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Supporting Information for

How the Electron-Deficient Cavity of Heterocalixarenes Recognizes Anions. Insights from Computation

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Contents

1. Comparison between the x-ray and calculated structures

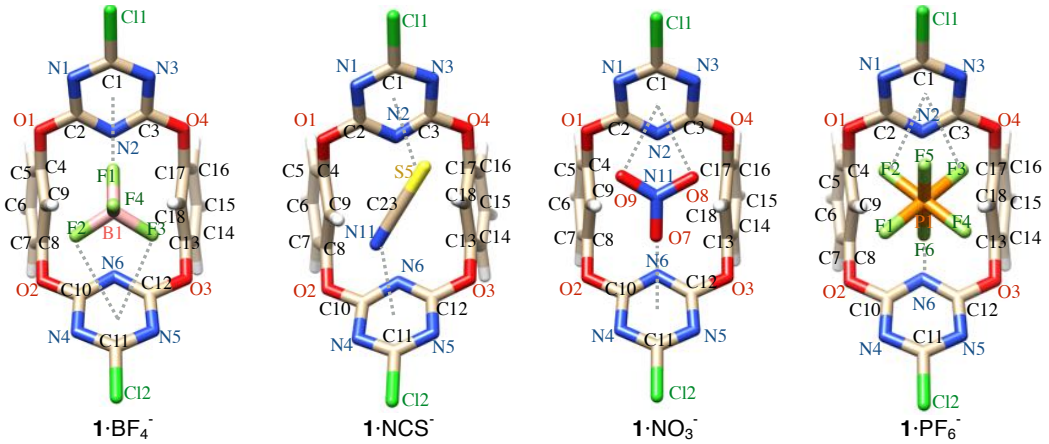


Figure S1. Minima structures of **1** which x-ray data are available.[1] Selected calculated by us at BP86-D3, {by others at wB97XD/*RI-MP2*}[2] and (Experimental)[1] bond lengths, in Å.

1·BF_4^-: 3.014, {2.969/*2.911*} (2.855) [F(1)···triazine(1) centroid], 3.333 (3.106) [F(2)···triazine (2) centroid], 3.342 [F(3)···triazine (2) centroid], 8.926 {8.789/*8.677*} (8.613) [C(1)···C(11)], 4.646 {4.602/*4.623*} (4.648) [N(2)···N(6)], 4.333 {4.338/*4.354*} (4.320) [C(9)···C(18)], 5.632 {5.722/*5.299*} (5.206) [C(6)···C(15)], 3.464 (3.581) [F(1)···C(9)], 3.073 (3.447) [F(3)···C(18)].

1·NCS^-: 3.042 (3.050) {2.991/*2.766*} [N(11)···triazine(2) centroid], 3.376 {3.460/*3.227*} (3.643) [S(5)···triazine(1) centroid], 3.553 [S(5)···N(2)], 3.041 [N(11)···N(6)], 3.525 (3.962) [C(23)···C(18)], 3.623 (3.916) [C(23)···C(9)], 8.847 {8.908/*8.782*} (9.055) [C(1)···C(11)], 4.633 {4.641/*4.678*} (4.688) [N(2)···N(6)], 4.311 {4.339/*4.343*} (4.406) [C(9)···C(18)], 5.749 {5.644/*5.245*} (4.870) [C(6)···C(15)].

1·NO_3^-: 3.306 [O(8)···triazine(1) centroid], 3.249 [O(9)···triazine(1) centroid], 3.074 {3.085/*2.926*} (3.084) [O(7)···triazine(2) centroid], 2.967 (3.243) [O(8)···C(3)], 2.926 [O(9)···C(2)], 8.977 {8.837/*8.680*} (8.964) [C(1)···C(11)], 4.657 {4.608/*4.618*} (4.668) [N(2)···N(6)], 5.393 {5.456/*5.081*} (4.569) [C(6)···C(15)]. 4.397 {4.410/*4.409*} (4.440) [C(9)···C(18)],

1·PF_6^-: 3.257 [F(2)···triazine centroid], 3.245 [F(3)···triazine centroid], 3.174 (3.216) [F(2)···C(9)], 3.169 [F(3)···C(18)], 9.001 {9.092/*8.255*} (8.475) [C(1)···C(11)], 4.659 {4.568/*4.495*} (4.639) [N(2)···N(6)], 4.341 {4.344/*4.570*} (4.478) [C(9)···C(18)], 5.598 {5.644/*4.712*} (4.653) [C(6)···C(15)].

2. Energy diagram of isomers of heterocalixarene 2

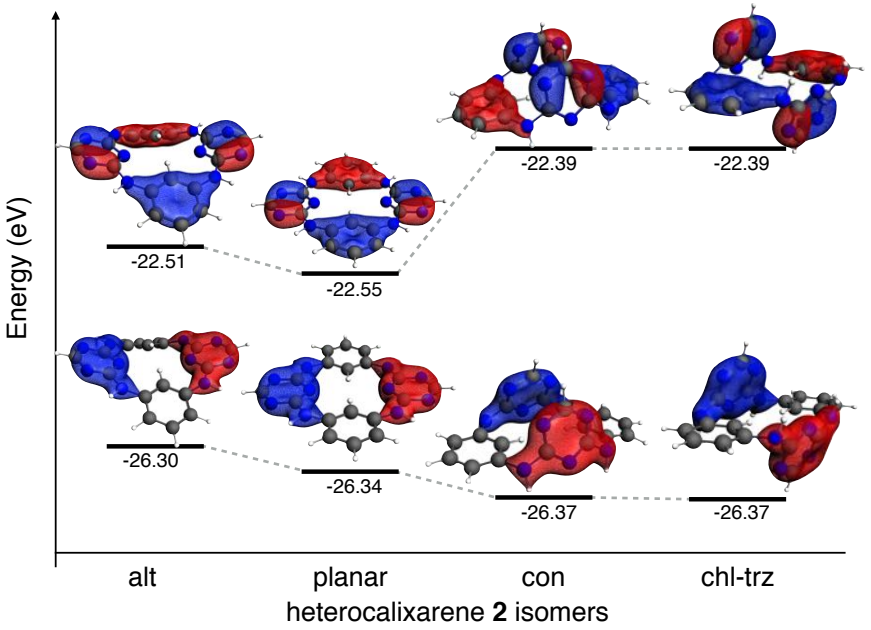
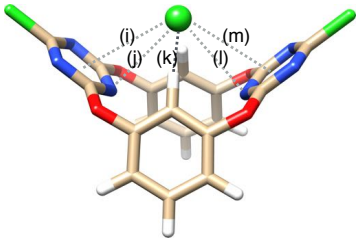


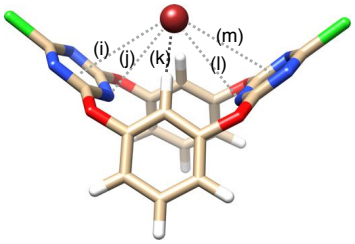
Figure S2. Energy diagram of selected molecular obitals involving aromatic stabilization of bridging N(H)- atoms for heteracalixarene **2** conformers. The lowers in energy are involved with the triazine units, whereas the highest in energy are involved with the arene units. The scale are qualitative in order to see the trends inside the same orbitals.

3. Optimized host-guest complex structures



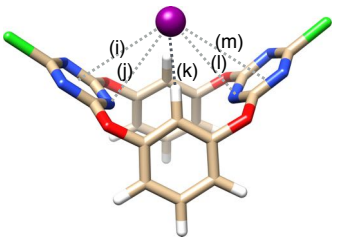
(i)=3.750, (j)=3.482, (k)=2.264, (l)=3.493, (m)=3.782

1·Cl^-



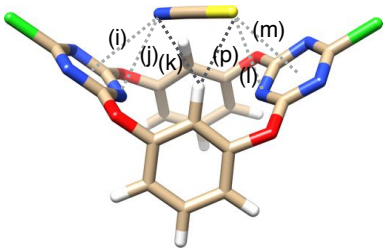
(i)=3.858, (j)=3.614, (k)=2.410, (l)=3.620, (m)=3.881

1·Br^-



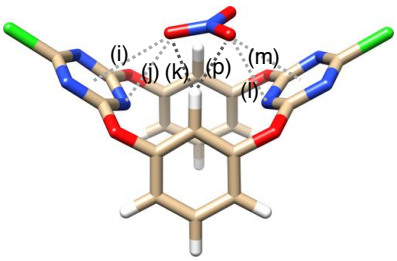
(i)=3.994, (j)=3.816, (k)=2.674, (l)=3.831, (m)=4.034

1·I^-



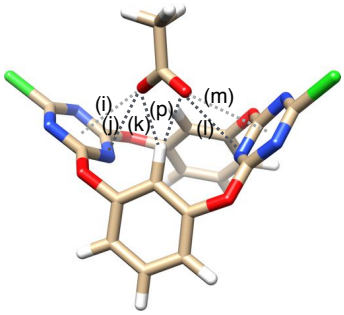
(i)=3.042, (j)=3.049, (k)=3.155, (l)=3.553, (m)=3.376, (p)=2.549

1·NCS^-



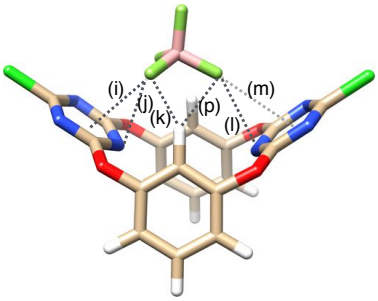
(i)=3.074, (j)=2.894, (k)=2.508, (l)=3.204, (m)=3.306, (p)=2.093

1·NO_3^-



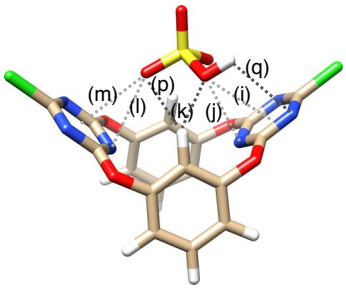
(i)=2.930, (j)=3.051, (k)=2.585, (l)=2.893, (m)=2.961, (p)=1.910

1·$CH_3CO_2^-$



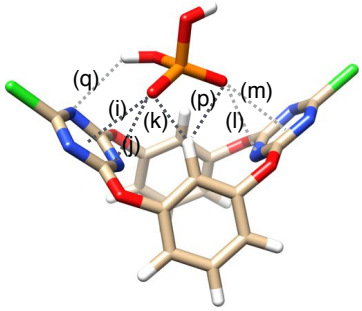
(i)=3.342, (j)=3.276, (k)=2.070, (l)=2.945, (m)=3.014, (p)=2.582

1·BF_4^-



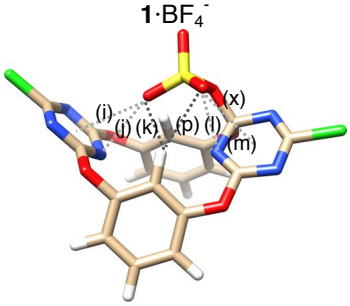
(i)=3.059, (j)=3.528, (k)=2.115, (l)=2.955, (m)=2.950, (p)=2.937, (q)=3.130

1·HSO_4^-



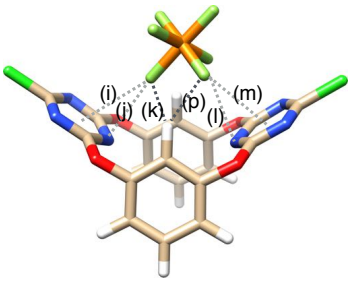
(i)=2.855, (j)=3.029, (k)=1.998, (l)=2.900, (m)=2.812, (p)=2.627, (q)=2.627

1·$H_2PO_4^-$



(x)=1.417, (i)=3.200, (j)=3.013, (k)=2.330, (l)=2.943, (m)=3.133, (p)=2.736

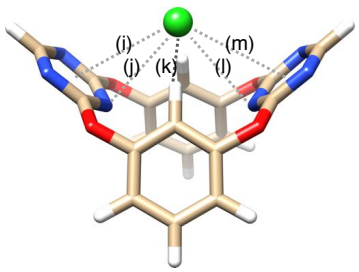
1·SO_4^{2-}



(i)=3.135, (j)=2.898, (k)=2.392, (l)=3.236, (m)=3.246, (p)=2.202

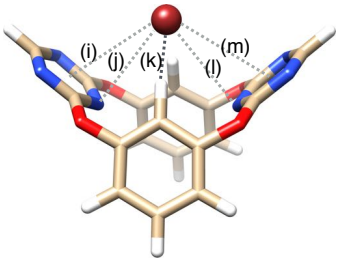
1·PF_6^-

Figure S3. Optimized structures for complexes of **1**, including selected geometrical parameters. Bond lengths are shown in Å.



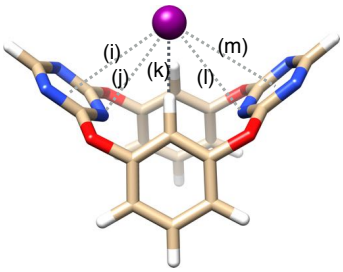
(i)=3.751, (j)=3.504, (k)=2.281,
(l)=3.506, (m)=3.753

2·Cl^-



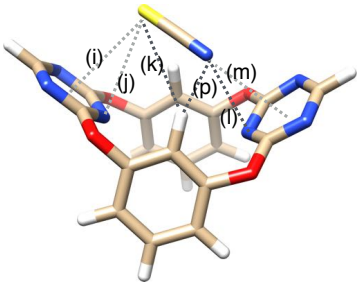
(i)=3.849, (j)=3.641, (k)=2.446,
(l)=3.642, (m)=3.849

2·Br^-



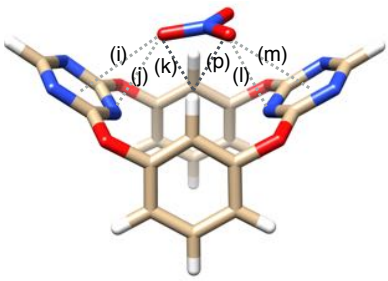
(i)=4.023, (j)=3.855, (k)=2.691,
(l)=3.845, (m)=4.007

2·I^-



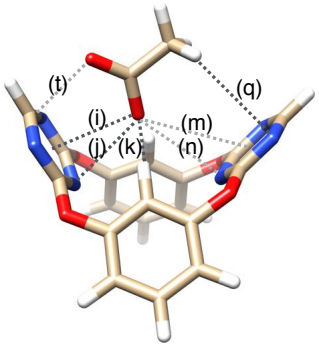
(i)=3.490, (j)=3.651, (k)=4.046,
(l)=3.109, (m)=3.135, (p)=2.075

2·NCS^-



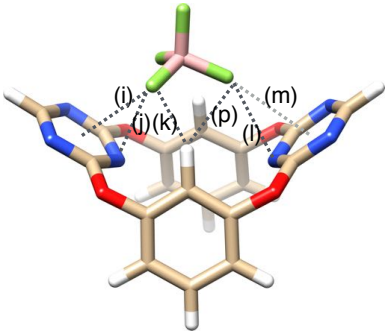
(i)=3.079, (j)=2.921, (k)=2.536,
(l)=3.224, (m)=3.333, (p)=2.109

2·NO_3^-



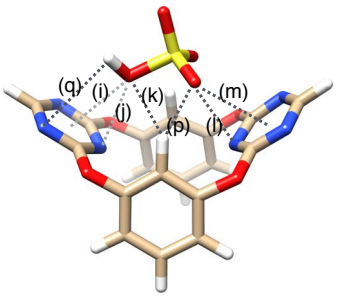
(i)=2.908, (j)=3.025, (k)=1.960,
(m)=3.723, (n)=3.327,
(q)=3.412, (t)=2.595

2·$CH_3CO_2^-$



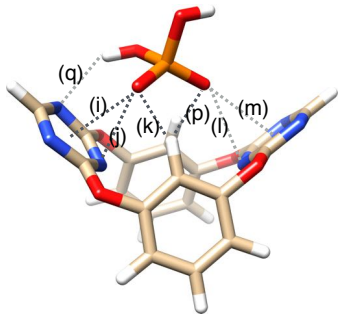
(i)=3.385, (j)=3.321, (k)=2.081,
(l)=2.966.
(m)=3.016, (p)=2.632

2·BF_4^-



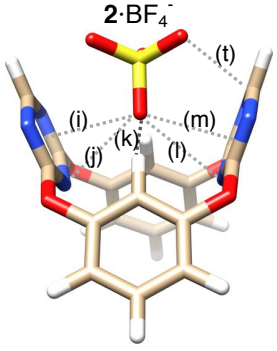
(i)=3.006, (j)=3.014, (k)=2.631,
(l)=3.243, (m)=3.230,
(p)=2.125.(q)=3.214

2·HSO_4^-



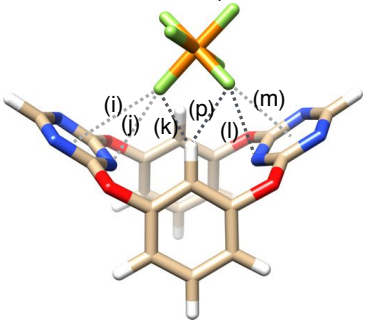
(i)=2.808, (j)=3.040, (k)=2.010,
(l)=2.949, (m)=2.954, (p)=2.923,
(q)=2.350

2·$H_2PO_4^-$



(i)=2.863, (j)=3.038, (k)=1.805,
(l)=3.041, (m)=2.866, (t)=2.405

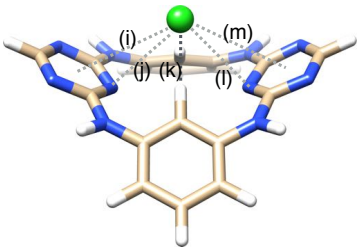
2·SO_4^{2-}



(i)=3.133, (j)=2.920, (k)=2.434,
(l)=3.267, (m)=3.271, (p)=2.217

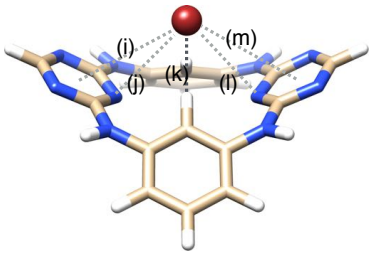
2·PF_6^-

Figure S4. Optimized structures for complexes of **2**, including selected geometrical parameters. Bond lengths are shown in Å.



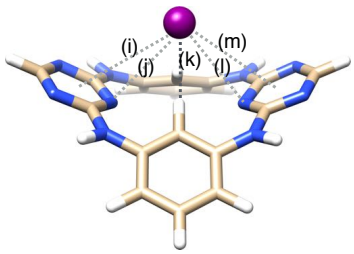
(i)=4.025, (j)=3.455, (k)=2.322, (l)=3.457, (m)=4.027

3·Cl^-



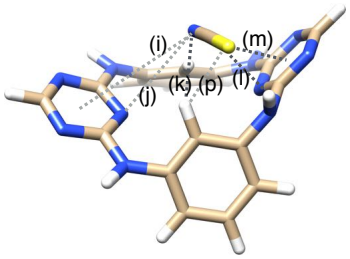
(i)=4.119, (j)=3.579, (k)=2.492, (l)=3.578, (m)=4.117

3·Br^-



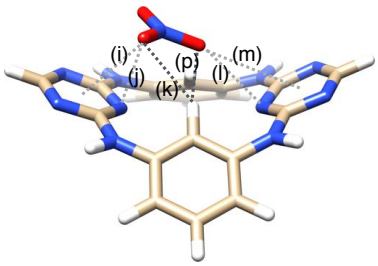
(i)=4.287, (j)=3.778, (k)=2.759, (l)=3.786, (m)=4.301

3·I^-



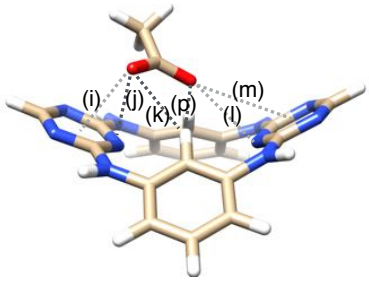
(i)=4.508, (j)=3.853, (k)=2.458, (l)=4.720, (m)=4.634, (p)=3.065

3·NCS^-



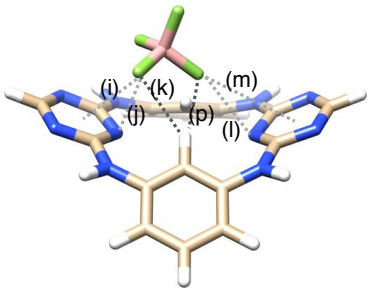
(i)=3.370, (j)=3.208, (k)=2.737, (l)=3.022, (m)=3.682, (p)=2.072

3·NO_3^-



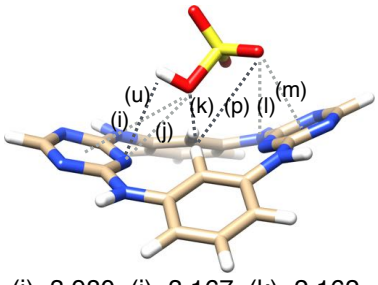
(i)=3.172, (j)=3.150, (k)=2.691, (l)=3.051, (m)=3.715, (p)=1.993

3·$CH_3CO_2^-$



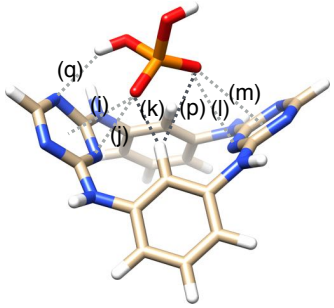
(i)=3.336, (j)=3.191, (k)=2.739, (l)=2.967, (m)=3.611, (p)=2.143

3·BF_4^-



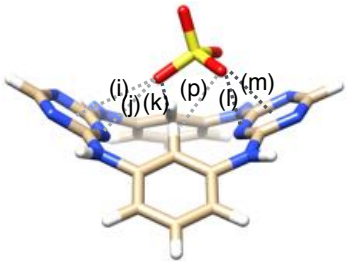
(i)=3.980, (j)=3.167, (k)=2.162, (l)=3.250, (m)=3.117, (p)=3.746, (u)=3.125

3·HSO_4^-



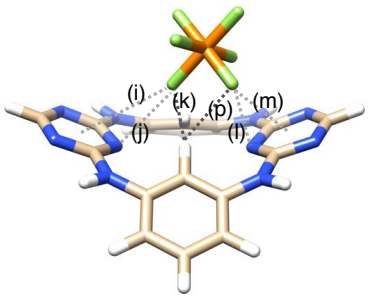
(i)=2.931, (j)=3.073, (k)=1.993, (l)=3.078, (m)=3.113, (p)=3.258, (q)=2.255

3·$H_2PO_4^-$



(i)=3.284, (j)=2.795, (k)=1.943, (l)=2.962, (m)=3.004, (p)=2.529

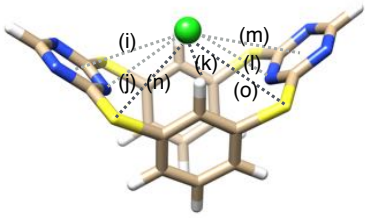
3·SO_4^{2-}



(i)=3.640, (j)=2.963, (k)=2.203, (l)=3.173, (m)=3.340, (p)=2.711

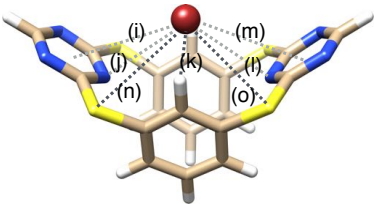
3·PF_6^-

Figure S5. Optimized structures for complexes of **3**, including selected geometrical parameters. Bond lengths are shown in Å.



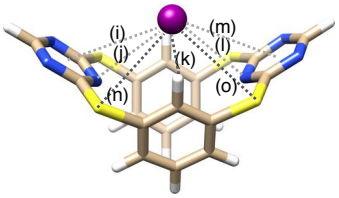
(i)=4.018, (j)=3.400, (k)=2.749, (l)=3.392, (m)=4.007, (n)=4.277, (o)=4.237

4·Cl$^-$



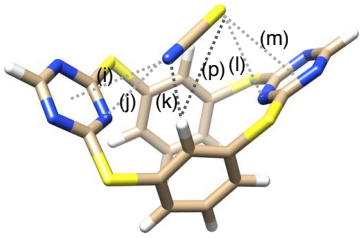
(i)=4.134, (j)=3.496, (k)=2.877, (l)=3.488, (m)=4.124, (n)=4.390, (o)=4.287

4·Br$^-$



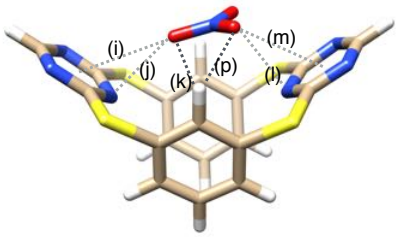
(i)=4.230, (j)=3.659, (k)=3.063, (l)=3.659, (m)=4.227, (n)=4.515, (o)=4.413

4·I$^-$



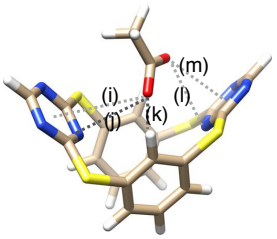
(i)=3.443, (j)=3.084, (k)=2.359, (l)=3.516, (m)=3.441, (p)=4.691

4·NCS$^-$



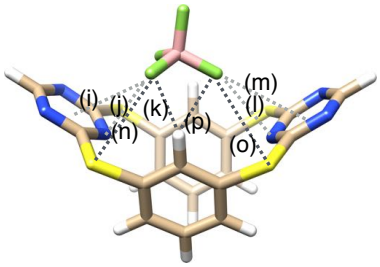
(i)=3.358, (j)=2.861, (k)=2.875, (l)=3.122, (m)=3.391, (p)=2.333

4·NO$_3^-$



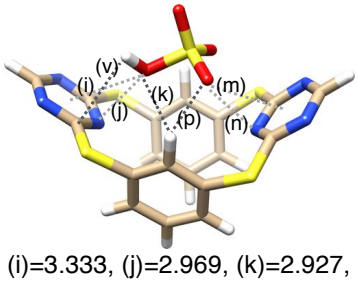
(i)=3.829, (j)=3.192, (k)=2.677, (l)=3.232, (m)=3.093

4·CH$_3$CO$_2^-$



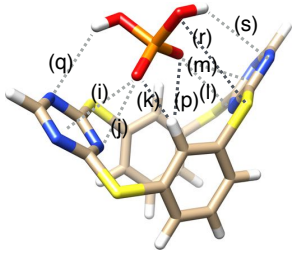
(i)=3.564, (j)=3.281, (k)=2.370, (l)=2.896, (m)=3.287, (n)=3.398, (o)=3.798 (p)=3.079

4·BF$_4^-$



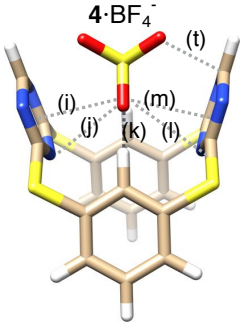
(i)=3.333, (j)=2.969, (k)=2.927, (m)=3.336, (n)=3.183, (p)=2.257, (v)=3.038

4·HSO$_4^-$



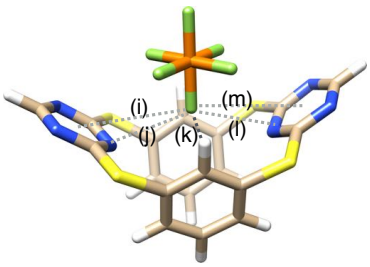
(i)=3.045, (j)=3.045, (k)=2.215, (l)=2.906, (m)=2.929, (q)=3.317, (r)=3.622, (s)=2.994

4·H$_2$PO$_4^-$



(i)=2.998, (j)=3.059, (k)=1.912, (l)=3.066, (m)=2.990, (t)=2.374

4·SO$_4^{2-}$



(i)=3.925, (j)=3.018, (k)=2.804, (l)=3.006, (m)=3.595

4·PF$_6^-$

Figure S6. Optimized structures for complexes of **4**, including selected geometrical parameters. Bond lengths are shown in Å.

4. Correlation between the C-H bond length and vibrational frequencies

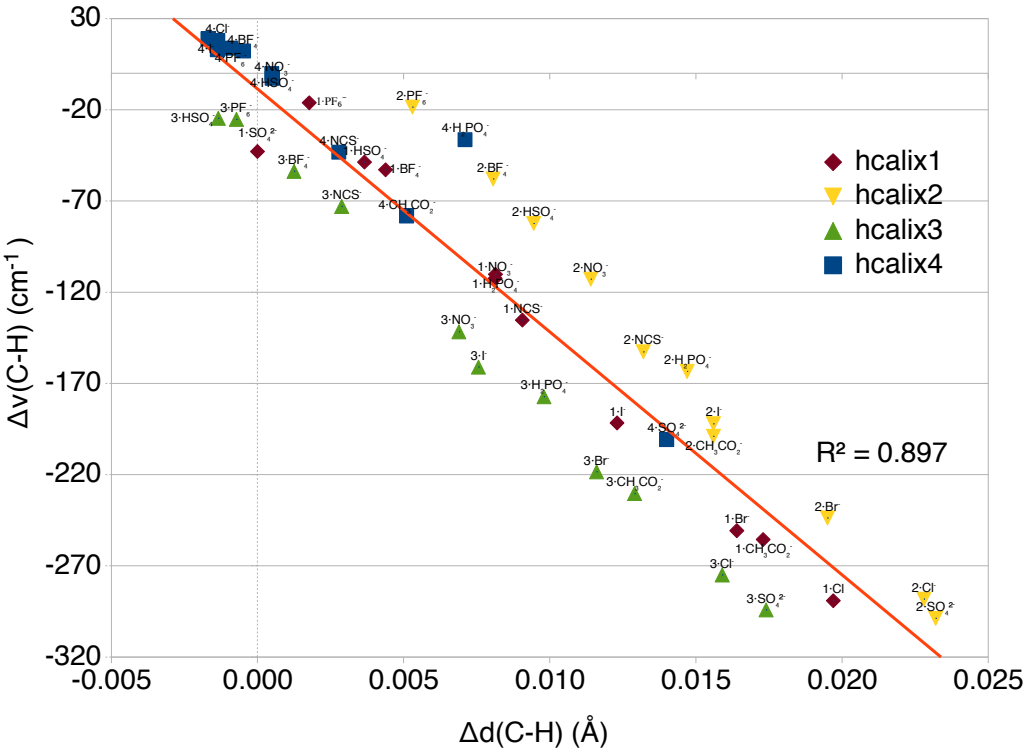


Figure S7. Correlation between the average values of Δd(C-H) bond length (Å) and (b) the Δν(C-H) vibrational frequencies (cm^{-1}), both relative to the respective values on the free heteracalixarenes.

