Supplementary information for the manuscript "Donor-Acceptor Complexes of Borazines" by Anna S. Lisovenko, Alexey Y. Timoshkin*

Table 1S. Total energies E^o_0, standard enthalpies H^o_{298} (in Hartree) and standard entropies S^o_{298}, kcal mol^{-1} for all considered molecules at B3LYP/TZVP level of theory. For structures of compounds, see Figure 3S.

N	Compound	E^o_0	H^o_{298}	S^o_{298}
1	H_2	-1.1795710	-1.166201	31.140
2	NH_3	-56.5836098	-56.545591	45.978
3	C_6H_6	-232.3283918	-232.222857	64.148
4	Py	-248.3673095	-248.273603	68.682
5	BH_3	-26.6229828	-26.592934	44.991
6	BF_3	-324.7022895	-324.685477	60.896
7	BCl_3	-1405.6489640	-1405.636110	69.186
8	$AlCl_3$	-1623.3325133	-1623.321482	75.029
9	$AlBr_3$	-7965.2001281	-7965.189673	83.330
10	$GaCl_3$	-3305.7373722	-3305.726907	78.040
11	HF	-100.4889021	-100.476331	41.499
12	HCl	-460.8301182	-460.820171	44.613
13	$BH_3{\cdot}NH_3$	-83.2546475	-83.180161	57.218
14	$BF_3{\cdot}NH_3$	-381.3192615	-381.260583	72.019
15	$BCl_3{\cdot}NH_3$	-1462.2693114	-1462.213574	78.936
16	$AlCl_3{\cdot}NH_3$	-1679.9748641	-1679.921782	90.895
17	$AlCl_3{\cdot}C_6H_6$	-1855.6702787	-1855.551401	110.513
18	$AlCl_3{\cdot}Py$	-1871.7590735	-1871.651234	113.281
19	$BCl_3{\cdot}Py$	-1654.0495565	-1653.939920	99.597
	Borazine and its derivatives			
20	$B_3N_3H_6$ (BZ)	-242.7619081	-242.662556	70.765
21	1-F-BZ	-342.1158685	-342.022024	75.575
22	1,2-F_2-BZ	-441.4694696	-441.381145	80.355
23	1,3,5-F_3-BZ	-540.8226012	-540.739832	82.982
24	1-Cl-BZ	-702.4357804	-702.342974	78.360
25	1,3,5-Cl_3-BZ	-1621.7805842	-1621.701072	91.298
26	1,3,5-Br_3-BZ	-7963.6347575	-7963.556209	101.920
27	1,3,5-F_3-2,4,6-$(CH_3)_3$-BZ	-658.7636172	-658.592405	114.843
28	2,4,6-$(CH_3)_3$-BZ	-360.7021010	-360.515372	103.061

29	1,3,5-$(CH_3)_3$-BZ	-360.7915520	-360.603325	105.754
30	1,2,3,4,5,6-$(CH_3)_6$-BZ	-478.7157611	-478.439224	122.964
31	1-CF_3-BZ	-579.9510873	-579.842490	98.129
32	1-CH_3-BZ	-282.1052837	-281.976313	83.441
	Binary complexes			
33	2-$AlCl_3$-BZ	-1866.1135578	-1866.000976	111.510
34	2-BCl_3-BZ	-1648.3943700	-1648.280255	104.845
35	2-$AlBr_3$-BZ	-8207.9767500	-8207.864830	120.718
36	2-$GaCl_3$-BZ	-3548.5107939	-3548.398765	115.967
37	2-BCl_3,5-F-BZ	-1747.7483952	-1747.639768	109.783
38	2-$AlCl_3$,5-F-BZ	-1965.4671124	-1965.360036	115.604
39	2-$AlCl_3$,5-Cl-BZ	-2325.7853367	-2325.679432	119.016
40	2-$AlCl_3$-1,3,5-F_3-BZ	-2164.1703412	-2164.074446	124.322
41	2-BCl_3-1,3,5-F_3-BZ	-1946.4525537	-1946.355236	118.013
42	2-$AlBr_3$-1,3,5-F_3-BZ	-8506.0334273	-8505.938165	132.369
43	2-$GaCl_3$-1,3,5-F_3-BZ	-3846.5679989	-3846.472694	129.016
44	2-$AlCl_3$-1,3,5-Br_3-BZ	-9586.9730523	-9586.881705	140.871
45	2-$AlBr_3$-1,3,5-Br_3-BZ	-15928.8356709	-15928.745014	149.791
46	2-$GaCl_3$-1,3,5-Br_3-BZ	-11269.3719336	-11269.281106	146.296
47	2-$AlCl_3$-1,3,5-F_3-2,4,6-$(CH_3)_3$-BZ	-2282.1086075	-2281.924268	148.710
48	2-BCl_3-1,3,5-F_3-2,4,6-$(CH_3)_3$-BZ	-2064.3911180	-2064.205259	141.855
49	2-$AlBr_3$-1,3,5-F_3-2,4,6-$(CH_3)_3$-BZ	-8623.9704652	-8623.786731	156.816
50	2-$GaCl_3$-1,3,5-F_3-2,4,6-$(CH_3)_3$-BZ	-3964.5067238	-3964.322958	153.513
51	2-$AlCl_3$-2,4,6-$(CH_3)_3$-BZ	-1984.4992600	-1983.849704	135.685
52	2-BCl_3-2,4,6-$(CH_3)_3$-BZ	-1766.3342194	-1766.132424	127.826
53	2-$AlBr_3$-2,4,6-$(CH_3)_3$-BZ	-8325.9121952	-8325.712558	143.159
54	2-$GaCl_3$-2,4,6-$(CH_3)_3$-BZ	-3666.4475007	-3666.248867	132.549
55	2-$AlCl_3$-1,3,5-$(CH_3)_3$-BZ	-1984.1501078	-1983.948662	139.327
56	2-BCl_3-1,3,5-$(CH_3)_3$-BZ	-1766.4312862	-1766.228315	131.603
57	2-$AlCl_3$-1,2,3,4,5,6-$(CH_3)_6$-BZ	-2102.0688414	-2101.779125	156.575
58	2-$AlBr_3$-1,2,3,4,5,6-$(CH_3)_6$-BZ	-8443.9305276	-8443.641411	163.777
59	2-$GaCl_3$-1,2,3,4,5,6-$(CH_3)_6$-BZ	-3784.4668676	-3784.177599	160.067
	Ternary complexes			
60	1-NH_3,4-$AlCl_3$-BZ	-1922.7017873	-1922.547551	122.350
61	1-NH_3,4-BCl_3-BZ	-1704.9846390	-1704.828545	114.107
62	1-NH_3,2-BCl_3-BZ	-1704.9922080	-1704.835567	113.611

63	1-NH_3,2-$AlCl_3$-BZ	-1922.7084850	-1922.553814	123.127
64	1-NH_3,4-BCl_3,1-F-BZ	-1804.3385230	-1804.188332	119.390
65	1-NH_3,2-BCl_3,1-F-BZ	-1804.3408868	-1804.190509	117.110
66	1-NH_3,4-BCl_3,1-Cl-BZ	-2164.6590134	-2164.509332	119.996
67	1-NH_3,2-BCl_3,1-Cl-BZ	-2164.6570815	-2164.507605	118.016
68	1-NH_3,2-BCl_3,5-Cl-BZ	-2164.6659424	-2164.515748	120.649
69	1-NH_3,2-BCl_3,1,3,5-F_3-BZ	-2003.0481519	-2002.908969	126.070
70	1-NH_3,2-BCl_3,1,3,5-Cl_3-BZ	-3083.9989792	-3083.862946	132.894
71	1-NH_3,4-BCl_3,1,3,5-Cl_3-BZ	-3083.9950256	-3083.859085	135.102
72	1-NH_3,2-BCl_3,5-F-BZ	-1804.3465906	-1804.195367	118.022
73	1-NH_3,2-$AlCl_3$,5-F-BZ	-2022.0624664	-2021.913272	128.543
74	1-NH_3,2-BCl_3,3,5-F_2-BZ	-1903.6998552	-1903.554258	122.176
75	1-NH_3,2-BCl_3,1,5- F_2-BZ	-1903.6949769	-1903.550168	122.078
76	1-NH_3,2-BCl_3,1,3- F_2-BZ	-1903.6944479	-1903.549765	121.600
77	1-NH_3,2-BCl_3,3-F-BZ	1804.3458506	-1804.194752	117.294
78	1-NH_3,2-BCl_3,5-CF_3-BZ	-2042.1808853	-2042.014852	135.623
79	1-NH_3,2-BCl_3,5-CH_3-BZ	-1744.3367727	-1744.150473	122.961
80	1-Py,2-BCl_3-BZ	-1896.781229	-1896.569863	129.584
81	1-Py,2-$AlCl_3$-BZ	-2114.4967397	-2114.287466	138.558
82	1-Py,2-BCl_3,5-F-BZ	-1996.1357939	-1995.929915	134.242
83	1-Py,2-$AlCl_3$,5-F-BZ	-2213.8511593	-2213.647346	143.047
84	1-Py,4-BCl_3-BZ	-1896.7713560	-1896.560598	132.696
85	1-Py,4-$AlCl_3$-BZ	-2114.4882762	-2114.279434	141.105
	Hydrogenation products			
86	3,4-H_2-BZ	-243.9004487	-243.780159	75.841
87	3,4,5,6-H_4-BZ	-245.0824694	-244.939259	78.643
88	1,3,4,6-H_4-BZ	-245.0632255	-244.924183	100.333
89	1,2,3,4,5,6-H_6-BZ	-246.283873	-246.117462	78.892
91	2-$AlCl_3$,4,5-H_2-BZ	-1867.2717346	-1867.137739	109.999
92	2-$AlCl_3$,3,4,5,6-H_4-BZ	-1868.4669762	-1868.309435	110.163
93	1-NH_3,2-$AlCl_3$,3,4-H_2-BZ	-1923.8841988	-1923.707413	120.777
94	1-NH_3,2-$AlCl_3$,5,6-H_2-BZ	-1923.8834207	-1923.706315	119.874
	Transition States leading to			
95	3,4-H_2-BZ	-243.8537145	-243.739637	74.792
96	3,4,5,6-H_4-BZ	-245.0118786	-244.875757	77.719
97	2-$AlCl_3$-3,4-H_2-BZ (H_2 in trans-position to $AlCl_3$)	-1867.2216778	-1867.093387	112.835

98	2-$AlCl_3$-3,4-H_2-BZ (H_2 in cis-position to $AlCl_3$)	-1867.2181017	-1867.089683	113.161
99	1-NH_3,2-$AlCl_3$-3,4-H_2-BZ (H_2 in trans-position to $AlCl_3$)	-1923.8192566	-1923.648808	120.747
100	1-NH_3,2-$AlCl_3$-3,4-H_2-BZ (H_2 in cis-position to $AlCl_3$)	-1923.8268399	-1923.656210	119.807
	Complex with benzene			
101	$AlCl_3$-C_6H_6…NH_3	-1912.2606055	-1912.101277	132.619

Table2S. Total energies E^{o}_{0} (in Hartree) for selected molecules at different levels of theory.

Compound	MP2/TZVP	B3LYP/aug-cc-pVTZ	MP2/aug-cc-pVTZ
BZ	-242.0132924	-242.7726571	-242.1667531
NH_3	-56.4160369	-56.5888573	-56.4605409
Py	-247.6176521	-248.3762575	-247.7775176
BCl_3	-1403.838477	-1405.68662	-1404.049084
$AlCl_3$	-1621.1346433	-1623.379611	-1621.358845
2-BCl_3-BZ	-1645.8576889	-1648.440982	-1646.223695
2-$AlCl_3$-BZ	-1863.1834584	-1866.16928	-1863.561601
1-NH_3,2-BCl_3-BZ	-1702.3004288	-1705.033098	-[a]
1-NH_3,2-$AlCl_3$-BZ	-1919.6224198	-1922.759427	-[a]
1-Py,2-BCl_3-BZ	-1893.5159584	-1896.835226	-[a]
1-Py,2-$AlCl_3$-BZ	-2110.8369597	-[a]	-[a]

[a)] Optimization did not converge.

Table 3S. Predicted structural and thermodynamic characteristics for gaseous ternary complexes of fluorine-substituted borazines 1-NH_3,2-BCl_3,1,3,5-F_n-BZ. B3LYP/TZVP level of theory.

Parameter	1-H	1-F	3-F	5-F	1,3-F_2	1,5-F_2	3,5-F_2	1,3,5-F_3
R (B–NH_3), Å	1.713	1.749	1.712	1.713	1.749	1.748	1.712	1.746
R (N–BCl_3), Å	1.650	1.665	1.660	1.652	1.676	1.667	1.662	1.677
q_{CT} (NH_3)	0.394	0.370	0.401	0.387	0.379	0.378	0.404	0.384
q_{CT} (BCl_3)	-0.344	-0.320	-0.330	-0.334	-0.304	-0.310	-0.320	-0.294
q_{CT} (ring)	-0.050	-0.050	-0.071	-0.053	-0.053	-0.068	-0.084	-0.089
$\Delta_{diss}H^o_{298}$, kJ mol^{-1}	-23	-35	-24	-22	-34	-33	-23	-33
$\Delta_{diss}S^o_{298}$, J mol^{-1} K^{-1}	303	308	307	304	309	307	307	302
$\Delta_{diss}G^o_{298}$, kJ mol^{-1}	-113	-127	-115	-113	-127	-125	-114	-123

Figure 1S. Position of points (denoted Bq) for NICS computation: (a) BZ; (b) 2-BCl_3-BZ; (c) 1-NH_3,4-BCl_3-BZ; (d) 1-NH_3,2-BCl_3-BZ.

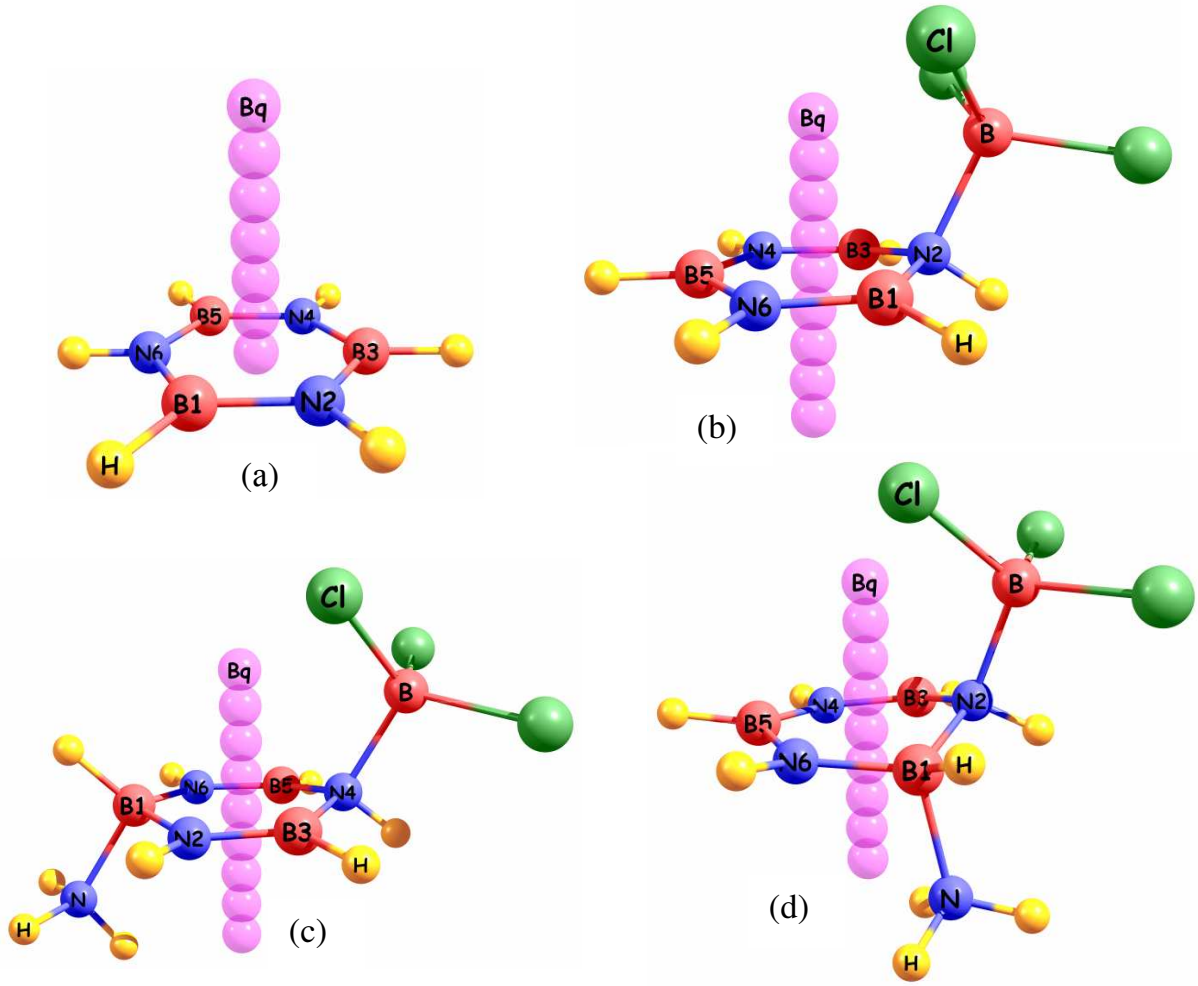


Figure 2S. NICS values for borazine and its donor-acceptor complexes computed at B3LYP/aug-cc-pVTZ level of theory.

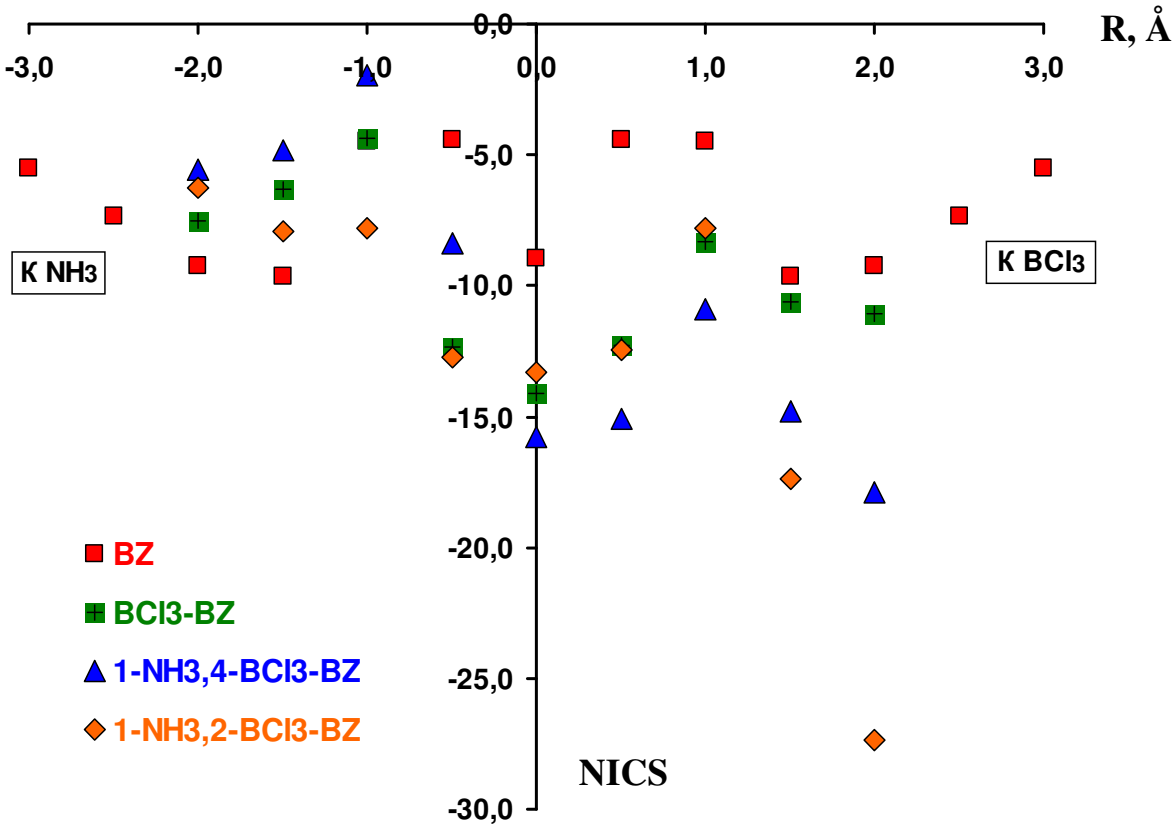
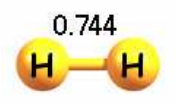


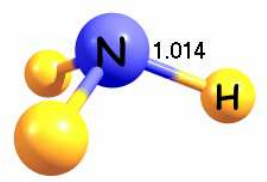
Figure 3S. Optimized geometries of considered compounds. B3LYP/TZVP level of theory. Cartesian xyz coordinates in Angstroms. Numbering of the compounds corresponds to Table 1S.

1) H_2



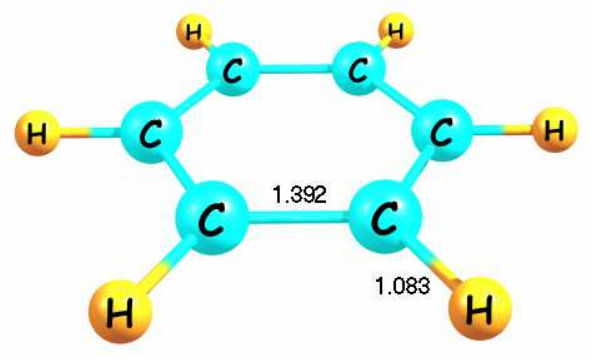
	X	Y	Z
H	0.000	0.000	0.372
H	0.000	0.000	-0.372

2) NH_3



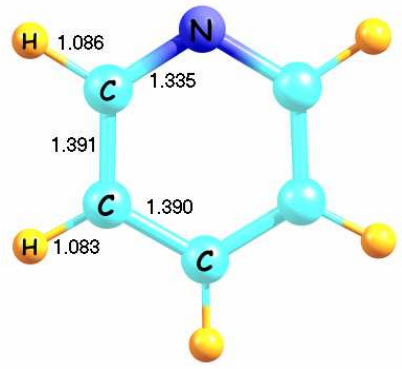
	X	Y	Z
N	0.000	0.000	0.110
H	0.000	0.945	-0.257
H	0.818	-0.472	-0.257
H	-0.818	-0.472	-0.257

3) C_6H_6



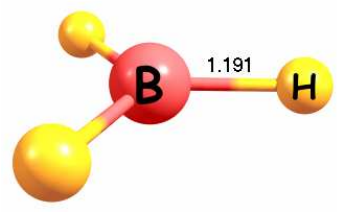
	X	Y	Z
C	1.392	0.000	0.000
C	0.696	-1.206	0.000
C	0.696	1.206	0.000
C	-1.392	0.000	0.000
C	-0.696	1.206	0.000
C	-0.696	-1.206	0.000
H	2.475	0.000	0.000
H	1.238	-2.144	0.000
H	1.238	2.144	0.000
H	-2.475	0.000	0.000
H	-1.238	2.144	0.000
H	-1.238	-2.144	0.000

4) Py



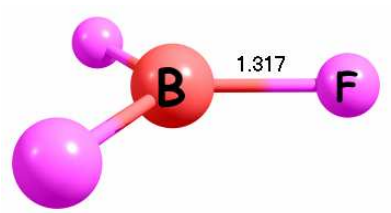
	X	Y	Z
N	-1.196	0.755	0.000
C	0.000	1.349	0.000
C	-1.218	-0.580	0.000
H	-0.008	2.434	0.000
H	-2.201	-1.040	0.000
C	1.205	0.652	0.000
C	-0.071	-1.368	0.000
H	2.145	1.189	0.000
H	-0.151	-2.448	0.000
C	1.167	-0.737	0.000
H	2.083	-1.315	0.000

5) BH_3



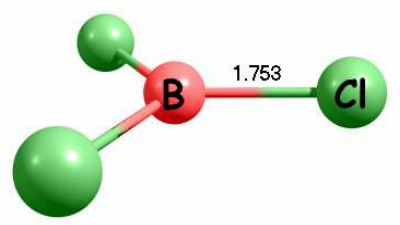
	X	Y	Z
B	0.000	0.000	0.000
H	0.595	1.031	0.000
H	0.598	-1.029	0.000
H	-1.191	-0.001	0.000

6) BF_3



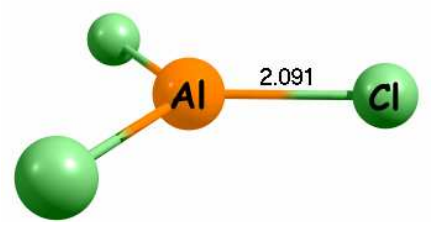
	X	Y	Z
B	0.000	0.000	0.000
F	-1.202	-0.209	0.000
F	0.824	-1.027	0.000
F	0.477	1.227	0.000

7) BCl_3



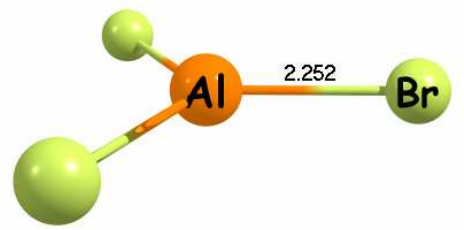
	X	Y	Z
B	0.000	0.000	0.000
Cl	0.000	1.753	0.000
Cl	1.518	-0.876	0.000
Cl	-1.518	-0.876	0.000

8) $AlCl_3$



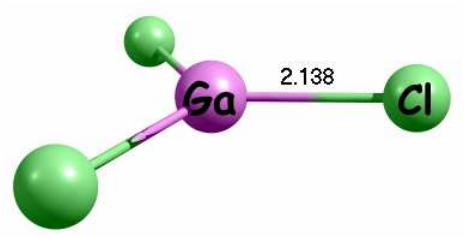
	X	Y	Z
Al	0.000	0.000	0.000
Cl	0.000	2.091	0.000
Cl	1.810	-1.045	0.000
Cl	-1.810	-1.045	0.000

9) $AlBr_3$



	X	Y	Z
Al	0.000	0.000	0.000
Br	0.000	2.252	0.000
Br	1.950	-1.126	0.000
Br	-1.950	-1.126	0.000

10) $GaCl_3$



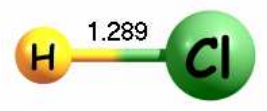
	X	Y	Z
Ga	0.000	0.000	0.000
Cl	0.000	2.138	0.000
Cl	1.851	-1.069	0.000
Cl	-1.851	-1.069	0.000

11) HF



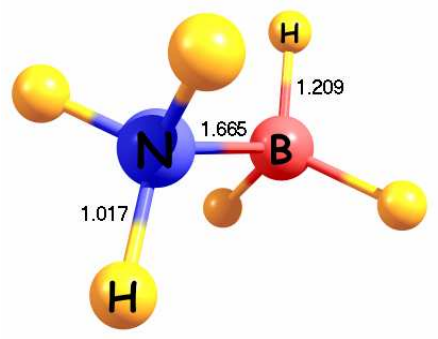
	X	Y	Z
F	0.000	0.000	0.093
H	0.000	0.000	-0.833

12) HCl



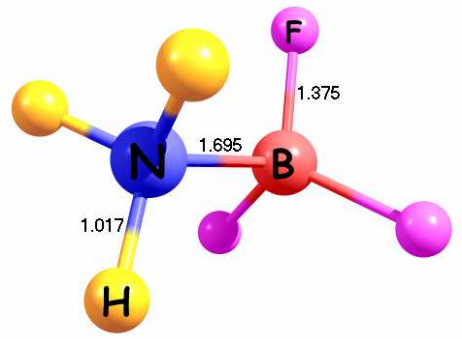
	X	Y	Z
Cl	0.000	0.000	0.072
H	0.000	0.000	-1.218

13) $BH_3 \cdot NH_3$



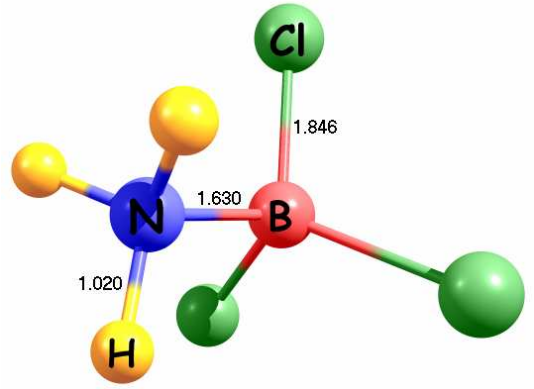
	X	Y	Z
B	0.000	0.000	-0.934
N	0.000	0.000	0.731
H	-1.012	0.584	-1.245
H	1.012	0.584	-1.245
H	0.000	-1.168	-1.245
H	0.000	0.948	1.097
H	-0.821	-0.474	1.097
H	0.821	-0.474	1.097

