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A Theoretical Study on Borenium Ion Affinities Toward Ammonia, Formaldehyde and Chloride Anion

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Supplementary Information

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Theory level employed in the study

The choice of the M06-2X functional has been made on the basis of literature data showing its ability to accurately model various amine-borane complexes when combined with the 6-311++G(3df,2p) basis set (ref. 2b, 6 and 13 in the manuscript). To make a compromise between the accuracy and computational time, we have chosen a smaller 6-311++G(d,p) basis set which was first tested by computing binding enthalpies of several amine-borane adducts and by comparing them with previously calculated and experimental data (Table S1). Our calculated values (the first row in the Table) are in excellent agreement with previous calculations and also with experimental data.

Table S1. Comparison of calculated binding enthalpies ΔH with experimental values and previuos calculations (kcal/mol).[a]

	BF_3–NH_3	BCl_3–NH_3	BH_3–NH_3	BMe_3–NH_3	BMe_3–NH_2Me	BMe_3–$NHMe_2$	BMe_3–NMe_3
Calc[b]	–22.4	–25.6	–27.0	–13.8	–17.9	–18.7	-17.3[c]
Calc[d]	–20.2	–25.1	–27.8	–14.2	–18.4	–19.2	–17.8
Exp[e]	/	–24.0	–27.5 ± 0.5	–13.8 ± 0.3	–17.6 ± 0.2	–19.3 ± 0.3	–17.6 ± 0.2

[a] Enthalpies are corrected for the BSSE by using the counterpoise method. Temperatures are 298.15 K for BF_3–NH_3, BCl_3–NH_3 and BH_3–NH_3, 373 K for BMe_3–NH_3, BMe_3–NH_2Me, BMe_3–$NHMe_2$ and BMe_3–NMe_3. [b] Calculated at the M06-2X/6-311++G(d,p)//M06-2X/6-311++G(d,p) level, this work. [c] Enthalpy corrections were obtained at the M06-2X/6-31++G(d,p) level, this work. [d] Data for BF_3–NH_3 and BCl_3–NH_3 are taken from ref. 6 in the manuscript. Data for BH_3–NH_3, BMe_3–NH_3, BMe_3–NH_2Me, BMe_3–$NHMe_2$ and BMe_3–NMe_3 are taken from ref. 13 in the manuscript. All these calculations were done at the M06-2X/6-311++G(3df,2p) level. Enthalpy corrections were obtained by using the B3LYP/6-31G(d). [e] Value for BCl_3–NH_3 is taken from ref. 6 and all others from ref. 13 in the manuscript.

Ammonia afinities of 4-8 at various theory levels and effect of inclusion of CP corrections in geometry optimization

We have also calculated NH_3 affinities of selected borenium cations **4**-**8** at the DFT level, using the same M06-2X functional and the correlation-consistent aug-cc-pVDZ basis set, and at the MP2 level using the same 6-311++G(d,p) basis set. The effect of CP corrections on molecular structure and thus obtained ΔHs/ΔEs was tested, too. All results are presented in Table S2, which also includes the M06-2X/6-311++G(d,p) data, presented in the manuscript.

The change of the basis set from 6-311++G(d,p) to aug-cc-pVDZ decreases slightly the B–N distancies (by up to 0.007 Å) and increases slightly ΔH and ΔE values, by up to 1.29 kcal/mol and 1.01 kcal/mol, respectively. At the MP2 level, the B–N distancies differ insignificantly (< 0.004 Å) from those obtained at the M06-2X/6-311++G(d,p) level and ΔHs/ΔEs decrease by up to 8.4 kcal/mol/6.9 kcal/mol. Both methods retain the same trend in ΔHs/ΔEs.

The CP corrections involved in geometry optimization increase the B–N bond lengths just slightly, by up to 0.005 Å. All other bond lengths change by less than 0.002 Å, while the NBN and RBR' bond angles differ by less than 0.3°. Changes in binding enthalpies do not exceed 0.03 kcal/mol, while binding energies vary by up to 0.28 kcal/mol.

Table S2. Calculated B-NH_3 distances (d_{BN}, Å) and counterpoise-corrected NH_3 affinities (ΔH at 298.15 K and ΔE, kcal/mol) at various levels of theory for borenium cations **4**-**8**.

	M06-2X/6-311++G(d,p)			M06-2X/6-311++G(d,p)[a]			M06-2X/aug-cc-pVDZ			MP2/6-311++G(d,p)		
ion	d_{BN}	ΔH	ΔE	d_{BN}	ΔH	ΔE	d_{BN}	ΔH	ΔE	d_{BN}	ΔH	ΔE
4	1.613	-54.37	-58.88	1.615	-54.39	-59.16	1.609	-54.84	-59.61	1.614	-51.23	-55.65
5	1.618	-49.82	-52.40	1.622	-49.84	-52.46	1.611	-49.90	-53.26	1.621	-42.67	-45.52
6	1.608	-44.83	-48.23	1.613	-44.86	-48.02	1.602	-46.01	-49.24	1.612	-36.47	-39.74
7	1.640	-36.69	-40.47	1.643	-36.72	-40.48	1.637	-36.81	-40.61	1.639	-33.37	-37.16
8	1.621	-33.85	-37.07	1.626	-33.84	-37.03	1.619	-35.14	-37.62	1.623	-27.96	-31.26

[a] Counterpoise corrections were included in geometry optimization.

Table S3. Calculated B–R/R' and B–L bond lengths (d_{BR}, $d_{BR'}$ and d_{BL}, Å), NBO charges at boron atom and electron occupancies of boron's p-orbital of borenium cations **4-29**.

ion	R	R'	L	d_{BR}	$d_{BR'}$	d_{BL}	charge at boron	electron occupancy
4	H	H	NH_3	1.175	1.175	1.552	0.687	0.023
5	F	F	NH_3	1.285	1.285	1.549	1.412	0.289
6	Cl	Cl	NH_3	1.701	1.701	1.564	0.566	0.460
7	Me	Me	NH_3	1.538	1.538	1.587	1.087	0.167
8	P	P	NH_3	1.864	1.864	1.562	0.124	0.501
9	Me	Ph	NH_3	1.545	1.517	1.592	1.041	0.249
10	Ph	Ph	NH_3	1.525	1.527	1.584	1.025	0.285
11	O	O	NH_3	1.342	1.342	1.535	1.185	0.438
12	P	S	NH_3	1.898	1.748	1.563	0.218	0.542
13	P	O	NH_3	1.907	1.320	1.561	0.781	0.378
14	S	S	NH_3	1.765	1.765	1.560	0.279	0.613
15	O	O	NH_3	1.328	1.328	1.541	1.205	0.411
16	O	S	NH_3	1.328	1.769	1.553	0.809	0.481
17	N	S	NH_3	1.376	1.784	1.557	0.691	0.536
18	N	O	NH_3	1.376	1.340	1.549	1.103	0.457
19	P	N	NH_3	1.913	1.369	1.564	0.631	0.462
20	N	N	NH_3	1.388	1.388	1.556	0.997	0.494
21	N	O	SMe_2	1.375	1.347	1.905	0.892	0.474
22	N	O	OMe_2	1.382	1.343	1.449	1.216	0.447
23	N	O	NMe_3	1.383	1.350	1.535	1.208	0.438
24	N	O	PMe_3	1.384	1.355	1.939	0.766	0.455
25	N	O	PH_3	1.377	1.344	1.956	0.784	0.478
26	N	O		1.390	1.361	1.582	0.959	0.441
27	N	O		1.395	1.363	1.575	0.947	0.436
28	N	O		1.395	1.362	1.584	0.957	0.430
29	N	O		1.386	1.351	1.521	1.187	0.438

Energy decomposition analysis of binding interactions in BF_3–NH_3 and BCl_3–NH_3

Table S4. Calculated B-N distances (d_{BN}, Å), NH_3 affinities (ΔE) and energy decomposition of binding interactions of BF_3 and BCl_3 with NH_3 (kcal/mol).[a-d]

	d_{BN}	ΔE	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{ex+rep}	ΔE_{oi}	ΔE_{disp}
BF_3	1.668	-24.74	23.57	-48.31	-95.35	144.50	-75.00	-22.46
					(49.5%)		(38.9%)	(11.6%)
BCl_3	1.617	-28.50	23.59	-52.09	-119.84	206.74	-113.05	-25.94
					(46.3%)		(43.7%)	(10.0%)

[a] Calculated at the M06-2X/6-311++G(d,p)//M06-2X/6-311++G(d,p) level. [b] Binding energies (ΔE) and all interaction energy terms are corrected for the BSSE by using the counterpoise method. [c] ΔE = total binding energy, ΔE_{def} = deformation energy, ΔE_{int} = interaction energy, ΔE_{elstat} = electrostatic energy, ΔE_{ex+rep} = exchange repulsion energy, ΔE_{oi} = orbital interaction energy, ΔE_{disp} = dispersion energy. [d] Values in parentheses are percentage contribution to all attractive interactions.

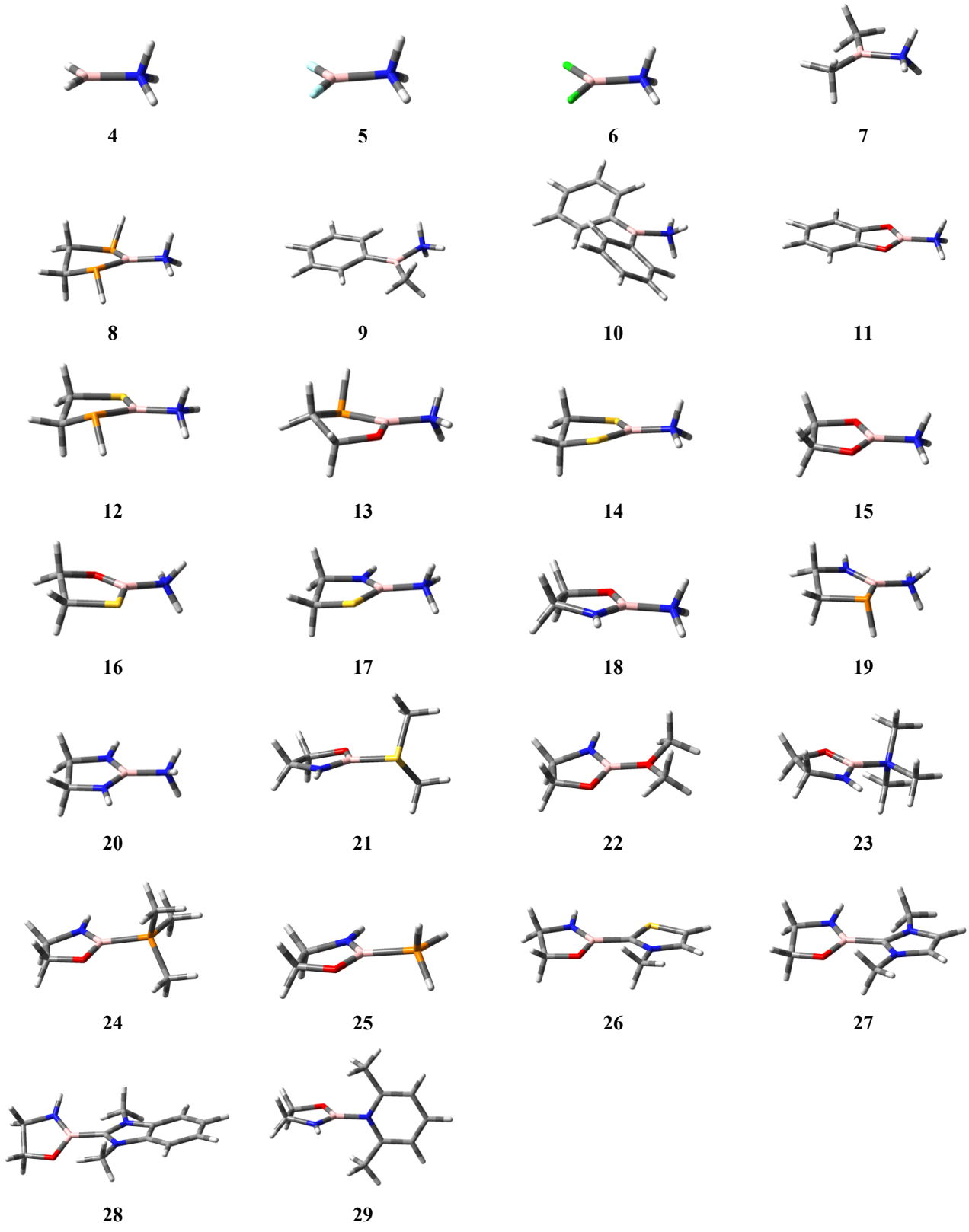


Figure S1. Optimized structures of borenium cations **4-29**.

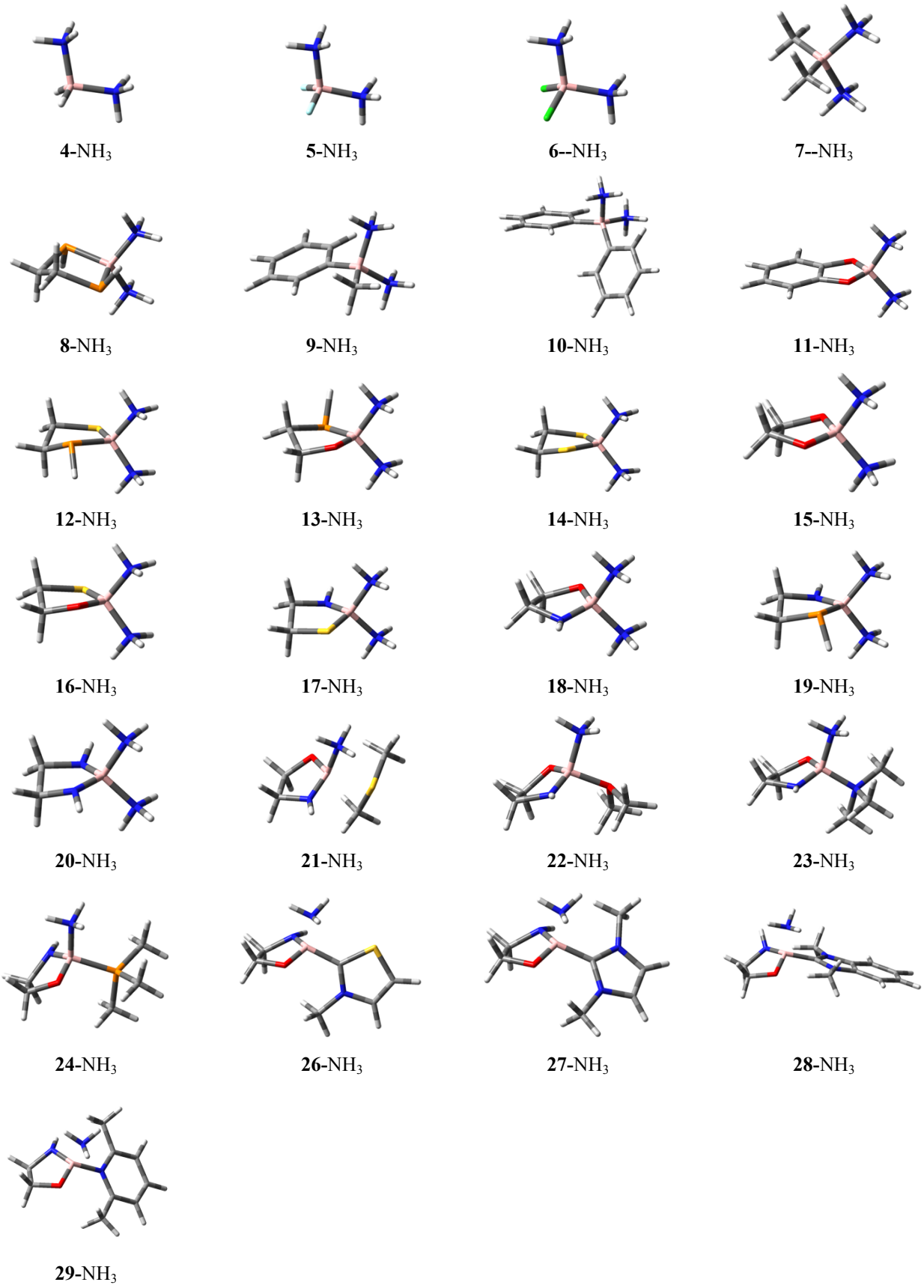


Figure S2. Optimized structures of NH_3-comlexes of borenium cations **4**-**29**.

