1.350639000
C	1.271956000	1.312798000	0.928732000
H	-0.979896000	-0.924090000	2.491712000
H	-1.510317000	-1.937902000	-1.636031000
C	1.120647000	-0.263810000	-2.866386000
H	2.126050000	-0.096002000	-3.290765000
H	0.396443000	-0.233501000	-3.698667000
C	1.126049000	-1.806960000	-2.310537000
H	2.173550000	-2.144880000	-2.293707000
H	0.587034000	-2.422079000	-3.049894000
C	-2.714438000	0.704762000	0.421409000
H	-3.520081000	1.012983000	-0.266653000
H	-2.968011000	1.098541000	1.417317000
C	-2.793347000	-0.915994000	0.499160000
H	-3.373713000	-1.275627000	-0.364417000
H	-3.353259000	-1.177418000	1.411301000
C	2.069111000	0.735464000	2.065046000
H	1.955325000	1.331779000	2.983976000
H	3.139065000	0.723582000	1.792278000
C	1.688451000	-0.799297000	2.469207000
H	1.163204000	-0.767266000	3.434799000

H	2.636137000	-1.342266000	2.617898000
H	2.432053000	-1.825494000	0.062530000
O	-0.520374000	5.970881000	1.236907000
O	0.031441000	4.582715000	3.211891000
S	-0.783425000	4.737973000	1.993105000
O	-0.198826000	3.562395000	0.914384000
O	-2.211239000	4.419510000	2.174437000

3·PO_4^{3-} (-2247.4996 a. u.)

C	-0.989189000	-1.628269000	-0.641009000
C	0.369774000	-1.916112000	-0.860925000
C	1.251542000	-1.786270000	0.228653000
C	0.818036000	-1.314517000	1.481188000
C	-0.547221000	-1.028554000	1.651269000
C	-1.468650000	-1.157445000	0.595229000
P	2.246633000	0.844006000	-0.624105000
C	1.114516000	0.683970000	-1.950550000
P	-0.611473000	1.035392000	-1.910225000
C	-1.113755000	1.460587000	-0.324837000
P	-0.221407000	1.910968000	1.207400000
C	1.477485000	1.371636000	0.827089000
H	-0.874340000	-0.548121000	2.574238000
H	-1.665808000	-1.626796000	-1.500081000
C	1.440856000	-0.505545000	-2.828367000
H	2.538643000	-0.597668000	-2.938359000
H	1.017079000	-0.401420000	-3.847739000
C	0.906786000	-1.943765000	-2.275215000
H	1.739451000	-2.667654000	-2.363617000

H	0.106114000	-2.286663000	-2.953064000
C	-2.552861000	1.133853000	-0.029936000
H	-3.144906000	1.125947000	-0.965553000
H	-2.961774000	1.881360000	0.678664000
C	-2.729083000	-0.334560000	0.652714000
H	-3.563933000	-0.838732000	0.133716000
H	-3.021862000	-0.175493000	1.700630000
C	2.192954000	0.842051000	2.048283000
H	1.964509000	1.455742000	2.933595000
H	3.288567000	0.853622000	1.891288000
C	1.809507000	-0.700329000	2.432870000
H	1.403329000	-0.702610000	3.456881000
H	2.746813000	-1.284696000	2.440456000
H	2.322720000	-1.924063000	0.060693000
P	-1.416412000	4.344021000	2.355339000
O	-1.465015000	5.749226000	1.758808000
O	-2.675952000	3.477197000	2.151987000
O	-0.217444000	3.532439000	1.203683000
O	-0.732818000	4.201880000	3.717207000

1c·BF_4^- (-2506.7308 a. u.)

C	-0.602830000	-2.463508000	-1.140625000
C	0.349922000	-1.438113000	-1.241264000
C	1.033373000	-1.041839000	-0.081487000
C	0.690616000	-1.560746000	1.175671000
C	-0.266912000	-2.584534000	1.242148000
C	-0.962065000	-3.010300000	0.100460000
C	-0.912789000	0.962315000	0.293639000
C	-1.517507000	0.495558000	-0.892292000
C	-2.545706000	-0.475122000	-0.771877000
C	-2.856698000	-1.096668000	0.456990000
C	-2.206755000	-0.603172000	1.617346000
C	-1.182423000	0.365540000	1.552045000
H	-3.029938000	-0.839460000	-1.678901000
H	-2.428674000	-1.068348000	2.578683000
H	-0.610776000	-2.924239000	2.224037000
H	-1.209282000	-2.708401000	-2.018118000
C	-0.808460000	0.683238000	-2.199225000
H	-0.285360000	1.646591000	-2.211087000
H	-1.517214000	0.645415000	-3.037901000
C	0.302117000	-0.478737000	-2.406201000
H	1.269544000	0.026289000	-2.517869000
H	0.064990000	-1.011091000	-3.338593000
C	-3.472277000	-2.464051000	0.470983000
H	-4.217191000	-2.557835000	-0.330801000
H	-3.986814000	-2.646734000	1.424137000
C	-2.341395000	-3.603105000	0.265294000

