

Electronic Supplementary Information (ESI)

Skeletally Substituted Aluminium and Gallium Carbenoids: A Computational Exploration

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Table S1 Calculated (M06-D3/Def2-TZVP) E–X bond lengths (r_1/r_2 in Å), Wiberg Bond Index (WBI) values and N–E–X bond angles (in degrees) of the singlet state geometry of **1-13** (X = C, N or Si and E = Al or Ga). The r_1 and r_2 are mentioned in Scheme 2.

Molecules	E-X (r_1/r_2)	WBI (r_1/r_2)	\angle N-E-X	Molecules	E-X (r_1/r_2)	WBI (r_1/r_2)	\angle N-E-X
1Al	2.012/2.012	0.252/0.252	88.6	1Ga	2.137/2.137	0.243/0.243	85.6
2Al	2.183/1.911	0.175/0.266	87.9	2Ga	2.416/2.024	0.142/0.283	84.2
3Al	2.058/1.980	0.239/0.225	94.4	3Ga	2.212/2.116	0.224/0.219	92.0
4Al	1.980/2.064	0.305/0.411	89.9	4Ga	2.106/2.130	0.303/0.441	87.4
5Al	2.063/1.946	0.203/0.276	86.4	5Ga	2.207/2.066	0.184/0.274	82.7
6Al	2.063/1.996	0.229/0.474	87.6	6Ga	2.216/2.054	0.211/0.521	84.4
7Al	1.907/2.006	0.308/0.269	88.3	7Ga	2.025/2.138	0.310/0.260	85.1
8Al	1.975/1.936	0.265/0.279	91.8	8Ga	2.189/2.067	0.230/0.277	88.8
9Al	1.923/1.973	0.309/0.242	93.1	9Ga	2.053/2.110	0.307/0.238	90.1
10Al	1.900/2.065	0.343/0.426	88.8	10Ga	2.012/2.131	0.357/0.461	86.1
11Al	1.919/1.955	0.282/0.289	86.4	11Ga	2.049/2.077	0.271/0.285	82.5
12Al	1.926/2.004	0.303/0.489	87.0	12Ga	2.057/2.060	0.299/0.542	84.0
13Al	1.910/1.910	0.322/0.322	87.6	13Ga	2.027/2.027	0.328/0.328	84.1

Table S2 Calculated (M06-D3/Def2-TZVP) natural valence population (NP_N) at the α -nitrogen atoms of ylidic Al(I)/Ga(I) carbenoids as well as their respective parent non-ylidic versions (It includes only the four-membered cyclic ylide decorate Al(I)/Ga(I) carbenoids and their respective parent non-ylidic versions).

Non-ylidic Molecule	NP_N	Ylide-decorated Molecule	NP_N
1Al/1Ga	5.70/5.65	7Al/7Ga	6.22/6.17
2Al/2Ga	5.55/5.49	8Al/8Ga	6.18/6.11
3Al/3Ga	5.71/5.65	9Al/9Ga	6.23/6.19
4Al/4Ga	5.71/5.65	10Al/10Ga	6.19/6.14
5Al/5Ga	5.66/5.61	11Al/11Ga	6.18/6.14
6Al/6Ga	5.64/5.58	12Al/12Ga	6.15/6.09
		13Al/13Ga	6.21/6.17

Table S3 Calculated (M06-D3/Def2-TZVP) natural charges (q) and occupancies of the formally vacant valence p- orbital (Occ) at the central atom (Al/Ga) for **1Al-13Al** and **1Ga-13Ga**. It also has the proton affinity (PA in kcal mol⁻¹) values for **1Al-13Al** and **1Ga-13Ga**.

Molecules	PA	q_{Al}	Occ_{Al}	Molecules	PA	q_{Ga}	Occ_{Ga}
1Al	255.9	0.719	0.101	1Ga	230.6	0.710	0.088
2Al	262.6	0.767	0.176	2Ga	236.1	0.736	0.120
3Al	265.2	0.759	0.063	3Ga	238.1	0.748	0.063
4Al	277.7	0.587	0.101	4Ga	260.6	0.550	0.101
5Al	253.7	0.736	0.060	5Ga	227.2	0.731	0.064
6Al	276.1	0.602	0.085	6Ga	258.1	0.564	0.092
7Al	270.3	0.698	0.113	7Ga	246.7	0.684	0.093
8Al	278.9	0.724	0.157	8Ga	253.9	0.713	0.127
9Al	275.5	0.733	0.075	9Ga	251.1	0.711	0.078
10Al	287.7	0.572	0.089	10Ga	271.6	0.523	0.094
11Al	267.9	0.703	0.070	11Ga	244.2	0.691	0.082
12Al	287.1	0.564	0.095	12Ga	270.8	0.515	0.100
13Al	278.9	0.667	0.088	13Ga	257.2	0.643	0.110

Table S4 Calculated (M06-D3/Def2-TZVP) Mulliken spin densities at the central atom (E =Al/Ga), α -nitrogen (N_α) and α -X atom (X_α) (where X=N, C, Si) with respect to the central atom for the molecules **1Al-13Al** and **1Ga-13Ga**.

Molecules	Al	Nα	Xα	Molecules	Ga	Nα	Xα
1Al	0.913	0.090	0.090	1Ga	0.159	0.284	0.260
2Al	1.021	0.069	0.060	2Ga	0.859	0.135	0.144
3Al	0.907	0.069	0.114	3Ga	0.715	0.125	0.214
4Al	0.910	0.094	0.090	4Ga	0.727	0.144	0.211
5Al	0.998	0.057	0.073	5Ga	0.856	0.133	0.142
6Al	0.918	0.070	0.085	6Ga	0.744	0.102	0.210
7Al	0.999	0.069	0.030	7Ga	0.029	0.092	0.184
8Al	1.691	0.030	0.071	8Ga	1.497	0.096	0.166
9Al	0.865	0.053	0.100	9Ga	0.019	0.045	0.174
10Al	1.040	0.064	0.057	10Ga	0.064	0.069	0.250
11Al	0.870	0.010	0.050	11Ga	0.664	0.246	0.106
12Al	1.609	0.002	0.034	12Ga	1.331	0.041	0.209
13Al	1.748	0.026	0.026	13Ga	0.050	0.018	-0.003

Table S5 Computed (**M06-D3/Def2-TZVP**) key geometrical parameters and occupancies of the formally vacant p- orbital (Occ_E) and natural charges at pseudo hydridic ($q_{\text{H}_{hy}}$) and the other hydrogen atom (q_{H}) of the transition states involved in the activation of dihydrogen by some of the representative Al(I) and Ga(I) carbenoids. Bond angles ($\angle X-E-N$, $E = \text{Al, Ga}$ and $X = \text{C, N, Si}$), bond lengths ($E-N/E-X$) are given in degree ($^\circ$) and in \AA respectively. Wiberg Bond Index (WBI) values are mentioned within parentheses.

Molecules	$\text{H}_{hy}-\text{H}$	$\text{E}-\text{H}$	$\text{E}-\text{H}_{hy}$	$\text{E}-\text{N}/\text{E}-\text{X}$	$\angle X-E-N$	Occ_E	$q_{\text{H}_{hy}}$	q_{H}
1AlTS^{H-H}	1.287 (0.220)	1.583 (0.731)	1.925 (0.709)	1.912/1.912	96.5	0.365	-0.221	-0.145
4AlTS^{H-H}	1.212 (0.256)	1.616 (0.667)	2.057 (0.598)	1.911/1.967	97.8	0.607	-0.265	-0.188
6AlTS^{H-H}	1.231 (0.247)	1.602 (0.697)	1.957 (0.656)	1.931/1.942	95.2	0.570	-0.220	-0.153
8AlTS^{H-H}	1.215 (0.256)	1.603 (0.685)	1.999 (0.648)	1.912/1.885	98.1	0.769	-0.253	-0.164
10AlTS^{H-H}	1.216 (0.257)	1.617 (0.682)	1.977 (0.665)	1.860/1.977	97.0	0.395	-0.229	-0.173
11AlTS^{H-H}	1.271 (0.229)	1.595 (0.710)	2.016 (0.685)	1.864/1.878	93.5	0.385	-0.272	-0.177
13AlTS^{H-H}	1.270 (0.229)	1.603 (0.713)	2.034 (0.670)	1.855/1.848	94.8	0.504	-0.286	-0.180
1GaTS^{H-H}	1.412 (0.162)	1.551 (0.778)	1.944 (0.756)	1.969/1.969	95.8	0.459	-0.227	-0.081
4GaTS^{H-H}	1.339 (0.191)	1.578 (0.731)	2.060 (0.679)	1.993/1.992	96.1	0.556	-0.274	-0.125
6GaTS^{H-H}	1.350 (0.185)	1.570 (0.741)	2.008 (0.702)	2.026/1.958	93.5	0.613	-0.249	-0.107
8GaTS^{H-H}	1.347 (0.187)	1.566 (0.743)	2.007 (0.696)	1.992/1.947	96.3	0.678	-0.275	-0.110
10GaTS^{H-H}	1.326 (0.198)	1.586 (0.730)	2.030 (0.695)	1.935/1.994	95.4	0.431	-0.259	-0.128
11GaTS^{H-H}	1.392 (0.172)	1.559 (0.763)	2.004 (0.720)	1.939/1.936	91.2	0.330	-0.277	-0.107
13GaTS^{H-H}	1.392 (0.173)	1.566 (0.759)	2.083 (0.693)	1.917/1.917	92.7	0.359	-0.328	-0.129

Table S6 Computed (M06-D3/Def2-TZVP) important geometrical parameters and natural charges (q) at the nitrogen atom of NH₃ and Al/Ga center for the loosely bound intermediate (**Int**) involved in the activation of N–H bond of NH₃ by some of the representative Al(I) and Ga(I) carbenoids. Bond lengths are given in Å and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	Al-NH ₃	q _{Al}	q _{NH₃}	Molecules	Ga-NH ₃	q _{Ga}	q _{NH₃}
1AlInt^{N-H}	2.306 (0.176)	0.659	-1.081	1GaInt^{N-H}	2.544 (0.140)	0.677	-1.061
4AlInt^{N-H}	2.271 (0.190)	0.536	-1.070	4GaInt^{N-H}	2.687 (0.125)	0.536	-1.045
6AlInt^{N-H}	2.282 (0.184)	0.553	-1.069	6GaInt^{N-H}	2.720 (0.116)	0.557	-1.048
8AlInt^{N-H}	2.233 (0.188)	0.648	-1.083	8GaInt^{N-H}	2.468 (0.153)	0.650	-1.060
10AlInt^{N-H}	2.263 (0.188)	0.522	-1.065	10GaInt^{N-H}	–	–	–
11AlInt^{N-H}	2.261 (0.188)	0.638	-1.078	11GaInt^{N-H}	2.892 (0.085)	0.673	-1.056
13AlInt^{N-H}	2.338 (0.166)	0.620	-1.065	13GaInt^{N-H}	–	–	–

Table S7 Computed (M06-D3/Def2-TZVP) key geometrical parameters, occupancies of the formally vacant p-orbital (Occ_E) and natural charges at negatively polarized amide NH_2 moiety ($q_{\text{NH}_2^{\delta-}}$) and hydrogen atom ($q_{\text{H}^{\delta+}}$) of the transition states involved in the activation of ammonia by some of the representative Al(I) and Ga(I) carbenoids. Bond angles ($\angle\text{X-E-N}$, $E = \text{Al, Ga}$ and $\text{X} = \text{C, N, Si}$), bond lengths ($E - \text{N}/E - \text{X}$) are given in degree ($^\circ$) and in \AA respectively. Wiberg Bond Index (WBI) values are mentioned within parentheses.

Molecules	$\text{H}_2 \text{N}^{\delta-}-\text{H}^{\delta+}$	$\text{H}_2 \text{N}^{\delta-}-E$	$E-\text{H}^{\delta+}$	$E-\text{N}/E-\text{X}$	$\angle\text{X-E-N}$	$q_{\text{NH}_2^{\delta-}}$	$q_{\text{H}^{\delta+}}$	Occ_E
1AlTS^{N-H}	1.414 (0.304)	1.936 (0.531)	1.710 (0.652)	1.952/ 1.959	93.4	-1.310	0.091	0.298
4AlTS^{N-H}	1.368 (0.311)	1.962 (0.514)	1.745 (0.641)	1.945/2.011	94.7	-1.322	0.087	0.310
6AlTS^{N-H}	1.379 (0.306)	1.966 (0.509)	1.733 (0.645)	1.988/1.966	91.9	-1.321	0.095	0.446
8AlTS^{N-H}	1.385 (0.305)	1.981 (0.486)	1.719 (0.648)	1.926/1.915	95.2	-1.329	0.090	0.564
10AlTS^{N-H}	1.361 (0.311)	1.979 (0.502)	1.748 (0.645)	1.876/2.010	93.9	-1.322	0.089	0.452
11AlTS^{N-H}	1.392 (0.305)	1.945 (0.524)	1.734 (0.653)	1.884/1.915	90.2	-1.325	0.086	0.378
13AlTS^{N-H}	1.382 (0.307)	1.958 (0.507)	1.737 (0.655)	1.882/1.877	91.6	-1.327	0.089	0.557
1GaTS^{N-H}	1.554 (0.241)	2.058 (0.544)	1.645 (0.709)	2.019/2.017	93.4	-1.286	0.056	0.313
4GaTS^{N-H}	1.536 (0.233)	2.102 (0.515)	1.649 (0.708)	2.016/2.026	94.2	-1.281	0.055	0.292
6GaTS^{N-H}	1.520 (0.240)	2.105 (0.505)	1.653 (0.695)	2.069/1.979	91.0	-1.290	0.059	0.340
8GaTS^{N-H}	1.556 (0.231)	2.056 (0.530)	1.641 (0.712)	2.031/1.967	93.5	-1.281	0.044	0.348
10GaTS^{N-H}	1.613 (0.203)	2.390 (0.431)	1.616 (0.740)	1.942/1.999	93.5	-1.255	-0.021	0.342
11GaTS^{N-H}	1.522 (0.246)	2.070 (0.535)	1.660 (0.701)	1.983/1.979	87.5	-1.300	0.052	0.177
13GaTS^{N-H}	1.518 (0.246)	2.076 (0.524)	1.665 (0.702)	1.953/1.947	89.1	-1.291	0.051	0.498

Table S8 Computed (M06-D3/Def2-TZVP) key geometrical parameters, occupancies of the formally vacant p-orbital (Occ_E) and natural charges at negatively polarized fluorine atom ($q_{F\delta^-}$) and ipso – C – atom of the cationic F_5C_6 moiety ($q_{C_6F_5}$) of the transition states involved in the activation of hexa-fluorobenzene by some of the representative Al(I) and Ga(I) carbenoids. Bond angles ($\angle X-E-N$, $E = \text{Al, Ga}$ and $X = \text{C, N, Si}$), bond lengths ($E - N/E - X$) are given in degree ($^\circ$) and in Å respectively. Wiberg Bond Index (WBI) values are mentioned within parentheses.