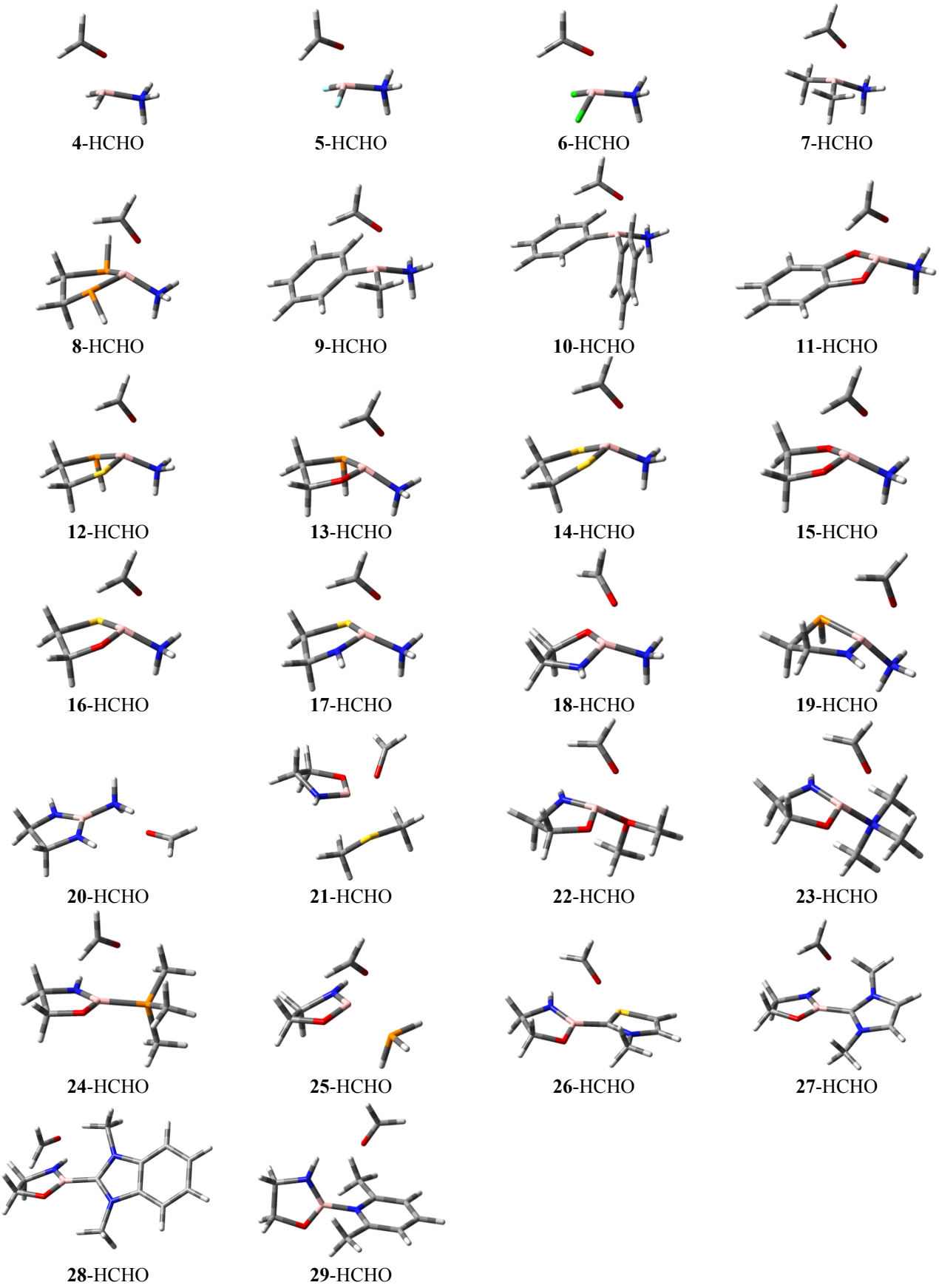


Figure S3. Optimized structures of HCHO-comlexes of borenium cations **4**-**29**.

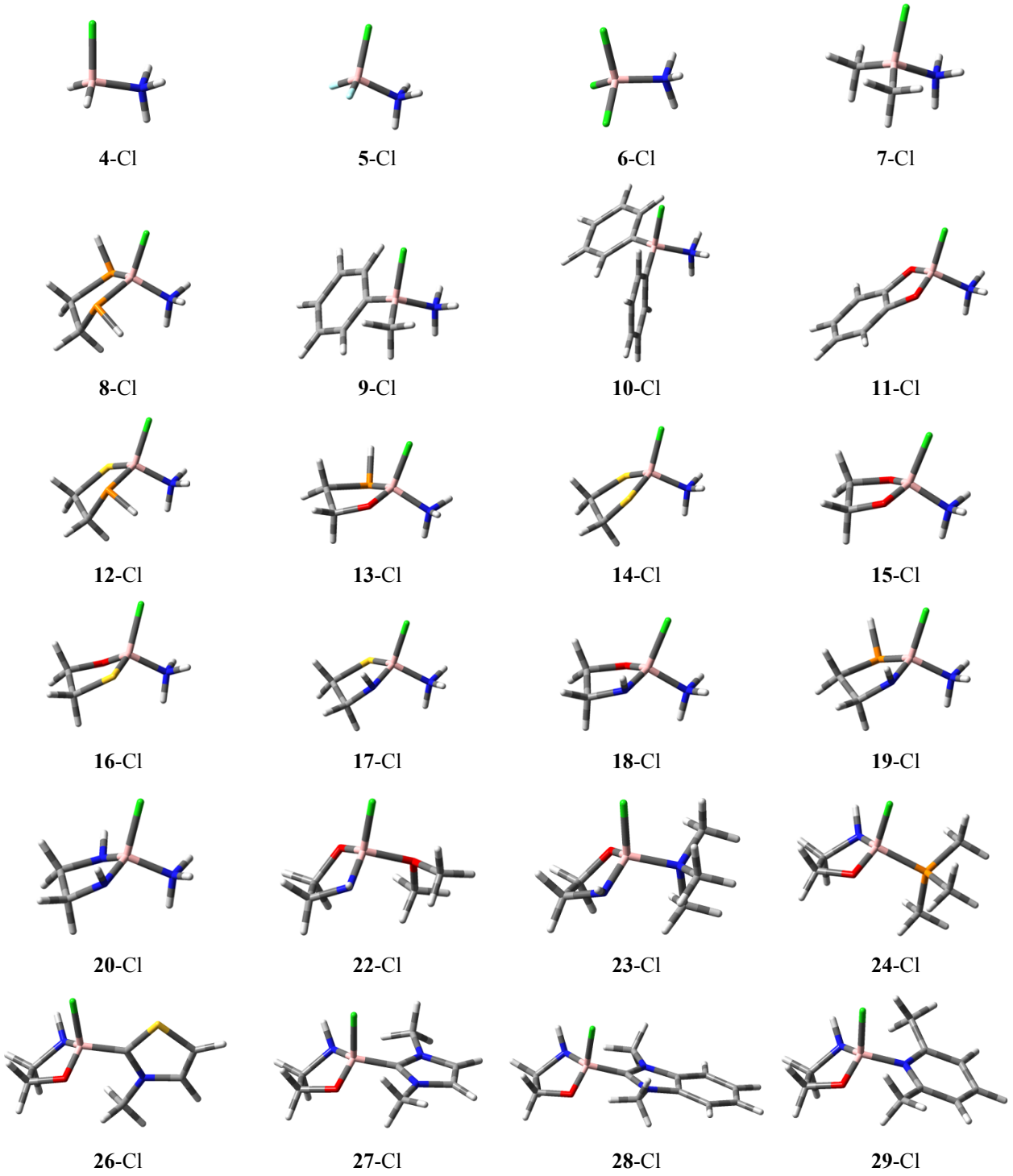
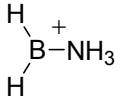


Figure S4. Optimized structures of Cl^--adducts of borenium cations **4**-**29**.

Absolute energies (a.u.) and x, y, z coordinates (Å) of the optimized structures



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E = -82.3196993 a.u. *i*: -140.23 cm^{-1}

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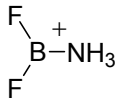
2	1	0	-1.417416	-1.064477	0.004699
3	1	0	-1.434012	1.058105	0.005894
4	7	0	0.631122	0.003601	-0.007513
5	1	0	1.046800	0.880182	-0.338392
6	1	0	0.959486	-0.127513	0.961461
7	1	0	1.032478	-0.776544	-0.540138



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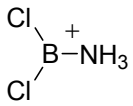
3	1	0	0.963946	-1.714558	0.000000
4	1	0	-0.457561	-1.740207	0.835703
5	9	0	-0.000966	0.760416	-1.154852
6	9	0	-0.000966	0.760416	1.154852
7	1	0	-0.457561	-1.740207	-0.835703



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3	17	0	-0.008701	-0.572486	-1.526059
4	7	0	0.025543	1.743781	0.000000
5	1	0	1.000699	2.073462	0.000000
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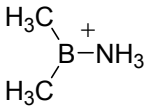
7	1	0	-0.420076	2.142665	0.834536



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3	1	0	0.972950	1.858295	0.031323
4	1	0	-0.442099	1.830152	-0.830858
5	6	0	1.376695	-0.806045	0.006570
6	1	0	2.065123	-0.376436	0.742619
7	1	0	1.319904	-1.882538	0.162246
8	1	0	1.852375	-0.644874	-0.973195
9	6	0	-1.410501	-0.747578	-0.007851
10	1	0	-1.450536	-1.606177	-0.684633
11	1	0	-1.577477	-1.179163	0.990930
12	1	0	-2.246473	-0.080328	-0.223535
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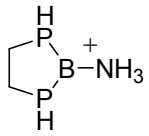

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4	1	0	1.745202	0.604424	-1.409327
5	6	0	1.677247	-0.697465	0.337720
6	1	0	2.527634	-1.289908	0.002068
7	1	0	1.718379	-0.613264	1.425036
8	15	0	0.097487	1.535257	0.182371
9	1	0	-0.267195	2.372979	-0.893955
10	7	0	-2.509133	0.007107	0.004552
11	1	0	-2.921659	0.878454	-0.340448
12	1	0	-2.901431	-0.762943	-0.545484
13	1	0	-2.845009	-0.118943	0.966203
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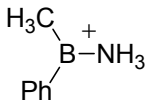

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4	1	0	2.171774	-1.818036	-0.847036
5	1	0	3.375655	-1.205409	0.103050
6	6	0	0.101802	0.036853	-0.002444
7	6	0	-0.611803	-1.180908	-0.008658
8	6	0	-0.638276	1.236435	0.005059
9	6	0	-1.995173	-1.200519	-0.008284
10	1	0	-0.095408	-2.137587	-0.018618
11	6	0	-2.024422	1.220299	0.008890
12	1	0	-0.121300	2.188646	0.009900
13	6	0	-2.700142	0.003461	0.001659
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15	1	0	-2.579538	2.149845	0.016635
16	1	0	-3.783734	-0.010624	0.003427
17	6	0	2.588553	1.310980	-0.013377
18	1	0	3.187910	1.319465	0.907243
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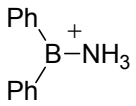

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4	1	0	-0.318713	2.786831	1.011672
5	1	0	0.913826	2.888802	-0.069306
6	6	0	-1.386848	0.259074	-0.012766
7	6	0	-1.531589	-1.050211	-0.512589
8	6	0	-2.547863	0.938150	0.409733
9	6	0	-2.779204	-1.652631	-0.581065
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11	6	0	-3.792073	0.332588	0.357592
12	1	0	-2.493075	1.946574	0.812867
13	6	0	-3.906080	-0.964788	-0.140629
14	1	0	-2.876978	-2.654377	-0.980674
15	1	0	-4.672266	0.862671	0.699539
16	1	0	-4.880127	-1.437171	-0.190699
17	6	0	1.384825	0.269226	0.024012
18	6	0	1.571783	-0.995863	0.615303
19	6	0	2.508855	0.913673	-0.529961
20	6	0	2.828118	-1.582105	0.658526
21	1	0	0.729065	-1.503914	1.070839
22	6	0	3.759182	0.317156	-0.511722
23	1	0	2.415924	1.873957	-1.032886
24	6	0	3.918777	-0.929485	0.090435
25	1	0	2.960252	-2.546660	1.133083
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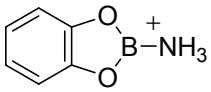

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4	6	0	0.002421	-2.587117	-0.697920
5	6	0	0.002421	-2.587117	0.697920
6	6	0	0.000433	-1.401879	1.435674
7	1	0	-0.000060	-1.389091	-2.517213
8	1	0	0.004112	-3.531681	-1.226516
9	1	0	0.004112	-3.531681	1.226516
10	1	0	-0.000060	-1.389091	2.517213
11	8	0	-0.004635	1.086029	-1.144644
12	8	0	-0.004635	1.086029	1.144644
13	5	0	-0.003382	1.786056	0.000000
14	7	0	0.003934	3.320591	0.000000
15	1	0	-0.463076	3.695113	-0.833003
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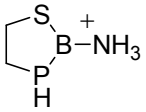
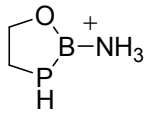


12

E = -899.9331582 a.u.

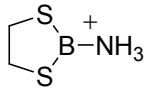
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.880086	0.074591	0.012863
2	6	0	-1.717855	0.499802	0.386706
3	1	0	-2.664500	0.934194	0.061887
4	1	0	-1.708648	0.454059	1.475942
5	6	0	-1.572401	-0.896496	-0.213385
6	1	0	-2.232867	-1.621022	0.260367
7	1	0	-1.755726	-0.901762	-1.288468
8	7	0	2.438156	0.181518	0.069585
9	1	0	2.899914	-0.709309	0.277246
10	1	0	2.801110	0.509783	-0.832424
11	1	0	2.745811	0.863185	0.770125
12	15	0	-0.291476	1.546494	-0.237715
13	1	0	0.061759	2.277567	0.921811
14	16	0	0.156206	-1.516720	0.020494



13

E = -576.9852181 a.u.

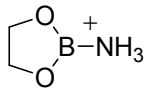
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.809960	-0.055339	0.002716
2	6	0	-1.705705	0.004190	0.301596
3	1	0	-2.667403	0.179318	-0.179122
4	1	0	-1.849892	0.019811	1.381540
5	6	0	-1.119751	-1.334361	-0.155215
6	1	0	-1.467424	-2.177697	0.437204
7	1	0	-1.312248	-1.529765	-1.210515
8	7	0	2.368713	-0.006192	0.076309
9	1	0	2.746489	-0.950068	0.214956
10	1	0	2.768141	0.368997	-0.790360
11	1	0	2.707378	0.591737	0.835657
12	15	0	-0.469470	1.342604	-0.209068
13	1	0	-0.219249	1.942783	1.047825
14	8	0	0.332276	-1.285389	-0.003400



14

E = -956.2086756 a.u.

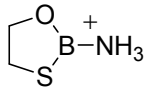
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.842181	0.006047	-0.012208
2	6	0	1.653180	0.695679	-0.279104
3	1	0	2.441055	1.296809	0.173478
4	1	0	1.774577	0.694321	-1.362196
5	6	0	1.641386	-0.711424	0.292839
6	1	0	2.429229	-1.321149	-0.148262
7	1	0	1.747873	-0.710869	1.377498
8	7	0	-2.401790	0.008341	0.005991
9	1	0	-2.795132	0.877611	-0.367152
10	1	0	-2.792734	-0.769017	-0.535724
11	1	0	-2.748838	-0.096927	0.965882
12	16	0	0.044928	1.529775	0.074987
13	16	0	0.030073	-1.527583	-0.085414



15

E = -310.3098535 a.u.

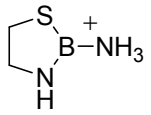
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.620284	0.000260	-0.003449
2	8	0	0.045672	1.148910	0.015117
3	8	0	0.045249	-1.148748	-0.022646
4	6	0	1.455061	-0.777276	0.023165
5	1	0	1.947154	-1.228449	-0.835212
6	1	0	1.871951	-1.179135	0.944162
7	6	0	1.455621	0.776838	-0.018295
8	1	0	1.940860	1.227478	0.844258
9	1	0	1.879978	1.178883	-0.935788
10	7	0	-2.161695	0.000987	0.000275
11	1	0	-2.534927	0.883561	-0.363359
12	1	0	-2.535034	-0.772894	-0.559099
13	1	0	-2.528150	-0.116326	0.951371



16

E = -633.2602732 a.u.

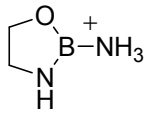
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.758640	0.114617	-0.007630
2	6	0	-1.699343	-0.180462	-0.225198
3	1	0	-2.545330	-0.510123	0.374108
4	1	0	-1.947001	-0.259854	-1.282280
5	6	0	-1.239294	1.224975	0.166452
6	1	0	-1.712712	1.996783	-0.436579
7	1	0	-1.408314	1.425908	1.224830
8	7	0	2.310898	0.111818	-0.045989
9	1	0	2.677623	-0.464270	-0.810003
10	1	0	2.658187	1.069163	-0.169508
11	1	0	2.711486	-0.257092	0.822739
12	16	0	-0.270043	-1.321499	0.088377
13	8	0	0.193635	1.315072	-0.053099



17

E = -613.3875825 a.u.