H	-2.617453000	-4.195932000	-0.618332000
H	-2.373575000	-4.273034000	1.136288000
C	-0.140435000	0.428647000	2.628047000
H	-0.593837000	0.288450000	3.619060000
H	0.373747000	1.396188000	2.605869000
C	0.975159000	-0.722695000	2.399392000
H	1.003276000	-1.349717000	3.302320000
H	1.938959000	-0.211047000	2.292919000
H	-0.119373000	1.707353000	0.215718000
H	1.710137000	-0.186935000	-0.136651000
F	2.238831000	1.910570000	0.827873000
B	2.490260000	2.431541000	-0.484102000
F	1.267226000	2.957948000	-0.995558000
F	3.471274000	3.428306000	-0.428617000
F	2.912639000	1.359067000	-1.321716000
O	-2.732306000	4.062782000	1.200890000
C	-2.872158000	2.927822000	0.968721000
Cr	-3.132626000	1.147555000	0.618521000
C	-4.421927000	1.605032000	-0.587144000
O	-5.255261000	1.888176000	-1.360308000
C	-4.409644000	1.114601000	1.917430000
O	-5.232336000	1.083943000	2.752088000

1c·Br^- (-4656.5252 a. u.)

C	-0.689310000	-1.738688000	-1.194616000
C	0.673713000	-1.492991000	-1.419877000
C	1.561212000	-1.620004000	-0.340230000
C	1.097127000	-1.879011000	0.958589000

C	-0.269702000	-2.125712000	1.150384000
C	-1.183150000	-1.997349000	0.093616000
C	1.212751000	1.108240000	0.208052000
C	0.352150000	1.158779000	-0.910695000
C	-1.036760000	0.993517000	-0.672101000
C	-1.544912000	0.643331000	0.597184000
C	-0.641090000	0.614233000	1.688822000
C	0.748472000	0.757233000	1.502193000
H	-1.720068000	1.025982000	-1.522040000
H	-1.022763000	0.293653000	2.669422000
H	-0.665554000	-2.198078000	2.173771000
H	-1.399298000	-1.537896000	-2.003289000
C	0.903826000	0.942959000	-2.288622000
H	1.883252000	1.430237000	-2.389234000
H	0.237630000	1.379284000	-3.045350000
C	1.074791000	-0.636191000	-2.597524000
H	2.125230000	-0.813738000	-2.869392000
H	0.460412000	-0.877150000	-3.476771000
C	-2.843023000	-0.096303000	0.719933000
H	-3.585687000	0.293483000	0.009801000
H	-3.232037000	-0.010880000	1.742886000
C	-2.619050000	-1.672761000	0.432525000
H	-3.291894000	-1.967315000	-0.386211000
H	-2.913112000	-2.194800000	1.352857000
C	1.681842000	0.133224000	2.496441000
H	1.248177000	0.192578000	3.502166000
H	2.656358000	0.641097000	2.499987000

C	1.913432000	-1.429942000	2.148145000
H	1.627772000	-2.000800000	3.040767000
H	2.986657000	-1.582856000	1.962797000
H	2.285080000	1.229379000	0.047552000
H	2.606147000	-1.325736000	-0.481449000
Br	-1.935018000	-1.434246000	4.243909000
O	-1.689745000	4.553043000	-1.152923000
C	-1.165535000	3.794208000	-0.428703000
Cr	-0.343634000	2.610192000	0.685468000
C	-1.224832000	3.378480000	2.096967000
O	-1.781849000	3.895265000	2.982999000
C	1.003371000	3.815750000	0.913571000
O	1.873543000	4.589211000	1.051469000

1c·Cl^- (-2542.3412 a. u.)

C	-0.503745000	-1.827867000	-1.321354000
C	0.885817000	-1.992392000	-1.429238000
C	1.649992000	-1.991429000	-0.252357000
C	1.065915000	-1.726271000	0.996282000
C	-0.325468000	-1.571459000	1.073397000
C	-1.114671000	-1.558499000	-0.086947000
C	2.010171000	0.771121000	-0.558563000
C	1.234159000	0.687112000	-1.741227000
C	-0.151708000	0.943202000	-1.625582000
C	-0.785297000	1.118566000	-0.370357000
C	0.032744000	1.203880000	0.777258000
C	1.423630000	0.950873000	0.714973000
H	-0.769469000	0.882618000	-2.523046000