14) $BF_3 \cdot NH_3$



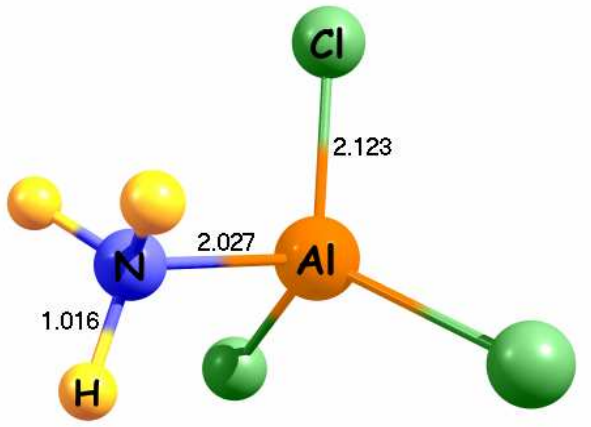
	X	Y	Z
B	-0.215	0.000	0.000
N	1.480	0.000	0.002
F	-0.546	-1.120	-0.726
F	-0.550	-0.068	1.331
F	-0.546	1.188	-0.608
H	1.832	-0.854	0.429
H	1.834	0.057	-0.950
H	1.832	0.796	0.529

15) $BCl_3 \cdot NH_3$



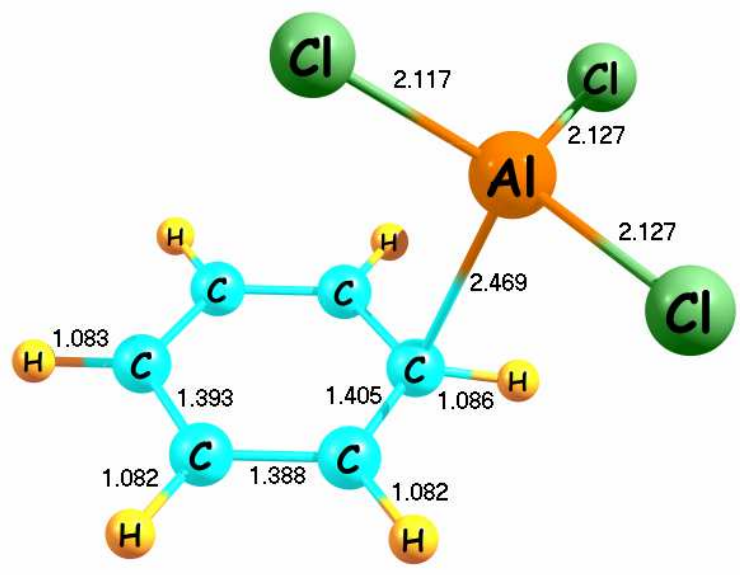
	X	Y	Z
B	0.000	0.000	0.107
N	-0.004	-0.003	1.737
Cl	-1.681	-0.595	-0.374
Cl	0.325	1.754	-0.370
Cl	1.358	-1.157	-0.371
H	-0.728	0.622	2.090
H	-0.186	-0.944	2.084
H	0.900	0.308	2.092

16) $AlCl_3 \cdot NH_3$



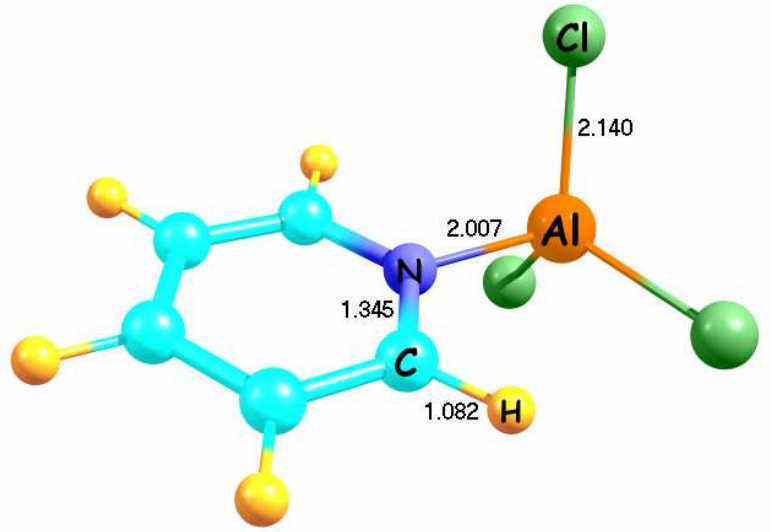
	X	Y	Z
Al	0.000	0.000	0.958
N	0.000	0.000	2.985
Cl	2.079	0.051	0.532
Cl	-0.995	-1.826	0.533
Cl	-1.084	1.775	0.534
H	0.371	-0.869	3.358
H	0.567	0.757	3.357
H	-0.939	0.112	3.356

17) $AlCl_3 \cdot C_6H_6$



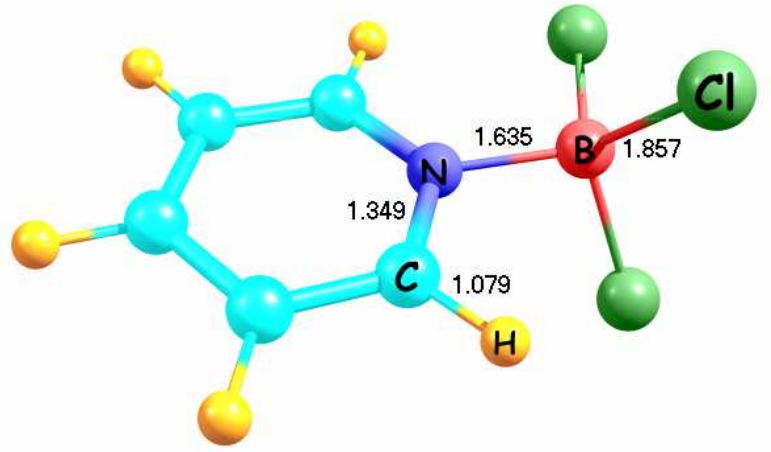
	X	Y	Z
H	1.413	0.456	-1.242
C	0.896	0.672	-0.311
C	0.827	1.874	1.785
C	-1.184	0.852	0.906
C	-0.532	1.586	1.894
C	-0.480	0.408	-0.204
C	1.540	1.435	0.678
H	-1.084	1.927	2.761
H	2.593	1.660	0.580
Al	1.753	-1.555	0.322
H	1.324	2.447	2.557
H	-2.240	0.634	1.000
H	-0.979	-0.156	-0.981
Cl	3.827	-1.165	0.063
Cl	0.847	-2.680	-1.239
Cl	1.076	-1.920	2.295

18) $AlCl_3 \cdot Py$



	X	Y	Z
N	-0.132	0.885	0.000
C	0.853	1.800	0.000
C	0.588	3.159	0.000
C	-0.733	3.587	0.000
C	-1.750	2.639	0.000
C	-1.414	1.298	0.000
H	1.862	1.409	0.000
H	1.410	3.862	0.000
H	-0.968	4.645	0.000
H	-2.792	2.928	0.000
H	-2.168	0.523	0.000
Al	0.230	-1.090	0.000
Cl	2.368	-1.228	0.000
Cl	-0.733	-1.748	1.794
Cl	-0.733	-1.748	-1.794

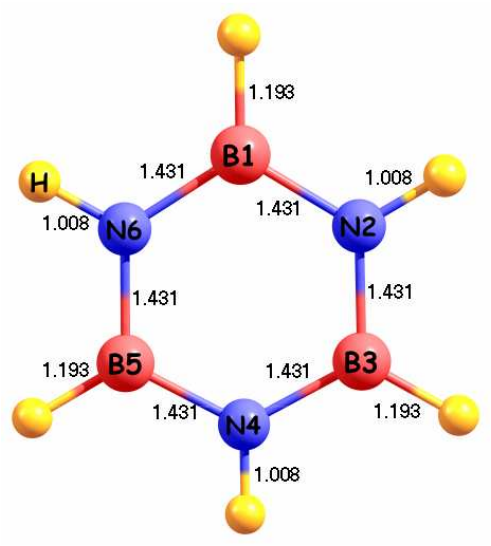
19) $BCl_3 \cdot Py$



	X	Y	Z
N	-0.054	0.621	0.000
C	0.945	1.518	0.000
C	0.695	2.880	0.000
C	-0.617	3.329	0.000
C	-1.646	2.393	0.000
C	-1.334	1.049	0.000
H	1.943	1.107	0.000
H	1.529	3.568	0.000
H	-0.838	4.389	0.000
H	-2.684	2.694	0.000
H	-2.089	0.279	0.000
B	0.198	-0.995	0.000
Cl	2.015	-1.341	0.000
Cl	-0.617	-1.636	1.540
Cl	-0.617	-1.636	-1.540

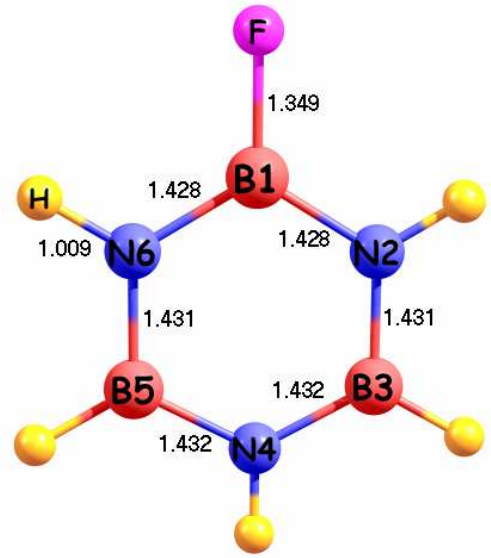
Borazine and its derivatives.

20) $B_3N_3H_6$ (in the following denoted as BZ)



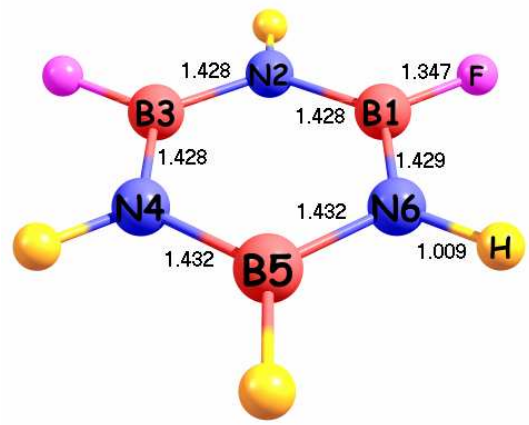
	X	Y	Z
B	0.000	0.000	-1.452
N	0.000	0.000	1.410
B	0.000	1.258	0.726
N	0.000	-1.221	-0.705
B	0.000	-1.258	0.726
N	0.000	1.221	-0.705
H	0.000	0.000	-2.645
H	0.000	0.000	2.418
H	0.000	2.291	1.323
H	0.000	-2.094	-1.209
H	0.000	-2.291	1.323
H	0.000	2.094	-1.209

21) 1-F-BZ



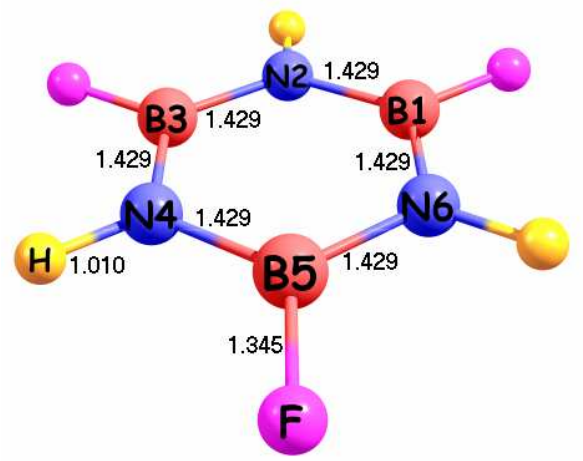
	X	Y	Z
B	-1.173	1.260	0.000
N	0.258	-1.228	0.000
B	0.987	0.000	0.000
N	-1.854	0.000	0.000
B	-1.173	-1.260	0.000
N	0.258	1.228	0.000
H	-1.768	2.293	0.000
H	0.772	-2.096	0.000
F	2.335	0.000	0.000
H	-2.862	0.000	0.000
H	-1.769	-2.293	0.000
H	0.772	2.096	0.000

22) 1,3-F_2-BZ



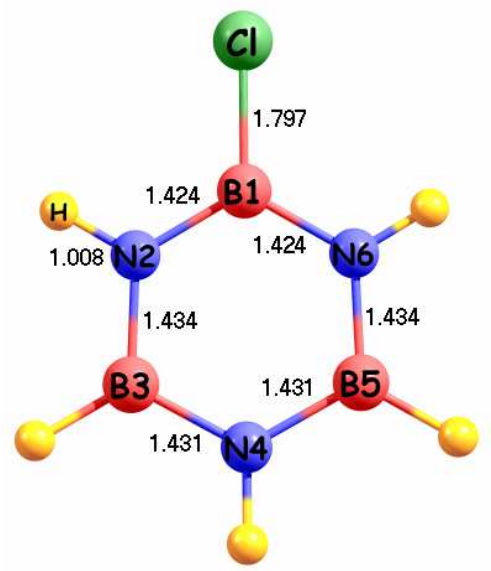
	X	Y	Z
B	1.243	-0.333	0.000
N	-1.222	1.095	0.000
B	-1.243	-0.333	0.000
N	1.222	1.095	0.000
B	0.000	1.842	0.000
N	0.000	-1.036	0.000
F	2.410	-1.007	0.000
H	-2.101	1.590	0.000
F	-2.410	-1.007	0.000
H	2.101	1.590	0.000
H	0.000	3.032	0.000
H	0.000	-2.046	0.000

23) 1,3,5-F_3-BZ



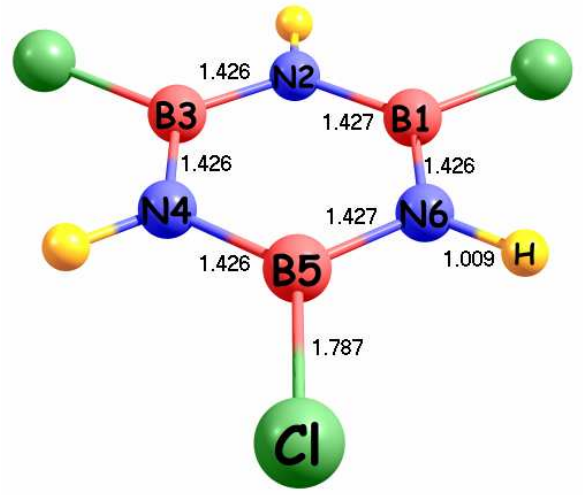
	X	Y	Z
B	0.000	0.000	1.438
N	0.000	0.000	-1.419
B	0.000	1.246	-0.719
N	0.000	-1.229	0.709
B	0.000	-1.246	-0.719
N	0.000	1.229	0.709
H	0.000	0.000	-2.429
H	0.000	-2.103	1.214
H	0.000	2.103	1.214
F	0.000	0.000	2.783
F	0.000	-2.410	-1.392
F	0.000	2.410	-1.392

24) 1-Cl-BZ



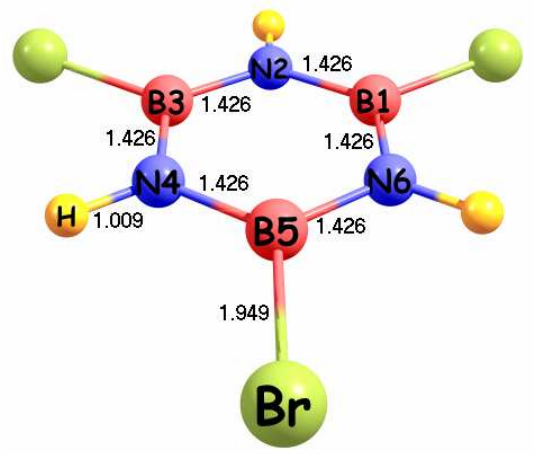
	X	Y	Z
B	0.000	0.000	1.436
N	0.000	0.000	-1.416
B	0.000	1.243	-0.718
N	0.000	-1.226	0.708
B	0.000	-1.243	-0.718
N	0.000	1.226	0.708
H	0.000	0.000	-2.425
H	0.000	-2.100	1.213
H	0.000	2.100	1.213
Br	0.000	0.000	3.384
Br	0.000	-2.931	-1.692
Br	0.000	2.931	-1.692

25) 1,3,5-Cl_3-BZ



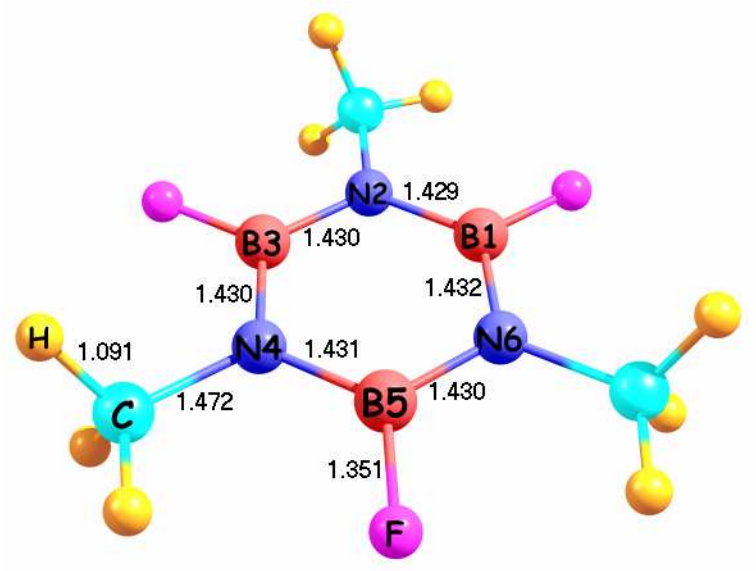
	X	Y	Z
B	0.000	-1.437	0.000
N	0.000	1.415	0.000
B	1.244	0.718	0.000
N	-1.226	-0.708	0.000
B	-1.245	0.719	0.000
N	1.226	-0.708	0.000
H	0.001	2.424	0.000
H	-2.100	-1.212	0.000
H	2.099	-1.213	0.000
Cl	0.000	-3.224	0.000
Cl	-2.792	1.613	0.000
Cl	2.792	1.612	0.000

26) 1,3,5-Br_3-BZ



	X	Y	Z
B	1.627	1.259	0.000
N	0.194	-1.225	0.001
B	-0.532	0.000	0.001
N	2.308	0.000	0.000
B	1.627	-1.258	0.000
N	0.194	1.224	0.001
H	2.218	2.293	0.000
H	-0.317	-2.094	0.001
Cl	-2.329	0.000	0.000
H	3.316	0.000	-0.001
H	2.219	-2.292	0.000
H	-0.318	2.094	0.001

27) 1,3,5-F_3-2,4,6-Me_3-BZ

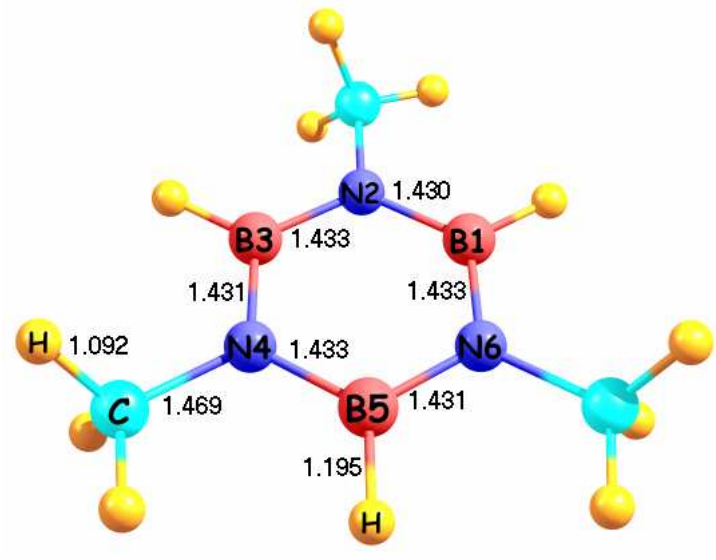


	X	Y	Z
B	1.042	0.970	-0.001
N	-1.048	-0.983	0.002
B	0.323	-1.393	0.001
N	-0.321	1.400	-0.002
B	-1.357	0.413	0.000
N	1.374	-0.422	0.000
C	-0.673	2.829	0.003
H	0.226	3.430	-0.108
H	-1.353	3.063	-0.817
H	-1.163	3.109	0.938
C	-2.140	-1.971	-0.003
H	-1.729	-2.973	0.094
H	-2.826	-1.793	0.826
H	-2.711	-1.919	-0.932
C	2.789	-0.829	0.000
H	2.860	-1.914	0.000
H	3.304	-0.447	-0.883
H	3.304	-0.448	0.884
F	2.038	1.881	-0.003
F	0.627	-2.709	0.003
F	-2.647	0.807	0.000

28) 2,4,6-Me_3-BZ

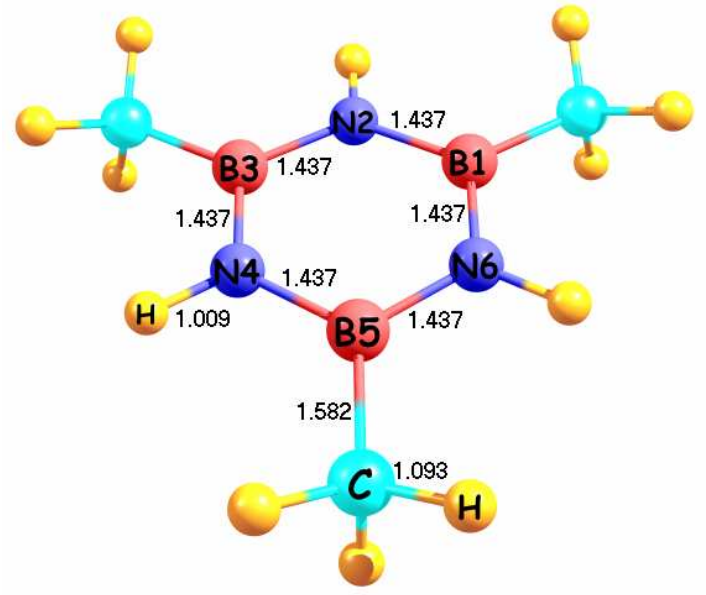
	X	Y	Z
B	1.017	1.014	-0.007
N	-1.006	-1.013	0.004
B	0.376	-1.389	0.007
N	-0.367	1.377	-0.005
B	-1.384	0.367	0.000
N	1.381	-0.372	0.000
C	-0.763	2.791	0.005
H	0.117	3.425	-0.104
H	-1.448	3.012	-0.816
H	-1.261	3.057	0.940
C	-2.053	-2.043	-0.004
H	-1.604	-3.031	0.091
H	-2.750	-1.902	0.825
H	-2.626	-2.018	-0.935
C	2.804	-0.737	0.000
H	2.909	-1.821	0.004
H	3.311	-0.348	-0.886
H	3.313	-0.341	0.882
H	1.862	1.859	-0.012
H	0.686	-2.544	0.011

H	-2.539	0.677	0.000



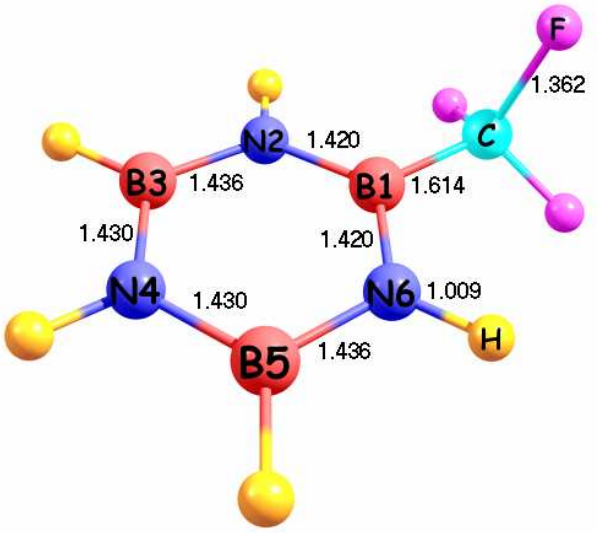
29) 1,3,5-Me_3-BZ

	X	Y	Z
B	-0.326	1.430	-0.020
N	0.312	-1.371	-0.026
B	1.402	-0.433	-0.020
N	-1.343	0.415	-0.028
B	-1.076	-0.997	-0.020
N	1.031	0.956	-0.027
C	-0.677	2.972	0.025
H	0.093	3.596	-0.435
H	-1.627	3.204	-0.464
H	-0.772	3.306	1.065
H	-2.307	0.712	-0.029
C	-2.235	-2.072	0.025
H	-1.947	-3.026	-0.424
H	-2.510	-2.287	1.065
H	-3.147	-1.734	-0.474
H	0.537	-2.355	-0.028
C	2.912	-0.899	0.025
H	3.588	-0.193	-0.466
H	3.250	-0.984	1.064
H	3.068	-1.879	-0.435
H	1.771	1.642	-0.027

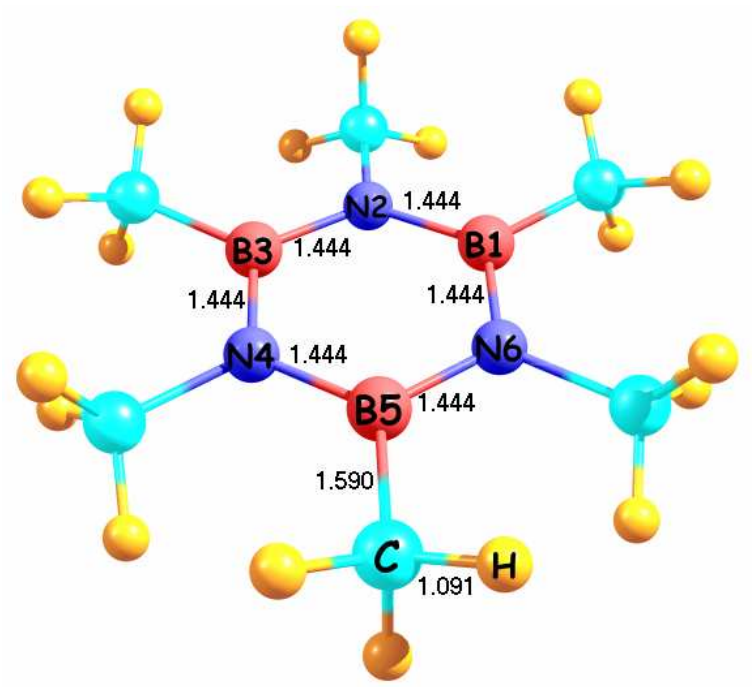


30) 1-CF_3-BZ

	X	Y	Z
B	-0.082	0.000	-0.028
N	-0.801	1.224	-0.025
B	-2.236	1.260	0.000
N	-2.913	0.001	0.018
B	-2.237	-1.260	0.000
N	-0.801	-1.225	-0.025
C	1.532	0.000	-0.003
H	-0.291	2.095	-0.049
H	-2.829	2.292	0.003
H	-3.922	0.001	0.036
H	-2.830	-2.291	0.004
H	-0.293	-2.097	-0.049
F	2.011	-0.042	1.272
F	2.071	-1.069	-0.647
F	2.069	1.111	-0.576

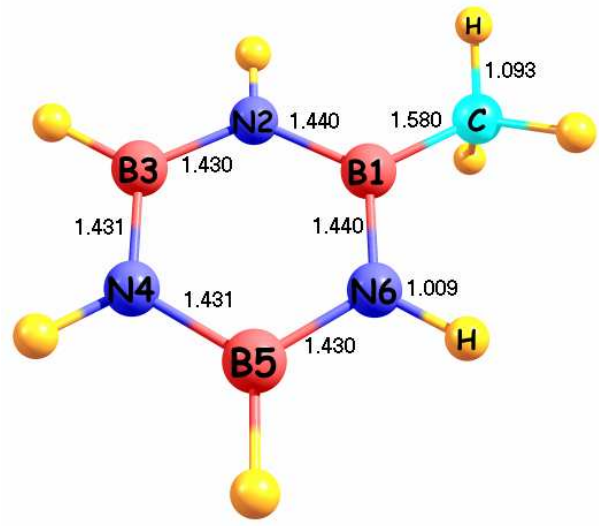


31) 1,2,3,4,5,6-Me_6-BZ



	X	Y	Z
B	-0.369	1.411	0.010
N	0.362	-1.382	-0.029
B	-1.037	-1.025	0.011
N	1.016	1.004	-0.029
B	1.406	-0.386	0.010
N	-1.377	0.377	-0.029
C	-0.771	2.946	0.107
H	-1.724	3.101	0.616
H	-0.026	3.543	0.636
H	-0.877	3.396	-0.889
C	2.061	2.036	-0.087
H	1.703	2.919	-0.614
H	2.389	2.349	0.910
H	2.934	1.672	-0.626
C	2.937	-0.805	0.107
H	3.081	-1.756	0.623
H	3.384	-0.923	-0.888
H	3.543	-0.064	0.630
C	0.734	-2.803	-0.090
H	-0.021	-3.377	-0.623
H	1.673	-2.933	-0.624
H	0.850	-3.243	0.906
C	-2.167	-2.140	0.109
H	-3.053	-1.793	0.644
H	-2.511	-2.451	-0.886
H	-1.825	-3.045	0.613
C	-2.794	0.766	-0.088
H	-3.380	0.012	-0.609
H	-3.227	0.900	0.909
H	-2.915	1.701	-0.632