5. Atom numbering scheme

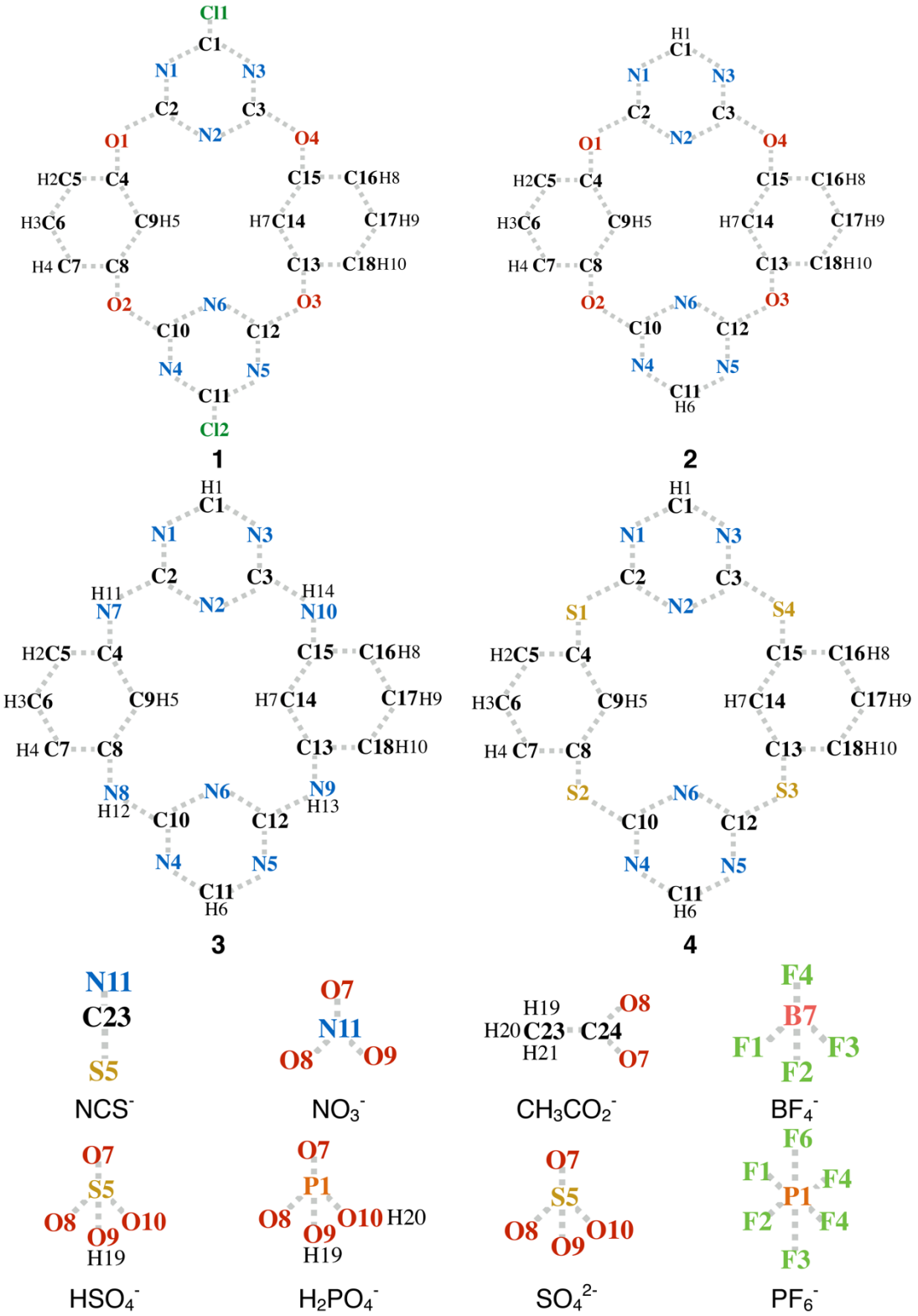


Figure S8. Atom numbering for complexes **1**-**4** and for polyatomic molecules. The spherical halides Cl^-, Br^- and I^- are classified as Cl(3), Br(1) and I(1), respectively.

6. NCI plots

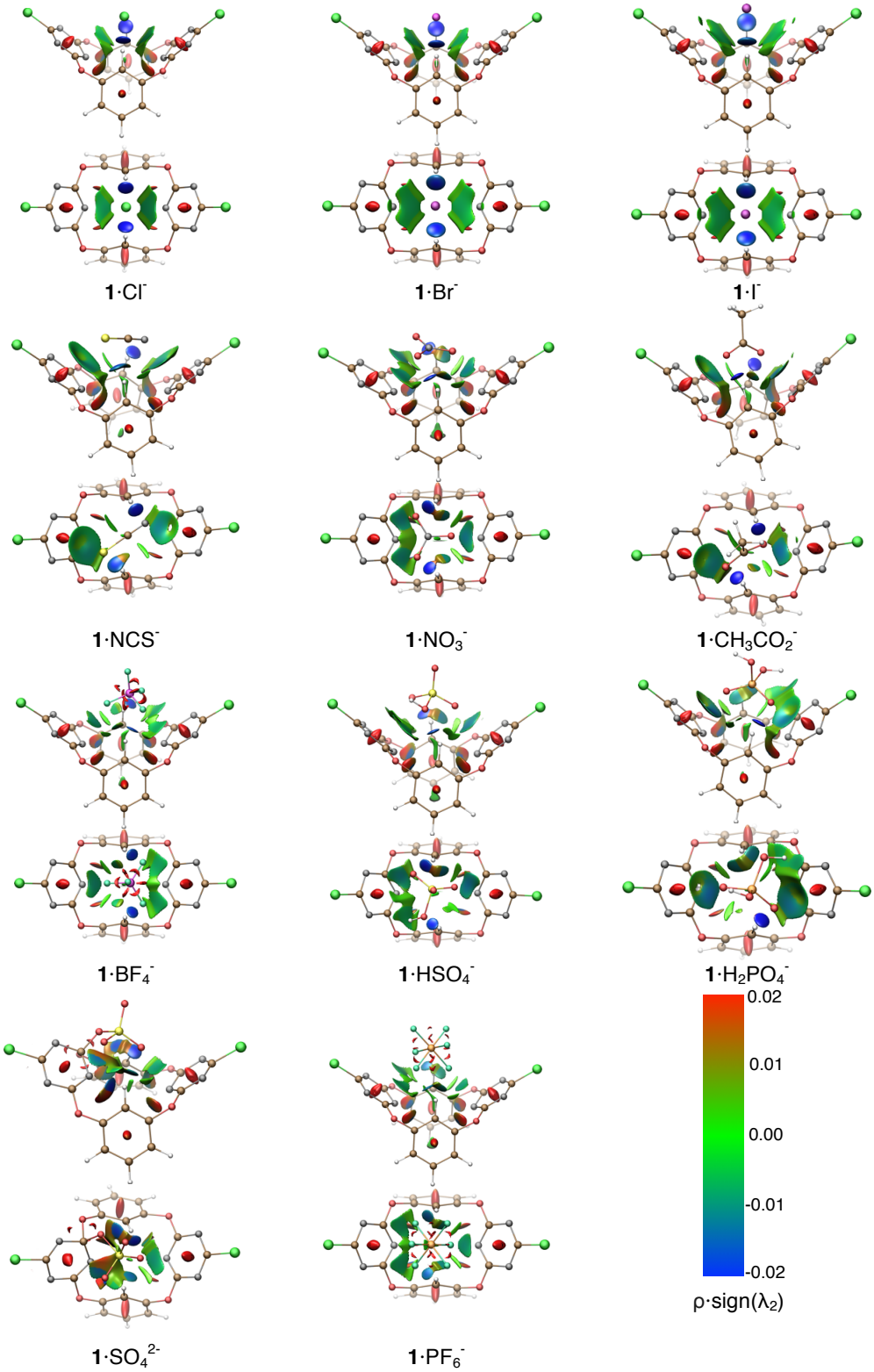


Figure S9. Upper and frontal vision of NCI plots for complexes of **1** interacting with different anions. Color scale of $-0.02<\rho<0.02$ a.u. Nitrogen atoms are shown in grey color in order to a clean vision of attractive interactions (blue surfaces).

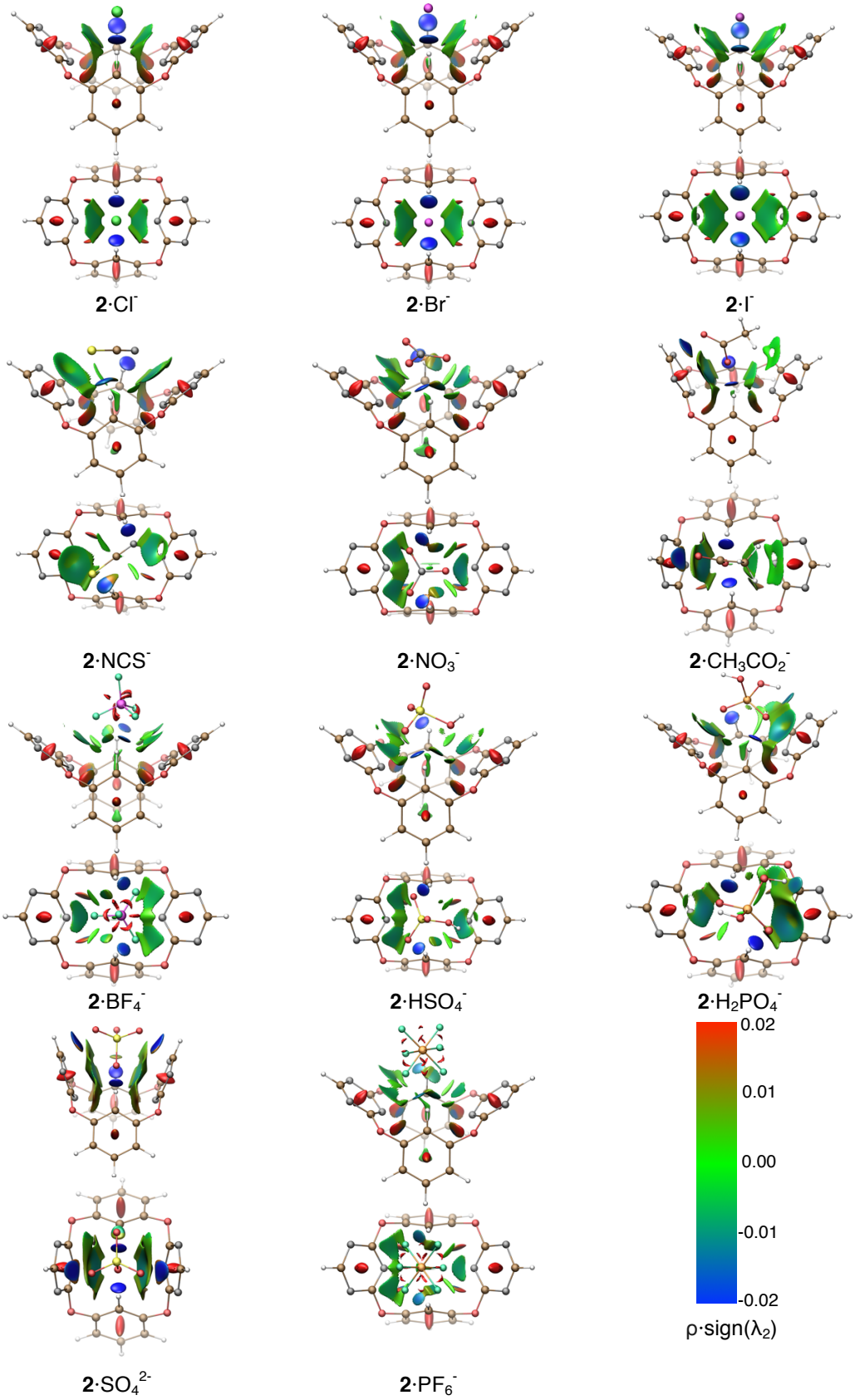


Figure S10. Upper and frontal vision of NCI plots for complexes of **2** interacting with different anions. Color scale of -0.02<ρ<0.02 a.u. Nitrogen atoms are shown in grey color in order to a clean vision of attractive interactions (blue surfaces).

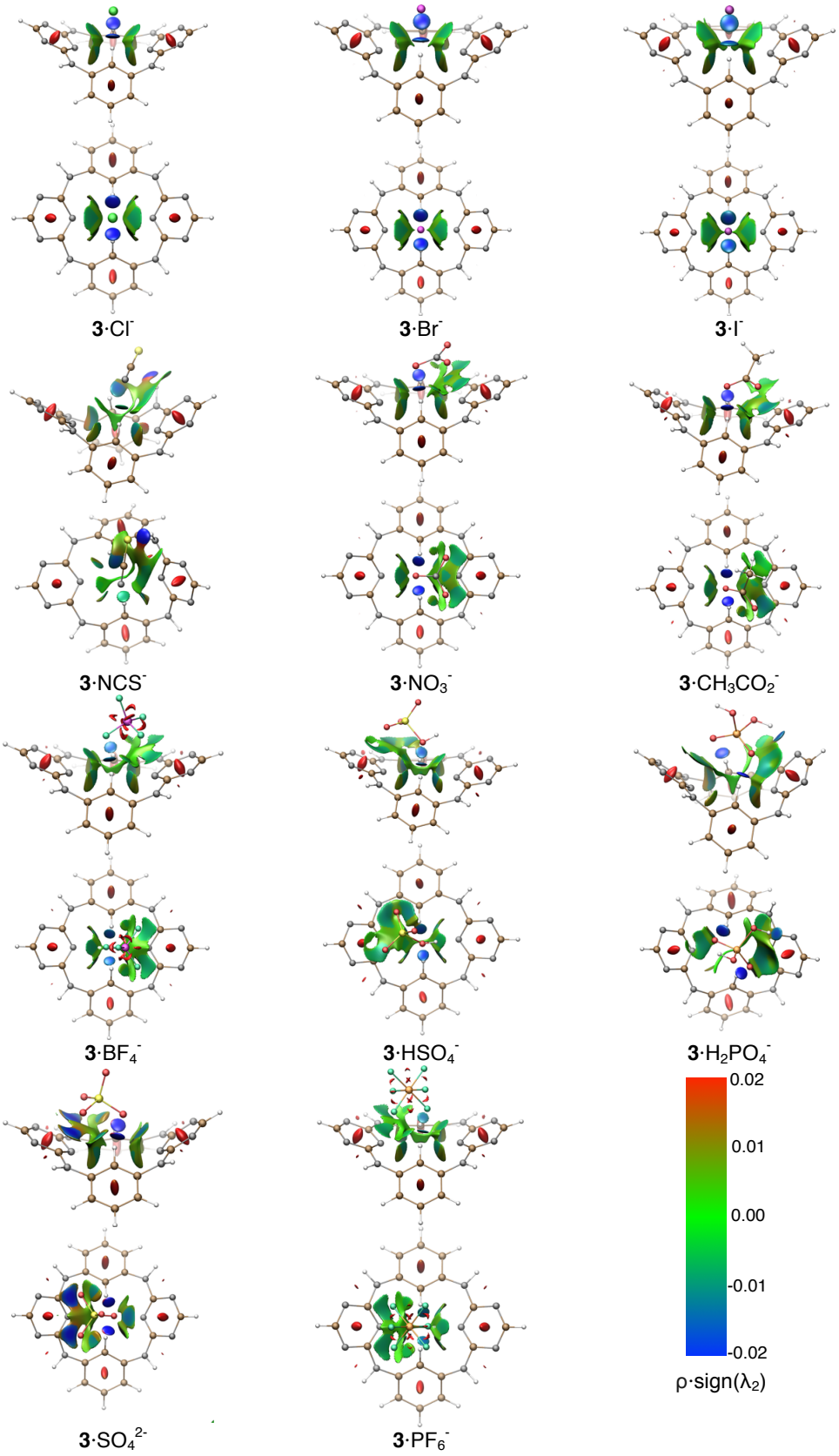


Figure S11. Upper and frontal vision of NCI plots for complexes of **3** interacting with different anions. Color scale of -0.02<ρ<0.02 a.u. Nitrogen atoms are shown in grey color in order to a clean vision of attractive interactions (blue surfaces).

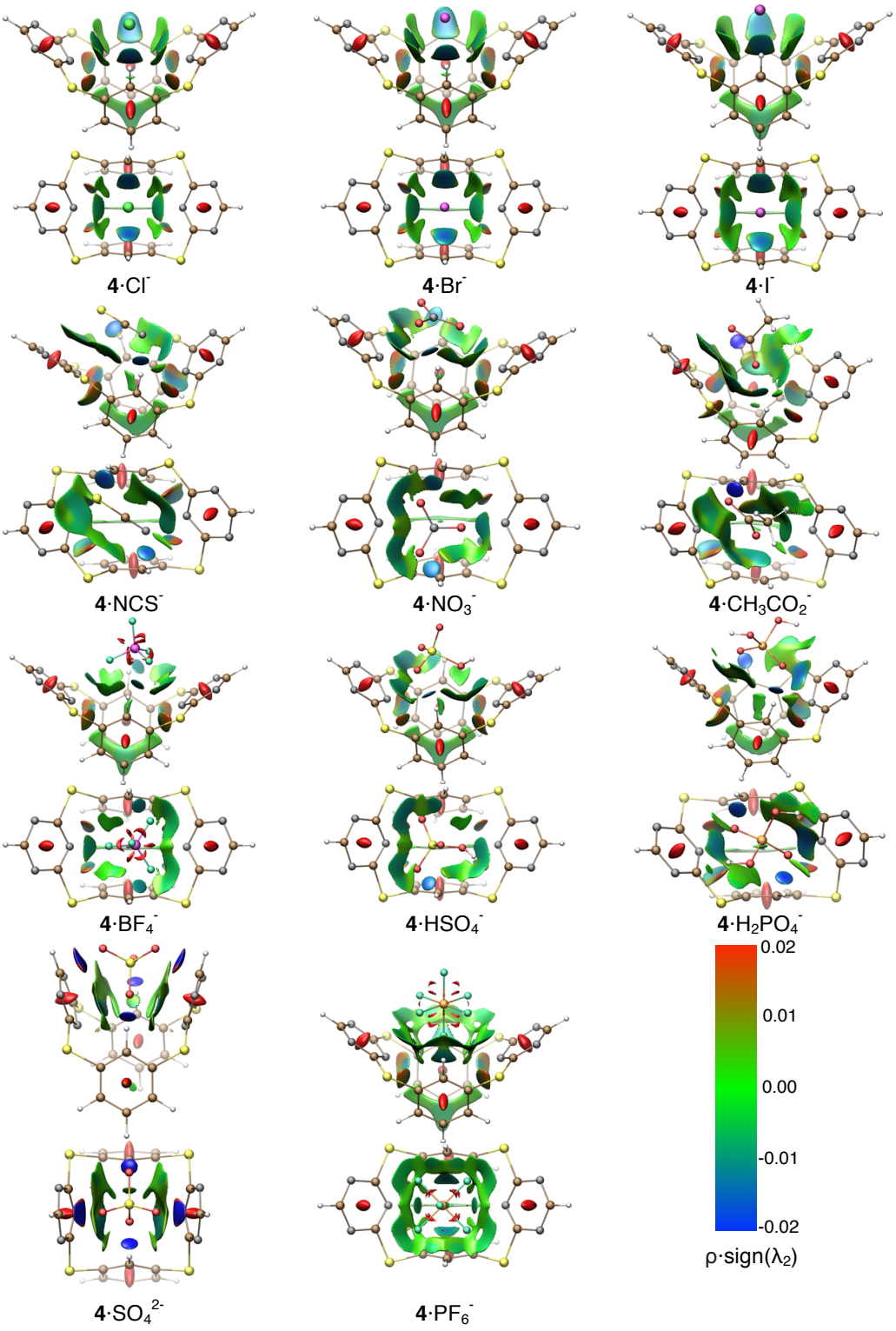


Figure S12. Upper and frontal vision of NCI plots for complexes of **4** interacting with different anions. Color scale of -0.02<ρ<0.02 a.u. Nitrogen atoms are shown in grey color in order to a clean vision of attractive interactions (blue surfaces).

7. Geometrical Parameters

Table S1. Selected bond lengths, in Å, for heterocalixarenes **1**-**4** and their complexes.

	C(1) •••C(11)	N(2) •••N(6)	C(9) •••C(18)	C(6) •••C(17)		C(1) •••C(11)	N(2) •••N(6)	C(9) •••C(18)	C(6) •••C(17)
1	9.256	4.679	4.490	4.900	**3**	9.785	4.535	4.343	9.471
1·Cl^-	8.661	4.620	4.233	6.231	**3**·Cl^-	9.375	4.613	4.287	8.852
1·Br^-	8.713	4.610	4.259	6.188	**3**·Br^-	9.386	4.595	4.294	8.944
1·I^-	8.735	4.621	4.342	5.745	**3**·I^-	9.446	4.579	4.299	9.028
1·BF_4^-	8.926	4.646	4.334	5.632	**3**·BF_4^-	9.535	4.591	4.314	9.084
1·$CH_3CO_2^-$	8.606	4.640	4.187	6.389	**3**·$CH_3CO_2^-$	9.429	4.611	4.285	8.908
1·$H_2PO_4^-$	8.656	4.665	4.304	5.771	**3**·$H_2PO_4^-$	8.794	4.683	4.283	7.791
1·HSO_4^-	8.740	4.628	4.361	5.544	**3**·HSO_4^-	9.637	4.544	4.305	9.438
1·NCS^-	8.847	4.634	4.311	5.749	**3**·NCS^-	9.197	4.671	4.297	7.642
1·NO_3^-	8.978	4.657	4.397	5.393	**3**·NO_3^-	9.534	4.595	4.320	9.000
1·PF_6^-	9.001	4.659	4.341	5.598	**3**·PF_6^-	9.581	4.579	4.322	9.181
1·SO_4^{2-}	8.830	4.297	4.167	6.723	**3**·SO_4^{2-}	9.271	4.647	4.299	9.060
2	9.269	4.661	4.490	4.850	**4**	10.322	5.533	5.024	3.347
2·Cl^-	8.607	4.621	4.203	6.323	**4**·Cl^-	9.815	5.633	4.798	3.464
2·Br^-	8.631	4.614	4.247	6.170	**4**·Br^-	10.007	5.630	4.860	3.384
2·I^-	8.701	4.619	4.309	5.866	**4**·I^-	10.028	5.627	4.935	3.347
2·BF_4^-	8.936	4.650	4.315	5.654	**4**·BF_4^-	10.015	5.621	4.891	3.401
2·$CH_3CO_2^-$	7.777	4.578	4.185	6.980	**4**·$CH_3CO_2^-$	9.290	5.430	4.764	3.592
2·$H_2PO_4^-$	8.668	4.667	4.246	5.999	**4**·$H_2PO_4^-$	9.327	5.491	4.656	3.791
2·HSO_4^-	8.943	4.660	4.352	5.460	**4**·HSO_4^-	9.923	5.603	4.878	3.431
2·NCS^-	8.873	4.630	4.325	5.646	**4**·NCS^-	9.771	5.487	4.796	3.550
2·NO_3^-	9.013	4.673	4.385	5.308	**4**·NO_3^-	9.929	5.616	4.886	3.425
2·PF_6^-	9.011	4.669	4.334	5.533	**4**·PF_6^-	9.990	5.587	5.047	3.356
2·SO_4^{2-}	6.379	4.568	4.328	7.560	**4**·SO_4^{2-}	6.507	5.043	4.807	6.005

Table S2. (a) C9-H5···A^- and (b) C14-H7···A^- bond angles (^{o}) for complexes **1**-**4**.

	1·Cl^-	**1**·Br^-	**1**·I^-	**1**·BF_4^-	**1**·$CH_3CO_2^-$	**1**·$H_2PO_4^-$	**1**·HSO_4^-	**1**·NCS^-	**1**·NO_3^-	**1**·PF_6^-	**1**·SO_4^{2-}
(a)	157.2	157.4	153.7	151.4	165.3	156.6	152.0	160.9	146.5	146.6	164.2
(b)	157.4	158.9	153.2	150.2	164.6	143.9	150.9	156.8	146.0	145.9	155.7
	2·Cl^-	**2**·Br^-	**2**·I^-	**2**·BF_4^-	**2**·$CH_3CO_2^-$	**2**·$H_2PO_4^-$	**2**·HSO_4^-	**2**·NCS^-	**2**·NO_3^-	**2**·PF_6^-	**2**·SO_4^{2-}
(a)	159.7	158.8	156.4	152.9	161.7	159.4	152.2	163.3	146.5	147.4	165.0
(b)	159.2	158.4	155.7	152.0	156.9	158.5	149.1	159.0	147.2	146.7	156.3
	3·Cl^-	**3**·Br^-	**3**·I^-	**3**·BF_4^-	**3**·$CH_3CO_2^-$	**3**·$H_2PO_4^-$	**3**·HSO_4^-	**3**·NCS^-	**3**·NO_3^-	**3**·PF_6^-	**3**·SO_4^{2-}
(a)	166.5	162.2	157.0	161.6	170.4	166.6	151.6	165.4	168.3	158.8	165.1
(b)	166.1	161.8	156.2	160.7	169.4	159.0	150.9	147.1	166.6	155.9	164.1
	4·Cl^-	**4**·Br^-	**4**·I^-	**4**·BF_4^-	**4**·$CH_3CO_2^-$	**4**·$H_2PO_4^-$	**4**·HSO_4^-	**4**·NCS^-	**4**·NO_3^-	**4**·PF_6^-	**4**·SO_4^{2-}
(a)	100.0	100.6	103.5	121.0	152.3	129.6	130.2	137.0	121.8	120.3	175.6
(b)	99.4	99.9	102.7	120.7	92.3	129.3	115.4	119.3	117.4	119.9	143.1

Table S3. C-H bond lengths (d, Å) and stretching vibrational frequencies (ν, cm^{-1}) for **1**-**4** and their complexes.

	1·Cl^-	**2**·Cl^-	**3**·Cl^-	**4**·Cl^-	**1**·Br^-	**2**·Br^-	**3**·Br^-	**4**·Br^-
d(C9-H5)	1.107	1.107	1.103	1.087	1.104	1.104	1.099	1.087
d(C14-H7)	1.108	1.107	1.104	1.087	1.104	1.104	1.099	1.087
ν(C9-H5)	2835.6	2838.7	2887.4	3136.7	2877.3	2886.9	2947.5	3138.0
ν(C14-H7)	2861.2	2863.4	2912.0	3136.2	2896.2	2904.1	2965.0	3136.6
	1·I^-	**2**·I^-	**3**·I^-	**4**·I^-	**1**·NCS^-	**2**·NCS^-	**3**·NCS^-	**4**·NCS^-
d(C9-H5)	1.100	1.100	1.095	1.087	1.096	1.096	1.089	1.089
d(C14-H7)	1.100	1.100	1.095	1.087	1.098	1.099	1.092	1.094
ν(C9-H5)	2940.7	2941.9	3008.2	3131.5	2988.5	2964.2	3086.8	3039.2
ν(C14-H7)	2950.9	2952.5	3019.2	3131.1	3015.9	3009.2	3116.7	3111.0
	1·NO_3^-	**2**·NO_3^-	**3**·NO_3^-	**4**·NO_3^-	**1**·$CH_3CO_2^-$	**2**·$CH_3CO_2^-$	**3**·$CH_3CO_2^-$	**4**·$CH_3CO_2^-$
d(C9-H5)	1.096	1.096	1.094	1.090	1.106	1.101	1.099	1.100
d(C14-H7)	1.096	1.096	1.094	1.089	1.104	1.099	1.102	1.087
ν(C9-H5)	3021.7	3023.1	3024.6	3122.2	2863.7	2940.3	2920.6	3136.5
ν(C14-H7)	3028.5	3029.9	3041.4	3109.0	2900.2	2940.3	2968.0	2943.8
	1·BF_4^-	**2**·BF_4^-	**3**·BF_4^-	**4**·BF_4^-	**1**·HSO_4^-	**2**·HSO_4^-	**3**·HSO_4^-	**4**·HSO_4^-
d(C9-H5)	1.092	1.092	1.089	1.088	1.090	1.094	1.087	1.090
d(C14-H7)	1.092	1.092	1.089	1.088	1.092	1.094	1.085	1.088
ν(C9-H5)	3082.1	3079.2	3114.8	3129.7	3099.0	3053.6	3163.4	3129.1
ν(C14-H7)	3087.1	3083.6	3127.2	3131.4	3078.7	3060.4	3136.7	3107.3
	1·H_2PO_4	**2**·H_2PO_4	**3**·H_2PO_4	**4**·H_2PO_4	**1**·SO_4^{2-}	**2**·SO_4^{2-}	**3**·SO_4^{2-}	**4**·SO_4^{2-}
d(C9-H5)	1.092	1.098	1.097	1.092	1.089	1.110	1.105	1.098
d(C14-H7)	1.099	1.100	1.098	1.099	1.089	1.105	1.105	1.107
ν(C9-H5)	2968.2	2961.5	2986.9	3080.6	3094.6	2796.8	2866.5	2846.8
ν(C14-H7)	3086.4	2990.3	3007.9	3083.3	3094.6	2884.3	2894.6	2988.4
	1·PF_6^-	**2**·PF_6^-	**3**·PF_6^-	**4**·PF_6^-	Free **1**	Free **2**	Free **3**	Free **4**
d(C9-H5)	1.089	1.090	1.087	1.088	1.088	1.084	1.088	1.089
d(C14-H7)	1.089	1.090	1.087	1.088	1.088	1.084	1.087	1.089
ν(C9-H5)	3121.2	3119.6	3144.5	3131.9	31374.8	3137.2	3174.7	3117.8
ν(C14-H7)	3121.5	3122.0	3154.3	3132.4	3137.3	3141.5	3174.7	3118.9

8. Charge analysis

Table S4. Hirshfeld charge analysis and the Natural Population Analysis (NPA) charges (in parenthesis) for complexes **1-4** considering the the anionic species as (f1) and the heterocalixarenes **1-4** as (f2).