H	-0.462638000	1.277400000	1.759726000
H	-0.780013000	-1.221060000	2.013405000
H	-1.092017000	-1.718741000	-2.238236000
C	1.762199000	-0.061725000	-2.928513000
H	2.832265000	0.143318000	-3.069824000
H	1.241431000	0.252652000	-3.843346000
C	1.560992000	-1.655954000	-2.737967000
H	2.551092000	-2.130559000	-2.796144000
H	0.967527000	-2.024522000	-3.587009000
C	-2.235988000	0.783905000	-0.194693000
H	-2.829884000	1.132738000	-1.051282000
H	-2.613634000	1.237747000	0.730635000
C	-2.428648000	-0.814868000	-0.040359000
H	-3.100798000	-1.158364000	-0.840631000
H	-2.910526000	-0.966952000	0.934211000
C	2.122509000	0.451879000	1.944608000
H	1.707990000	0.938844000	2.835483000
H	3.200654000	0.659630000	1.896250000
C	1.906637000	-1.143560000	2.108661000
H	1.410037000	-1.301309000	3.074235000
H	2.898229000	-1.618552000	2.141253000
H	3.081967000	0.576879000	-0.623136000
H	2.741559000	-2.009458000	-0.334952000
Cl	-1.795679000	0.388435000	3.433598000
Cr	0.886052000	2.676721000	-0.707190000
C	2.475863000	3.486126000	-1.070615000
O	3.501595000	4.001779000	-1.312025000

C	0.112214000	3.708571000	-1.993710000
O	-0.380360000	4.368279000	-2.828687000
C	0.531245000	3.992776000	0.516867000
O	0.317479000	4.850136000	1.280246000

1c·SO_4^{2-} (-2781.3445 a. u.)

C	-0.888193000	-1.669964000	-0.786033000
C	0.474375000	-1.867908000	-1.127964000
C	1.437672000	-1.571356000	-0.138474000
C	1.089833000	-0.979720000	1.104451000
C	-0.277768000	-0.837947000	1.415849000
C	-1.278718000	-1.089229000	0.438461000
C	1.646043000	0.964360000	-1.291532000
C	0.653951000	0.615510000	-2.223626000
C	-0.687266000	0.876887000	-1.898484000
C	-1.051896000	1.387890000	-0.641400000
C	-0.035306000	1.754508000	0.257014000
C	1.311309000	1.477797000	-0.028213000
H	-1.470646000	0.494600000	-2.562939000
H	-0.311437000	2.068205000	1.272363000
H	-0.597287000	-0.369933000	2.362042000
H	-1.650548000	-1.869716000	-1.541004000
C	0.955666000	-0.471375000	-3.228915000
H	1.962865000	-0.343395000	-3.655602000
H	0.237358000	-0.435475000	-4.062543000
C	0.881030000	-1.945252000	-2.570480000
H	1.865662000	-2.426546000	-2.661013000
H	0.163453000	-2.552930000	-3.140674000

C	-2.423425000	1.138387000	-0.063008000
H	-3.206551000	1.264398000	-0.828079000
H	-2.581392000	1.828231000	0.787005000
C	-2.576958000	-0.352706000	0.559704000
H	-3.381928000	-0.881611000	0.026780000
H	-2.819826000	-0.212591000	1.626564000
C	2.251591000	1.298227000	1.140657000
H	2.011958000	2.025414000	1.927044000
H	3.299496000	1.411552000	0.817795000
C	2.092205000	-0.150011000	1.848092000
H	1.723554000	0.048465000	2.862571000
H	3.076857000	-0.641808000	1.874379000
H	2.678622000	0.648994000	-1.480875000
H	2.493550000	-1.694609000	-0.385132000
Cr	0.011960000	-3.022266000	0.752584000
C	-0.806301000	-4.410855000	-0.074106000
C	-0.728714000	-3.569918000	2.335319000
O	-1.188456000	-3.979346000	3.329698000
O	-1.325704000	-5.317389000	-0.621746000
O	2.344354000	-4.820315000	1.274276000
C	1.426417000	-4.106555000	1.079726000
O	-1.971814000	2.741774000	2.606479000
S	-1.384678000	1.803560000	3.638778000
O	-2.059231000	0.449726000	3.520635000
O	0.094895000	1.605912000	3.311118000
O	-1.537808000	2.358515000	5.009910000

2c·BF_4^- (-2566.3746 a. u.)

C	-0.592601000	-0.956677000	-1.065191000
C	1.729022000	-1.423952000	-0.568900000
C	1.505100000	-1.210941000	0.810141000
C	0.177482000	-0.947631000	1.225958000
C	-0.869076000	-0.722584000	0.303233000
N	2.333879000	1.263637000	-0.780429000
C	1.289229000	1.376946000	-1.626264000
N	0.039696000	1.697510000	-1.269487000
C	-0.178278000	1.833568000	0.056459000
N	0.793075000	1.705736000	0.986180000
C	2.007073000	1.385648000	0.522772000
H	-0.011755000	-0.761183000	2.282446000
H	-1.382962000	-0.776878000	-1.793055000
C	1.454586000	0.744861000	-2.985057000
H	2.492660000	0.856481000	-3.319053000
H	0.781006000	1.232808000	-3.698508000
C	1.095860000	-0.826112000	-2.932813000
H	1.969258000	-1.396663000	-3.274083000
H	0.270362000	-1.020825000	-3.628966000
C	-1.593522000	1.710538000	0.529775000
H	-2.256687000	2.204184000	-0.187401000
H	-1.696534000	2.220380000	1.492868000
C	-2.018299000	0.163481000	0.686606000
H	-2.888832000	-0.026103000	0.046142000
H	-2.316062000	-0.013182000	1.727768000
C	2.958107000	0.764245000	1.513901000
H	2.841531000	1.254299000	2.487014000