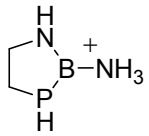
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.779158	0.178519	0.013368
2	6	0	1.685346	-0.301975	0.239565
3	1	0	2.515880	-0.724950	-0.320414
4	1	0	1.887124	-0.381575	1.306649
5	6	0	1.384608	1.139756	-0.175467
6	1	0	1.971895	1.839527	0.419357
7	1	0	1.607865	1.298280	-1.233514
8	7	0	-2.335901	0.156499	0.044626
9	1	0	-2.753506	1.080904	0.178343
10	1	0	-2.709576	-0.225785	-0.830363
11	1	0	-2.675979	-0.450820	0.797040
12	16	0	0.174563	-1.325244	-0.094444
13	7	0	-0.058669	1.350312	0.051679
14	1	0	-0.398652	2.301366	0.068437



18

E = -290.436977 a.u.

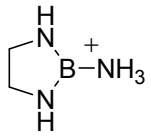
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.551584	0.692279	0.056442
2	6	0	1.402352	-0.849947	-0.049785
3	1	0	2.160912	1.093477	-0.752743
4	1	0	1.983357	0.996063	1.010993
5	1	0	1.901018	-1.379692	0.758008
6	1	0	1.748995	-1.233945	-1.007777
7	8	0	-0.022395	-1.133201	0.039155
8	7	0	0.153411	1.164351	-0.047768
9	1	0	-0.045998	2.151440	-0.055397
10	5	0	-0.650958	0.049072	-0.006033
11	7	0	-2.199642	0.006977	0.003219
12	1	0	-2.515343	-0.900036	-0.356319
13	1	0	-2.569784	0.096609	0.954740
14	1	0	-2.629216	0.743044	-0.562681



19

E = -557.11482 a.u.

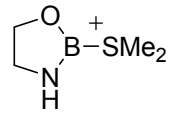
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.833703	0.120484	0.016585
2	6	0	1.714118	-0.140101	0.296265
3	1	0	2.658912	-0.413963	-0.169996
4	1	0	1.839223	-0.172312	1.378349
5	6	0	1.277479	1.261835	-0.150148
6	1	0	1.748911	2.038552	0.452503
7	1	0	1.530450	1.438181	-1.198460
8	7	0	-2.395407	0.062664	0.071458
9	1	0	-2.714614	-0.530944	0.842850
10	1	0	-2.841906	0.977148	0.182142
11	1	0	-2.765033	-0.360029	-0.786363
12	7	0	-0.193467	1.330898	0.003053
13	1	0	-0.607185	2.254858	-0.015104
14	15	0	0.359207	-1.356652	-0.213584
15	1	0	0.104178	-1.969461	1.036628



20

E = -270.5601548 a.u.

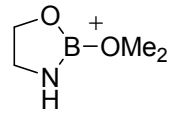
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.679999	0.002445	-0.008538
2	6	0	1.501339	-0.769819	0.101114
3	1	0	2.146062	-1.266624	-0.622348
4	1	0	1.825562	-1.040103	1.108455
5	6	0	1.505597	0.766291	-0.093652
6	1	0	2.142687	1.260413	0.638335
7	1	0	1.843734	1.035866	-1.096545
8	7	0	-2.235976	0.001016	0.003730
9	1	0	-2.623388	0.857288	-0.400447
10	1	0	-2.616146	-0.787644	-0.526094
11	1	0	-2.597976	-0.073022	0.959203
12	7	0	0.088668	1.154939	0.078961
13	7	0	0.085573	-1.153144	-0.090972
14	1	0	-0.161236	2.129524	0.049333
15	1	0	-0.168770	-2.126436	-0.054011



21

E = -711.8501378 a.u.

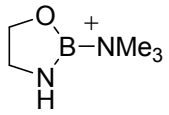
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.673884	0.440897	-0.061647
2	6	0	2.215190	-1.007476	0.252957
3	1	0	3.371023	0.467966	-0.898739
4	1	0	3.137826	0.920412	0.801821
5	1	0	2.603375	-1.380284	1.197628
6	1	0	2.469078	-1.702058	-0.546740
7	7	0	1.404607	1.113916	-0.402020
8	1	0	1.395444	2.070414	-0.717682
9	8	0	0.760990	-0.969351	0.346149
10	5	0	0.382662	0.246351	-0.094625
11	6	0	-1.979905	0.120879	1.462277
12	1	0	-1.519370	-0.833044	1.712543
13	1	0	-1.646090	0.909112	2.134802
14	1	0	-3.066780	0.060708	1.471770
15	6	0	-1.996864	-0.879048	-1.157487
16	1	0	-3.083778	-0.923553	-1.116284
17	1	0	-1.669955	-0.742946	-2.186900
18	1	0	-1.537401	-1.758777	-0.711128
19	16	0	-1.485043	0.599136	-0.224976



22

E = -388.877197 a.u.

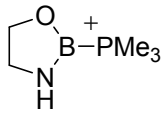
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.275398	0.705417	-0.041276
2	6	0	-2.137820	-0.831520	0.096028
3	1	0	-2.885968	1.124650	0.757753
4	1	0	-2.702530	0.991655	-1.003882
5	1	0	-2.708362	-1.377249	-0.651118
6	1	0	-2.407865	-1.179965	1.092222
7	7	0	-0.873880	1.164363	0.057760
8	1	0	-0.672495	2.149194	0.090795
9	8	0	-0.729570	-1.134155	-0.101116
10	5	0	-0.079544	0.039551	-0.054312
11	6	0	2.095088	-1.260009	0.064539
12	1	0	2.496046	-1.256545	1.076374
13	1	0	1.368880	-2.053296	-0.081528
14	1	0	2.877953	-1.285066	-0.689148
15	6	0	2.157763	1.227656	0.036556
16	1	0	3.109476	1.054630	-0.459399
17	1	0	1.614265	2.027214	-0.458544
18	1	0	2.285256	1.413722	1.101592
19	8	0	1.367373	0.008341	-0.129254



23

E = -408.3454785 a.u.

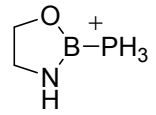
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.479343	-0.713151	0.064581
2	6	0	-2.338613	0.825182	-0.066128
3	1	0	-3.099249	-1.128360	-0.729684
4	1	0	-2.898888	-1.004722	1.029063
5	1	0	-2.869365	1.365692	0.714051
6	1	0	-2.663324	1.184661	-1.042055
7	7	0	-1.081848	-1.173241	-0.049009
8	1	0	-0.876676	-2.158631	-0.051712
9	8	0	-0.924048	1.118572	0.059413
10	5	0	-0.265721	-0.058516	0.005631
11	7	0	1.268858	-0.016358	0.001151
12	6	0	1.864176	-1.385486	0.012350
13	1	0	1.534488	-1.924939	-0.874807
14	1	0	2.950258	-1.294718	0.004586
15	1	0	1.544766	-1.906574	0.913967
16	6	0	1.722932	0.744670	1.214512
17	1	0	2.810802	0.810745	1.192852
18	1	0	1.276460	1.736577	1.189746
19	1	0	1.398326	0.211161	2.107625
20	6	0	1.709054	0.716396	-1.234687
21	1	0	2.797104	0.783172	-1.227804
22	1	0	1.374243	0.162230	-2.111422
23	1	0	1.263740	1.709234	-1.226634



24

E = -694.9474197 a.u.

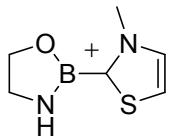
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.881644	-0.701965	0.059669
2	6	0	-2.714171	0.833036	-0.064547
3	1	0	-3.506430	-1.104391	-0.737628
4	1	0	-3.308080	-0.990999	1.022106
5	1	0	-3.228698	1.379229	0.722821
6	1	0	-3.039970	1.204169	-1.035829
7	7	0	-1.491728	-1.185754	-0.052730
8	1	0	-1.300005	-2.173881	-0.058275
9	8	0	-1.292223	1.102481	0.051451
10	5	0	-0.649196	-0.088721	-0.001996
11	15	0	1.288401	-0.019049	0.001255
12	6	0	1.821937	1.014681	1.388243
13	1	0	2.907024	1.128086	1.369766
14	1	0	1.346725	1.992912	1.298757
15	1	0	1.518844	0.555946	2.330264
16	6	0	2.043004	-1.657837	0.152016
17	1	0	1.745752	-2.281111	-0.692800
18	1	0	3.129992	-1.560941	0.157080
19	1	0	1.721077	-2.129044	1.081870
20	6	0	1.862205	0.754041	-1.532988
21	1	0	2.947719	0.863213	-1.505904
22	1	0	1.579772	0.138056	-2.387664
23	1	0	1.398141	1.736779	-1.630261



25

E = -576.9710838 a.u.

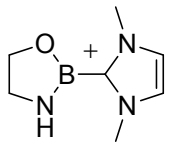
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.024297	0.678806	0.057404
2	6	0	1.856003	-0.858593	-0.058114
3	1	0	2.639146	1.078485	-0.748509
4	1	0	2.456046	0.973893	1.014966
5	1	0	2.358415	-1.401485	0.738652
6	1	0	2.183301	-1.239549	-1.024364
7	7	0	0.631854	1.169206	-0.045951
8	1	0	0.442028	2.158127	-0.058591
9	8	0	0.427215	-1.126225	0.049460
10	5	0	-0.190848	0.066236	-0.000025
11	15	0	-2.145762	0.006619	0.000256
12	1	0	-2.647355	-0.666043	-1.118051
13	1	0	-2.639788	-0.684756	1.110497
14	1	0	-2.773623	1.254947	0.011926



26

E = -842.2141202 a.u.

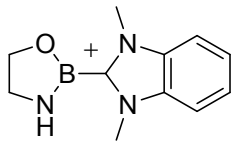
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.224492	-0.799631	-0.187739
2	6	0	-3.109053	0.678392	0.244582
3	1	0	-3.614580	-0.899535	-1.203144
4	1	0	-3.860426	-1.367741	0.491312
5	1	0	-3.389212	0.819334	1.288960
6	1	0	-3.690219	1.352185	-0.380962
7	7	0	-1.824855	-1.250869	-0.125879
8	1	0	-1.605599	-2.215573	-0.312740
9	8	0	-1.708165	1.029196	0.120822
10	5	0	-1.009452	-0.131344	-0.012947
11	6	0	0.572580	-0.120367	-0.014069
12	16	0	1.508989	-1.532108	0.079336
13	6	0	2.704276	0.686791	-0.027055
14	6	0	2.968950	-0.637017	0.049987
15	1	0	3.412926	1.500206	-0.063382
16	1	0	3.933265	-1.118959	0.091652
17	7	0	1.352971	0.957108	-0.061948
18	6	0	0.841318	2.343578	-0.124487
19	1	0	0.427049	2.614467	0.844794
20	1	0	1.673759	2.993735	-0.380026
21	1	0	0.063524	2.404611	-0.880202



27

E = -538.7032982 a.u.

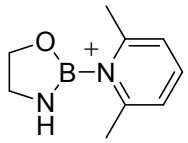
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.143739	0.702771	-0.231897
2	6	0	3.014582	-0.752074	0.262118
3	1	0	3.503829	0.753351	-1.262271
4	1	0	3.810057	1.285830	0.403917
5	1	0	3.295812	-0.849446	1.311546
6	1	0	3.588682	-1.458121	-0.333844
7	7	0	1.753801	1.181587	-0.146744
8	1	0	1.551006	2.133281	-0.400003
9	8	0	1.611934	-1.088564	0.153801
10	5	0	0.917484	0.073754	-0.003704
11	6	0	-2.730913	-0.767951	-0.037322
12	6	0	-2.805610	0.588237	0.029918
13	1	0	-3.506674	-1.514068	-0.072412
14	1	0	-3.656775	1.246892	0.067109
15	6	0	-0.656562	0.022035	-0.005857
16	7	0	-1.517351	1.055032	0.048944
17	7	0	-1.401029	-1.096983	-0.056010
18	6	0	-1.145196	2.469805	0.113671
19	1	0	-0.785480	2.803527	-0.859700
20	1	0	-2.028477	3.042787	0.385310
21	1	0	-0.381639	2.608175	0.877373
22	6	0	-0.888749	-2.474741	-0.110428
23	1	0	-0.356947	-2.702207	0.810368
24	1	0	-1.741420	-3.138448	-0.230161
25	1	0	-0.210561	-2.577751	-0.953672



28

E = -692.3270179 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.065211	-0.732737	0.065412
2	6	0	4.083858	0.672322	-0.039428
3	6	0	2.919513	1.415371	-0.098330
4	6	0	1.724935	0.696671	-0.047622
5	6	0	1.706619	-0.693499	0.054954
6	6	0	2.881019	-1.444000	0.114965
7	1	0	5.005584	-1.267408	0.108143
8	1	0	5.038098	1.182574	-0.073318
9	1	0	2.938962	2.495116	-0.172786
10	1	0	2.868275	-2.523447	0.195421
11	7	0	0.398917	1.102808	-0.084809
12	7	0	0.372505	-1.071117	0.073364
13	6	0	-0.400214	0.023634	-0.004629
14	6	0	-0.060679	-2.465845	0.176714
15	1	0	-1.143342	-2.511849	0.112475
16	1	0	0.375842	-3.026978	-0.649416
17	1	0	0.284822	-2.874376	1.126511
18	6	0	-0.012429	2.497669	-0.224087
19	1	0	-1.044746	2.537157	-0.562481
20	1	0	0.095884	3.015506	0.729861
21	1	0	0.622965	2.971765	-0.971218
22	5	0	-1.984085	0.034825	0.006463
23	7	0	-2.819245	1.029196	0.516791
24	8	0	-2.679817	-1.011735	-0.518620
25	6	0	-4.083147	-0.661410	-0.496804
26	1	0	-4.654466	-1.529503	-0.175419
27	1	0	-4.369987	-0.395149	-1.514938
28	6	0	-4.206588	0.537670	0.463902
29	1	0	-4.542824	0.232233	1.457654
30	1	0	-4.889787	1.293719	0.076995
31	1	0	-2.600148	1.819111	1.101456



29

E = -560.7780695 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.201650	0.134268	0.683389
2	6	0	-3.057391	-0.140874	-0.834142
3	1	0	-3.843878	-0.602934	1.165161
4	1	0	-3.601549	1.131286	0.880777
5	1	0	-3.602671	0.571397	-1.449135
6	1	0	-3.366679	-1.153434	-1.095088
7	7	0	-1.808975	0.030157	1.150944
8	1	0	-1.589464	0.102941	2.130746
9	8	0	-1.646281	-0.023812	-1.139786
10	5	0	-0.984382	0.004852	0.037669
11	7	0	0.536520	0.002732	0.037852
12	6	0	1.184864	-1.193269	0.033918
13	6	0	1.192915	1.193478	-0.004633
14	6	0	2.576635	1.197090	-0.023858
15	1	0	3.099664	2.143321	-0.056662
16	6	0	2.568575	-1.206746	0.015109
17	1	0	3.085283	-2.156989	0.014100
18	6	0	3.267433	-0.007289	-0.010115
19	1	0	4.350992	-0.011203	-0.026462
20	6	0	0.372089	2.445235	-0.045483
21	1	0	-0.277355	2.443613	-0.925044
22	1	0	-0.257792	2.527241	0.843726
23	1	0	1.020219	3.317489	-0.092761
24	6	0	0.355517	-2.440073	0.037614
25	1	0	-0.267155	-2.490411	0.934141
26	1	0	-0.301556	-2.459436	-0.836163
27	1	0	0.997366	-3.317784	0.010243

4-NH_3 complex

E = -138.9623591 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.691857
2	1	0	-1.014971	0.000000	1.314694
3	1	0	1.014971	0.000000	1.314694
4	7	0	0.000000	1.309833	-0.249280
5	1	0	0.000000	2.115837	0.380614
6	1	0	0.826447	1.414601	-0.839998
7	1	0	-0.826447	1.414601	-0.839998
8	7	0	0.000000	-1.309833	-0.249280
9	1	0	0.826447	-1.414601	-0.839998
10	1	0	-0.826447	-1.414601	-0.839998
11	1	0	0.000000	-2.115837	0.380614

5-NH_3 complex

E =-337.5834906 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.162248
2	7	0	0.000000	1.332228	-0.755555
3	1	0	0.000000	2.115781	-0.093424
4	1	0	0.832145	1.448117	-1.337601
5	9	0	-1.163878	0.000000	0.850210
6	9	0	1.163878	0.000000	0.850210
7	1	0	-0.832145	1.448117	-1.337601
8	7	0	0.000000	-1.332228	-0.755555
9	1	0	-0.832145	-1.448117	-1.337601
10	1	0	0.000000	-2.115781	-0.093424
11	1	0	0.832145	-1.448117	-1.337601

6-NH_3 complex

E = -1058.2536466 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.202655
2	17	0	1.541939	0.000000	-0.730879
3	17	0	-1.541939	0.000000	-0.730879
4	7	0	0.000000	1.307223	1.138396
5	1	0	0.000000	2.113058	0.503605
6	1	0	-0.834837	1.402919	1.722962
7	1	0	0.834837	1.402919	1.722962
8	7	0	0.000000	-1.307223	1.138396
9	1	0	0.000000	-2.113058	0.503605
10	1	0	-0.834837	-1.402919	1.722962
11	1	0	0.834837	-1.402919	1.722962