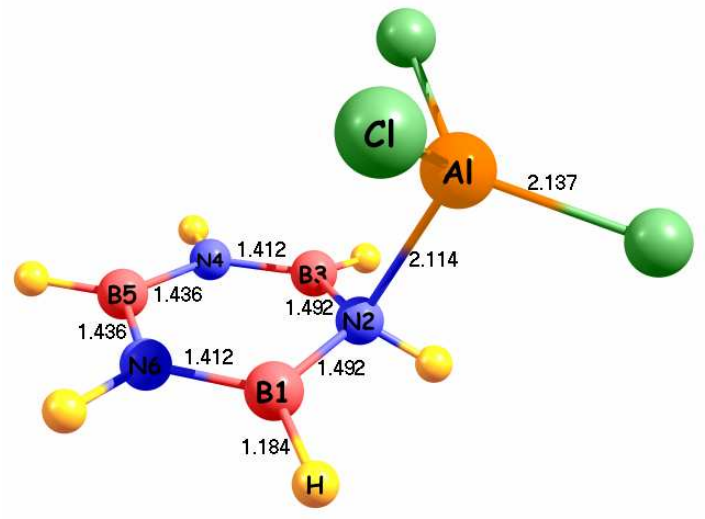
32) 1-CH_3-BZ



	X	Y	Z
B	0.950	0.000	-0.016
N	0.182	1.217	-0.013
B	-1.248	1.255	0.002
N	-1.935	0.000	0.011
B	-1.247	-1.255	0.002
N	0.182	-1.217	-0.013
Cl	2.530	0.000	0.010
H	0.679	2.095	-0.020
H	-1.842	2.290	0.005
H	-2.943	0.000	0.021
H	-1.841	-2.291	0.006
H	0.679	-2.095	-0.020
H	2.889	-0.008	1.046
H	2.961	-0.879	-0.476
H	2.962	0.886	-0.462

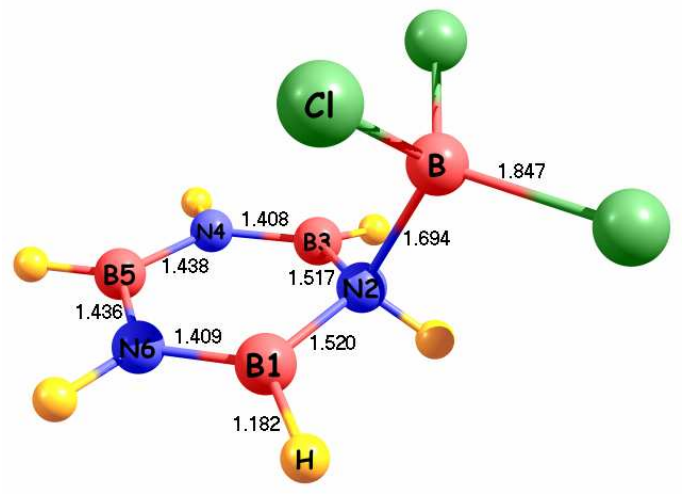
Binary complexes of BZ

33) 2-$AlCl_3$-BZ



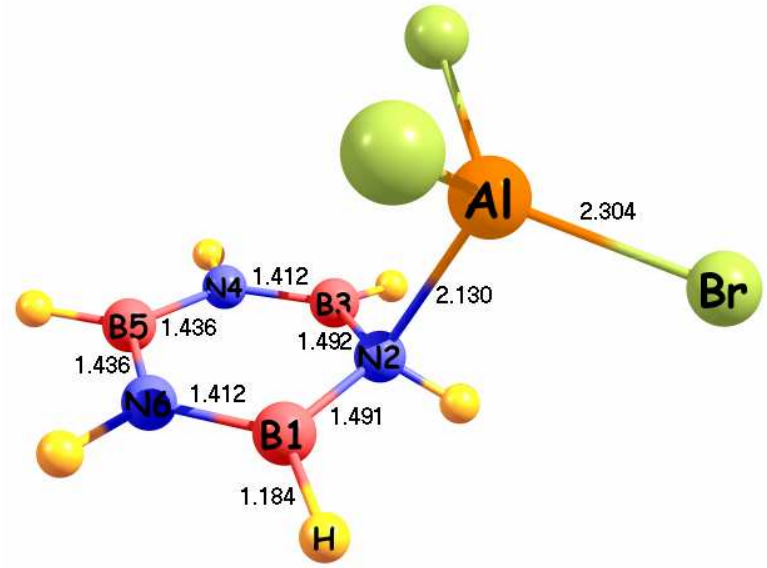
	X	Y	Z
B	-3.233	0.000	-0.227
N	-2.608	-1.225	0.187
B	-1.406	-1.286	0.924
N	-0.679	0.000	1.135
B	-1.406	1.286	0.924
N	-2.608	1.225	0.187
H	-4.245	0.000	-0.850
H	-3.069	-2.094	-0.037
H	-0.977	-2.282	1.398
H	-0.112	0.000	1.981
H	-0.977	2.283	1.398
H	-3.069	2.095	-0.037
Al	1.005	0.000	-0.143
Cl	0.817	1.793	-1.282
Cl	2.535	0.000	1.349
Cl	0.817	-1.793	-1.282

34) 2-BCl_3-BZ



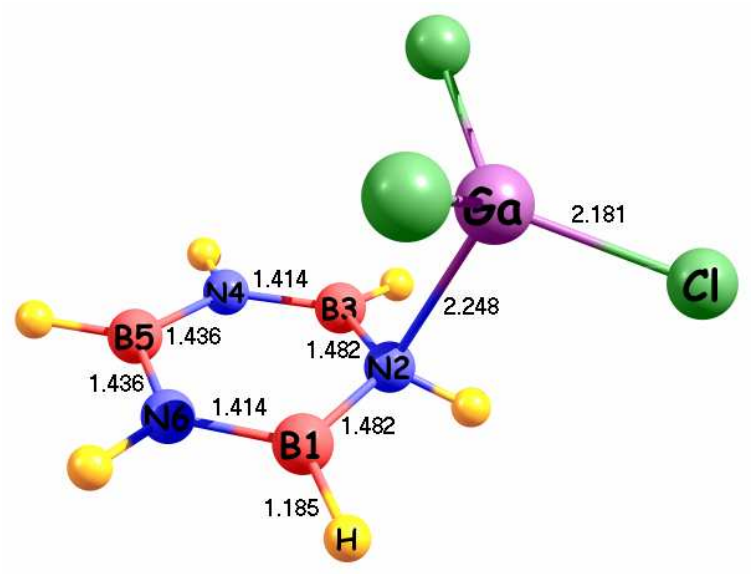
	X	Y	Z
B	-3.056	0.007	0.228
N	-2.401	1.233	-0.143
B	-1.179	1.295	-0.841
N	-0.402	0.000	-0.982
B	-1.147	-1.305	-0.751
N	-2.420	-1.222	-0.152
H	-4.108	0.015	0.779
H	-2.891	2.099	0.026
H	-0.793	2.261	-1.402
H	0.069	-0.025	-1.885
H	-0.679	-2.306	-1.172
H	-2.901	-2.087	0.048
B	0.945	0.006	0.045
Cl	0.620	-1.241	1.385
Cl	2.378	-0.468	-1.018
Cl	1.122	1.707	0.759

35) 2-$AlBr_3$-BZ



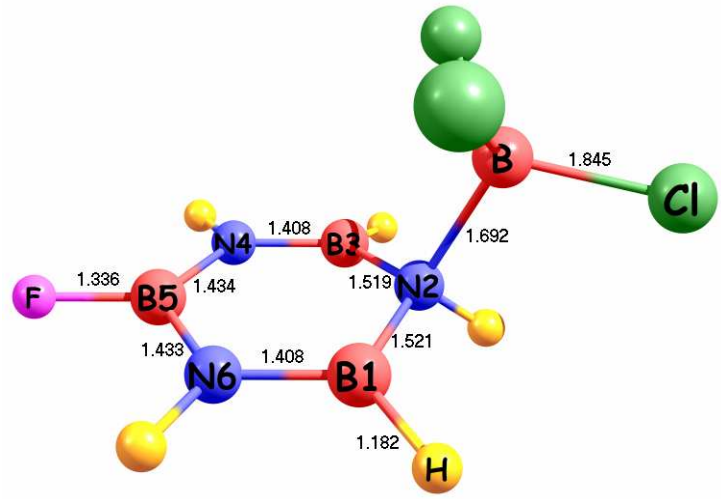
	X	Y	Z
B	-3.716	0.000	0.580
N	-3.026	-1.225	0.873
B	-1.711	-1.285	1.386
N	-0.959	0.000	1.465
B	-1.711	1.285	1.386
N	-3.026	1.225	0.873
H	-4.825	0.000	0.155
H	-3.520	-2.094	0.739
H	-1.208	-2.281	1.782
H	-0.252	0.000	2.199
H	-1.208	2.281	1.782
H	-3.520	2.094	0.739
Al	0.506	0.000	-0.081
Br	0.132	1.926	-1.277
Br	2.385	0.000	1.252
Br	0.132	-1.926	-1.277

36) 2-$GaCl_3$-BZ



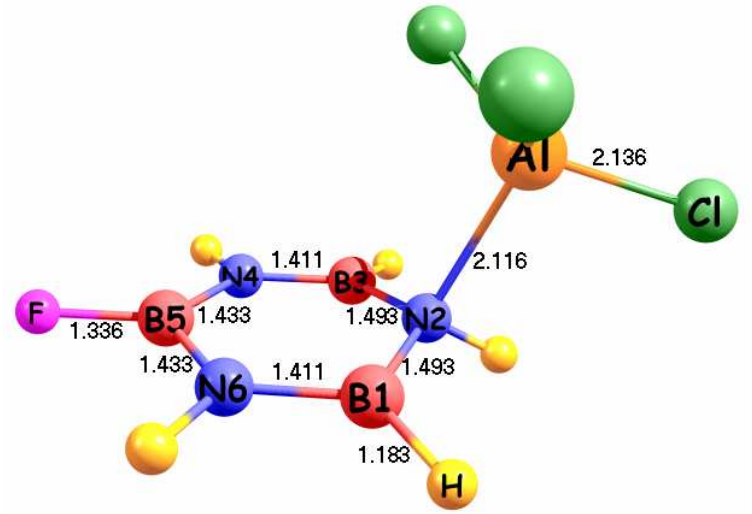
	X	Y	Z
B	-1.666	-2.971	0.000
N	-1.689	-2.221	1.224
B	-1.689	-0.809	1.282
N	-1.507	-0.089	0.000
B	-1.689	-0.809	-1.282
N	-1.689	-2.221	-1.224
H	-1.666	-4.159	0.000
H	-1.733	-2.731	2.095
H	-1.843	-0.197	2.285
H	-1.866	0.862	0.000
H	-1.843	-0.197	-2.285
H	-1.733	-2.731	-2.095
Ga	0.609	0.670	0.000
Cl	1.457	-0.129	-1.837
Cl	0.098	2.790	0.000
Cl	1.457	-0.129	1.837

37) 2-BCl_3,5-F-BZ



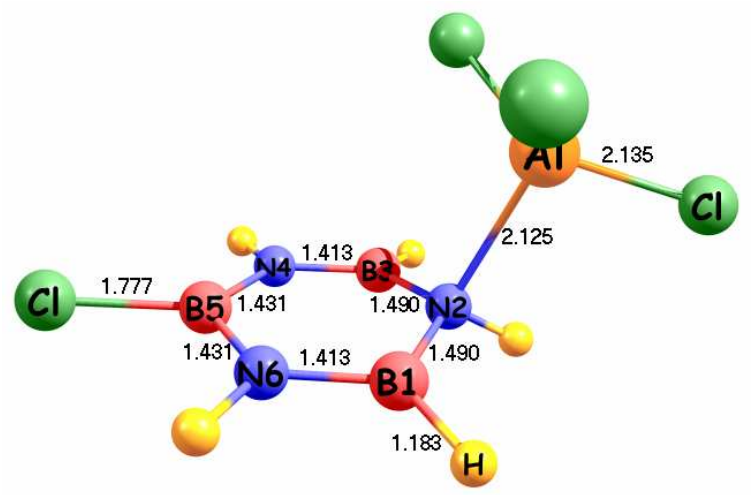
	X	Y	Z
B	-2.713	0.000	-0.047
N	-2.054	1.234	-0.367
B	-0.781	1.296	-0.964
N	0.000	-0.004	-1.055
B	-0.759	-1.312	-0.893
N	-2.067	-1.236	-0.375
F	-3.937	0.006	0.488
H	-2.568	2.094	-0.233
H	-0.351	2.263	-1.489
H	0.538	-0.023	-1.920
H	-0.273	-2.307	-1.308
H	-2.572	-2.096	-0.212
B	1.258	0.005	0.076
Cl	0.894	-1.330	1.318
Cl	2.795	-0.334	-0.887
Cl	1.280	1.671	0.892

38) 2-$AlCl_3$,5-F-BZ



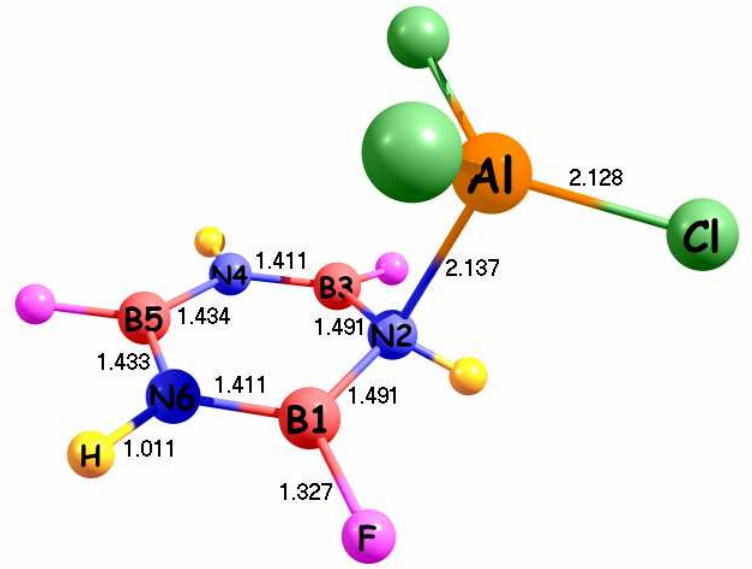
	X	Y	Z
B	2.911	0.000	-0.080
N	2.270	-1.232	-0.434
B	1.013	-1.289	-1.072
N	0.275	0.000	-1.224
B	1.013	1.289	-1.072
N	2.270	1.232	-0.434
F	4.104	0.000	0.523
H	2.759	-2.096	-0.246
H	0.549	-2.284	-1.513
H	-0.356	0.000	-2.024
H	0.549	2.284	-1.513
H	2.759	2.096	-0.246
Al	-1.305	0.000	0.184
Cl	-1.014	1.793	1.302
Cl	-2.949	-0.001	-1.180
Cl	-1.014	-1.793	1.302

39) 2-$AlCl_3$,5-Cl-BZ



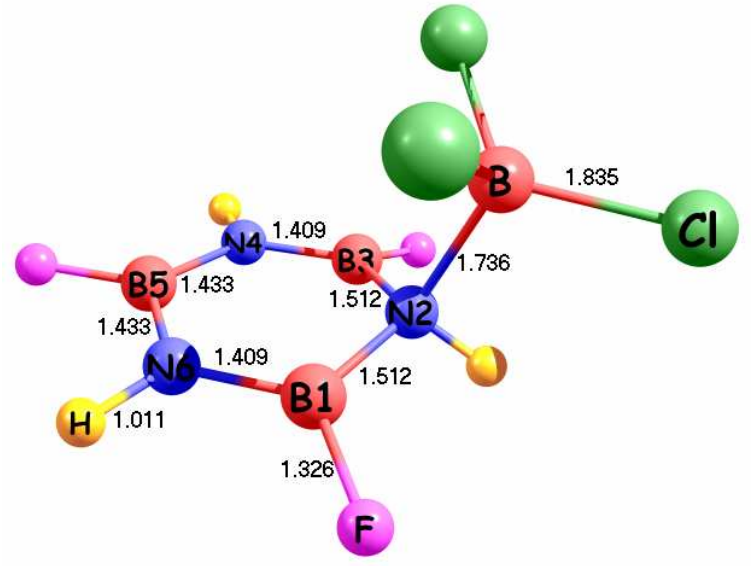
	X	Y	Z
B	2.575	0.000	-0.296
N	1.912	-1.228	-0.611
B	0.618	-1.286	-1.176
N	-0.128	0.000	-1.286
B	0.618	1.286	-1.176
N	1.912	1.228	-0.611
Cl	4.207	0.000	0.408
H	2.406	-2.095	-0.454
H	0.132	-2.284	-1.585
H	-0.809	0.000	-2.043
H	0.132	2.284	-1.585
H	2.406	2.095	-0.454
Al	-1.622	0.000	0.224
Cl	-1.258	1.794	1.316
Cl	-3.344	0.000	-1.039
Cl	-1.258	-1.794	1.316

40) 2-$AlCl_3$,1,3,5-F_3-BZ



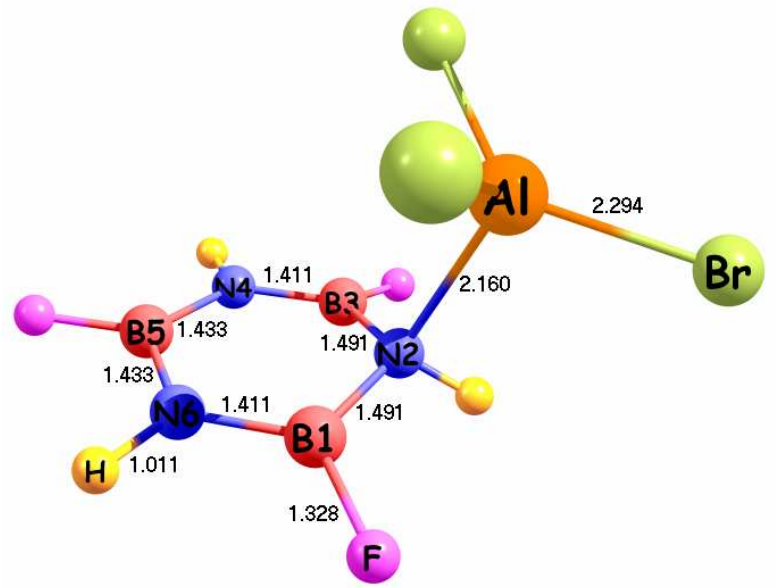
	X	Y	Z
B	2.825	0.000	0.227
N	2.201	-1.232	-0.159
B	0.983	-1.269	-0.869
N	0.217	0.000	-1.033
B	0.983	1.269	-0.869
N	2.201	1.232	-0.159
F	3.983	0.000	0.889
H	2.668	-2.103	0.052
F	0.514	-2.365	-1.453
H	-0.362	0.000	-1.874
F	0.514	2.365	-1.453
H	2.668	2.103	0.052
Al	-1.405	0.000	0.358
Cl	-1.079	1.793	1.461
Cl	-3.024	0.000	-1.023
Cl	-1.079	-1.793	1.461

41) 2-BCl_3,1,3,5-F_3-BZ



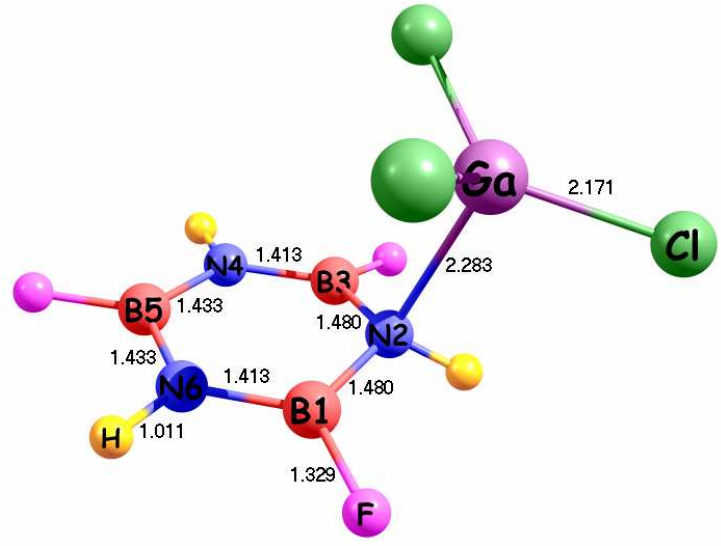
	X	Y	Z
B	-2.647	0.000	0.235
N	-2.010	1.234	-0.123
B	-0.757	1.280	-0.765
N	0.038	0.000	-0.889
B	-0.757	-1.280	-0.765
N	-2.010	-1.234	-0.123
F	-3.839	0.000	0.834
H	-2.499	2.101	0.051
F	-0.300	2.354	-1.395
H	0.578	0.000	-1.755
F	-0.300	-2.354	-1.395
H	-2.499	-2.101	0.051
B	1.319	0.000	0.283
Cl	1.112	-1.528	1.304
Cl	2.862	0.000	-0.710
Cl	1.112	1.528	1.304

42) 2-$AlBr_3$,1,3,5-F_3-BZ



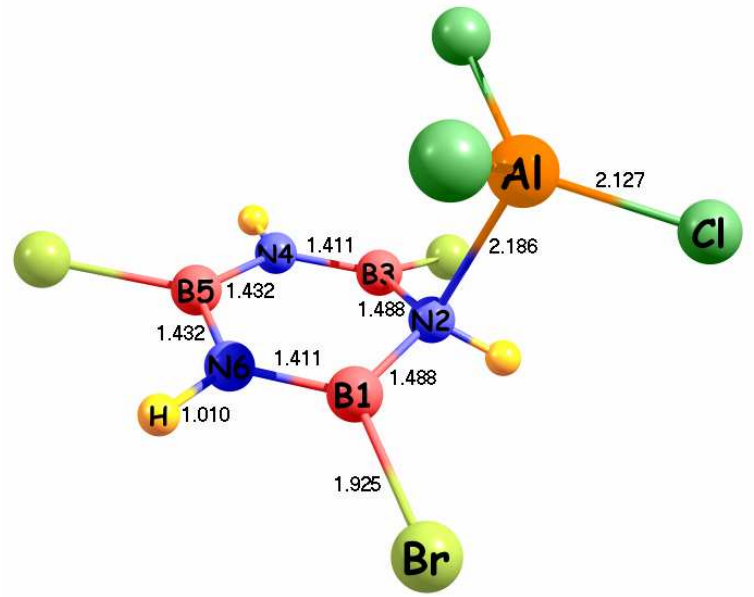
	X	Y	Z
B	-2.186	0.000	-0.019
N	-1.492	1.228	-0.265
B	-0.145	1.264	-0.685
N	0.636	0.000	-0.616
B	-0.145	-1.264	-0.685
N	-1.492	-1.228	-0.265
Br	-4.035	0.000	0.542
H	-2.001	2.097	-0.193
Br	0.664	2.842	-1.436
H	1.449	0.000	-1.230
Br	0.664	-2.842	-1.436
H	-2.001	-2.097	-0.194
Al	1.785	0.000	1.244
Cl	1.165	-1.782	2.226
Cl	3.723	-0.001	0.367
Cl	1.166	1.782	2.226

43) 2-$GaCl_3$,1,3,5-F_3-BZ



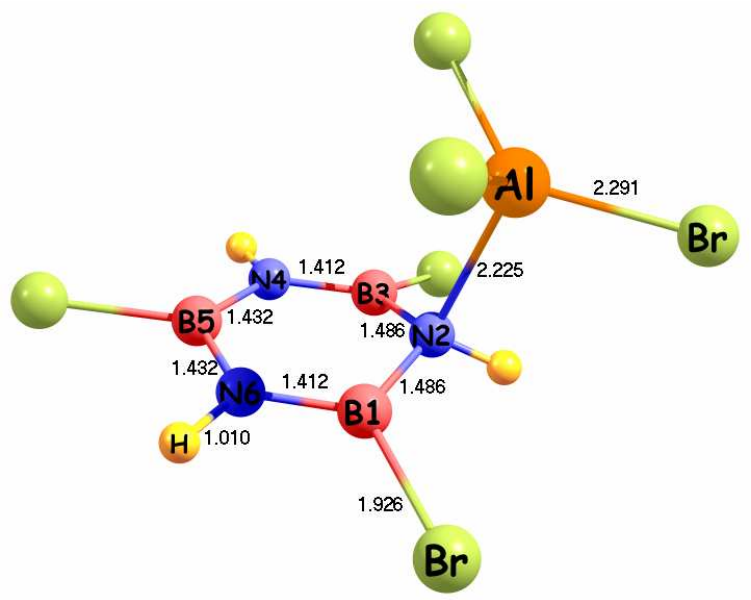
	X	Y	Z
B	-2.727	1.304	0.000
N	-1.996	1.350	1.232
B	-0.584	1.409	1.265
N	0.159	1.218	0.000
B	-0.584	1.409	-1.265
N	-1.996	1.350	-1.232
F	-4.061	1.261	0.000
H	-2.506	1.375	2.104
F	0.102	1.669	2.374
H	1.090	1.630	0.000
F	0.102	1.669	-2.374
H	-2.506	1.375	-2.104
Ga	0.950	-0.924	0.000
Cl	0.102	-1.710	-1.838
Cl	3.060	-0.413	0.000
Cl	0.102	-1.710	1.838

44) 2-$AlCl_3$,1,3,5-Br_3-BZ



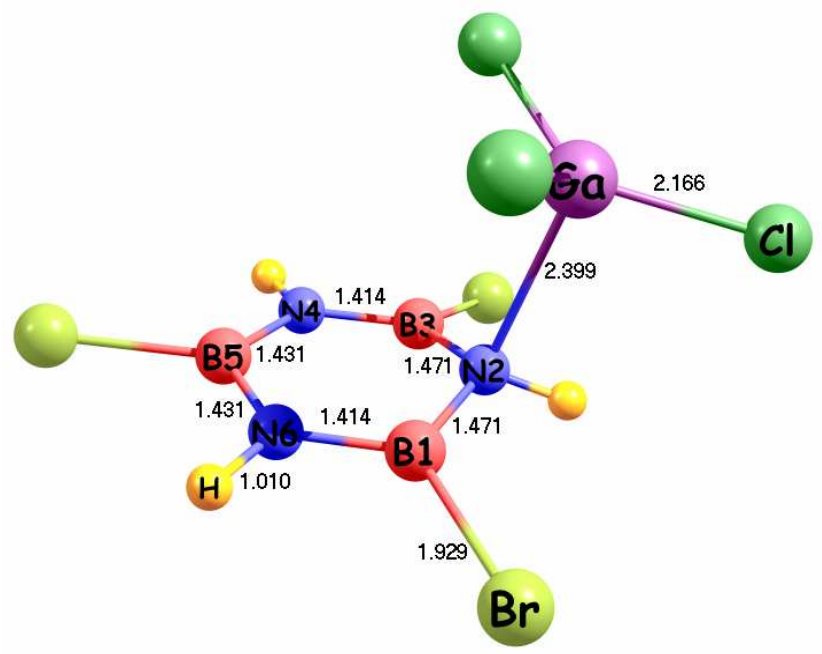
	X	Y	Z
B	3.378	0.000	0.175
N	2.731	1.232	0.520
B	1.472	1.267	1.156
N	0.696	0.000	1.269
B	1.472	-1.267	1.156
N	2.731	-1.232	0.520
F	4.577	0.000	-0.410
H	3.212	2.103	0.343
F	0.973	2.361	1.720
H	0.064	0.000	2.071
F	0.973	-2.361	1.720
H	3.212	-2.103	0.343
Al	-0.874	0.000	-0.214
Br	-0.498	-1.926	-1.402
Br	-2.675	-0.001	1.207
Br	-0.499	1.926	-1.401

45) 2-$AlBr_3$,1,3,5-Br_3-BZ



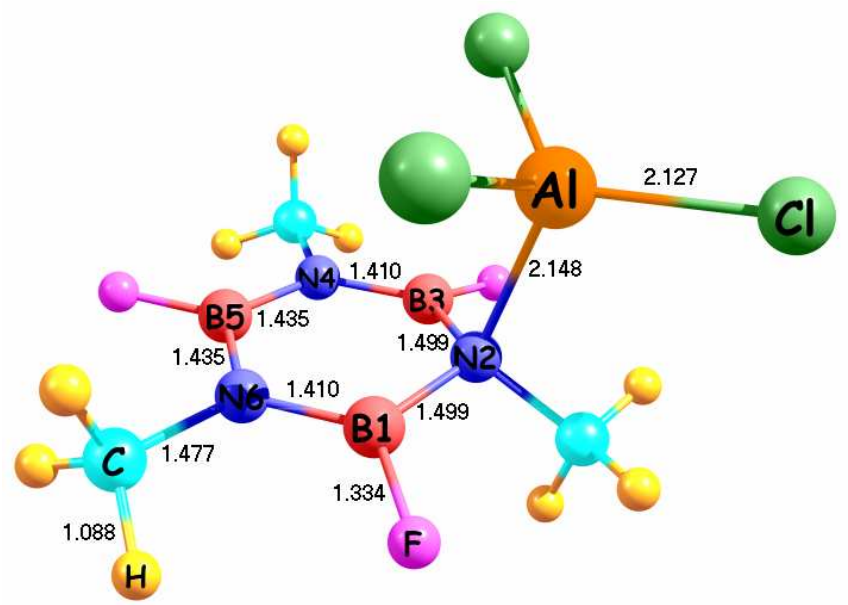
	X	Y	Z
B	1.153	-2.389	0.000
N	0.563	-1.949	1.228
B	-0.538	-1.066	1.262
N	-0.910	-0.375	0.000
B	-0.538	-1.066	-1.262
N	0.563	-1.949	-1.228
Br	2.647	-3.617	0.000
H	0.903	-2.335	2.097
Br	-1.623	-0.826	2.835
H	-1.870	-0.034	0.000
Br	-1.623	-0.826	-2.835
H	0.903	-2.335	-2.097
Al	0.000	1.655	0.000
Br	1.255	1.727	-1.913
Br	-1.964	2.835	0.000
Br	1.255	1.727	1.913