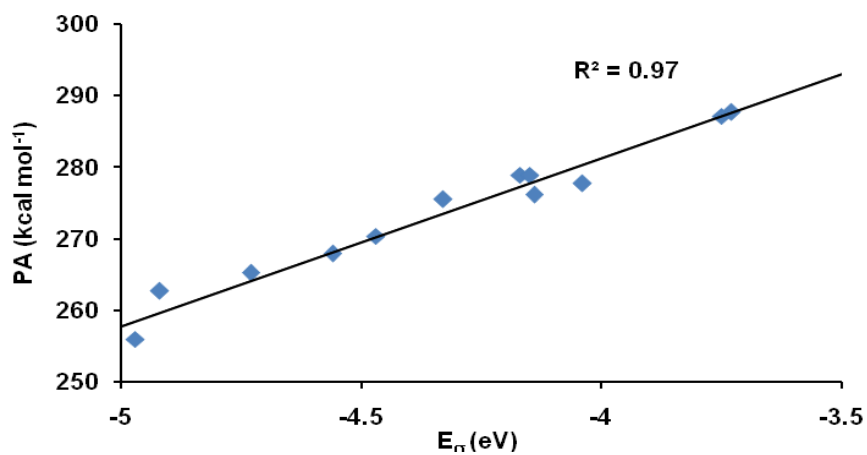
Molecules	$F_5 C_6-F\delta^-$	$F_5 C_6-E$	$E-F\delta^-$	$E-N/E-X$	$\angle X-E-N$	$q_{C_6F_5}$	$q_{F\delta^-}$	Occ_E
1AlTS^{C-F}	1.458 (0.707)	2.350 (0.417)	2.215 (0.159)	1.941/ 1.941	93.2	0.054	-0.399	0.227
4AlTS^{C-F}	1.372 (0.831)	2.518 (0.319)	2.895 (0.062)	1.941/2.014	93.5	0.136	-0.351	0.325
6AlTS^{C-F}	1.409 (0.778)	2.400 (0.412)	2.483 (0.109)	1.967/1.941	92.6	0.086	-0.367	0.209
8AlTS^{C-F}	1.393 (0.790)	2.502 (0.370)	2.710 (0.081)	1.888/1.870	96.9	0.130	-0.378	0.145
10AlTS^{C-F}	1.378 (0.818)	2.610 (0.362)	2.795 (0.079)	1.861/2.000	93.6	0.176	-0.357	0.132
11AlTS^{C-F}	1.388 (0.808)	2.419 (0.400)	2.603 (0.096)	1.877/1.887	91.6	0.098	-0.350	0.153
13AlTS^{C-F}	1.386 (0.806)	2.518 (0.373)	2.681 (0.086)	1.857/1.860	92.1	0.145	-0.360	0.150
1GaTS^{C-F}	1.588 (0.553)	2.201 (0.532)	2.169 (0.212)	1.993/1.992	93.1	-0.029	-0.477	0.186
6GaTS^{C-F}	1.492 (0.658)	2.207 (0.535)	2.377 (0.147)	2.038/1.948	92.5	-0.014	-0.427	0.182
8GaTS^{C-F}	1.477 (0.671)	2.289 (0.479)	2.382 (0.139)	1.997/1.951	96.3	0.032	-0.429	0.133
10GaTS^{C-F}	1.382 (0.802)	2.487 (0.412)	2.817 (0.077)	1.940/2.028	92.0	0.160	-0.368	0.158
11GaTS^{C-F}	1.624 (0.494)	1.977 (0.649)	2.557 (0.112)	1.888/1.884	94.9	-0.252	-0.529	0.149

Table S9 Computed (M06-D3/Def2-TZVP) key geometrical parameters, occupancies of the formally vacant p-orbital (Occ_E) and natural charges at negatively polarized hydrogen atom (q_{H^δ}) and cationic BPin moiety (q_{BPin}) of the transition states involved in the activation of pinacolborane by some of the representative Al(I) and Ga(I) carbenoids. Bond angles ($\angle\text{X-E-N}$, E = Al, Ga and X = C, N, Si), bond lengths (E – N/E – X) are given in degree ($^\circ$) and in Å respectively. Wiberg Bond Index (WBI) values are mentioned within parentheses.

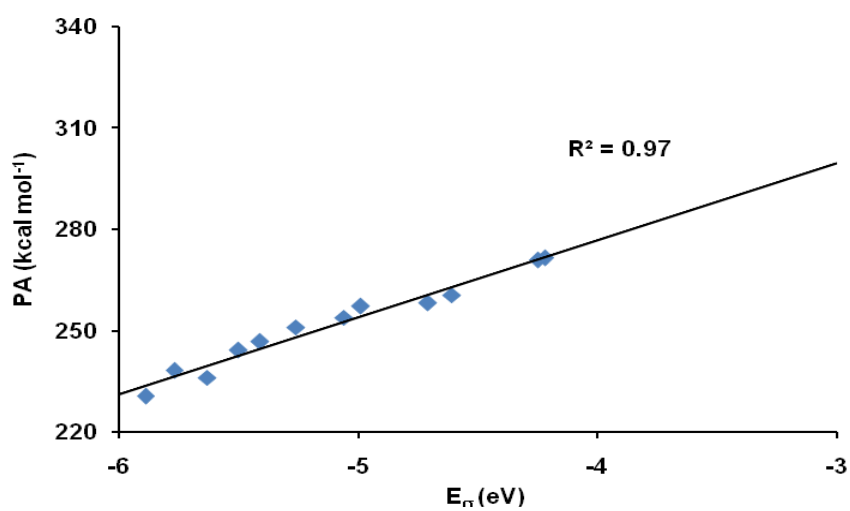
Molecules	$\text{H}^\delta\text{-B}_{\text{pin}}$	E-B_{Pin}	E-H^δ	E-N/E-X	$\angle\text{X-E-N}$	q_{H^δ}	q_{BPin}	Occ_E
1AITS^{B-H}	1.494 (0.567)	2.021 (0.973)	1.814 (0.355)	1.909/1.910	96.5	-0.158	0.319	0.504
4AITS^{B-H}	1.485 (0.595)	2.014 (0.961)	1.841 (0.319)	1.891/1.966	99.2	-0.165	0.257	0.471
6AITS^{B-H}	1.518 (0.554)	2.020 (0.965)	1.819 (0.344)	1.917/1.920	96.1	-0.176	0.319	0.499
8AITS^{B-H}	1.525 (0.564)	2.013 (0.944)	1.847 (0.332)	1.876/1.856	100.1	-0.202	0.277	0.444
10AITS^{B-H}	1.531 (0.569)	2.012 (0.952)	1.841 (0.326)	1.828/1.952	98.2	-0.198	0.268	0.469
11AITS^{B-H}	1.538 (0.555)	2.003 (0.969)	1.817 (0.346)	1.833/1.863	94.2	-0.190	0.293	0.490
13AITS^{B-H}	1.548 (0.557)	2.008 (0.958)	1.841 (0.331)	1.828/1.831	95.7	-0.215	0.280	0.472
1GaTS^{B-H}	1.661 (0.444)	1.999 (1.005)	1.806 (0.471)	1.969/1.968	95.0	-0.162	0.460	0.545
4GaTS^{B-H}	1.653 (0.469)	1.993 (1.006)	1.831 (0.434)	1.955/1.982	98.0	-0.173	0.410	0.521
6GaTS^{B-H}	1.683 (0.438)	1.998 (0.997)	1.827 (0.451)	2.005/1.937	94.3	-0.184	0.454	0.540
8GaTS^{B-H}	1.705 (0.426)	1.992 (0.985)	1.825 (0.459)	1.966/1.917	98.1	-0.217	0.448	0.502
10GaTS^{B-H}	1.695 (0.452)	1.992 (0.997)	1.846 (0.432)	1.904/1.970	96.2	-0.205	0.420	0.514
11GaTS^{B-H}	1.718 (0.427)	1.982 (1.010)	1.811 (0.466)	1.908/1.921	92.6	-0.195	0.456	0.542
13GaTS^{B-H}	1.722 (0.435)	1.985 (1.000)	1.843 (0.439)	1.898/1.892	93.1	-0.229	0.439	0.513

Table S10 Comparison of the Activation Energy Barriers ($\Delta G_{\text{TS}}^0 \text{X-Y}^\ddagger$) and Reaction Free Energies for the formation of the Intermediates ($\Delta G_{\text{Int}}^0 \text{X-Y}$), van der Waals complexes ($\Delta G_{\text{V}}^0 \text{X-Y}$) and the X–Y (**X = B, C, H, N** and **Y = F, H**) bond splitting products ($\Delta G_{\text{Total}}^0 \text{X-Y}$) for the activation of H₂, NH₃, C₆F₆ and pinacolborane by some of the representative Al(I) and Ga(I) carbenoids calculated at different levels of theory (in gas-phase) using **Def2-TZVP** basis set. The energies are given in kcal mol⁻¹.

Substrates	Molecules	Level of Theory	$\Delta G_{\text{Int}}^0 \text{X-Y}$	$\Delta G_{\text{V}}^0 \text{X-Y}$	$\Delta G_{\text{TS}}^0 \text{X-Y}^\ddagger$	$\Delta G_{\text{Total}}^0 \text{X-Y}$
H ₂	1Al	PBE0-D3	–	–	39.6	-28.5
		M062X-D3	–	–	46.1	-25.2
		B3PW91-D3	–	–	40.5	-27.4
		M06-D3	–	–	41.5	-29.2
	4Al	PBE0-D3	–	–	31.8	-30.3
		M062X-D3	–	–	37.6	-27.6
		B3PW91-D3	–	–	32.5	-29.6
		M06-D3	–	–	33.3	-30.9
NH ₃	6Al	PBE0-D3	2.7	–	26.9	-44.2
		M062X-D3	2.9	–	29.5	-46.4
		B3PW91-D3	3.6	–	27.4	-44.1
		M06-D3	3.2	–	29.2	-45.7
C ₆ F ₆	1Al	PBE0-D3	–	–	18.7	-103.4
		M062X-D3	–	–	21.1	-107.1
		B3PW91-D3	–	–	18.7	-103.8
		M06-D3	–	–	20.1	-100.2
HB _{Pin}	4Al	PBE0-D3	–	3.6	4.9	-20.0
		M062X-D3	–	4.2	8.8	-17.5
		B3PW91-D3	–	3.4	5.3	-20.0
		M06-D3	–	1.9	7.8	-18.2

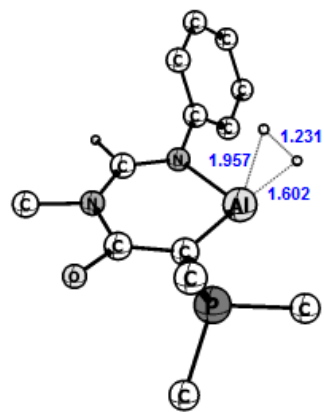


(a)

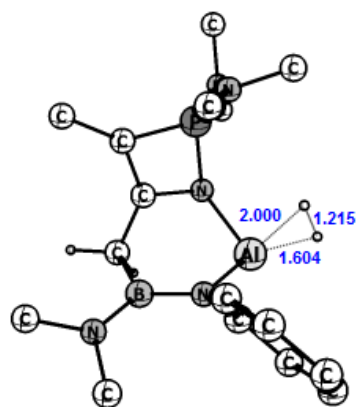


(b)

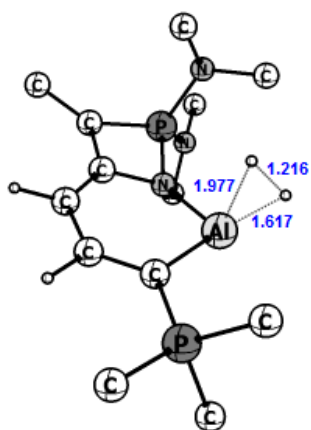
Fig. S1 Correlation plots between the E_{σ} (eV) and PA (kcal mol⁻¹) for (a) Al(I) carbenoids (1Al–13Al) and (b) Ga(I) carbenoids (1Ga–13Ga).