7-NH_3 complex

E = -217.6003603 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.120450
2	7	0	0.000000	1.299670	-0.880258
3	1	0	0.000000	2.124836	-0.276361
4	1	0	0.828308	1.383368	-1.472216
5	1	0	-0.828308	1.383368	-1.472216
6	7	0	0.000000	-1.299670	-0.880258
7	1	0	-0.828308	-1.383368	-1.472216
8	1	0	0.828308	-1.383368	-1.472216
9	6	0	-1.371055	0.000000	0.932170
10	1	0	-1.440933	-0.870883	1.591024
11	1	0	-1.440933	0.870883	1.591024
12	1	0	-2.272049	0.000000	0.306408
13	6	0	1.371055	0.000000	0.932170
14	1	0	1.440933	-0.870883	1.591024
15	1	0	2.272049	0.000000	0.306408
16	1	0	1.440933	0.870883	1.591024
17	1	0	0.000000	-2.124836	-0.276361

8-NH_3 complex

E = -900.2601184 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.845324
2	6	0	0.000000	0.765420	-1.888131
3	1	0	0.535476	1.151062	-2.756486
4	1	0	-1.021069	1.150807	-1.929315
5	6	0	0.000000	-0.765420	-1.888131
6	1	0	-0.535476	-1.151062	-2.756486
7	1	0	1.021069	-1.150807	-1.929315
8	7	0	-1.127368	0.636783	1.820928
9	1	0	-1.586906	-0.036596	2.440348
10	1	0	-0.816966	1.430750	2.385536
11	1	0	-1.866157	0.990457	1.207606
12	15	0	0.873448	1.325410	-0.325627
13	1	0	0.112214	2.475300	0.005692
14	7	0	1.127368	-0.636783	1.820928
15	1	0	1.586906	0.036596	2.440348
16	1	0	0.816966	-1.430750	2.385536
17	1	0	1.866157	-0.990457	1.207606
18	15	0	-0.873448	-1.325410	-0.325627
19	1	0	-0.112214	-2.475300	0.005692

9-NH_3 complex

E = -409.310618 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.698220	-1.263672	0.000000
2	7	0	-0.129221	-2.077964	1.302663
3	1	0	-0.477358	-1.567219	2.117563
4	1	0	-0.459714	-3.039773	1.397998
5	1	0	0.888814	-2.071606	1.387863
6	7	0	-0.129221	-2.077964	-1.302663
7	1	0	-0.477358	-1.567219	-2.117563
8	1	0	0.888814	-2.071606	-1.387863
9	1	0	-0.459714	-3.039773	-1.397998
10	6	0	0.003172	0.167101	0.000000
11	6	0	1.402119	0.287620	0.000000
12	6	0	-0.746951	1.347768	0.000000
13	6	0	2.029249	1.527907	0.000000
14	1	0	2.041412	-0.598138	0.000000
15	6	0	-0.129221	2.595300	0.000000
16	1	0	-1.830704	1.297344	0.000000
17	6	0	1.257812	2.686737	0.000000
18	1	0	3.110590	1.593585	0.000000
19	1	0	-0.730986	3.496269	0.000000
20	1	0	1.739230	3.657140	0.000000
21	6	0	-2.287000	-1.367776	0.000000
22	1	0	-2.723798	-0.874024	-0.873246
23	1	0	-2.660322	-2.399035	0.000000
24	1	0	-2.723798	-0.874024	0.873246

10-NH_3 complex

E = -601.018362 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.021237	0.980172	0.072970
2	7	0	0.003190	1.821094	1.479459
3	1	0	-0.076700	1.114304	2.214825
4	1	0	0.845875	2.358884	1.688925
5	1	0	-0.813023	2.426872	1.582622
6	7	0	0.111839	2.103565	-1.104487
7	1	0	0.059278	1.586352	-1.986133
8	1	0	-0.635744	2.799536	-1.124663
9	1	0	1.013104	2.584439	-1.114678
10	6	0	1.375692	0.139960	0.003246
11	6	0	1.389805	-1.173721	-0.480234
12	6	0	2.608653	0.715467	0.349538
13	6	0	2.580446	-1.883969	-0.604484
14	1	0	0.456596	-1.650272	-0.761352
15	6	0	3.802559	0.012121	0.233659
16	1	0	2.668328	1.740730	0.717930
17	6	0	3.786894	-1.294305	-0.244516
18	1	0	2.565314	-2.900191	-0.979750
19	1	0	4.739211	0.478635	0.514258
20	1	0	4.713207	-1.848508	-0.335693
21	6	0	-1.377718	0.222281	-0.002930
22	6	0	-2.425302	0.584244	-0.857133
23	6	0	-1.606568	-0.843959	0.881451
24	6	0	-3.647292	-0.085301	-0.836819
25	1	0	-2.315950	1.393479	-1.575898
26	6	0	-2.824163	-1.511393	0.916139
27	1	0	-0.806424	-1.180651	1.537488
28	6	0	-3.849171	-1.131576	0.053581
29	1	0	-4.437600	0.210784	-1.516036
30	1	0	-2.972150	-2.332749	1.606915
31	1	0	-4.797705	-1.654207	0.072602

11-NH_3 complex

E = -519.3141097 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.695464	-0.526772
2	6	0	0.000000	-0.695464	-0.526772
3	6	0	0.000000	-1.426004	-1.692167
4	6	0	0.000000	-0.695488	-2.886139
5	6	0	0.000000	0.695488	-2.886139
6	6	0	0.000000	1.426004	-1.692167
7	1	0	0.000000	-2.507973	-1.679161
8	1	0	0.000000	-1.228621	-3.828157
9	1	0	0.000000	1.228621	-3.828157
10	1	0	0.000000	2.507973	-1.679161
11	8	0	0.000000	-1.166477	0.782061
12	8	0	0.000000	1.166477	0.782061
13	5	0	0.000000	0.000000	1.578324
14	7	0	1.312802	0.000000	2.541000
15	1	0	1.413343	0.831820	3.125711
16	1	0	1.413343	-0.831820	3.125711
17	7	0	-1.312802	0.000000	2.541000
18	1	0	-1.413343	-0.831820	3.125711
19	1	0	-1.413343	0.831820	3.125711
20	1	0	2.109157	0.000000	1.897071
21	1	0	-2.109157	0.000000	1.897071

12-NH_3 complex

E = -956.5332267 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.810305	0.041083	-0.008442
2	6	0	1.902176	0.579227	-0.350139
3	1	0	2.826198	1.071461	-0.040773
4	1	0	1.893375	0.522452	-1.439763
5	6	0	1.826926	-0.816451	0.253942
6	1	0	2.556816	-1.491310	-0.191962
7	1	0	1.992997	-0.796684	1.331625
8	7	0	-1.691251	0.155822	-1.365902
9	1	0	-2.290493	-0.654535	-1.547317
10	1	0	-2.259436	1.001460	-1.453289
11	1	0	-1.013397	0.174017	-2.131792
12	15	0	0.433013	1.540839	0.300832
13	1	0	0.120085	2.325246	-0.839219
14	16	0	0.167580	-1.552400	-0.067507
15	7	0	-1.885634	-0.023045	1.210251
16	1	0	-2.478716	0.803260	1.320517
17	1	0	-2.482197	-0.854061	1.203231
18	1	0	-1.326604	-0.086990	2.065329

13-NH_3 complex

E = -633.5809987 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.688836	-0.046166	0.026238
2	6	0	-1.933529	0.008204	0.270436
3	1	0	-2.903921	0.139203	-0.208027
4	1	0	-2.072155	0.073828	1.350449
5	6	0	-1.311877	-1.333332	-0.112280
6	1	0	-1.751007	-2.166638	0.434912
7	1	0	-1.433773	-1.526217	-1.183929
8	7	0	1.620852	0.196996	1.336894
9	1	0	2.230203	-0.602343	1.532586
10	1	0	2.181099	1.050084	1.349917
11	7	0	1.738332	-0.159523	-1.232352
12	1	0	2.299522	0.671147	-1.427139
13	1	0	2.357912	-0.970468	-1.162088
14	1	0	0.972841	0.255171	2.125462
15	1	0	1.162779	-0.310513	-2.064446
16	15	0	-0.711772	1.307498	-0.335076
17	1	0	-0.564295	2.067712	0.850622
18	8	0	0.088918	-1.296768	0.201987

14-NH_3 complex

E = -1012.805259 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.778773
2	6	0	-0.359257	0.667628	-1.849037
3	1	0	-0.006027	1.308475	-2.657454
4	1	0	-1.437022	0.538439	-1.946399
5	6	0	0.359257	-0.667628	-1.849037
6	1	0	0.006027	-1.308475	-2.657454
7	1	0	1.437022	-0.538439	-1.946399
8	7	0	-1.294471	-0.043623	1.760257
9	1	0	-1.374832	-0.884383	2.338274
10	1	0	-1.398390	0.777473	2.361179
11	7	0	1.294471	0.043623	1.760257
12	1	0	1.374832	0.884383	2.338274
13	1	0	1.398390	-0.777473	2.361179
14	1	0	-2.104846	-0.047423	1.135434
15	1	0	2.104846	0.047423	1.135434
16	16	0	0.000000	1.544671	-0.275346
17	16	0	0.000000	-1.544671	-0.275346

15-NH_3 complex

E = -366.9040217 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.742953	0.190684	-1.652972
2	6	0	0.742953	-0.190684	-1.652972
3	1	0	-1.347491	-0.415531	-2.325143
4	1	0	-0.890877	1.246908	-1.895317
5	1	0	1.347491	0.415531	-2.325143
6	1	0	0.890877	-1.246908	-1.895317
7	8	0	1.157560	0.050039	-0.296267
8	8	0	-1.157560	-0.050039	-0.296267
9	5	0	0.000000	0.000000	0.484758
10	7	0	0.000000	-1.305770	1.475102
11	1	0	0.099926	-2.111757	0.853712
12	1	0	0.771147	-1.354053	2.142157
13	1	0	-0.881121	-1.437088	1.974956
14	7	0	0.000000	1.305770	1.475102
15	1	0	-0.771147	1.354053	2.142157
16	1	0	0.881121	1.437088	1.974956
17	1	0	-0.099926	2.111757	0.853712

16-NH_3 complex

E = -689.8554498 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.660511	0.083626	0.033078
2	6	0	1.914852	-0.130722	0.234714
3	1	0	2.805798	-0.381224	-0.338428
4	1	0	2.135267	-0.226911	1.297493
5	6	0	1.381449	1.253207	-0.112421
6	1	0	1.893324	2.043080	0.436304
7	1	0	1.483109	1.445391	-1.185450
8	7	0	-1.644105	-0.147080	1.305408
9	1	0	-2.225201	0.668263	1.516650
10	1	0	-2.235913	-0.978229	1.268783
11	7	0	-1.639339	0.207674	-1.273985
12	1	0	-2.156237	-0.638216	-1.520775
13	1	0	-2.293914	0.992131	-1.227716
14	1	0	-1.018039	-0.272747	2.104585
15	1	0	-1.010533	0.392830	-2.059544
16	16	0	0.572870	-1.310611	-0.213180
17	8	0	-0.004341	1.293526	0.249983

17-NH_3 complex

E = -669.9699672 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.674446	0.144858	-0.035860
2	6	0	-1.925103	-0.256750	-0.237184
3	1	0	-2.790971	-0.621729	0.311442
4	1	0	-2.113669	-0.341941	-1.306878
5	6	0	-1.547576	1.166099	0.149741
6	1	0	-2.174862	1.886659	-0.378762
7	1	0	-1.695744	1.309417	1.227265
8	7	0	1.683477	-0.085172	-1.308477
9	1	0	2.326049	0.684693	-1.507520
10	1	0	2.217109	-0.955826	-1.288068
11	7	0	1.676533	0.207932	1.277044
12	1	0	2.158865	-0.668855	1.485432
13	1	0	2.369507	0.959168	1.277618
14	1	0	1.050202	-0.150275	-2.108854
15	1	0	1.049312	0.376261	2.067130
16	16	0	-0.479256	-1.317939	0.189531
17	7	0	-0.141928	1.327868	-0.240276
18	1	0	0.209566	2.274684	-0.205382

18-NH_3 complex

E = -347.0187072 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.762692	-0.397010	-0.556548
2	6	0	-1.617282	0.459055	0.704883
3	1	0	-2.532131	-0.006980	-1.223786
4	1	0	-2.018869	-1.431856	-0.300204
5	1	0	-2.246553	0.131017	1.529923
6	1	0	-1.827806	1.511035	0.491709
7	8	0	-0.236546	0.325868	1.090245
8	7	0	-0.418404	-0.281872	-1.143274
9	1	0	-0.240659	-0.796140	-1.991553
10	5	0	0.503021	-0.016390	-0.050095
11	7	0	1.496461	-1.256226	0.411194
12	1	0	1.952682	-1.062432	1.305143
13	1	0	0.869965	-2.045967	0.578999
14	1	0	2.203674	-1.570370	-0.253555
15	7	0	1.539924	1.219693	-0.411123
16	1	0	2.079274	1.554711	0.388828
17	1	0	2.175514	1.068272	-1.194962
18	1	0	0.916151	1.980274	-0.689621

19-NH_3 complex

E = -613.6962911 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.707397	0.115026	0.025516
2	6	0	1.950747	-0.152066	0.284255
3	1	0	2.912022	-0.416098	-0.154726
4	1	0	2.041197	-0.196791	1.370363
5	6	0	1.503732	1.242496	-0.153686
6	1	0	2.052371	2.014616	0.388826
7	1	0	1.707684	1.382129	-1.222673
8	7	0	-1.641034	-0.102277	1.364550
9	1	0	-2.292320	0.662403	1.558535
10	1	0	-2.157358	-0.981634	1.418647
11	7	0	-1.801814	0.147487	-1.214993
12	1	0	-2.330115	-0.716736	-1.349387
13	1	0	-2.465518	0.924624	-1.196172
14	1	0	-0.969639	-0.101904	2.135146
15	1	0	-1.239608	0.264896	-2.061193
16	7	0	0.066118	1.338148	0.141223
17	1	0	-0.319679	2.270569	0.074882
18	15	0	0.606784	-1.320894	-0.317471
19	1	0	0.406431	-2.093885	0.853356

20-NH_3 complex

E = -327.1324432 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.521429
2	6	0	0.731466	0.222652	-1.731813
3	1	0	1.323361	-0.321270	-2.468239
4	1	0	0.799426	1.294316	-1.954321
5	6	0	-0.731466	-0.222652	-1.731813
6	1	0	-1.323361	0.321270	-2.468239
7	1	0	-0.799426	-1.294316	-1.954321
8	7	0	0.000000	1.305760	1.557743
9	1	0	-0.840104	1.390585	2.132059
10	1	0	0.812070	1.413294	2.166577
11	7	0	0.000000	-1.305760	1.557743
12	1	0	0.840104	-1.390585	2.132059
13	1	0	-0.812070	-1.413294	2.166577
14	1	0	-0.013725	2.104703	0.920583
15	1	0	0.013725	-2.104703	0.920583
16	7	0	-1.163731	0.081410	-0.356644
17	7	0	1.163731	-0.081410	-0.356644
18	1	0	-2.101108	-0.205213	-0.117041
19	1	0	2.101108	0.205213	-0.117041

21-NH_3 complex

E = -768.4371438 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.484688	-0.545826	-0.297039
2	6	0	1.832660	-0.734876	1.081982
3	1	0	2.838758	-1.494199	-0.704008
4	1	0	3.334142	0.143164	-0.240647
5	1	0	2.513337	-0.541251	1.908919
6	1	0	1.420767	-1.740749	1.190880
7	7	0	1.376293	0.014912	-1.081807
8	1	0	1.536427	0.239187	-2.050208
9	8	0	0.755458	0.221428	1.139676
10	5	0	0.425790	0.585857	-0.165086
11	16	0	-1.525372	-0.110903	-0.612215
12	6	0	-2.414303	0.282966	0.918974
13	1	0	-2.773419	1.309875	0.854199
14	1	0	-3.275900	-0.377806	1.001021
15	1	0	-1.739727	0.151434	1.765504
16	6	0	-1.176641	-1.864087	-0.335670
17	1	0	-0.804862	-1.992253	0.680284
18	1	0	-2.092376	-2.430404	-0.492669
19	1	0	-0.420055	-2.154120	-1.062830
20	7	0	0.178044	2.192232	-0.201961
21	1	0	1.089171	2.637275	-0.068525
22	1	0	-0.216466	2.546994	-1.073900
23	1	0	-0.415229	2.497520	0.572323