46) 2-$GaCl_3$,1,3,5-Br_3-BZ



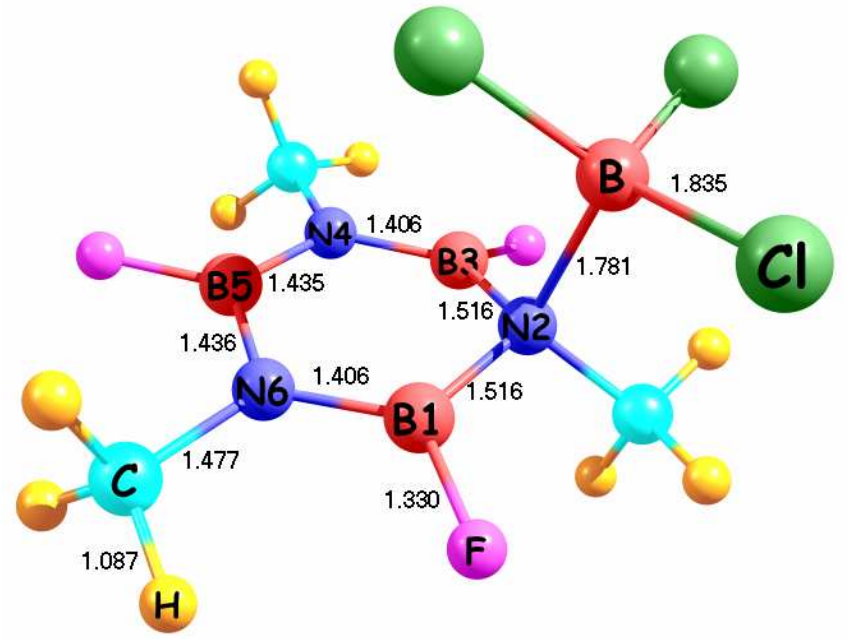
	X	Y	Z
B	-0.614	2.271	0.000
N	-0.723	1.545	-1.228
B	-0.893	0.141	-1.260
N	-0.723	-0.599	0.000
B	-0.893	0.141	1.260
N	-0.723	1.545	1.228
Br	-0.400	4.195	0.000
H	-0.735	2.057	-2.098
Br	-1.408	-0.796	-2.865
H	-1.107	-1.540	0.000
Br	-1.408	-0.796	2.865
H	-0.735	2.057	2.098
Ga	1.528	-1.428	0.000
Cl	2.331	-0.586	1.826
Cl	0.925	-3.509	0.000
Cl	2.331	-0.586	-1.826

47) 2-$AlCl_3$,1,3,5-F_3,2,4,6-$(CH_3)_3$-BZ



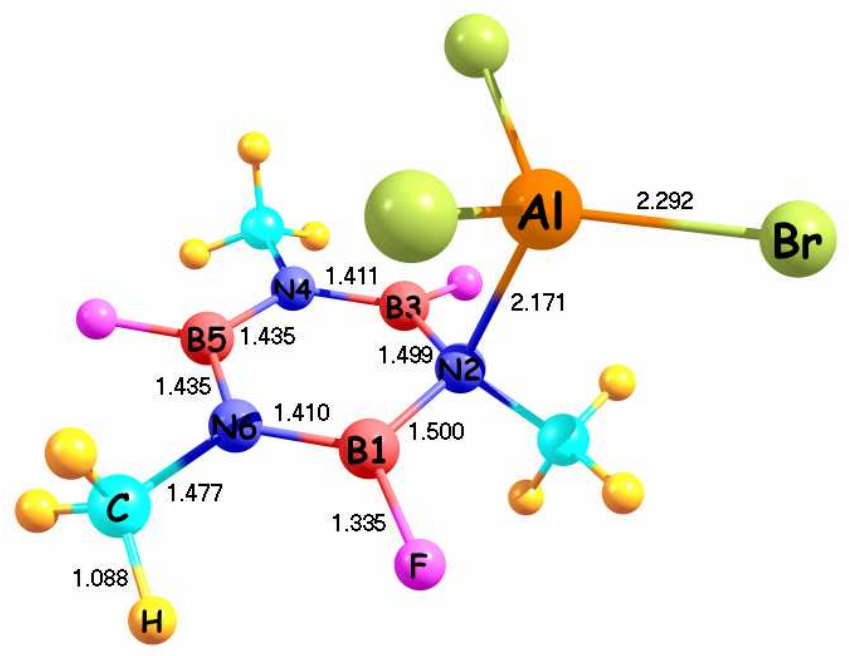
	X	Y	Z
B	2.476	0.000	-0.188
N	1.874	1.248	0.186
B	0.639	1.260	0.865
N	-0.146	0.000	1.072
B	0.639	-1.260	0.865
N	1.874	-1.248	0.186
F	3.640	0.000	-0.852
F	0.157	2.373	1.423
F	0.157	-2.373	1.423
Al	-1.580	0.000	-0.528
Cl	-1.098	-1.791	-1.593
Cl	-3.500	0.000	0.387
Cl	-1.098	1.791	-1.593
C	-0.898	0.000	2.390
H	-1.523	-0.884	2.453
H	-0.185	0.000	3.215
H	-1.523	0.884	2.453
C	2.524	-2.524	-0.179
H	2.283	-3.287	0.558
H	2.176	-2.861	-1.156
H	3.604	-2.395	-0.216
C	2.524	2.524	-0.179
H	3.603	2.395	-0.217
H	2.174	2.862	-1.155
H	2.285	3.287	0.559

48) 2-BCl_3,1,3,5-F_3,2,4,6-$(CH_3)_3$-BZ



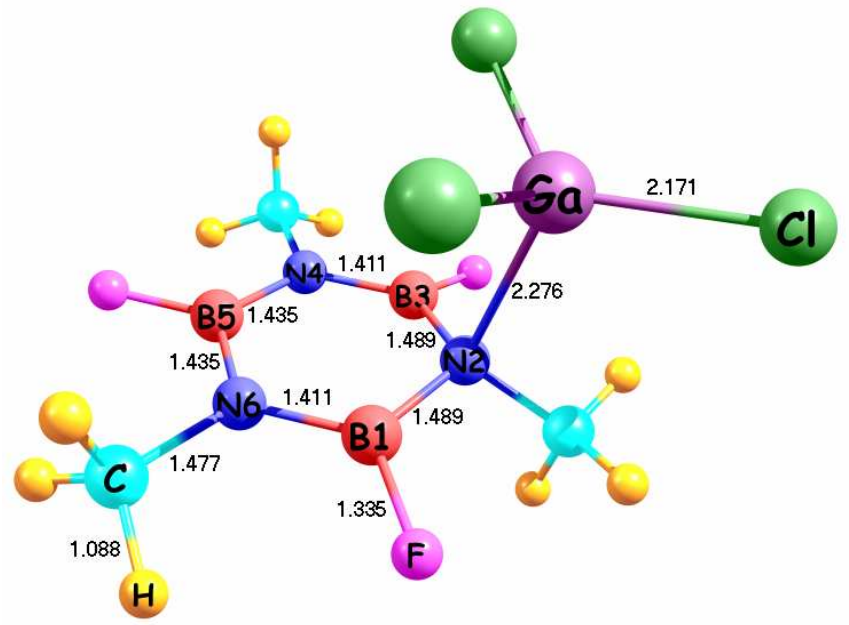
	X	Y	Z
B	2.321	-0.001	-0.183
N	1.696	1.250	0.142
B	0.444	1.258	0.782
N	-0.391	-0.004	0.874
B	0.439	-1.268	0.766
N	1.733	-1.249	0.218
F	3.512	-0.001	-0.792
F	-0.009	2.346	1.399
F	-0.087	-2.388	1.255
B	-1.510	0.001	-0.512
Cl	-0.498	-0.275	-2.036
Cl	-2.712	-1.360	-0.249
Cl	-2.313	1.656	-0.524
C	-1.208	0.005	2.152
H	-1.766	-0.921	2.224
H	-0.541	0.105	3.008
H	-1.892	0.847	2.125
C	2.458	-2.509	-0.043
H	2.022	-3.313	0.545
H	2.394	-2.772	-1.100
H	3.508	-2.402	0.226
C	2.407	2.512	-0.150
H	3.429	2.472	0.225
H	2.437	2.686	-1.226
H	1.889	3.342	0.325

49) 2-$AlBr_3$,1,3,5-F_3,2,4,6-$(CH_3)_3$-BZ



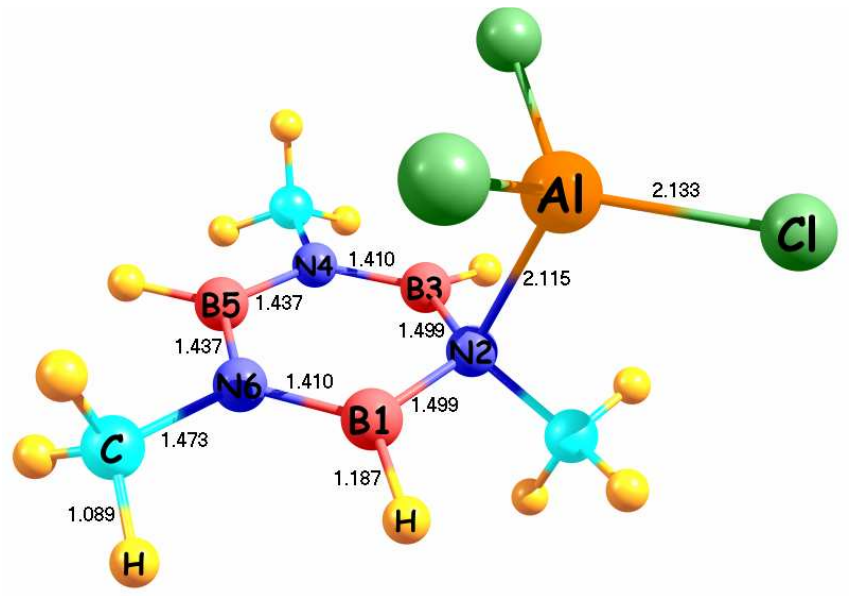
	X	Y	Z
B	3.015	-0.007	0.014
N	2.419	1.243	0.392
B	1.203	1.257	1.108
N	0.418	-0.001	1.328
B	1.196	-1.263	1.104
N	2.425	-1.253	0.412
F	4.164	-0.008	-0.674
F	0.752	2.365	1.700
F	0.720	-2.377	1.665
Al	-1.083	0.003	-0.242
Br	-0.567	-1.859	-1.498
Br	-3.126	-0.111	0.792
Br	-0.699	1.982	-1.356
C	-0.287	0.000	2.672
H	-0.901	-0.889	2.763
H	0.456	0.012	3.470
H	-0.917	0.879	2.754
C	3.072	-2.530	0.046
H	2.852	-3.286	0.797
H	2.703	-2.879	-0.919
H	4.150	-2.396	-0.017
C	3.068	2.516	0.018
H	4.148	2.389	-0.013
H	2.723	2.842	-0.965
H	2.821	3.286	0.745

50) 2-$GaCl_3$,1,3,5-F_3,2,4,6-$(CH_3)_3$-BZ



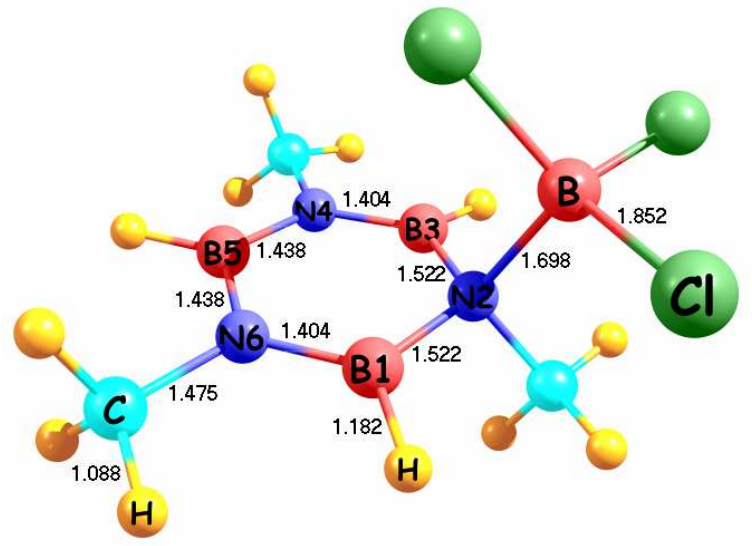
	X	Y	Z
B	-2.635	0.000	-0.222
N	-2.056	-1.248	0.186
B	-0.863	-1.258	0.940
N	-0.108	0.000	1.196
B	-0.863	1.258	0.940
N	-2.056	1.248	0.186
F	-3.756	0.000	-0.956
F	-0.399	-2.377	1.502
F	-0.399	2.376	1.502
Ga	1.453	0.000	-0.461
Cl	0.977	1.836	-1.538
Cl	3.353	0.000	0.588
Cl	0.976	-1.836	-1.539
C	0.642	0.000	2.504
H	1.268	0.883	2.569
H	-0.067	0.000	3.333
H	1.268	-0.884	2.569
C	-2.683	2.522	-0.221
H	-2.458	3.296	0.509
H	-2.302	2.840	-1.193
H	-3.762	2.403	-0.289
C	-2.682	-2.523	-0.221
H	-3.761	-2.401	-0.298
H	-2.295	-2.845	-1.189
H	-2.464	-3.295	0.514

51) 2-$AlCl_3$,2,4,6-$(CH_3)_3$-BZ



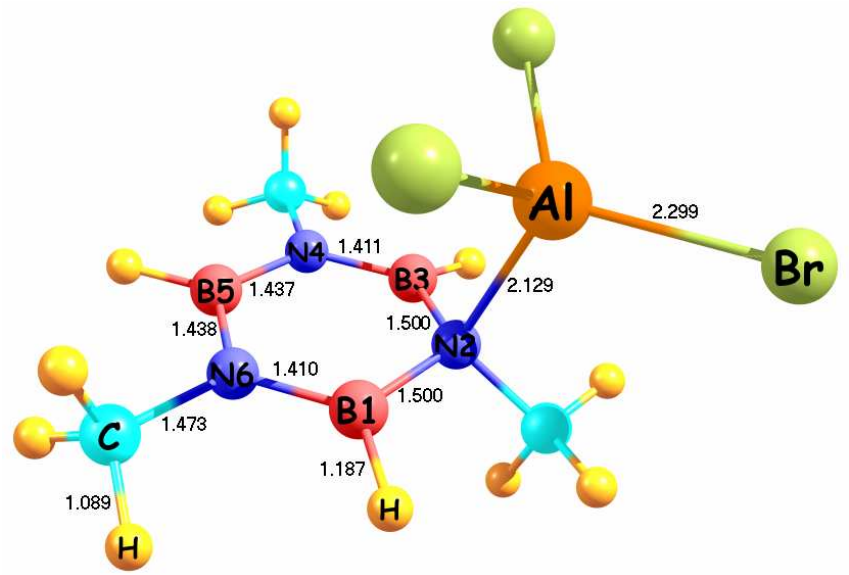
	X	Y	Z
B	2.743	0.000	-0.199
N	2.133	1.243	0.186
B	0.920	1.276	0.904
N	0.178	0.000	1.165
B	0.920	-1.276	0.904
N	2.133	-1.243	0.186
H	3.773	0.000	-0.796
H	0.490	2.277	1.376
H	0.490	-2.277	1.376
Al	-1.338	0.000	-0.309
Cl	-0.972	-1.792	-1.428
Cl	-3.203	-0.001	0.727
Cl	-0.973	1.793	-1.427
C	-0.477	0.000	2.526
H	-1.098	-0.884	2.640
H	0.292	-0.001	3.300
H	-1.097	0.885	2.641
C	2.773	-2.512	-0.205
H	2.516	-3.296	0.505
H	2.433	-2.821	-1.195
H	3.856	-2.398	-0.228
C	2.773	2.512	-0.205
H	3.856	2.398	-0.229
H	2.432	2.822	-1.195
H	2.517	3.296	0.506

52) 2-BCl_3,2,4,6-$(CH_3)_3$-BZ



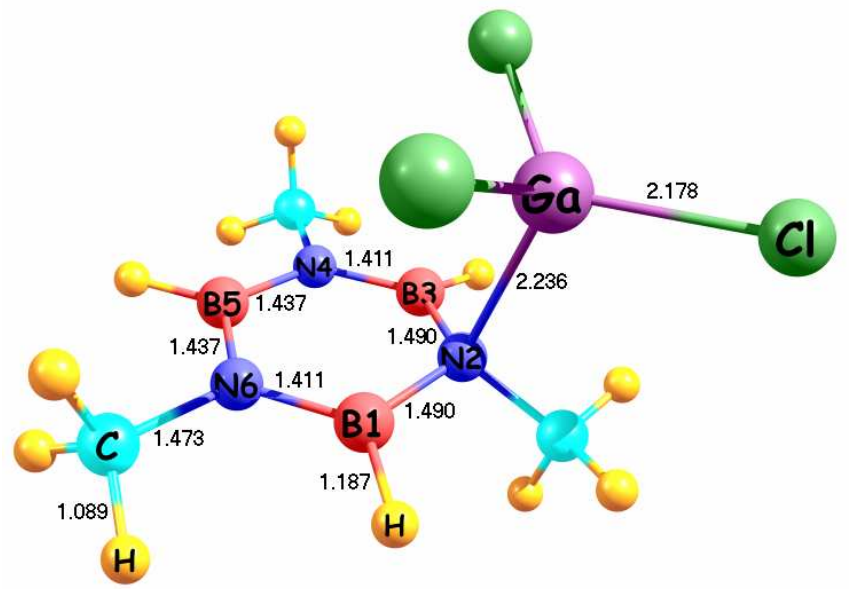
	X	Y	Z
B	-2.659	0.000	-0.188
N	-2.014	-1.245	0.135
B	-0.719	-1.285	0.674
N	0.072	0.000	0.874
B	-0.719	1.285	0.674
N	-2.014	1.245	0.134
H	-3.746	0.000	-0.674
H	-0.229	-2.296	1.042
H	-0.229	2.297	1.042
B	1.345	0.000	-0.249
Cl	0.549	-0.001	-1.931
Cl	2.365	1.524	0.010
Cl	2.365	-1.523	0.012
C	0.640	0.000	2.279
H	1.251	0.888	2.413
H	-0.176	0.001	3.002
H	1.250	-0.888	2.413
C	-2.731	2.503	-0.144
H	-2.204	3.338	0.313
H	-2.790	2.678	-1.219
H	-3.744	2.464	0.257
C	-2.731	-2.503	-0.144
H	-3.744	-2.464	0.257
H	-2.789	-2.679	-1.219
H	-2.204	-3.338	0.314

53) 2-$AlBr_3$,2,4,6-$(CH_3)_3$-BZ



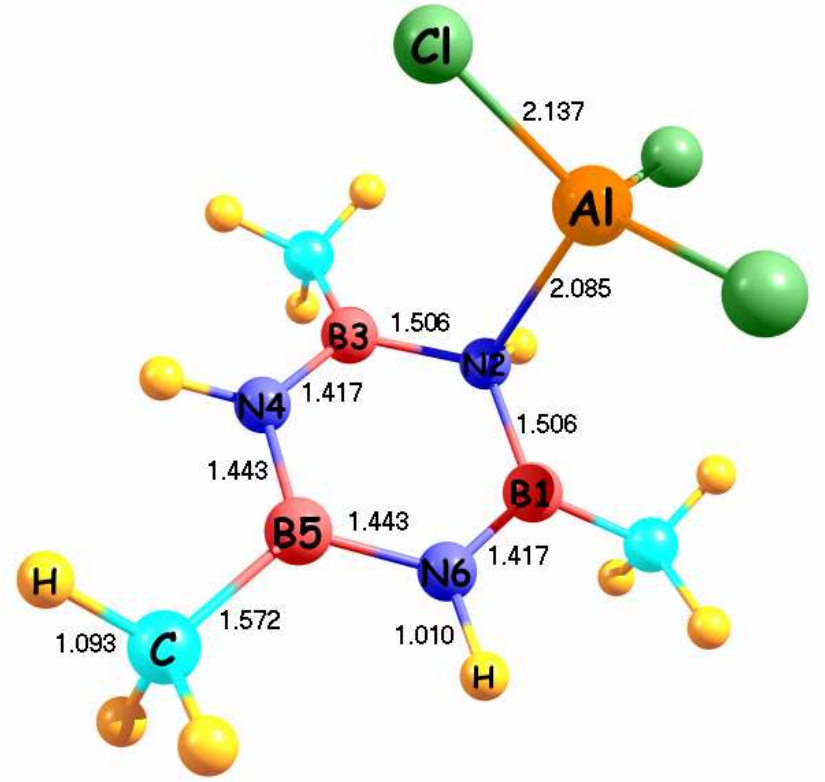
	X	Y	Z
B	3.294	-0.017	0.164
N	2.665	1.229	0.507
B	1.432	1.266	1.193
N	0.672	-0.007	1.419
B	1.418	-1.287	1.182
N	2.672	-1.258	0.538
H	4.349	-0.021	-0.387
H	1.008	2.262	1.677
H	0.952	-2.288	1.617
Al	-0.812	0.003	-0.107
Br	-0.275	-1.781	-1.473
Br	-2.855	-0.243	0.919
Br	-0.550	2.046	-1.152
C	-0.013	-0.003	2.765
H	-0.622	-0.896	2.875
H	0.740	0.018	3.555
H	-0.649	0.873	2.857
C	3.328	-2.528	0.183
H	3.044	-3.308	0.888
H	3.028	-2.845	-0.818
H	4.411	-2.412	0.203
C	3.323	2.496	0.141
H	4.405	2.373	0.137
H	3.003	2.818	-0.851
H	3.059	3.276	0.855

54) 2-$GaCl_3$,2,4,6-$(CH_3)_3$-BZ



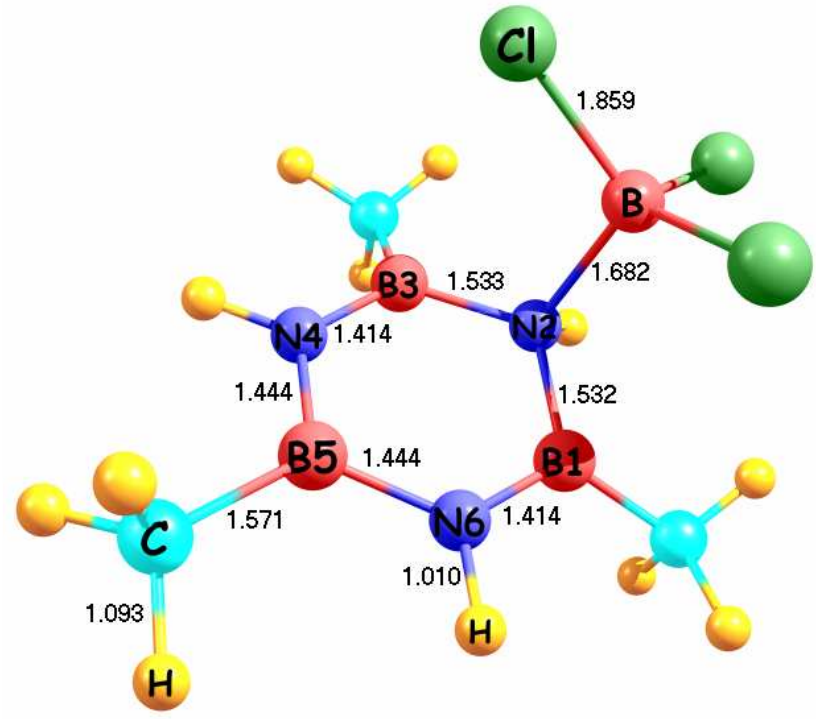
	X	Y	Z
B	-2.895	0.000	-0.226
N	-2.306	-1.243	0.191
B	-1.133	-1.273	0.976
N	-0.419	0.000	1.273
B	-1.133	1.273	0.976
N	-2.306	1.243	0.191
H	-3.889	0.000	-0.881
H	-0.716	-2.277	1.453
H	-0.717	2.277	1.453
Ga	1.194	0.000	-0.276
Cl	0.829	1.838	-1.405
Cl	3.053	-0.004	0.858
Cl	0.825	-1.834	-1.410
C	0.261	0.000	2.612
H	0.884	0.884	2.716
H	-0.491	0.000	3.403
H	0.884	-0.884	2.716
C	-2.922	2.511	-0.237
H	-2.682	3.303	0.471
H	-2.548	2.805	-1.220
H	-4.005	2.406	-0.294
C	-2.923	-2.511	-0.237
H	-4.005	-2.405	-0.296
H	-2.546	-2.806	-1.219
H	-2.684	-3.302	0.472

55) 2-$AlCl_3$,1,3,5-$(CH_3)_3$-BZ



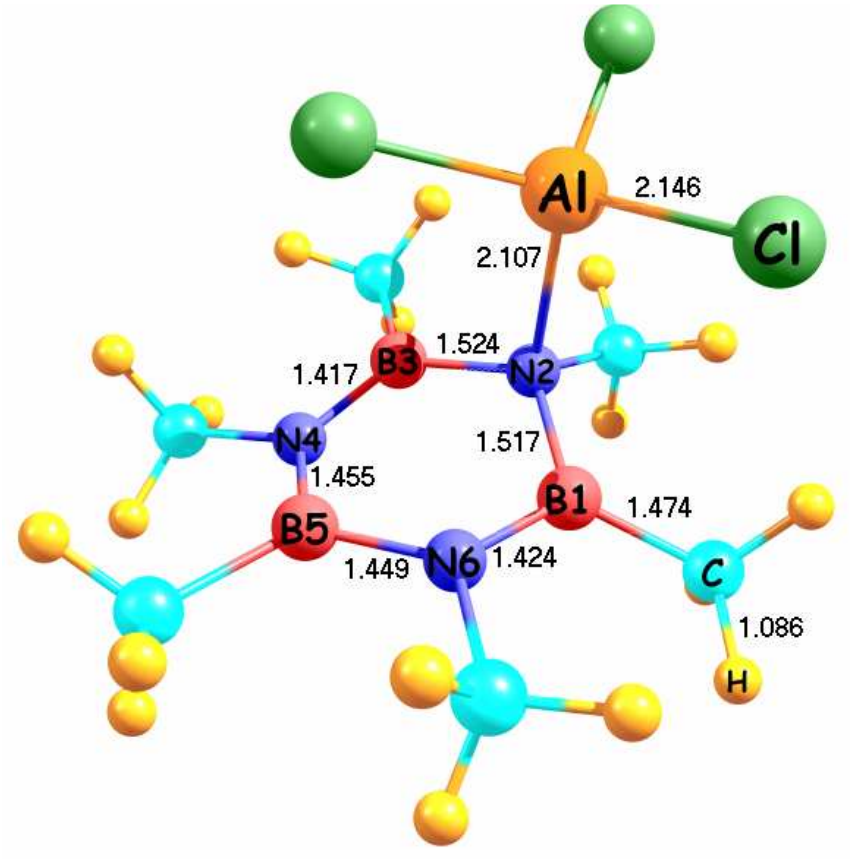
	X	Y	Z
B	-2.821	0.000	-0.206
N	-2.170	-1.221	0.205
B	-0.946	-1.298	0.914
N	-0.191	0.000	1.031
B	-0.946	1.298	0.914
N	-2.170	1.221	0.205
Al	1.336	0.000	-0.389
Cl	1.085	1.788	-1.532
Cl	3.024	0.000	0.935
Cl	1.085	-1.788	-1.532
C	-4.196	0.000	-0.969
H	-4.328	0.882	-1.599
H	-4.329	-0.883	-1.598
H	-5.024	0.001	-0.250
H	-2.644	-2.091	0.007
C	-2.645	2.090	0.007
H	-0.412	-2.588	1.626
H	0.678	-2.646	1.662
H	-0.764	-2.597	2.666
H	-0.780	-3.503	1.159
C	-0.412	2.588	1.626
H	-0.780	3.503	1.159
H	-0.765	2.597	2.665
H	0.677	2.646	1.662
H	0.435	0.000	1.836