	1·Cl^-	**1**·Br^-	**1**·I^-	**1**·BF_4^-	**1**·$CH_3CO_2^-$	**1**·$H_2PO_4^-$	**1**·HSO_4^-	**1**·NCS^-	**1**·NO_3^-	**1**·PF_6^-	**1**·SO_4^{2-}
q_{f1}	-0.870	-0.900	-0.921	-0.928	-0.868	-0.909	-0.915	-0.915	-0.889	-0.940	-1.296
	(-0.861)	*(-0.862)*	*(-0.877)*	*(-0.952)*	*(-0.887)*	*(-0.934)*	*(-0.940)*	*(-0.921)*	*(-0.900)*	*(-0.963)*	*(-1.174)*
q_{f2}	-0.130	-0.100	-0.079	-0.072	-0.132	-0.091	-0.085	-0.085	-0.111	-0.061	-0.704
	(0.139)	*(0.138)*	*(0.123)*	*(0.048)*	*(0.113)*	*(0.066)*	*(0.060)*	*(0.079)*	*(0.100)*	*(0.037)*	*(0.826)*
	2·Cl^-	**2**·Br^-	**2**·I^-	**2**·BF_4^-	**2**·$CH_3CO_2^-$	**2**·$H_2PO_4^-$	**2**·HSO_4^-	**2**·NCS^-	**2**·NO_3^-	**2**·PF_6^-	**2**·SO_4^{2-}
q_{f1}	-0.876	-0.908	-0.930	-0.933	-0.843	-0.913	-0.920	-0.917	-0.897	-0.945	-1.613
	(-0.869)	*(-0.875)*	*(-0.888)*	*(-0.956)*	*(-0.859)*	*(-0.933)*	*(-0.942)*	*(-0.922)*	*(-0.908)*	*(-0.967)*	*(-1.628)*
q_{f2}	-0.124	-0.092	-0.070	-0.067	-0.157	-0.087	-0.080	-0.083	-0.103	-0.056	-0.387
	(0.131)	*(0.125)*	*(0.112)*	*(0.044)*	*(0.141)*	*(0.067)*	*(0.058)*	*(0.078)*	*(0.092)*	*(0.033)*	*(0.372)*
	3·Cl^-	**3**·Br^-	**3**·I^-	**3**·BF_4^-	**3**·$CH_3CO_2^-$	**3**·$H_2PO_4^-$	**3**·HSO_4^-	**3**·NCS^-	**3**·NO_3^-	**3**·PF_6^-	**3**·SO_4^{2-}
q_{f1}	-0.880	-0.910	-0.930	-0.939	-0.885	-0.925	-0.933	-0.891	-0.902	-0.950	-1.683
	(-0.875)	*(-0.882)*	*(-0.896)*	*(-0.961)*	*(-0.899)*	*(-0.943)*	*(-0.951)*	*(-0.893)*	*(-0.914)*	*(-0.969)*	*(-1.713)*
q_{f2}	-0.120	-0.090	-0.070	-0.062	-0.116	-0.075	-0.068	-0.109	-0.098	-0.050	-0.317
	(0.125)	*(0.118)*	*(0.104)*	*(0.039)*	*(0.101)*	*(0.057)*	*(0.049)*	*(0.107)*	*(0.086)*	*(0.031)*	*(0.287)*
	4·Cl^-	**4**·Br^-	**4**·I^-	**4**·BF_4^-	**4**·$CH_3CO_2^-$	**4**·$H_2PO_4^-$	**4**·HSO_4^-	**4**·NCS^-	**4**·NO_3^-	**4**·PF_6^-	**4**·SO_4^{2-}
q_{f1}	-0.833	-0.862	-0.880	-0.941	-0.870	-0.901	-0.921	-0.909	-0.887	-0.935	-1.551
	(-0.842)	*(-0.833)*	*(-0.830)*	*(-0.968)*	*(-0.897)*	*(-0.929)*	*(-0.948)*	*(-0.915)*	*(-0.909)*	*(-0.966)*	*(-1.544)*
q_{f2}	-0.166	-0.139	-0.121	-0.059	-0.130	-0.100	-0.079	-0.092	-0.113	-0.065	-0.449
	(0.158)	*(0.167)*	*(0.170)*	*(0.032)*	*(0.103)*	*(0.071)*	*(0.052)*	*(0.085)*	*(0.091)*	*(0.034)*	*(0.456)*

Table S5. Atomic charges derived from the Natural Population Analysis (NPA), for the heterocalixarene atoms in **1** and in their complexes.

	1	**1**·Cl^-	**1**·Br^-	**1**·I^-	**1**·BF_4^-	**1**·$CH_3CO_2^-$	**1**·$H_2PO_4^-$	**1**·HSO_4^-	**1**·NCS^-	**1**·NO_3^-	**1**·PF_6^-	**1**·SO_4^{2-}
Cl1	0.071	0.015	0.017	0.013	0.023	0.009	0.009	0.021	0.019	0.012	0.028	-0.028
Cl2	0.070	0.014	0.017	0.014	0.021	0.012	0.019	0.021	0.022	0.014	0.029	-0.129
N1	-0.487	-0.495	-0.494	-0.476	-0.494	-0.491	-0.499	-0.498	-0.491	-0.495	-0.490	-0.506
N2	-0.542	-0.513	-0.517	-0.475	-0.522	-0.511	-0.522	-0.524	-0.524	-0.538	-0.532	-0.506
N3	-0.488	-0.495	-0.494	-0.518	-0.494	-0.499	-0.489	-0.487	-0.493	-0.495	-0.490	-0.510
N4	-0.488	-0.496	-0.495	-0.475	-0.491	-0.492	-0.517	-0.509	-0.495	-0.498	-0.493	-0.610
N5	-0.488	-0.496	-0.495	-0.475	-0.491	-0.519	-0.488	-0.488	-0.493	-0.498	-0.492	-0.530
N6	-0.542	-0.513	-0.516	-0.518	-0.531	-0.495	-0.526	-0.530	-0.531	-0.518	-0.524	-0.592
O1	-0.406	-0.413	-0.413	-0.395	-0.413	-0.411	-0.421	-0.419	-0.412	-0.413	-0.411	-0.413
O2	-0.406	-0.413	-0.413	-0.396	-0.411	-0.417	-0.415	-0.416	-0.415	-0.413	-0.411	-0.441
O3	-0.406	-0.413	-0.413	-0.396	-0.411	-0.415	-0.414	-0.411	-0.412	-0.414	-0.411	-0.470
O4	-0.406	-0.413	-0.413	-0.395	-0.412	-0.421	-0.412	-0.410	-0.417	-0.413	-0.411	-0.418
H5	0.247	0.306	0.298	0.285	0.301	0.313	0.313	0.296	0.288	0.299	0.296	0.313
H7	0.247	0.306	0.298	0.285	0.301	0.311	0.298	0.305	0.299	0.299	0.295	0.296
C1	0.370	0.385	0.386	0.378	0.385	0.388	0.393	0.388	0.390	0.389	0.385	0.392
C2	0.664	0.681	0.681	0.660	0.680	0.699	0.680	0.672	0.685	0.691	0.684	0.689
C3	0.664	0.681	0.681	0.660	0.681	0.674	0.704	0.699	0.689	0.689	0.684	0.680
C4	0.274	0.268	0.269	0.266	0.271	0.270	0.277	0.276	0.274	0.275	0.276	0.256
C5	-0.245	-0.261	-0.260	-0.254	-0.257	-0.262	-0.259	-0.258	-0.256	-0.257	-0.255	-0.289
C6	-0.185	-0.209	-0.208	-0.204	-0.204	-0.209	-0.204	-0.203	-0.204	-0.206	-0.203	-0.224
C7	-0.244	-0.261	-0.260	-0.254	-0.257	-0.263	-0.258	-0.257	-0.259	-0.258	-0.256	-0.270
C8	0.274	0.268	0.269	0.266	0.276	0.272	0.273	0.275	0.275	0.271	0.271	0.299
C9	-0.261	-0.274	-0.274	-0.274	-0.261	-0.275	-0.264	-0.264	-0.264	-0.265	-0.257	-0.268
C10	0.664	0.681	0.681	0.660	0.687	0.693	0.679	0.680	0.686	0.683	0.677	0.641
C11	0.370	0.385	0.385	0.378	0.386	0.393	0.394	0.387	0.390	0.384	0.382	0.408
C12	0.664	0.681	0.681	0.660	0.686	0.680	0.703	0.698	0.679	0.683	0.677	0.703
C13	0.274	0.268	0.269	0.266	0.276	0.271	0.272	0.273	0.271	0.271	0.271	0.320
C14	-0.261	-0.274	-0.274	-0.274	-0.261	-0.280	-0.269	-0.262	-0.267	-0.265	-0.258	-0.306
C15	0.274	0.268	0.269	0.266	0.271	0.274	0.273	0.273	0.275	0.276	0.276	0.255
C16	-0.244	-0.261	-0.260	-0.254	-0.258	-0.264	-0.258	-0.256	-0.259	-0.256	-0.255	-0.316
C17	-0.185	-0.209	-0.208	-0.204	-0.204	-0.208	-0.207	-0.206	-0.206	-0.206	-0.203	-0.223
C18	-0.244	-0.261	-0.260	-0.254	-0.257	-0.264	-0.261	-0.259	-0.259	-0.257	-0.256	-0.280

Table S6. Atomic charges derived from the Natural Population Analysis (NPA), for the heterocalixarene atoms in **2** and in their complexes.

	2	**2**·Cl^-	**2**·Br^-	**2**·I^-	**2**·BF_4^-	**2**·$CH_3CO_2^-$	**2**·$H_2PO_4^-$	**2**·HSO_4^-	**2**·NCS^-	**2**·NO_3^-	**2**·PF_6^-	**2**·SO_4^{2-}
N1	-0.481	-0.491	-0.489	-0.473	-0.487	-0.488	-0.495	-0.486	-0.485	-0.494	-0.485	-0.486
N2	-0.481	-0.513	-0.517	-0.518	-0.530	-0.522	-0.518	-0.534	-0.522	-0.520	-0.532	-0.523
N3	-0.540	-0.491	-0.489	-0.473	-0.487	-0.486	-0.486	-0.488	-0.490	-0.494	-0.486	-0.483
N4	-0.481	-0.491	-0.489	-0.473	-0.489	-0.491	-0.519	-0.493	-0.490	-0.491	-0.488	-0.487
N5	-0.481	-0.491	-0.489	-0.473	-0.489	-0.495	-0.483	-0.499	-0.488	-0.491	-0.488	-0.483
N6	-0.540	-0.513	-0.517	-0.518	-0.522	-0.508	-0.525	-0.522	-0.530	-0.538	-0.524	-0.523
O1	-0.411	-0.420	-0.420	-0.402	-0.417	-0.438	-0.425	-0.417	-0.417	-0.420	-0.417	-0.452
O2	-0.411	-0.420	-0.420	-0.402	-0.419	-0.415	-0.419	-0.418	-0.421	-0.419	-0.417	-0.452
O3	-0.411	-0.420	-0.420	-0.402	-0.419	-0.420	-0.422	-0.418	-0.418	-0.420	-0.417	-0.449
O4	-0.411	-0.420	-0.420	-0.402	-0.417	-0.435	-0.417	-0.420	-0.424	-0.420	-0.417	-0.450
H1	0.197	0.179	0.180	0.175	0.181	0.201	0.177	0.181	0.181	0.179	0.183	0.204
H5	0.246	0.305	0.297	0.284	0.300	0.306	0.306	0.302	0.287	0.297	0.293	0.327
H6	0.197	0.179	0.180	0.175	0.181	0.181	0.182	0.180	0.180	0.178	0.183	0.204
H7	0.246	0.305	0.297	0.284	0.300	0.307	0.312	0.302	0.300	0.298	0.294	0.325
C1	0.265	0.262	0.264	0.258	0.265	0.309	0.264	0.266	0.268	0.260	0.268	0.302
C2	0.655	0.671	0.670	0.651	0.675	0.654	0.669	0.680	0.674	0.672	0.673	0.652
C3	0.655	0.671	0.671	0.652	0.675	0.664	0.686	0.680	0.674	0.673	0.673	0.658
C4	0.274	0.270	0.271	0.268	0.277	0.289	0.277	0.282	0.274	0.273	0.277	0.291
C5	-0.246	-0.264	-0.263	-0.257	-0.259	-0.268	-0.264	-0.257	-0.256	-0.259	-0.257	-0.297
C6	-0.187	-0.211	-0.210	-0.205	-0.206	-0.207	-0.208	-0.207	-0.207	-0.208	-0.205	-0.221
C7	-0.246	-0.264	-0.263	-0.257	-0.260	-0.277	-0.262	-0.261	-0.260	-0.258	-0.258	-0.297
C8	0.274	0.270	0.271	0.268	0.273	0.268	0.273	0.269	0.276	0.277	0.273	0.291
C9	-0.262	-0.276	-0.275	-0.275	-0.262	-0.295	-0.272	-0.264	-0.264	-0.266	-0.258	-0.323
C10	0.655	0.671	0.671	0.651	0.670	0.667	0.671	0.669	0.674	0.679	0.666	0.651
C11	0.265	0.262	0.264	0.257	0.265	0.258	0.276	0.256	0.269	0.265	0.264	0.302
C12	0.655	0.671	0.670	0.651	0.671	0.661	0.689	0.675	0.668	0.679	0.667	0.658
C13	0.274	0.270	0.271	0.268	0.273	0.269	0.275	0.270	0.273	0.277	0.273	0.287
C14	-0.262	-0.277	-0.275	-0.275	-0.262	-0.289	-0.271	-0.264	-0.270	-0.266	-0.258	-0.305
C15	0.274	0.270	0.271	0.268	0.277	0.287	0.274	0.281	0.276	0.273	0.277	0.287
C16	-0.246	-0.264	-0.263	-0.257	-0.259	-0.267	-0.260	-0.258	-0.262	-0.259	-0.257	-0.292
C17	-0.187	-0.211	-0.210	-0.205	-0.206	-0.207	-0.209	-0.207	-0.208	-0.208	-0.205	-0.224
C18	-0.246	-0.264	-0.263	-0.257	-0.260	-0.273	-0.264	-0.260	-0.261	-0.259	-0.258	-0.292

Table S7. Atomic charges derived from the Natural Population Analysis (NPA), for the heterocalixarene atoms in **3** and in their complexes.

	3	**3**·Cl^-	**3**·Br^-	**3**·I^-	**3**·BF_4^-	**3**·$CH_3CO_2^-$	**3**·$H_2PO_4^-$	**3**·HSO_4^-	**3**·NCS^-	**3**·NO_3^-	**3**·PF_6^-	**3**·SO_4^{2-}
N1	-0.526	-0.539	-0.538	-0.522	-0.531	-0.545	-0.533	-0.528	-0.539	-0.533	-0.535	-0.551
N2	-0.532	-0.491	-0.495	-0.492	-0.511	-0.491	-0.512	-0.516	-0.513	-0.517	-0.506	-0.514
N3	-0.526	-0.539	-0.538	-0.522	-0.532	-0.539	-0.559	-0.525	-0.540	-0.533	-0.536	-0.552
N4	-0.526	-0.539	-0.538	-0.522	-0.537	-0.545	-0.531	-0.537	-0.495	-0.541	-0.530	-0.553
N5	-0.526	-0.539	-0.538	-0.522	-0.538	-0.525	-0.539	-0.544	-0.546	-0.541	-0.531	-0.552
N6	-0.532	-0.491	-0.495	-0.492	-0.500	-0.507	-0.508	-0.511	-0.515	-0.497	-0.512	-0.484
N7	-0.519	-0.535	-0.534	-0.507	-0.529	-0.536	-0.560	-0.524	-0.552	-0.530	-0.528	-0.544
N8	-0.519	-0.536	-0.534	-0.508	-0.531	-0.544	-0.550	-0.518	-0.605	-0.532	-0.529	-0.540
N9	-0.526	-0.536	-0.534	-0.507	-0.530	-0.529	-0.561	-0.526	-0.557	-0.532	-0.529	-0.539
N10	-0.526	-0.536	-0.534	-0.507	-0.529	-0.531	-0.568	-0.529	-0.539	-0.530	-0.530	-0.544
H5	0.269	0.311	0.304	0.292	0.300	0.314	0.298	0.300	0.294	0.302	0.294	0.335
H7	0.260	0.311	0.304	0.292	0.300	0.316	0.310	0.299	0.278	0.302	0.294	0.335
C1	0.258	0.251	0.252	0.246	0.259	0.249	0.267	0.266	0.252	0.259	0.253	0.253
C2	0.542	0.555	0.555	0.535	0.568	0.548	0.571	0.573	0.546	0.565	0.550	0.599
C3	0.544	0.555	0.555	0.534	0.567	0.555	0.566	0.569	0.550	0.565	0.549	0.598
C4	0.151	0.141	0.143	0.139	0.152	0.143	0.140	0.164	0.123	0.150	0.144	0.163
C5	-0.258	-0.265	-0.265	-0.263	-0.262	-0.268	-0.251	-0.259	-0.238	-0.262	-0.266	-0.277
C6	-0.193	-0.218	-0.217	-0.210	-0.212	-0.215	-0.219	-0.212	-0.222	-0.215	-0.210	-0.234
C7	-0.258	-0.265	-0.265	-0.263	-0.268	-0.267	-0.251	-0.271	-0.216	-0.268	-0.262	-0.291
C8	0.151	0.141	0.143	0.139	0.142	0.146	0.137	0.135	0.153	0.140	0.152	0.134
C9	-0.263	-0.230	-0.232	-0.237	-0.224	-0.235	-0.208	-0.223	-0.193	-0.225	-0.225	-0.226
C10	0.542	0.555	0.556	0.534	0.550	0.548	0.564	0.543	0.565	0.550	0.564	0.560
C11	0.258	0.251	0.252	0.246	0.252	0.257	0.260	0.247	0.254	0.249	0.259	0.243
C12	0.543	0.555	0.555	0.534	0.550	0.579	0.563	0.540	0.542	0.550	0.563	0.561
C13	0.147	0.141	0.143	0.139	0.143	0.147	0.138	0.144	0.152	0.141	0.153	0.134
C14	-0.242	-0.230	-0.232	-0.238	-0.227	-0.223	-0.200	-0.245	-0.222	-0.226	-0.229	-0.226
C15	0.146	0.141	0.143	0.139	0.153	0.136	0.133	0.159	0.142	0.150	0.146	0.162
C16	-0.254	-0.265	-0.265	-0.263	-0.263	-0.266	-0.233	-0.266	-0.267	-0.262	-0.268	-0.278
C17	-0.193	-0.218	-0.216	-0.210	-0.212	-0.219	-0.221	-0.209	-0.211	-0.215	-0.209	-0.234
C18	-0.254	-0.265	-0.265	-0.263	-0.269	-0.260	-0.240	-0.273	-0.261	-0.268	-0.264	-0.291
H11	0.416	0.406	0.407	0.403	0.409	0.405	0.404	0.409	0.409	0.408	0.409	0.398
H12	0.416	0.406	0.407	0.403	0.408	0.406	0.407	0.409	0.437	0.407	0.410	0.398
H13	0.417	0.406	0.407	0.403	0.408	0.407	0.406	0.408	0.403	0.407	0.409	0.398
H14	0.417	0.406	0.407	0.403	0.408	0.406	0.414	0.408	0.406	0.408	0.409	0.398

Table S8. Atomic charges derived from the Natural Population Analysis (NPA), for the heterocalixarene atoms in **4** and in their complexes.

	4	**4**·Cl^-	**4**·Br^-	**4**·I^-	**4**·BF_4^-	**4**·$CH_3CO_2^-$	**4**·$H_2PO_4^-$	**4**·HSO_4^-	**4**·NCS^-	**4**·NO_3^-	**4**·PF_6^-	**4**·SO_4^{2-}
N1	-0.482	-0.496	-0.496	-0.479	-0.492	-0.485	-0.494	-0.490	-0.496	-0.495	-0.491	-0.484
N2	-0.482	-0.468	-0.471	-0.471	-0.479	-0.483	-0.491	-0.492	-0.482	-0.475	-0.482	-0.499
N3	-0.500	-0.496	-0.496	-0.479	-0.491	-0.488	-0.495	-0.492	-0.485	-0.496	-0.491	-0.492
N4	-0.482	-0.496	-0.496	-0.479	-0.491	-0.490	-0.491	-0.493	-0.484	-0.496	-0.490	-0.484
N5	-0.482	-0.496	-0.497	-0.479	-0.490	-0.501	-0.494	-0.499	-0.494	-0.495	-0.490	-0.491
N6	-0.500	-0.468	-0.471	-0.471	-0.486	-0.477	-0.487	-0.481	-0.494	-0.496	-0.483	-0.498
S1	0.359	0.327	0.330	0.336	0.337	0.296	0.300	0.349	0.307	0.339	0.344	0.242
S2	0.358	0.329	0.336	0.342	0.341	0.381	0.373	0.336	0.371	0.332	0.339	0.242
S3	0.359	0.327	0.329	0.336	0.341	0.301	0.302	0.351	0.312	0.339	0.340	0.240
S4	0.358	0.328	0.335	0.343	0.341	0.348	0.374	0.326	0.383	0.332	0.341	0.239
H1	0.197	0.179	0.179	0.174	0.182	0.179	0.180	0.180	0.181	0.180	0.182	0.200
H5	0.244	0.275	0.273	0.266	0.279	0.303	0.293	0.274	0.284	0.284	0.269	0.311
H6	0.197	0.179	0.179	0.174	0.181	0.180	0.180	0.184	0.181	0.178	0.182	0.200
H7	0.244	0.275	0.273	0.265	0.278	0.257	0.293	0.288	0.277	0.280	0.269	0.320
C1	0.262	0.249	0.249	0.243	0.255	0.264	0.258	0.259	0.253	0.251	0.256	0.304
C2	0.247	0.261	0.260	0.249	0.263	0.282	0.274	0.281	0.266	0.263	0.265	0.279
C3	0.247	0.263	0.262	0.249	0.264	0.278	0.280	0.282	0.263	0.261	0.265	0.286
C4	-0.186	-0.193	-0.195	-0.189	-0.185	-0.176	-0.178	-0.174	-0.184	-0.184	-0.185	-0.166
C5	-0.185	-0.190	-0.191	-0.190	-0.192	-0.217	-0.214	-0.185	-0.211	-0.193	-0.189	-0.231
C6	-0.206	-0.233	-0.232	-0.225	-0.222	-0.229	-0.223	-0.221	-0.224	-0.225	-0.222	-0.236
C7	-0.185	-0.190	-0.190	-0.189	-0.191	-0.197	-0.188	-0.196	-0.187	-0.194	-0.190	-0.232
C8	-0.186	-0.193	-0.193	-0.187	-0.180	-0.179	-0.183	-0.190	-0.183	-0.182	-0.185	-0.166
C9	-0.196	-0.155	-0.163	-0.177	-0.176	-0.193	-0.191	-0.180	-0.184	-0.181	-0.168	-0.197
C10	0.247	0.262	0.260	0.249	0.271	0.251	0.275	0.256	0.262	0.276	0.267	0.279
C11	0.262	0.249	0.249	0.243	0.258	0.248	0.257	0.250	0.261	0.258	0.257	0.304
C12	0.247	0.262	0.260	0.249	0.270	0.257	0.271	0.253	0.274	0.277	0.267	0.287
C13	-0.186	-0.195	-0.196	-0.189	-0.180	-0.189	-0.179	-0.187	-0.180	-0.181	-0.184	-0.165
C14	-0.197	-0.154	-0.162	-0.177	-0.177	-0.168	-0.190	-0.180	-0.199	-0.180	-0.168	-0.200
C15	-0.186	-0.193	-0.193	-0.187	-0.184	-0.167	-0.184	-0.177	-0.185	-0.185	-0.184	-0.165
C16	-0.185	-0.190	-0.190	-0.189	-0.191	-0.183	-0.187	-0.196	-0.185	-0.193	-0.190	-0.244
C17	-0.206	-0.234	-0.233	-0.225	-0.222	-0.220	-0.224	-0.224	-0.222	-0.224	-0.222	-0.231
C18	-0.184	-0.191	-0.191	-0.190	-0.191	-0.207	-0.214	-0.192	-0.208	-0.190	-0.190	-0.244

Table S9. Atomic charges derived from the Natural Population Analysis (NPA), for the anion atoms in complexes **1**-**4**.

			Anion on heterocalixarene			
anion	atom	free anion	**1**	**2**	**3**	**4**
Cl^-	Cl1	-1.000	-0.861	-0.869	-0.875	-0.842
Br^-	Br1	-1.000	-0.862	-0.875	-0.882	-0.833
I^-	I1	-1.000	-0.877	-0.888	-0.896	-0.830
BF_4^-	B7	1.204	1.216	1.214	1.213	1.217
	F1	-0.551	-0.546	-0.553	-0.551	-0.549
	F2	-0.551	-0.523	-0.545	-0.545	-0.550
	F3	-0.551	-0.545	-0.545	-0.534	-0.535
	F4	-0.551	-0.554	-0.527	-0.544	-0.551
$CH_3CO_2^-$	C23	-0.767	-0.745	-0.747	-0.753	-0.751
	C24	0.676	0.704	0.704	0.693	0.693
	O7	-0.746	-0.729	-0.665	-0.751	-0.736
	O8	-0.746	-0.760	-0.789	-0.712	-0.734
$H_2PO_4^-$	P1	2.337	2.376	2.375	2.368	2.378
	O7	-1.156	-1.154	-1.155	-1.148	-1.154
	O8	-1.120	-1.148	-1.150	-1.143	-1.152
	O9	-1.007	-1.000	-0.982	-0.984	-0.987
	O10	-0.993	-0.980	-0.998	-1.010	-0.988
	H19	0.471	0.490	0.482	0.494	0.486
	H20	0.468	0.482	0.495	0.480	0.488
HSO_4^-	S5	2.382	2.391	2.386	2.378	2.387
	O7	-0.984	-0.935	-0.963	-0.954	-0.966
	O8	-0.985	-0.979	-0.953	-0.962	-0.959
	O9	-0.906	-0.924	-0.930	-0.928	-0.916
	O10	-0.986	-0.976	-0.966	-0.969	-0.972
	H19	0.462	0.483	0.484	0.484	0.478
NCS^-	N11	-0.561	-0.584	-0.582	-0.536	-0.567
	C23	-0.009	0.009	0.012	-0.007	0.014
	S5	-0.430	-0.346	-0.352	-0.350	-0.362
NO_3^-	N11	0.616	0.613	0.613	0.611	0.613
	O7	-0.539	-0.499	-0.513	-0.496	-0.505
	O8	-0.539	-0.501	-0.503	-0.497	-0.510
	O9	-0.539	-0.513	-0.505	-0.532	-0.507
PF_6^-	P1	2.439	2.447	2.446	2.446	2.444
	F1	-0.574	-0.559	-0.561	-0.564	-0.571
	F2	-0.574	-0.576	-0.575	-0.573	-0.572
	F3	-0.574	-0.556	-0.559	-0.563	-0.560
	F4	-0.574	-0.584	-0.582	-0.578	-0.565
	F5	-0.574	-0.559	-0.561	-0.564	-0.571
	F6	-0.574	-0.576	-0.575	-0.573	-0.571
SO_4^{2-}	S5	2.395	2.394	2.424	2.419	2.424
	O7	-1.098	-0.939	-0.980	-1.030	-0.955
	O8	-1.099	-0.701	-0.980	-1.012	-0.956
	O9	-1.099	-0.985	-1.086	-1.059	-1.054
	O10	-1.099	-0.943	-1.006	-1.031	-1.003

9. NBO second order stabilization energies

Table S10. Donor-acceptor $i \rightarrow j^*$ second order stabilization estimation (kcal.mol^{-1}), showing the contributions for the HB ($A^- \rightarrow$H-C), the donation to the triazine rings, and some backdonation from the heterocalixarenes to the anion molecules. The energetic contribution are the sum of all donor-acceptor NBOs.

		Cl^-		
	1·Cl^-	**2**·Cl^-	**3**·Cl^-	**4**·Cl^-
$A^- \rightarrow$H-C	Cl(lp) → C-H (σ*)	Cl(lp) → C-H(σ*)	Cl(lp) → C-H(σ*)	Cl(lp) → C-H(σ*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	27.37	26.59	23.12	6.26
$A^- \rightarrow$C-N	Cl(lp) → C-N(π*)	Cl(lp) → C-N(π*)	Cl(lp) → C-N(π*)	Cl(lp) → C-N(π*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	0.60	0.37	0.32	0.95
calix$\rightarrow A^-$	-	-	-	-
$\Delta E^{(2)}_{i \rightarrow j^*}$	-	-	-	-
		Br^-		
	1·Br^-	**2**·Br^-	**3**·Br^-	**4**·Br^-
$A^- \rightarrow$H-C	Br(lp) → C-H(σ*)	Br(lp) → C-H(σ*)	Br(lp) → C-H(σ*)	Br(lp) → C-H(σ*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	25.85	23.55	19.70	6.18
$A^- \rightarrow$C-N	Br(lp) → C-N(π*)	Br(lp) → C-N(π*)	Br(lp) → C-N(π*)	Br(lp) → C-N(π*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	0.66	0.60	0.36	1.12
calix$\rightarrow A^-$	-	-	-	-
$\Delta E^{(2)}_{i \rightarrow j^*}$	-	-	-	-
		I^-		
	1·I^-	**2**·I^-	**3**·I^-	**4**·I^-
$A^- \rightarrow$H-C	(a)	-	-	-
$\Delta E^{(2)}_{i \rightarrow j^*}$	-	-	-	-
$A^- \rightarrow$C-N	-	-	-	-
$\Delta E^{(2)}_{i \rightarrow j^*}$	-	-	-	-
calix$\rightarrow A^-$	-	-	-	-
$\Delta E^{(2)}_{i \rightarrow j^*}$	-	-	-	-
		NCS^-		
	1·NCS^-	**2**·NCS^-	**3**·NCS^-	**4**·NCS^-
$A^- \rightarrow$H-C	C-N(π) → C-H(σ*) C-S(σ)→ C-H(σ*) S(lp) → C-H(σ*)	C-N(π) → C-H(σ*) C-S(σ)→ C-H(σ*) S(lp) → C-H(σ*)	C-N(π) → C-H(σ*) C-S(σ)→ C-H(σ*) S(lp) → C-H(σ*)	C-N(π) → C-H(σ*) C-S(σ)→ C-H(σ*) S(lp) → C-H(σ*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	10.69	12.10	3.52	6.12
$A^- \rightarrow$C-N	N(lp) → C-N(π*)S(lp) → C-N(π*) C-N(π) → C-N(π*)	N(lp) → C-N(π*) S(lp) → C-N(π*) C-N(π) → C-N(π*)	N(lp) → C-N(π*) S(lp) → C-N(π*) C-N(π) → C-N(π*)	N(lp) → C-N(π*) S(lp) → C-N(π*) C-N(π) → C-N(π*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	2.04	1.34	3.32	1.99
calix$\rightarrow A^-$	C-N(π) → C-N(π*) C-H(σ) → C-N(π*) C-H(σ) → C-S(σ*)	C-N(π) → C-N(π*) C-H(σ) → C-N(π*) C-H(σ) → C-S(σ*)	C-N(π) → C-N(π*) C-H(σ) → C-N(π*) C-H(σ) → C-S(σ*)	C-N(π) → C-N(π*) C-H(σ) → C-N(π*) C-H(σ) → C-S(σ*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	1.15	1.36	0.81	1.06
		NO_3^-		
	1·NO_3^-	**2**·NO_3^-	**3**·NO_3^-	**4**·NO_3^-
$A^- \rightarrow$H-C	N-O(σ) → C-H(σ*) O(lp) → C-H(σ*)	N-O(σ) → C-H(σ*) O(lp) → C-N(π*) O(lp) → C-H(σ*)	N-O(σ) → C-H(σ*) O(lp) → C-H(σ*)	N-O(σ) → C-H(σ*) O(lp) → C-N(π*) O(lp) → C-H(σ*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	13.79	16.85	15.25	8.61
$A^- \rightarrow$C-N	N-O(BD) → C-N(π*) O-O(BD) → C-N(π*) O(lp) → C-N(π*)	O(lp) → C-N(π*)	N-O(BD) → C-N(π*) O(lp) → C-N(π*)	O(lp) → C-N(π*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	2.55	0.99	1.46	0.65
calix$\rightarrow A^-$	C-H(σ) → N-O (σ*) C-N(π) → N-O (σ*)	C-N(π) → N-O (σ*) N(lp) → N-O (σ*)	C-N(π) → N-O (σ*) N(lp) → N-O(σ*)	C-N(π) → N-O(σ*) N(lp) → N-O(σ*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	1.86	0.36	0.27	0.17

(a)Second order stabilization estimation was not reliable due the use of ECP on iodine atom.