22-NH_3 complex

E = -445.4621287 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.084549	-0.123129	0.951349
2	6	0	-1.923896	-0.917278	-0.349672
3	1	0	-2.372436	-0.766425	1.783653
4	1	0	-2.841071	0.660994	0.839363
5	1	0	-2.830387	-0.956750	-0.950064
6	1	0	-1.581245	-1.937268	-0.150601
7	7	0	-0.733968	0.434685	1.126373
8	1	0	-0.600632	1.077000	1.891177
9	8	0	-0.906800	-0.218654	-1.091118
10	5	0	-0.115016	0.473265	-0.180347
11	6	0	1.453973	-1.584125	-0.516569
12	1	0	0.956320	-2.153448	0.270777
13	1	0	0.940567	-1.695295	-1.465555
14	1	0	2.502154	-1.865068	-0.598978
15	6	0	2.171262	0.101921	1.027853
16	1	0	3.209766	-0.159220	0.833070
17	1	0	2.092502	1.167880	1.237098
18	1	0	1.758975	-0.472094	1.857724
19	8	0	1.408008	-0.172750	-0.168527
20	7	0	0.260352	1.900035	-0.859075
21	1	0	0.937564	2.480817	-0.365795
22	1	0	0.612642	1.740642	-1.805441
23	1	0	-0.604739	2.435760	-0.946382

23-NH_3 complex

E = -464.9212122 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.421122	-0.202132	0.670985
2	6	0	-2.128236	-0.678925	-0.753808
3	1	0	-2.931651	-0.967670	1.257241
4	1	0	-3.051807	0.695979	0.657340
5	1	0	-2.929047	-0.462006	-1.458707
6	1	0	-1.920751	-1.753476	-0.770752
7	7	0	-1.066167	0.067215	1.174203
8	1	0	-1.008186	0.490968	2.087651
9	8	0	-0.946847	0.034958	-1.151087
10	5	0	-0.242638	0.408963	0.012418
11	7	0	1.241518	-0.282304	0.044716
12	6	0	1.935290	-0.026451	1.332643
13	1	0	2.900180	-0.535956	1.336734
14	1	0	2.106984	1.043355	1.461288
15	1	0	1.314766	-0.405127	2.143437
16	6	0	1.018646	-1.755336	-0.089241
17	1	0	0.569333	-1.949259	-1.061366
18	1	0	1.979083	-2.265799	-0.007931
19	1	0	0.347420	-2.074517	0.705436
20	6	0	2.086021	0.165194	-1.094727
21	1	0	2.408453	1.195644	-0.939253
22	1	0	2.974805	-0.463818	-1.159553
23	1	0	1.504800	0.078333	-2.013264
24	7	0	0.034529	2.043332	-0.183116
25	1	0	-0.884434	2.470880	-0.058808
26	1	0	0.672998	2.509445	0.460853
27	1	0	0.322265	2.256745	-1.139468

24-NH_3 complex

E = -751.5204965 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.374209	0.929075	0.613873
2	6	0	-2.485623	0.411692	-0.821924
3	1	0	-3.342972	0.934993	1.116146
4	1	0	-1.971768	1.949382	0.629627
5	1	0	-2.673140	1.196463	-1.553257
6	1	0	-3.270862	-0.345839	-0.905526
7	7	0	-1.454228	-0.048465	1.211112
8	1	0	-1.141792	0.152909	2.148874
9	8	0	-1.213012	-0.195024	-1.105585
10	5	0	-0.616981	-0.573100	0.123099
11	15	0	1.263822	0.158501	-0.002461
12	6	0	1.042621	1.956861	-0.067817
13	1	0	2.001402	2.454869	-0.219371
14	1	0	0.370696	2.193162	-0.894388
15	1	0	0.597397	2.303717	0.866288
16	6	0	2.418770	-0.178238	1.364434
17	1	0	2.661319	-1.241639	1.406320
18	1	0	3.343941	0.382817	1.220335
19	1	0	1.968898	0.122644	2.312268
20	6	0	2.110177	-0.314740	-1.540576
21	1	0	3.016339	0.278601	-1.674570
22	1	0	2.384976	-1.370992	-1.516198
23	1	0	1.431410	-0.139297	-2.377171
24	7	0	-0.553381	-2.221680	0.190310
25	1	0	-1.529861	-2.517919	0.260837
26	1	0	-0.162210	-2.639210	-0.654820
27	1	0	-0.069268	-2.603366	1.002807

26-NH_3 complex

E = -898.7804041 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.763297	0.538937	0.985237
2	6	0	-2.909811	0.504280	-0.541201
3	1	0	-3.684429	0.222698	1.479254
4	1	0	-2.526541	1.550581	1.337502
5	1	0	-3.248175	1.449470	-0.965511
6	1	0	-3.612912	-0.279624	-0.845849
7	7	0	-1.663554	-0.405827	1.205954
8	1	0	-1.243939	-0.393650	2.122430
9	8	0	-1.605786	0.201572	-1.049373
10	5	0	-0.908627	-0.536271	-0.056406
11	6	0	0.690661	-0.151445	-0.029178
12	16	0	1.989271	-1.237284	0.161937
13	6	0	2.531974	1.214378	-0.012361
14	6	0	3.153752	0.028115	0.135745
15	1	0	2.984098	2.193028	-0.068753
16	1	0	4.210649	-0.163603	0.230252
17	7	0	1.155670	1.091638	-0.098724
18	6	0	0.283305	2.272827	-0.256503
19	1	0	0.881856	3.160320	-0.066845
20	1	0	-0.128391	2.283679	-1.262923
21	1	0	-0.524938	2.206781	0.467508
22	7	0	-0.970422	-2.156141	-0.546941
23	1	0	-1.968237	-2.370716	-0.567105
24	1	0	-0.600156	-2.318557	-1.483823
25	1	0	-0.549169	-2.825330	0.097440

27-NH_3 complex

E = -595.2653379 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.653909	-0.308215	1.269374
2	6	0	-2.894664	0.745089	0.188868
3	1	0	-3.549289	-0.901933	1.462353
4	1	0	-2.346186	0.171945	2.204802
5	1	0	-3.287428	1.684076	0.576389
6	1	0	-3.585499	0.369506	-0.576222
7	7	0	-1.567101	-1.114416	0.685389
8	1	0	-1.048686	-1.623867	1.386009
9	8	0	-1.608546	0.977251	-0.394043
10	5	0	-0.867921	-0.231828	-0.288878
11	6	0	2.896894	-0.318236	0.361682
12	6	0	2.696619	1.017956	0.272605
13	1	0	3.787495	-0.889526	0.562982
14	1	0	3.382143	1.841113	0.381195
15	6	0	0.730767	0.024635	-0.079829
16	7	0	1.674034	-0.913026	0.140859
17	7	0	1.360695	1.209817	-0.002967
18	6	0	1.466269	-2.360488	0.158077
19	1	0	0.404846	-2.577390	0.053732
20	1	0	2.023301	-2.822965	-0.657170
21	1	0	1.813724	-2.764035	1.108668
22	6	0	0.748145	2.539126	-0.145437
23	1	0	0.117792	2.562276	-1.028701
24	1	0	0.139822	2.759537	0.728748
25	1	0	1.555195	3.262640	-0.236095
26	7	0	-1.017647	-0.959082	-1.830507
27	1	0	-1.994585	-1.249196	-1.889457
28	1	0	-0.839943	-0.291969	-2.581060
29	1	0	-0.455321	-1.791327	-2.000900

28-NH_3 complex

E = -748.8859931 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.722471	0.971841	-0.863532
2	6	0	-3.738372	-0.551595	-1.017081
3	1	0	-4.698297	1.360951	-0.569899
4	1	0	-3.431363	1.454465	-1.801145
5	1	0	-3.933991	-0.888569	-2.034092
6	1	0	-4.481064	-1.006503	-0.349110
7	7	0	-2.703968	1.192401	0.175263
8	1	0	-2.963859	1.804391	0.932214
9	8	0	-2.425932	-0.977508	-0.634923
10	5	0	-1.901647	-0.042850	0.299935
11	6	0	1.867454	0.719789	0.008309
12	6	0	1.865019	-0.670005	-0.060451
13	6	0	-0.255897	0.024350	0.167814
14	7	0	0.535713	-1.060801	0.039896
15	7	0	0.539725	1.109376	0.146323
16	6	0	0.118732	-2.458882	-0.038530
17	1	0	0.597377	-2.915704	-0.904957
18	1	0	0.432286	-2.990601	0.862445
19	1	0	-0.957732	-2.505555	-0.181830
20	6	0	0.148567	2.516820	0.214475
21	1	0	0.448876	2.935036	1.176321
22	1	0	0.657479	3.051554	-0.587491
23	1	0	-0.925584	2.586556	0.074832
24	6	0	3.041100	-1.402005	-0.209692
25	1	0	3.042179	-2.483242	-0.264213
26	6	0	3.047290	1.457519	-0.065958
27	1	0	3.052818	2.538594	-0.010384
28	6	0	4.217901	0.733192	-0.212312
29	1	0	5.161641	1.260009	-0.274583
30	6	0	4.214937	-0.671631	-0.283333
31	1	0	5.156478	-1.193200	-0.399443
32	7	0	-2.141614	-0.721600	1.855975
33	1	0	-3.145804	-0.876266	1.951910
34	1	0	-1.682280	-1.625368	1.970376
35	1	0	-1.848016	-0.124226	2.628312

29-NH_3 complex

E = -617.3377707 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.652104	-0.377738	-1.392386
2	6	0	2.971697	0.796965	-0.475590
3	1	0	3.543542	-0.956827	-1.638264
4	1	0	2.195190	-0.026840	-2.325029
5	1	0	3.225190	1.712296	-1.008891
6	1	0	3.786761	0.550236	0.212604
7	7	0	1.708027	-1.146164	-0.569045
8	1	0	1.239256	-1.879809	-1.073300
9	8	0	1.770502	1.010042	0.275623
10	5	0	1.032257	-0.188214	0.326508
11	6	0	-1.357309	-1.095727	-0.034475
12	6	0	-1.156245	1.256306	0.043645
13	6	0	-2.703385	-0.989631	-0.347026
14	6	0	-2.501901	1.376631	-0.286832
15	6	0	-3.283316	0.256950	-0.500737
16	1	0	-3.280846	-1.896924	-0.469807
17	1	0	-2.925685	2.368795	-0.362516
18	1	0	-4.330519	0.353184	-0.761503
19	7	0	-0.584799	0.016741	0.129791
20	6	0	-0.805187	-2.492941	0.112415
21	1	0	-0.698070	-2.950981	-0.875009
22	1	0	0.158615	-2.565644	0.607139
23	1	0	-1.527314	-3.096224	0.663676
24	6	0	-0.395640	2.522793	0.321511
25	1	0	0.187876	2.462207	1.237671
26	1	0	0.305845	2.747838	-0.480719
27	1	0	-1.112082	3.337282	0.409334
28	7	0	1.130391	-0.665852	1.941021
29	1	0	0.411755	-1.282366	2.317204
30	1	0	2.029441	-1.141878	2.031342
31	1	0	1.165492	0.171666	2.523020

4-HCHO complex

E = -196.8794261 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.472941	0.691627	0.072711
2	1	0	0.482864	1.224666	1.135526
3	1	0	0.345364	1.361101	-0.902714
4	7	0	1.751269	-0.248646	-0.062824
5	1	0	2.590400	0.335551	-0.053663
6	1	0	1.840493	-0.906111	0.714282
7	1	0	1.773236	-0.784583	-0.932079
8	8	0	-0.703939	-0.356716	0.104633
9	6	0	-1.874091	-0.043761	-0.071575
10	1	0	-2.146376	0.990693	-0.303224
11	1	0	-2.633509	-0.822634	0.010472

5-HCHO complex

E = -395.502908 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.373854	-0.190353	-0.015937
2	7	0	1.514006	0.901733	0.180727
3	1	0	2.415642	0.420006	0.252118
4	1	0	1.576163	1.540815	-0.615858
5	1	0	1.397968	1.456118	1.032026
6	8	0	-0.934545	0.691757	-0.234560
7	6	0	-2.041440	0.223771	0.018780
8	1	0	-2.135787	-0.775318	0.455885
9	1	0	-2.918617	0.834249	-0.200794
10	9	0	0.190991	-0.888689	1.120161
11	9	0	0.578156	-0.857191	-1.158491

6-HCHO complex

E = -1116.1706334 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.053900	-0.212170	0.208643
2	7	0	0.244835	-0.998251	1.574444
3	1	0	0.481265	-1.972394	1.362883
4	1	0	1.009197	-0.615316	2.138359
5	1	0	-0.608193	-1.007735	2.141001
6	8	0	-0.285076	1.240256	0.745960
7	6	0	-0.536037	2.172130	-0.014457
8	1	0	-0.539603	2.022641	-1.099160
9	1	0	-0.752886	3.145483	0.427449
10	17	0	1.607098	-0.131714	-0.678694
11	17	0	-1.376292	-0.837633	-0.669294

7-HCHO complex

E = -275.5207574 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.394645	0.000008	0.140841
2	7	0	1.411935	-0.000100	-1.115222
3	1	0	2.372557	-0.000465	-0.767309
4	1	0	1.308091	-0.826399	-1.707061
5	1	0	1.308601	0.826451	-1.706797
6	8	0	-0.998169	-0.000070	-0.711538
7	6	0	-2.094850	0.000011	-0.174220
8	1	0	-2.184034	0.000146	0.917053
9	1	0	-2.985557	-0.000065	-0.805005
10	6	0	0.482420	1.377501	0.921254
11	1	0	-0.253693	1.432998	1.728795
12	1	0	1.456729	1.479915	1.409267
13	1	0	0.341666	2.259635	0.287802
14	6	0	0.482386	-1.377350	0.921485
15	1	0	0.342176	-2.259627	0.288117
16	1	0	1.456460	-1.479432	1.410030
17	1	0	-0.254148	-1.432901	1.728642

8-HCHO complex

E = -958.1814135 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.651825	0.056243	0.392333
2	6	0	1.893295	0.604955	-0.717790
3	1	0	2.821156	1.178362	-0.722565
4	1	0	1.623754	0.407032	-1.758314
5	6	0	2.066552	-0.706457	0.054650
6	1	0	2.806527	-1.347847	-0.425529
7	1	0	2.403955	-0.510850	1.074545
8	15	0	0.568082	1.587473	0.170342
9	1	0	-0.067714	2.239422	-0.914803
10	7	0	-1.371177	0.137759	1.824413
11	1	0	-1.967774	0.964824	1.916988
12	1	0	-1.937670	-0.682334	2.051839
13	1	0	-0.648705	0.218482	2.543311
14	15	0	0.403109	-1.566565	0.041227
15	1	0	0.381912	-2.168784	1.322381
16	8	0	-1.914814	0.087753	-0.527403
17	6	0	-1.939980	-0.211563	-1.720373
18	1	0	-1.034594	-0.552487	-2.229450
19	1	0	-2.892036	-0.128603	-2.244189

9-HCHO complex

E = -467.2326493 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.298705	0.337046	0.224304
2	7	0	1.804626	0.007887	1.722305
3	1	0	1.376868	-0.832738	2.114630
4	1	0	2.820027	-0.086491	1.788556
5	1	0	1.529237	0.784771	2.326512
6	6	0	-0.275195	0.186180	0.134485
7	6	0	-0.920335	-0.990520	0.552052
8	6	0	-1.070417	1.219526	-0.372211
9	6	0	-2.300197	-1.129914	0.469787
10	1	0	-0.345339	-1.831794	0.939774
11	6	0	-2.454807	1.089707	-0.454127
12	1	0	-0.607360	2.142415	-0.706073
13	6	0	-3.069524	-0.083838	-0.034054
14	1	0	-2.776253	-2.046164	0.797953
15	1	0	-3.052007	1.903923	-0.846505
16	1	0	-4.146163	-0.186459	-0.098159
17	6	0	2.035032	1.624896	-0.330459
18	1	0	1.727536	2.520508	0.218671
19	1	0	3.125718	1.560771	-0.265650
20	1	0	1.784153	1.806221	-1.379578
21	8	0	1.984193	-0.940264	-0.534547
22	6	0	1.534960	-1.381322	-1.583330
23	1	0	2.077138	-2.188210	-2.079553
24	1	0	0.609890	-0.973371	-2.004715

10-HCHO complex

E = -658.9397699 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.001781	0.766441	0.428611
2	7	0	-0.040497	1.383000	1.922334
3	1	0	-0.220260	0.611213	2.568139
4	1	0	0.826722	1.832143	2.221103
5	1	0	-0.810105	2.046573	2.033075
6	6	0	-1.412069	0.098701	0.141703
7	6	0	-1.676093	-1.152233	0.722577
8	6	0	-2.437520	0.704418	-0.593246
9	6	0	-2.909150	-1.774299	0.569591
10	1	0	-0.897891	-1.662566	1.285388
11	6	0	-3.672488	0.081179	-0.757671
12	1	0	-2.294983	1.680785	-1.046482
13	6	0	-3.910184	-1.157658	-0.175944
14	1	0	-3.086215	-2.742439	1.022787
15	1	0	-4.449242	0.567089	-1.335880
16	1	0	-4.870698	-1.642219	-0.303010
17	6	0	1.347438	-0.027223	0.171890
18	6	0	2.584337	0.493468	0.588110
19	6	0	1.358087	-1.233339	-0.540648
20	6	0	3.778090	-0.166223	0.322659
21	1	0	2.640812	1.442215	1.120317
22	6	0	2.550492	-1.899834	-0.811566
23	1	0	0.422113	-1.658528	-0.887503
24	6	0	3.759763	-1.370255	-0.376617
25	1	0	4.718565	0.252974	0.659782
26	1	0	2.534103	-2.832520	-1.362484
27	1	0	4.687371	-1.890212	-0.583624
28	8	0	0.065194	2.159927	-0.401255
29	6	0	0.503026	2.196492	-1.543547
30	1	0	0.465819	3.147254	-2.078744
31	1	0	0.922341	1.296451	-2.005967