56) 2-BCl_3,1,3,5-$(CH_3)_3$-BZ



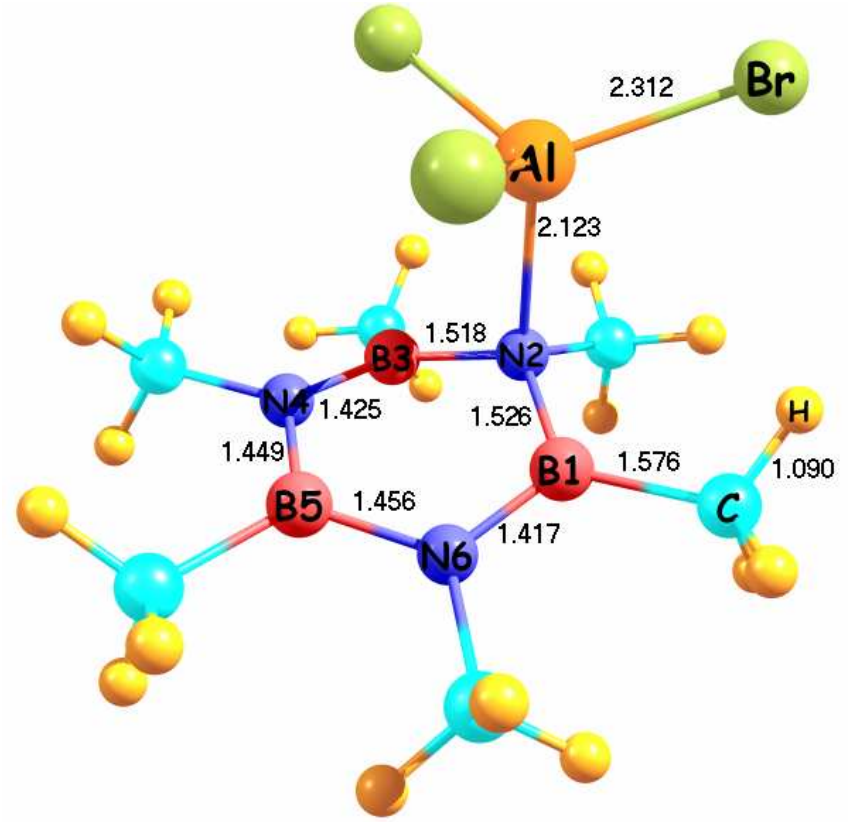
	X	Y	Z
B	-2.657	-0.004	-0.167
N	-1.986	-1.224	0.213
B	-0.709	-1.309	0.812
N	0.081	0.004	0.863
B	-0.715	1.312	0.809
N	-1.986	1.221	0.196
B	1.265	0.002	-0.332
Cl	1.097	1.544	-1.356
Cl	2.881	-0.041	0.583
Cl	1.042	-1.501	-1.404
C	-4.048	-0.009	-0.897
H	-4.648	0.879	-0.684
H	-3.886	-0.024	-1.981
H	-4.653	-0.888	-0.661
H	-2.486	-2.091	0.074
C	-2.488	2.086	0.050
H	-0.154	-2.568	1.557
H	0.935	-2.634	1.542
H	-0.460	-2.525	2.611
H	-0.555	-3.500	1.152
C	-0.179	2.572	1.566
H	-0.568	3.503	1.150
H	-0.514	2.529	2.611
H	0.910	2.638	1.580
H	0.667	0.006	1.696

57) 2-$AlCl_3$,1,2,3,4,5,6-$(CH_3)_6$-BZ



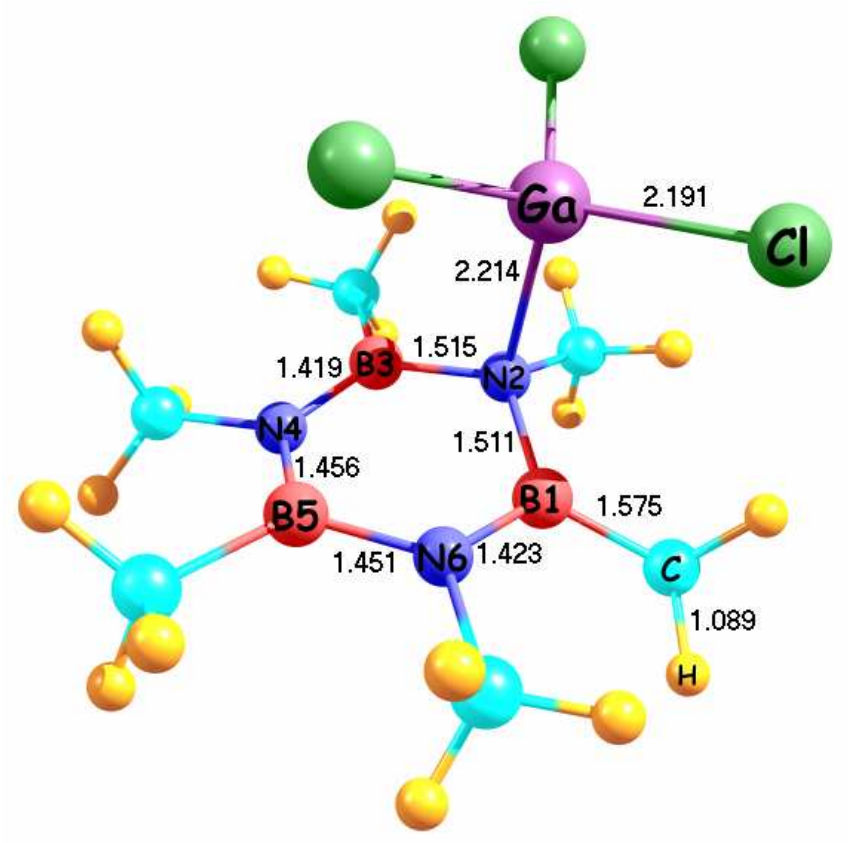
	X	Y	Z
B	-2.373	0.101	-0.195
N	-1.938	-1.175	0.351
B	-0.637	-1.360	0.883
N	0.210	-0.115	1.117
B	-0.534	1.208	1.100
N	-1.636	1.285	0.200
Al	1.445	0.009	-0.586
Cl	1.898	2.097	-0.790
Cl	3.178	-1.171	-0.140
Cl	0.322	-0.784	-2.231
C	-3.654	0.197	-1.112
H	-3.636	1.055	-1.783
H	-3.796	-0.694	-1.724
H	-4.558	0.303	-0.499
C	-2.799	-2.352	0.143
H	-3.847	-2.064	0.171
H	-2.600	-2.831	-0.820
H	-2.640	-3.086	0.930
C	-2.133	2.601	-0.239
H	-1.458	3.390	0.079
H	-2.181	2.638	-1.327
H	-3.128	2.812	0.159
C	-0.050	-2.776	1.245
H	1.032	-2.838	1.117
H	-0.256	-3.028	2.293
H	-0.489	-3.569	0.640
C	-0.119	2.357	2.093
H	-0.743	3.245	2.004
H	-0.219	2.004	3.125
H	0.920	2.671	1.973
C	1.128	-0.259	2.304
H	0.547	-0.270	3.226
H	1.702	-1.175	2.232
H	1.825	0.574	2.340

58) 2-$AlBr_3$,1,2,3,4,5,6-$(CH_3)_6$-BZ



	X	Y	Z
B	2.887	0.070	-0.022
N	2.169	1.269	0.358
B	1.111	1.228	1.312
N	0.356	-0.086	1.404
B	1.187	-1.344	1.173
N	2.468	-1.184	0.588
Al	-0.979	-0.006	-0.245
Br	0.096	-0.937	-2.065
Br	-2.846	-1.228	0.360
Br	-1.475	2.233	-0.546
C	4.135	0.125	-0.986
H	4.242	-0.783	-1.580
H	4.107	0.967	-1.677
H	5.062	0.229	-0.407
C	2.655	2.569	-0.139
H	2.686	2.565	-1.228
H	1.981	3.366	0.160
H	3.656	2.798	0.235
C	3.312	-2.374	0.385
H	3.185	-3.077	1.205
H	3.067	-2.887	-0.550
H	4.362	-2.092	0.355
C	0.773	2.403	2.304
H	-0.275	2.705	2.280
H	0.979	2.078	3.331
H	1.374	3.294	2.133
C	0.613	-2.745	1.607
H	1.011	-3.556	0.996
H	0.884	-2.971	2.646
H	-0.474	-2.804	1.548
C	-0.490	-0.186	2.648
H	0.147	-0.164	3.532
H	-1.185	0.648	2.697
H	-1.064	-1.104	2.646

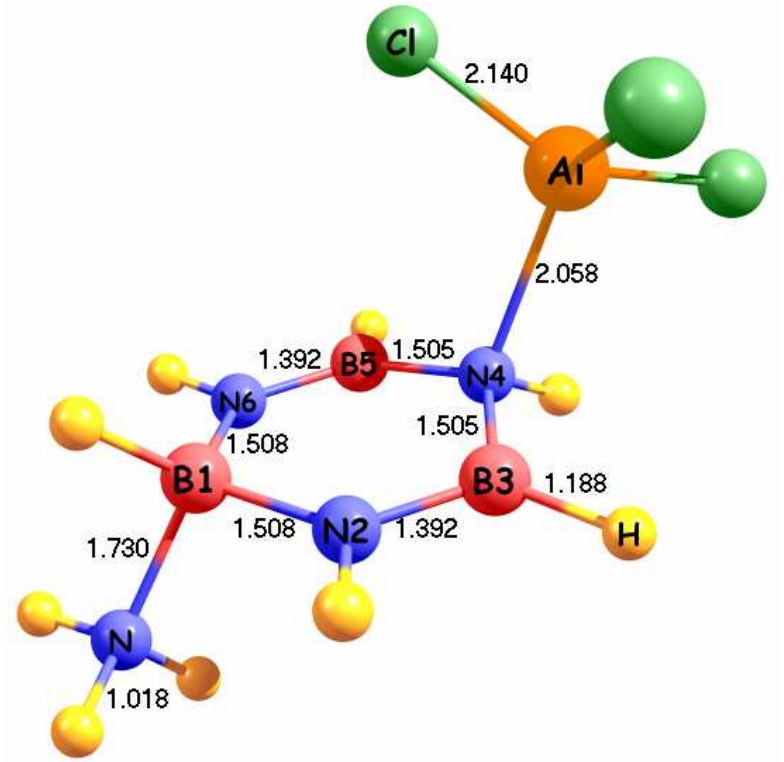
59) 2-$GaCl_3$,1,2,3,4,5,6-$(CH_3)_6$-BZ



	X	Y	Z
B	-2.464	0.097	-0.246
N	-2.067	-1.185	0.319
B	-0.843	-1.359	1.016
N	-0.010	-0.117	1.261
B	-0.746	1.202	1.212
N	-1.800	1.284	0.259
Ga	1.293	0.006	-0.524
Cl	2.103	2.039	-0.427
Cl	2.812	-1.536	-0.188
Cl	0.080	-0.379	-2.304
C	-3.645	0.196	-1.287
H	-3.585	1.084	-1.915
H	-3.687	-0.670	-1.949
H	-4.614	0.244	-0.773
C	-2.903	-2.362	0.020
H	-3.942	-2.066	-0.107
H	-2.576	-2.864	-0.895
H	-2.866	-3.077	0.838
C	-2.293	2.600	-0.185
H	-1.713	3.398	0.267
H	-2.189	2.694	-1.266
H	-3.344	2.745	0.076
C	-0.320	-2.748	1.543
H	0.744	-2.891	1.343
H	-0.439	-2.816	2.632
H	-0.843	-3.599	1.112
C	-0.357	2.357	2.210
H	-1.063	3.187	2.197
H	-0.327	1.982	3.237
H	0.635	2.767	2.003
C	0.955	-0.240	2.401
H	0.418	-0.291	3.349
H	1.561	-1.132	2.291
H	1.618	0.622	2.422

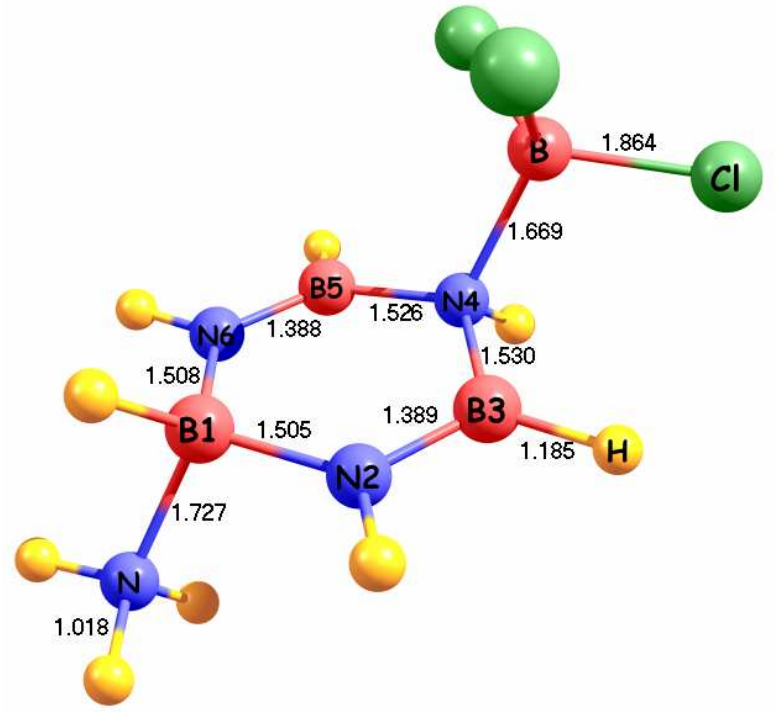
Ternary complexes of BZ

60) 1-NH_3,4-$AlCl_3$-BZ



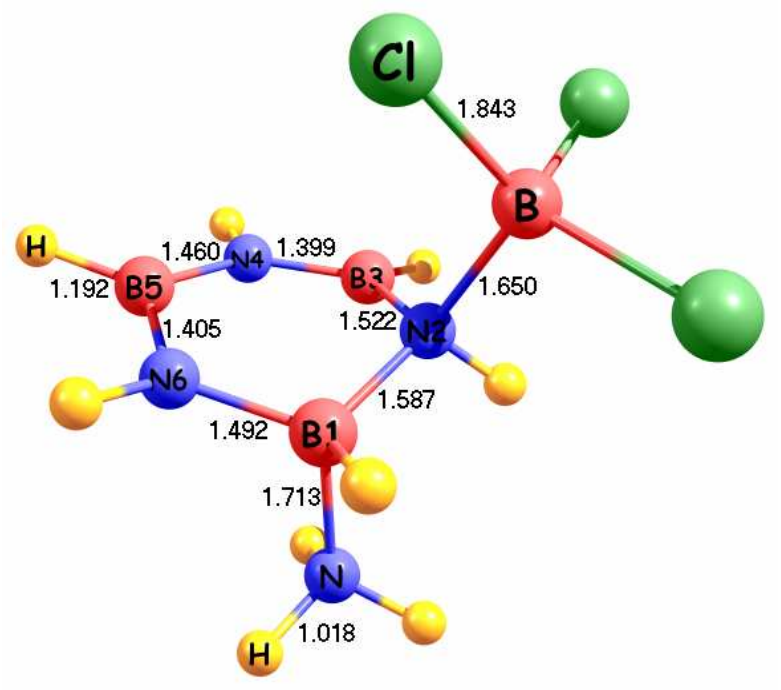
	X	Y	Z
B	-1.060	-1.285	0.800
N	-0.311	0.000	1.033
B	-1.060	1.285	0.800
N	-2.235	1.239	0.055
B	-2.904	0.000	-0.484
N	-2.235	-1.240	0.055
H	-0.625	-2.286	1.271
H	0.170	0.000	1.932
H	-0.625	2.286	1.271
H	-2.604	2.135	-0.232
H	-3.177	0.000	-1.661
H	-2.604	-2.135	-0.232
N	-4.481	0.000	0.227
H	-4.399	0.000	1.243
H	-5.015	0.821	-0.051
H	-5.015	-0.821	-0.051
Al	1.414	0.000	-0.089
Cl	1.373	1.789	-1.262
Cl	2.868	0.000	1.495
Cl	1.374	-1.789	-1.262

61) 1-NH_3,4-BCl_3-BZ



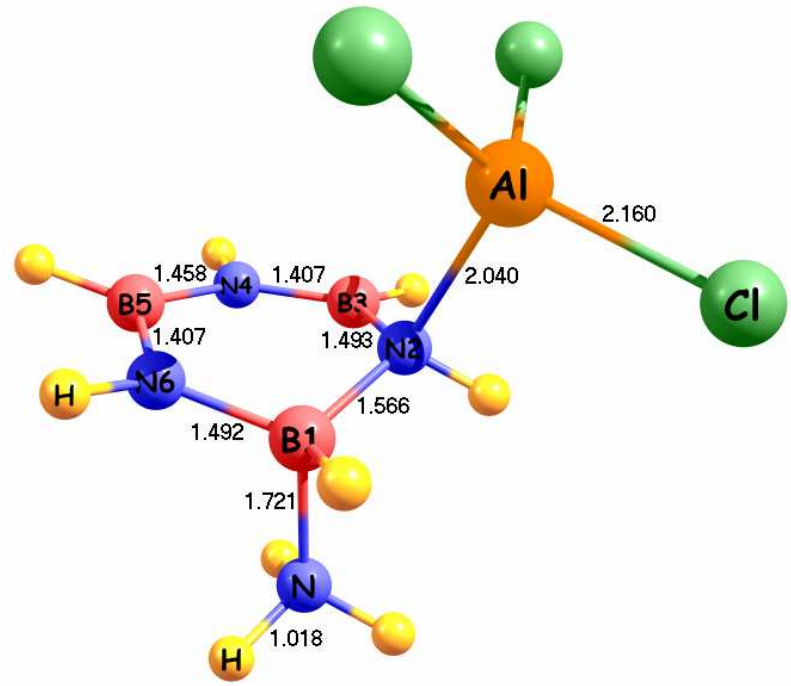
	X	Y	Z
B	-0.845	1.311	-0.673
N	-0.035	0.030	-0.848
B	-0.784	-1.275	-0.573
N	-2.037	-1.222	0.025
B	-2.751	0.012	0.508
N	-2.051	1.252	0.011
H	-0.440	2.306	-1.173
H	0.345	0.006	-1.795
H	-0.276	-2.288	-0.919
H	-2.407	-2.117	0.314
H	-3.111	0.013	1.660
H	-2.472	2.146	0.224
N	-4.266	0.002	-0.322
H	-4.108	0.000	-1.329
H	-4.810	-0.825	-0.083
H	-4.830	0.816	-0.088
B	1.393	0.009	0.014
Cl	1.020	-0.695	1.690
Cl	2.549	-1.081	-0.962
Cl	2.064	1.731	0.139

62) 1-NH_3,2-BCl_3-BZ



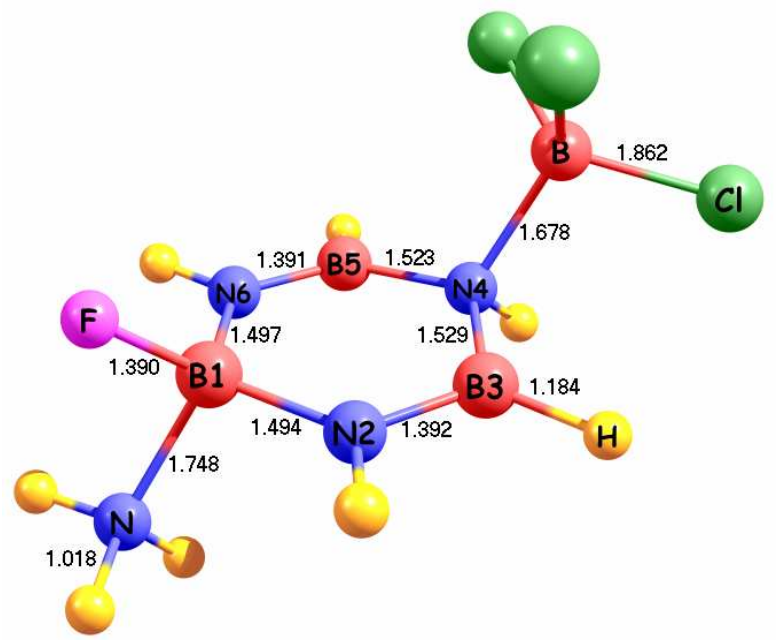
	X	Y	Z
B	-0.554	1.309	-0.836
N	0.260	0.026	-0.944
B	-0.493	-1.282	-0.700
N	-1.799	-1.225	-0.222
B	-2.553	0.011	0.148
N	-1.816	1.250	-0.256
H	-0.110	2.302	-1.304
H	0.713	-0.007	-1.858
H	0.050	-2.296	-0.982
H	-2.204	-2.110	0.051
F	-3.139	0.022	1.408
H	-2.269	2.138	-0.085
N	-3.999	-0.010	-0.834
H	-3.767	-0.022	-1.824
H	-4.559	-0.834	-0.624
H	-4.580	0.805	-0.647
B	1.628	0.010	0.029
Cl	1.148	-0.784	1.634
Cl	2.880	-0.999	-0.909
Cl	2.226	1.742	0.286

63) 1-NH_3,2-$AlCl_3$-BZ



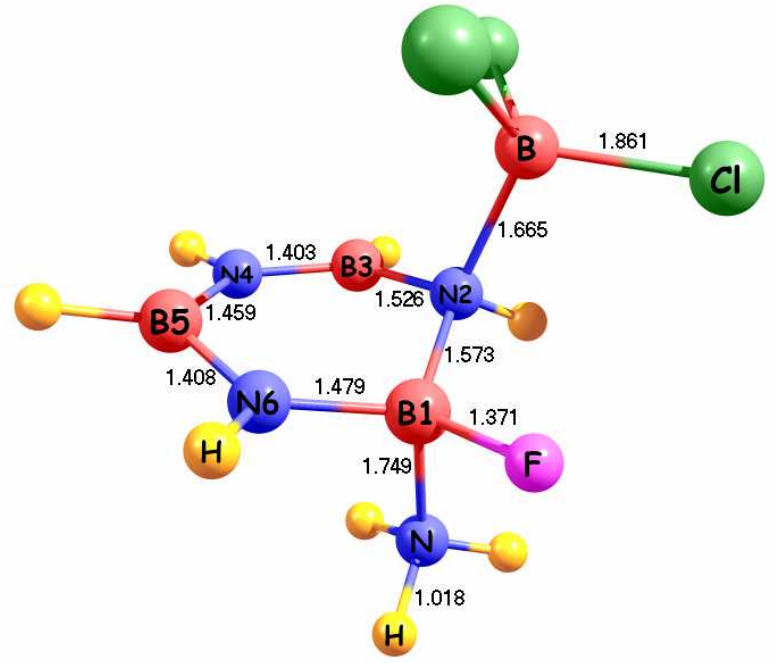
	X	Y	Z
B	2.666	-1.276	0.629
N	2.149	-1.688	-0.670
B	1.172	-0.970	-1.383
N	0.652	0.286	-0.764
B	1.598	1.021	0.243
N	2.400	0.045	1.037
H	3.300	-2.036	1.292
H	2.428	-2.588	-1.031
H	0.786	-1.301	-2.456
H	0.295	0.915	-1.482
H	1.066	1.904	0.854
H	2.639	0.301	1.982
N	2.719	1.889	-0.733
H	3.267	1.272	-1.331
H	2.283	2.605	-1.313
H	3.369	2.357	-0.105
Al	-1.183	0.018	0.087
Cl	-1.025	-0.149	2.211
Cl	-2.117	1.834	-0.614
Cl	-1.956	-1.759	-0.837

64) 1-NH_3,4-BCl_3,1-F-BZ



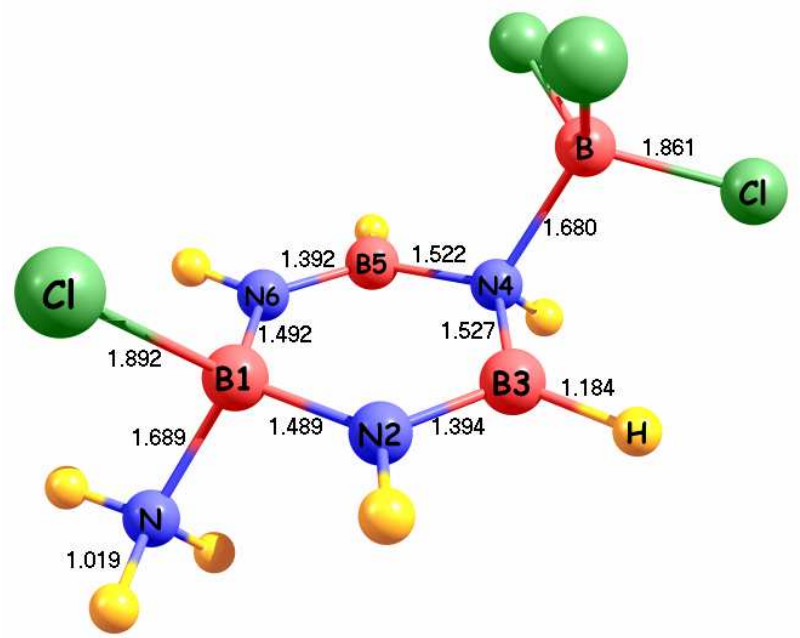
	X	Y	Z
B	-0.554	1.309	-0.836
N	0.260	0.026	-0.944
B	-0.493	-1.282	-0.700
N	-1.799	-1.225	-0.222
B	-2.553	0.011	0.148
N	-1.816	1.250	-0.256
H	-0.110	2.302	-1.304
H	0.713	-0.007	-1.858
H	0.050	-2.296	-0.982
H	-2.204	-2.110	0.051
F	-3.139	0.022	1.408
H	-2.269	2.138	-0.085
N	-3.999	-0.010	-0.834
H	-3.767	-0.022	-1.824
H	-4.559	-0.834	-0.624
H	-4.580	0.805	-0.647
B	1.628	0.010	0.029
Cl	1.148	-0.784	1.634
Cl	2.880	-0.999	-0.909
Cl	2.226	1.742	0.286

65) 1-NH_3,2-BCl_3,1-F-BZ



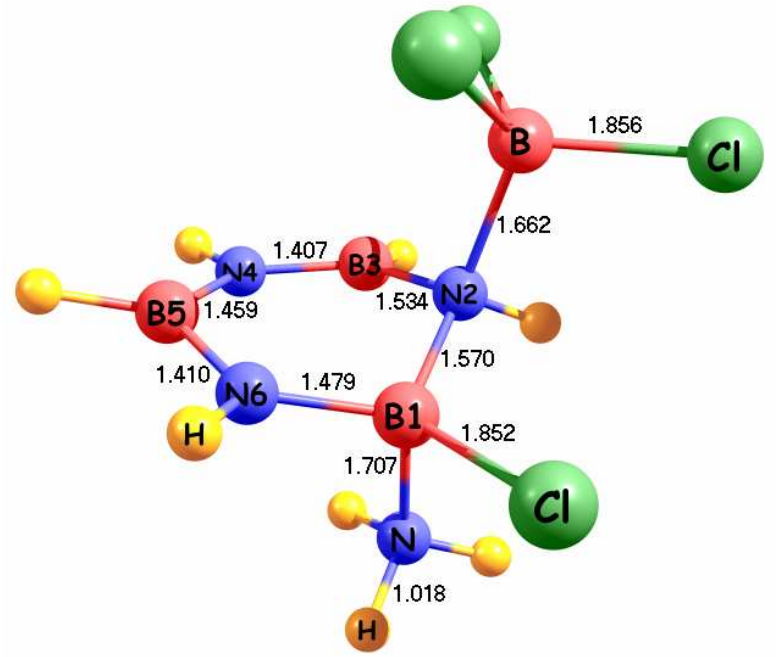
	X	Y	Z
B	-2.208	1.525	0.811
N	-1.543	2.086	-0.361
B	-0.643	1.380	-1.173
N	-0.283	-0.038	-0.738
B	-1.451	-0.772	0.019
N	-2.189	0.124	0.935
H	-2.777	2.234	1.579
H	-1.706	3.058	-0.580
H	-0.269	1.781	-2.223
H	-0.019	-0.569	-1.566
F	-1.144	-2.019	0.499
H	-2.536	-0.293	1.787
N	-2.568	-1.198	-1.257
H	-2.944	-0.392	-1.753
H	-2.176	-1.852	-1.934
H	-3.348	-1.665	-0.798
B	1.193	-0.040	0.034
Cl	1.004	0.135	1.854
Cl	2.005	-1.640	-0.457
Cl	2.149	1.421	-0.662

66) 1-NH_3,4-BCl_3,1-Cl-BZ



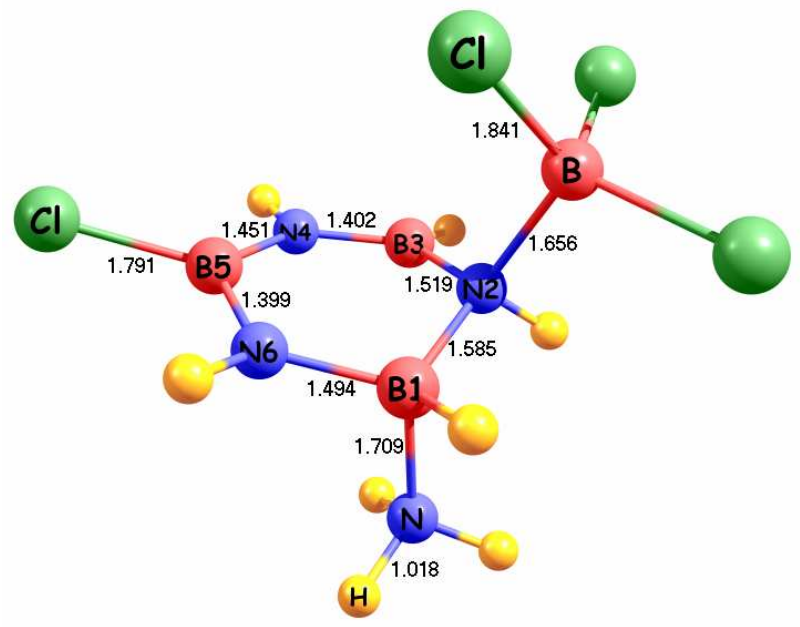
	X	Y	Z
B	0.224	-0.252	-1.642
N	-0.601	0.690	-0.777
B	0.172	1.537	0.231
N	1.529	1.282	0.426
B	2.322	0.197	-0.216
N	1.552	-0.486	-1.296
H	-0.266	-0.707	-2.618
H	-1.152	1.300	-1.383
H	-0.398	2.427	0.765
H	1.955	1.776	1.198
Cl	3.215	-0.960	0.985
H	2.020	-1.219	-1.812
N	3.646	0.937	-0.960
H	3.334	1.612	-1.657
H	4.219	1.419	-0.270
H	4.243	0.246	-1.413
B	-1.855	-0.062	0.049
Cl	-1.200	-0.514	1.723
Cl	-3.209	1.212	0.142
Cl	-2.404	-1.556	-0.890