H	3.988784000	0.882677000	1.159876000
C	2.652706000	-0.809074000	1.690961000
H	2.420595000	-1.004420000	2.745463000
H	3.558031000	-1.373295000	1.432504000
H	2.746799000	-1.609629000	-0.910819000
C	-0.335831000	-3.687996000	1.524804000
C	1.201522000	-4.161688000	-0.464757000
C	-1.277461000	-3.668007000	-0.857169000
O	-0.600362000	-4.260985000	2.509168000
O	-2.146842000	-4.228640000	-1.402149000
O	1.922681000	-5.035563000	-0.757716000
C	0.714756000	-1.219198000	-1.534669000
Cr	0.083511000	-2.796203000	-0.010613000
B	-1.766283000	5.009501000	0.595896000
F	-2.781734000	4.539845000	-0.283985000
F	-1.724122000	6.416000000	0.587309000
F	-2.029170000	4.531142000	1.910890000
F	-0.504045000	4.487369000	0.161117000

2c·Br^- (-4765.8674 a. u.)

C	-1.006304000	-1.648484000	-0.758802000
C	1.332286000	-1.519415000	-0.157141000
C	1.005798000	-1.464053000	1.216089000
C	-0.354844000	-1.600859000	1.569469000
C	-1.385484000	-1.612199000	0.601641000
N	1.175687000	1.193051000	-0.168479000
C	0.183453000	1.121518000	-1.047728000
N	-1.140697000	1.137161000	-0.754685000

C	-1.395663000	1.045614000	0.574356000
N	-0.493359000	1.112828000	1.545899000
C	0.810248000	1.269823000	1.150740000
H	-0.628021000	-1.549239000	2.622467000
H	-1.785718000	-1.632552000	-1.519839000
C	0.547637000	0.652138000	-2.438181000
H	1.515564000	1.081116000	-2.722753000
H	-0.222713000	0.984777000	-3.144525000
C	0.656532000	-0.949405000	-2.512810000
H	1.672087000	-1.224825000	-2.825692000
H	-0.043404000	-1.322550000	-3.272049000
C	-2.751587000	0.492925000	0.951496000
H	-3.496660000	0.833351000	0.222082000
H	-3.023885000	0.855380000	1.949660000
C	-2.750574000	-1.113832000	0.973387000
H	-3.505863000	-1.483810000	0.267534000
H	-3.030265000	-1.457968000	1.977642000
C	1.845777000	0.767960000	2.135490000
H	1.578996000	1.134781000	3.131025000
H	2.816021000	1.189657000	1.856819000
C	1.964461000	-0.835995000	2.182200000
H	1.755345000	-1.175476000	3.205511000
H	2.996921000	-1.120389000	1.938651000
H	2.374830000	-1.403937000	-0.450150000
C	-0.225701000	-4.401751000	1.663063000
C	1.561086000	-4.315519000	-0.164431000
C	-0.915238000	-4.454606000	-0.800701000

O	-0.424262000	-5.093343000	2.587266000
O	-1.557279000	-5.180409000	-1.459321000
O	2.512372000	-4.951415000	-0.414549000
C	0.341491000	-1.529141000	-1.165678000
Cr	0.081627000	-3.327090000	0.225002000
Br	1.268903000	3.834980000	1.714636000

2c·Cl^- (-2603.6635 a. u.)

C	-1.104575000	-0.450722000	-1.105564000
C	1.233170000	-0.323955000	-0.502570000
C	0.905367000	-0.271511000	0.869469000
C	-0.454675000	-0.407491000	1.222638000
C	-1.484114000	-0.419195000	0.254456000
N	1.089873000	2.387179000	-0.504222000
C	0.097593000	2.316091000	-1.377623000
N	-1.229028000	2.336276000	-1.087641000
C	-1.480761000	2.238172000	0.243334000
N	-0.584495000	2.304689000	1.215378000
C	0.726353000	2.494352000	0.823903000
H	-0.727721000	-0.356968000	2.275628000
H	-1.883735000	-0.432434000	-1.866742000
C	0.457775000	1.847937000	-2.771747000
H	1.426883000	2.274534000	-3.056681000
H	-0.312641000	2.188259000	-3.474668000
C	0.559898000	0.247920000	-2.856688000
H	1.573955000	-0.031681000	-3.171210000
H	-0.142291000	-0.119995000	-3.616562000
C	-2.839972000	1.684718000	0.615614000

H	-3.582542000	2.034492000	-0.112241000
H	-3.112228000	2.041654000	1.615994000
C	-2.848586000	0.079254000	0.626728000
H	-3.603184000	-0.284154000	-0.083417000
H	-3.131439000	-0.271567000	1.627935000
C	1.756975000	1.949514000	1.800724000
H	1.495436000	2.311853000	2.799678000
H	2.730817000	2.365303000	1.524334000
C	1.864977000	0.349522000	1.838871000
H	1.652547000	0.003729000	2.859656000
H	2.895863000	0.057773000	1.596135000
H	2.275778000	-0.207848000	-0.794786000
C	-0.319908000	-3.211890000	1.313319000
C	1.462715000	-3.121597000	-0.516367000
C	-1.013928000	-3.259706000	-1.150473000
O	-0.515773000	-3.905805000	2.237158000
O	-1.655377000	-3.984114000	-1.812181000
O	2.414434000	-3.756462000	-0.770313000
C	0.243136000	-0.333904000	-1.511325000
Cr	-0.016185000	-2.135728000	-0.123095000
Cl	1.116526000	4.761884000	1.312411000

2c·NO_3^- (-2410.6880 a. u.)