11-HCHO complex

E = -577.236997 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.648820	0.384686	0.579550
2	6	0	-0.679250	-0.694649	-0.297200
3	6	0	-1.850849	-1.137039	-0.868289
4	6	0	-3.013244	-0.441856	-0.518773
5	6	0	-2.981339	0.637286	0.360284
6	6	0	-1.783655	1.077250	0.934553
7	1	0	-1.864493	-1.981606	-1.544526
8	1	0	-3.959473	-0.755711	-0.940709
9	1	0	-3.902125	1.149028	0.609026
10	1	0	-1.746833	1.910116	1.624658
11	8	0	0.601857	-1.205069	-0.453891
12	8	0	0.664103	0.609179	0.992631
13	5	0	1.412264	-0.312552	0.250319
14	7	0	2.572911	-1.029577	1.047886
15	1	0	3.165201	-1.590043	0.430043
16	1	0	3.168331	-0.376043	1.561019
17	1	0	2.151661	-1.665672	1.729642
18	8	0	2.321656	0.523269	-0.856405
19	6	0	1.912894	1.595820	-1.284091
20	1	0	1.018197	2.057701	-0.853696
21	1	0	2.462490	2.074006	-2.097128

12-HCHO complex

E = -1014.4561727 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.600988	0.180845	0.360232
2	6	0	1.897424	0.319266	-0.797061
3	1	0	2.873143	0.804176	-0.880741
4	1	0	1.628264	-0.019996	-1.801441
5	6	0	1.957509	-0.854629	0.169078
6	1	0	2.502688	-1.704125	-0.243924
7	1	0	2.426138	-0.567349	1.110637
8	7	0	-1.424956	0.604989	1.667438
9	1	0	-1.932654	1.486287	1.554087
10	1	0	-2.097299	-0.108694	1.959865
11	1	0	-0.767635	0.720436	2.441393
12	8	0	-1.833975	0.073575	-0.654974
13	6	0	-1.845284	-0.611691	-1.672323
14	1	0	-2.721313	-0.548832	-2.318678
15	1	0	-0.998286	-1.265560	-1.901604
16	16	0	0.256166	-1.453588	0.546417
17	15	0	0.628398	1.587268	-0.274755
18	1	0	1.155865	1.806629	1.027458

13-HCHO complex

E = -691.5066133 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.453409	0.376667	0.174756
2	8	0	-0.038410	-0.483456	1.177388
3	6	0	1.887399	-0.662561	-0.261152
4	1	0	2.967975	-0.519938	-0.296350
5	1	0	1.663721	-1.567554	-0.833398
6	6	0	1.374839	-0.776856	1.170206
7	1	0	1.500651	-1.774980	1.590960
8	1	0	1.878226	-0.058753	1.823064
9	7	0	-1.252261	1.632081	0.778083
10	1	0	-1.743937	2.180359	0.069548
11	1	0	-1.930646	1.336416	1.485446
12	1	0	-0.588130	2.253134	1.244138
13	8	0	-1.698553	-0.323934	-0.601849
14	6	0	-1.850857	-1.539269	-0.594202
15	1	0	-2.672620	-1.959829	-1.176115
16	1	0	-1.174222	-2.170067	-0.009935
17	15	0	1.001739	0.768192	-1.097335
18	1	0	1.533191	1.781657	-0.251113

14-HCHO complex

E = -1070.7251365 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.565987	0.113147	0.385844
2	6	0	1.868105	0.512574	-0.755883
3	1	0	2.769687	1.125461	-0.727401
4	1	0	1.661361	0.248209	-1.793523
5	6	0	2.012793	-0.721075	0.114192
6	1	0	2.654160	-1.467732	-0.355108
7	1	0	2.419040	-0.469781	1.093459
8	7	0	-1.311286	0.407829	1.771258
9	1	0	-1.863933	1.269234	1.753451
10	1	0	-1.925173	-0.355954	2.064305
11	1	0	-0.596308	0.518335	2.493473
12	8	0	-1.901169	-0.005871	-0.537154
13	6	0	-1.868647	-0.433151	-1.684592
14	1	0	-2.795550	-0.433667	-2.259844
15	1	0	-0.931185	-0.809005	-2.105767
16	16	0	0.496327	1.548568	-0.111731
17	16	0	0.363216	-1.495364	0.346972

15-HCHO complex

E = -424.827162 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.208435	0.446943	-0.002058
2	8	0	-0.370635	-0.137388	-1.116580
3	8	0	-0.631066	0.489316	1.089704
4	6	0	-1.725872	-0.389848	0.781136
5	1	0	-2.639820	0.012371	1.213551
6	1	0	-1.530383	-1.375533	1.213758
7	6	0	-1.739473	-0.427332	-0.754903
8	1	0	-2.021919	-1.396572	-1.163114
9	1	0	-2.384539	0.343615	-1.180121
10	7	0	0.929718	1.846699	-0.238160
11	1	0	1.458709	2.137073	0.587484
12	1	0	1.557567	1.848501	-1.043601
13	1	0	0.210353	2.554116	-0.402411
14	8	0	1.586803	-0.438915	0.378320
15	6	0	1.722492	-1.585553	-0.021002
16	1	0	2.594417	-2.154040	0.309844
17	1	0	0.981712	-2.018846	-0.700921

16-HCHO complex

E = -747.7770928 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.419267	0.356177	0.178507
2	8	0	0.032394	-0.508321	1.159326
3	6	0	1.908554	-0.603307	-0.325377
4	1	0	2.961867	-0.340205	-0.407586
5	1	0	1.731630	-1.528334	-0.875573
6	6	0	1.457065	-0.705392	1.125724
7	1	0	1.668446	-1.682339	1.559926
8	1	0	1.932328	0.067105	1.735213
9	7	0	-1.136417	1.662453	0.772807
10	1	0	-1.620228	2.214265	0.061148
11	1	0	-1.805956	1.432704	1.511184
12	1	0	-0.415330	2.260129	1.182646
13	8	0	-1.735212	-0.318933	-0.511298
14	6	0	-1.902557	-1.531691	-0.497699
15	1	0	-2.765730	-1.939547	-1.026377
16	1	0	-1.197504	-2.174100	0.038090
17	16	0	0.900369	0.745790	-1.067560

17-HCHO complex

E = -727.8942931 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.438637	0.379845	0.207735
2	6	0	1.933950	-0.543866	-0.361449
3	1	0	2.939211	-0.240812	-0.646536
4	1	0	1.767785	-1.569234	-0.693243
5	6	0	1.684212	-0.389543	1.132667
6	1	0	2.072159	-1.251258	1.679505
7	1	0	2.185370	0.510413	1.504483
8	7	0	-1.239719	1.739392	0.506452
9	1	0	-1.733915	2.081004	-0.321321
10	1	0	-1.925557	1.659834	1.260109
11	1	0	-0.560054	2.455821	0.769527
12	16	0	0.729336	0.555482	-1.220265
13	7	0	0.224925	-0.289815	1.291831
14	1	0	-0.100853	-0.260496	2.248647
15	6	0	-1.767765	-1.711715	-0.313385
16	1	0	-2.643582	-2.263227	-0.661605
17	1	0	-0.847032	-2.228024	-0.020927
18	8	0	-1.828569	-0.494656	-0.246007

18-HCHO complex (hydrogen-bonded)

E = -404.9532897 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.611262	0.563784	0.015759
2	8	0	1.891323	0.975057	0.011328
3	6	0	2.706413	-0.221872	-0.113101
4	1	0	3.491539	-0.175410	0.637720
5	1	0	3.151865	-0.208926	-1.107232
6	6	0	1.750162	-1.428977	0.083326
7	1	0	1.886080	-2.177581	-0.696885
8	1	0	1.888712	-1.903518	1.056466
9	7	0	-0.499191	1.627045	0.041255
10	1	0	-0.410737	2.260516	-0.757480
11	1	0	-1.433677	1.180191	0.022785
12	1	0	-0.421468	2.206130	0.881557
13	8	0	-2.601956	-0.231227	0.009854
14	6	0	-3.772395	-0.527412	-0.048555
15	1	0	-4.555766	0.239895	-0.131057
16	1	0	-4.089048	-1.579160	-0.021199
17	7	0	0.420144	-0.799042	0.000778
18	1	0	-0.430498	-1.338152	0.042828

18-HCHO complex

E = -404.9456366 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.816245	0.403270	-0.712940
2	6	0	1.730570	0.364551	0.818631
3	1	0	2.788993	0.066752	-1.072245
4	1	0	1.637892	1.416011	-1.095053
5	1	0	1.999845	1.305710	1.294756
6	1	0	2.344796	-0.437713	1.231483
7	8	0	0.344844	0.068497	1.112872
8	7	0	0.741415	-0.525894	-1.088139
9	1	0	0.565041	-0.675138	-2.069095
10	5	0	-0.211825	-0.488738	-0.024358
11	7	0	-1.068898	-1.804331	0.247801
12	1	0	-0.419927	-2.587363	0.349282
13	1	0	-1.602496	-1.728639	1.116077
14	1	0	-1.718568	-2.032266	-0.506699
15	8	0	-1.598306	0.511585	-0.416750
16	6	0	-1.677410	1.647323	0.021006
17	1	0	-0.940360	2.006045	0.747993
18	1	0	-2.492445	2.290355	-0.321493

19-HCHO complex (hydrogen-bonded)

E = -671.6300092 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.348766	0.737256	0.346295
2	6	0	-1.959471	-1.102246	-0.499831
3	1	0	-2.836647	-1.699496	-0.253817
4	1	0	-1.422508	-1.615758	-1.299835
5	6	0	-2.341833	0.312022	-0.943323
6	1	0	-2.556197	0.353420	-2.012018
7	1	0	-3.219798	0.672980	-0.400573
8	7	0	0.847277	1.596626	0.824299
9	1	0	1.717634	1.107681	0.529014
10	1	0	0.865590	2.543705	0.441230
11	1	0	0.874453	1.670939	1.843461
12	7	0	-1.195386	1.191345	-0.629559
13	1	0	-1.170020	2.088806	-1.097219
14	6	0	3.598091	-0.785098	-0.626797
15	1	0	4.459715	-0.832537	0.055036
16	1	0	3.612946	-1.429018	-1.517202
17	8	0	2.663685	-0.051946	-0.411442
18	15	0	-0.770380	-1.043370	0.959613
19	1	0	-1.679075	-0.544750	1.934321

19-HCHO complex

E = -671.6211904 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.522906	0.894707	1.011431
2	6	0	-2.157617	0.069048	-0.110376
3	1	0	-2.149681	0.888823	1.904488
4	1	0	-1.411480	1.939720	0.697759
5	1	0	-2.950772	0.623782	-0.610429
6	1	0	-2.579083	-0.851810	0.293847
7	15	0	-0.762092	-0.317166	-1.311213
8	1	0	-0.974753	-1.704116	-1.499030
9	7	0	-0.217365	0.280980	1.305973
10	1	0	0.163996	0.456853	2.225019
11	5	0	0.439920	-0.399360	0.239695
12	7	0	1.155681	-1.780793	0.634173
13	1	0	1.782768	-1.692026	1.437548
14	1	0	0.431080	-2.454614	0.886566
15	1	0	1.697976	-2.180034	-0.134164
16	8	0	1.921525	0.365794	-0.213203
17	6	0	1.919640	1.557206	-0.472681
18	1	0	0.995574	2.140410	-0.390537
19	1	0	2.851034	2.033873	-0.786980

20-HCHO complex (hydrogen-bonded)

E = -385.0756649 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.625935	0.612188	0.000236
2	6	0	-1.673828	-1.453470	-0.095907
3	1	0	-1.798919	-2.256300	0.629780
4	1	0	-1.730572	-1.876866	-1.101745
5	6	0	-2.736735	-0.343180	0.099747
6	1	0	-3.547600	-0.434413	-0.621878
7	1	0	-3.157115	-0.377187	1.107753
8	7	0	0.511740	1.659713	0.001087
9	1	0	1.430888	1.181796	0.000421
10	1	0	0.462135	2.264904	-0.821246
11	1	0	0.466457	2.265266	0.823376
12	8	0	2.634297	-0.198695	-0.005712
13	6	0	3.790098	-0.550592	0.003426
14	1	0	4.054445	-1.617177	-0.004636
15	1	0	4.612534	0.179459	0.020227
16	7	0	-1.983184	0.913276	-0.092500
17	1	0	-2.471247	1.791349	-0.035853
18	7	0	-0.389703	-0.752836	0.087145
19	1	0	0.485118	-1.249829	0.034585

21-HCHO complex

E = -826.3575992 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.374120	-1.004222	-0.327864
2	6	0	1.781454	-1.004224	1.085943
3	1	0	2.756971	-1.987081	-0.604778
4	1	0	3.190300	-0.277169	-0.415074
5	1	0	2.494334	-0.727484	1.860681
6	1	0	1.341601	-1.974435	1.329711
7	7	0	1.204015	-0.622627	-1.129168
8	1	0	1.306567	-0.532630	-2.127547
9	8	0	0.721579	-0.019100	1.053501
10	5	0	0.345295	0.141677	-0.276892
11	16	0	-1.601844	-0.203799	-0.601871
12	6	0	-2.367320	0.716046	0.759722
13	1	0	-2.434232	1.760439	0.459071
14	1	0	-3.371294	0.324362	0.913885
15	1	0	-1.759264	0.597972	1.656748
16	6	0	-1.618414	-1.879036	0.086500
17	1	0	-1.208335	-1.850634	1.095561
18	1	0	-2.644329	-2.241536	0.085001
19	1	0	-0.999046	-2.492448	-0.565500
20	8	0	0.324152	1.778794	-0.595289
21	6	0	0.868432	2.570477	0.161110
22	1	0	1.313035	2.214974	1.095824
23	1	0	0.893143	3.624663	-0.123159

22-HCHO complex

E = -503.3826523 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.733075	-0.879016	1.085894
2	6	0	-1.872506	-1.298883	-0.382504
3	1	0	-1.818188	-1.705919	1.787868
4	1	0	-2.467781	-0.111443	1.347914
5	1	0	-2.907481	-1.253690	-0.722752
6	1	0	-1.497859	-2.317373	-0.536154
7	8	0	-0.413151	-0.315419	1.187147
8	7	0	-1.023254	-0.296349	-1.047993
9	1	0	-0.878720	-0.390798	-2.041494
10	5	0	-0.054010	0.134378	-0.072140
11	8	0	1.457781	-0.116044	-0.331080
12	6	0	2.345813	0.307784	0.754079
13	1	0	2.140508	-0.312014	1.626101
14	1	0	3.364167	0.186168	0.393678
15	1	0	2.130658	1.351638	0.954693
16	6	0	1.738803	-1.489291	-0.731384
17	1	0	2.793699	-1.537777	-0.990280
18	1	0	1.500922	-2.149790	0.103356
19	1	0	1.121257	-1.707657	-1.596292
20	8	0	0.065732	1.798961	-0.045525
21	6	0	-0.874287	2.494352	-0.395462
22	1	0	-1.773594	2.023706	-0.806943
23	1	0	-0.786148	3.577829	-0.291113

23-HCHO complex

E = -522.8478599 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.127259	-1.125153	0.683450
2	6	0	2.142394	-0.824305	-0.820759
3	1	0	3.079057	-0.879310	1.156566
4	1	0	1.906940	-2.181645	0.869996
5	1	0	2.448587	-1.671329	-1.431328
6	1	0	2.790200	0.028098	-1.050267
7	7	0	1.031294	-0.254763	1.143812
8	1	0	0.750263	-0.338611	2.107764
9	8	0	0.786333	-0.479564	-1.147263
10	5	0	0.185532	-0.008778	0.005461
11	7	0	-1.374126	-0.260504	0.025331
12	6	0	-2.052477	0.435261	1.153435
13	1	0	-1.953758	1.511427	1.026523
14	1	0	-3.108775	0.163908	1.153566
15	1	0	-1.600776	0.123055	2.094619
16	6	0	-1.553407	-1.739029	0.182933
17	1	0	-2.619513	-1.966794	0.173894
18	1	0	-1.053361	-2.238106	-0.644922
19	1	0	-1.112568	-2.052753	1.127909
20	6	0	-1.998789	0.154237	-1.271134
21	1	0	-3.047454	-0.144871	-1.261437
22	1	0	-1.918684	1.233119	-1.377469
23	1	0	-1.468469	-0.339263	-2.082899
24	8	0	0.105566	1.799337	-0.221380
25	6	0	1.052280	2.478982	0.124449
26	1	0	1.873883	2.022651	0.690175
27	1	0	1.067845	3.543036	-0.129096