67) 1-NH_3,2-BCl_3,1-Cl-BZ



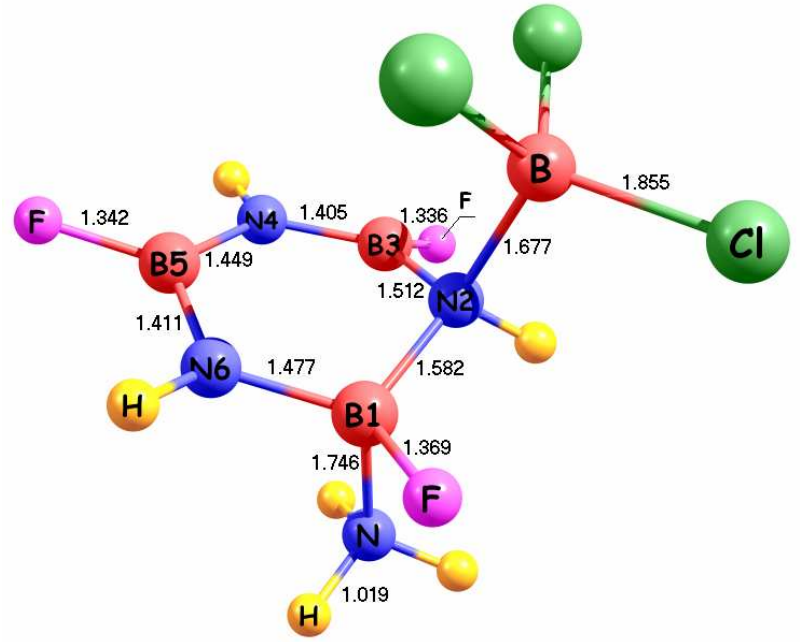
	X	Y	Z
B	-1.582	2.052	0.988
N	-0.812	2.540	-0.151
B	-0.109	1.714	-1.047
N	-0.152	0.208	-0.757
B	-1.524	-0.220	-0.124
N	-1.951	0.692	0.958
H	-1.922	2.793	1.855
H	-0.707	3.538	-0.261
H	0.320	2.094	-2.084
H	-0.005	-0.298	-1.629
Cl	-1.712	-2.028	0.227
H	-2.391	0.284	1.769
N	-2.643	-0.010	-1.395
H	-2.707	0.964	-1.694
H	-2.461	-0.600	-2.205
H	-3.551	-0.281	-1.021
B	1.264	-0.191	0.019
Cl	1.061	-0.343	1.835
Cl	1.855	-1.759	-0.777
Cl	2.449	1.232	-0.373

68) 1-NH_3,2-BCl_3,5-Cl-BZ



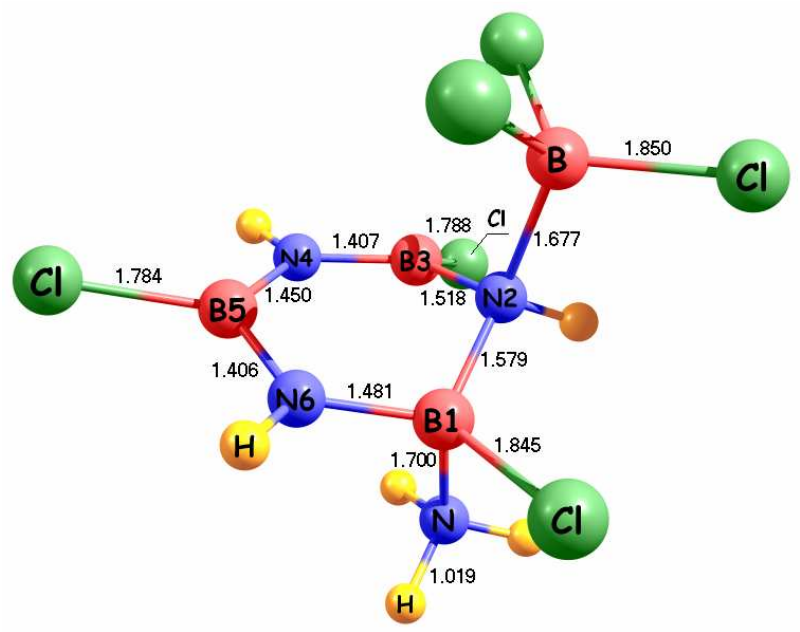
	X	Y	Z
B	-2.285	-0.111	0.092
N	-1.640	-0.527	1.323
B	-0.331	-0.164	1.670
N	0.474	0.635	0.659
B	-0.382	1.533	-0.328
N	-1.702	0.916	-0.658
Cl	-3.836	-0.875	-0.377
H	-2.151	-1.129	1.952
H	0.121	-0.379	2.742
H	1.124	1.220	1.183
H	0.243	1.954	-1.252
H	-2.070	1.086	-1.582
N	-0.718	2.952	0.563
H	-1.240	2.780	1.422
H	0.118	3.489	0.790
H	-1.305	3.537	-0.029
B	1.595	-0.296	-0.126
Cl	0.816	-1.171	-1.546
Cl	2.932	0.898	-0.663
Cl	2.281	-1.510	1.116

69) 1-NH_3,2-BCl_3,1,3,5-F_3-BZ



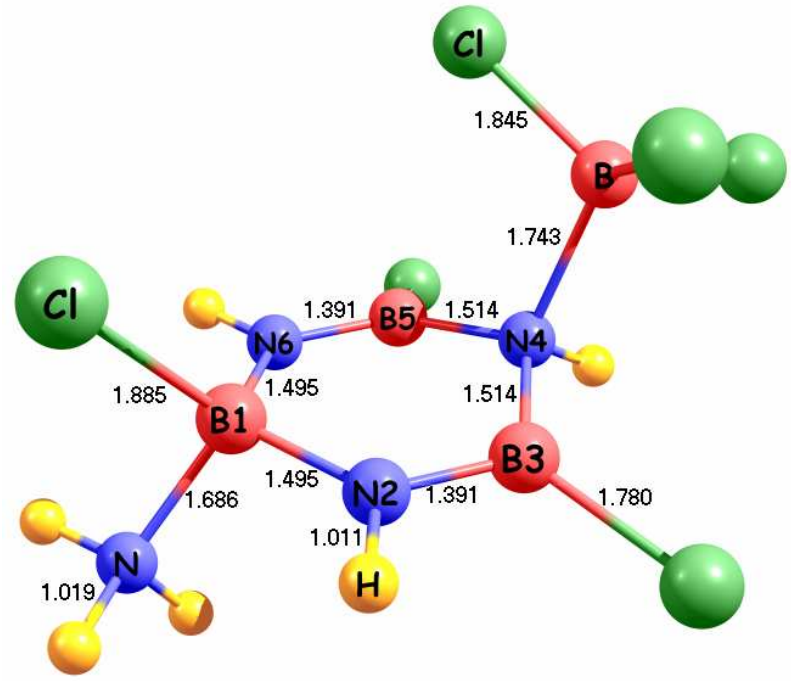
	X	Y	Z
B	2.325	-0.586	0.656
N	1.705	-1.476	-0.304
B	0.611	-1.074	-1.089
N	-0.085	0.221	-0.738
B	0.920	1.335	-0.237
N	1.982	0.783	0.629
F	3.259	-1.071	1.488
H	2.092	-2.400	-0.437
F	0.306	-1.656	-2.252
H	-0.591	0.547	-1.562
F	0.327	2.496	0.179
H	2.292	1.366	1.393
N	1.691	1.893	-1.701
H	2.214	1.176	-2.201
H	1.042	2.338	-2.348
H	2.359	2.603	-1.405
B	-1.387	-0.090	0.272
Cl	-0.940	0.114	2.041
Cl	-2.715	1.083	-0.280
Cl	-1.866	-1.869	-0.077

70) 1-NH_3,2-BCl_3,1,3,5-Cl_3-BZ



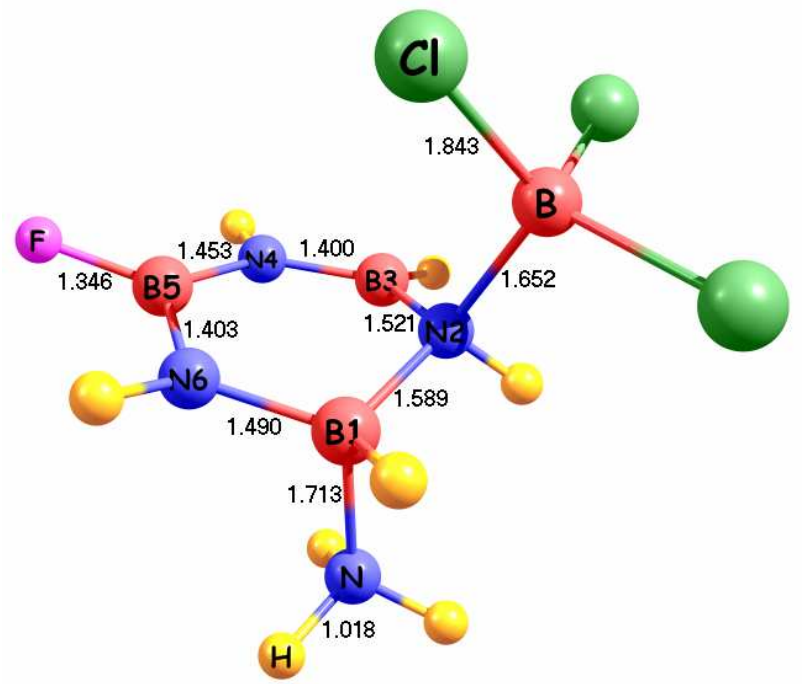
	X	Y	Z
B	2.214	0.003	-0.352
N	1.622	1.256	0.072
B	0.348	1.327	0.664
N	-0.503	0.070	0.635
B	0.390	-1.202	0.913
N	1.628	-1.193	0.100
Cl	3.712	0.023	-1.321
H	2.156	2.107	-0.038
Cl	-0.077	2.627	1.815
H	-1.229	0.141	1.346
Cl	-0.523	-2.805	0.957
H	1.944	-2.069	-0.287
N	0.860	-1.031	2.538
H	1.396	-0.181	2.717
H	0.074	-1.066	3.187
H	1.460	-1.827	2.748
B	-1.457	0.116	-0.744
Cl	-0.788	-0.907	-2.105
Cl	-3.143	-0.409	-0.195
Cl	-1.447	1.938	-1.237

71) 1-NH_3,4-BCl_3,1,3,5-Cl_3-BZ



	X	Y	Z
B	0.233	-1.262	-0.813
N	-0.590	0.008	-0.758
B	0.238	1.275	-0.798
N	1.558	1.236	-0.362
B	2.319	-0.002	-0.014
N	1.556	-1.232	-0.385
Cl	-0.483	-2.688	-1.603
H	-1.282	0.014	-1.506
Cl	-0.465	2.708	-1.586
H	2.008	2.130	-0.217
Cl	3.099	-0.020	1.703
H	2.002	-2.129	-0.252
N	3.699	0.006	-0.981
H	3.445	0.016	-1.969
H	4.277	0.821	-0.782
H	4.275	-0.815	-0.797
B	-1.644	-0.001	0.631
Cl	-1.312	1.530	1.605
Cl	-3.339	-0.030	-0.097
Cl	-1.266	-1.512	1.619

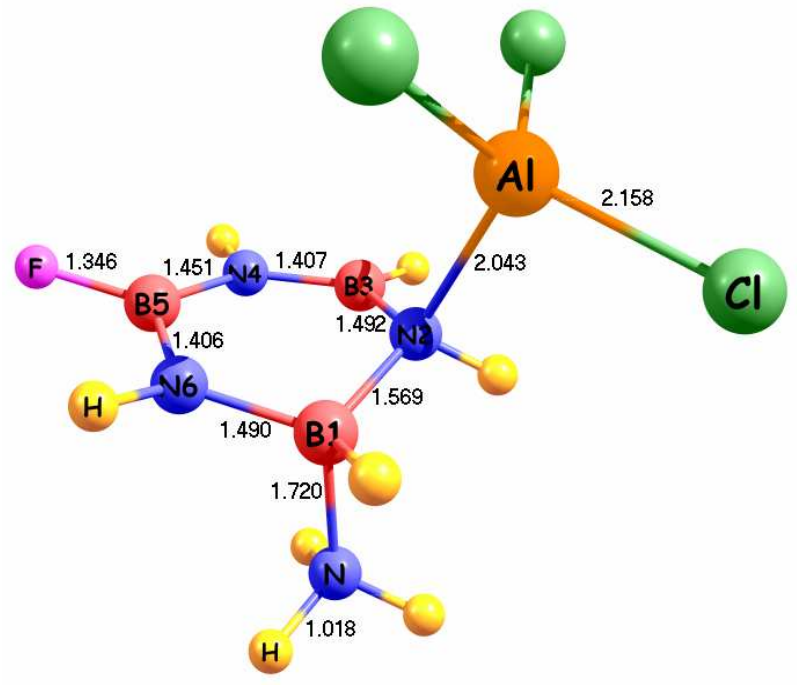
72) 1-NH_3,2-BCl_3, 5-F-BZ



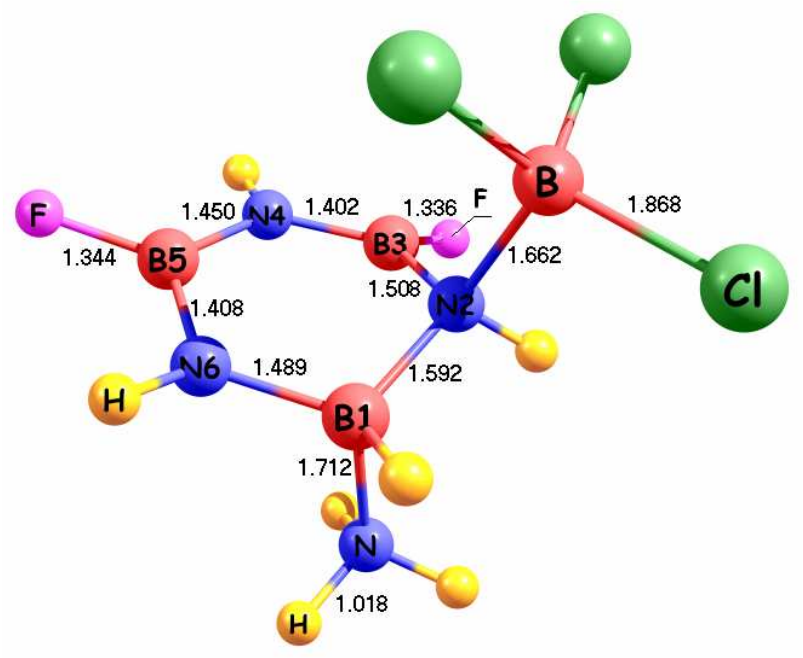
	X	Y	Z
B	2.512	-0.573	0.126
N	1.873	-1.004	-1.105
B	0.664	-0.474	-1.571
N	-0.057	0.525	-0.679
B	0.876	1.375	0.287
N	2.071	0.609	0.741
F	3.545	-1.292	0.603
H	2.318	-1.734	-1.643
H	0.240	-0.706	-2.652
H	-0.584	1.151	-1.288
H	0.274	1.961	1.133
H	2.409	0.795	1.673
N	1.452	2.653	-0.698
H	1.977	2.335	-1.512
H	0.713	3.283	-1.008
H	2.093	3.195	-0.122
B	-1.341	-0.157	0.106
Cl	-0.774	-1.025	1.629
Cl	-2.504	1.260	0.478
Cl	-2.150	-1.352	-1.082

73) 1-NH_3,2-$AlCl_3$, 5-F-BZ

	X	Y	Z
B	2.667	-0.639	0.109
N	2.099	-0.948	-1.190
B	0.927	-0.338	-1.674
N	0.243	0.643	-0.781
B	1.120	1.378	0.293
N	2.204	0.492	0.802
F	3.644	-1.429	0.594
H	2.525	-1.684	-1.736
H	0.500	-0.546	-2.761
H	-0.308	1.298	-1.334
H	0.483	1.969	1.118
H	2.487	0.598	1.765
N	1.885	2.668	-0.549
H	2.466	2.341	-1.321
H	1.229	3.361	-0.906
H	2.499	3.139	0.112
Al	-1.397	-0.163	0.131
Cl	-0.917	-0.777	2.119
Cl	-2.709	1.544	-0.016
Cl	-1.968	-1.795	-1.139

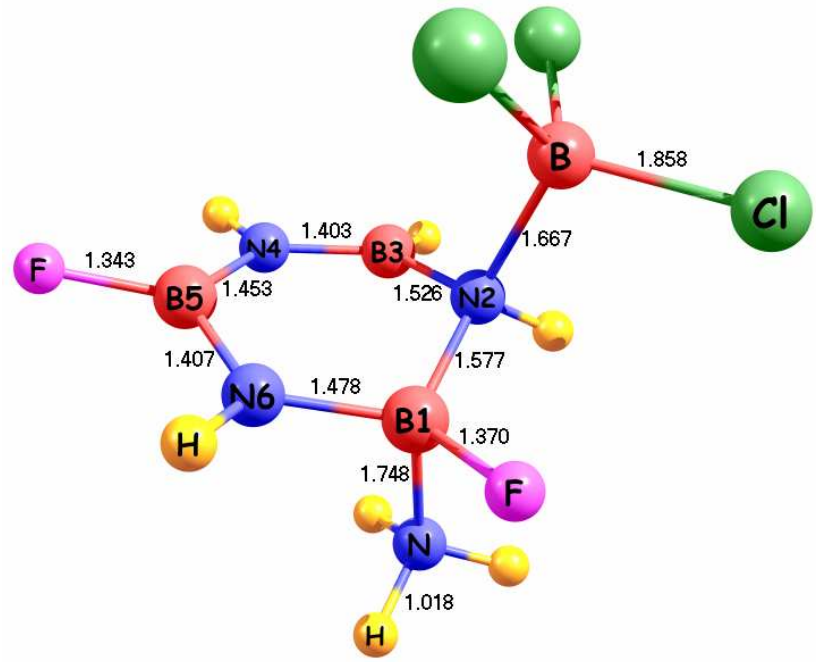

Al
2.158
Cl
2.043
F
1.346
1.451
N4
1.407
B3
B5
1.492
N2
1.406
H
N6
1.569
1.490
B1
1.720
N
1.018
H

74) 1-NH_3,2-BCl_3,3,5-F_2-BZ



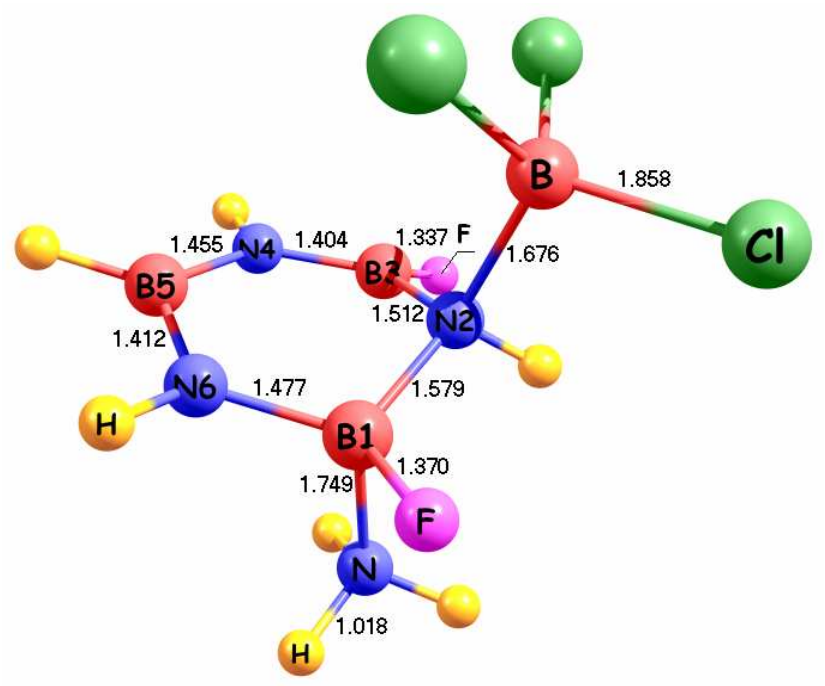
	X	Y	Z
B	2.430	-0.376	0.570
N	1.831	-1.231	-0.437
B	0.695	-0.835	-1.156
N	-0.078	0.373	-0.690
B	0.838	1.518	-0.071
N	1.999	0.960	0.676
F	3.424	-0.871	1.328
H	2.277	-2.109	-0.664
F	0.368	-1.376	-2.334
H	-0.600	0.734	-1.489
H	0.208	2.371	0.475
H	2.302	1.468	1.494
N	1.469	2.344	-1.431
H	2.022	1.755	-2.052
H	0.753	2.818	-1.981
H	2.095	3.059	-1.066
B	-1.361	-0.030	0.286
Cl	-0.850	-0.110	2.053
Cl	-2.628	1.306	-0.028
Cl	-1.978	-1.689	-0.299

75) 1-NH_3,2-BCl_3,1,5-F_2-BZ



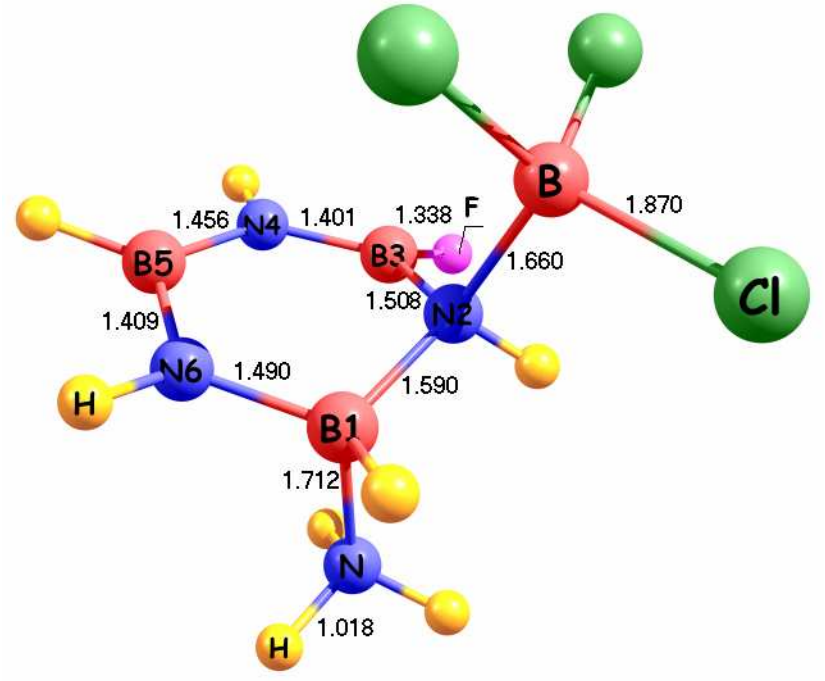
	X	Y	Z
B	2.375	-0.825	0.201
N	1.725	-1.358	-0.984
B	0.574	-0.794	-1.554
N	-0.075	0.361	-0.796
B	0.948	1.258	0.001
N	2.033	0.472	0.624
F	3.329	-1.552	0.805
H	2.119	-2.185	-1.411
H	0.183	-1.081	-2.633
H	-0.589	0.932	-1.465
F	0.385	2.235	0.780
H	2.367	0.790	1.523
N	1.688	2.245	-1.237
H	2.179	1.710	-1.951
H	1.029	2.876	-1.691
H	2.379	2.819	-0.757
B	-1.368	-0.211	0.088
Cl	-0.851	-0.700	1.783
Cl	-2.624	1.158	0.077
Cl	-2.015	-1.705	-0.849

76) 1-NH_3,2-BCl_3,1,3-F_2-BZ



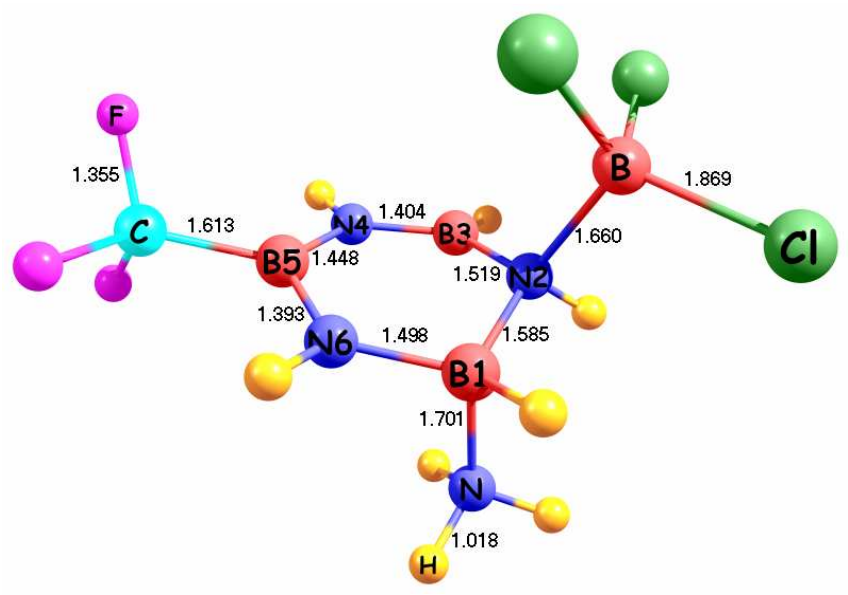
	X	Y	Z
B	-2.147	0.817	1.518
N	-1.545	1.823	0.657
B	-0.735	1.494	-0.443
N	-0.280	0.061	-0.600
B	-1.389	-0.967	-0.145
N	-2.100	-0.521	1.071
H	-2.698	1.138	2.522
H	-1.718	2.799	0.848
F	-0.531	2.330	-1.467
H	-0.037	-0.093	-1.579
F	-1.009	-2.282	-0.198
H	-2.401	-1.248	1.704
N	-2.553	-0.931	-1.450
H	-2.990	-0.022	-1.591
H	-2.170	-1.253	-2.338
H	-3.287	-1.583	-1.181
B	1.235	-0.146	0.085
Cl	1.127	-0.790	1.801
Cl	2.123	-1.304	-1.065
Cl	2.025	1.554	0.075

77) 1-NH_3,2-BCl_3,3-F-BZ



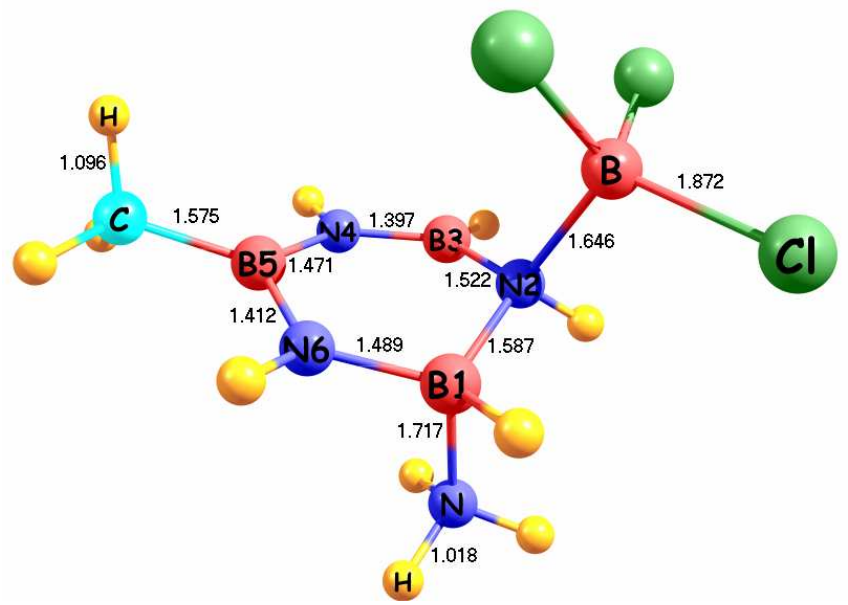
	X	Y	Z
B	-2.401	0.341	1.418
N	-1.896	1.456	0.629
B	-0.990	1.283	-0.426
N	-0.321	-0.056	-0.607
B	-1.257	-1.281	-0.215
N	-2.137	-0.959	0.943
H	-3.050	0.547	2.395
H	-2.227	2.389	0.828
F	-0.816	2.202	-1.382
H	-0.034	-0.131	-1.583
H	-0.672	-2.320	-0.179
H	-2.365	-1.724	1.560
N	-2.283	-1.483	-1.571
H	-2.860	-0.665	-1.769
H	-1.786	-1.746	-2.421
H	-2.918	-2.244	-1.341
B	1.181	-0.133	0.097
Cl	1.068	-0.678	1.852
Cl	2.131	-1.347	-0.961
Cl	1.921	1.574	-0.019