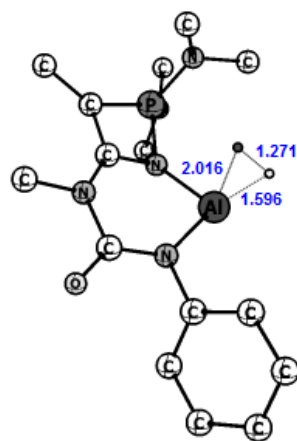
6AITSH-H



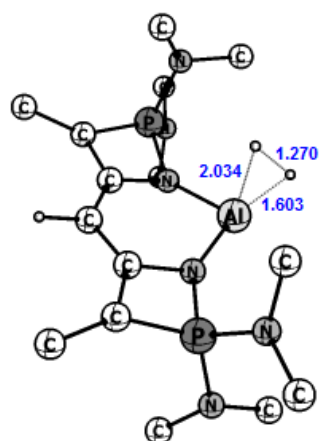
8AITSH-H



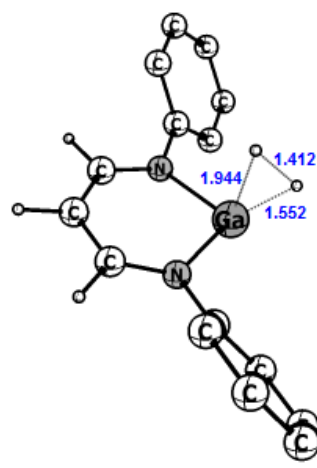
10AITSH-H



11AITSH-H



13AITSH-H



1GaTSH-H

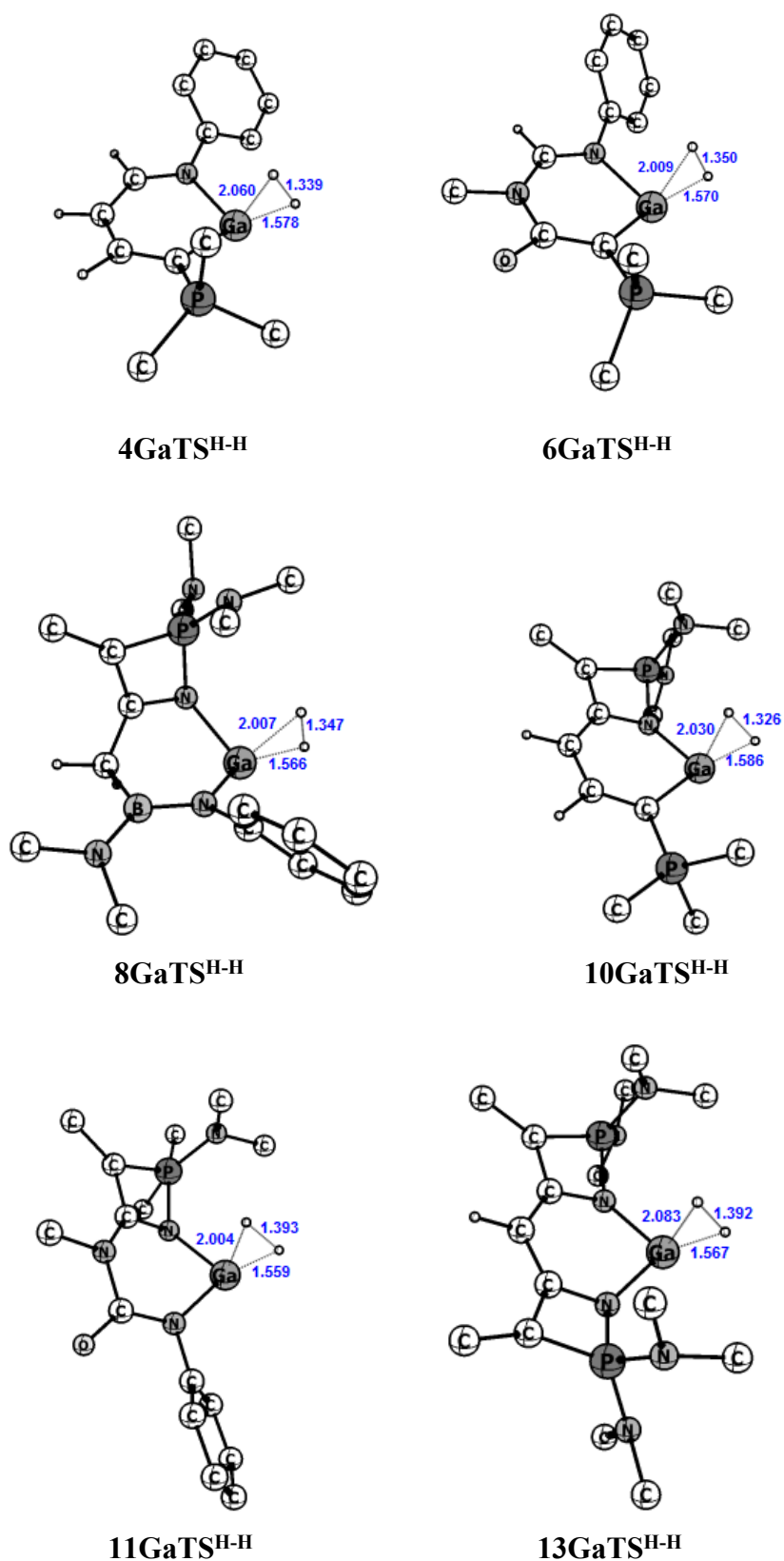
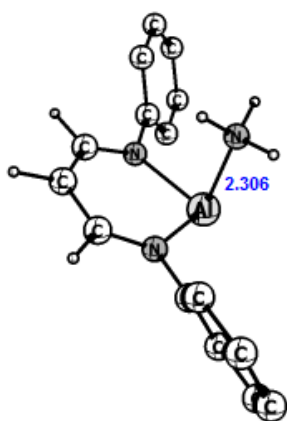
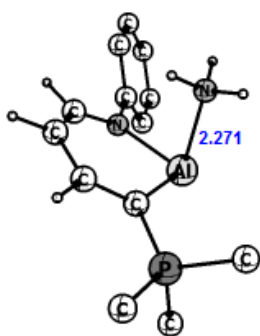


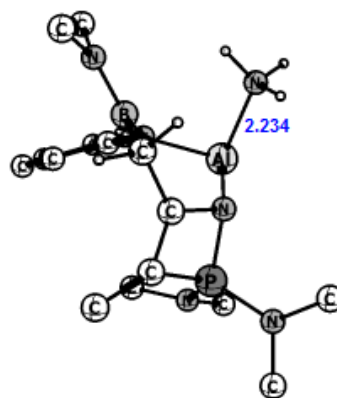
Fig. S2 Optimized geometries (at M06-D3/Def2-TZVP level theory) for the transition states involved in the activation of dihydrogen by some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



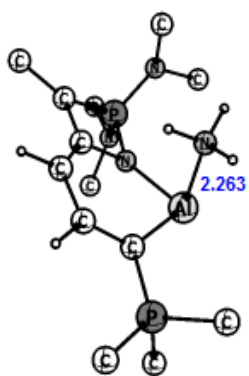
1AlInt^{N-H}



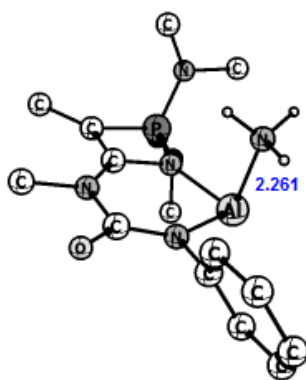
4AlInt^{N-H}



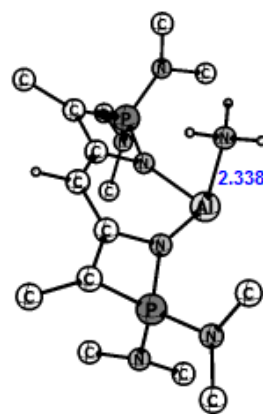
8AlInt^{N-H}



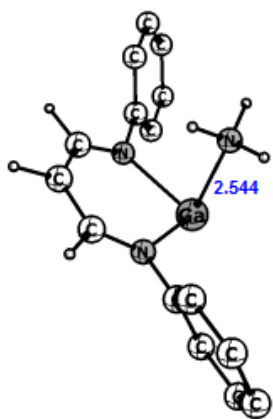
10AlInt^{N-H}



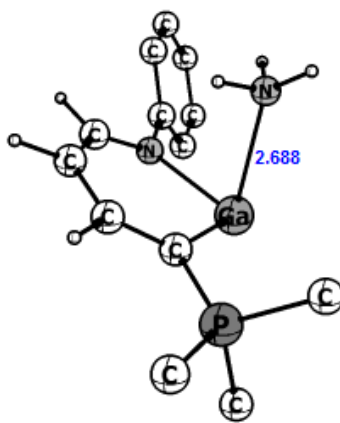
11AlInt^{N-H}



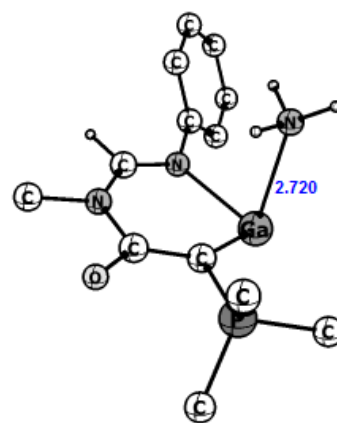
13AlInt^{N-H}



1GaInt^{N-H}



4GaInt^{N-H}



6GaInt^{N-H}

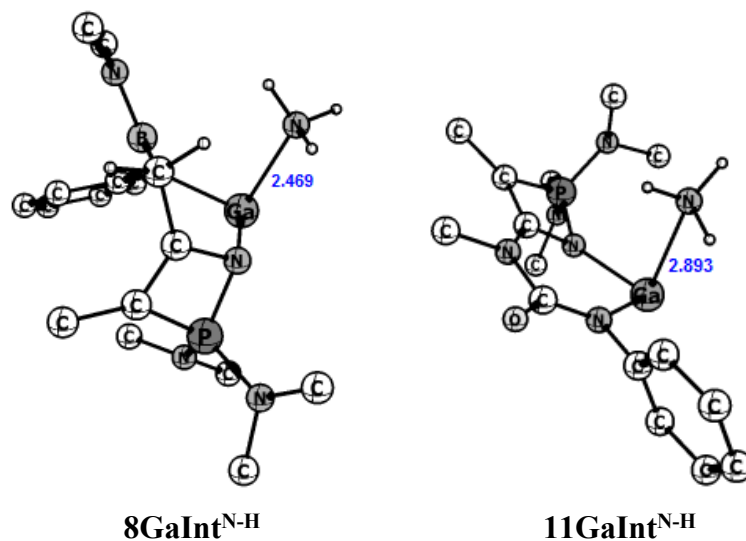
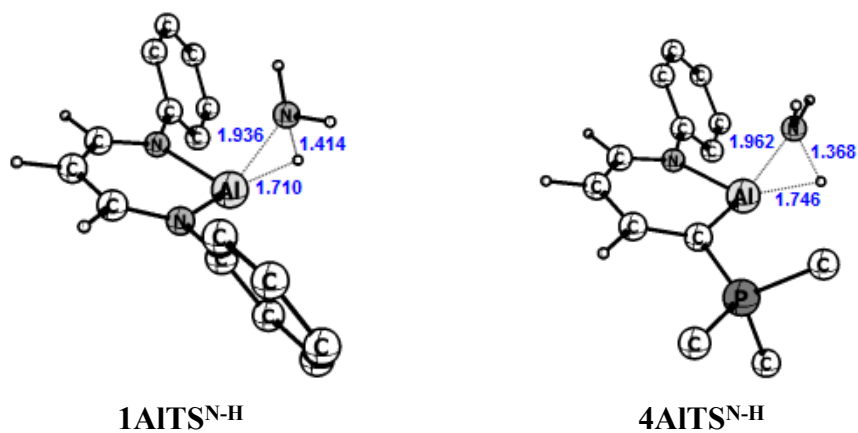
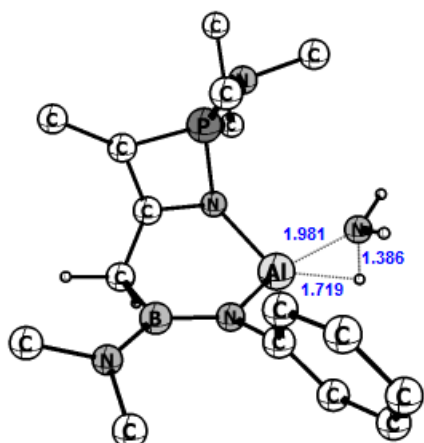
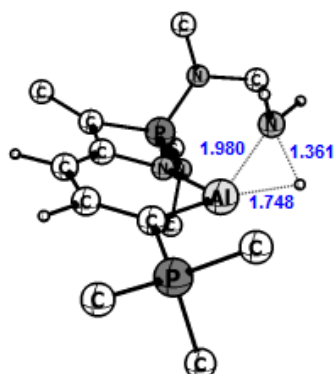


Fig. S3 Optimized geometries (at **M06-D3/Def2-TZVP** level theory) for the loosely bound intermediates involved in the activation of N–H bond of ammonia by some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.

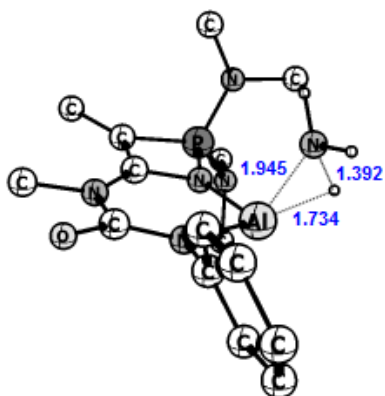




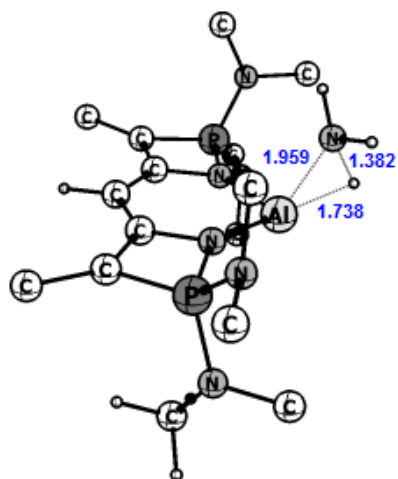
8AITS^{N-H}



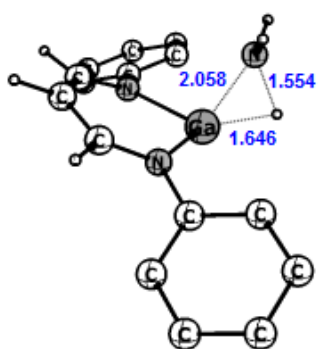
10AITS^{N-H}



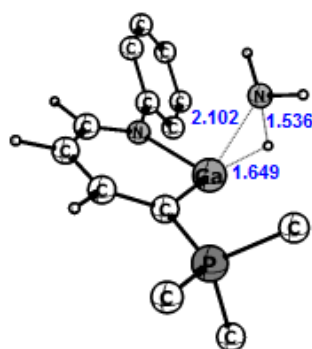
11AITS^{N-H}



13AITS^{N-H}



1GaTS^{N-H}



4GaTS^{N-H}

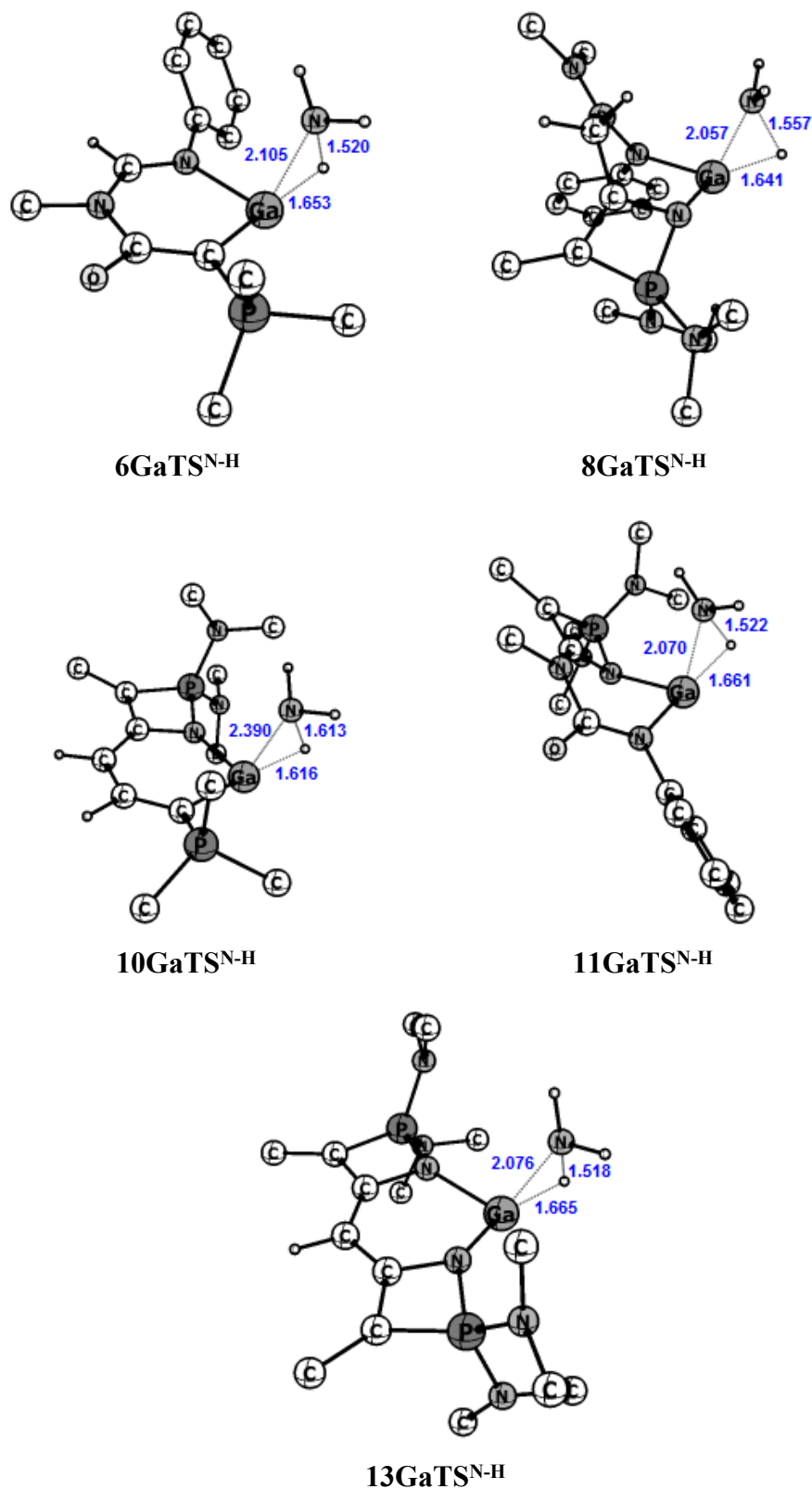
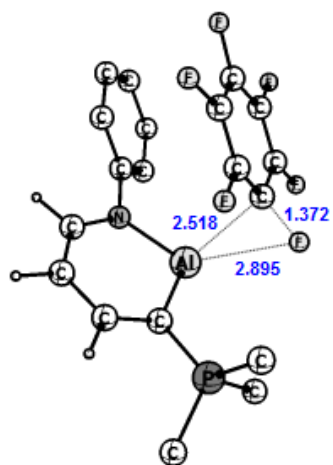
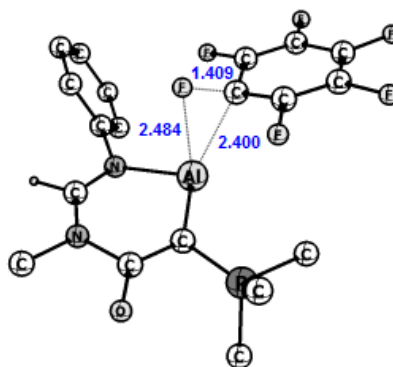