C	-0.996212000	-1.198275000	-1.044949000
C	1.317765000	-0.837862000	-0.435989000
C	0.956833000	-0.609306000	0.912946000
C	-0.400856000	-0.779960000	1.261914000
C	-1.407848000	-0.990443000	0.290177000

N	0.979239000	1.840858000	-0.915561000
C	-0.013834000	1.567780000	-1.760342000
N	-1.327981000	1.520508000	-1.443858000
C	-1.571022000	1.630668000	-0.116521000
N	-0.660223000	1.889296000	0.819629000
C	0.623976000	2.021059000	0.387339000
H	-0.699389000	-0.592503000	2.292532000
H	-1.758320000	-1.338051000	-1.810920000
C	0.377081000	0.914266000	-3.065237000
H	1.288309000	1.383623000	-3.454365000
H	-0.437807000	1.035641000	-3.788811000
C	0.660124000	-0.656804000	-2.862771000
H	1.712631000	-0.862055000	-3.096642000
H	0.040285000	-1.221705000	-3.571592000
C	-2.889087000	1.071670000	0.365873000
H	-3.674396000	1.291054000	-0.367641000
H	-3.142350000	1.533515000	1.326933000
C	-2.807375000	-0.523239000	0.565856000
H	-3.517128000	-1.006609000	-0.118062000
H	-3.108196000	-0.765773000	1.593318000
C	1.704579000	1.772071000	1.404494000
H	1.481809000	2.372586000	2.294945000
H	2.651158000	2.115766000	0.973817000
C	1.841819000	0.222363000	1.796111000
H	1.555797000	0.089880000	2.847703000
H	2.894549000	-0.073667000	1.693329000
H	2.357269000	-0.696584000	-0.729502000

C	-0.181648000	-3.548867000	1.728957000
C	1.730723000	-3.580810000	0.027348000
C	-0.676363000	-3.972960000	-0.748660000
O	-0.407135000	-4.128240000	2.720480000
O	-1.217647000	-4.822417000	-1.345959000
O	2.730853000	-4.180814000	-0.072058000
C	0.352280000	-1.049825000	-1.446657000
Cr	0.168796000	-2.648926000	0.179457000
N	0.745818000	5.037391000	1.462329000
O	0.544737000	6.264175000	1.328374000
O	0.840788000	4.500574000	2.597657000
O	0.862764000	4.313026000	0.396838000

2c·SO_4^{2-} (-2842.5146 a. u.)

C	1.341956000	-1.297333000	0.068725000
C	0.966580000	-1.612097000	1.392203000
C	-0.407230000	-1.776863000	1.663681000
C	-1.396118000	-1.582350000	0.676481000
N	1.219740000	1.332837000	0.653971000
C	0.224471000	1.787980000	-0.314909000
N	-1.140160000	1.351107000	-0.045107000
C	-0.967788000	-1.265742000	-0.629897000
C	-1.408428000	1.009044000	1.185928000
N	-0.538944000	0.904341000	2.242020000
C	0.764972000	0.987053000	1.829921000
H	-0.719632000	-1.978145000	2.687283000
H	-1.716278000	-1.062476000	-1.393467000
C	0.647254000	1.349657000	-1.743503000

H	1.617524000	1.822873000	-1.928564000
H	-0.076295000	1.814949000	-2.422612000
C	0.755172000	-0.190021000	-2.105490000
H	1.782215000	-0.413285000	-2.429579000
H	0.091698000	-0.405116000	-2.955878000
C	-2.770450000	0.373113000	1.427613000
H	-3.511333000	0.867036000	0.786209000
H	-3.046538000	0.515644000	2.481504000
C	-2.778864000	-1.192678000	1.100681000
H	-3.501973000	-1.398395000	0.299143000
H	-3.090085000	-1.761170000	1.988909000
C	1.763225000	0.323409000	2.769167000
H	1.437694000	0.487452000	3.805712000
H	2.749363000	0.781828000	2.620441000
C	1.890808000	-1.250430000	2.513980000
H	1.628054000	-1.802644000	3.427636000
H	2.930172000	-1.499875000	2.257913000
H	2.392925000	-1.118041000	-0.150588000
C	-0.284684000	-4.561199000	1.061913000
C	1.592789000	-4.053400000	-0.591303000
C	-0.826172000	-4.013784000	-1.373268000
O	-0.529832000	-5.466861000	1.775952000
O	-1.420182000	-4.567919000	-2.226183000
O	2.558445000	-4.631412000	-0.939738000
C	0.391066000	-1.059086000	-0.943361000
Cr	0.097218000	-3.183532000	-0.053178000
O	-0.058926000	5.597719000	-0.705955000

S	0.133302000	4.356205000	-1.466405000
O	-1.024791000	3.946788000	-2.282910000
O	0.252550000	3.252508000	-0.190785000
O	1.420710000	4.277792000	-2.185337000

2c·PO_4^{3-} (-2785.1633 a. u.)