78) 1-NH_3,2-BCl_3,5-CF_3-BZ



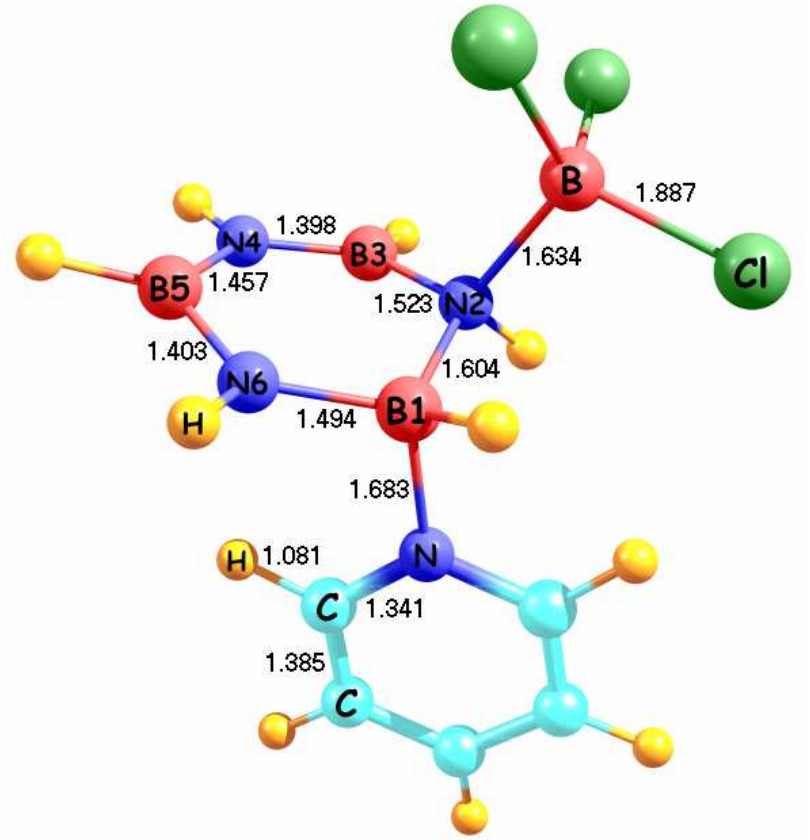
	X	Y	Z
B	-1.777	0.145	0.206
N	-1.130	-0.339	1.407
B	0.214	-0.075	1.712
N	1.044	0.661	0.675
B	0.241	1.618	-0.300
N	-1.143	1.113	-0.570
C	-3.261	-0.374	-0.154
H	-1.657	-0.907	2.056
H	0.683	-0.325	2.769
H	1.754	1.192	1.178
H	0.866	1.955	-1.258
H	-1.549	1.334	-1.468
N	0.066	3.076	0.559
H	-0.436	2.977	1.441
H	0.959	3.533	0.740
H	-0.481	3.704	-0.026
B	2.070	-0.360	-0.137
Cl	1.176	-1.186	-1.519
Cl	2.704	-1.610	1.095
Cl	3.471	0.726	-0.730
F	-4.168	0.097	0.757
F	-3.692	0.044	-1.372
F	-3.375	-1.724	-0.139

79) 1-NH_3,2-BCl_3,5-CH_3-BZ



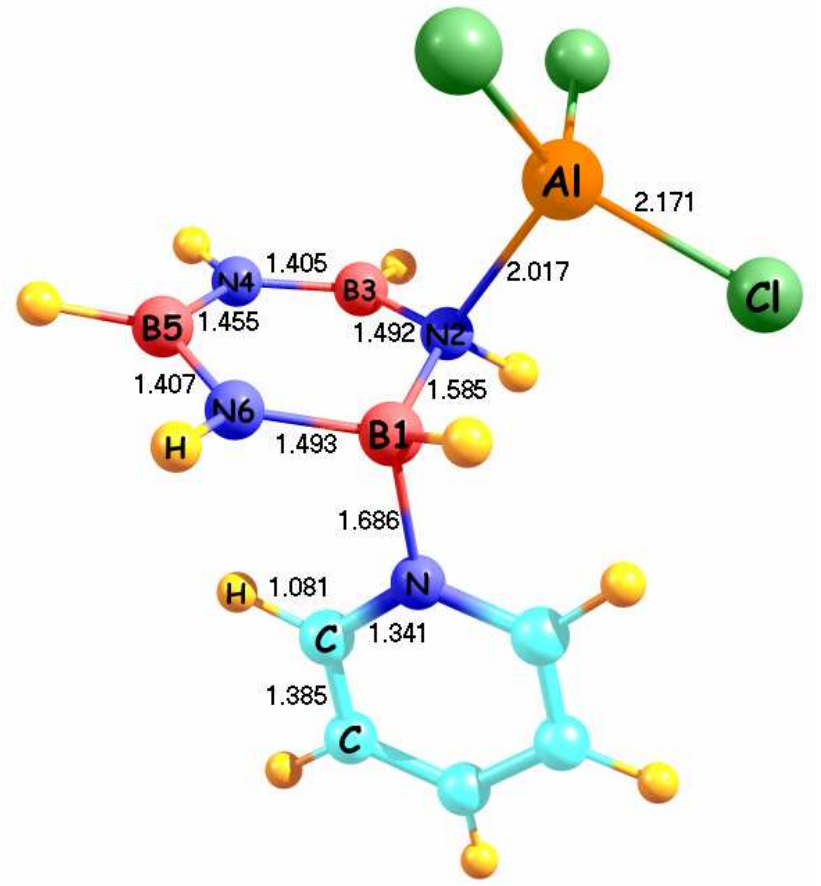
	X	Y	Z
B	-2.548	-0.465	-0.061
N	-1.893	-0.788	1.216
B	-0.642	-0.312	1.616
N	0.121	0.582	0.650
B	-0.803	1.408	-0.340
N	-2.026	0.659	-0.739
C	-3.756	-1.333	-0.577
H	-2.348	-1.451	1.826
H	-0.200	-0.508	2.698
H	0.684	1.221	1.211
H	-0.200	1.943	-1.220
H	-2.362	0.822	-1.676
N	-1.335	2.741	0.602
H	-1.865	2.460	1.426
H	-0.579	3.362	0.891
H	-1.964	3.280	0.011
B	1.357	-0.199	-0.105
Cl	0.727	-1.168	-1.544
Cl	2.166	-1.322	1.151
Cl	2.557	1.142	-0.622
H	-4.512	-1.488	0.201
H	-4.260	-0.903	-1.445
H	-3.406	-2.330	-0.865

80) 1-Py,2-BCl_3-BZ



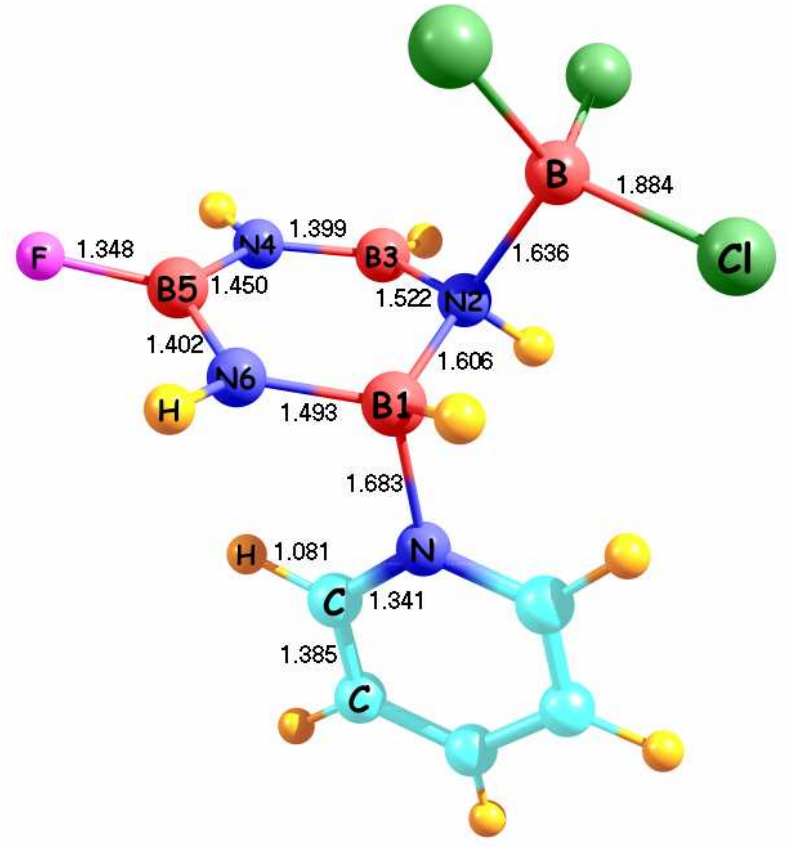
	X	Y	Z
B	-0.089	2.949	-0.410
N	-0.538	2.613	0.936
B	-0.669	1.306	1.414
N	-0.478	0.156	0.434
B	0.466	0.465	-0.826
N	0.472	1.916	-1.177
H	-0.158	4.073	-0.801
H	-0.769	3.368	1.565
H	-0.859	1.062	2.557
H	-0.069	-0.604	0.977
H	0.252	-0.272	-1.738
H	0.679	2.128	-2.142
B	-1.887	-0.557	0.015
Cl	-2.729	0.420	-1.303
Cl	-1.433	-2.294	-0.565
Cl	-2.958	-0.688	1.541
N	1.996	-0.020	-0.321
C	2.937	0.857	0.057
C	2.275	-1.337	-0.331
H	2.643	1.896	0.014
H	1.469	-1.983	-0.659
C	4.198	0.443	0.454
C	3.512	-1.818	0.057
H	4.933	1.178	0.752
H	3.700	-2.883	0.037
C	4.492	-0.915	0.457
H	5.470	-1.266	0.760

81) 1-Py,2-$AlCl_3$-BZ



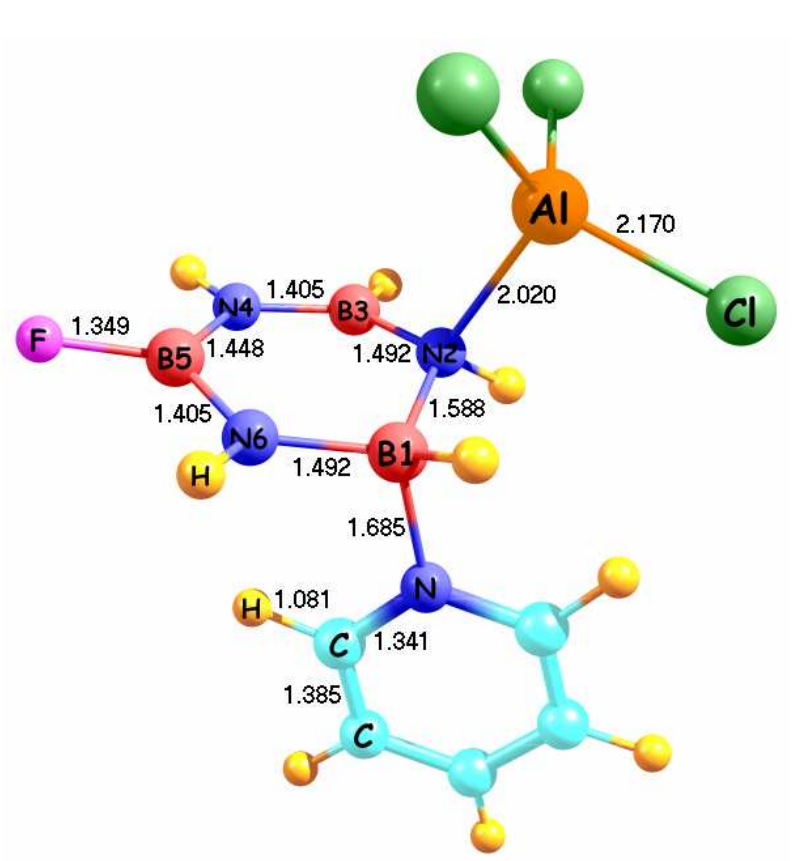
	X	Y	Z
B	0.232	3.019	-0.384
N	-0.216	2.749	0.973
B	-0.390	1.453	1.486
N	-0.227	0.299	0.553
B	0.672	0.499	-0.738
N	0.711	1.936	-1.142
H	0.219	4.134	-0.809
H	-0.440	3.530	1.571
H	-0.649	1.246	2.626
H	0.076	-0.512	1.090
H	0.391	-0.268	-1.616
H	0.913	2.115	-2.114
Al	-1.977	-0.518	-0.029
Cl	-2.714	0.488	-1.763
Cl	-1.336	-2.570	-0.335
Cl	-3.284	-0.345	1.667
N	2.209	-0.036	-0.296
C	3.190	0.814	0.040
C	2.443	-1.360	-0.296
H	2.929	1.863	-0.007
H	1.609	-1.986	-0.593
C	4.448	0.364	0.403
C	3.675	-1.878	0.060
H	5.216	1.078	0.666
H	3.827	-2.948	0.049
C	4.696	-1.003	0.415
H	5.672	-1.382	0.692

82) 1-Py,2-BCl_3,5-F-BZ



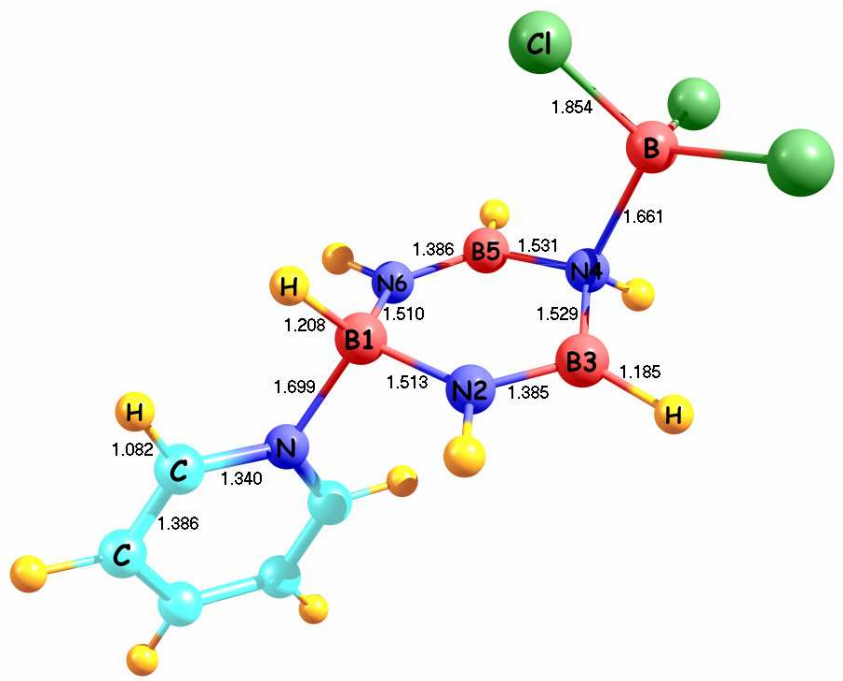
	X	Y	Z
B	-0.162	2.701	-0.130
N	-0.602	2.266	1.182
B	-0.676	0.920	1.553
N	-0.458	-0.134	0.477
B	0.477	0.299	-0.756
N	0.442	1.773	-0.990
F	-0.285	4.005	-0.453
H	-0.842	2.971	1.864
H	-0.836	0.579	2.675
H	-0.037	-0.932	0.950
H	0.280	-0.368	-1.724
H	0.602	2.075	-1.940
B	-1.860	-0.824	-0.007
Cl	-2.706	0.255	-1.240
Cl	-1.387	-2.499	-0.727
Cl	-2.932	-1.088	1.501
N	2.020	-0.184	-0.292
C	2.946	0.687	0.132
C	2.327	-1.491	-0.392
H	2.630	1.721	0.158
H	1.534	-2.132	-0.758
C	4.220	0.277	0.488
C	3.579	-1.968	-0.049
H	4.942	1.008	0.826
H	3.790	-3.025	-0.142
C	4.543	-1.072	0.399
H	5.533	-1.419	0.669

83) 1-Py,2-$AlCl_3$,5-F-BZ



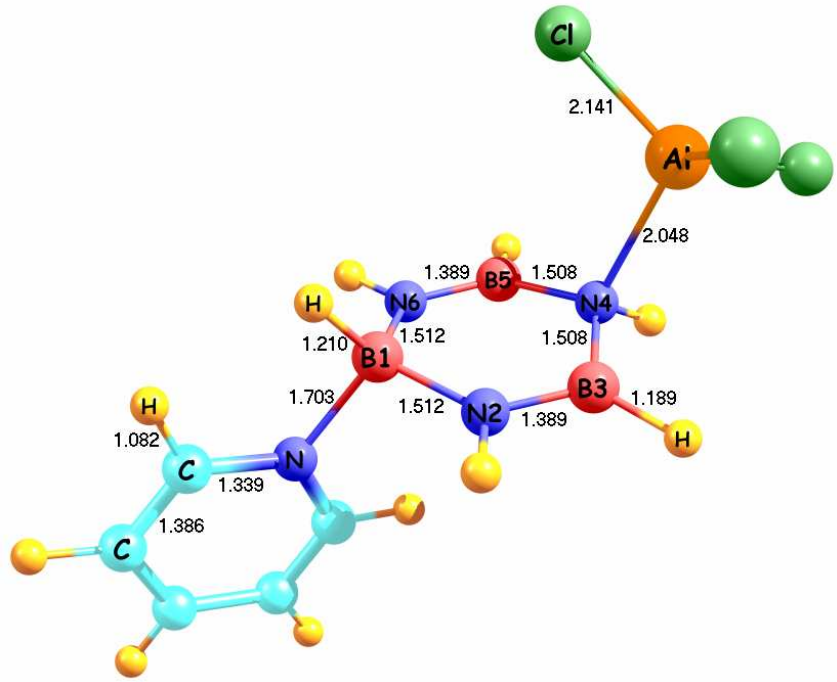
	X	Y	Z
B	0.250	2.803	-0.093
N	-0.226	2.445	1.227
B	-0.410	1.111	1.627
N	-0.240	0.040	0.602
B	0.670	0.335	-0.666
N	0.733	1.799	-0.948
F	0.261	4.104	-0.447
H	-0.439	3.186	1.879
H	-0.680	0.814	2.744
H	0.055	-0.814	1.074
H	0.380	-0.348	-1.607
H	0.916	2.067	-1.904
Al	-1.996	-0.714	-0.056
Cl	-2.707	0.454	-1.695
Cl	-1.369	-2.735	-0.533
Cl	-3.305	-0.672	1.646
N	2.194	-0.262	-0.265
C	3.199	0.543	0.110
C	2.396	-1.589	-0.346
H	2.964	1.599	0.125
H	1.546	-2.177	-0.674
C	4.449	0.042	0.432
C	3.618	-2.156	-0.034
H	5.237	0.722	0.728
H	3.744	-3.227	-0.110
C	4.664	-1.329	0.362
H	5.632	-1.746	0.606

84) 1-Py,4-BCl_3-BZ



	X	Y	Z
B	0.552	1.264	0.601
N	1.304	0.612	-0.563
B	0.486	-0.386	-1.384
N	-0.662	-0.922	-0.826
B	-1.281	-0.560	0.506
N	-0.648	0.711	1.020
H	1.016	2.246	1.077
H	1.651	1.343	-1.186
H	0.836	-0.622	-2.491
H	-1.106	-1.659	-1.356
H	-1.384	-1.458	1.308
H	-1.032	1.105	1.868
B	2.753	0.007	-0.022
Cl	2.435	-0.907	1.559
Cl	3.464	-1.113	-1.322
Cl	3.858	1.489	0.236
N	-2.912	-0.202	0.192
C	-3.232	0.829	-0.604
C	-3.883	-0.953	0.729
H	-2.396	1.392	-0.996
H	-3.548	-1.763	1.362
C	-4.547	1.146	-0.892
C	-5.223	-0.696	0.483
H	-4.768	1.986	-1.536
H	-5.980	-1.324	0.934
C	-5.562	0.370	-0.339
H	-6.600	0.596	-0.547

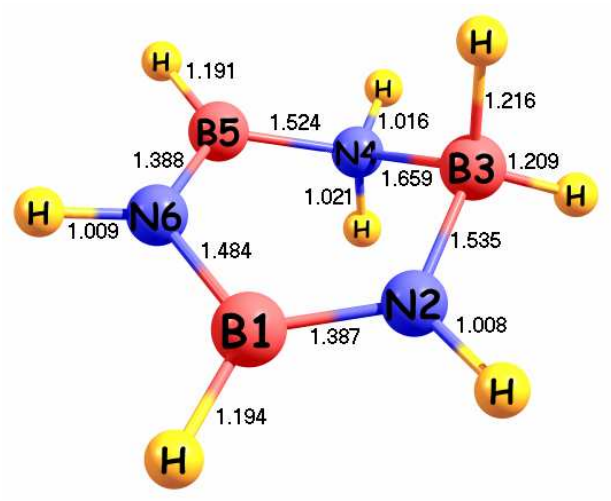
85) 1-Py,4-$AlCl_3$-BZ



	X	Y	Z
B	0.244	-0.327	-1.446
N	1.000	-0.949	-0.298
B	0.249	-1.098	1.001
N	-0.889	-0.325	1.198
B	-1.497	0.644	0.209
N	-0.895	0.415	-1.159
H	0.643	-0.514	-2.550
H	1.442	-1.825	-0.576
H	0.650	-1.886	1.796
H	-1.278	-0.339	2.130
H	-1.565	1.796	0.571
H	-1.290	0.934	-1.930
Al	2.757	0.056	0.014
Cl	2.750	1.735	-1.314
Cl	2.793	0.607	2.083
Cl	4.160	-1.489	-0.511
N	-3.148	0.244	0.086
C	-3.515	-0.996	-0.271
C	-4.087	1.167	0.335
H	-2.703	-1.687	-0.455
H	-3.715	2.143	0.618
C	-4.844	-1.357	-0.389
C	-5.439	0.878	0.236
H	-5.103	-2.367	-0.678
H	-6.168	1.649	0.445
C	-5.825	-0.404	-0.132
H	-6.874	-0.659	-0.217

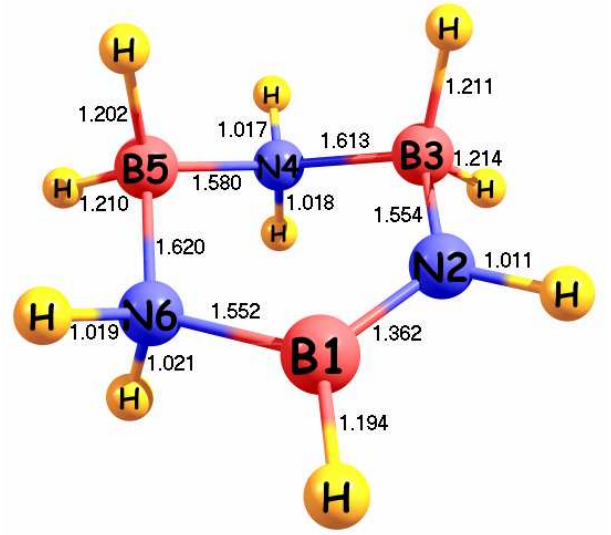
Hydrogenation products

86) 3,4-H_2-BZ



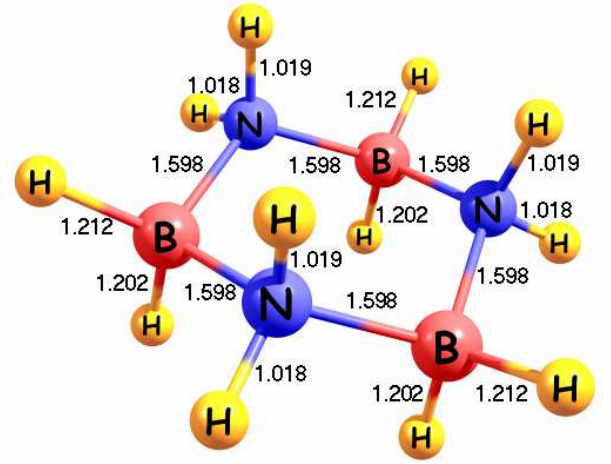
	X	Y	Z
B	1.202	-0.829	0.362
N	-1.234	0.769	0.100
B	-0.037	1.471	0.108
N	-0.151	-1.418	-0.058
B	-1.333	-0.694	-0.127
N	1.202	0.688	-0.308
H	2.149	-1.418	-0.106
H	-2.086	1.277	0.282
H	0.066	2.625	0.382
H	-0.189	-2.413	-0.215
H	-2.404	-1.170	-0.355
H	2.063	1.173	-0.075
H	1.207	0.554	-1.321
H	1.312	-0.638	1.558

87) 3,4,5,6-H_4-BZ



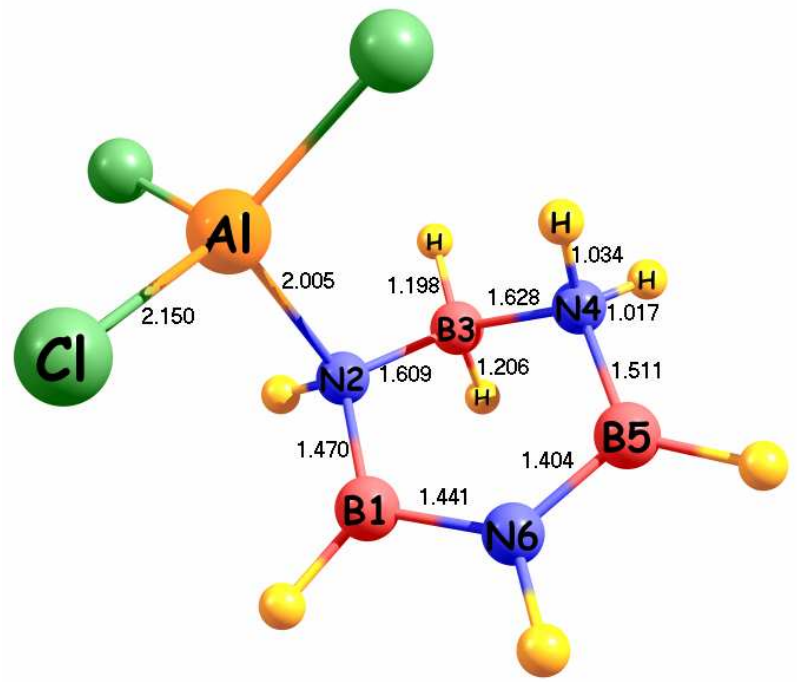
	X	Y	Z
B	0.579	-1.372	0.333
N	-0.499	1.383	0.041
B	0.859	1.300	-0.032
N	-0.859	-1.118	-0.269
B	-1.579	0.269	0.125
N	1.498	-0.113	-0.105
H	1.074	-2.374	-0.131
H	-0.882	2.319	0.075
H	1.613	2.225	-0.069
H	-0.853	-1.222	-1.282
H	-2.469	0.477	-0.674
H	2.330	-0.130	0.481
H	1.862	-0.253	-1.049
H	0.516	-1.374	1.534
H	-1.462	-1.866	0.064
H	-2.006	0.149	1.253

88) 1,2,3,4,5,6-H_6-BZ



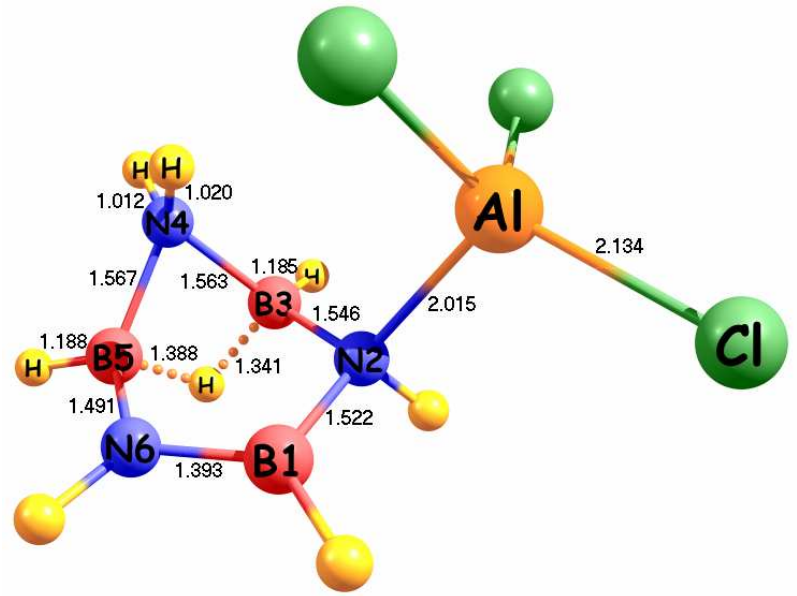
	X	Y	Z
B	-1.512	-0.461	0.247
N	-1.086	1.014	-0.196
B	0.357	1.540	0.247
N	1.421	0.433	-0.196
B	1.156	-1.079	0.247
N	-0.335	-1.447	-0.196
H	-1.602	-0.488	1.445
H	-2.532	-0.772	-0.330
H	-1.219	1.138	-1.199
H	-1.764	1.647	0.222
H	0.378	1.632	1.445
H	0.597	2.578	-0.331
H	1.595	0.486	-1.199
H	2.308	0.704	0.222
H	1.225	-1.143	1.445
H	1.934	-1.806	-0.331
H	-0.376	-1.624	-1.199
H	-0.544	-2.351	0.222