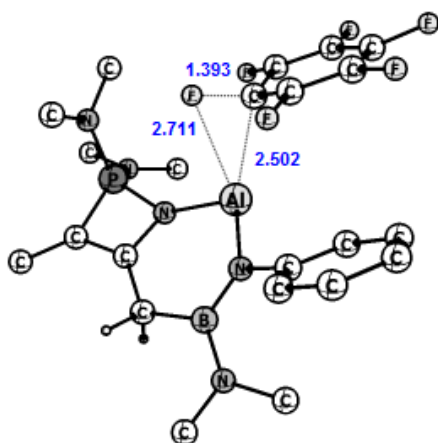
Fig. S4 Optimized geometries (at M06-D3/Def2-TZVP level theory) for the transition states involved in the activation of N–H bond of ammonia by some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



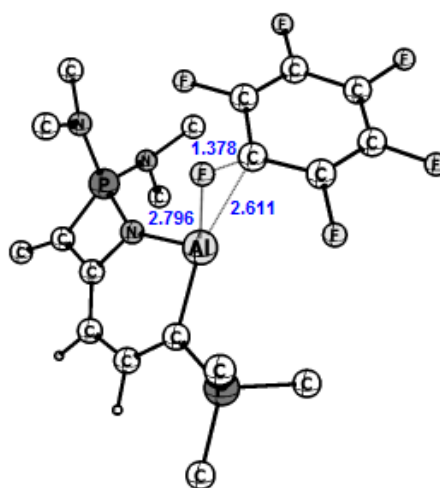
4AITS^{C-F}



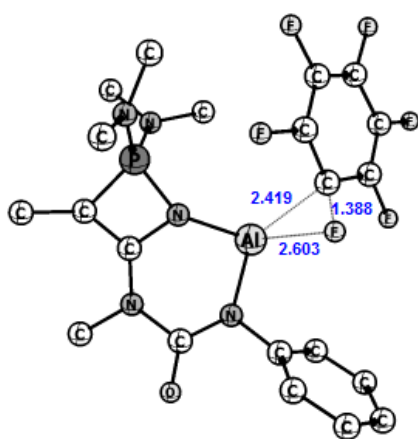
6AITS^{C-F}



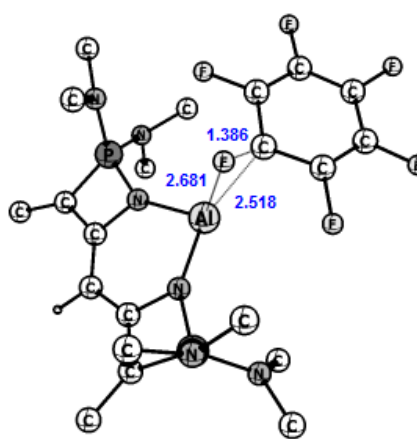
8AITS^{C-F}



10AITS^{C-F}



11AITS^{C-F}



13AITS^{C-F}

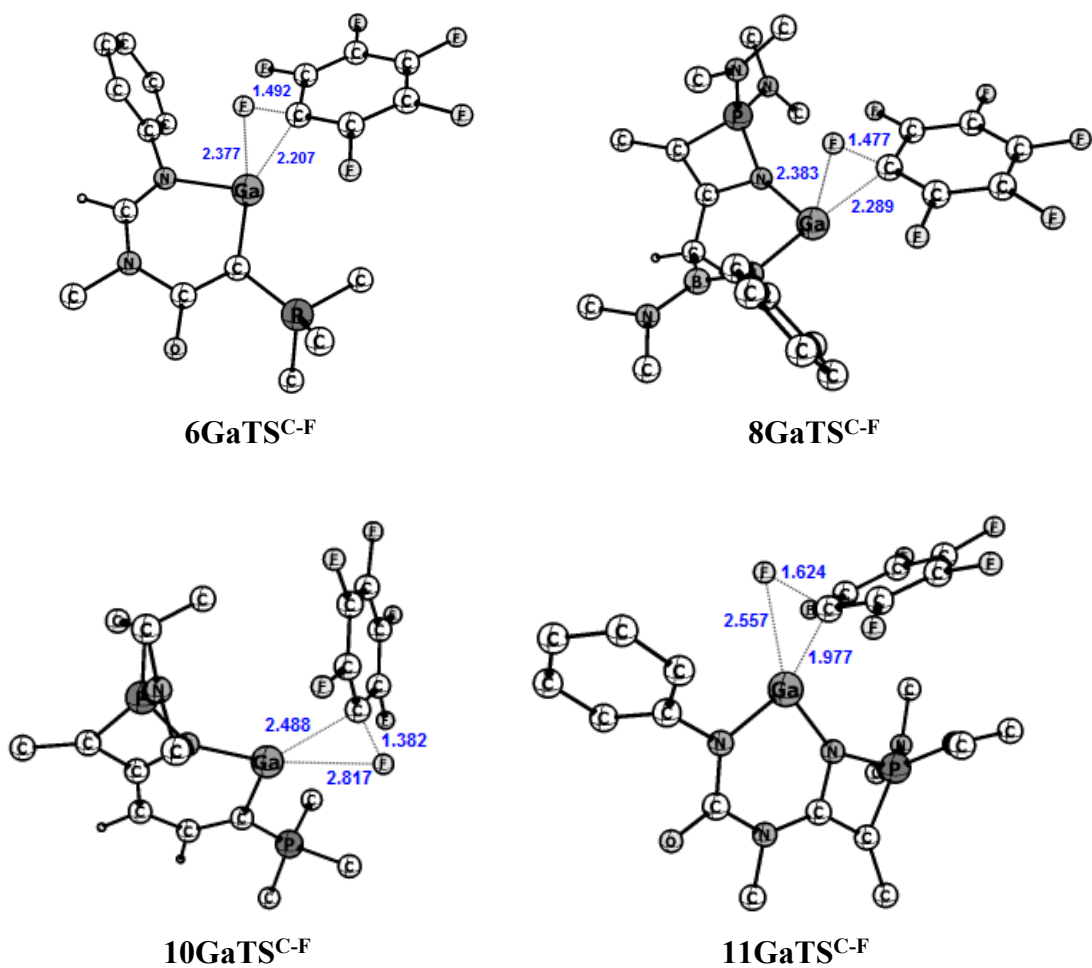
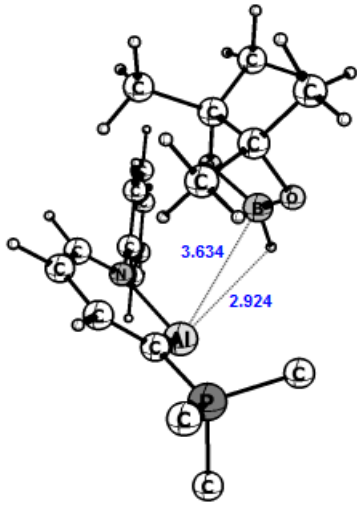
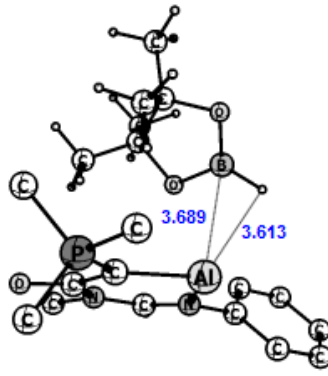


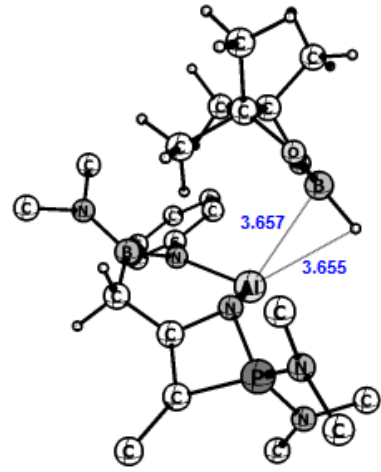
Fig. S5 Optimized geometries (at M06-D3/Def2-TZVP level theory) for the transition states involved in the activation of C–F bond of hexa-fluorobenzene by some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