C	-0.784077000	-1.478391000	-0.810448000
C	1.506388000	-1.852525000	-0.133520000
C	1.145934000	-1.768964000	1.226477000
C	-0.217141000	-1.546780000	1.535069000
C	-1.187585000	-1.331474000	0.533962000
N	1.938263000	0.821390000	-0.172016000
C	0.908169000	0.914160000	-1.081744000
N	-0.345374000	1.189622000	-0.862451000
C	-0.716163000	1.595206000	0.518499000
N	0.257327000	1.115806000	1.534920000
C	1.461297000	0.846089000	1.120280000
H	-0.505847000	-1.412526000	2.575859000
H	-1.515310000	-1.291452000	-1.594643000
C	1.245532000	0.343135000	-2.456199000
H	2.294941000	0.576083000	-2.696478000
H	0.588504000	0.811419000	-3.202223000
C	1.043465000	-1.240129000	-2.515800000
H	1.991438000	-1.735747000	-2.778888000
H	0.307860000	-1.493065000	-3.295328000
C	-2.123026000	1.014596000	0.857265000
H	-2.804490000	1.519696000	0.155886000
H	-2.357748000	1.430730000	1.847898000

C	-2.416939000	-0.541497000	0.851343000
H	-3.199678000	-0.765107000	0.108280000
H	-2.809257000	-0.842618000	1.836434000
C	2.399418000	0.200820000	2.136689000
H	2.205673000	0.638677000	3.125912000
H	3.441113000	0.406363000	1.844119000
C	2.191399000	-1.380057000	2.226719000
H	1.872695000	-1.657055000	3.243563000
H	3.140300000	-1.901048000	2.021424000
H	2.557109000	-1.979650000	-0.391731000
C	-0.790634000	-4.371165000	1.650629000
C	1.010287000	-4.735490000	-0.105148000
C	-1.391516000	-4.291171000	-0.810949000
O	-1.181529000	-5.021641000	2.561713000
O	-2.167305000	-4.889683000	-1.478693000
O	1.780108000	-5.614045000	-0.321358000
C	0.566084000	-1.698382000	-1.171717000
Cr	-0.196220000	-3.430113000	0.230517000
P	-2.110869000	4.059451000	0.951631000
O	-3.168920000	3.734192000	-0.116998000
O	-2.522094000	3.668290000	2.380911000
O	-0.726998000	2.993614000	0.564022000
O	-1.436047000	5.423016000	0.811549000

3c·BF_4^- (-3430.0241 a. u.)

C	-0.548045000	-0.967574000	-0.962921000
C	0.841291000	-1.129916000	-1.138709000
C	1.615871000	-1.467182000	0.006743000

C	1.054626000	-1.549045000	1.298816000
C	-0.354501000	-1.386136000	1.415758000
C	-1.169754000	-1.050476000	0.313479000
P	2.504140000	1.254943000	0.425538000
C	1.371430000	1.579658000	-0.855750000
P	-0.334907000	1.961499000	-0.857454000
C	-0.901806000	1.666063000	0.772180000
P	-0.068315000	1.365994000	2.265062000
C	1.621836000	1.108571000	1.918772000
H	-0.812115000	-1.472480000	2.400050000
H	-1.161560000	-0.719998000	-1.828077000
C	1.837914000	1.013752000	-2.182932000
H	2.926784000	1.130888000	-2.292425000
H	1.353610000	1.536119000	-3.020278000
C	1.511398000	-0.570873000	-2.354348000
H	2.454947000	-1.096428000	-2.550966000
H	0.865404000	-0.692975000	-3.233043000
C	-2.340379000	1.199289000	0.808458000
H	-2.932402000	1.741304000	0.058945000
H	-2.781955000	1.394435000	1.796994000
C	-2.498348000	-0.396659000	0.529719000
H	-3.136942000	-0.525561000	-0.353270000
H	-3.012006000	-0.845686000	1.389635000
C	2.261473000	0.126057000	2.880091000
H	1.906205000	0.294515000	3.907967000
H	3.357108000	0.229174000	2.877895000
C	1.930369000	-1.425366000	2.508976000

H	1.444376000	-1.886592000	3.378577000
H	2.882648000	-1.944693000	2.339426000
H	2.687781000	-1.617818000	-0.111109000
Cr	-0.024949000	-2.969175000	-0.117800000
C	-0.322378000	-4.219212000	1.176930000
C	-1.377086000	-3.700670000	-1.102071000
C	1.147191000	-4.114319000	-0.919743000
O	1.902013000	-4.846597000	-1.433252000
O	-0.509741000	-5.017883000	2.011719000
O	-2.244803000	-4.169365000	-1.730702000
B	-1.518494000	4.937378000	-1.138529000
F	-2.575157000	4.112208000	-0.680069000
F	-1.495657000	4.978951000	-2.539193000
F	-1.601190000	6.216297000	-0.579805000
F	-0.255474000	4.329623000	-0.679808000

3c·Br^- (-5629.5375 a. u.)