Table S11. Donor-acceptor $i \rightarrow j^*$ second order stabilization estimation (kcal.mol^{-1}), showing the contributions for the HB ($A^- \rightarrow$H-C), the donation to the triazine rings, and some backdonation from the heterocalixarenes to the anion molecules. The energetic contribution are the sum of all donor-acceptor NBOs.

			$CH_3CO_2^-$	
	1·$CH_3CO_2^-$	**2**·$CH_3CO_2^-$	**3**·$CH_3CO_2^-$	**4**·$CH_3CO_2^-$
$A^-\rightarrow$H-C	O(lp) → C-H(σ*) C-C(σ) → C-H(σ*) C-O(π) → C-H(σ*)	O(lp) → C-H(σ*) C-C(σ) → C-H(σ*) C-O(π) → C-H(σ*)	O(lp) → C-H(σ*) C-C(σ) → C-H(σ*) C-O(π)→ C-H(σ*)	O(lp) → C-H(σ*) C-C(σ) → C-H(σ*) C-O(π) → C-H(σ*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	24.79	18.10	19.70	10.54
$A^-\rightarrow$C-N	O(lp) → C-N(π*) C-O(π) → C-N(π*)	O(lp) → C-N(π*) C-O(π) → C-N(π*)	O(lp) → C-N(π*) C-O(π)→ C-N(π*)	O(lp) → C-N(π*) C-O(π) → C-N(π*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	2.04	8.03	1.00	2.12
calix$\rightarrow A^-$	C-N(π) → O-C (σ*) C-H(σ) → O-C (σ*)	C-H(σ) → O-C (BD*)	C-N(π) → O-C (σ*) C-H(σ) → O-C (σ*) N(lp) → C-H(σ*)	C-C(σ) → O-C (σ*) C-H(σ) → O-C (σ*) S(lp) → O-C (σ*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	0.44	0.58	0.30	0.73
			BF_4^-	
	1·BF_4^-	**2**·BF_4^-	**3**·BF_4^-	**4**·BF_4^-
$A^-\rightarrow$H-C	F(lp) → C-H(σ*)	F(lp) → C-H(σ*)	F(lp) → C-H(σ*)	F(lp) → C-H(σ*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	6.37	4.71	7.44	2.39
$A^-\rightarrow$C-N	F(lp) → C-N(π*)	F(lp) → C-N(π*)	F(lp) → C-N(π*)	F(lp) → C-N(π*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	4.62	0.83	1.08	0.92
calix$\rightarrow A^-$	-	-	-	-
$\Delta E^{(2)}_{i\rightarrow j^*}$	-	-	-	-
			HSO_4^-	
	1·HSO_4^-	**2**·HSO_4^-	**3**·HSO_4^-	**4**·HSO_4^-
$A^-\rightarrow$H-C	O(lp) → C-H(σ*) O-S(σ) → C-H(σ*)	O(lp) → C-H(σ*) O-S(σ) → C-H(σ*)	S-O(σ) → C-H(σ*) O(lp) → C-H(σ*) O(lp) → C-C (BD*)	O(lp) → C-H(σ*) O(lp) → C-C (BD*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	11.28	12.81	7.62	4.94
$A^-\rightarrow$C-N	O(lp) → C-N(π*)	O(lp) → C-N(π*)	O(lp) → C-N(π*)	O(lp) → C-N(π*) O-H(σ) → C-N(π*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	2.43	1.93	1.64	1.70
calix$\rightarrow A^-$	C-H(σ) → S-O(σ*) C-H(σ) → O-H(σ*) C-N(π) → S-O(σ*)	C-H(σ) → S-O(σ*) C-H(σ) → O-H(σ*)	C-H(σ) → S-O(σ*) C-N(π) → S-O(σ*)	C-N(π) → S-O(σ*) S(lp) → S-O(σ*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	0.34	0.23	0.34	0.61
			$H_2PO_4^-$	
	1·$H_2PO_4^-$	**2**·$H_2PO_4^-$	**3**·$H_2PO_4^-$	**4**·$H_2PO_4^-$
$A^-\rightarrow$H-C	O(lp) → C-H(σ*) O-P(σ) → C-H(σ*)	O(lp) → C-H(σ*) O-P(σ) → C-H(σ*)	O(lp) → C-H(σ*) O-P(σ) → C-H(σ*)	O(lp) → C-H(σ*) O-P (σ) → C-H(σ*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	12.28	15.47	16.54	6.61
$A^-\rightarrow$C-N	O(lp) → C-N(π*)	O(lp) → C-N(π*)	O(lp) → C-N(π*)	O(lp) → C-N(π*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	2.51	1.59	1.04	15.73
calix$\rightarrow A^-$	C-N(π) → O-P(σ*) C-N(π) → O-H(σ*)	C-N(π) → O-P(σ*) C-N(π) → O-H(σ*)	C-N(π) → O-P(σ*) C-N(π) → O-H(σ*) N(lp) → O-H(σ*)	C-N(π) → O-P(σ*) S(lp) → O-P(σ*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	0.36	1.37	2.41	0.64
			SO_4^{2-}	
	1·SO_4^{2-}	**2**·SO_4^{2-}	**3**·SO_4^{2-}	**4**·SO_4^{2-}
$A^-\rightarrow$H-C	-	S-O(σ) → C-H(σ*) O(lp) → C-H(σ*)	S-O(σ) → C-H(σ*) O(lp) → C-H(σ*)	S-O(σ) → C-H(σ*) O(lp) → C-H(σ*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	-	21.31	29.1	22.41
$A^-\rightarrow$C-N	-	S-O(σ) → C-N(π*) O(lp) → C-N(π*)	S-O(σ) → C-N(π*) O(lp) → C-N(π*)	S-O(σ) → C-N(π*) O(lp) → C-N(π*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	-	22.18	16.44	15.66
calix$\rightarrow A^-$	-	C-H(σ) → S-O(σ*) C-N(π) → S-O(σ*)	N(lp) → S-O(σ*) C-N(π) → S-O(σ*)	C-H(σ) → S-O(σ*) C-N(π) → S-O(σ*)
$\Delta E^{(2)}_{i\rightarrow j^*}$	-	1.42	0.58	1.61

Table S12. Donor-acceptor $i \rightarrow j^*$ second order stabilization estimation (kcal.mol^{-1}), showing the contributions for the HB ($A^- \rightarrow$H-C), the donation to the triazine rings, and some backdonation from the heterocalixarenes to the anion molecules. The energetic contribution are the sum of all donor-acceptor NBOs.

	PF_6^-			
	1·PF_6^-	**2**·PF_6^-	**3**·PF_6^-	**4**·PF_6^-
$A^- \rightarrow$H-C	F(lp) → C-H(σ*)	F(lp) → C-H(σ*)	F(lp) → C-H(σ*)	F(lp) → C-H(σ*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	7.29	6.74	5.56	1.82
$A^- \rightarrow$C-N	F(lp) → C-N(π*)	F(lp) → C-N(π*)	F(lp) → C-N(π*)	F(lp) → C-N(π*)
$\Delta E^{(2)}_{i \rightarrow j^*}$	1.07	0.91	0.56	0.72
calix$\rightarrow A^-$	-	C-H(σ) → P(lp*)	-	-
$\Delta E^{(2)}_{i \rightarrow j^*}$	-	0.05	-	-

10. EDA analysis of x-ray structures

Table S13. EDA analysis (in kcal.mol^{-1}) for x-ray structures of $[Et_4N^+][\mathbf{1}\cdot BF_4^-]$,[1] varying the anion···Et_4N^+ counterion, ranging the equilibrium position from -2.0 to +10.0 Å. The equilibrium position (pointed as zero angstrom) is exaclty the found in x-ray data. The % values of each term are relative to the equilibrium position.

Dist (Å)	ΔE^{int}		ΔE^{Pauli}		ΔV^{elstat}		ΔE^{oi}		ΔE^{disp}	
-2.00	341.9	*-438.9%*	1016.3	*9963.7%*	-344.2	*510.7%*	-317.5	*2461.2%*	-12.6	*163.6%*
-1.75	110.0	*-141.2%*	502.7	*4928.4%*	-239.4	*355.2%*	-141.5	*1096.9%*	-11.7	*151.9%*
-1.50	-3.6	*4.6%*	231.9	*2273.5%*	-158.9	*235.8%*	-65.7	*509.3%*	-10.9	*141.6%*
-1.25	-54.5	*70.0%*	105.2	*1031.4%*	-114.1	*169.3%*	-35.4	*274.4%*	-10.2	*132.5%*
-1.00	-74.8	*96.0%*	49.5	*485.3%*	-91.6	*135.9%*	-23.1	*179.1%*	-9.5	*123.4%*
-0.75	-81.2	*104.2%*	25.9	*253.9%*	-80.3	*119.1%*	-17.8	*138.0%*	-9.0	*116.9%*
-0.50	-81.8	*105.0%*	16.0	*156.9%*	-74.1	*109.9%*	-15.2	*117.8%*	-8.5	*110.4%*
-0.25	-80.2	*103.0%*	11.9	*116.7%*	-70.2	*104.2%*	-13.8	*107.0%*	-8.0	*103.9%*
0.00	**-77.9**	***100.0%***	**10.2**	***100.0%***	**-67.4**	***100.0%***	**-12.9**	***100.0%***	**-7.7**	***100.0%***
0.25	-75.5	*96.9%*	9.4	*92.2%*	-65.2	*96.7%*	-12.4	*96.1%*	-7.4	*96.1%*
0.50	-73.2	*94.0%*	9.0	*88.2%*	-63.2	*93.8%*	-11.9	*92.2%*	-7.1	*92.2%*
1.00	-69.2	*88.8%*	8.7	*85.3%*	-59.7	*88.6%*	-11.4	*88.4%*	-6.8	*88.3%*
2.00	-62.9	*80.7%*	8.5	*83.3%*	-54.1	*80.3%*	-10.9	*84.5%*	-6.5	*84.4%*
3.00	-58.1	*74.6%*	8.5	*83.3%*	-49.6	*73.6%*	-10.6	*82.2%*	-6.4	*83.1%*
4.00	-54.3	*69.7%*	8.5	*83.3%*	-46.0	*68.2%*	-10.5	*81.4%*	-6.4	*83.1%*
5.00	-51.3	*65.9%*	8.5	*83.3%*	-43.0	*63.8%*	-10.4	*80.6%*	-6.3	*81.8%*
7.50	-45.7	*58.7%*	8.5	*83.3%*	-37.5	*55.6%*	-10.4	*80.6%*	-6.3	*81.8%*
10.00	-41.9	*53.8%*	8.5	*83.3%*	-33.7	*50.0%*	-10.3	*79.8%*	-6.3	*81.8%*

Table S14. EDA analysis (in kcal.mol^{-1}) for x-ray structures of $[Et_4N^+][\mathbf{1}\cdot NCS^-]$,[1] varying the anion···Et_4N^+ counterion, ranging the equilibrium position from -2.0 to +10.0 Å. The equilibrium position (pointed as zero angstrom) is exaclty the found in x-ray data. The % values of each term are relative to the equilibrium position.

Dist (Å)	ΔE^{int}		ΔE^{Pauli}		ΔV^{elstat}		ΔE^{oi}		ΔE^{disp}	
-2.00	117.2	*-133.5%*	550.7	*3933.6%*	-264.5	*354.1%*	-150.5	*1016.9%*	-18.5	*150.4%*
-1.75	15.5	*-17.7%*	315.4	*2252.9%*	-197.1	*263.9%*	-84.0	*567.6%*	-18.8	*152.8%*
-1.50	-43.2	*49.2%*	177.3	*1266.4%*	-150.0	*200.8%*	-52.3	*353.4%*	-18.3	*148.8%*
-1.25	-73.9	*84.2%*	99.5	*710.7%*	-120.0	*160.6%*	-36.0	*243.2%*	-17.3	*140.7%*
-1.00	-87.8	*100.0%*	57.1	*407.9%*	-101.7	*136.1%*	-27.0	*182.4%*	-16.2	*131.7%*
-0.75	-92.7	*105.6%*	34.6	*247.1%*	-90.5	*121.2%*	-21.7	*146.6%*	-15.1	*122.8%*
-0.50	-92.8	*105.7%*	22.9	*163.6%*	-83.3	*111.5%*	-18.4	*124.3%*	-14.0	*113.8%*
-0.25	-90.8	*103.4%*	17.0	*121.4%*	-78.4	*105.0%*	-16.2	*109.5%*	-13.1	*106.5%*
0.00	**-87.8**	***100.0%***	**14.0**	***100.0%***	**-74.7**	***100.0%***	**-14.8**	***100.0%***	**-12.3**	***100.0%***
0.25	-84.7	*96.5%*	12.4	*88.6%*	-71.7	*96.0%*	-13.7	*92.6%*	-11.7	*95.1%*
0.50	-81.7	*93.1%*	11.7	*83.6%*	-69.3	*92.8%*	-13.0	*87.8%*	-11.2	*91.1%*
1.00	-76.4	*87.0%*	11.0	*78.6%*	-65.1	*87.1%*	-12.0	*81.1%*	-10.4	*84.6%*
2.00	-68.5	*78.0%*	10.7	*76.4%*	-58.5	*78.3%*	-11.0	*74.3%*	-9.7	*78.9%*
3.00	-62.9	*71.6%*	10.7	*76.4%*	-53.5	*71.6%*	-10.6	*71.6%*	-9.5	*77.2%*
4.00	-58.6	*66.7%*	10.7	*76.4%*	-49.5	*66.3%*	-10.4	*70.3%*	-9.4	*76.4%*
5.00	-55.2	*62.9%*	10.7	*76.4%*	-46.2	*61.8%*	-10.3	*69.6%*	-9.4	*76.4%*
7.50	-49.0	*55.8%*	10.7	*76.4%*	-40.2	*53.8%*	-10.2	*68.9%*	-9.3	*75.6%*
10.00	-44.9	*51.1%*	10.7	*76.4%*	-36.1	*48.3%*	-10.2	*68.9%*	-9.3	*75.6%*

Table S15. EDA analysis (in kcal.mol^{-1}) for x-ray structures of $[Et_4N^+][\mathbf{1}\cdot NO_3^-]$,[1] varying the anion···Et_4N^+ counterion, ranging the equilibrium position from -2.0 to +10.0 Å. The equilibrium position (pointed as zero angstrom) is exaclty the found in x-ray data. The % values of each term are relative to the equilibrium position.

Dist (Å)	ΔE^{int}		ΔE^{Pauli}		ΔV^{elstat}		ΔE^{oi}		ΔE^{disp}	
-2.00	36.8	*-44.2%*	377.5	*2621.5%*	-223.8	*313.0%*	-104.6	*618.9%*	-12.2	*134.1%*
-1.75	-34.1	*41.0%*	189.8	*1318.1%*	-156.4	*218.7%*	-55.9	*330.8%*	-11.7	*128.6%*
-1.50	-69.6	*83.7%*	98.7	*685.4%*	-120.2	*168.1%*	-36.7	*217.2%*	-11.4	*125.3%*
-1.25	-84.7	*101.8%*	54.5	*378.5%*	-100.3	*140.3%*	-28.0	*165.7%*	-10.9	*119.8%*
-1.00	-89.7	*107.8%*	33.1	*229.9%*	-89.0	*124.5%*	-23.3	*137.9%*	-10.5	*115.4%*
-0.75	-90.0	*108.2%*	22.7	*157.6%*	-82.1	*114.8%*	-20.6	*121.9%*	-10.1	*111.0%*
-0.50	-88.3	*106.1%*	17.8	*123.6%*	-77.5	*108.4%*	-18.9	*111.8%*	-9.7	*106.6%*
-0.25	-85.8	*103.1%*	15.5	*107.6%*	-74.2	*103.8%*	-17.7	*104.7%*	-9.4	*103.3%*
0.00	**-83.2**	***100.0%***	**14.4**	***100.0%***	**-71.5**	***100.0%***	**-16.9**	***100.0%***	**-9.1**	***100.0%***
0.25	-80.6	*96.9%*	13.8	*95.8%*	-69.2	*96.8%*	-16.3	*96.4%*	-8.9	*97.8%*
0.50	-78.3	*94.1%*	13.6	*94.4%*	-67.2	*94.0%*	-15.9	*94.1%*	-8.8	*96.7%*
1.00	-74.2	*89.2%*	13.3	*92.4%*	-63.7	*89.1%*	-15.3	*90.5%*	-9.7	*106.6%*
2.00	-67.9	*81.6%*	13.2	*91.7%*	-58.0	*81.1%*	-14.8	*87.6%*	-8.3	*91.2%*
3.00	-63.2	*76.0%*	13.2	*91.7%*	-53.7	*75.1%*	-14.5	*85.8%*	-8.2	*90.1%*
4.00	-59.8	*71.9%*	13.1	*91.0%*	-50.2	*70.2%*	-14.6	*86.4%*	-8.2	*90.1%*
5.00	-57.2	*68.8%*	13.1	*91.0%*	-47.3	*66.2%*	-14.9	*88.2%*	-8.2	*90.1%*
7.50	-51.2	*61.5%*	13.1	*91.0%*	-42.0	*58.7%*	-14.2	*84.0%*	-8.2	*90.1%*
10.00	-47.5	*57.1%*	13.1	*91.0%*	-38.3	*53.6%*	-14.2	*84.0%*	-8.2	*90.1%*

Table S16. EDA analysis (in kcal.mol^{-1}) for x-ray structures of $[Et_4N^+][\mathbf{1}\cdot PF_6^-]$,[1] varying the anion···Et_4N^+ counterion, ranging the equilibrium position from -2.0 to +10.0 Å. The equilibrium position (pointed as zero angstrom) is exaclty the found in x-ray data. The % values of each term are relative to the equilibrium position.

Dist (Å)	ΔE^{int}		ΔE^{Pauli}		ΔV^{elstat}		ΔE^{oi}		ΔE^{disp}	
-2.00	361.1	*-481.5%*	998.8	*12485.0%*	-410.5	*646.5%*	-208.7	*2151.5%*	-18.5	*188.8%*
-1.75	126.4	*-168.5%*	491.3	*6141.3%*	-247.5	*389.8%*	-100.3	*1034.0%*	-17.1	*174.5%*
-1.50	5.3	*-7.1%*	230.2	*2877.5%*	-157.7	*248.3%*	-51.3	*528.9%*	-15.8	*161.2%*
-1.25	-49.9	*66.5%*	105.6	*1320.0%*	-111.6	*175.7%*	-29.4	*303.1%*	-14.6	*149.0%*
-1.00	-72.1	*96.1%*	49.4	*617.5%*	-88.6	*139.5%*	-19.4	*200.0%*	-13.5	*137.8%*
-0.75	-79.0	*105.3%*	24.9	*311.3%*	-76.9	*121.1%*	-14.6	*150.5%*	-12.4	*126.5%*
-0.50	-79.6	*106.1%*	14.4	*180.0%*	-70.5	*111.0%*	-12.1	*124.7%*	-11.4	*116.3%*
-0.25	-77.7	*103.6%*	10.0	*125.0%*	-66.4	*104.6%*	-10.6	*109.3%*	-10.6	*108.2%*
0.00	**-75.0**	***100.0%***	**8.0**	***100.0%***	**-63.5**	***100.0%***	**-9.7**	***100.0%***	**-9.8**	***100.0%***
0.25	-72.4	*96.5%*	7.2	*90.0%*	-61.2	*96.4%*	-9.1	*93.8%*	-9.2	*93.9%*
0.50	-69.9	*93.2%*	6.7	*83.8%*	-59.2	*93.2%*	-8.7	*89.7%*	-8.7	*88.8%*
1.00	-65.5	*87.3%*	6.3	*78.8%*	-55.7	*87.7%*	-8.1	*83.5%*	-8.1	*82.7%*
2.00	-58.8	*78.4%*	6.1	*76.3%*	-49.9	*78.6%*	-7.5	*77.3%*	-7.5	*76.5%*
3.00	-53.8	*71.7%*	6.0	*75.0%*	-45.4	*71.5%*	-7.2	*74.2%*	-7.3	*74.5%*
4.00	-50.0	*66.7%*	6.0	*75.0%*	-41.7	*65.7%*	-7.1	*73.2%*	-7.2	*73.5%*
5.00	-46.9	*62.5%*	6.0	*75.0%*	-38.7	*60.9%*	-7.0	*72.2%*	-7.2	*73.5%*
7.50	-41.2	*54.9%*	6.0	*75.0%*	-33.1	*52.1%*	-6.9	*71.1%*	-7.2	*73.5%*
10.00	-37.3	*49.7%*	6.0	*75.0%*	-29.3	*46.1%*	-6.9	*71.1%*	-7.2	*73.5%*

XYZ coordinates

Heterocalixarene conformation XYZ coordinates

Heterocalixarene **1** (1,3-alternate conformation) E= -6199.70 kcal/mol

C	1.130647196	-0.162000621	-2.835717436
C	0.339902913	0.745093702	-2.139397554
C	-0.783186803	0.251470353	-1.486644571
C	-1.132597158	-1.093377712	-1.529152756
C	0.819281734	-1.514757904	-2.904048278
C	-0.321899158	-1.974773014	-2.245005060
H	-0.582852992	-3.031123385	-2.291722241
O	-1.639852871	1.158850224	-0.826482727
C	-1.372045919	1.426949855	0.467566530
N	-0.318283350	0.841174808	1.044364055
C	-0.150750734	1.186378787	2.324405871
N	-0.919969095	2.022245397	3.033919718
N	-2.226577286	2.281106372	1.045179142
C	-1.929468322	2.519478350	2.321352136
O	0.885462892	0.661987575	3.011010292
C	1.753226791	-0.198232369	2.304122234
C	2.810012619	0.354138180	1.589351661
C	3.682637589	-0.519124981	0.951453256
C	3.532853895	-1.899498115	1.025121367
C	1.565608263	-1.571432205	2.404224743
C	2.466841886	-2.420041791	1.759357813
Cl	-2.987673058	3.614985482	3.158497022
H	4.244579641	-2.547891795	0.517636131
H	0.728702810	-1.961325276	2.980405647
O	4.800764777	0.010961867	0.271644512
C	4.641012012	0.306603150	-1.035019049
N	3.441265923	0.127385178	-1.595198096
C	3.403247159	0.453361780	-2.890393212
N	4.420709341	0.915931336	-3.628462929
N	5.745484046	0.761822002	-1.640710279
C	5.547691213	1.037810827	-2.928622023
O	2.241670343	0.316573105	-3.562951769
H	2.944929374	1.431485442	1.524805319
H	1.461582269	-2.188187989	-3.468477306
H	-2.026484300	-1.435227223	-1.010891092
H	0.594467907	1.801775516	-2.100703994
Cl	6.928124967	1.629759618	-3.801813627
H	2.336583486	-3.499064528	1.830206548

Heterocalixarene **2** (1,3-alternate conformation) E= -6265.39 kcal/mol

C	1.146960303	-0.123039241	-2.831652342
C	0.322465910	0.747951126	-2.128803798
C	-0.784897719	0.210640623	-1.483480481
C	-1.089477679	-1.144596777	-1.544753665
C	0.880796220	-1.484549492	-2.915787646
C	-0.248483715	-1.989474959	-2.269342594
H	-0.478100322	-3.052338216	-2.334425108
O	-1.672567941	1.079282505	-0.816273940
C	-1.410292513	1.352944971	0.481298713
N	-0.329351397	0.805900834	1.045637803
C	-0.163824802	1.147075462	2.326970290
N	-0.953488441	1.953001816	3.047224253
N	-2.293291263	2.168045771	1.070982786
C	-1.995843980	2.424232658	2.351053825
O	0.898305754	0.647176334	2.998278023
C	1.764618090	-0.205622393	2.284302359

C	2.824014240	0.352231670	1.578859242
C	3.700485676	-0.513372790	0.934928776
C	3.549462321	-1.894184910	0.993402756
C	1.575633416	-1.579955152	2.366644981
C	2.479737365	-2.421894299	1.717427307
H	-2.677450622	3.090443559	2.885526965
H	4.263003873	-2.538383994	0.482146555
H	0.736790254	-1.975586817	2.936014244
O	4.818746524	0.025693615	0.266141306
C	4.654333996	0.366041640	-1.032070305
N	3.458566389	0.175945730	-1.597149762
C	3.404017841	0.555408826	-2.877213601
N	4.402057323	1.081087017	-3.597517773
N	5.745278976	0.869105763	-1.622535773
C	5.541170108	1.202579985	-2.903196622
O	2.240429437	0.404726538	-3.548605206
H	2.959415744	1.430126641	1.526529164
H	1.547662081	-2.129952081	-3.483942416
H	-1.974033113	-1.522967473	-1.034840203
H	0.538610496	1.812313860	-2.081410997
H	6.397298115	1.616220862	-3.441137137
H	2.350553057	-3.502109211	1.778120021

Heterocalixarene **3** (1,3-alternate conformation) E= -6797.24 kcal/mol

C	-0.767498138	2.976486219	0.288932998
C	-1.269190550	1.712173096	0.621775627
C	-2.650917438	1.500748254	0.530871397
C	-3.506138081	2.515561341	0.068940749
C	-1.621320848	3.991344831	-0.175047838
C	-2.985331216	3.753138655	-0.286543709
H	-3.646907829	4.536277314	-0.658410308
N	-3.287632506	0.337125968	0.989456036
C	-2.930249886	-0.977986444	1.035521906
N	-1.726146253	-1.393887536	0.598908691
C	-1.606762635	-2.733711674	0.600149013
N	-2.527210920	-3.626081025	1.060542613
N	-3.926602977	-1.762138052	1.528269305
C	-3.641492500	-3.063135510	1.521122250
N	-0.509708035	-3.360010769	0.087164918
C	0.717473049	-2.950044582	-0.449880160
C	1.291740661	-1.685525378	-0.249097326
C	2.598214769	-1.473635409	-0.714918044
C	3.288222107	-2.480445808	-1.415131036
C	1.407588163	-3.953384802	-1.155635843
C	2.685611665	-3.710759825	-1.639153659
H	-4.402264922	-3.736285950	1.926999962
H	4.296997513	-2.284866860	-1.779983386
H	0.930047618	-4.920393773	-1.316611661
N	3.353118700	-0.320978461	-0.463682450
C	3.081350611	0.952476045	-0.058702718
N	1.821172353	1.389501542	0.116271615
C	1.760788137	2.703567540	0.402977097
N	2.817193912	3.536496844	0.603368895
N	4.219524451	1.683503011	0.103369819
C	4.003094272	2.949662444	0.450649978
N	0.567736549	3.358235756	0.492965453
H	0.753317175	-0.904092024	0.275671512
H	-1.203702212	4.961716748	-0.445441473
H	-4.576066693	2.320746486	-0.009436411
H	-0.611245587	0.932474287	0.988711424
H	4.886441477	3.573131213	0.618369750
H	3.215516002	-4.485924481	-2.192250118
H	-0.649749521	-4.367793518	0.104801164

H	4.353546503	-0.427118583	-0.616176557
H	0.721162770	4.357609358	0.603630581
H	-4.263789712	0.449703512	1.254129944

Heterocalixarene **4** (1,3-alternate conformation) E= -6008.65 kcal/mol

C	-0.502270760	2.565540148	-0.009018762
C	-1.486743457	1.950260460	0.770581857
C	-2.389649257	1.069214223	0.167865484
C	-2.301399069	0.792162907	-1.199872908
C	-0.410801510	2.291191377	-1.377080258
C	-1.304591462	1.397166136	-1.963312147
H	-1.238653690	1.188719717	-3.030530885
S	-3.723022817	0.396880941	1.145380044
C	-3.227276931	-1.282547695	1.369812003
N	-2.071726559	-1.734675474	0.864291789
C	-1.843419104	-3.029339579	1.121957150
N	-2.649665305	-3.860085207	1.812288966
N	-4.123295461	-1.999561778	2.076536647
C	-3.767667282	-3.276375731	2.257061680
S	-0.374203797	-3.825192063	0.555047436
C	0.440034167	-2.537183746	-0.373817960
C	1.601643039	-1.963104230	0.150652464
C	2.319765098	-1.038777990	-0.613670053
C	1.873736234	-0.679608256	-1.889254175
C	-0.009173953	-2.181250542	-1.649211007
C	0.704341509	-1.244866010	-2.395427560
H	-4.460384151	-3.905784236	2.821711926
H	2.448392144	0.032229516	-2.480015144
H	-0.907880883	-2.645237387	-2.052685776
S	3.877174434	-0.432868782	0.012960062
C	3.485574270	1.214342419	0.511649548
N	2.242094419	1.697436775	0.387861064
C	2.113122163	2.962508340	0.811069691
N	3.092014466	3.736980268	1.319451217
N	4.553004769	1.874664487	1.002904371
C	4.280644514	3.126943437	1.385295405
S	0.554311147	3.788394726	0.747332768
H	1.950994311	-2.242396139	1.143299193
H	0.354148769	2.783912610	-1.975239688
H	-3.017161219	0.111323838	-1.658088755
H	-1.554201832	2.161479065	1.836353241
H	5.112206631	3.710598120	1.788852440
H	0.360006418	-0.973074667	-3.392991371

Heterocalixarene **1** (chair-like-arene conformation) E= -6191.44 kcal/mol

C	0.933594604	-0.406905059	-3.012092178
C	0.450265620	0.824598616	-2.585380165
C	-0.799382602	0.838387654	-1.976334066
C	-1.558837580	-0.315476235	-1.807610608
C	0.207228349	-1.584632564	-2.863256434
C	-1.046087212	-1.531741933	-2.255996805
H	-1.629821147	-2.443307921	-2.136030753
O	-1.365457037	2.059991183	-1.549289083
C	-1.257351469	2.329024343	-0.229028656
N	-0.278949977	1.742707703	0.467147120
C	-0.299175047	2.033368970	1.770738812
N	-1.201017328	2.795719257	2.402134842
N	-2.173144882	3.182296193	0.248232795
C	-2.083077176	3.347095732	1.566859958
O	0.670707132	1.517078675	2.562357785
C	1.951160814	1.415815144	1.974768376
C	2.405623063	0.213116134	1.440714328
C	3.700598491	0.199788933	0.930241301

C	4.522005065	1.324615804	0.947658876
C	2.741793738	2.562064079	2.009962576
C	4.033416601	2.511877546	1.490545215
Cl	-3.244574005	4.421292487	2.285684245
H	5.533124120	1.252585366	0.550354897
H	2.340390110	3.472753785	2.451950582
O	4.271342511	-0.987330009	0.417030805
O	2.179107474	-0.487566623	-3.673251526
H	1.769570637	-0.667745383	1.398575481
H	0.624577604	-2.522398426	-3.224330491
H	-2.536830033	-0.250381124	-1.333849159
H	1.037192536	1.733011969	-2.694805609
H	4.665073613	3.399458495	1.516676822
C	4.234153645	-1.124533934	-0.929849937
N	3.159156097	-0.679826576	-1.586823718
C	3.237065833	-0.839421550	-2.911282210
N	4.282920907	-1.321934496	-3.595142178
N	5.307986531	-1.715134370	-1.468658701
C	5.264054909	-1.744883059	-2.801208231
Cl	6.662015490	-2.403368806	-3.593934308