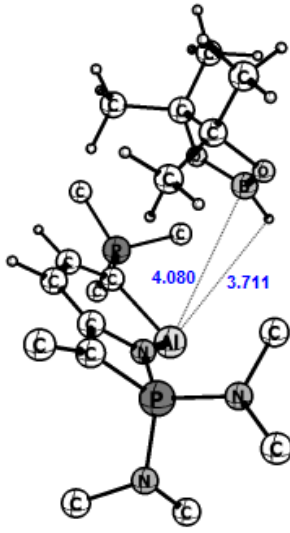
4Alv^{B-H}



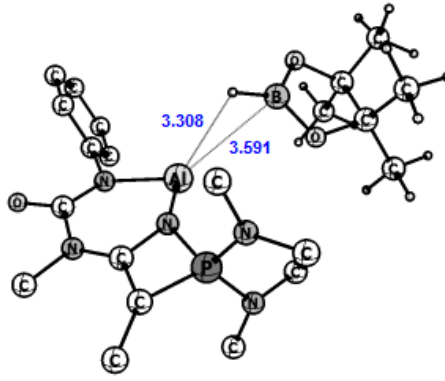
6Alv^{B-H}



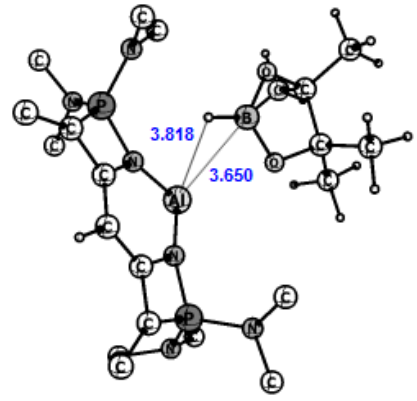
8Alv^{B-H}



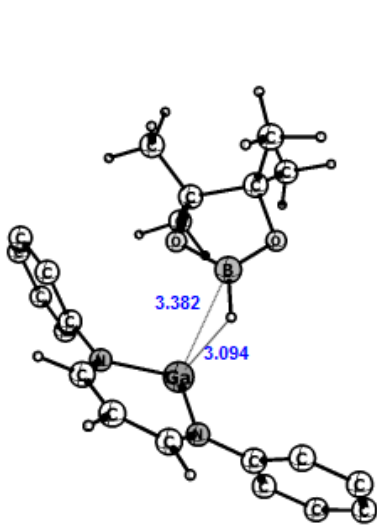
10Alv^{B-H}



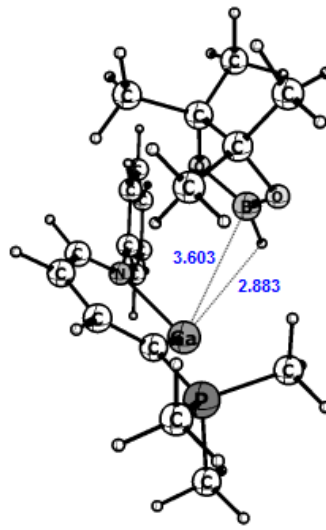
11Alv^{B-H}



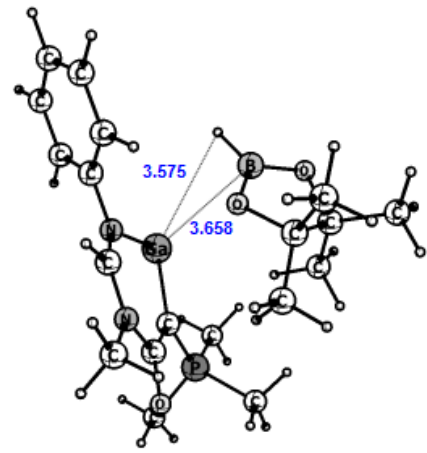
13Alv^{B-H}



1Gav^{B-H}



4Gav^{B-H}



6Gav^{B-H}

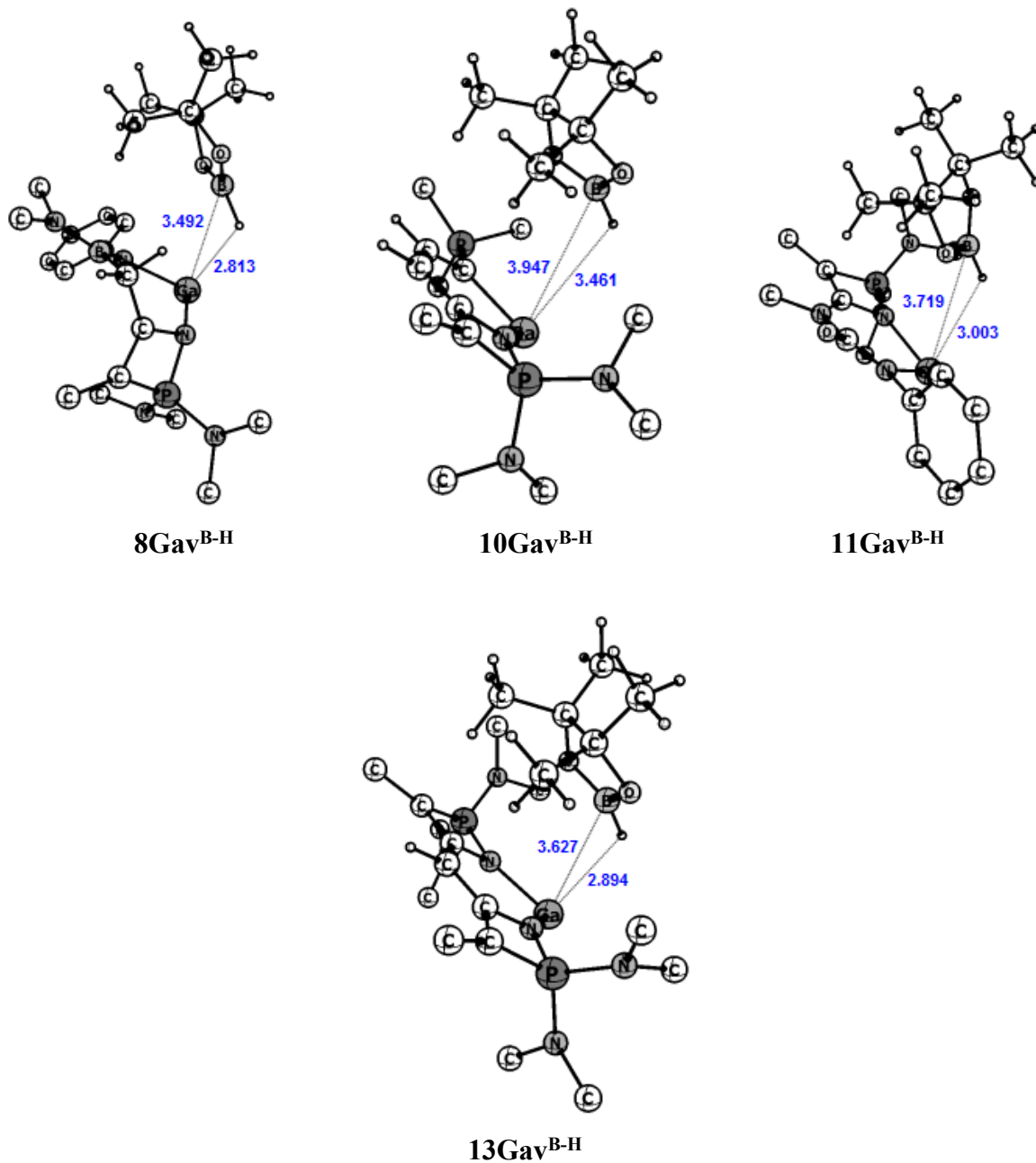
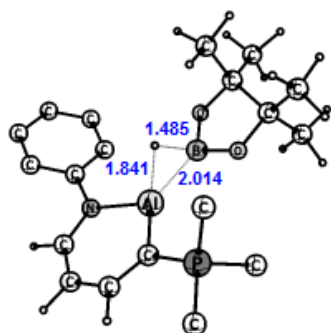
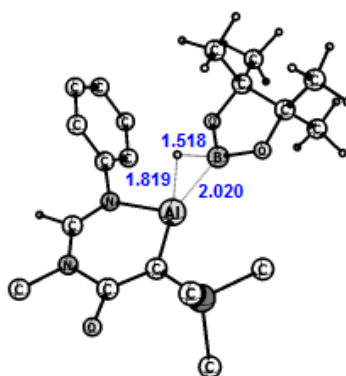


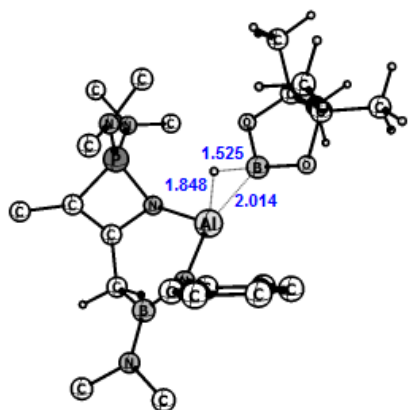
Fig. S6 Optimized geometries (at **M06-D3/Def2-TZVP** level theory) for the van der Waals complexes involved in the activation of B–H bond of pinacolborane by some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



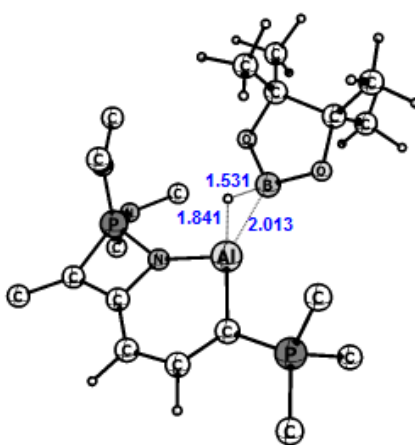
4AITS^{B-H}



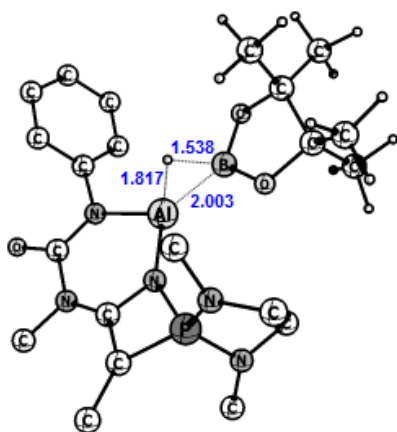
6AITS^{B-H}



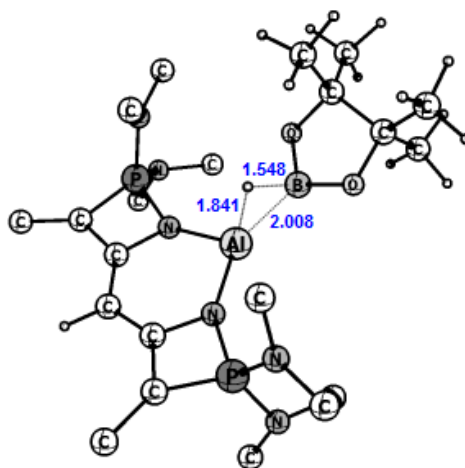
8AITS^{B-H}



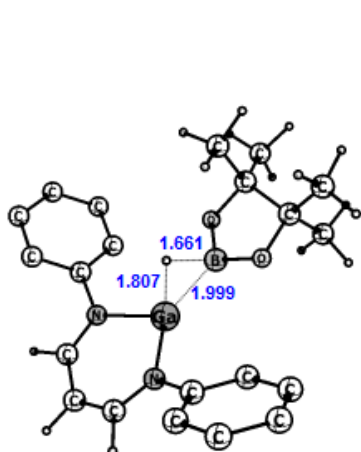
10AITS^{B-H}



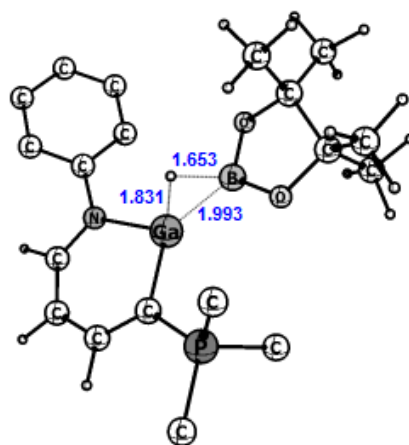
11AITS^{B-H}



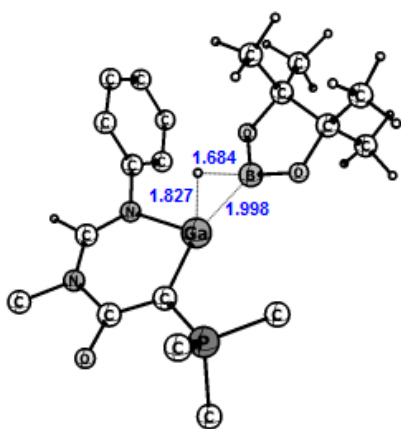
13AITS^{B-H}



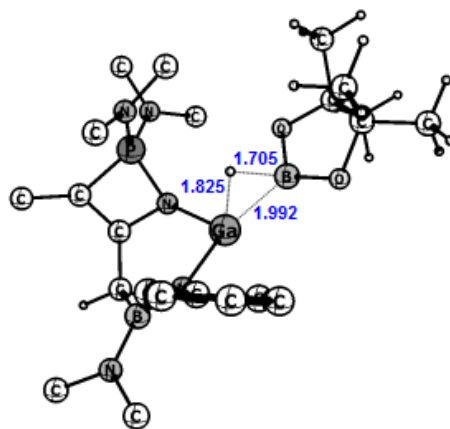
1GaTS^{B-H}



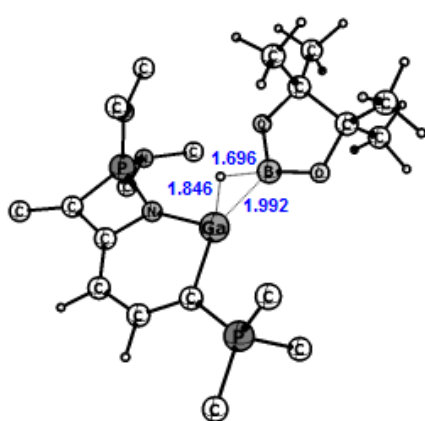
4GaTS^{B-H}



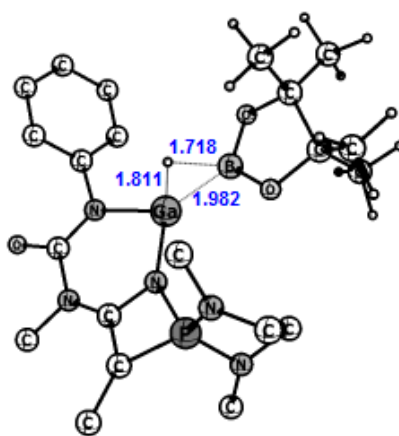
6GaTS^{B-H}



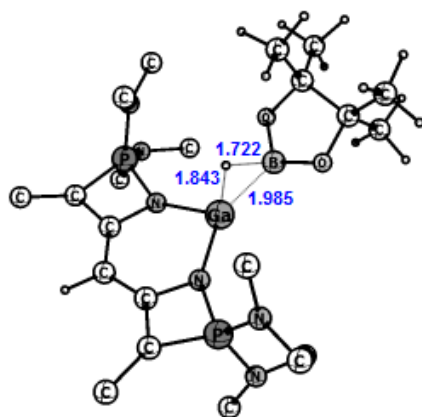
8GaTS^{B-H}



10GaTS^{B-H}

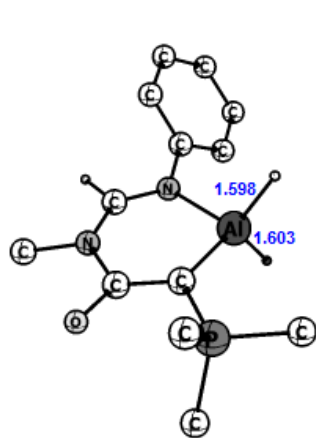


11GaTS^{B-H}

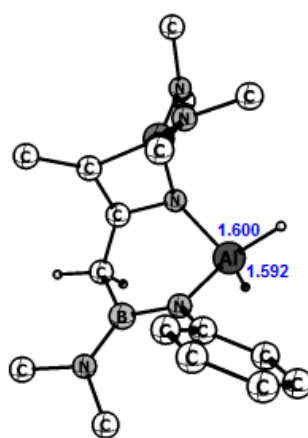


13GaTS^{B-H}

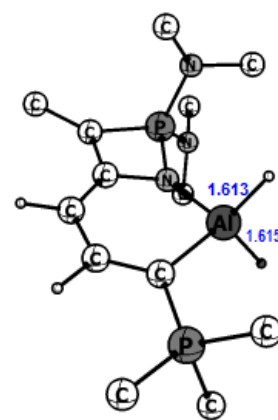
Fig. S7 Optimized geometries (at M06-D3/Def2-TZVP level theory) for the transition states involved in the activation of B–H bond of pinacolborane by some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



6AlP^{H-H}



8AlP^{H-H}



10AlP^{H-H}

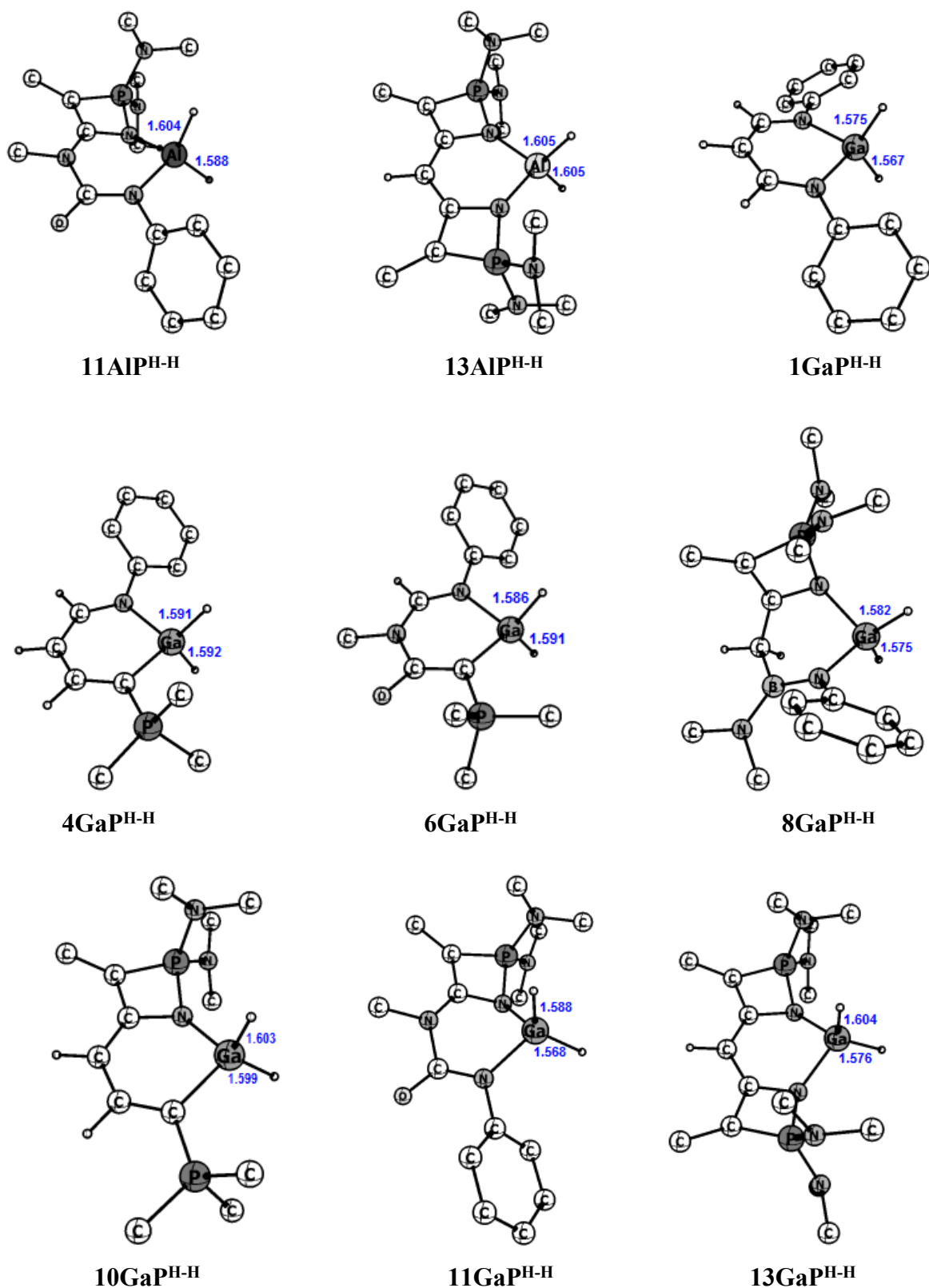
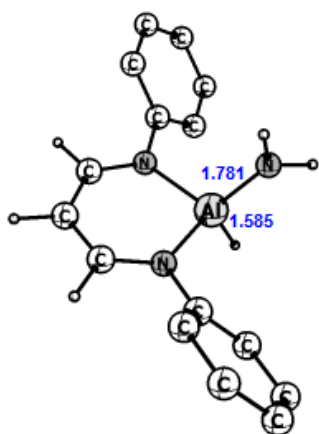
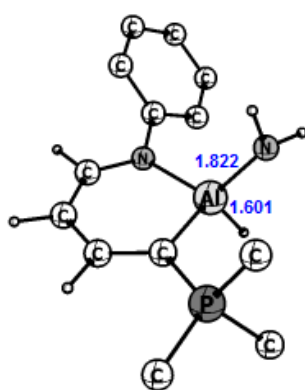