89) 2-$AlCl_3$,3,4-H_2-BZ



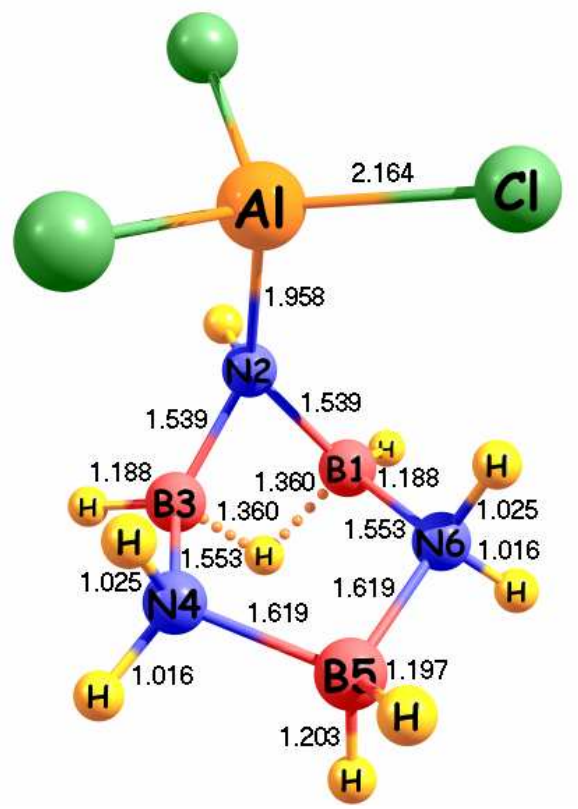
	X	Y	Z
B	-3.120	0.093	0.296
N	-2.526	1.254	-0.224
B	-1.344	1.299	-1.047
N	-0.570	0.059	-1.197
B	-1.469	-1.274	-1.241
N	-2.363	-1.202	0.119
H	-4.172	0.096	0.846
H	-3.024	2.124	-0.098
H	-1.053	2.295	-1.620
H	-0.046	0.095	-2.072
H	-0.793	-2.262	-1.203
H	-1.700	-1.328	0.902
Al	0.980	0.007	0.074
Cl	0.358	-1.152	1.806
Cl	2.560	-0.867	-1.061
Cl	1.267	2.064	0.630
H	-2.231	-1.229	-2.174
H	-2.985	-2.007	0.157

90) 2-$AlCl_3$,4,5-H_2-BZ



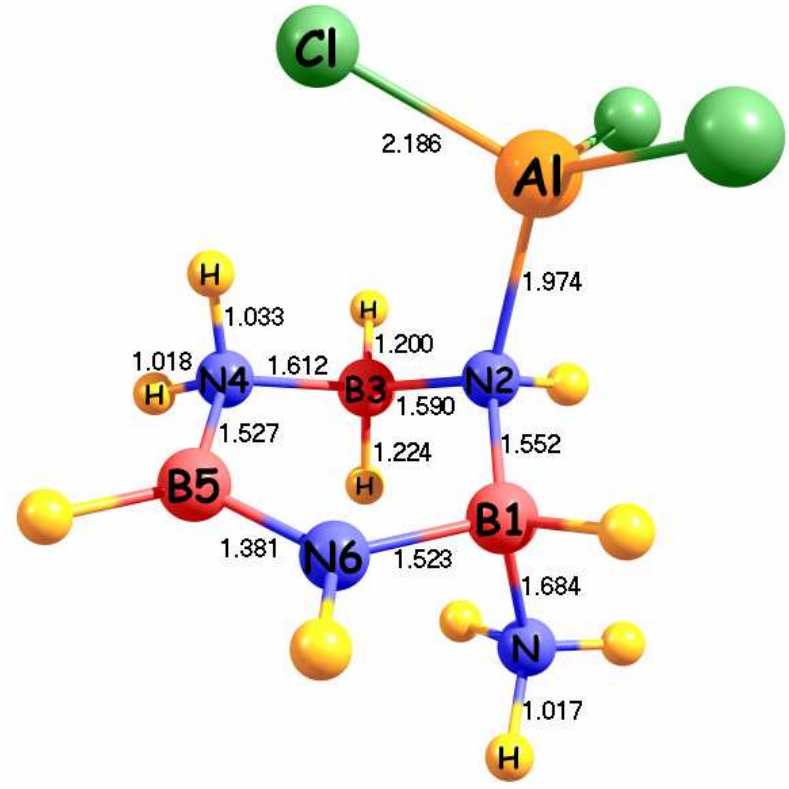
	X	Y	Z
B	-3.198	0.112	-0.303
N	-2.228	1.154	0.351
B	-1.610	0.891	-1.061
N	-0.654	-0.322	-1.000
B	-1.389	-1.557	-0.499
N	-2.699	-1.280	-0.113
H	-2.761	0.439	-1.580
H	-2.574	2.094	0.495
H	-1.353	1.827	-1.740
H	-0.245	-0.512	-1.916
H	-0.865	-2.619	-0.487
H	-3.314	-2.006	0.220
Al	1.032	0.009	0.052
Cl	0.346	-0.185	2.099
Cl	2.371	-1.512	-0.616
Cl	1.624	2.011	-0.415
H	-4.354	0.384	-0.344
H	-1.688	0.841	1.158

91) 2-$AlCl_3$,3,4,5,6-H_4-BZ



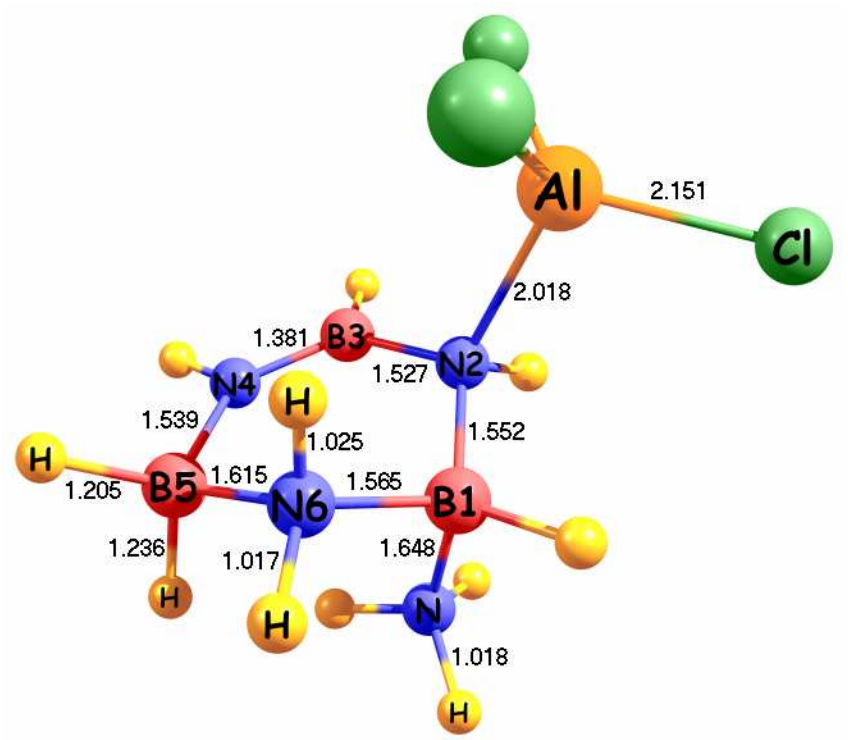
	X	Y	Z
B	-3.003	0.000	-0.654
N	-2.248	-1.278	-0.007
B	-1.632	-0.938	1.377
N	-0.418	0.000	1.243
B	-1.632	0.938	1.377
N	-2.248	1.278	-0.007
H	-4.129	0.000	-0.231
H	-2.921	-2.034	0.078
H	-2.491	0.000	1.860
H	0.091	0.000	2.124
H	-1.644	1.755	2.240
H	-2.921	2.034	0.078
Al	1.034	0.000	-0.070
Cl	0.780	1.784	-1.268
Cl	2.786	0.000	1.154
Cl	0.779	-1.784	-1.268
H	-2.907	0.000	-1.848
H	-1.508	-1.628	-0.625
H	-1.644	-1.755	2.240
H	-1.508	1.628	-0.625

92) 1-NH_3,2-$AlCl_3$,3,4-H_2-BZ



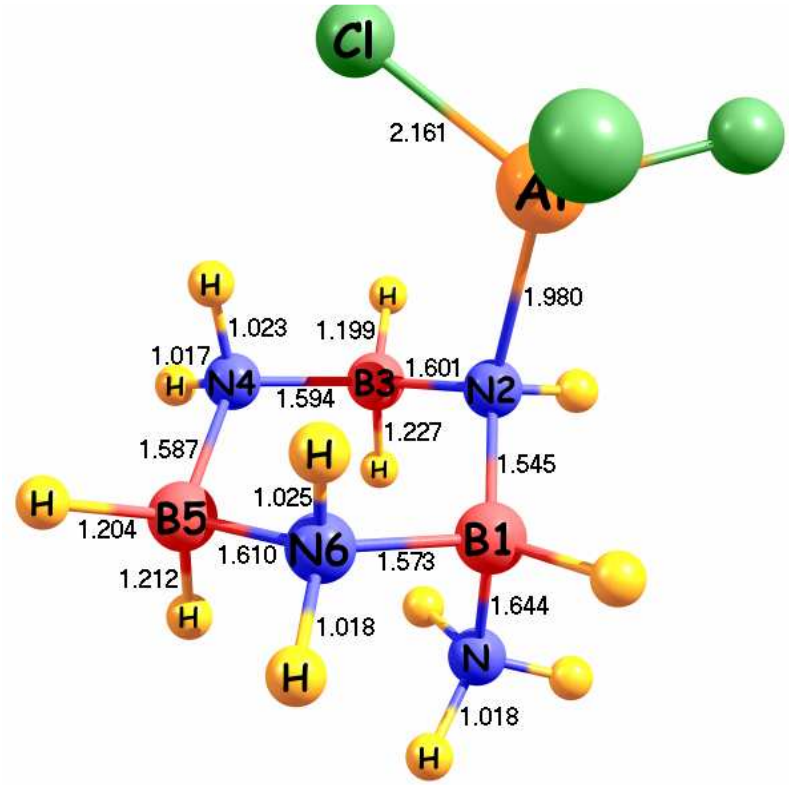
	X	Y	Z
B	2.561	1.268	-0.724
N	1.801	1.761	0.505
B	1.309	0.625	1.538
N	0.634	-0.508	0.649
B	1.654	-1.149	-0.329
N	2.457	-0.071	-1.047
H	3.190	2.056	-1.357
H	0.951	2.241	0.167
H	2.313	0.212	2.102
H	0.323	-1.216	1.317
H	1.221	-1.994	-1.059
H	2.886	-0.350	-1.918
N	2.747	-1.979	0.646
H	3.006	-1.372	1.429
H	2.351	-2.842	1.014
H	3.589	-2.222	0.129
Al	-1.159	-0.064	-0.046
Cl	-1.185	2.056	-0.579
Cl	-1.602	-1.262	-1.772
Cl	-2.432	-0.524	1.630
H	2.329	2.475	1.003
H	0.540	1.107	2.323

93) 1-NH3,2-$AlCl_3$,5,6-H_2-BZ



	X	Y	Z
B	3.090	-0.923	0.543
N	2.302	-1.552	-0.619
B	1.169	-1.104	-1.268
N	0.534	0.205	-0.805
B	1.479	1.126	0.013
N	2.148	0.253	1.126
H	4.123	-0.372	0.145
H	2.673	-2.433	-0.946
H	0.680	-1.658	-2.200
H	0.178	0.707	-1.620
H	0.965	2.130	0.414
H	1.392	-0.150	1.687
N	2.734	1.587	-0.950
H	3.452	0.845	-0.926
H	2.453	1.753	-1.913
H	3.159	2.446	-0.608
Al	-1.283	0.000	0.049
Cl	-0.939	-0.260	2.169
Cl	-2.197	1.875	-0.475
Cl	-2.227	-1.693	-0.846
H	3.364	-1.696	1.425
H	2.678	0.819	1.785

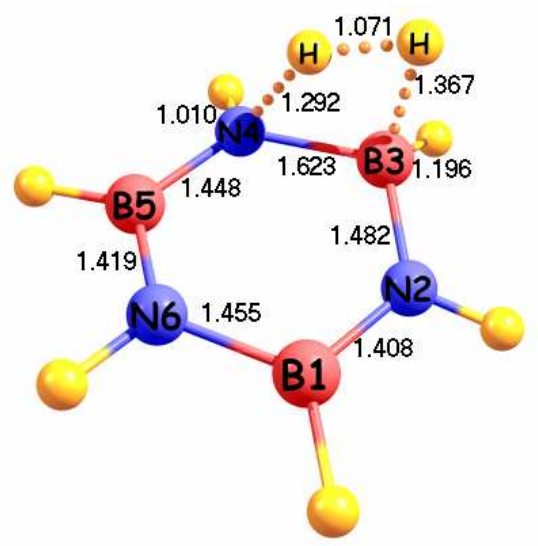
94) 1-NH3,2-$AlCl_3$,3,4,5,6-H_4-BZ



	X	Y	Z
B	-2.788	1.092	0.561
N	-1.828	1.670	-0.563
B	-1.243	0.629	-1.621
N	-0.534	-0.531	-0.776
B	-1.505	-1.259	0.180
N	-2.056	-0.193	1.196
H	-3.810	0.706	0.036
H	-1.041	2.185	-0.160
H	-2.195	0.190	-2.258
H	-0.187	-1.203	-1.462
H	-1.070	-2.235	0.723
H	-1.254	0.080	1.774
N	-2.793	-1.771	-0.706
H	-2.962	-1.079	-1.450
H	-2.587	-2.670	-1.136
H	-3.649	-1.875	-0.166
Al	1.220	-0.045	0.002
Cl	1.144	-0.547	2.118
Cl	2.605	-1.240	-1.122
Cl	1.519	2.090	-0.139
H	-2.991	1.904	1.426
H	-2.694	-0.617	1.867
H	-2.353	2.370	-1.082
H	-0.468	1.1571	-2.369

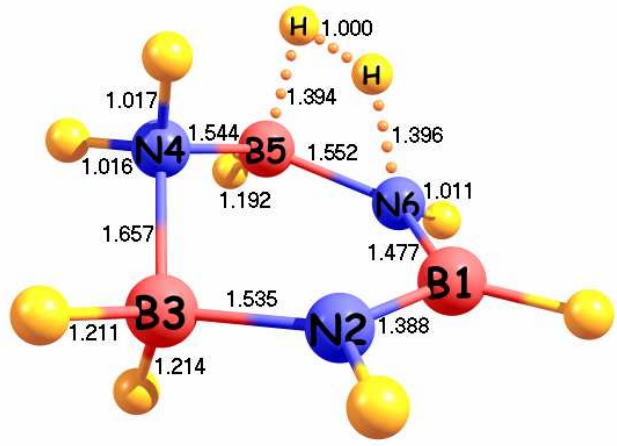
Transition states

95) TS – 3,4-H_2-BZ



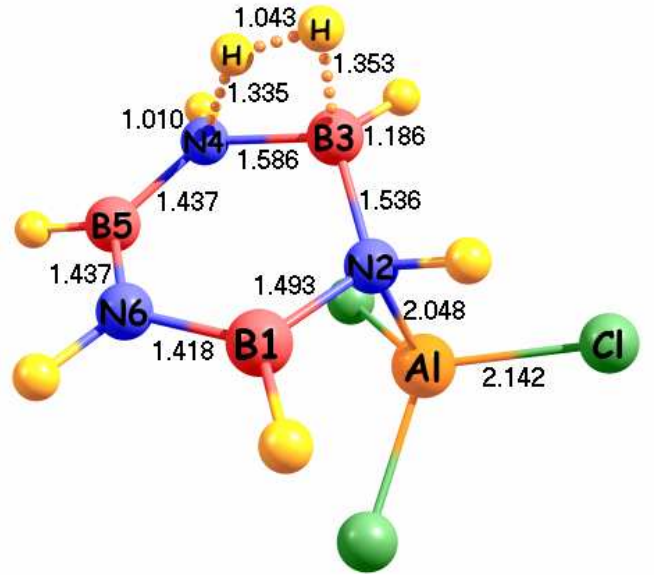
	X	Y	Z
B	0.741	-1.297	-0.094
N	1.469	-0.102	0.139
B	0.878	1.218	-0.017
N	-0.523	1.325	-0.120
B	-1.477	0.202	0.032
N	-0.705	-1.221	-0.089
H	1.280	-2.341	-0.303
H	2.475	-0.162	0.181
H	1.586	2.176	-0.093
H	-0.915	2.239	-0.282
H	-2.541	0.221	-0.514
H	-1.231	-1.997	-0.465
H	-1.808	0.043	1.349
H	-1.243	-0.801	1.009

96) TS – 3,4,5,6-H_4-BZ



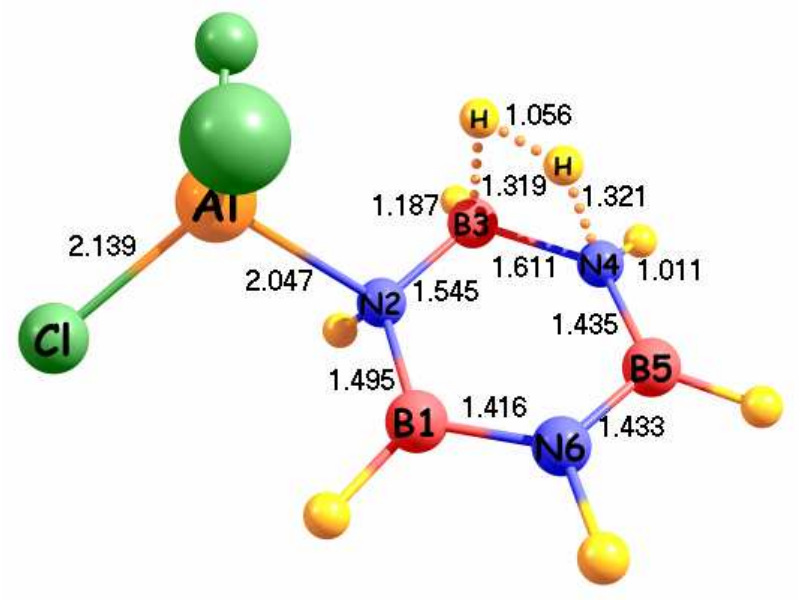
	X	Y	Z
B	1.441	-0.293	0.167
N	0.865	1.148	0.151
B	-0.561	1.448	-0.093
N	-1.447	0.379	-0.125
B	-1.113	-1.041	0.352
N	0.396	-1.347	-0.260
H	2.190	-0.599	1.043
H	1.409	1.853	0.629
H	-0.879	2.590	-0.259
H	-2.409	0.564	-0.359
H	-0.983	-1.145	1.555
H	-1.851	-1.882	-0.109
H	0.685	-2.272	0.043
H	0.285	-1.398	-1.270
H	2.277	-0.188	-0.943
H	1.737	0.644	-0.815

97) TS – 2-$AlCl_3$,3,4-H_4-BZ (trans)



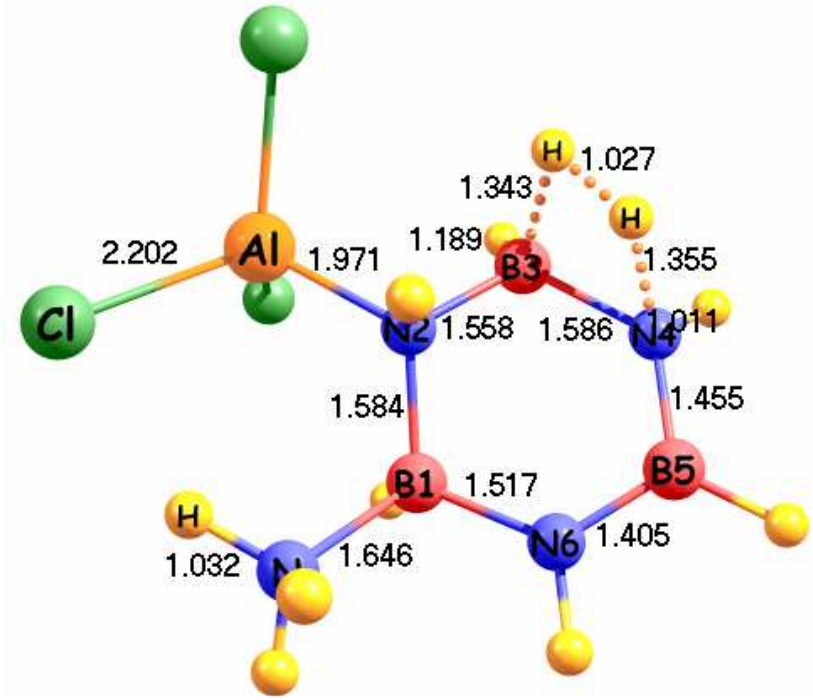
	X	Y	Z
B	-3.001	0.143	0.483
N	-2.508	1.274	-0.254
B	-1.353	1.264	-1.078
N	-0.583	-0.011	-1.172
B	-1.402	-1.303	-1.036
N	-2.547	-1.150	0.050
H	-3.771	0.259	1.380
H	-2.939	2.171	-0.084
H	-1.005	2.214	-1.694
H	-0.034	-0.034	-2.031
H	-0.836	-2.345	-1.024
H	-2.721	-1.956	0.633
H	-2.204	-1.389	-2.122
H	-2.777	-1.319	-1.254
Al	0.997	0.000	0.132
Cl	0.481	-1.252	1.789
Cl	2.542	-0.753	-1.147
Cl	1.187	2.068	0.667

98) TS – 2-$AlCl_3$,3,4-H_4-BZ (cis)



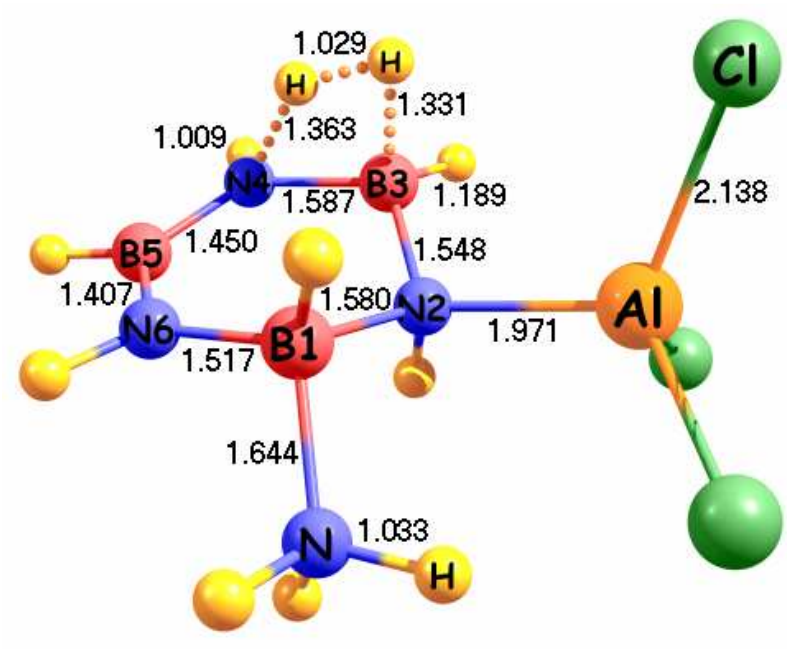
	X	Y	Z
B	3.565	-0.154	-0.012
N	2.669	-1.273	-0.034
B	1.371	-1.250	-0.597
N	0.694	0.055	-0.871
B	1.453	1.377	-0.619
N	3.007	1.144	-0.260
H	4.732	-0.293	0.166
H	3.055	-2.182	0.176
H	0.814	-2.249	-0.907
H	0.333	0.037	-1.826
H	1.266	2.276	-1.371
H	3.633	1.908	-0.470
H	1.063	1.826	0.558
H	2.084	1.558	0.591
Al	-1.113	-0.015	0.088
Cl	-0.557	-0.801	2.005
Cl	-1.842	1.995	0.125
Cl	-2.251	-1.314	-1.175

99) TS – 1-NH_3,2-$AlCl_3$,3,4-H_4-BZ (trans)



	X	Y	Z
B	3.696	-0.481	-0.043
N	3.082	0.780	0.024
B	1.617	0.985	0.365
N	0.730	-0.144	-0.304
B	1.268	-1.577	-0.012
N	2.850	-1.664	-0.072
H	4.883	-0.613	-0.041
H	3.713	1.555	0.172
H	1.357	1.095	1.535
H	0.803	-0.012	-1.314
H	0.746	-2.207	0.852
H	3.257	-2.518	0.284
H	1.002	-2.260	-1.137
H	2.012	-2.104	-1.042
Al	-1.208	-0.145	0.055
Cl	-1.580	-0.345	2.146
Cl	-1.890	1.815	-0.684
Cl	-2.007	-1.688	-1.208
N	1.180	2.425	-0.301
H	0.153	2.521	-0.348
H	1.540	3.191	0.264
H	1.548	2.537	-1.246

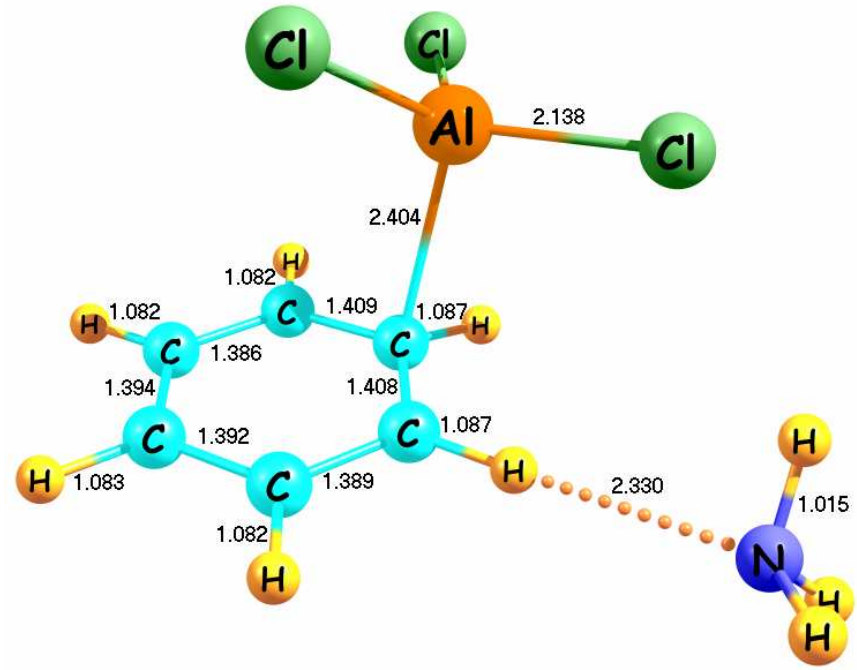
100) TS – 1-NH_3,2-$AlCl_3$,3,4-H_4-BZ (cis)



	X	Y	Z
B	3.697	-0.443	-0.207
N	3.086	0.776	0.143
B	1.614	0.986	0.446
N	0.734	-0.126	-0.251
B	1.295	-1.549	-0.012
N	2.865	-1.630	-0.224
H	4.859	-0.525	-0.464
H	3.718	1.538	0.343
H	1.317	1.090	1.611
H	0.825	-0.025	-1.267
H	0.702	-2.466	-0.479
H	3.228	-2.490	-0.610
H	1.245	-1.753	1.303
H	2.215	-1.794	0.963
Al	-1.220	-0.155	0.010
Cl	-1.667	-1.181	1.831
Cl	-1.893	1.935	0.101
Cl	-1.954	-1.046	-1.802
N	1.197	2.432	-0.216
H	0.176	2.570	-0.144
H	1.647	3.191	0.290
H	1.470	2.510	-1.195

Benzene complexes

101) $AlCl_3 \cdot C_6H_6 \cdot NH_3$



	X	Y	Z
H	1.379	0.446	-1.260
C	0.877	0.651	-0.318
C	0.845	1.860	1.778
C	-1.186	0.859	0.919
C	-0.515	1.583	1.901
C	-0.504	0.406	-0.204
C	1.540	1.413	0.664
H	-1.055	1.931	2.774
N	-2.260	-1.457	-2.461
H	2.594	1.630	0.553
Al	1.740	-1.499	0.323
H	1.356	2.428	2.544
H	-2.244	0.658	1.020
H	-1.038	-0.138	-0.978
Cl	3.830	-1.119	0.143
Cl	0.967	-2.706	-1.263
Cl	1.011	-1.929	2.267
H	-2.294	-1.191	-3.439
H	-3.166	-1.844	-2.223
H	-1.576	-2.201	-2.370