24-HCHO complex

E = -809.4543222 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.621586	-1.057252	0.691123
2	6	0	2.504798	-0.935281	-0.841505
3	1	0	3.172881	-0.220186	1.129153
4	1	0	3.107073	-1.987893	0.984783
5	1	0	2.553762	-1.909819	-1.329043
6	1	0	3.254746	-0.278259	-1.278406
7	7	0	1.209008	-1.020657	1.106485
8	1	0	0.966376	-1.149507	2.074555
9	8	0	1.191059	-0.378989	-1.100987
10	5	0	0.464309	-0.525764	0.042069
11	15	0	-1.448871	-0.231566	-0.026216
12	6	0	-2.276978	-1.822808	-0.303560
13	1	0	-3.356671	-1.671408	-0.351246
14	1	0	-1.931414	-2.254845	-1.244048
15	1	0	-2.043609	-2.509348	0.511246
16	6	0	-2.093614	0.468628	1.512729
17	1	0	-1.602034	1.422559	1.703253
18	1	0	-3.171190	0.615253	1.420154
19	1	0	-1.898842	-0.217250	2.338750
20	6	0	-1.874772	0.851063	-1.410416
21	1	0	-2.955064	0.837877	-1.563376
22	1	0	-1.545017	1.865091	-1.189327
23	1	0	-1.370371	0.493505	-2.309355
24	8	0	0.390715	2.095855	0.422190
25	6	0	1.364004	2.619977	-0.057607
26	1	0	1.968634	2.099025	-0.818867
27	1	0	1.674868	3.631220	0.245060

25-HCHO complex

E = -691.4765369 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.014646	-0.886341	-0.515595
2	6	0	-1.979055	-0.107104	0.805124
3	1	0	-2.905256	-0.645333	-1.096992
4	1	0	-1.994493	-1.967235	-0.340018
5	1	0	-2.386550	-0.658600	1.649481
6	1	0	-2.499365	0.849998	0.712756
7	7	0	-0.790974	-0.410273	-1.172137
8	1	0	-0.584897	-0.715703	-2.108894
9	8	0	-0.577134	0.155429	1.059925
10	5	0	0.100043	0.038211	-0.147595
11	15	0	1.778079	-1.143149	0.184864
12	1	0	2.683277	-0.792057	1.196412
13	1	0	1.346288	-2.416069	0.575130
14	1	0	2.616303	-1.412693	-0.905690
15	8	0	0.850416	1.442859	-0.540395
16	6	0	0.517788	2.481363	0.014397
17	1	0	-0.235864	2.460475	0.807873
18	1	0	0.995196	3.411500	-0.299871

26-HCHO complex

E = -956.7185318 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.999506	1.247473	-0.197067
2	6	0	-2.915099	-0.021653	-1.069553
3	1	0	-3.776790	1.159437	0.562935
4	1	0	-3.194150	2.141219	-0.795179
5	1	0	-3.392787	0.093355	-2.040075
6	1	0	-3.337286	-0.890038	-0.559474
7	7	0	-1.653320	1.296107	0.394991
8	1	0	-1.426320	2.019910	1.056665
9	8	0	-1.508188	-0.275493	-1.273659
10	5	0	-0.825530	0.443010	-0.339728
11	6	0	0.748609	0.342709	-0.231001
12	16	0	1.705825	1.516439	0.533911
13	6	0	2.849104	-0.515649	-0.427355
14	6	0	3.139818	0.622798	0.239647
15	1	0	3.535885	-1.279495	-0.758444
16	1	0	4.107403	0.976577	0.558655
17	7	0	1.501416	-0.652261	-0.686152
18	6	0	0.952741	-1.838072	-1.376550
19	1	0	1.789316	-2.454663	-1.694429
20	1	0	0.320051	-2.378759	-0.675453
21	1	0	0.367084	-1.513011	-2.232184
22	8	0	-0.536377	-1.580043	1.390303
23	6	0	-1.329583	-1.625562	2.294074
24	1	0	-2.072066	-0.821890	2.439204
25	1	0	-1.342548	-2.465618	3.005647

27-HCHO complex

E = -653.2058751 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.993853	-0.226014	1.182425
2	6	0	2.889421	-0.967111	-0.165357
3	1	0	3.735295	0.572648	1.143055
4	1	0	3.249389	-0.903159	2.001558
5	1	0	3.404307	-1.925700	-0.168479
6	1	0	3.263358	-0.354297	-0.987852
7	7	0	1.630332	0.298713	1.346046
8	1	0	1.408643	0.848416	2.158376
9	8	0	1.482243	-1.193457	-0.392176
10	5	0	0.794246	-0.357297	0.440545
11	6	0	-2.881649	0.404160	0.437690
12	6	0	-2.871514	-0.803022	-0.186034
13	1	0	-3.695258	1.066847	0.678801
14	1	0	-3.675188	-1.394879	-0.589888
15	6	0	-0.775796	-0.292615	0.338707
16	7	0	-1.579650	0.698612	0.754826
17	7	0	-1.563466	-1.215778	-0.236826
18	8	0	0.411738	1.735118	-1.346577
19	6	0	0.852263	2.108331	-2.402227
20	1	0	1.469719	1.447742	-3.032867
21	1	0	0.656801	3.124255	-2.781081
22	6	0	-1.136226	1.922717	1.423867
23	1	0	-0.227634	2.274258	0.938855
24	1	0	-1.915851	2.672842	1.312405
25	1	0	-0.971433	1.727744	2.483880
26	6	0	-1.108692	-2.460764	-0.868776
27	1	0	-0.658903	-2.238374	-1.834490
28	1	0	-0.372242	-2.943186	-0.232068
29	1	0	-1.974554	-3.106873	-0.992990

28-HCHO complex

E = -806.8309559 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.869200	-0.176519	1.344413
2	6	0	3.853846	-0.800343	-0.063282
3	1	0	4.614145	0.615660	1.423211
4	1	0	4.063959	-0.922904	2.118936
5	1	0	4.390246	-1.744911	-0.123558
6	1	0	4.256307	-0.106056	-0.804683
7	7	0	2.498181	0.341483	1.454782
8	1	0	2.210701	0.810533	2.297759
9	8	0	2.464048	-1.030715	-0.385350
10	5	0	1.721081	-0.249249	0.458005
11	6	0	-1.943717	0.590313	0.306055
12	6	0	-1.975872	-0.766614	-0.012659
13	6	0	0.145136	-0.177530	0.323391
14	7	0	-0.658651	-1.204041	0.003929
15	7	0	-0.610219	0.914629	0.511637
16	6	0	-0.262657	-2.585131	-0.265874
17	1	0	-0.680616	-3.236117	0.502288
18	1	0	-0.645540	-2.875792	-1.244075
19	1	0	0.821686	-2.651346	-0.269746
20	6	0	-0.146434	2.267602	0.809986
21	1	0	-0.525665	2.942969	0.043545
22	1	0	-0.514345	2.568034	1.791633
23	1	0	0.938871	2.288013	0.780813
24	6	0	-3.171363	-1.433512	-0.276249
25	1	0	-3.198305	-2.488176	-0.519682
26	6	0	-3.105410	1.358250	0.371251
27	1	0	-3.083309	2.412256	0.617765
28	6	0	-4.292482	0.698307	0.107986
29	1	0	-5.223537	1.249298	0.147735
30	6	0	-4.325251	-0.673277	-0.208391
31	1	0	-5.280708	-1.143787	-0.402978
32	8	0	1.536779	1.551451	-1.545605
33	6	0	2.036987	1.191874	-2.579505
34	1	0	2.501772	0.195330	-2.668565
35	1	0	2.045223	1.842324	-3.467948

29-HCHO hydrogen-bonded

E = -675.2829898 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.187040	0.835561	-0.198137
2	6	0	3.387813	-0.615969	0.305535
3	1	0	3.753195	1.024172	-1.110669
4	1	0	3.482776	1.571038	0.554116
5	1	0	4.018881	-0.676374	1.189516
6	1	0	3.795479	-1.262866	-0.472394
7	7	0	1.737997	0.882906	-0.434160
8	1	0	1.271498	1.697873	-0.802750
9	8	0	2.072835	-1.118725	0.645991
10	5	0	1.174570	-0.241867	0.138335
11	6	0	-1.048609	-0.000979	1.211538
12	6	0	-0.846697	-1.375361	-0.724336
13	6	0	-2.403257	-0.279622	1.279972
14	6	0	-2.200975	-1.655152	-0.679697
15	6	0	-2.982511	-1.106974	0.328881
16	1	0	-2.988384	0.152616	2.080514
17	1	0	-2.627614	-2.309240	-1.428057
18	1	0	-4.042010	-1.330555	0.375787
19	7	0	-0.310452	-0.555204	0.217359
20	6	0	-0.353655	0.897155	2.185105
21	1	0	0.551020	0.425916	2.577606
22	1	0	-0.070988	1.827128	1.685739
23	1	0	-1.013014	1.130181	3.018575
24	6	0	0.069369	-1.944161	-1.763105
25	1	0	0.574219	-1.145017	-2.312251
26	1	0	0.832978	-2.568154	-1.291668
27	1	0	-0.494088	-2.551106	-2.468225
28	8	0	-0.859051	2.256845	-0.819293
29	6	0	-1.595698	3.065794	-1.322467
30	1	0	-1.226094	3.813794	-2.041359
31	1	0	-2.670709	3.089306	-1.081864

4-Cl^- complex

E = -542.8504246 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.930627	0.000000
2	1	0	-0.161850	1.537693	1.017968
3	1	0	-0.161850	1.537693	-1.017968
4	7	0	1.552552	0.425928	0.000000
5	1	0	1.730959	-0.149108	-0.821802
6	1	0	2.203220	1.209117	0.000000
7	1	0	1.730959	-0.149108	0.821802
8	17	0	-0.953488	-0.683583	0.000000

5-Cl^- complex

E = -741.4835101 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.335558	-0.178683	0.000000
2	9	0	-0.846184	-0.711989	1.150464
3	9	0	-0.846184	-0.711989	-1.150464
4	7	0	-0.846184	1.385215	0.000000
5	1	0	-0.497214	1.865749	-0.827224
6	1	0	-1.865251	1.417501	0.000000
7	1	0	-0.497214	1.865749	0.827224
8	17	0	1.511298	-0.066840	0.000000

6-Cl^- complex

E = -1462.1566323 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.108667
2	7	0	0.000000	0.000000	1.725497
3	1	0	-0.830566	0.479527	2.074575
4	1	0	0.000000	-0.959055	2.074575
5	1	0	0.830566	0.479527	2.074575
6	17	0	0.000000	1.769103	-0.369520
7	17	0	-1.532088	-0.884551	-0.369520
8	17	0	1.532088	-0.884551	-0.369520

7-Cl^- complex

E = -621.4867284 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.340511	-0.157815	0.000000
2	7	0	-0.843362	1.413570	0.000000
3	1	0	-1.859950	1.479543	0.000000
4	1	0	-0.481549	1.891999	0.823637
5	1	0	-0.481549	1.891999	-0.823637
6	6	0	-0.843362	-0.819053	-1.365700
7	1	0	-0.458900	-1.838891	-1.446937
8	1	0	-1.937546	-0.889393	-1.409901
9	1	0	-0.501457	-0.282221	-2.257330
10	6	0	-0.843362	-0.819053	1.365700
11	1	0	-0.458900	-1.838891	1.446937
12	1	0	-0.501457	-0.282221	2.257330
13	1	0	-1.937546	-0.889393	1.409901
14	17	0	1.549723	0.087070	0.000000

8-Cl^- complex

E = -1304.1525343 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.604232	-0.052515	0.162278
2	6	0	2.090830	0.762480	-0.412023
3	1	0	2.956993	1.336623	-0.078906
4	1	0	2.113018	0.724971	-1.503335
5	6	0	2.122713	-0.660944	0.157237
6	1	0	3.009572	-1.198140	-0.185185
7	1	0	2.166977	-0.627529	1.251350
8	15	0	0.503263	1.593720	0.163961
9	1	0	0.057861	2.135795	-1.060393
10	7	0	-1.042614	-0.294799	1.715346
11	1	0	-1.577774	0.506418	2.055548
12	1	0	-1.625943	-1.127556	1.798425
13	1	0	-0.225364	-0.406914	2.314594
14	15	0	0.565149	-1.510923	-0.470977
15	1	0	0.377786	-2.436817	0.597240
16	17	0	-2.249477	0.092244	-0.698481

9-Cl^- complex

E = -813.1953111 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.207064	0.366472	0.046515
2	7	0	1.567018	0.238139	1.652740
3	1	0	1.095494	0.968130	2.185302
4	1	0	1.257543	-0.667554	2.003940
5	1	0	2.573116	0.310801	1.798990
6	6	0	-0.379094	0.131317	-0.044750
7	6	0	-0.952480	-1.135138	0.142129
8	6	0	-1.254874	1.205659	-0.240940
9	6	0	-2.330880	-1.319477	0.145588
10	1	0	-0.303257	-1.999334	0.254122
11	6	0	-2.637339	1.031726	-0.244454
12	1	0	-0.853281	2.200026	-0.408249
13	6	0	-3.179503	-0.232551	-0.045659
14	1	0	-2.744896	-2.312094	0.284230
15	1	0	-3.290194	1.881816	-0.408138
16	1	0	-4.254177	-0.373522	-0.050034
17	6	0	1.790044	1.765351	-0.459077
18	1	0	1.354295	2.623594	0.067117
19	1	0	2.877119	1.822719	-0.343320
20	1	0	1.577333	1.900926	-1.522605
21	17	0	2.198307	-1.090362	-0.657655

10-Cl^- complex

E = -1004.9028623 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.028803	0.818708	0.246489
2	7	0	0.061974	1.309396	1.818838
3	1	0	-0.021563	0.513018	2.449576
4	1	0	0.932024	1.799048	2.024755
5	1	0	-0.716485	1.945322	1.989879
6	6	0	-1.380120	0.071953	0.068898
7	6	0	-1.667484	-1.053633	0.858172
8	6	0	-2.370087	0.493299	-0.823537
9	6	0	-2.884725	-1.721081	0.772055
10	1	0	-0.912575	-1.443517	1.539780
11	6	0	-3.589245	-0.173026	-0.924533
12	1	0	-2.180533	1.357904	-1.449459
13	6	0	-3.853038	-1.278744	-0.124655
14	1	0	-3.075233	-2.588109	1.394594
15	1	0	-4.335742	0.175624	-1.629354
16	1	0	-4.802509	-1.795884	-0.201181
17	6	0	1.362580	-0.042653	0.009445
18	6	0	2.623564	0.514012	0.271382
19	6	0	1.331492	-1.358610	-0.462678
20	6	0	3.796315	-0.209923	0.094143
21	1	0	2.697927	1.555819	0.577173
22	6	0	2.501642	-2.091306	-0.652899
23	1	0	0.377114	-1.817715	-0.697295
24	6	0	3.736632	-1.522224	-0.367658
25	1	0	4.756120	0.251111	0.298544
26	1	0	2.446805	-3.107130	-1.027784
27	1	0	4.648178	-2.089735	-0.515132
28	17	0	0.115499	2.483326	-0.648660

11-Cl^- complex

E = -923.2065699 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.057612	0.782017	0.698556
2	6	0	-0.057612	0.782017	-0.698556
3	6	0	-0.059490	1.954942	-1.420809
4	6	0	-0.063925	3.153751	-0.694808
5	6	0	-0.063925	3.153751	0.694808
6	6	0	-0.059490	1.954942	1.420809
7	1	0	-0.052562	1.939802	-2.503048
8	1	0	-0.064476	4.095158	-1.230127
9	1	0	-0.064476	4.095158	1.230127
10	1	0	-0.052562	1.939802	2.503048
11	8	0	-0.057612	-0.501047	-1.166967
12	8	0	-0.057612	-0.501047	1.166967
13	5	0	-0.071265	-1.341493	0.000000
14	7	0	-1.518655	-2.128104	0.000000
15	1	0	-1.596751	-2.716657	-0.827936
16	1	0	-1.596751	-2.716657	0.827936
17	1	0	-2.278974	-1.448791	0.000000
18	17	0	1.163976	-2.720905	0.000000

12-Cl^- complex

E = -1360.4227621 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.585068	0.027049	0.151240
2	6	0	-2.132528	0.621463	0.171830
3	1	0	-3.024673	1.134947	-0.194533
4	1	0	-2.203375	0.556250	1.260960
5	6	0	-2.046047	-0.779084	-0.426129
6	1	0	-2.837095	-1.428988	-0.051419
7	1	0	-2.124508	-0.736992	-1.514157
8	7	0	1.013894	0.147558	1.724173
9	1	0	1.557281	-0.673680	1.995400
10	1	0	1.585199	0.976214	1.890746
11	1	0	0.181946	0.183435	2.311728
12	15	0	-0.583932	1.523256	-0.395424
13	1	0	-0.396722	2.353418	0.746755
14	16	0	-0.440327	-1.562798	0.002100
15	17	0	2.242060	-0.025360	-0.696902