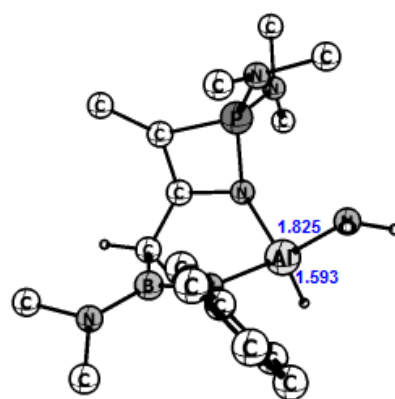
Fig. S8 Optimized geometries (at M06-D3/Def2-TZVP level theory) of the H-H splitting products attained for the reactions of dihydrogen with some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



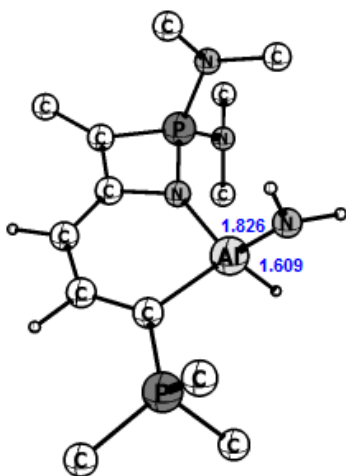
1AIP^{N-H}



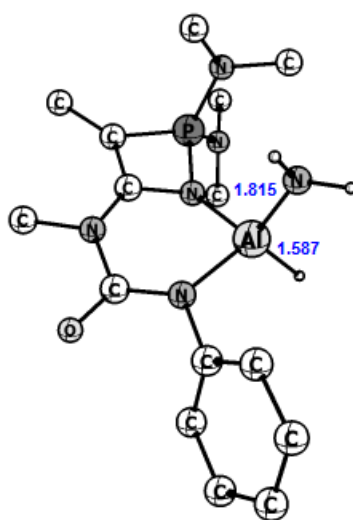
4AIP^{N-H}



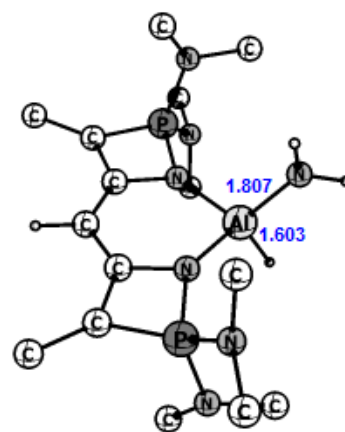
8AIP^{N-H}



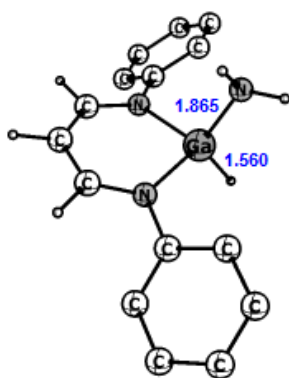
10AIP^{N-H}



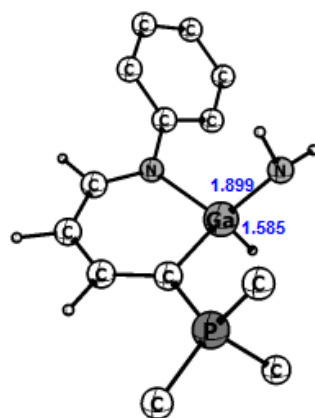
11AIP^{N-H}



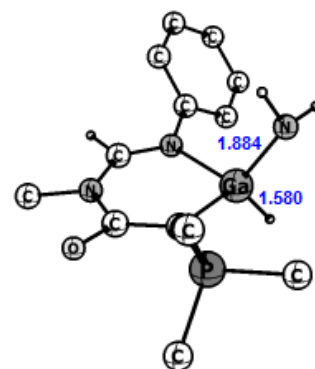
13AIP^{N-H}



1GaP^{N-H}



4GaP^{N-H}



6GaP^{N-H}

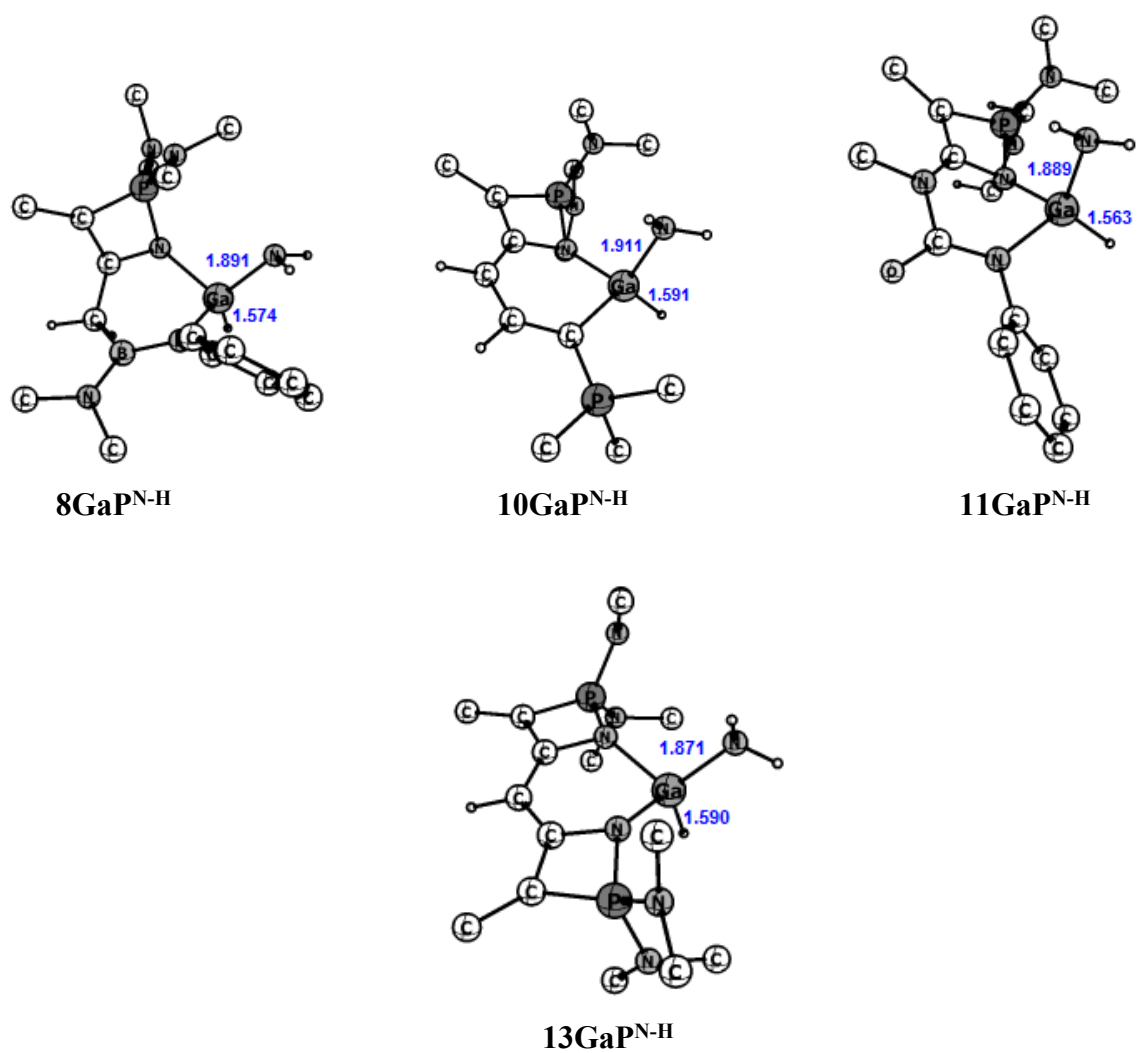
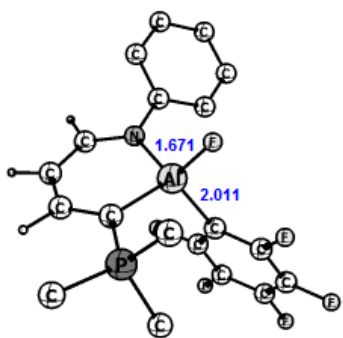
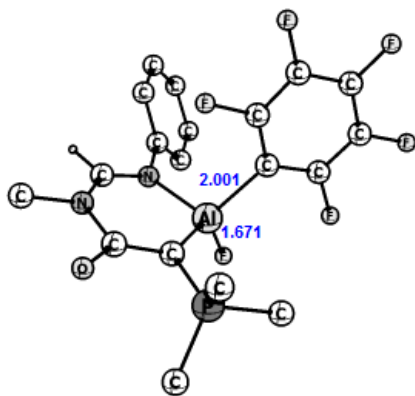


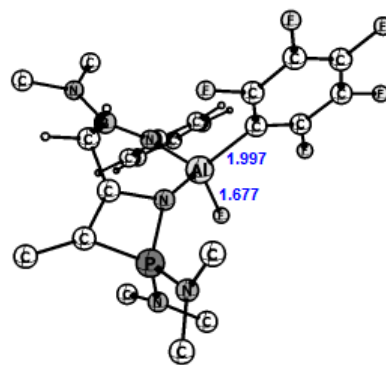
Fig. S9 Optimized geometries (at **M06-D3/Def2-TZVP** level theory) of the N-H splitting products attained for the reactions of ammonia with some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