C	-0.887548000	-1.484048000	-0.872308000
C	0.504340000	-1.398318000	-1.086137000
C	1.350624000	-1.399591000	0.053302000
C	0.845047000	-1.442988000	1.364141000
C	-0.567240000	-1.530136000	1.529387000
C	-1.452526000	-1.496591000	0.433926000
P	1.664883000	1.683735000	0.103675000
C	0.469761000	1.382629000	-1.174509000
P	-1.258283000	1.344288000	-1.133213000
C	-1.812259000	1.281658000	0.517381000
P	-0.881169000	1.279856000	1.991736000

C	0.806233000	1.323872000	1.617779000
H	-0.976682000	-1.576351000	2.536550000
H	-1.553441000	-1.495534000	-1.732868000
C	1.033904000	0.729386000	-2.418481000
H	2.071082000	1.054718000	-2.588433000
H	0.443122000	1.022043000	-3.300473000
C	1.036019000	-0.895422000	-2.388592000
H	2.064043000	-1.247211000	-2.546292000
H	0.422680000	-1.262224000	-3.222349000
C	-3.106215000	0.495976000	0.649951000
H	-3.790698000	0.734553000	-0.179032000
H	-3.624388000	0.737492000	1.591239000
C	-2.890038000	-1.118915000	0.636698000
H	-3.511545000	-1.544436000	-0.162638000
H	-3.249530000	-1.522923000	1.592400000
C	1.647124000	0.620441000	2.661762000
H	1.242843000	0.824158000	3.666012000
H	2.685504000	0.982633000	2.638786000
C	1.703776000	-0.994029000	2.501675000
H	1.373653000	-1.451435000	3.443693000
H	2.745670000	-1.293884000	2.329375000
H	2.426768000	-1.311864000	-0.091901000
Cr	0.048338000	-3.216600000	0.187895000
C	0.173702000	-4.311298000	1.638739000
C	-1.227718000	-4.314196000	-0.508358000
C	1.329041000	-4.206604000	-0.646266000
O	2.151596000	-4.843418000	-1.186066000

O	0.259612000	-5.014560000	2.572503000
O	-2.052222000	-5.018434000	-0.953964000
Br	1.768479000	4.160710000	0.152776000

3c·Cl^- (-3467.3380 a. u.)

C	-0.896248000	-1.481887000	-0.869345000
C	0.495508000	-1.400306000	-1.089365000
C	1.345255000	-1.395034000	0.046478000
C	0.845255000	-1.439912000	1.358747000
C	-0.566436000	-1.523463000	1.530209000
C	-1.456658000	-1.489509000	0.438192000
P	1.664973000	1.748657000	0.100951000
C	0.479097000	1.387989000	-1.177851000
P	-1.248825000	1.339110000	-1.130773000
C	-1.801670000	1.293033000	0.521622000
P	-0.862612000	1.279901000	1.990642000
C	0.823951000	1.334383000	1.615844000
H	-0.971164000	-1.570526000	2.539113000
H	-1.564716000	-1.495795000	-1.727805000
C	1.048616000	0.721561000	-2.412559000
H	2.094355000	1.027912000	-2.564969000
H	0.478071000	1.027256000	-3.303404000
C	1.021074000	-0.902367000	-2.394386000
H	2.040803000	-1.271092000	-2.567490000
H	0.389528000	-1.254053000	-3.220931000
C	-3.097596000	0.511894000	0.664456000
H	-3.790828000	0.754593000	-0.155763000
H	-3.603593000	0.753179000	1.612018000

C	-2.891571000	-1.105100000	0.644660000
H	-3.515742000	-1.523227000	-0.156663000
H	-3.252955000	-1.510901000	1.599123000
C	1.667541000	0.617450000	2.648597000
H	1.271881000	0.822800000	3.655737000
H	2.708850000	0.971941000	2.619195000
C	1.711454000	-0.996827000	2.491985000
H	1.381209000	-1.450609000	3.435934000
H	2.750234000	-1.305161000	2.314808000
H	2.420653000	-1.305331000	-0.103254000
Cr	0.047304000	-3.214781000	0.187733000
C	0.137327000	-4.308894000	1.642060000
C	-1.207686000	-4.314443000	-0.543496000
C	1.350966000	-4.200772000	-0.613515000
O	2.190066000	-4.833517000	-1.132768000
O	0.199908000	-5.011383000	2.578419000
O	-2.017515000	-5.020524000	-1.012812000
Cl	1.608279000	4.000898000	0.160126000

3c·NO_3^- (-3285.5738 a. u.)