13-Cl^- complex

E = -1037.4697067 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.449476	0.201286	0.188582
2	6	0	-1.982210	-0.351407	-0.574263
3	1	0	-3.048908	-0.510244	-0.413966
4	1	0	-1.696822	-0.782416	-1.535318
5	6	0	-1.639100	1.137994	-0.544560
6	1	0	-1.920669	1.635457	-1.474972
7	1	0	-2.168844	1.633086	0.279157
8	7	0	1.300854	0.808179	1.444607
9	1	0	1.915703	0.110645	1.859088
10	1	0	1.873024	1.577003	1.093825
11	1	0	0.666955	1.165588	2.157815
12	15	0	-0.930537	-1.090230	0.797867
13	1	0	-0.472487	-2.247422	0.132897
14	8	0	-0.238844	1.305075	-0.360479
15	17	0	1.829138	-0.473651	-0.913231

14-Cl^- complex

E = -1416.6959521 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.569186	0.003059	0.172917
2	6	0	2.093097	-0.696424	0.086324
3	1	0	2.854380	-1.311854	-0.396476
4	1	0	2.330438	-0.617518	1.149299
5	6	0	2.012505	0.680832	-0.548749
6	1	0	2.883428	1.287902	-0.296655
7	1	0	1.935383	0.597401	-1.633379
8	7	0	-1.124548	-0.056799	1.710114
9	1	0	-1.682933	0.769097	1.929105
10	1	0	-1.705900	-0.884542	1.842730
11	1	0	-0.334334	-0.096340	2.352555
12	16	0	0.483737	-1.533762	-0.150440
13	16	0	0.529611	1.547684	0.077642
14	17	0	-2.141757	0.029939	-0.814309

15-Cl^- complex

E = -770.7889313 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.228647	0.242846	0.019230
2	8	0	-0.578757	0.049133	1.168692
3	8	0	-0.590440	0.249330	-1.137560
4	6	0	-1.915663	-0.062459	-0.724993
5	1	0	-2.355007	-0.787070	-1.412434
6	1	0	-2.528454	0.846802	-0.728080
7	6	0	-1.742922	-0.613622	0.696999
8	1	0	-2.584575	-0.391835	1.354247
9	1	0	-1.572263	-1.695874	0.680248
10	7	0	0.941424	1.701625	0.185484
11	1	0	1.526825	1.704445	1.019063
12	1	0	1.526680	1.894630	-0.625124
13	1	0	0.227353	2.422776	0.271676
14	17	0	1.725372	-0.908865	-0.119719

16-Cl^- complex

E = -1093.7443949 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.430957	0.008469	0.254964
2	6	0	-2.173596	0.016994	-0.128469
3	1	0	-2.907329	-0.002157	-0.933671
4	1	0	-2.663185	0.326275	0.796285
5	6	0	-1.478509	-1.331172	0.038609
6	1	0	-2.083483	-2.037884	0.609815
7	1	0	-1.253404	-1.762733	-0.943217
8	7	0	1.096566	0.698641	1.567533
9	1	0	1.700588	0.019129	2.030944
10	1	0	1.653124	1.513202	1.315987
11	1	0	0.354205	0.981994	2.205215
12	16	0	-0.830106	1.189140	-0.561397
13	8	0	-0.274841	-1.105468	0.751631
14	17	0	1.927164	-0.368711	-0.812967

17-Cl^- complex

E = -1073.8591905 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.452298	0.128737	0.170727
2	6	0	-2.081626	-0.218491	-0.560462
3	1	0	-3.064699	-0.558377	-0.234323
4	1	0	-2.032269	-0.255857	-1.650418
5	6	0	-1.742455	1.180242	-0.040501
6	1	0	-2.257328	1.959124	-0.608589
7	1	0	-2.082411	1.258658	0.998987
8	7	0	1.027650	0.186305	1.709231
9	1	0	1.514969	-0.670352	1.967223
10	1	0	1.670250	0.973271	1.794821
11	1	0	0.243580	0.320166	2.345800
12	16	0	-0.795878	-1.328591	0.126088
13	7	0	-0.293950	1.378118	-0.100502
14	1	0	-0.003848	1.843509	-0.949618
15	17	0	2.017230	-0.057520	-0.834721

18-Cl^- complex

E = -750.9047721 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.243270	0.250609	0.015009
2	8	0	0.568134	0.204879	-1.148629
3	6	0	1.748532	-0.506917	-0.797591
4	1	0	2.558221	-0.209769	-1.465835
5	1	0	1.572621	-1.584257	-0.904557
6	6	0	1.992855	-0.136063	0.672545
7	1	0	2.502327	-0.930938	1.220334
8	1	0	2.610020	0.766886	0.739931
9	7	0	-0.964550	1.719920	-0.040757
10	1	0	-1.475255	1.822030	-0.916183
11	1	0	-1.612212	1.831975	0.735671
12	1	0	-0.242115	2.435392	0.015445
13	7	0	0.642123	0.120241	1.199044
14	1	0	0.353954	-0.540839	1.904422
15	17	0	-1.752212	-0.912106	0.025119

19-Cl^- complex

E = -1017.5858895 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.468871	0.153358	0.189162
2	6	0	-2.081425	-0.236043	-0.581678
3	1	0	-3.123149	-0.474834	-0.361036
4	1	0	-1.901945	-0.380242	-1.648981
5	6	0	-1.732038	1.205681	-0.180764
6	1	0	-2.199381	1.934354	-0.847204
7	1	0	-2.130473	1.400123	0.823704
8	7	0	1.180703	0.413492	1.655716
9	1	0	1.698533	-0.400182	1.983522
10	1	0	1.820582	1.203249	1.574044
11	1	0	0.463645	0.645507	2.341253
12	7	0	-0.277128	1.380270	-0.178448
13	1	0	0.060550	1.849214	-1.006727
14	15	0	-0.892153	-1.292019	0.418362
15	1	0	-0.429231	-2.159003	-0.594968
16	17	0	1.960857	-0.198756	-0.897122

20-Cl^- complex

E = -731.0193002 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.256052	0.240236	0.036832
2	6	0	-1.845256	-0.646600	0.651303
3	1	0	-2.716090	-0.487530	1.293070
4	1	0	-1.709491	-1.728432	0.508624
5	6	0	-1.993285	0.045127	-0.709964
6	1	0	-2.544005	-0.563376	-1.429038
7	1	0	-2.538229	0.987758	-0.585072
8	7	0	0.987023	1.704667	0.259718
9	1	0	1.579714	1.712570	1.087223
10	1	0	1.550760	1.944104	-0.553186
11	1	0	0.245041	2.393116	0.371175
12	7	0	-0.618663	0.316221	-1.162524
13	7	0	-0.639886	-0.009418	1.193703
14	1	0	-0.337141	-0.260028	-1.941845
15	1	0	-0.250605	-0.500917	1.986493
16	17	0	1.786571	-0.892346	-0.153289

22-Cl^- complex

E = -849.3413437 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.154909	-0.008449	0.941426
2	6	0	-2.161454	-0.506638	-0.507995
3	1	0	-2.648978	-0.714638	1.613932
4	1	0	-2.669672	0.957716	1.011554
5	1	0	-3.041278	-0.186875	-1.067196
6	1	0	-2.105814	-1.602383	-0.541734
7	7	0	-0.718930	0.116712	1.209617
8	1	0	-0.500360	0.741447	1.972117
9	8	0	-0.996595	0.050360	-1.108116
10	5	0	-0.090917	0.386196	-0.094340
11	6	0	0.741109	-2.083415	-0.561425
12	1	0	0.152172	-2.453718	0.282899
13	1	0	0.133602	-2.010154	-1.458351
14	1	0	1.606814	-2.722949	-0.736255
15	6	0	2.134735	-0.759391	0.827498
16	1	0	2.986994	-1.384184	0.558996
17	1	0	2.453318	0.269633	0.969968
18	1	0	1.635840	-1.138500	1.722598
19	8	0	1.209077	-0.762707	-0.266092
20	17	0	0.848689	1.961340	-0.325147

23-Cl^- complex

E = -868.8015143 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.447591	-0.235364	0.655655
2	6	0	-2.172690	-0.823953	-0.728930
3	1	0	-3.061648	-0.900205	1.268922
4	1	0	-2.966370	0.727021	0.553431
5	1	0	-2.958057	-0.600778	-1.452859
6	1	0	-2.052067	-1.914322	-0.666554
7	7	0	-1.089108	-0.072985	1.187507
8	1	0	-1.054423	0.602996	1.938562
9	8	0	-0.952285	-0.232049	-1.152438
10	5	0	-0.261070	0.252085	-0.008376
11	7	0	1.199332	-0.543134	0.056124
12	6	0	1.938868	-0.196622	1.291191
13	1	0	2.871598	-0.764498	1.328083
14	1	0	2.148182	0.871276	1.289931
15	1	0	1.313314	-0.451193	2.146518
16	6	0	0.902469	-1.998901	0.064867
17	1	0	0.406558	-2.253875	-0.870006
18	1	0	1.837076	-2.556026	0.159750
19	1	0	0.241290	-2.208591	0.903616
20	6	0	2.023020	-0.235656	-1.139613
21	1	0	2.324875	0.808140	-1.106544
22	1	0	2.901515	-0.885340	-1.148553
23	1	0	1.412177	-0.407698	-2.025183
24	17	0	0.195505	2.104993	-0.154245

24-Cl^- complex

E = -1155.3976469 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.402576	-1.083559	0.669317
2	6	0	2.529522	-0.648543	-0.795991
3	1	0	3.332410	-0.950093	1.225484
4	1	0	2.125627	-2.143049	0.726864
5	1	0	2.859711	-1.445379	-1.464774
6	1	0	3.211170	0.205603	-0.891037
7	7	0	1.318689	-0.240995	1.198061
8	1	0	1.631337	0.441529	1.873340
9	8	0	1.211354	-0.250757	-1.160623
10	5	0	0.608594	0.309685	0.004514
11	15	0	-1.283004	-0.331411	-0.012406
12	6	0	-1.292825	-2.148187	0.045077
13	1	0	-2.306722	-2.547143	0.098656
14	1	0	-0.791812	-2.524419	-0.848029
15	1	0	-0.723654	-2.457519	0.923880
16	6	0	-2.223979	0.232585	1.435328
17	1	0	-2.286078	1.321391	1.406923
18	1	0	-3.225842	-0.198892	1.454224
19	1	0	-1.674926	-0.062341	2.331287
20	6	0	-2.233002	0.154900	-1.483770
21	1	0	-3.237058	-0.272147	-1.473597
22	1	0	-2.290819	1.244093	-1.511629
23	1	0	-1.691788	-0.184467	-2.368426
24	17	0	0.426772	2.214436	0.021125

26-Cl^- complex

E = -1302.6478631 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.708603	-1.103789	0.606957
2	6	0	2.765385	-0.625614	-0.851438
3	1	0	3.637008	-0.895486	1.143059
4	1	0	2.540453	-2.189028	0.646613
5	1	0	3.116176	-1.387910	-1.550249
6	1	0	3.400826	0.263812	-0.943096
7	7	0	1.563409	-0.377725	1.175404
8	1	0	1.816897	0.225802	1.943708
9	8	0	1.422158	-0.285341	-1.165169
10	5	0	0.870657	0.293934	0.021335
11	6	0	-0.754600	0.030455	0.001394
12	16	0	-1.970527	1.217968	-0.033658
13	6	0	-2.684588	-1.209389	-0.008993
14	6	0	-3.219260	0.028067	-0.033477
15	1	0	-3.197745	-2.158681	-0.001749
16	1	0	-4.264891	0.288899	-0.049868
17	7	0	-1.301369	-1.181035	0.010367
18	6	0	-0.480398	-2.400793	0.053423
19	1	0	0.127530	-2.368067	0.957054
20	1	0	-1.145671	-3.261173	0.051881
21	1	0	0.171488	-2.409792	-0.818532
22	17	0	1.044158	2.224407	0.086282

27-Cl^- complex

E = -999.1337217 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.684100	0.930285	1.072818
2	6	0	2.754912	-0.595271	0.958582
3	1	0	3.627595	1.416558	0.817588
4	1	0	2.421465	1.217142	2.096696
5	1	0	3.108439	-1.090732	1.865004
6	1	0	3.387218	-0.894341	0.112791
7	7	0	1.601708	1.313059	0.148886
8	1	0	1.974476	1.711642	-0.703098
9	8	0	1.410544	-0.980816	0.710321
10	5	0	0.829831	0.041868	-0.105484
11	6	0	-2.926874	0.649216	0.331646
12	6	0	-2.860458	-0.698527	0.445621
13	1	0	-3.765316	1.323114	0.362982
14	1	0	-3.630697	-1.434395	0.599415
15	6	0	-0.780850	0.058043	0.146970
16	7	0	-1.634102	1.095771	0.153272
17	7	0	-1.531635	-1.041961	0.329501
18	6	0	-1.274195	2.488243	-0.106198
19	1	0	-0.231550	2.623927	0.175938
20	1	0	-1.405181	2.704691	-1.167228
21	1	0	-1.922841	3.130681	0.488114
22	6	0	-1.012915	-2.409855	0.350635
23	1	0	-0.293091	-2.522346	-0.458086
24	1	0	-0.512851	-2.602045	1.297195
25	1	0	-1.852599	-3.088267	0.209628
26	17	0	0.888665	-0.409373	-2.027891

28-Cl^- complex

E = -1152.758439 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.573724	1.181814	-0.951206
2	6	0	-3.628797	-0.318615	-1.251887
3	1	0	-4.541523	1.586134	-0.648690
4	1	0	-3.239776	1.730253	-1.838776
5	1	0	-3.897765	-0.553752	-2.283371
6	1	0	-4.323605	-0.827233	-0.571378
7	7	0	-2.571384	1.298621	0.122320
8	1	0	-3.010040	1.462832	1.018891
9	8	0	-2.302608	-0.764371	-1.004349
10	5	0	-1.797447	0.005875	0.091757
11	6	0	1.977396	0.739107	0.002859
12	6	0	1.952559	-0.638798	-0.211831
13	6	0	-0.160950	0.076894	-0.030375
14	7	0	0.616334	-1.003552	-0.236765
15	7	0	0.652962	1.141632	0.103159
16	6	0	0.157949	-2.384257	-0.351328
17	1	0	0.699191	-2.861432	-1.169119
18	1	0	0.348886	-2.907090	0.587025
19	1	0	-0.906974	-2.382112	-0.565405
20	6	0	0.261147	2.525607	0.345829
21	1	0	0.587569	2.822987	1.343882
22	1	0	0.738413	3.161542	-0.401364
23	1	0	-0.822723	2.587309	0.261749
24	6	0	3.124001	-1.375793	-0.353210
25	1	0	3.105859	-2.446738	-0.510355
26	6	0	3.172015	1.447053	0.080404
27	1	0	3.188605	2.516228	0.250320
28	6	0	4.341670	0.714458	-0.063009
29	1	0	5.295851	1.223236	-0.006251
30	6	0	4.317586	-0.672767	-0.274819
31	1	0	5.254286	-1.206358	-0.376811
32	17	0	-1.976391	-0.920314	1.818593

29-Cl^- complex

E = -1021.2109716 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.585128	0.651347	-1.519315
2	6	0	-2.740822	-0.806756	-1.087205
3	1	0	-3.532279	1.193921	-1.520559
4	1	0	-2.161936	0.706103	-2.528354
5	1	0	-2.948438	-1.495565	-1.908213
6	1	0	-3.523025	-0.908255	-0.324502
7	7	0	-1.640156	1.202245	-0.538904
8	1	0	-2.079133	1.858545	0.091068
9	8	0	-1.480572	-1.128914	-0.520561
10	5	0	-0.984715	0.036516	0.128174
11	6	0	1.366552	1.170099	-0.078526
12	6	0	1.321221	-1.181529	-0.060069
13	6	0	2.723725	1.154920	-0.379688
14	6	0	2.679134	-1.219384	-0.361360
15	6	0	3.383637	-0.046967	-0.560495
16	1	0	3.247614	2.098648	-0.452027
17	1	0	3.167444	-2.183058	-0.419518
18	1	0	4.438427	-0.068557	-0.808505
19	7	0	0.668290	0.008249	-0.000828
20	6	0	0.717294	2.489439	0.224115
21	1	0	0.134743	2.841142	-0.625514
22	1	0	0.042420	2.397096	1.075352
23	1	0	1.498413	3.210153	0.465687
24	6	0	0.630676	-2.477007	0.259622
25	1	0	-0.102958	-2.345600	1.052733
26	1	0	0.098604	-2.860995	-0.609589
27	1	0	1.387510	-3.196280	0.572865
28	17	0	-1.239643	0.042530	2.036374