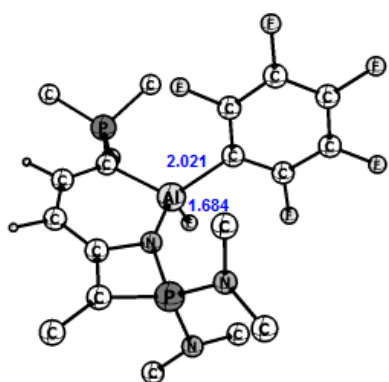
4AIPC-F



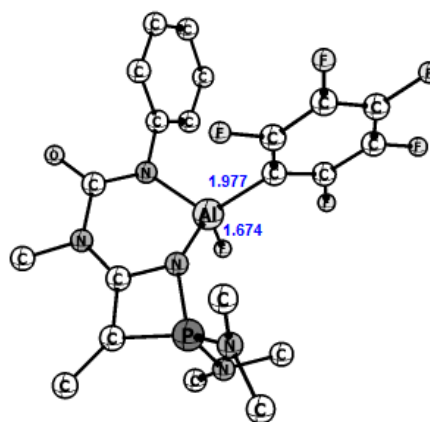
6AIPC-F



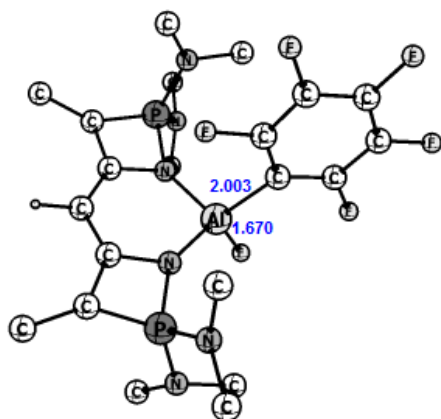
8AIPC-F



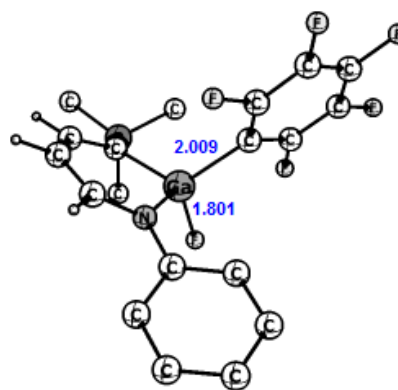
10AIPC-F



11AIPC-F



13AIPC-F



4GaPC-F

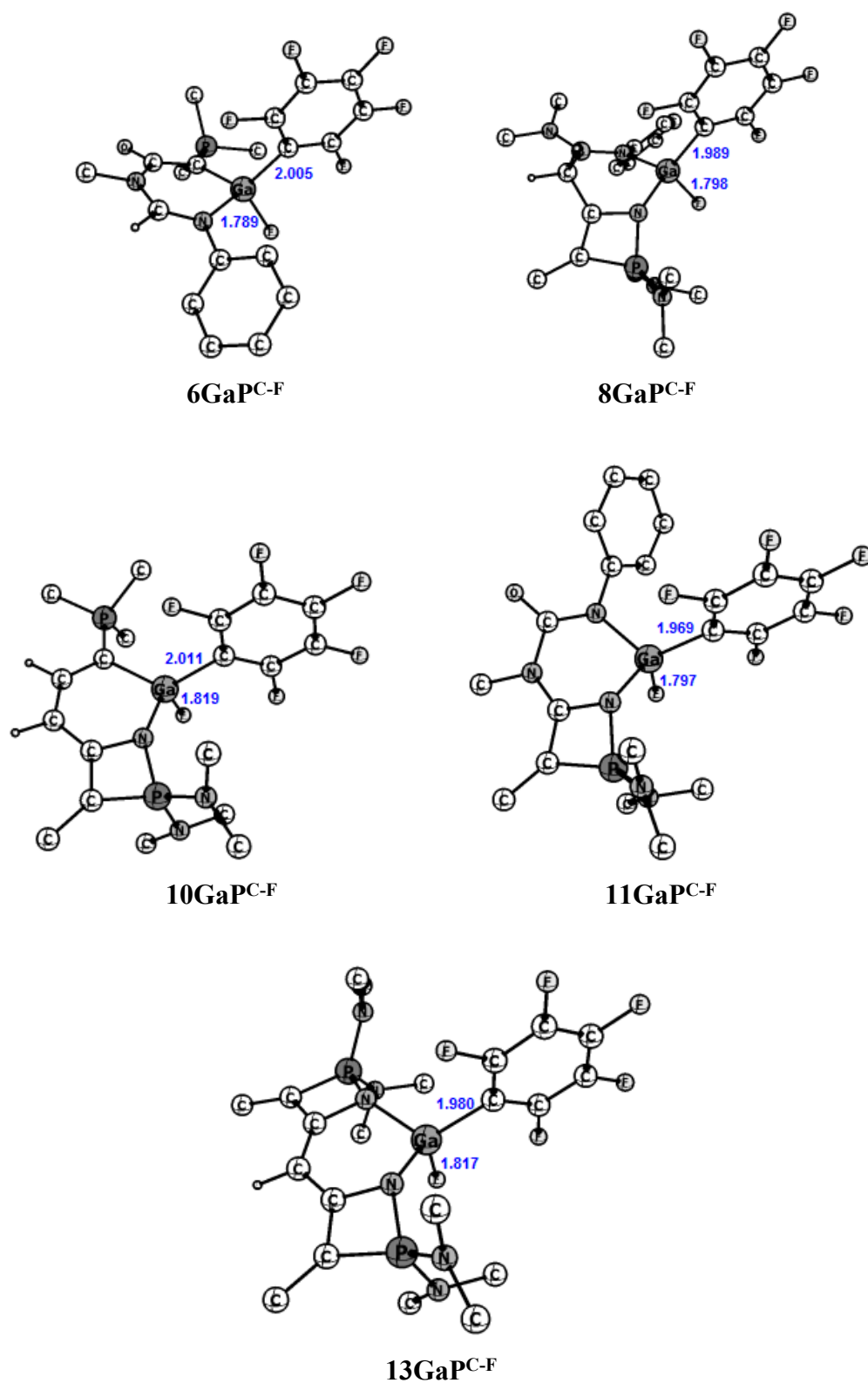
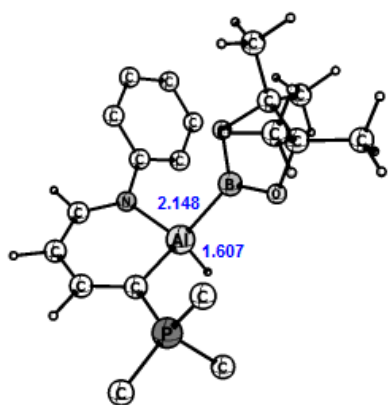
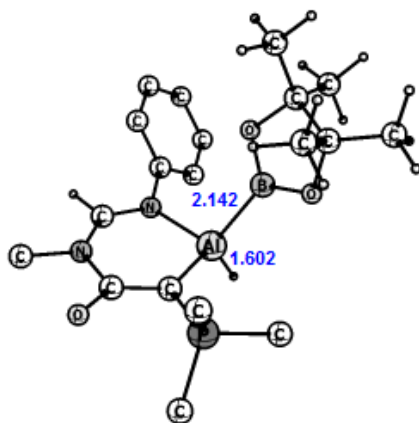


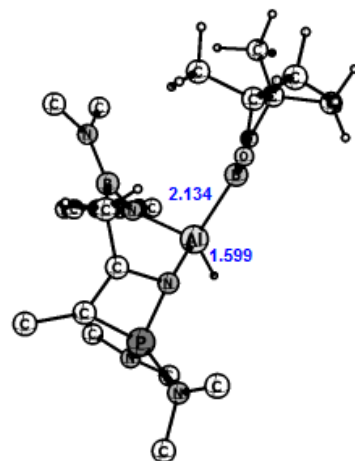
Fig. S10 Optimized geometries (at M06-D3/Def2-TZVP level theory) of the C-F splitting products attained for the reactions of hexafluorobenzene with some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



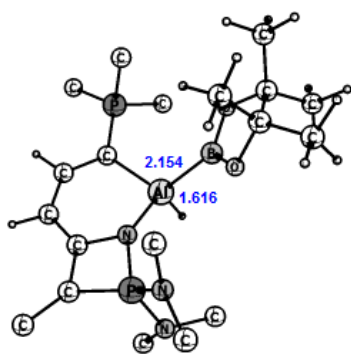
4AIPB-H



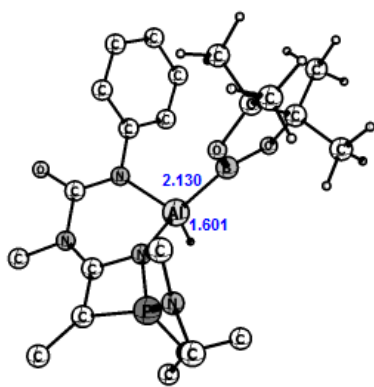
6AIPB-H



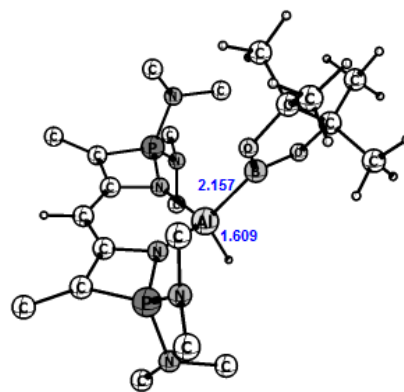
8AIPB-H



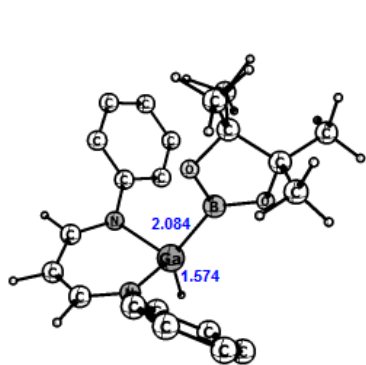
10AIPB-H



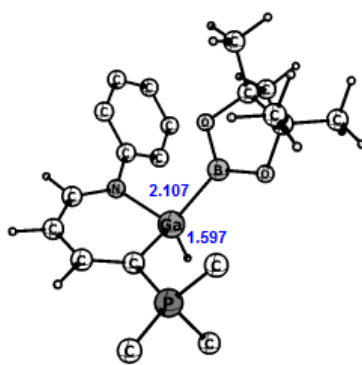
11AIPB-H



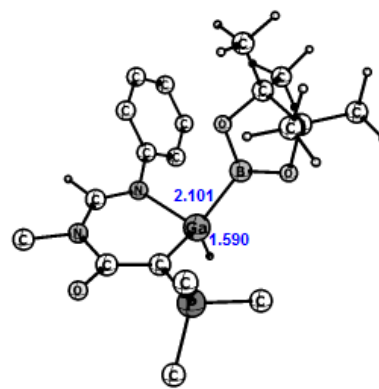
13AIPB-H



1GaPB-H



4GaPB-H



6GaPB-H

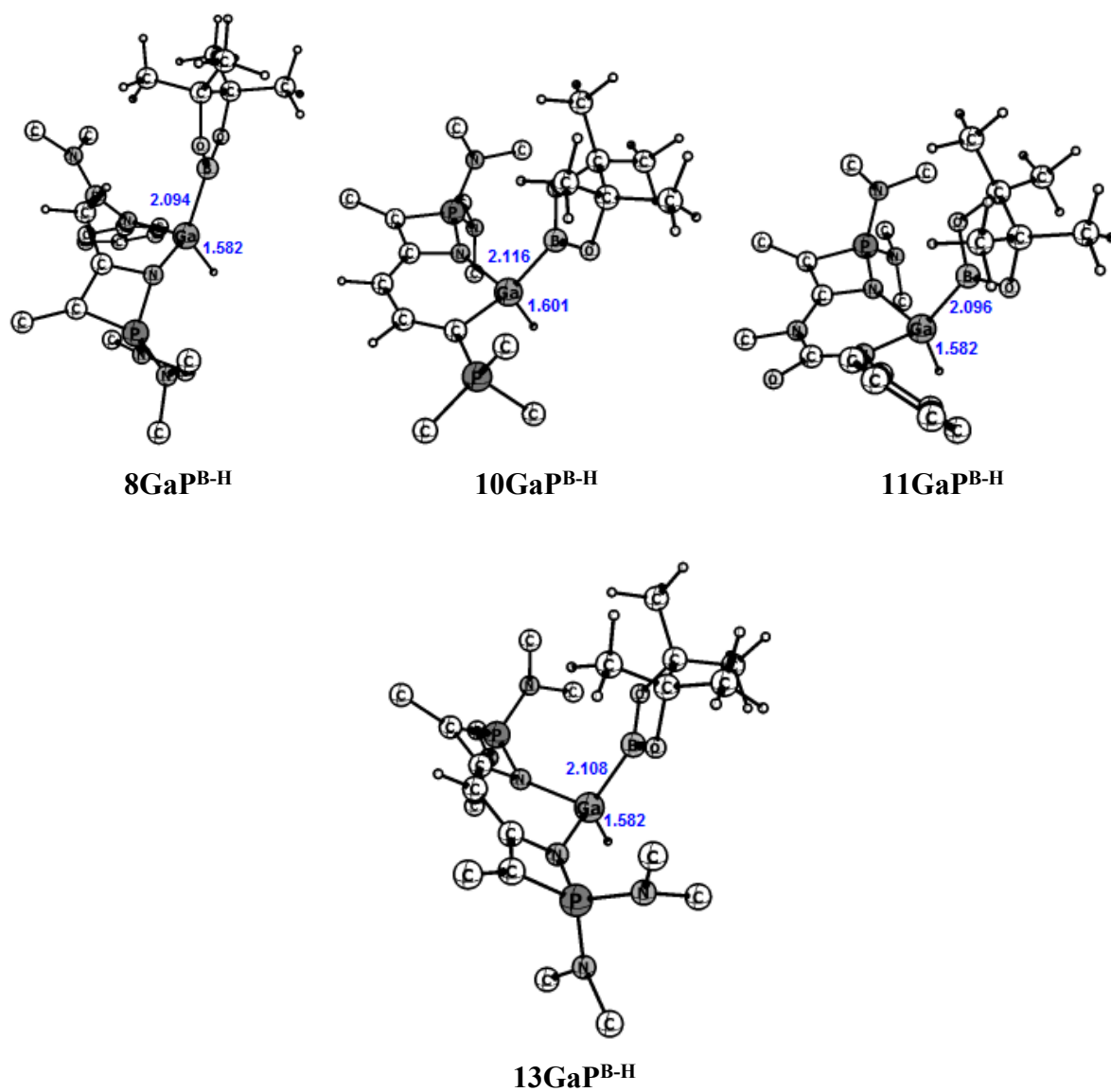
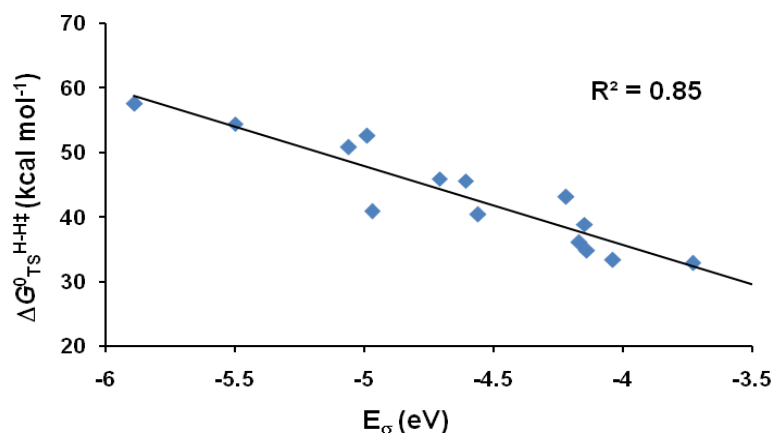
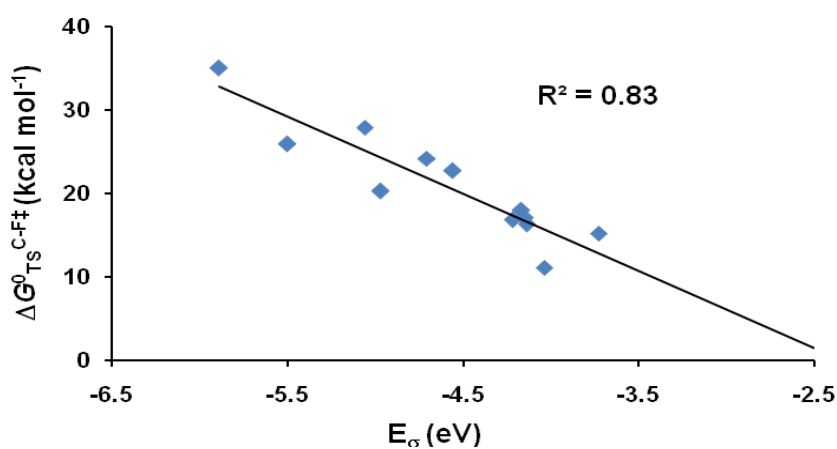


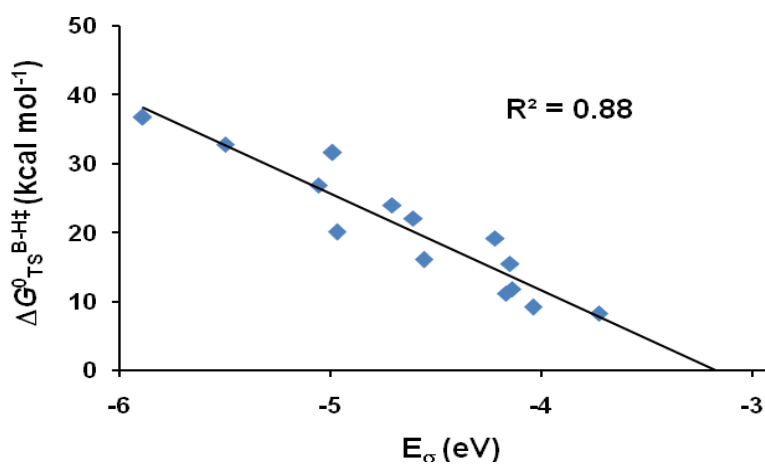
Fig. S11 Optimized geometries (at M06-D3/Def2-TZVP level theory) of the B–H splitting products attained for the reactions of pinacolborane with some of the representative Al(I) and Ga(I) carbenoids. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



(a) Correlation plot between E_σ values and $\Delta G_{TS}^{0, H-H^\ddagger}$ values obtained for Al/Ga carbenoids.



(b) Correlation plot between E_σ values and $\Delta G_{TS}^{0, C-F^\ddagger}$ values obtained for Al/Ga carbenoids.



(c) Correlation plot between E_σ values and $\Delta G_{TS}^{0, B-H^\ddagger}$ values obtained for Al/Ga carbenoids.

Fig. S12 Correlation plots between E_σ values and $\Delta G_{TS}^{0, X-Y^\ddagger}$ values obtained for Al/Ga carbenoids (where, X = B, C, H and Y = H, F) for activation of H_2 , C_6F_6 and H-BPin.