Heterocalixarene **2** (chair-like-arene conformation) E= -6257.55 kcal/mol

C	1.086423685	-0.203573759	-3.040557971
C	0.466788826	0.926375956	-2.516182569
C	-0.778379767	0.749366511	-1.922129924
C	-1.401148562	-0.494406878	-1.857555167
C	0.497264776	-1.463855028	-2.993900360
C	-0.754406354	-1.604570491	-2.397299386
H	-1.229887314	-2.583525831	-2.357066981
O	-1.485619243	1.851691927	-1.396094774
C	-1.435527819	1.988147141	-0.047698019
N	-0.358122771	1.528515457	0.593982809
C	-0.425119574	1.654014301	1.922233682
N	-1.460824006	2.130021034	2.624208456
N	-2.496468345	2.585745194	0.508257199
C	-2.447684644	2.598457230	1.847303533
O	0.646554195	1.266438054	2.657597239
C	1.894567694	1.364019793	2.006820408
C	2.512531648	0.229181734	1.491922867
C	3.754341703	0.401257930	0.889599457
C	4.375176817	1.644690832	0.807760981
C	2.482845577	2.624298034	1.944009035
C	3.730244676	2.760156812	1.338233184
H	-3.305410599	3.037777143	2.361986558
H	5.351971718	1.724601391	0.333837931
H	1.960705795	3.479429112	2.370048161
O	4.457283741	-0.705153625	0.366125930
O	2.336217419	-0.096758352	-3.688339965
H	2.029952787	-0.744399422	1.524926022
H	1.019602396	-2.315420736	-3.426538528
H	-2.382114541	-0.577709551	-1.392702856
H	0.951262915	1.899161690	-2.538419894
H	4.204447732	3.738791715	1.283618379
C	4.415639179	-0.829242721	-0.984209392
N	3.332220623	-0.382326898	-1.624113701
C	3.409196459	-0.481004476	-2.953602473
N	4.457682247	-0.924569190	-3.657491893
N	5.488524295	-1.400769798	-1.543330139
C	5.446720177	-1.392748803	-2.883017703
H	6.313215609	-1.810624363	-3.400467206

Heterocalixarene **3** (planar conformation) E= -6797.67 kcal/mol

C	0.740744000	-0.638949000	-3.342787000

C	0.210198000	0.019780000	-2.222417000
C	-1.152355000	0.357671000	-2.245720000
C	-1.955891000	0.051898000	-3.360615000
C	-0.068798000	-0.948329000	-4.452797000
C	-1.410483000	-0.600565000	-4.455454000
H	-2.033954000	-0.836828000	-5.316602000
N	-1.844156000	0.997804000	-1.213826000
C	-1.558779000	1.493244000	0.024261000
N	-0.317276000	1.471659000	0.548607000
C	-0.265215000	2.023943000	1.776916000
N	-1.312553000	2.544475000	2.476006000
N	-2.679215000	1.992964000	0.615988000
C	-2.474905000	2.491277000	1.832376000
N	0.893301000	2.130111000	2.488443000
C	2.237671000	1.794615000	2.309719000
C	2.766546000	1.128219000	1.192737000
C	4.143782000	0.855753000	1.184204000
C	4.965550000	1.241761000	2.260525000
C	3.064208000	2.180719000	3.382585000
C	4.421837000	1.902400000	3.351634000
H	-3.346871000	2.896452000	2.353221000
H	6.031774000	1.016166000	2.229141000
H	2.627468000	2.699591000	4.236729000
N	4.831335000	0.197259000	0.161665000
N	2.068308000	-1.052751000	-3.483422000
H	2.132364000	0.833128000	0.364497000
H	0.369277000	-1.460430000	-5.310340000
H	-3.009946000	0.330720000	-3.354580000
H	0.830826000	0.254713000	-1.365135000
H	5.059358000	2.201123000	4.182867000
C	4.533373000	-0.355054000	-1.049525000
N	3.288052000	-0.351320000	-1.565352000
C	3.227356000	-0.945198000	-2.773603000
N	4.265887000	-1.507485000	-3.453190000
N	5.647639000	-0.884237000	-1.627308000
C	5.432144000	-1.436608000	-2.817875000
H	6.297767000	-1.873239000	-3.323838000
H	5.827789000	0.084973000	0.338468000
H	0.693262000	2.580452000	3.379513000
H	2.264266000	-1.522781000	-4.365407000
H	-2.837612000	1.124564000	-1.397649000

Heterocalixarene **4** (chair-like-arene conformation) E= -6002.57 kcal/mol

C	1.193690371	0.140521645	-3.109220468
C	0.465848914	1.261663109	-2.694688668
C	-0.679181753	1.078296500	-1.912260208
C	-1.076078966	-0.206668774	-1.524302567
C	0.799691331	-1.144639409	-2.720717396
C	-0.321038094	-1.310477945	-1.911105118
H	-0.625676253	-2.311512765	-1.605995681
S	-1.708441180	2.472861059	-1.484564713
C	-1.724095175	2.341304395	0.281884957
N	-0.743203488	1.673258710	0.899548052
C	-0.877199165	1.600184485	2.228923464
N	-1.921293316	2.063699051	2.942285212
N	-2.764189031	2.951282986	0.883623292
C	-2.811332672	2.743055444	2.206225410
S	0.408025136	0.844854473	3.189097519
C	1.792204249	1.026340911	2.073877996
C	2.531586097	-0.092246483	1.674593771
C	3.667408368	0.092550572	0.878061905
C	4.042847464	1.375477224	0.463233238
C	2.166051145	2.309804767	1.658975896

C	3.276947509	2.476403203	0.836496779
H	-3.660939799	3.173673474	2.740950271
H	4.934689344	1.506740784	-0.147795251
H	1.588324359	3.172944569	1.986223194
S	4.711681252	-1.294831815	0.460712345
S	2.586365972	0.323355332	-4.213499281
H	2.224636204	-1.093237132	1.974059002
H	1.368699325	-2.010002179	-3.056502253
H	-1.976053808	-0.337048718	-0.925165424
H	0.789082856	2.263784583	-2.971792912
H	3.565959088	3.475500390	0.510145575
C	4.712301170	-1.183589545	-1.307752792
N	3.721366970	-0.531811073	-1.925462764
C	3.865257102	-0.439255954	-3.252770252
N	4.918213634	-0.884084641	-3.964173004
N	5.756328329	-1.786508847	-1.910563045
C	5.805645419	-1.570908005	-3.231377679
H	6.656551093	-1.999244381	-3.767408399

Heterocalixarene **1** (pinched-cone conformation) E= -6178.97 kcal/mol

C	0.646302677	0.938428494	-3.317023118
C	0.143011919	1.027329370	-2.023005339
C	-1.234871610	1.069172663	-1.833815026
C	-2.111542668	1.079631989	-2.912687719
C	-0.195357994	0.947468518	-4.422679553
C	-1.573676359	1.031530294	-4.202092889
H	-2.248044934	1.034912864	-5.057423889
O	-1.727786038	1.173004621	-0.521555401
C	-1.079411176	0.359481048	0.360613917
N	-0.461430945	0.969832391	1.378451822
C	0.312030958	0.138077597	2.085695188
N	0.401610153	-1.191033501	1.940395520
N	-1.081234551	-0.952761908	0.093544034
C	-0.357118974	-1.666335087	0.954960686
O	1.124584377	0.718909671	3.012695812
C	2.483792527	0.404643725	2.830241886
C	3.011391553	0.498339487	1.546228477
C	4.354971917	0.199234944	1.343234216
C	5.189247875	-0.133345317	2.404464349
C	3.283341179	0.076615213	3.918646043
C	4.639353766	-0.176995283	3.688993792
Cl	-0.391365630	-3.386832586	0.762702088
H	6.237330629	-0.361553396	2.223234154
H	2.850326873	0.010878009	4.914340424
O	4.873738539	0.306225286	0.040980476
C	4.054613922	-0.233903379	-0.906271517
N	3.621248318	0.602782777	-1.855696285
C	2.672564741	0.061136197	-2.628184973
N	2.252054368	-1.211071932	-2.606973320
N	3.726089177	-1.524631231	-0.764014551
C	2.858515489	-1.951115977	-1.680811662
O	2.042826929	0.912330216	-3.485847722
H	2.386031494	0.821577294	0.716442135
H	0.219764079	0.879706058	-5.425869610
H	-3.185416854	1.114900507	-2.742581120
H	0.819080471	1.086128467	-1.172507684
Cl	2.465853319	-3.637737010	-1.654201224
H	5.278920484	-0.440581095	4.530367581

Heterocalixarene **2** (pinched-cone conformation) E= -6243.64 kcal/mol

C	0.654063937	0.916494980	-3.326659627
C	0.155501784	1.022469054	-2.031845757
C	-1.220782533	1.088140287	-1.837040216

C	-2.100528008	1.107113007	-2.913593151
C	-0.192119538	0.933644885	-4.429259604
C	-1.567999154	1.042964722	-4.204569509
H	-2.245156680	1.052342219	-5.057633321
O	-1.707220761	1.202804040	-0.524506809
C	-1.069487625	0.373688080	0.355345997
N	-0.434697932	0.973335786	1.368453933
C	0.317135193	0.129546668	2.084583135
N	0.379372978	-1.200796822	1.945617829
N	-1.098945575	-0.939078946	0.093761020
C	-0.382300151	-1.673622015	0.952357829
O	1.132936067	0.704648939	3.016966323
C	2.490569615	0.394370803	2.829955721
C	3.013112428	0.466272636	1.542228411
C	4.357909117	0.171951182	1.337497110
C	5.198943459	-0.134135164	2.401943090
C	3.298484103	0.092487789	3.920523600
C	4.655224623	-0.155988834	3.689671432
H	-0.408512217	-2.757746094	0.820300996
H	6.248049897	-0.357641837	2.220354570
H	2.870651461	0.044371794	4.919515100
O	4.872173112	0.255602877	0.033533981
C	4.041187344	-0.289871558	-0.904678000
N	3.612227034	0.542888466	-1.859127763
C	2.661346989	0.004868829	-2.631134809
N	2.227076739	-1.261691670	-2.599082835
N	3.700774606	-1.575615884	-0.751827532
C	2.816347146	-2.008079276	-1.658232237
O	2.047363539	0.860332325	-3.500990406
H	2.382217942	0.768653202	0.709040901
H	0.218430936	0.851905086	-5.433298465
H	-3.173086007	1.160299778	-2.739832892
H	0.835096196	1.073124151	-1.183911214
H	2.537936217	-3.063534568	-1.615635771
H	5.300833717	-0.397388916	4.533348941

Heterocalixarene **3** (pinched-cone conformation) E= -6764.98 kcal/mol

C	0.724638407	0.903530189	-3.443857109
C	0.157856662	0.901976001	-2.170955933
C	-1.198497392	1.156691576	-1.977013777
C	-2.002679552	1.464123763	-3.076521365
C	-0.072800951	1.207382074	-4.549055683
C	-1.425491672	1.502271998	-4.350067639
H	-2.051005588	1.737239790	-5.210831051
N	-1.705724034	1.151406571	-0.628767729
C	-1.091507765	0.272301138	0.250604028
N	-0.586168258	0.784534754	1.392057966
C	0.223004691	-0.068428650	2.053029687
N	0.406103476	-1.371101312	1.755261395
N	-0.979323256	-1.009815059	-0.154658904
C	-0.257805342	-1.773972998	0.668652976
N	1.002833469	0.453590766	3.075548603
C	2.423992235	0.271440157	2.956363167
C	2.976252231	0.163888726	1.680946176
C	4.350821606	0.034542460	1.490704229
C	5.200929316	0.044602065	2.599219359
C	3.267408347	0.282298815	4.070105999
C	4.648376619	0.183019395	3.876385944
H	-0.190287746	-2.835491890	0.418777515
H	6.276161172	-0.061604189	2.462538208
H	2.846151591	0.360216656	5.071470619
N	4.855251866	-0.017255557	0.144439183
C	4.003755694	-0.539608063	-0.818260263

N	3.710568349	0.243756248	-1.876877484
C	2.678322999	-0.211813528	-2.615732593
N	2.067315928	-1.405010294	-2.463343422
N	3.476746266	-1.755814585	-0.568421316
C	2.549366964	-2.132683964	-1.453070168
N	2.137318119	0.648019410	-3.560700818
H	2.322738429	0.212607178	0.813861897
H	0.358303355	1.203241359	-5.549391573
H	-3.065011396	1.657645351	-2.935991628
H	0.791981145	0.717609888	-1.306923202
H	2.132295155	-3.134988449	-1.327536121
H	5.308484898	0.189072297	4.743297205
H	5.274370328	0.859446304	-0.165667705
H	0.732872278	1.411155869	3.301524389
H	-1.805692463	2.081181797	-0.221414743
H	2.699493820	1.493275941	-3.661448316

Heterocalixarene **4** (pinched-cone conformation) E= -5991.9 kcal/mol

C	0.965567133	0.856188755	-3.856102284
C	0.206426024	1.346927345	-2.791519058
C	-1.157655677	1.055152672	-2.713071357
C	-1.781231896	0.336017628	-3.735806948
C	0.352016898	0.133875008	-4.882999661
C	-1.023472717	-0.102579211	-4.824867943
H	-1.505458074	-0.669926411	-5.620930157
S	-2.040190091	1.641003949	-1.266919888
C	-1.177025812	0.637976330	-0.072175460
N	-0.882784639	1.225013989	1.099754269
C	-0.079148478	0.489540548	1.887019413
N	0.319535339	-0.772162345	1.645549751
N	-0.839594403	-0.613228760	-0.433206110
C	-0.130719474	-1.269531276	0.489614896
S	0.546896946	1.299977116	3.345080127
C	2.170148183	0.538762808	3.342592280
C	3.036366321	0.887936255	2.304356605
C	4.283188618	0.267117568	2.195388091
C	4.697744837	-0.650710121	3.163455949
C	2.575131037	-0.378162612	4.316401465
C	3.846126944	-0.951267141	4.229576704
H	0.100224044	-2.317372785	0.280268462
H	5.665680824	-1.140467042	3.068269899
H	1.894419521	-0.654632186	5.119912749
S	5.289306175	0.693735297	0.773150638
C	4.216542402	-0.019960126	-0.460050749
N	4.087130594	0.666330630	-1.607239046
C	3.125600496	0.190715298	-2.416060715
N	2.421835707	-0.939169722	-2.223725847
N	3.573976188	-1.159511944	-0.146571869
C	2.728059235	-1.579814748	-1.092085302
S	2.725191326	1.195179092	-3.831457328
H	2.728026016	1.624639707	1.563504405
H	0.948684419	-0.253651790	-5.707279406
H	-2.843017727	0.104106229	-3.667361748
H	0.683811973	1.935439785	-2.009096597
H	2.238565092	-2.542135445	-0.921742031
H	4.163406697	-1.671202345	4.983723799

Heterocalixarene **1** (chair-like-triazine conformation) E= -6177.70 kcal/mol

C	0.964843000	-0.207795000	-3.107968000
N	0.330922000	0.931818000	-2.812804000
C	-0.740348000	0.742739000	-2.032798000
N	-1.249152000	-0.434102000	-1.644614000
N	0.567675000	-1.449243000	-2.803709000

C	-0.565934000	-1.481747000	-2.102896000
Cl	-1.207826000	-3.049239000	-1.736183000
O	-1.337507000	1.870006000	-1.558030000
C	-1.388769000	1.944562000	-0.154946000
C	-0.258430000	1.578027000	0.570079000
C	-0.274279000	1.701982000	1.956371000
C	-1.396606000	2.186156000	2.621906000
C	-2.527136000	2.435552000	0.471377000
C	-2.513056000	2.549833000	1.865063000
O	0.830068000	1.275646000	2.707891000
C	2.028720000	1.399515000	2.067622000
N	2.660644000	0.257200000	1.780955000
C	3.729114000	0.437867000	0.995567000
N	4.238446000	1.610259000	0.596426000
N	2.424429000	2.637281000	1.748946000
C	3.556685000	2.662769000	1.045722000
H	-3.397092000	2.930213000	2.374967000
O	4.320623000	-0.694194000	0.525802000
O	2.166090000	-0.077560000	-3.741753000
Cl	4.196624000	4.224636000	0.657296000
C	4.371421000	-0.775267000	-0.876856000
C	3.249072000	-0.392323000	-1.605414000
C	3.264295000	-0.521787000	-2.991382000
C	4.377969000	-1.028221000	-3.653917000
C	5.501646000	-1.289549000	-1.500298000
C	5.486980000	-1.409224000	-2.893462000
H	6.364766000	-1.807834000	-3.400532000
H	-1.387541000	2.275359000	3.706185000
H	-3.397889000	2.713378000	-0.118547000
H	0.621986000	1.206273000	0.052135000
H	2.374352000	-0.000271000	-1.092618000
H	6.366366000	-1.582615000	-0.908381000
H	4.368820000	-1.121542000	-4.737868000

Heterocalixarene **2** (chair-like-triazine conformation) E= -6243.37 kcal/mol

C	1.006861000	-0.083855000	-3.127669000
N	0.363994000	1.041720000	-2.797719000
C	-0.737155000	0.820118000	-2.071269000
N	-1.264820000	-0.370050000	-1.761697000
N	0.599917000	-1.336295000	-2.892163000
C	-0.562474000	-1.408143000	-2.231689000
H	-0.965807000	-2.405696000	-2.044714000
O	-1.347827000	1.932255000	-1.565185000
C	-1.394491000	1.971145000	-0.164279000
C	-0.301536000	1.507511000	0.562524000
C	-0.318110000	1.602299000	1.951220000
C	-1.406448000	2.150276000	2.622502000
C	-2.498941000	2.528508000	0.470905000
C	-2.488245000	2.609471000	1.866257000
O	0.752992000	1.076581000	2.687060000
C	1.971764000	1.241909000	2.091394000
N	2.615441000	0.116789000	1.762152000
C	3.715828000	0.338859000	1.034956000
N	4.242918000	1.529118000	0.725437000
N	2.378270000	2.494390000	1.856074000
C	3.540740000	2.566935000	1.196015000
H	-3.346789000	3.042033000	2.378529000
O	4.325793000	-0.772896000	0.527096000
O	2.224646000	0.080963000	-3.725464000
H	3.944239000	3.564491000	1.010140000
C	4.377540000	-0.803596000	-0.874270000
C	3.278658000	-0.351582000	-1.599762000
C	3.299416000	-0.435227000	-2.988981000

C	4.397318000	-0.962583000	-3.661640000
C	5.491479000	-1.339700000	-1.510732000
C	5.484277000	-1.411189000	-2.906750000
H	6.350217000	-1.826821000	-3.420562000
H	-1.397895000	2.218804000	3.708186000
H	-3.343785000	2.881563000	-0.116398000
H	0.555260000	1.077259000	0.050093000
H	2.415113000	0.061450000	-1.084528000
H	6.340914000	-1.683291000	-0.924449000
H	4.392138000	-1.022662000	-4.747768000

Heterocalixarene **3** (chair-like-triazine conformation) E= -6764.65 kcal/mol

C	0.981103000	-0.201870000	-3.089334000
N	0.214065000	0.890373000	-2.896538000
C	-0.794974000	0.695054000	-2.022926000
N	-1.162634000	-0.493617000	-1.497201000
N	0.716433000	-1.442055000	-2.624776000
C	-0.389034000	-1.512156000	-1.878695000
H	-0.679743000	-2.505723000	-1.527507000
N	-1.463896000	1.815353000	-1.554318000
C	-1.514507000	1.961034000	-0.119413000
C	-0.410056000	1.547173000	0.622797000
C	-0.376545000	1.674743000	2.009997000
C	-1.471374000	2.228892000	2.675101000
C	-2.612756000	2.518075000	0.537236000
C	-2.579366000	2.646095000	1.929855000
N	0.792798000	1.198549000	2.709252000
C	2.001098000	1.369013000	2.051805000
N	2.765456000	0.274662000	1.859612000
C	3.776692000	0.467622000	0.988527000
N	4.149860000	1.655961000	0.465493000
N	2.269184000	2.608140000	1.587352000
C	3.377405000	2.676243000	0.844899000
H	-3.435349000	3.080253000	2.445917000
N	4.442276000	-0.654482000	0.518892000
N	2.188777000	-0.029158000	-3.747276000
H	3.671746000	3.669193000	0.494844000
C	4.495419000	-0.792697000	-0.918136000
C	3.390721000	-0.379158000	-1.659781000
C	3.359197000	-0.503312000	-3.047234000
C	4.456407000	-1.051361000	-3.712648000
C	5.595921000	-1.344133000	-1.575150000
C	5.565022000	-1.467113000	-2.968060000
H	6.423416000	-1.895824000	-3.484622000
H	4.118090000	-1.498990000	0.991554000
H	0.694291000	0.244475000	3.058166000
H	2.286392000	0.924913000	-4.096334000
H	-1.153796000	2.660143000	-2.036165000
H	-1.448810000	2.342352000	3.758228000
H	-3.483852000	2.834338000	-0.034954000
H	0.444913000	1.114509000	0.107259000
H	2.534113000	0.049543000	-1.143713000
H	6.467460000	-1.658584000	-1.002505000
H	4.433256000	-1.163449000	-4.795751000

Heterocalixarene **4** (chair-like-triazine conformation) E= -5988.53 kcal/mol

C	1.047899000	-0.001919000	-3.175924000
N	0.252948000	1.068915000	-3.016039000
C	-0.710501000	0.901679000	-2.093151000
N	-0.974873000	-0.238525000	-1.431808000
N	0.883513000	-1.197722000	-2.583597000
C	-0.160228000	-1.252157000	-1.747847000
H	-0.361513000	-2.214670000	-1.270765000

S	-1.635684000	2.370817000	-1.702461000
C	-1.761923000	2.240493000	0.073374000
C	-0.716069000	1.700176000	0.820494000
C	-0.756611000	1.728478000	2.214397000
C	-1.843842000	2.316374000	2.872473000
C	-2.869711000	2.801345000	0.721120000
C	-2.894224000	2.840003000	2.116392000
S	0.495693000	0.887570000	3.170324000
C	1.925497000	1.149307000	2.139491000
N	2.717374000	0.076318000	1.978994000
C	3.682518000	0.242824000	1.057679000
N	3.953695000	1.384649000	0.401771000
N	2.095178000	2.346300000	1.550918000
C	3.142336000	2.400214000	0.719585000
H	-3.748193000	3.287580000	2.624626000
S	4.596452000	-1.230560000	0.656884000
S	2.472219000	0.261698000	-4.214254000
H	3.349223000	3.364144000	0.247159000
C	4.742503000	-1.071270000	-1.114586000
C	3.692102000	-0.538735000	-1.861531000
C	3.738878000	-0.553619000	-3.255061000
C	4.842099000	-1.112475000	-3.912900000
C	5.864455000	-1.603318000	-1.761161000
C	5.898436000	-1.623391000	-3.156956000
H	6.763938000	-2.047698000	-3.665540000
H	-1.869452000	2.360602000	3.960369000
H	-3.697843000	3.206653000	0.141439000
H	0.132312000	1.252927000	0.314471000
H	2.832562000	-0.115746000	-1.353592000
H	6.695626000	-2.001369000	-1.180872000
H	4.874621000	-1.145032000	-5.001066000

Host-guest complexes XYZ coordinates

1·Cl^- E= -6323.62 kcal/mol

Cl	0.064516710	0.070995093	2.538028627
C	-1.171546535	2.406222177	-0.710869276
C	0.021267213	2.145022900	-0.046890884
C	1.192186573	2.405734498	-0.749630106
C	1.199365401	2.877569348	-2.059442068
C	-1.221309741	2.877612914	-2.019907840
C	-0.021680314	3.104181299	-2.696485718
H	-0.038554183	3.469952891	-3.723095346
O	2.432153366	2.339846956	-0.082363588
C	2.877406582	1.147805246	0.357393232
N	2.327798010	0.026167990	-0.108142640
C	2.874529185	-1.080567470	0.394974830
N	3.911873259	-1.147267742	1.247065366
N	3.915742796	1.240580594	1.205814861
C	4.361307766	0.052241418	1.588623327
O	2.427470690	-2.285491306	-0.005674528
C	1.189378858	-2.370419616	-0.674420467
C	0.016958259	-2.087829717	0.016889540
C	-1.174124365	-2.368304605	-0.642379860
C	-1.220588158	-2.879130165	-1.936470491
C	1.199943009	-2.881413337	-1.969169349
C	-0.019350661	-3.126038454	-2.602847864
Cl	5.733597630	0.069338168	2.682344334
H	-2.184246498	-3.084187722	-2.400316573
H	2.150359195	-3.087972015	-2.458808810
O	-2.394321878	-2.282855576	0.058802323

C	-2.832915452	-1.078338630	0.468556616
N	-2.291644391	0.028749008	-0.039640921
C	-2.830720052	1.150164049	0.438221802
N	-3.855457668	1.242472866	1.303493518
N	-3.857425394	-1.145397640	1.336390969
C	-4.298906155	0.054037038	1.688408001
O	-2.389529171	2.342526293	-0.003358121
H	0.031762166	-1.616998687	1.018837493
H	-2.186029366	3.069485535	-2.487133002
H	2.148472545	3.069323887	-2.557734090
H	0.037509493	1.702604496	0.968305181
Cl	-5.657461713	0.070655376	2.799687322
H	-0.033617011	-3.521747359	-3.618175798

2·Cl^- E= -6385.17 kcal/mol

Cl	0.00159581	0.03538822	2.63004316
C	-1.18475594	2.39909770	-0.65441472
C	-0.00099575	2.11834343	0.01962492
C	1.18175575	2.40113622	-0.65540875
C	1.20772589	2.90780958	-1.95261611
C	-1.21276845	2.90570576	-1.95162232
C	-0.00300855	3.15044635	-2.60302211
H	-0.00374638	3.54369986	-3.61972275
O	2.40970822	2.33055930	0.02846086
C	2.84661798	1.13578761	0.48325768
N	2.31083528	0.01724096	-0.00576716
C	2.84781246	-1.09329629	0.49995253
N	3.85748024	-1.16860853	1.37966892
N	3.85634955	1.22547258	1.36143352
C	4.30351152	0.03161632	1.76275536
O	2.41307046	-2.29512909	0.06274083
C	1.18535368	-2.37963339	-0.61992705
C	0.00171446	-2.08439402	0.04823775
C	-1.18093444	-2.38163261	-0.62077520
C	-1.20698148	-2.91589495	-1.90680735
C	1.21327604	-2.91388127	-1.90592490
C	0.00359665	-3.17219101	-2.55215036
H	5.12664151	0.03746716	2.48251534
H	-2.16391436	-3.13295612	-2.37908465
H	2.17094448	-3.12942780	-2.37745887
O	-2.40932963	-2.29929886	0.06090904
C	-2.84582949	-1.09833618	0.49893595
N	-2.30996565	0.01333224	-0.00547258
C	-2.84736923	1.13078635	0.48428017
N	-3.85750959	1.21836188	1.36225234
N	-3.85577867	-1.17574248	1.37812295
C	-4.30338752	0.02361732	1.76224101
O	-2.41194751	2.32646353	0.03063640
H	0.00108261	-1.60443965	1.04604730
H	-2.17046172	3.11029987	-2.42798265
H	2.16462777	3.11403920	-2.42984681
H	-0.00037464	1.65812850	1.02646540
H	-5.12674190	0.02773200	2.48172367
H	0.00428555	-3.58757263	-3.55993466

3·Cl^- E= -6905.71 kcal/mol

Cl	0.001869403	0.025605206	2.468352529
C	-1.192723852	2.748002917	-0.610887581
C	0.002982336	2.156280063	-0.187274678
C	1.201102470	2.746156922	-0.607779812
C	1.209963097	3.867157681	-1.456036311
C	-1.196809970	3.868318029	-1.459647084
C	0.007740748	4.425860092	-1.877057626

H	0.009572884	5.296804123	-2.534239512
N	2.452020471	2.352943041	-0.093249086
C	2.953639307	1.130383271	0.241539062
N	2.307033383	0.011352745	-0.105515416
C	2.951534649	-1.106712006	0.248477465
N	4.161427854	-1.179748037	0.874333484
N	4.162976067	1.204971543	0.868081294
C	4.687921288	0.012946984	1.146081517
N	2.447279680	-2.330671506	-0.077374879
C	1.193466552	-2.728128946	-0.581505933
C	-0.002262598	-2.130198988	-0.167235464
C	-1.200538566	-2.726424011	-0.578048837
C	-1.209401812	-3.860795003	-1.407924968
C	1.197227338	-3.861710336	-1.411941106
C	-0.007325746	-4.426419137	-1.819599330
H	5.659968790	0.013489299	1.649544314
H	-2.163201633	-4.290664591	-1.716704541
H	2.149156271	-4.292282370	-1.723915352
N	-2.451911254	-2.325478778	-0.070740500
C	-2.953339605	-1.099455855	0.251878161
N	-2.306126680	0.016140606	-0.104969635
C	-2.950357238	1.137649476	0.238769428
N	-4.159867477	1.216799980	0.864614171
N	-4.163502072	-1.167885604	0.877967906
C	-4.687527943	0.026762950	1.146046961
N	-2.445973597	2.358135765	-0.099272477
H	-0.000583286	-1.301626362	0.560748177
H	-2.148939226	4.294782550	-1.778276150
H	2.163849066	4.292702064	-1.771789416
H	0.001376763	1.337813290	0.552963652
H	-5.659855891	0.031027919	1.649237758
H	-0.009267439	-5.306151242	-2.462471211
H	-3.107842430	-3.069198178	0.147751019
H	3.101608577	-3.076345108	0.139255516
H	-3.099237377	3.106607428	0.110792417
H	3.106828697	3.099512114	0.118712077

4·Cl^- E= -6120.91 kcal/mol

Cl	-0.004733743	0.038962668	2.049047050
C	-1.199215390	2.274756005	-0.691960626
C	0.009006938	2.404298851	0.002787346
C	1.208199850	2.278859865	-0.708107123
C	1.204944751	1.925243960	-2.058840885
C	-1.212955866	1.920968156	-2.042733402
C	-0.008200323	1.719974298	-2.717691719
H	-0.014967710	1.424601950	-3.766823830
S	2.724353158	2.710967062	0.123872040
C	3.366259498	1.143290227	0.611995199
N	2.816518531	0.016854394	0.151415474
C	3.355134724	-1.092241425	0.663505895
N	4.416901061	-1.154801057	1.496663831
N	4.428797775	1.234082040	1.440349151
C	4.908403926	0.045193344	1.820057622
S	2.704011585	-2.675239023	0.247051585
C	1.200030308	-2.272353980	-0.622516063
C	-0.007634263	-2.392872829	0.073514675
C	-1.207056759	-2.276891118	-0.637554098
C	-1.204957557	-1.940469100	-1.992830681
C	1.213718925	-1.936147005	-1.977596002
C	0.008207948	-1.743860808	-2.654181811
H	5.788313904	0.055967489	2.470432221
H	-2.151578054	-1.834314830	-2.521702650
H	2.166269866	-1.826667979	-2.494477090