C	-0.940488000	-1.349883000	-0.868836000
C	0.419975000	-1.083319000	-1.133656000
C	1.297234000	-0.946269000	-0.026734000
C	0.849875000	-1.047483000	1.301080000
C	-0.531423000	-1.321262000	1.519943000
C	-1.451807000	-1.420433000	0.457146000
P	1.175487000	2.233708000	0.004599000
C	0.039782000	1.687855000	-1.249437000

P	-1.661227000	1.385087000	-1.147376000
C	-2.160015000	1.293276000	0.519014000
P	-1.187522000	1.411678000	1.963078000
C	0.463769000	1.702871000	1.547414000
H	-0.893000000	-1.414109000	2.541929000
H	-1.626831000	-1.465409000	-1.705124000
C	0.673233000	1.075724000	-2.482669000
H	1.675876000	1.499309000	-2.642808000
H	0.068579000	1.310258000	-3.372592000
C	0.830959000	-0.539033000	-2.460669000
H	1.877985000	-0.789726000	-2.677213000
H	0.209818000	-0.968361000	-3.257787000
C	-3.336823000	0.347700000	0.702822000
H	-4.070042000	0.480001000	-0.107524000
H	-3.854189000	0.537880000	1.655712000
C	-2.917401000	-1.228045000	0.708215000
H	-3.507755000	-1.745082000	-0.060293000
H	-3.187399000	-1.654012000	1.683750000
C	1.433711000	1.113487000	2.548205000
H	1.054863000	1.279588000	3.568604000
H	2.412861000	1.607324000	2.471320000
C	1.682899000	-0.481937000	2.404137000
H	1.442840000	-0.965121000	3.360513000
H	2.747730000	-0.653061000	2.198365000
H	2.345267000	-0.712740000	-0.212381000
Cr	0.262384000	-2.924860000	0.167219000
C	0.617891000	-3.969906000	1.617914000

C	-0.884618000	-4.199176000	-0.450136000
C	1.620841000	-3.739343000	-0.731565000
O	2.493644000	-4.260877000	-1.314154000
O	0.850569000	-4.639527000	2.550942000
O	-1.625163000	-5.017158000	-0.845580000
N	1.293752000	4.883863000	0.746580000
O	0.586956000	4.009928000	-0.045093000
O	0.993497000	6.065380000	0.612466000
O	2.146122000	4.425364000	1.509468000

3c·SO_4^{2-} (-3689.4120 a. u.)

C	-0.775835000	-1.207349000	-0.754219000
C	0.608188000	-1.297060000	-0.975326000
C	1.441017000	-1.605810000	0.138560000
C	0.925027000	-1.759258000	1.440300000
C	-0.484665000	-1.686925000	1.602566000
C	-1.351561000	-1.387251000	0.528781000
P	2.186643000	1.106606000	0.648883000
C	1.039347000	1.421815000	-0.601431000
P	-0.690828000	1.927922000	-0.534791000
C	-1.217066000	1.334294000	1.086288000
P	-0.326468000	1.017065000	2.529599000
C	1.383399000	0.910877000	2.187053000
H	-0.907349000	-1.831450000	2.594426000
H	-1.423002000	-0.928726000	-1.584211000
C	1.502869000	0.897341000	-1.943056000
H	2.595391000	1.018221000	-2.031213000
H	1.029767000	1.453211000	-2.765594000

C	1.197322000	-0.677014000	-2.199974000
H	2.134565000	-1.177430000	-2.481843000
H	0.495677000	-0.769936000	-3.039553000
C	-2.613942000	0.756509000	1.130539000
H	-3.267364000	1.279812000	0.418114000
H	-3.039365000	0.880125000	2.139871000
C	-2.711449000	-0.834154000	0.796106000
H	-3.359336000	-0.971610000	-0.079840000
H	-3.177791000	-1.346151000	1.649489000
C	2.080739000	-0.103749000	3.075882000
H	1.732693000	-0.015691000	4.118610000
H	3.172784000	0.049937000	3.073941000
C	1.832156000	-1.651092000	2.632318000
H	1.399750000	-2.196931000	3.483250000
H	2.803693000	-2.109972000	2.399067000
H	2.514340000	-1.689844000	-0.016370000
Cr	-0.124423000	-3.240703000	-0.004208000
C	-0.231153000	-4.546157000	1.256145000
C	-1.494153000	-4.029171000	-0.902185000
C	1.051373000	-4.264131000	-0.939901000
O	1.805083000	-4.934705000	-1.546562000
O	-0.295570000	-5.398304000	2.066362000
O	-2.376378000	-4.552831000	-1.477603000
O	-1.127878000	5.934657000	-0.645258000
S	-1.475801000	4.632516000	-1.225190000
O	-2.865363000	4.201719000	-0.996831000
O	-0.533440000	3.587450000	-0.256118000

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O       -0.988671000      4.413360000     -2.596572000
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References

(1) Gilli, G. *The nature of the hydrogen bond : outline of a comprehensive hydrogen bond theory*; Oxford University Press: Oxford New York, 2009.