S	-2.721560041	-2.683766733	0.211856840
C	-3.364727315	-1.102230747	0.646800771
N	-2.816354599	0.009414871	0.151142169
C	-3.354854823	1.133715382	0.629911569
N	-4.414400602	1.221381579	1.462409237
N	-4.428291160	-1.168114947	1.477331552
C	-4.906861839	0.031404234	1.821551763
S	-2.704515795	2.703604280	0.160977519
H	-0.012524824	-2.574611015	1.145533712
H	-2.166047721	1.807499444	-2.558412952
H	2.151308668	1.815960219	-2.586613663
H	0.015474468	2.608199211	1.070768591
H	-5.786524214	0.040506512	2.472273892
H	0.014296719	-1.461003444	-3.706827108

1·Br^- E= -6317.1 kcal/mol

Br	0.060352109	0.082781883	2.722718932
C	-1.174169172	2.411333984	-0.703491680
C	0.017572988	2.170969263	-0.030850913
C	1.191832493	2.410844947	-0.734092449
C	1.202729949	2.854377966	-2.053005099
C	-1.219028636	2.854437311	-2.021920090
C	-0.016610982	3.068864192	-2.697566840
H	-0.030011100	3.414602922	-3.730881562
O	2.428701664	2.348035736	-0.060910445
C	2.881617589	1.153562258	0.364687097
N	2.322676050	0.033746261	-0.096067799
C	2.881312700	-1.075595383	0.388569545
N	3.933399471	-1.146748391	1.221051615
N	3.934713118	1.241759444	1.194339648
C	4.386805158	0.051339427	1.563276023
O	2.429808043	-2.279498794	-0.012231432
C	1.191316742	-2.364499686	-0.678352177
C	0.017750909	-2.087469374	0.013059954
C	-1.174714760	-2.362978416	-0.645413268
C	-1.220662235	-2.871650878	-1.940022131
C	1.200220290	-2.873464804	-1.973586730
C	-0.019405676	-3.118721776	-2.606039247
Cl	5.776097601	0.062422179	2.634035196
H	-2.184121804	-3.077223519	-2.403691473
H	2.150206564	-3.080399895	-2.463640413
O	-2.394166279	-2.277155822	0.055271418
C	-2.838369180	-1.072890351	0.461849975
N	-2.287351523	0.035875298	-0.032504179
C	-2.839444389	1.156166607	0.435051835
N	-3.879453588	1.245334706	1.281387875
N	-3.876898036	-1.143007248	1.311806546
C	-4.325406471	0.055370811	1.659343495
O	-2.393684270	2.350120562	0.001166767
H	0.031146342	-1.636157545	1.020309407
H	-2.181762063	3.034665398	-2.497440179
H	2.153066585	3.034530773	-2.552821355
H	0.031131300	1.764045462	0.995696364
Cl	-5.699179468	0.067805510	2.750267625
H	-0.033848032	-3.516201020	-3.620479854

2·Br^- E= -6378.83 kcal/mol

Br	-0.00383454	0.04220261	2.80567188
C	-1.18788510	2.38482710	-0.67760463
C	-0.00300250	2.13667843	0.00625109
C	1.18141448	2.38795656	-0.67725589
C	1.20713428	2.84476497	-1.99264318
C	-1.21467893	2.84162851	-1.99294160

C	-0.00396576	3.06405832	-2.65089892
H	-0.00424153	3.41950201	-3.68151561
O	2.40720739	2.32903288	0.01105785
C	2.84767673	1.13594165	0.46919580
N	2.30579376	0.01519707	-0.00923372
C	2.84901482	-1.09370845	0.49459251
N	3.86502575	-1.16546860	1.36637741
N	3.86367232	1.22883158	1.33883316
C	4.31265609	0.03638338	1.74306357
O	2.41075631	-2.29738736	0.06366299
C	1.18639374	-2.37516148	-0.62538372
C	-0.00003647	-2.10988457	0.04921874
C	-1.18275688	-2.37850014	-0.63071683
C	-1.20532772	-2.86928499	-1.93374258
C	1.21630691	-2.86587235	-1.92829233
C	0.00729922	-3.10506752	-2.58335080
H	5.13910722	0.04502750	2.45874725
H	-2.16073888	-3.06837583	-2.41677614
H	2.17445821	-3.06242199	-2.40695743
O	-2.41044339	-2.30391029	0.05252592
C	-2.85106062	-1.10175437	0.48593359
N	-2.30864462	0.00903677	-0.01451305
C	-2.85262826	1.12797686	0.46577633
N	-3.87002815	1.21733448	1.33422201
N	-3.86817692	-1.17701523	1.35598528
C	-4.31799779	0.02342846	1.73491140
O	-2.41353559	2.32260006	0.01078136
H	-0.00271030	-1.67325656	1.06297504
H	-2.17170581	3.02513692	-2.47905575
H	2.16374913	3.03073832	-2.47863665
H	-0.00303892	1.72505451	1.03040046
H	-5.14548319	0.02918431	2.44941155
H	0.01011403	-3.48746437	-3.60416274

3·Br^- E= -6900.12 kcal/mol

Br	-0.005286485	0.030940755	2.615807083
C	-1.193178840	2.760905365	-0.629029720
C	0.004948550	2.156334290	-0.232699992
C	1.202201006	2.752851384	-0.643932345
C	1.206372241	3.893703660	-1.466042159
C	-1.200667330	3.902232992	-1.449839164
C	0.002215900	4.465225316	-1.863576715
H	0.001205512	5.351814259	-2.497872453
N	2.455399847	2.347326753	-0.148138295
C	2.952075984	1.125486875	0.198393702
N	2.296430261	0.003992605	-0.125212595
C	2.945321467	-1.111855953	0.230820183
N	4.159919864	-1.179843590	0.846861108
N	4.166766510	1.203909673	0.811862439
C	4.690225587	0.014272110	1.102873358
N	2.441290264	-2.339974107	-0.079579617
C	1.192425828	-2.749859791	-0.582911219
C	-0.006373727	-2.137274879	-0.201451171
C	-1.203041265	-2.742310688	-0.602635144
C	-1.205753147	-3.899642943	-1.400783012
C	1.201192966	-3.907196331	-1.380265071
C	-0.001006470	-4.478816003	-1.784191584
H	5.663988656	0.018560283	1.602928455
H	-2.157564569	-4.337991340	-1.704344799
H	2.154991909	-4.351110776	-1.667678425
N	-2.457572313	-2.327290172	-0.118941288
C	-2.954925731	-1.100122609	0.207808046
N	-2.298080361	0.016363634	-0.130517631

C	-2.947583579	1.137457695	0.208412752
N	-4.163607468	1.214592140	0.821217143
N	-4.172122215	-1.169328351	0.818437155
C	-4.695968971	0.024427894	1.091544186
N	-2.442715135	2.360553965	-0.119438822
H	-0.008387140	-1.292594050	0.501701314
H	-2.154035815	4.340743542	-1.747705394
H	2.158726279	4.325711976	-1.776754659
H	0.005814207	1.326003278	0.487158501
H	-5.672127297	0.027546328	1.588221674
H	0.000927396	-5.378483223	-2.399723389
H	3.099589190	-3.080265428	0.143905471
H	3.118324568	3.089654722	0.054148811
H	-3.100289600	3.104761558	0.092969254
H	-3.121716536	-3.065842818	0.092954031

4·Br^- E= -6116.86 kcal/mol

Br	-0.007098486	0.071085061	2.213679512
C	-1.202359811	2.265630887	-0.696957194
C	0.014526058	2.434706660	-0.026332211
C	1.205382247	2.279764129	-0.745920682
C	1.185669950	1.872956466	-2.081787048
C	-1.231639373	1.859572044	-2.032805267
C	-0.035002245	1.638220492	-2.715203673
H	-0.054496480	1.306013949	-3.753084885
S	2.735900514	2.729012145	0.049865867
C	3.397553570	1.170271323	0.539734054
N	2.814113639	0.034419859	0.149348994
C	3.381658471	-1.064454448	0.653912978
N	4.490921052	-1.108692440	1.423539813
N	4.508433464	1.277991147	1.300147985
C	5.001953002	0.097618819	1.688486987
S	2.702664471	-2.655777525	0.329266558
C	1.201812587	-2.280186184	-0.557373545
C	-0.014752860	-2.422554724	0.119465387
C	-1.205951238	-2.298120944	-0.605041084
C	-1.186959491	-1.949342069	-1.956920823
C	1.230920530	-1.932121748	-1.909258129
C	0.033727653	-1.742944564	-2.600509611
H	5.916157790	0.121699230	2.289109174
H	-2.127233279	-1.837214623	-2.495280838
H	2.189532313	-1.806420031	-2.410713213
S	-2.736380030	-2.694325006	0.220931310
C	-3.399998593	-1.108366223	0.606704253
N	-2.816134946	0.001871096	0.148263819
C	-3.382984208	1.129235858	0.585564753
N	-4.492063223	1.220726687	1.350951590
N	-4.512479881	-1.169113304	1.370184529
C	-5.005248160	0.032711502	1.686424456
S	-2.702891822	2.698587862	0.161536354
H	-0.032526382	-2.628245342	1.186584303
H	-2.190797905	1.717665041	-2.529178009
H	2.126045552	1.741539984	-2.615874358
H	0.033546514	2.692743265	1.029477073
H	-5.920339352	0.045271461	2.286026397
H	0.052658386	-1.453445793	-3.651045577

1·I^- E= -6308.31 kcal/mol

I	0.076736078	0.075757110	2.997860891
C	-1.173250571	2.374304596	-0.700475288
C	0.024171235	2.202294303	-0.017522635
C	1.196183801	2.372574278	-0.744356999
C	1.198354032	2.696764083	-2.097381186

C	-1.224949189	2.699029789	-2.052533372
C	-0.025705530	2.855383712	-2.750116297
H	-0.045190981	3.107135289	-3.810147352
O	2.433098567	2.341366497	-0.068242251
C	2.893086773	1.150735921	0.365772459
N	2.329024574	0.028378352	-0.082765617
C	2.887632859	-1.079301420	0.406975330
N	3.941461899	-1.146120141	1.235838436
N	3.947728354	1.243270608	1.190912489
C	4.397794073	0.054072209	1.569998064
O	2.423761371	-2.283140937	0.016260233
C	1.191297681	-2.335773633	-0.666536241
C	0.014806122	-2.139476449	0.046194996
C	-1.178371808	-2.333689513	-0.638522903
C	-1.221409436	-2.705745730	-1.978609037
C	1.202099325	-2.708034772	-2.007112092
C	-0.017710142	-2.888531089	-2.661941372
Cl	5.783208821	0.070890460	2.641776618
H	-2.183382823	-2.852712564	-2.467062264
H	2.152163834	-2.856603985	-2.517847549
O	-2.395131180	-2.279827789	0.072196783
C	-2.848119517	-1.076734573	0.476673908
N	-2.291781049	0.031923999	-0.013434360
C	-2.843553264	1.153699659	0.451560437
N	-3.885512714	1.244902746	1.293372202
N	-3.890037552	-1.144753746	1.320753977
C	-4.336135374	0.055161984	1.669672121
O	-2.384985916	2.345292779	0.020611615
H	0.028018082	-1.796812050	1.091360086
H	-2.190039616	2.829737777	-2.539373001
H	2.145120763	2.825311451	-2.619489398
H	0.043181672	1.896550515	1.038827969
Cl	-5.709016603	0.070407622	2.758166680
H	-0.030476651	-3.178357349	-3.712436081

2·I^- E= -6370.33 kcal/mol

I	-0.01089453	0.04568166	3.07457003
C	-1.18779009	2.36256992	-0.67539328
C	0.00026359	2.16983267	0.01979590
C	1.18470124	2.36661824	-0.68055874
C	1.20693006	2.73201601	-2.02346658
C	-1.21645358	2.72793951	-2.01830368
C	-0.00652776	2.90764142	-2.69111253
H	-0.00929783	3.19203201	-3.74327746
O	2.40919670	2.32989034	0.01231406
C	2.86353117	1.13785198	0.46049191
N	2.30901519	0.01665526	-0.00358141
C	2.86242201	-1.09326244	0.48793959
N	3.89449086	-1.16527039	1.33971052
N	3.89651047	1.22980493	1.30908867
C	4.35010718	0.03672867	1.70751953
O	2.40956368	-2.29570487	0.06739955
C	1.18811898	-2.35272089	-0.62895218
C	-0.00041821	-2.13851872	0.05921298
C	-1.18427937	-2.35657263	-0.63609379
C	-1.20489314	-2.76221169	-1.96767567
C	1.21814193	-2.75822084	-1.96044737
C	0.00894763	-2.95770380	-2.62882373
H	5.18805450	0.04490873	2.40932824
H	-2.15955986	-2.92628523	-2.46501779
H	2.17630072	-2.91915464	-2.45208054
O	-2.41006407	-2.30322058	0.05252351
C	-2.86374830	-1.10286277	0.47895048

N	-2.31005576	0.00943994	-0.00671898
C	-2.86379845	1.12826986	0.46404002
N	-3.89669794	1.21591999	1.31318552
N	-3.89626802	-1.17930372	1.32959972
C	-4.35124034	0.02090943	1.70437957
O	-2.40927661	2.32260128	0.02234731
H	-0.00397107	-1.77817406	1.09852225
H	-2.17402909	2.87321485	-2.51586239
H	2.16194822	2.88039123	-2.52499024
H	0.00379983	1.83891380	1.06858061
H	-5.18939023	0.02552882	2.40595907
H	0.01262152	-3.27378606	-3.67200632

3·I^- E= -6892.55 kcal/mol

I	0.008773614	0.067730062	2.879395620
C	-1.178598015	2.771253486	-0.673099804
C	0.015216916	2.154627344	-0.280803285
C	1.219234951	2.756717518	-0.664200393
C	1.233939683	3.915140889	-1.462276894
C	-1.173360273	3.928815007	-1.472586394
C	0.035147488	4.496048565	-1.862010324
H	0.042731175	5.395223537	-2.478295376
N	2.466008190	2.337604210	-0.168014853
C	2.963068222	1.112217465	0.165915649
N	2.289482902	-0.007016899	-0.131910333
C	2.947870639	-1.125324508	0.200194104
N	4.180146530	-1.197186324	0.778869939
N	4.195851079	1.185586791	0.743834360
C	4.722221154	-0.005212967	1.022088474
N	2.433762272	-2.353643214	-0.096120955
C	1.178228029	-2.771032693	-0.570722549
C	-0.015448991	-2.143803499	-0.195986790
C	-1.219766158	-2.756225859	-0.560698015
C	-1.235133102	-3.937681650	-1.323630009
C	1.172457082	-3.951782821	-1.335079371
C	-0.036437427	-4.530255876	-1.706397876
H	5.709577056	-0.004389592	1.495375644
H	-2.191106570	-4.383745755	-1.601001069
H	2.120625559	-4.409104482	-1.621403328
N	-2.465742848	-2.320625300	-0.076365428
C	-2.963453694	-1.083428197	0.209987551
N	-2.289030657	0.023525098	-0.129182750
C	-2.947758313	1.153886207	0.158318838
N	-4.180216433	1.248179134	0.733668619
N	-4.197228409	-1.134241539	0.788165491
C	-4.723109295	0.066575574	1.021151189
N	-2.434363760	2.369866271	-0.185535986
H	-0.008128137	-1.278732859	0.474863379
H	-2.121739148	4.378208674	-1.770929558
H	2.189773468	4.353607664	-1.752409887
H	0.008190038	1.308752710	0.414754956
H	-5.710951978	0.084174058	1.493185939
H	-0.044413283	-5.447011858	-2.296051107
H	-3.143667628	-3.048575397	0.130526152
H	3.101049576	-3.092029092	0.108047755
H	3.143187516	3.072702218	0.014525630
H	-3.101839016	3.115047898	-0.008646956

4·I^- E= -6110.85 kcal/mol

I	-0.001033815	0.009848265	2.466529197
C	-1.200020950	2.296734029	-0.634187319
C	0.017110929	2.481196234	0.032565306
C	1.209412476	2.313765502	-0.681987842

C	1.189962621	1.904270479	-2.016736196
C	-1.227784535	1.887364942	-1.968630418
C	-0.030381672	1.672379236	-2.651662525
H	-0.049084397	1.336898201	-3.688165527
S	2.743472804	2.726729888	0.127662277
C	3.403110505	1.146106092	0.549886112
N	2.813040423	0.024211166	0.127472749
C	3.385144547	-1.092092509	0.588985913
N	4.501218745	-1.163242441	1.345696780
N	4.519690930	1.226336468	1.304946461
C	5.014698839	0.033151309	1.649480151
S	2.701220172	-2.675455458	0.225755140
C	1.199293975	-2.276034868	-0.646365153
C	-0.017899663	-2.453749548	0.022277307
C	-1.210280081	-2.292840328	-0.694065050
C	-1.190690077	-1.898207257	-2.033385787
C	1.227053340	-1.881568019	-1.985301274
C	0.029742581	-1.673854285	-2.671020250
H	5.932212237	0.036186511	2.245318818
H	-2.131171853	-1.767470723	-2.567722920
H	2.185469484	-1.737644465	-2.482348514
S	-2.743244251	-2.706921905	0.116116421
C	-3.403821918	-1.128255703	0.545082147
N	-2.814000833	-0.004321809	0.127636468
C	-3.384490626	1.109636730	0.596647239
N	-4.498303319	1.176901284	1.357383583
N	-4.520167100	-1.212241533	1.299679668
C	-5.012991411	-0.020686664	1.653416389
S	-2.702843975	2.694491866	0.238015838
H	-0.036191085	-2.708094088	1.079252331
H	-2.186093682	1.735989731	-2.463982781
H	2.130343232	1.766766923	-2.549159482
H	0.035421785	2.744742304	1.087292502
H	-5.929596614	-0.026566976	2.250633794
H	0.048472232	-1.352058583	-3.711911554

1·BF_4^- E= -6936.95 kcal/mol

B	-0.344605716	0.089509398	3.182836576
F	0.941502013	0.063200362	2.560812174
F	-1.059915695	-1.083313484	2.788407425
F	-0.218116124	0.140769915	4.572575350
F	-1.054032450	1.233331403	2.702706204
C	1.172776168	-2.366495634	-0.575974225
C	-0.021669757	-2.166050330	0.105864688
C	-1.197405510	-2.367864779	-0.609882019
C	-1.202753516	-2.742374305	-1.949956461
C	1.218282486	-2.740490264	-1.915511302
C	0.017538268	-2.923975749	-2.602011094
H	0.032843644	-3.215846233	-3.651807961
O	-2.435787483	-2.314286894	0.057859508
C	-2.920577562	-1.107315427	0.411235602
N	-2.318800441	-0.005330170	-0.038035111
C	-2.913951340	1.122997027	0.351606668
N	-4.029567846	1.225948780	1.090628030
N	-4.036841633	-1.164324640	1.154371263
C	-4.511257408	0.040987295	1.442406692
O	-2.421944130	2.305891278	-0.065853500
C	-1.188622631	2.310336988	-0.745827535
C	-0.008950093	2.165624000	-0.023311797
C	1.181906047	2.309717873	-0.725539097
C	1.219724958	2.576584328	-2.090495147
C	-1.201751643	2.577150056	-2.111298271
C	0.014923426	2.705180421	-2.782639854

Cl	-5.981586329	0.070907290	2.395885180
H	2.180494270	2.682925824	-2.591113017
H	-2.153864368	2.684386736	-2.628118589
O	2.403621875	2.305300464	-0.020463577
C	2.889045016	1.120377113	0.399021157
N	2.327056992	-0.007427990	-0.036907736
C	2.881390293	-1.107366368	0.473385281
N	3.946443110	-1.163982640	1.289673436
N	3.954691382	1.224539885	1.209259150
C	4.413966682	0.040072863	1.592569504
O	2.391127073	-2.314769892	0.132617942
H	-0.036871131	1.936277635	1.043834965
H	2.181815884	-2.888593039	-2.400073446
H	-2.152070841	-2.892108901	-2.461376491
H	-0.054683702	-1.858444076	1.153304768
Cl	5.826551690	0.070454685	2.629298358
H	0.024166069	2.910839198	-3.852543692

2·BF_4^- E= -6999.02 kcal/mol

B	-0.32710229	0.09602382	3.22197779
F	0.96579475	0.08006806	2.61874098
F	-1.02883610	-1.08158065	2.82168217
F	-0.21800764	0.14670885	4.61662324
F	-1.03848097	1.23590465	2.73781648
C	1.17297261	-2.36451952	-0.57764911
C	-0.02352800	-2.15813557	0.10052780
C	-1.19957758	-2.36630240	-0.61374212
C	-1.20260724	-2.74907272	-1.95230727
C	1.21787602	-2.74699335	-1.91560772
C	0.01795094	-2.93461131	-2.60247130
H	0.03418099	-3.23323117	-3.65071353
O	-2.43684657	-2.31662397	0.05241415
C	-2.92684980	-1.10944835	0.41386070
N	-2.32755309	-0.00722491	-0.03934632
C	-2.92491585	1.12148834	0.34725645
N	-4.03331325	1.22705031	1.09188418
N	-4.03493844	-1.16827517	1.16451994
C	-4.52174371	0.03995191	1.46665096
O	-2.43196831	2.30355780	-0.08626218
C	-1.19496707	2.30596429	-0.75546342
C	-0.01935975	2.15499650	-0.02640253
C	1.17753471	2.30651486	-0.71797727
C	1.22331361	2.58387520	-2.08149107
C	-1.19737308	2.58303718	-2.11980499
C	0.02376679	2.71681991	-2.78181935
H	-5.42274846	0.05915423	2.08543771
H	2.18802095	2.69559478	-2.57367907
H	-2.14632487	2.69460978	-2.64189643
O	2.39363324	2.30543088	-0.00762304
C	2.88288051	1.12033188	0.42090944
N	2.32221123	-0.00744569	-0.01775141
C	2.87981846	-1.10841111	0.48729077
N	3.93889986	-1.16830098	1.30634115
N	3.94289288	1.22600059	1.23383215
C	4.41294824	0.03899948	1.63116007
O	2.38988670	-2.31614960	0.12884401
H	-0.05405656	1.92214739	1.04016541
H	2.18235141	-2.89894036	-2.39747684
H	-2.15201958	-2.90278550	-2.46276719
H	-0.05732046	-1.84680078	1.14714240
H	5.28027603	0.05758598	2.29631095
H	0.04072917	2.93105597	-3.85032859

3·BF_4^- E= -7521.38 kcal/mol

B	-0.696751825	0.073543812	2.995756049
F	0.420274759	0.067150097	2.089242791
F	-1.464098224	-1.098994724	2.765933641
F	-0.224026423	0.098852554	4.320936749
F	-1.484494793	1.223111161	2.727222931
C	1.217882622	-2.803276451	-0.508153348
C	0.019522016	-2.175271462	-0.149946721
C	-1.182035184	-2.802342208	-0.503824672
C	-1.181651879	-4.008876321	-1.228364857
C	1.224557511	-4.006362923	-1.235614039
C	0.020729506	-4.604615489	-1.591518527
H	0.019869490	-5.537964537	-2.155093631
N	-2.436796503	-2.358421047	-0.063861839
C	-2.942424465	-1.118531181	0.198775464
N	-2.258304479	-0.013277755	-0.127728830
C	-2.937694734	1.116265322	0.111679366
N	-4.194842748	1.211882597	0.625298576
N	-4.199072458	-1.167989117	0.720086545
C	-4.741194880	0.032266960	0.911753233
N	-2.426349716	2.331427813	-0.242385229
C	-1.171469575	2.742426423	-0.711481242
C	0.030850609	2.134854636	-0.325713496
C	1.228453910	2.736423154	-0.730476709
C	1.232768105	3.893282402	-1.528945134
C	-1.172485422	3.902715735	-1.508383250
C	0.028502504	4.473516459	-1.911545661
H	-5.748038835	0.051325651	1.340892669
H	2.184573461	4.328160476	-1.836095548
H	-2.124902609	4.346931920	-1.800585779
N	2.489458796	2.324714259	-0.260132285
C	3.005931915	1.108825253	0.074979067
N	2.332496616	-0.020603368	-0.177116362
C	2.998393135	-1.127473042	0.177734435
N	4.246055534	-1.178633932	0.727521810
N	4.254904956	1.201965272	0.615348876
C	4.793951105	0.020600291	0.910569925
N	2.474923833	-2.364442364	-0.048798843
H	0.036093013	1.282029454	0.350958825
H	2.177032010	-4.461750272	-1.509629493
H	-2.133208442	-4.468318177	-1.497431598
H	0.023357156	-1.282771941	0.473274827
H	5.795987430	0.037365016	1.350380556
H	0.026350079	5.372005392	-2.529894975
H	-3.118977823	-3.082461854	0.141626924
H	3.148250775	-3.094638362	0.165173431
H	-3.108436508	3.069636540	-0.095323965
H	3.169526678	3.065467882	-0.115650654

4·BF_4^- E= -6735.94 kcal/mol

B	-0.349872308	0.072716495	2.968262579
F	0.917774648	0.015139955	2.324687267
F	-1.091641205	-1.102438815	2.642431164
F	-0.181551172	0.161354426	4.363584902
F	-1.062225792	1.214917183	2.493460304
C	1.179307199	-2.314458397	-0.566805339
C	-0.043306658	-2.467004808	0.092840797
C	-1.228010475	-2.331903925	-0.637318415
C	-1.195659794	-1.990103361	-1.991926037
C	1.221695796	-1.971491228	-1.921629872
C	0.031328968	-1.790210876	-2.624030615
H	0.060140552	-1.508365799	-3.676759722
S	-2.771794390	-2.718232515	0.170530636

C	-3.418121331	-1.120244600	0.535096360
N	-2.817813442	-0.020377752	0.070698309
C	-3.406048529	1.116034658	0.455190170
N	-4.532439598	1.224348049	1.189409761
N	-4.547078373	-1.163705772	1.272430133
C	-5.044634484	0.044550726	1.552665795
S	-2.750349655	2.678010179	-0.029639273
C	-1.212400787	2.235187878	-0.818683179
C	-0.022093218	2.419327212	-0.108362742
C	1.195449053	2.245720500	-0.772121719
C	1.228642824	1.836840668	-2.108950306
C	-1.189113751	1.825008947	-2.154471733
C	0.033640964	1.607084400	-2.788973233
H	-5.965521420	0.070588938	2.142304971
H	2.188014549	1.702059700	-2.606650341
H	-2.127745431	1.681269265	-2.687982607
S	2.699495852	2.694018513	0.078101509
C	3.371766368	1.131278357	0.540265766
N	2.802953189	-0.003958627	0.126719158
C	3.360905993	-1.102279437	0.643535249
N	4.461631579	-1.147724684	1.423291286
N	4.473127992	1.238493833	1.312561951
C	4.969560810	0.057921563	1.695521390
S	2.676228926	-2.694498451	0.326904996
H	-0.053330850	2.667207663	0.950679774
H	2.184035339	-1.846661254	-2.415774694
H	-2.129925573	-1.879802949	-2.540758603
H	-0.082186477	-2.655584239	1.163960219
H	5.879418113	0.081422386	2.302100012
H	0.055225997	1.276565995	-3.827596029

1·$CH_3CO_2^-$ E= -7244.47 kcal/mol

O	0.995023421	-0.831045768	2.603680156
C	-0.109500904	0.283616811	4.421412856
C	-0.013977355	-0.146402400	2.945412163
O	-0.954893464	0.241885471	2.180514669
H	-1.146774799	0.209876727	4.773316918
H	0.190952844	1.339330596	4.498510280
H	0.556488853	-0.316212252	5.052914682
C	-1.329517569	2.312704288	-1.030822478
C	-0.311859708	2.044412496	-0.115645265
C	0.973716702	2.411207430	-0.490418857
C	1.268779453	2.988112682	-1.723466284
C	-1.085807045	2.883867851	-2.277288213
C	0.225931915	3.213816466	-2.621879141
H	0.434639596	3.659551698	-3.594199846
O	2.019207484	2.335575364	0.455799201
C	2.606093588	1.145281182	0.684871822
N	2.240803339	0.081389799	-0.027126611
C	2.893546223	-1.031351732	0.313086343
N	3.910828467	-1.130418392	1.181311449
N	3.571017486	1.192832879	1.620585707
C	4.169884903	0.022643944	1.783081612
O	2.584824740	-2.191690665	-0.303931832
C	1.288921096	-2.350447448	-0.826822856
C	0.182034196	-2.111897229	-0.016088536
C	-1.056418755	-2.431865058	-0.551696542
C	-1.217902058	-2.955479019	-1.832731661
C	1.185938388	-2.869176312	-2.114170290
C	-0.082987478	-3.167645252	-2.616139585
Cl	5.493283889	-0.002750732	2.936762821
H	-2.216333399	-3.192273284	-2.197452818
H	2.087940033	-3.039333246	-2.700211016

O	-2.201256241	-2.351810764	0.273816044
C	-2.796634917	-1.158428561	0.421647097
N	-2.386482908	-0.118392712	-0.306956604
C	-3.043945657	1.005493312	-0.039748413
N	-4.104062736	1.146704592	0.771824740
N	-3.834784147	-1.171810623	1.278094553
C	-4.426816993	0.007086903	1.372931658
O	-2.675973358	2.147640474	-0.668801453
H	0.308261949	-1.675824444	0.992620029
H	-1.918698542	3.071350201	-2.952762616
H	2.296641380	3.257977514	-1.960109059
H	-0.509912702	1.528031331	0.839446689
Cl	-5.823297423	0.080036642	2.436444641
H	-0.186391867	-3.573787739	-3.622488526

2·$CH_3CO_2^-$ E= -7302.47 kcal/mol

H	-0.14555762	4.10199669	1.68113820
H	-1.57784048	4.11766687	0.64365535
H	-0.35273215	5.41711725	0.47286847
O	0.80695056	4.03454595	-1.32386216
C	-0.50257519	4.34855283	0.67098844
C	0.22611842	3.46347035	-0.36386127
O	0.15818724	2.20518187	-0.14279105
C	2.64464530	-0.51686616	0.78281746
C	1.53360439	0.00518407	1.44637662
C	1.04103301	-0.72310534	2.52407878
C	1.58696636	-1.94362657	2.91881304
C	3.22436454	-1.73134145	1.14638404
C	2.68149470	-2.44597739	2.21449811
H	3.12121843	-3.39946410	2.50734428
O	0.07663221	-0.17051848	3.38420655
C	-1.04349184	0.40407102	2.89246699
N	-1.52235286	0.01150461	1.71079682
C	-2.65243460	0.63170435	1.36108830
N	-3.31369451	1.55563511	2.08018769
N	-1.59729225	1.29856650	3.72714812
C	-2.72724810	1.82968039	3.24768750
O	-3.27828388	0.29690195	0.21753245
C	-2.62226779	-0.47945059	-0.75985017
C	-1.51385885	0.03256445	-1.42109125
C	-1.03757703	-0.69145965	-2.51671677
C	-1.62091697	-1.89582429	-2.91421044
C	-3.23798469	-1.67450503	-1.12320854
C	-2.71910967	-2.38449059	-2.20721490
H	-3.22220194	2.57172257	3.88010289
H	-1.21300008	-2.42551462	-3.77362435
H	-4.10916853	-2.02296982	-0.57132344
O	-0.04225791	-0.17525664	-3.33600430
C	0.95878303	0.55505457	-2.73629993
N	1.55688647	0.00519091	-1.67754016
C	2.56566633	0.74947456	-1.21722617
N	2.99779332	1.91061113	-1.69663581
N	1.25063052	1.70605925	-3.32443477
C	2.24512421	2.37557780	-2.70758385
O	3.30341803	0.24664819	-0.18033388
H	-1.02635079	0.96101265	-1.08640653
H	4.09013020	-2.09398818	0.59513513
H	1.16411445	-2.47005420	3.77288121
H	1.07839469	0.94838921	1.11314531
H	2.51315051	3.34667776	-3.11767376
H	-3.18137157	-3.32449385	-2.50859892

3·$CH_3CO_2^-$ E= -7825.52 kcal/mol

H	1.984054789	3.259714465	0.586660028
H	0.778043932	4.447621501	1.095126047
H	1.546397667	4.594783749	-0.525245299
O	-0.240996868	3.122661934	-1.574575478
C	1.161123836	3.894120686	0.225859370
C	0.041083092	2.996025945	-0.355032703
O	-0.480874427	2.181061031	0.476075163
C	2.654342830	-0.200335742	1.056577999
C	1.363470379	-0.032210590	1.575113344
C	1.061788068	-0.667150754	2.786701719
C	2.002715379	-1.482767864	3.440661149
C	3.602974572	-1.010223692	1.706456497
C	3.272112664	-1.647680676	2.897546894
H	4.004365318	-2.278875026	3.401543112
N	-0.126511888	-0.417916025	3.497097772
C	-1.384497937	-0.082403465	3.087488994
N	-1.752942762	-0.247822264	1.814717926
C	-3.024271173	0.098552946	1.574390124
N	-3.919333967	0.558632548	2.498191468
N	-2.177354735	0.347709708	4.110973377
C	-3.417943916	0.644671473	3.726641373
N	-3.567563993	-0.058182033	0.339597855
C	-3.003643312	-0.452047074	-0.893306447
C	-1.776930778	0.050686270	-1.339688451
C	-1.391324560	-0.259255372	-2.650454894
C	-2.192764903	-1.071685775	-3.473464802
C	-3.813823747	-1.262163614	-1.706453095
C	-3.402879416	-1.567065610	-3.000461595
H	-4.098817628	0.997724796	4.508237567
H	-1.855874985	-1.300615131	-4.485423053
H	-4.758637375	-1.641659398	-1.315147862
N	-0.271999386	0.316186678	-3.272549427
C	0.917897322	0.753368362	-2.780921180
N	1.327850329	0.390619851	-1.556010114
C	2.538661410	0.856483645	-1.242826721
N	3.344200774	1.618531933	-2.032026431
N	1.644698060	1.457556894	-3.693214491
C	2.822796266	1.862456627	-3.235461350
N	3.122558816	0.530590888	-0.049080096
H	-1.209819806	0.762550549	-0.719058280
H	4.593552279	-1.130240737	1.266230815
H	1.727257446	-1.973628671	4.374913669
H	0.652227444	0.663255595	1.107934949
H	3.437601588	2.454701364	-3.920700269
H	-4.024266469	-2.195325612	-3.639208107
H	-0.039087428	-0.369072475	4.507414874
H	4.096309565	0.816224506	-0.021943399
H	-4.566078932	0.124999929	0.341395382
H	-0.393559645	0.593101206	-4.241768710

4·$CH_3CO_2^-$ E= -7042.08 kcal/mol

H	-0.229536219	4.390450155	1.219505329
H	-1.833342094	3.975252538	0.583101980
H	-0.777287381	5.051603060	-0.368121800
O	-0.245033213	2.924198053	-1.677491326
C	-0.789225280	4.179832064	0.298087952
C	-0.230951005	2.922059149	-0.406315301
O	0.147787324	1.980173097	0.350354256
C	2.291040888	-0.197662109	0.899614916
C	1.560272322	0.064358814	2.058286425
C	0.827498807	-0.965754645	2.655210413
C	0.788395578	-2.237667940	2.081498020
C	2.267960285	-1.472501846	0.322615446

C	1.505307307	-2.480795785	0.908496126
H	1.462867157	-3.465241012	0.442883936
S	-0.061445615	-0.612358815	4.164691831
C	-1.438850881	0.282893231	3.497414671
N	-1.713027886	0.160595171	2.199111209
C	-2.684716001	0.969145675	1.762485220
N	-3.402987202	1.822130827	2.533359855
N	-2.106800882	1.043481621	4.389132470
C	-3.077573022	1.778065924	3.826231223
S	-3.154039482	0.990332907	0.076569553
C	-2.127904485	-0.260624726	-0.675396681
C	-1.318852739	0.142039706	-1.736140271
C	-0.640239608	-0.839800253	-2.470649692
C	-0.724561953	-2.187846648	-2.120389077
C	-2.235539152	-1.610465696	-0.316828506
C	-1.516441537	-2.566060917	-1.030889151
H	-3.658056777	2.415980356	4.499584446
H	-0.167982451	-2.932266524	-2.689371578
H	-2.868205360	-1.902320660	0.519708002
S	0.269890405	-0.324225697	-3.922774230
C	1.477323170	0.726884091	-3.157944616
N	1.834096543	0.459958501	-1.900677852
C	2.695116484	1.331751076	-1.379408998
N	3.240207418	2.385793742	-2.021055390
N	1.978158811	1.702202057	-3.937066946
C	2.846290191	2.492841297	-3.293634057
S	3.300439488	1.122345445	0.263928193
H	-1.159718030	1.208181969	-1.956546456
H	2.825662087	-1.660490781	-0.591567368
H	0.184789187	-3.019288817	2.540736470
H	1.527146231	1.074653928	2.458770350
H	3.276468622	3.316285724	-3.870857441
H	-1.578670047	-3.616277308	-0.743351557

1·$H_2PO_4^-$ E= -7256.17 kcal/mol

O	-0.085238020	-0.292104123	4.751234820
O	-0.786302960	1.618990586	3.147817516
P	-0.205282621	0.061632534	3.143886383
O	-1.277102232	-0.839289722	2.590138756
H	-1.759730670	1.588453102	3.193255550
H	0.795325745	0.009006401	5.036832274
O	1.172698162	0.166991209	2.551657053
C	-1.107036630	2.387791389	-0.576698630
C	0.154050079	2.194514066	-0.029177049
C	1.244918910	2.355725111	-0.879738675
C	1.100104173	2.685339257	-2.223776028
C	-1.302055183	2.720834537	-1.914585528
C	-0.185713874	2.864407049	-2.738542548
H	-0.317434201	3.118312320	-3.790323969
O	2.545313497	2.303958819	-0.352724825
C	2.942743328	1.143407139	0.224003983
N	2.320688517	0.015134737	-0.107125264
C	2.765823871	-1.049178922	0.563498052
N	3.807749485	-1.079477054	1.412283022
N	3.988191676	1.275523234	1.052133682
C	4.347651854	0.114314992	1.588574254
O	2.199831222	-2.249571547	0.350970254
C	1.071427337	-2.312200863	-0.493310753
C	-0.187814655	-2.095330133	0.047091787
C	-1.275823390	-2.298328224	-0.797230697
C	-1.138793347	-2.693546806	-2.123343326
C	1.263762704	-2.709643358	-1.814645001
C	0.147072247	-2.896425259	-2.629627223

Cl	5.731977497	0.177350637	2.667912694
H	-2.025584483	-2.841190368	-2.737513801
H	2.274287162	-2.870163526	-2.186634523
O	-2.579892763	-2.217083219	-0.269503081
C	-2.963738972	-1.047169346	0.277355239
N	-2.343575841	0.075884454	-0.092803444
C	-2.764439777	1.153416220	0.563883536
N	-3.729478838	1.197270726	1.499633659
N	-4.013289645	-1.142961157	1.107533887
C	-4.307287919	0.014003302	1.679742430
O	-2.229338706	2.356507389	0.276457490
H	-0.346445430	-1.764014411	1.083334347
H	-2.313229571	2.861125447	-2.292871260
H	1.985471739	2.798818332	-2.846949922
H	0.281518817	1.920996995	1.020432492
Cl	-5.638881279	-0.011624420	2.818811004
H	0.278008721	-3.205780047	-3.666411427

2·$H_2PO_4^-$ E= -7318.03 kcal/mol

O	0.03013347	-0.24266948	4.79617900
O	-1.08187783	1.62565585	3.41198338
P	-0.31084244	0.17445048	3.23323552
O	-1.30307028	-0.82822277	2.70729956
H	-2.03465999	1.49524409	3.24295435
H	0.95156594	0.03165703	4.94804501
O	0.99427687	0.46763228	2.53565037
C	-1.11010382	2.33552180	-0.51454125
C	0.17364627	2.11179940	-0.03411418
C	1.22559244	2.33288863	-0.92273630
C	1.01959671	2.73873282	-2.23855476
C	-1.36490763	2.74468827	-1.82185481
C	-0.28776901	2.94013791	-2.68560978
H	-0.46659925	3.25497378	-3.71369909
O	2.55240775	2.27894192	-0.47229871
C	2.96399602	1.16573829	0.18880590
N	2.33946701	0.01500966	-0.05000305
C	2.78756834	-0.99728706	0.69429067
N	3.82197933	-0.96294598	1.54885596
N	4.01831884	1.35834168	0.99007542
C	4.38851941	0.24198937	1.63185822
O	2.21557687	-2.21107801	0.56523592
C	1.11942930	-2.33461063	-0.31319628
C	-0.16205707	-2.11599616	0.17173541
C	-1.21712450	-2.37392239	-0.70186514
C	-1.02200135	-2.82370348	-2.00377355
C	1.36660314	-2.78607269	-1.60854272
C	0.28441240	-3.02728416	-2.45429426
H	5.24940302	0.33090919	2.29993233
H	-1.88343750	-3.01097740	-2.64285324
H	2.39303011	-2.94285499	-1.93644424
O	-2.54067385	-2.29446127	-0.23482759
C	-2.94229427	-1.13072953	0.32719738
N	-2.32782334	-0.00142535	-0.03312534
C	-2.73356401	1.06426276	0.65321009
N	-3.67578175	1.08760102	1.61127638
N	-3.98350968	-1.24483526	1.16057420
C	-4.27191701	-0.09922184	1.78262656
O	-2.19871729	2.27170159	0.37872883
H	-0.35787769	-1.74577259	1.18881392
H	-2.39245068	2.90582912	-2.14364080
H	1.87732963	2.89684958	-2.89039923
H	0.35971593	1.75705664	0.98836136
H	-5.07931445	-0.13332248	2.51823455

H	0.45822444	-3.37752313	-3.47171056

3·$H_2PO_4^-$ E= -7837.09 kcal/mol

O	0.018409916	-0.175331451	4.719890040
O	-1.232489632	1.655907229	3.394470538
P	-0.240871937	0.343570492	3.166560073
O	-1.050257445	-0.719902692	2.473462146
H	-2.143322277	1.371552940	3.174708299
H	0.873650690	0.208048090	4.981803678
O	1.062681363	0.871062186	2.627290229
C	-1.155807029	2.580806072	-0.525594967
C	0.128068962	2.197023305	-0.144305508
C	1.209850657	2.602680082	-0.935125376
C	1.004601358	3.361538724	-2.094283796
C	-1.374907117	3.336296917	-1.683385957
C	-0.288750490	3.728617648	-2.464684940
H	-0.449664346	4.314629195	-3.370319189
N	2.538786527	2.335451322	-0.526055507
C	2.967916673	1.203740554	0.116890753
N	2.295250957	0.064502632	-0.075326495
C	2.792100295	-0.974680851	0.605749718
N	3.892134102	-0.953266040	1.410490217
N	4.103797703	1.358758097	0.843841512
C	4.483890910	0.237211990	1.462012186
N	2.225608742	-2.203348801	0.462332001
C	1.125579319	-2.574046472	-0.356424802
C	-0.152112772	-2.076362871	-0.098754047
C	-1.226798542	-2.587162678	-0.837286680
C	-1.023115729	-3.549305919	-1.835671737
C	1.339883132	-3.547745403	-1.342007444
C	0.260721404	-4.033233250	-2.078437870
H	5.385082393	0.306269485	2.079904737
H	-1.877657756	-3.918835489	-2.403773648
H	2.351676668	-3.910926822	-1.523140764
N	-2.569418465	-2.267724990	-0.499182678
C	-2.984568491	-1.117323235	0.122506662
N	-2.386632860	0.035789355	-0.188174924
C	-2.778338558	1.065630462	0.573495248
N	-3.696755955	1.011028722	1.581028531
N	-4.029242802	-1.276593346	0.976982635
C	-4.297320495	-0.176716040	1.680273280
N	-2.274302622	2.301023655	0.321049756
H	-0.328465671	-1.392356435	0.741361979
H	-2.394956945	3.607032483	-1.954746659
H	1.863446892	3.652410927	-2.700411314
H	0.310517278	1.646368336	0.786463975
H	-5.088666780	-0.259214572	2.431565521
H	0.421121255	-4.786350922	-2.850084725
H	-2.508253789	2.986083113	1.034582278
H	-3.148781980	-3.060765504	-0.234918959
H	2.750694311	-2.941451766	0.919786485
H	3.146378980	3.133071538	-0.363464492

4·$H_2PO_4^-$ E= -7056.42 kcal/mol

O	0.492298098	-0.662967853	4.321015742
O	-0.898989890	1.482958657	4.039422920
P	-0.146349852	0.311952631	3.143504873
O	-1.225616206	-0.474784157	2.444016198
H	-1.854161516	1.321436659	3.938121137
H	1.452764180	-0.505981093	4.298392314
O	1.012553854	0.956718578	2.426406387
C	-0.912606602	2.141720977	-0.526362163
C	0.434685224	2.322043547	-0.212347414

C	1.386267588	2.228694134	-1.237444190
C	1.004981237	1.912205053	-2.541428413
C	-1.309924077	1.831055335	-1.834692901
C	-0.347008048	1.700420557	-2.831034564
H	-0.649564194	1.435707170	-3.844823069
S	3.096475220	2.584206290	-0.854871373
C	3.442185701	1.228672933	0.235069084
N	2.694587538	0.130755617	0.132453760
C	2.921717242	-0.775630257	1.085798551
N	3.874806330	-0.695580093	2.040227784
N	4.456277575	1.426040555	1.098332803
C	4.614370424	0.412765075	1.961458420
S	1.979315974	-2.255174724	1.160042572
C	0.846507410	-2.100397562	-0.207530642
C	-0.511330168	-2.227150888	0.082907126
C	-1.427627820	-2.289242369	-0.976587491
C	-0.999344765	-2.175000682	-2.299587217
C	1.290860634	-1.993250114	-1.533069581
C	0.363613474	-2.014310297	-2.570675678
H	5.429611435	0.510990784	2.684228317
H	-1.728790330	-2.198933022	-3.108451417
H	2.353506767	-1.885633820	-1.741163279
S	-3.149832950	-2.588775944	-0.602402779
C	-3.518802412	-1.104004901	0.296065630
N	-2.793724763	-0.016788617	0.040635523
C	-3.020137287	0.997160608	0.879750495
N	-3.970246742	1.029478752	1.840499939
N	-4.527074968	-1.202273309	1.182263331
C	-4.698561707	-0.087002916	1.905760961
S	-2.089704154	2.482292525	0.767989858
H	-0.849091741	-2.205030905	1.120921280
H	-2.364275683	1.681633532	-2.059050161
H	1.762331718	1.818816024	-3.318572263
H	0.735121091	2.463698087	0.827345816
H	-5.512086944	-0.100567947	2.636898956
H	0.702464105	-1.910242611	-3.602325180

1·HSO_4^- E= -7067.33 kcal/mol

O	0.187991199	0.184002118	4.771698247
O	1.340354063	1.114298666	2.788759689
S	0.265009652	0.246083488	3.312025733
O	0.729899262	-1.319545798	2.839596435
H	1.511551817	-1.531861357	3.384682886
O	-1.008091101	0.367982191	2.589508994
C	-1.127806400	2.371130125	-0.483811221
C	0.106743134	2.190956079	0.124548190
C	1.234131427	2.367393779	-0.670213847
C	1.157674152	2.711617480	-2.015457981
C	-1.257860958	2.717011401	-1.826113570
C	-0.103124751	2.884649641	-2.591069925
H	-0.185461085	3.154117311	-3.643779648
O	2.511329725	2.302891267	-0.076342137
C	2.933951021	1.107153378	0.374853103
N	2.304530229	0.000191126	-0.028990689
C	2.812214452	-1.118438411	0.482569621
N	3.851298043	-1.213723808	1.329121504
N	4.029616523	1.164527733	1.148162344
C	4.395308213	-0.029383569	1.590854742
O	2.304370862	-2.309628234	0.102505768
C	1.133080311	-2.301601783	-0.682369628
C	-0.094888851	-2.161507285	-0.049504114
C	-1.235259789	-2.281675155	-0.835922350
C	-1.173228555	-2.524148071	-2.204349819

C	1.246152828	-2.545365575	-2.048229693
C	0.079954721	-2.651947051	-2.807522444
Cl	5.790413135	-0.057717592	2.651194653
H	-2.094457013	-2.609549420	-2.778112261
H	2.231990253	-2.647609683	-2.498681967
O	-2.497852150	-2.270875775	-0.215861379
C	-2.914756298	-1.105388676	0.333128832
N	-2.323551877	0.028700028	-0.035294578
C	-2.813987721	1.107519879	0.580418192
N	-3.852523435	1.135968181	1.431044298
N	-3.944179987	-1.239188001	1.181219352
C	-4.344550323	-0.069568880	1.670577546
O	-2.294886000	2.316836008	0.306425066
H	-0.140521990	-1.958108906	1.020874464
H	-2.250321111	2.850980745	-2.253197324
H	2.072320722	2.841206242	-2.591687093
H	0.203341875	1.907540888	1.174797943
Cl	-5.709698839	-0.136640936	2.766980929
H	0.147394585	-2.837147467	-3.879543579

2·HSO_4^- E= -7129.26 kcal/mol

O	0.68012173	1.27169663	2.81666815
O	-0.09728926	-0.00353799	4.81434641
S	0.22145632	-0.00662535	3.38128423
O	-1.30377899	-0.20321303	2.64414226
H	-1.85995501	-0.51995362	3.37935563
O	0.99065917	-1.17328490	2.91245447
C	1.17429891	-2.40077888	-0.56951646
C	-0.01246134	-2.23772608	0.14060676
C	-1.19753306	-2.42745775	-0.55861685
C	-1.22747510	-2.76015117	-1.91032466
C	1.19386673	-2.73230844	-1.92137860
C	-0.01868654	-2.90893033	-2.59057564
H	-0.02147158	-3.16658747	-3.64976388
O	-2.42285678	-2.39816474	0.14207986
C	-2.97830628	-1.19654610	0.39664728
N	-2.44175004	-0.10235386	-0.14528390
C	-3.05980508	1.02608266	0.20484539
N	-4.17400840	1.13297464	0.94515643
N	-4.07533900	-1.25056950	1.16910094
C	-4.62008671	-0.04852600	1.38347262
O	-2.57335664	2.20454451	-0.23838695
C	-1.28766136	2.20912960	-0.82047553
C	-0.16937336	2.10958479	-0.00146214
C	1.07449267	2.24288983	-0.61018435
C	1.21421616	2.46027039	-1.97856554
C	-1.19700794	2.42536331	-2.19169459
C	0.06796165	2.54733131	-2.76896923
H	-5.52896712	-0.02944187	1.99074793
H	2.21096064	2.55831423	-2.40548657
H	-2.10644873	2.49603554	-2.78600197
O	2.23083467	2.27159668	0.18678512
C	2.73748816	1.08894379	0.60578217
N	2.20987076	-0.04004344	0.12963572
C	2.82792139	-1.14082233	0.56003848
N	3.90383057	-1.19761100	1.35379771
N	3.79316930	1.19621300	1.42304812
C	4.31484064	0.01059288	1.75470629
O	2.40099538	-2.34533363	0.11104100
H	-0.22904968	1.91992241	1.07414781
H	2.14913026	-2.85098141	-2.43008006
H	-2.18511640	-2.90064201	-2.40933848
H	0.01345810	-1.96326619	1.19895878

H	5.17996515	0.03139474	2.42244097
H	0.15989946	2.71338414	-3.84215952

3·HSO_4^- E= -7649.81 kcal/mol

O	1.198883343	1.802311889	2.419808803
O	0.124725810	0.715976115	4.377985896
S	0.877860110	0.550530801	3.122854899
O	-0.281035163	-0.204185179	2.107858658
H	-1.104148195	-0.100892268	2.618920401
O	1.969529479	-0.428370933	3.145597361
C	1.034250359	-2.981615325	-0.341809240
C	-0.195226511	-2.314870897	-0.237569543
C	-1.342306650	-2.970720529	-0.700206764
C	-1.262035249	-4.240544167	-1.303162567
C	1.115461120	-4.258372284	-0.930268982
C	-0.032277614	-4.878370051	-1.408775029
H	0.032036864	-5.864400603	-1.869345084
N	-2.650597400	-2.496553603	-0.498247715
C	-3.177053445	-1.289921372	-0.139186089
N	-2.449165477	-0.166361780	-0.200738461
C	-3.130404032	0.933269164	0.166554901
N	-4.422860594	0.965005720	0.612530685
N	-4.487119390	-1.387271136	0.233229351
C	-5.020225592	-0.223001737	0.604740032
N	-2.574922929	2.169659399	0.090741788
C	-1.356620976	2.656395260	-0.430960467
C	-0.139648989	1.989258196	-0.274001732
C	1.028482050	2.646717316	-0.683638060
C	0.962813001	3.919946350	-1.280998718
C	-1.427984909	3.931905859	-1.017117360
C	-0.261016992	4.556535047	-1.442266769
H	-6.062885950	-0.247964204	0.937692615
H	1.886298205	4.410494094	-1.591403716
H	-2.396522769	4.421454364	-1.129720485
N	2.319284177	2.168857191	-0.443194559
C	2.806692393	0.976041202	0.014700139
N	2.093126613	-0.155198918	-0.091033781
C	2.763809880	-1.239757977	0.318402427
N	4.036013791	-1.274653524	0.795371051
N	4.083289811	1.082463244	0.470868924
C	4.612188545	-0.077155671	0.855178967
N	2.222865167	-2.492511703	0.210411930
H	-0.091040434	1.039197396	0.247721465
H	2.085746019	-4.749905796	-1.007352735
H	-2.171429108	-4.721591432	-1.666276975
H	-0.257635411	-1.362038665	0.282050016
H	5.633051406	-0.043520538	1.248055600
H	-0.305149034	5.547612845	-1.894364973
H	2.911676315	-3.195165559	0.464835582
H	-3.368320095	-3.216479876	-0.479259340
H	-3.256688734	2.884786545	0.330805057
H	3.025137186	2.892367731	-0.335107405

4·HSO_4^- E= -6866.8 kcal/mol

O	0.861526441	1.181394706	2.627014764
O	-0.069099019	-0.080097964	4.568394176
S	0.334350968	-0.084861200	3.154554688
O	-1.143170608	-0.222057264	2.328446109
H	-1.717934430	-0.649607236	2.990067587
O	1.102997314	-1.275281752	2.740447409
C	1.227363983	-2.346237414	-0.666291120
C	0.061510841	-2.459280493	0.100846267
C	-1.176590097	-2.354406688	-0.537224651

C	-1.257397926	-2.089167060	-1.908661595
C	1.156974683	-2.078544817	-2.034872522
C	-0.088304128	-1.932966758	-2.649327086
H	-0.146959708	-1.714744900	-3.715896993
S	-2.648024859	-2.726520702	0.400992355
C	-3.443705815	-1.163334662	0.542909147
N	-2.929170163	-0.075592043	-0.039421650
C	-3.576471438	1.054136346	0.260066875
N	-4.724394780	1.153337342	0.965486520
N	-4.570657537	-1.209234482	1.288399879
C	-5.166684782	-0.020325029	1.426960448
S	-2.946849028	2.611334386	-0.270120100
C	-1.332041769	2.185427338	-0.903053069
C	-0.215295010	2.406750630	-0.090150397
C	1.060619625	2.218615319	-0.629627346
C	1.217401403	1.755079227	-1.939375594
C	-1.183767406	1.726501285	-2.214967789
C	0.094015187	1.492377634	-2.721870453
H	-6.105807031	-0.004868252	1.987844226
H	2.220039934	1.600829320	-2.334916464
H	-2.067618752	1.551255526	-2.827095659
S	2.471710353	2.691571047	0.351685836
C	3.149723009	1.128124832	0.800516285
N	2.664074075	-0.000982535	0.276766994
C	3.290431637	-1.101877790	0.699320983
N	4.352451900	-1.150762979	1.527162910
N	4.194761579	1.230967490	1.646329319
C	4.741253206	0.052904325	1.960194100
S	2.797698674	-2.691632093	0.111474177
H	-0.322547665	2.693131013	0.954431232
H	2.077192282	-1.986506443	-2.610747365
H	-2.233305373	-2.008057409	-2.384809378
H	0.138153273	-2.589833723	1.180190960
H	5.598075124	0.075722455	2.639849056
H	0.215101833	1.118701467	-3.738873071

1·NCS^- E= -6740.74 kcal/mol

C	-0.123673000	-0.008345000	2.883664000
N	-1.102589000	0.579853000	2.560769000
S	1.238212000	-0.842460000	3.291849000
C	1.276818000	-2.355157000	-0.687371000
C	0.162626000	-2.189943000	0.129262000
C	-1.079672000	-2.415222000	-0.444732000
C	-1.232100000	-2.796401000	-1.775639000
C	1.176008000	-2.733141000	-2.021973000
C	-0.092243000	-2.953007000	-2.563285000
H	-0.191087000	-3.249398000	-3.607044000
O	-2.224457000	-2.364636000	0.372565000
C	-2.819677000	-1.170643000	0.544501000
N	-2.365386000	-0.113928000	-0.126727000
C	-3.023980000	1.009687000	0.147522000
N	-4.109870000	1.133492000	0.921870000
N	-3.875122000	-1.199054000	1.372357000
C	-4.455802000	-0.014695000	1.488353000
O	-2.628934000	2.159293000	-0.437686000
C	-1.318701000	2.237354000	-0.934963000
C	-0.243263000	2.097866000	-0.061829000
C	1.022329000	2.322456000	-0.583149000
C	1.235891000	2.666173000	-1.916007000
C	-1.157127000	2.577782000	-2.273660000
C	0.134030000	2.788251000	-2.761849000
Cl	-5.875437000	0.041123000	2.512529000
H	2.250471000	2.837613000	-2.271054000

H	-2.033399000	2.678208000	-2.911372000
O	2.133013000	2.327473000	0.284040000
C	2.729111000	1.155027000	0.562812000
N	2.263875000	0.038245000	0.005996000
C	2.945170000	-1.052981000	0.356859000
N	4.053420000	-1.097703000	1.109555000
N	3.794802000	1.261755000	1.371402000
C	4.390399000	0.096173000	1.578329000
O	2.562355000	-2.248422000	-0.133624000
H	-0.404821000	1.792979000	0.980101000
H	2.080250000	-2.852385000	-2.615981000
H	-2.230011000	-2.964819000	-2.176258000
H	0.279948000	-1.896585000	1.178550000
Cl	5.818949000	0.139735000	2.588120000
H	0.280452000	3.054998000	-3.808072000

2·NCS^- E= -6802.95 kcal/mol

S	1.512584000	-0.960225000	3.374241000
C	0.216830000	-0.007354000	3.001747000
N	-0.714388000	0.665448000	2.704664000
C	-1.252493000	2.301594000	-0.810960000
C	-0.141903000	2.156752000	0.018178000
C	1.104349000	2.364158000	-0.554515000
C	1.266577000	2.694120000	-1.898763000
C	-1.140626000	2.628168000	-2.158758000
C	0.132210000	2.820156000	-2.700604000
H	0.239047000	3.074214000	-3.755109000
O	2.249623000	2.364862000	0.268693000
C	2.865638000	1.186545000	0.507955000
N	2.362034000	0.072038000	-0.023407000
C	3.073720000	-1.022173000	0.257729000
N	4.232167000	-1.074632000	0.926458000
N	3.978349000	1.287134000	1.249372000
C	4.605342000	0.116874000	1.407253000
O	2.650163000	-2.214273000	-0.226709000
C	1.324916000	-2.297955000	-0.687165000
C	0.274950000	-2.143773000	0.213627000
C	-1.010797000	-2.329005000	-0.272230000
C	-1.266583000	-2.663708000	-1.600170000
C	1.118619000	-2.629326000	-2.021998000
C	-0.190450000	-2.812417000	-2.474213000
H	5.530236000	0.136887000	1.988907000
H	-2.294432000	-2.797780000	-1.933189000
H	1.973462000	-2.737988000	-2.687371000
O	-2.091242000	-2.271574000	0.630663000
C	-2.678334000	-1.069683000	0.822264000
N	-2.265312000	-0.027177000	0.101230000
C	-2.906878000	1.105369000	0.387622000
N	-3.935188000	1.253862000	1.230236000
N	-3.675450000	-1.077880000	1.718226000
C	-4.255952000	0.116543000	1.859969000
O	-2.544466000	2.238903000	-0.262844000
H	0.472529000	-1.885484000	1.260240000
H	-2.040559000	2.730655000	-2.763103000
H	2.267475000	2.850761000	-2.297600000
H	-0.255780000	1.856570000	1.069211000
H	-5.085136000	0.172779000	2.569670000
H	-0.371491000	-3.069203000	-3.517748000

3·NCS^- E= -7323.78 kcal/mol

S	-0.949058311	-2.228838815	-3.783563038
C	-0.613722701	-0.755230566	-3.100619207
N	-0.374330180	0.268637602	-2.553577156

C	-1.297252163	2.390904733	1.383596013
C	-0.167489086	1.991097701	0.649019643
C	1.066808400	2.565320646	0.971662324
C	1.190811284	3.489713757	2.021469612
C	-1.172782972	3.303427403	2.445643557
C	0.065729211	3.853761780	2.755771715
H	0.156481688	4.563589998	3.578372252
N	2.226916890	2.348193158	0.186214071
C	2.868454621	1.183657166	-0.117741645
N	2.312372745	0.010127711	0.196761704
C	3.083473620	-1.051371791	-0.090508156
N	4.329507387	-1.014510568	-0.638057059
N	4.089793473	1.364381562	-0.699256987
C	4.743497907	0.223199414	-0.916784337
N	2.625007624	-2.292942251	0.223191892
C	1.283490317	-2.619503455	0.564964247
C	0.234237272	-2.191418063	-0.251432869
C	-1.070708109	-2.559447329	0.071119836
C	-1.328733366	-3.328498536	1.211124625
C	1.037734231	-3.398479406	1.699519195
C	-0.275062177	-3.745830216	2.023217564
H	5.734795452	0.311411361	-1.372801930
H	-2.359502435	-3.598719250	1.439525618
H	1.872194598	-3.708266621	2.329773426
N	-2.158056090	-2.233071809	-0.794566315
C	-2.783363845	-1.028004154	-0.712516470
N	-2.356674885	-0.134830882	0.206373613
C	-3.024546174	1.015893489	0.192929801
N	-4.117425075	1.311731115	-0.553882700
N	-3.825331429	-0.836637434	-1.567058804
C	-4.439343868	0.329733136	-1.408938569
N	-2.615068496	2.034163294	1.028991366
H	0.419726548	-1.564897198	-1.122442159
H	-2.063640413	3.580225362	3.011061703
H	2.171029429	3.906129510	2.255621638
H	-0.254243597	1.314263097	-0.203097835
H	-5.303872476	0.517297108	-2.053598979
H	-0.475310634	-4.342628493	2.914440179
H	2.823672842	3.156314403	0.035657415
H	-3.273779966	2.808845083	1.014067575
H	-2.056789880	-2.556586769	-1.782562687
H	3.276202789	-3.042175986	0.009736319

4·NCS^- E= -6866.8kcal/mol

S	1.227483257	-1.113289457	-3.063086642
C	0.023772468	-0.088448295	-2.573232608
N	-0.849436409	0.638979225	-2.233580945
C	-1.361762911	2.265070108	1.285612779
C	-0.414201708	2.335106756	0.255484794
C	0.932018112	2.132818799	0.561311331
C	1.328532807	1.822936542	1.868697131
C	-0.978495170	1.949473425	2.589293103
C	0.370272780	1.715091551	2.872477281
H	0.674764845	1.456125632	3.886780776
S	2.124464878	2.448463865	-0.726074958
C	3.040307775	0.950190252	-0.817014861
N	2.679249433	-0.114582471	-0.096752878
C	3.426334130	-1.198554150	-0.320063330
N	4.521647084	-1.266681688	-1.099263229
N	4.094370050	1.019879719	-1.658053825
C	4.789930457	-0.117029342	-1.732112316
S	2.995887594	-2.720285842	0.475333705
C	1.326858207	-2.346690740	0.995881471

C	0.303910750	-2.402276515	0.041953030
C	-1.009553849	-2.155609434	0.441661345
C	-1.301330643	-1.844697653	1.776754038
C	1.049661897	-2.029871573	2.325423855
C	-0.270007541	-1.772827445	2.707914963
H	5.669359305	-0.111776263	-2.381907976
H	-2.328707902	-1.649535432	2.075899942
H	1.862469250	-1.972746366	3.048480493
S	-2.289495901	-2.384186463	-0.775395493
C	-3.190182116	-0.879330868	-0.700376197
N	-2.799116589	0.117522849	0.098878437
C	-3.543848442	1.218355152	0.004131299
N	-4.663003048	1.366275635	-0.730901066
N	-4.280633097	-0.867932753	-1.499784385
C	-4.968955855	0.274449630	-1.446540251
S	-3.065075829	2.659388740	0.915536205
H	0.542295451	-2.567735092	-1.012465111
H	-1.733224948	1.879493186	3.371758433
H	2.382076766	1.661722791	2.089262576
H	-0.720919899	2.490486994	-0.778109409
H	-5.876114059	0.329011459	-2.055331411
H	-0.494371380	-1.512144467	3.742199900

1·NO_3^- E= -6847.90 kcal/mol

N	0.179633000	-0.234848000	2.714291000
O	0.782730000	-1.351248000	2.790007000
O	0.812499000	0.846936000	2.929358000
O	-1.050490000	-0.197741000	2.391412000
C	1.177564000	-2.306267000	-0.653060000
C	-0.060196000	-2.236550000	-0.022772000
C	-1.183501000	-2.301902000	-0.837390000
C	-1.104293000	-2.435437000	-2.220172000
C	1.309415000	-2.439653000	-2.032293000
C	0.156030000	-2.503178000	-2.815678000
H	0.239685000	-2.605958000	-3.897797000
O	-2.461949000	-2.344039000	-0.238190000
C	-2.992760000	-1.180488000	0.184552000
N	-2.409054000	-0.031564000	-0.157919000
C	-3.007233000	1.043301000	0.355819000
N	-4.142868000	1.059834000	1.075973000
N	-4.125728000	-1.322809000	0.892767000
C	-4.626557000	-0.157555000	1.279893000
O	-2.493017000	2.265236000	0.119210000
C	-1.218891000	2.335936000	-0.485009000
C	-0.087935000	2.148659000	0.300146000
C	1.144321000	2.334188000	-0.317502000
C	1.263767000	2.695011000	-1.656894000
C	-1.151696000	2.696863000	-1.827193000
C	0.103438000	2.874563000	-2.411385000
Cl	-6.135069000	-0.237126000	2.175256000
H	2.253072000	2.833106000	-2.090324000
H	-2.070842000	2.834635000	-2.394531000
O	2.321374000	2.266252000	0.452913000
C	2.793107000	1.047885000	0.784207000
N	2.229936000	-0.037569000	0.250633000
C	2.807852000	-1.179694000	0.628221000
N	3.884631000	-1.307614000	1.419122000
N	3.868371000	1.077736000	1.588025000
C	4.333089000	-0.136148000	1.849092000
O	2.348424000	-2.345813000	0.129867000
H	-0.142866000	1.849433000	1.352904000
H	2.302937000	-2.492575000	-2.474522000
H	-2.018044000	-2.484358000	-2.810385000

H	-0.123257000	-2.113414000	1.064157000
Cl	5.750483000	-0.200856000	2.883133000
H	0.177509000	3.156688000	-3.461691000

2·NO_3^- E= -6906.66 kcal/mol

N	0.155568144	-0.237136871	2.742928954
O	0.769290765	-1.349316662	2.805134348
O	0.781379394	0.849173521	2.960258075
O	-1.078330596	-0.208514710	2.436868254
C	1.177254673	-2.293086014	-0.654814570
C	-0.063597517	-2.229739083	-0.029248045
C	-1.185787163	-2.287878879	-0.847127592
C	-1.099827200	-2.402660484	-2.231409208
C	1.313013784	-2.408124333	-2.035493807
C	0.162553170	-2.460820189	-2.823620098
H	0.250270997	-2.546335680	-3.906780673
O	-2.464436388	-2.340554607	-0.254037946
C	-3.001457164	-1.180131548	0.181679778
N	-2.415423218	-0.030483919	-0.154039104
C	-3.011251391	1.044073799	0.363503857
N	-4.140468863	1.062632302	1.088171042
N	-4.130756975	-1.326221538	0.890894874
C	-4.639246478	-0.159463702	1.301547470
O	-2.486886313	2.264901083	0.120754926
C	-1.216067323	2.323018001	-0.488018772
C	-0.081707219	2.143465937	0.294695656
C	1.149676358	2.321410172	-0.328004707
C	1.263862566	2.663433451	-1.672916714
C	-1.151544076	2.664747428	-1.835702386
C	0.101568080	2.832440127	-2.426668471
H	-5.566308331	-0.210817785	1.879054684
H	2.252238050	2.793724578	-2.110796565
H	-2.072544015	2.794163332	-2.401944615
O	2.328604956	2.266207468	0.438315522
C	2.808255587	1.048640727	0.778763322
N	2.239283288	-0.037786902	0.253514761
C	2.816226648	-1.180468329	0.630815043
N	3.890509581	-1.311145931	1.420731225
N	3.883086713	1.081904472	1.578440665
C	4.357076719	-0.136834439	1.858348650
O	2.344742030	-2.344806413	0.129815955
H	-0.133730233	1.855101661	1.350520272
H	2.308431330	-2.453214673	-2.474381966
H	-2.011673420	-2.443232674	-2.825039637
H	-0.130624712	-2.114897137	1.058314093
H	5.231890443	-0.177023954	2.512925682
H	0.172735321	3.097558397	-3.481532231

3·NO_3^- E= -7430.03 kcal/mol

O	-1.170424323	-1.446466892	-2.682783739
O	-1.185729554	0.745182103	-2.918078813
N	-0.614582958	-0.318613947	-2.535947271
O	0.535304134	-0.248214634	-1.962227609
C	-1.151142346	2.782658239	0.263813096
C	0.082386418	2.169411673	0.007217809
C	1.241754981	2.843648571	0.407163574
C	1.181672605	4.082954677	1.067406482
C	-1.219357158	4.026430280	0.919477705
C	-0.053645253	4.672235246	1.315024971
H	-0.108339291	5.635724914	1.822189098
N	2.532566064	2.404106222	0.049734492
C	3.088355285	1.165066332	-0.049178824
N	2.427049755	0.078248989	0.371537235

C	3.126913115	-1.056367074	0.236372792
N	4.399816356	-1.169547470	-0.246512321
N	4.360284324	1.195585582	-0.545993386
C	4.933964769	-0.004607751	-0.608038708
N	2.616603843	-2.248349608	0.653999803
C	1.335696545	-2.639380774	1.092878832
C	0.158630870	-2.115998973	0.545408581
C	-1.055613081	-2.704370229	0.923921555
C	-1.089827735	-3.767248856	1.846800855
C	1.309363570	-3.700147846	2.015144393
C	0.092201844	-4.262673729	2.385047484
H	5.956682823	-0.036691591	-0.998087291
H	-2.052154046	-4.197095529	2.128389980
H	2.246843446	-4.076033533	2.426773201
N	-2.284917048	-2.376848632	0.333390905
C	-2.800771495	-1.207670625	-0.144512555
N	-2.154180864	-0.047436035	0.035495158
C	-2.842150523	1.015870574	-0.404109532
N	-4.076560143	0.998022392	-0.979154549
N	-4.030468890	-1.368973148	-0.706264702
C	-4.584181882	-0.226311495	-1.105101740
N	-2.370197934	2.281884149	-0.215995102
H	0.203833691	-1.353633043	-0.238111339
H	-2.195706712	4.473102557	1.114167400
H	2.107678120	4.571781314	1.374240533
H	0.154247979	1.252452716	-0.585831705
H	-5.569466967	-0.299267423	-1.576189833
H	0.065120797	-5.091021980	3.093433568
H	-2.937536968	-3.144753288	0.204726272
H	-3.056055874	2.972953938	-0.504838339
H	3.200664072	3.130565957	-0.190880940
H	3.309315639	-2.989632316	0.591652523

4·NO_3^- E= -6644.53 kcal/mol

N	0.257925453	-0.253119955	2.430499861
O	0.884259292	-1.356581585	2.541895772
O	0.843557643	0.837467679	2.722753627
O	-0.944633999	-0.240847679	2.019751864
C	1.220337027	-2.239917416	-0.798907937
C	-0.008969995	-2.448471396	-0.164635785
C	-1.185362682	-2.239623316	-0.889079728
C	-1.142423571	-1.773823517	-2.206580868
C	1.274042206	-1.772964076	-2.115048600
C	0.089606643	-1.521997388	-2.808302770
H	0.127590413	-1.145217876	-3.830834942
S	-2.732318286	-2.722545742	-0.142133083
C	-3.454752885	-1.182009481	0.311149390
N	-2.894819884	-0.028338143	-0.063099535
C	-3.497114607	1.050446018	0.443055699
N	-4.639015353	1.063194073	1.164777371
N	-4.590122047	-1.321492663	1.029711052
C	-5.133789171	-0.156866515	1.395392174
S	-2.823468145	2.658200163	0.187118547
C	-1.235344054	2.312269769	-0.550661494
C	-0.096300688	2.419427317	0.252099000
C	1.163735816	2.312150466	-0.343952137
C	1.284209586	2.041174711	-1.710077143
C	-1.125098684	2.042626960	-1.917672165
C	0.137738330	1.887535492	-2.489003445
H	-6.074759287	-0.207311571	1.951518455
H	2.275174002	1.950007760	-2.152725785
H	-2.026371821	1.952491883	-2.522521928
S	2.604094971	2.652946793	0.652374199

C	3.227841627	1.038082762	0.983902642
N	2.704161787	-0.032327354	0.378667521
C	3.275194317	-1.185896136	0.736134751
N	4.330304619	-1.332318237	1.563732560
N	4.277476157	1.042159283	1.831290476
C	4.772478463	-0.176180732	2.067225182
S	2.711734075	-2.714454181	0.061829514
H	-0.176366370	2.539581003	1.331183807
H	2.242130754	-1.608620750	-2.586582761
H	-2.072454647	-1.609655200	-2.749201824
H	-0.035611484	-2.723331257	0.889447949
H	5.632004299	-0.232904219	2.741904128
H	0.229370180	1.662954253	-3.552083612

1·PF_6^- E= -7091.59 kcal/mol

F	-0.464653767	-1.088415981	4.380307055
F	1.251037582	-1.092934733	2.815767764
F	1.499253239	0.092542138	4.800208757
P	0.386674508	0.072204888	3.614668462
F	-0.719925366	0.051524636	2.373339269
F	-0.479984226	1.238381426	4.354217180
F	1.236672571	1.229212391	2.789488475
C	-1.184543776	2.357821283	-0.673439622
C	0.004012163	2.205713862	0.031947764
C	1.187597439	2.358580220	-0.682952629
C	1.204729170	2.642744006	-2.045302218
C	-1.216287240	2.641750296	-2.035174093
C	-0.008690177	2.779245785	-2.720389724
H	-0.013312015	2.999362349	-3.787510202
O	2.419250296	2.344465571	-0.001920995
C	2.922598331	1.152789462	0.379189969
N	2.320419279	0.032366996	-0.023883753
C	2.927819519	-1.077644398	0.399265384
N	4.054381723	-1.148377206	1.124620303
N	4.048598804	1.242249208	1.103077383
C	4.536150059	0.050917345	1.428190245
O	2.430345732	-2.278599023	0.040540915
C	1.192368295	-2.316108597	-0.627833301
C	0.014715666	-2.134802714	0.090561340
C	-1.179645918	-2.315029915	-0.597748904
C	-1.222929180	-2.653134115	-1.946855589
C	1.198004250	-2.653979204	-1.977838731
C	-0.021216053	-2.818015263	-2.636261276
Cl	6.019325054	0.063197723	2.357875912
H	-2.185882174	-2.788153476	-2.436283706
H	2.147980364	-2.789742738	-2.491860181
O	-2.399832439	-2.277672709	0.108805261
C	-2.903362405	-1.076143470	0.450605677
N	-2.338182710	0.031816851	-0.031353429
C	-2.909714382	1.153735635	0.408862314
N	-3.994238897	1.245045305	1.195101662
N	-3.986714022	-1.144004190	1.240892457
C	-4.464204888	0.055268521	1.549639747
O	-2.410298377	2.344374741	0.024418552
H	0.037843617	-1.854132626	1.142929666
H	-2.175048978	2.755310660	-2.538094851
H	2.159054031	2.757080283	-2.556460323
H	0.018667138	1.964521001	1.094242860
Cl	-5.905261684	0.069900343	2.543354330
H	-0.034940153	-3.081872566	-3.693395174

2·PF_6^- E= -7154.21 kcal/mol

F	-0.45550313	-1.08624243	4.43285379

F	1.23796092	-1.08990932	2.84367240
F	1.51247306	0.09800997	4.82333690
P	0.38286169	0.07491713	3.64972812
F	-0.74032731	0.05168901	2.42717189
F	-0.47474983	1.23997375	4.40565062
F	1.21927294	1.23324661	2.81594085
C	-1.18674608	2.34819679	-0.67407330
C	0.00472284	2.20165092	0.02847797
C	1.18787747	2.34839058	-0.68930140
C	1.20061517	2.61861615	-2.05479371
C	-1.22004396	2.61861560	-2.03883327
C	-0.01419416	2.74849590	-2.72846016
H	-0.02130266	2.95726346	-3.79799719
O	2.41886640	2.34364844	-0.01024422
C	2.92945411	1.15320689	0.37894969
N	2.32867373	0.03203685	-0.02448161
C	2.93589866	-1.07842450	0.39797538
N	4.05479037	-1.15133597	1.12962182
N	4.04739097	1.24490596	1.11001104
C	4.54403812	0.05110369	1.45199724
O	2.43186071	-2.27862803	0.03005546
C	1.19401046	-2.30624042	-0.63528868
C	0.01763890	-2.13179426	0.08775915
C	-1.18038153	-2.30535143	-0.59690627
C	-1.22679985	-2.62769355	-1.95020351
C	1.19366038	-2.62806219	-1.98964990
C	-0.02768123	-2.78402991	-2.64589986
H	5.45237461	0.05879127	2.05950469
H	-2.19161421	-2.75654196	-2.43777970
H	2.14201572	-2.75726037	-2.50846928
O	-2.39606690	-2.27781105	0.11395950
C	-2.90468090	-1.07680068	0.46621721
N	-2.34022125	0.03173185	-0.01584189
C	-2.91218466	1.15434379	0.42296755
N	-3.98912833	1.24845658	1.21497013
N	-3.98039447	-1.14707409	1.26265715
C	-4.46596819	0.05580114	1.58825238
O	-2.40917233	2.34388507	0.02581569
H	0.04399662	-1.86110628	1.14288824
H	-2.18012820	2.72695253	-2.54046874
H	2.15386924	2.72723067	-2.56928844
H	0.02155556	1.96989408	1.09298455
H	-5.34806116	0.06532946	2.23347980
H	-0.04512676	-3.03477675	-3.70632061

3·PF_6^- E= -7677.66 kcal/mol

F	-0.360105525	-1.040081400	4.168366379
F	1.450516295	-1.116696358	2.718271186
F	1.615721907	0.068764999	4.713416555
P	0.585551393	0.083464820	3.444715331
F	-0.448555498	0.097202373	2.144246850
F	-0.287484026	1.283165423	4.136080116
F	1.522272066	1.205948370	2.685077881
C	-1.216102354	2.802885147	-0.676682429
C	-0.017852803	2.178140044	-0.310610227
C	1.184926106	2.798902613	-0.673955630
C	1.186997014	3.994449187	-1.416509643
C	-1.218086869	3.997135044	-1.420160021
C	-0.014044320	4.587276665	-1.785150679
H	-0.012194591	5.513181874	-2.360979939
N	2.441047179	2.364416563	-0.231843026
C	2.948869973	1.142280707	0.102928132
N	2.260927649	0.016516918	-0.132388795

C	2.943998982	-1.092726017	0.185990200
N	4.203698260	-1.148312457	0.699804834
N	4.210721310	1.230400650	0.606659602
C	4.754328666	0.048413727	0.887966734
N	2.431379985	-2.331570477	-0.065106073
C	1.176319378	-2.777672316	-0.501382732
C	-0.023752912	-2.141601770	-0.158781473
C	-1.224253760	-2.770173612	-0.508248638
C	-1.231428886	-3.984565400	-1.218123213
C	1.174489286	-3.994045421	-1.208612736
C	-0.029298052	-4.591115416	-1.563965024
H	5.764012059	0.061972616	1.310393245
H	-2.184457120	-4.441573301	-1.487031336
H	2.125175373	-4.459657123	-1.469727174
N	-2.481642009	-2.320934647	-0.065896332
C	-3.005116360	-1.082817497	0.155675680
N	-2.317798416	0.026256090	-0.153875188
C	-3.003213997	1.155023913	0.075742811
N	-4.274148852	1.244921893	0.563504468
N	-4.274595915	-1.135617612	0.651895309
C	-4.826764478	0.062836200	0.827186689
N	-2.477713572	2.375544771	-0.227837510
H	-0.022119993	-1.238179454	0.445282702
H	-2.169289130	4.452341658	-1.699054879
H	2.139442985	4.448672311	-1.692539190
H	-0.019360559	1.291533737	0.317481155
H	-5.845582996	0.077777593	1.226849685
H	-0.031015493	-5.531966901	-2.115031782
H	3.115730137	-3.055017445	0.135497432
H	3.133561371	3.093144232	-0.085129484
H	-3.168573944	3.109054180	-0.097654306
H	-3.170704941	-3.045609695	0.114464481

4·PF_6^- E= -6894.5 kcal/mol

F	-0.874657155	-1.148471447	3.035637309
F	1.445539242	-1.130380038	2.851428312
F	0.405992861	0.024409128	4.583591251
P	0.276946130	0.025633457	2.956539043
F	0.146737831	0.026329708	1.320603893
F	-0.892351631	1.181962811	3.037571411
F	1.428828547	1.198163248	2.854500918
C	-1.184583253	2.350775347	-0.528289461
C	0.065134787	2.551220128	0.064237898
C	1.220061322	2.355061945	-0.697642849
C	1.131481614	1.936393487	-2.028010981
C	-1.281269536	1.931186063	-1.858142521
C	-0.120706996	1.714694127	-2.599499832
H	-0.192825402	1.382252783	-3.635222197
S	2.797500915	2.738074127	0.043089866
C	3.464062229	1.146027181	0.407980907
N	2.857781162	0.029057112	-0.005493435
C	3.463965702	-1.092471053	0.395819261
N	4.619266989	-1.171636488	1.088264134
N	4.620929379	1.217356871	1.099415974
C	5.139698135	0.021166398	1.392287067
S	2.797846159	-2.680048156	0.009288304
C	1.212807815	-2.290771324	-0.709120329
C	0.067773993	-2.495779701	0.065640580
C	-1.189294534	-2.296493124	-0.511038422
C	-1.303564584	-1.869142629	-1.837246666
C	1.106859529	-1.861490711	-2.034698558
C	-0.153061032	-1.641568556	-2.590232792
H	6.085577162	0.017968106	1.941441744

H	-2.291810982	-1.712564682	-2.267578851
H	2.010788467	-1.698593122	-2.619936609
S	-2.636566647	-2.679921584	0.457123508
C	-3.268679943	-1.087841321	0.877654697
N	-2.714447054	0.029562447	0.397168590
C	-3.273206374	1.151263049	0.861459739
N	-4.347127880	1.229919476	1.674923245
N	-4.342166788	-1.158576023	1.692532492
C	-4.829830616	0.037145607	2.035693358
S	-2.644964301	2.739720453	0.418918265
H	0.155061447	-2.772224548	1.114085841
H	-2.263664177	1.774777663	-2.301880624
H	2.042782099	1.783774059	-2.604682542
H	0.138654350	2.822340911	1.115075616
H	-5.712719614	0.040087217	2.681489988
H	-0.239159367	-1.301018402	-3.622126541

1·SO_4^{2-} E= -6961.30 kcal/mol

O	0.196219132	0.793277423	4.480217823
O	1.423041050	1.216913520	2.414994664
S	0.448043541	0.059677780	3.239993509
O	-0.743352605	-0.083499997	2.368004921
O	1.251354155	-1.162385814	3.356379857
C	-1.114753336	2.344921037	-0.850685564
C	-0.095347948	1.957770666	0.004867778
C	1.230129901	2.285696103	-0.343851586
C	1.467834340	2.963603792	-1.560048365
C	-0.908006801	3.014935725	-2.054148128
C	0.413828587	3.316571840	-2.397653521
H	0.620905887	3.832791774	-3.337469273
O	2.313293767	2.046594800	0.424899474
C	2.314419583	0.832083573	1.381879559
N	1.879837926	-0.276450927	0.621611158
C	2.774962462	-1.176611400	0.378781246
N	4.070233498	-1.240486712	0.748173124
N	3.663698635	0.843232639	1.871038872
C	4.365942529	-0.163935397	1.490370743
O	2.430746382	-2.281019265	-0.414769099
C	1.132735446	-2.474914881	-0.820525565
C	0.005554641	-2.208104298	-0.028600611
C	-1.233637152	-2.525877917	-0.564130038
C	-1.412352308	-3.100036723	-1.819745641
C	0.991141782	-3.056931777	-2.088482329
C	-0.274228467	-3.369055964	-2.582031181
Cl	6.097579457	-0.159655751	2.055838322
H	-2.416621526	-3.321593616	-2.178003171
H	1.891829333	-3.247020167	-2.671251921
O	-2.394666107	-2.368468812	0.234664320
C	-2.878887911	-1.133904893	0.433164122
N	-2.335762722	-0.087817835	-0.189511519
C	-2.921682416	1.076277946	0.095217599
N	-4.025717394	1.245168052	0.858721448
N	-3.964656340	-1.111519241	1.237577992
C	-4.458984144	0.105864118	1.370279664
O	-2.469989653	2.218428944	-0.440608063
H	0.081069241	-1.740150626	0.951932180
H	-1.752658170	3.292032067	-2.683004932
H	2.500184068	3.193559952	-1.822890207
H	-0.317622914	1.422809557	0.927386553
Cl	-5.923331359	0.226991784	2.361091302
H	-0.375715208	-3.815776589	-3.572281217

2·SO_4^{2-} E= -7003.29 kcal/mol

O	1.22700051	-0.15727146	4.13700459
O	-1.23907450	-0.13366195	4.13757014
S	-0.00098632	0.41630240	3.46657186
O	-0.00557875	-0.03496376	2.00613674
O	0.01329369	1.90593204	3.49239355
C	-1.18394963	2.59438063	-0.58347015
C	0.00374702	2.20223181	0.03069226
C	1.19810394	2.59242677	-0.57178594
C	1.22732127	3.34470326	-1.75022772
C	-1.19968549	3.34688536	-1.76226850
C	0.01698862	3.71892108	-2.33809604
H	0.02205820	4.29990210	-3.26269108
O	2.41794499	2.34264557	0.05127269
C	2.55591523	1.13650775	0.70814282
N	2.28223623	0.03269245	0.00344920
C	2.54453835	-1.08270036	0.69258475
N	3.01986107	-1.18505952	1.92338541
N	3.04353183	1.21143337	1.93823807
C	3.18435443	0.00884618	2.53365712
O	2.41290086	-2.28012088	0.00960531
C	1.18208583	-2.56995253	-0.56521123
C	-0.00719793	-2.12599448	0.01075333
C	-1.20116495	-2.56812229	-0.55681594
C	-1.22794768	-3.41804574	-1.66753781
C	1.19881886	-3.41998309	-1.67635585
C	-0.01682431	-3.84029516	-2.21851706
H	3.55482635	0.00133991	3.55445822
H	-2.18708448	-3.73419587	-2.07631785
H	2.15438023	-3.73788658	-2.09211547
O	-2.42696811	-2.27667517	0.02901296
C	-2.55597820	-1.07222929	0.69857710
N	-2.28564197	0.03571905	0.00017536
C	-2.55406546	1.14705079	0.69451109
N	-3.04124828	1.23600159	1.92375464
N	-3.03764624	-1.16049152	1.92833555
C	-3.19411078	0.03914185	2.52821557
O	-2.41095109	2.34650673	0.02545706
H	-0.00424410	-1.45732836	0.89639098
H	-2.15407577	3.62627447	-2.20774815
H	2.18663207	3.62223413	-2.18621263
H	-0.00072742	1.59376991	0.95330966
H	-3.56615426	0.04304201	3.54850280
H	-0.02045815	-4.50204241	-3.08678431

3·SO_4^{2-} E= -7519.89 kcal/mol

O	1.166815339	1.233803668	2.482042270
O	-0.115871838	0.018033753	4.206765084
S	0.367477360	-0.011993923	2.797877190
O	-0.819211027	-0.061257020	1.831926207
O	1.218506802	-1.237269506	2.549564511
C	1.040698701	-2.849687175	-0.469317784
C	-0.188994381	-2.243715848	-0.160060748
C	-1.351523754	-2.893756294	-0.585854970
C	-1.313929356	-4.089727919	-1.328238709
C	1.089041334	-4.052047617	-1.206972859
C	-0.084179898	-4.668995667	-1.628324351
H	-0.039528906	-5.598396656	-2.199430508
N	-2.638413635	-2.485335495	-0.168664474
C	-3.160820197	-1.258804446	0.110710575
N	-2.577279810	-0.143875421	-0.339915432
C	-3.205530137	0.975808882	0.030727732
N	-4.400693613	1.049006925	0.693290014
N	-4.350389616	-1.331503603	0.782521659

C	-4.896293010	-0.141741584	1.017118252
N	-2.727978037	2.199664598	-0.330359759
C	-1.451048555	2.629091249	-0.757475590
C	-0.271208166	2.052780298	-0.276973907
C	0.939478343	2.685465011	-0.608342633
C	0.952880629	3.842984545	-1.416037581
C	-1.447568099	3.777220918	-1.572743122
C	-0.236379316	4.386009394	-1.890600330
H	-5.860822748	-0.142378936	1.538752571
H	1.911861824	4.303331890	-1.662466801
H	-2.394376100	4.178363657	-1.938865405
N	2.173999188	2.297984273	-0.090814828
C	2.627649716	1.089358508	0.379182795
N	2.058356443	-0.047679216	-0.030185326
C	2.675263490	-1.142265551	0.420601396
N	3.880297135	-1.181540837	1.066314445
N	3.827922586	1.203117523	1.024743257
C	4.368381581	0.027060924	1.328451444
N	2.266034185	-2.387963898	0.009567112
H	-0.313368736	1.208421048	0.433939923
H	2.061762550	-4.489940899	-1.439257634
H	-2.248964909	-4.549424637	-1.653392929
H	-0.257759661	-1.360686215	0.500458155
H	5.340130203	0.057317462	1.836980711
H	-0.218490406	5.279850277	-2.517292537
H	2.924652177	-3.099060828	0.309611907
H	-3.250416877	-3.226897304	0.155932464
H	-3.370290445	2.937324329	-0.059225631
H	2.805511646	3.047247365	0.172794176

4·SO_4^{2-} E= -6738.77 kcal/mol

O	1.218056012	0.074651621	4.172637648
O	-1.223271496	0.089744541	4.176809604
S	-0.002546975	0.443572334	3.347399583
O	-0.009179594	-0.343373269	2.064877985
O	0.006409964	1.908681740	3.032658161
C	-1.196238718	2.608335151	-0.640534198
C	0.004354339	2.487379046	0.071136388
C	1.208184581	2.607009941	-0.635454696
C	1.218360306	2.800104194	-2.023311611
C	-1.200544201	2.801120612	-2.028499378
C	0.010431494	2.893497577	-2.716718651
H	0.012827866	3.027222206	-3.800473335
S	2.741354815	2.739025113	0.270951577
C	2.801864043	1.152952528	1.104661745
N	2.518823150	0.060220500	0.376708486
C	2.744470056	-1.074202286	1.054326770
N	3.123175558	-1.199962011	2.322309215
N	3.228184628	1.193277950	2.364127753
C	3.246391397	-0.015447044	2.967891011
S	2.734333100	-2.612036598	0.118485126
C	1.197849371	-2.542441181	-0.780030018
C	-0.005336038	-2.316552326	-0.100737281
C	-1.210598607	-2.541139775	-0.776747799
C	-1.218944952	-2.924851713	-2.126506264
C	1.201770418	-2.925841385	-2.129923273
C	-0.009613452	-3.111082271	-2.797701226
H	3.559701973	-0.047758516	4.008020358
H	-2.171333336	-3.072407050	-2.636515552
H	2.152556576	-3.074086808	-2.642679102
S	-2.744250360	-2.608293997	0.126912079
C	-2.754729622	-1.065853119	1.054062837
N	-2.524335003	0.065213510	0.372702742

C	-2.803416231	1.161768818	1.096224126
N	-3.231468207	1.208233515	2.355116428
N	-3.138614514	-1.185275397	2.321640338
C	-3.260313506	0.001473935	2.961613304
S	-2.733233358	2.745449047	0.259053725
H	-0.003954362	-1.969809538	0.941082729
H	-2.152390347	2.871057700	-2.555359202
H	2.172470895	2.869031237	-2.546228452
H	0.002313250	2.328040302	1.166902205
H	-3.573569326	-0.025555987	4.002005221
H	-0.011231586	-3.393232852	-3.852917104

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