Cartesian coordinates of Al(I) carbenoids (**1Al-13Al**) and Ga(I) carbenoids (**1Ga-13Ga**) in their optimized singlet (S) and triplet (T) states and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1Al-S (T.E = -930.860673)

7	1.405380000	0.449777000	-0.240373000
6	1.222861000	1.704534000	-0.603896000
6	0.000073000	2.327014000	-0.789412000
7	-1.405381000	0.449957000	-0.240238000
1	0.000161000	3.355712000	-1.120609000
1	2.116270000	2.303937000	-0.794826000
6	2.741688000	0.023199000	-0.040966000
6	3.155885000	-1.193303000	-0.572987000
6	3.638014000	0.774148000	0.712979000
6	4.449209000	-1.638677000	-0.368793000
1	2.457476000	-1.778008000	-1.161286000
6	4.931915000	0.326469000	0.908413000
1	3.304935000	1.699950000	1.169624000
6	5.343236000	-0.880482000	0.368245000
1	4.760976000	-2.585098000	-0.794770000
1	5.619262000	0.919623000	1.500469000
1	6.355412000	-1.232391000	0.527570000
6	-2.741700000	0.023356000	-0.040837000
6	-3.156065000	-1.192678000	-0.573781000
6	-3.637839000	0.773740000	0.713864000
6	-4.449382000	-1.638138000	-0.369771000
1	-2.457756000	-1.776969000	-1.162619000
6	-4.931746000	0.325989000	0.909126000
1	-3.304647000	1.699150000	1.171230000
6	-5.343250000	-0.880480000	0.368022000
1	-4.761249000	-2.584203000	-0.796465000
1	-5.618948000	0.918717000	1.501775000
1	-6.355436000	-1.232424000	0.527197000
6	-1.222760000	1.704849000	-0.603234000
1	-2.116120000	2.304633000	-0.793249000
13	-0.000088000	-0.897538000	0.268339000

1Al-T (T.E = -930.816029)

7	1.447836000	0.506075000	-0.304398000
6	1.244391000	1.877415000	-0.440456000
6	0.000000000	2.470866000	-0.515400000
7	-1.447836000	0.506074000	-0.304399000
1	0.000000000	3.542303000	-0.676675000
1	2.133587000	2.484857000	-0.565853000

6	2.734221000	0.013554000	-0.058394000
6	3.059197000	-1.286448000	-0.455253000
6	3.710738000	0.764033000	0.598650000
6	4.302239000	-1.824120000	-0.186199000
1	2.328591000	-1.866907000	-1.014831000
6	4.959213000	0.224164000	0.848103000
1	3.475496000	1.762917000	0.945571000
6	5.266465000	-1.070357000	0.463942000
1	4.525957000	-2.834979000	-0.507358000
1	5.699315000	0.824138000	1.365817000
1	6.246258000	-1.486004000	0.664182000
6	-2.734221000	0.013554000	-0.058394000
6	-3.059197000	-1.286447000	-0.455254000
6	-3.710738000	0.764033000	0.598651000
6	-4.302240000	-1.824120000	-0.186199000
1	-2.328591000	-1.866907000	-1.014832000
6	-4.959213000	0.224164000	0.848104000
1	-3.475495000	1.762917000	0.945572000
6	-5.266465000	-1.070356000	0.463942000
1	-4.525958000	-2.834979000	-0.507358000
1	-5.699314000	0.824138000	1.365818000
1	-6.246258000	-1.486004000	0.664183000
6	-1.244391000	1.877415000	-0.440457000
1	-2.133587000	2.484856000	-0.565857000
13	0.000000000	-0.584576000	-0.229932000

2AI-S (T.E = -1052.125003)

7	1.789469000	0.424458000	0.465922000
6	1.544922000	1.674932000	0.452996000
6	0.239836000	2.229833000	0.858310000
7	-1.031328000	0.034092000	0.397259000
1	0.242527000	3.302950000	0.680230000
1	2.324566000	2.365965000	0.109392000
6	3.056439000	-0.069112000	0.087426000
6	3.099635000	-1.186148000	-0.737799000
6	4.237819000	0.499036000	0.544894000
6	4.317800000	-1.705752000	-1.131990000
1	2.168313000	-1.627327000	-1.078176000
6	5.454214000	-0.029728000	0.150472000
1	4.198338000	1.337149000	1.232084000
6	5.497777000	-1.128235000	-0.690925000
1	4.346248000	-2.570233000	-1.784524000
1	6.374049000	0.413431000	0.513609000
1	6.451763000	-1.542909000	-0.993593000
6	-2.183271000	-0.750039000	0.232564000
6	-2.125946000	-1.945345000	-0.486236000
6	-3.396457000	-0.410945000	0.836731000
6	-3.241021000	-2.757077000	-0.615794000

1	-1.191973000	-2.214831000	-0.971256000
6	-4.510016000	-1.215840000	0.696199000
1	-3.447944000	0.502109000	1.421355000
6	-4.441649000	-2.394462000	-0.032740000
1	-3.168591000	-3.677901000	-1.183665000
1	-5.441205000	-0.926640000	1.170965000
1	-5.315783000	-3.025845000	-0.137272000
5	-0.987821000	1.434752000	0.156948000
7	-1.886298000	2.168634000	-0.670732000
6	-2.775541000	1.563022000	-1.637208000
1	-2.529036000	0.517569000	-1.806145000
1	-3.826573000	1.617544000	-1.324488000
1	-2.688426000	2.090813000	-2.594712000
6	-2.046018000	3.601754000	-0.666616000
1	-3.100283000	3.866973000	-0.515586000
1	-1.478910000	4.075128000	0.131812000
1	-1.737448000	4.048003000	-1.621637000
13	0.319541000	-0.927710000	1.347295000
1	0.131399000	2.088873000	1.943198000

2Al-T (T.E = -1052.090789)

7	-1.808961000	0.269477000	-0.285931000
6	-1.503554000	1.606122000	-0.348319000
6	-0.222891000	2.051185000	-0.951308000
7	1.118621000	-0.036882000	-0.257757000
1	-0.211065000	3.140610000	-0.964816000
1	-2.160023000	2.300761000	0.166987000
6	-3.132067000	-0.135311000	-0.064903000
6	-3.388399000	-1.371120000	0.531313000
6	-4.217881000	0.657435000	-0.436262000
6	-4.682450000	-1.808727000	0.730275000
1	-2.550739000	-1.981437000	0.864410000
6	-5.511715000	0.222019000	-0.215026000
1	-4.035137000	1.605590000	-0.928656000
6	-5.756225000	-1.011511000	0.364635000
1	-4.853969000	-2.773726000	1.193328000
1	-6.341368000	0.852768000	-0.514408000
1	-6.771872000	-1.348088000	0.533295000
6	2.304157000	-0.782901000	-0.201617000
6	2.354329000	-1.992811000	0.492268000
6	3.454636000	-0.369453000	-0.875719000
6	3.504793000	-2.762520000	0.507501000
1	1.477534000	-2.313355000	1.050855000
6	4.606642000	-1.131362000	-0.844017000
1	3.427939000	0.562571000	-1.430603000
6	4.641162000	-2.334902000	-0.156126000
1	3.513540000	-3.698376000	1.054678000
1	5.486869000	-0.786360000	-1.375052000

1	5.544740000	-2.931969000	-0.138944000
5	1.031764000	1.412177000	-0.185430000
7	1.932780000	2.198673000	0.572628000
6	2.839814000	1.669499000	1.566125000
1	2.619788000	0.628399000	1.791445000
1	3.887022000	1.734012000	1.243232000
1	2.744359000	2.244220000	2.494830000
6	2.046123000	3.634226000	0.483178000
1	3.084959000	3.923912000	0.281371000
1	1.430232000	4.037268000	-0.317106000
1	1.751842000	4.118463000	1.423041000
13	-0.441077000	-0.919398000	-0.553107000
1	-0.185408000	1.717929000	-2.004912000

3Al-S (T.E = -1221.556766)

7	1.669504000	0.439520000	-0.148929000
6	1.575320000	1.754021000	-0.274712000
6	0.419438000	2.512227000	-0.361409000
7	-1.281461000	0.169278000	-0.065365000
1	0.536196000	3.578864000	-0.506840000
1	2.524721000	2.296698000	-0.337671000
6	2.983971000	-0.078248000	-0.023713000
6	3.381437000	-1.147034000	-0.820864000
6	3.878024000	0.433916000	0.911613000
6	4.652322000	-1.678236000	-0.694922000
1	2.686976000	-1.547720000	-1.550714000
6	5.150648000	-0.095747000	1.028340000
1	3.557818000	1.237919000	1.565801000
6	5.543498000	-1.153748000	0.226091000
1	4.949130000	-2.506818000	-1.327323000
1	5.834954000	0.313151000	1.762910000
1	6.537977000	-1.572526000	0.323296000
6	-2.540227000	-0.463757000	0.057587000
6	-2.957695000	-1.384235000	-0.900801000
6	-3.366001000	-0.221253000	1.152795000
6	-4.177384000	-2.025628000	-0.774333000
1	-2.312124000	-1.583826000	-1.749162000
6	-4.587260000	-0.859712000	1.272203000
1	-3.025502000	0.464171000	1.923234000
6	-5.000504000	-1.763626000	0.307734000
1	-4.485786000	-2.737964000	-1.530973000
1	-5.215477000	-0.656173000	2.131894000
1	-5.955012000	-2.266956000	0.403414000
14	-1.171355000	1.801644000	-0.273851000
6	-2.693923000	2.832722000	-0.432788000
1	-3.446935000	2.309156000	-1.024341000
1	-3.131434000	3.033423000	0.546904000
1	-2.458165000	3.786410000	-0.906050000

13 0.270411000 -1.046337000 0.120973000

3AI-T (T.E = -1221.519050)

7	1.678749000	0.463392000	-0.207467000
6	1.559236000	1.833452000	-0.368322000
6	0.407855000	2.521828000	-0.491607000
7	-1.332974000	0.246987000	-0.100047000
1	0.529491000	3.590531000	-0.649938000
1	2.511768000	2.360532000	-0.417488000
6	2.957523000	-0.098871000	-0.029013000
6	3.222664000	-1.361337000	-0.559049000
6	3.963627000	0.540053000	0.694040000
6	4.446692000	-1.973015000	-0.360978000
1	2.461721000	-1.850125000	-1.162254000
6	5.193489000	-0.067672000	0.869973000
1	3.769900000	1.506320000	1.145074000
6	5.443316000	-1.327105000	0.350476000
1	4.627456000	-2.954320000	-0.784190000
1	5.961460000	0.445558000	1.437609000
1	6.406669000	-1.799755000	0.497583000
6	-2.522287000	-0.501661000	0.022379000
6	-2.693780000	-1.681330000	-0.702630000
6	-3.543378000	-0.108336000	0.887086000
6	-3.837938000	-2.446370000	-0.560502000
1	-1.920357000	-1.980036000	-1.405254000
6	-4.692296000	-0.867348000	1.015024000
1	-3.414398000	0.791036000	1.477802000
6	-4.846863000	-2.041439000	0.295876000
1	-3.944285000	-3.360169000	-1.133909000
1	-5.470975000	-0.542412000	1.695855000
1	-5.746252000	-2.635582000	0.403190000
14	-1.311556000	1.910793000	-0.653556000
6	-2.501671000	3.051181000	0.249598000
1	-3.545501000	2.817443000	0.040717000
1	-2.339136000	3.013807000	1.330746000
1	-2.311081000	4.072754000	-0.087448000
13	0.232903000	-0.617810000	0.080013000

4AI-S (T.E = -1143.637336)

7	1.203669000	0.444784000	-0.193836000
6	0.954265000	1.737590000	-0.410704000
6	-0.275676000	2.349128000	-0.478124000
6	-1.500074000	1.688357000	-0.308921000
6	-1.650434000	0.341668000	-0.078396000
6	2.567422000	0.086352000	-0.072420000
6	3.049743000	-1.038129000	-0.736484000

6	3.440618000	0.814864000	0.731670000
6	4.374443000	-1.413575000	-0.608496000
1	2.371761000	-1.608451000	-1.361686000
6	4.766510000	0.438958000	0.850937000
1	3.063241000	1.666293000	1.287711000
6	5.241031000	-0.676369000	0.181521000
1	4.733592000	-2.288638000	-1.138038000
1	5.430393000	1.015767000	1.485038000
1	6.278557000	-0.972970000	0.279743000
1	1.825059000	2.377329000	-0.570348000
15	-3.226960000	-0.305096000	0.098392000
6	-4.606802000	0.851569000	-0.058513000
1	-5.549461000	0.315759000	0.066403000
1	-4.535144000	1.627589000	0.704534000
1	-4.592142000	1.322019000	-1.042392000
6	-3.547477000	-1.605316000	-1.106634000
1	-3.509022000	-1.184467000	-2.111975000
1	-2.757917000	-2.355850000	-1.014805000
1	-4.520395000	-2.070567000	-0.935727000
6	-3.451121000	-1.109580000	1.694833000
1	-3.346148000	-0.371160000	2.490480000
1	-4.430108000	-1.588997000	1.760059000
1	-2.663474000	-1.858494000	1.812170000
1	-2.374710000	2.345503000	-0.378293000
1	-0.282995000	3.412559000	-0.681628000
13	-0.102852000	-1.008722000	0.125240000

4Al-T (T.E = -1143.598381)

7	1.277489000	0.475587000	-0.264521000
6	0.966349000	1.831748000	-0.351571000
6	-0.303688000	2.365052000	-0.332603000
6	-1.523730000	1.706996000	-0.198384000
6	-1.684647000	0.278166000	-0.062643000
6	2.605938000	0.087828000	-0.101244000
6	3.006643000	-1.188718000	-0.515334000
6	3.572048000	0.911197000	0.486983000
6	4.302273000	-1.627729000	-0.333971000
1	2.284059000	-1.830279000	-1.014410000
6	4.871643000	0.467927000	0.651397000
1	3.289815000	1.891779000	0.850249000
6	5.251670000	-0.801282000	0.248215000
1	4.578401000	-2.621237000	-0.669621000
1	5.597186000	1.125989000	1.117437000
1	6.271661000	-1.140628000	0.381007000
1	1.805843000	2.500297000	-0.512679000
15	-3.227589000	-0.374451000	0.112739000
6	-4.145005000	0.232995000	1.554653000
1	-5.160939000	-0.166117000	1.585617000

1	-3.608211000	-0.048358000	2.461255000
1	-4.189151000	1.322614000	1.508335000
6	-4.366961000	-0.025898000	-1.255535000
1	-4.420708000	1.054506000	-1.401260000
1	-3.972397000	-0.474072000	-2.168121000
1	-5.369285000	-0.410903000	-1.056386000
6	-3.216633000	-2.166584000	0.274577000
1	-2.626300000	-2.457202000	1.144585000
1	-4.238851000	-2.529697000	0.395250000
1	-2.777170000	-2.618089000	-0.615747000
1	-2.412897000	2.340587000	-0.212688000
1	-0.343957000	3.442994000	-0.452015000
13	-0.096238000	-0.732671000	-0.120577000

5A1-S (T.E = -1061.439221)

7	1.476485000	0.148275000	-0.103583000
6	1.283430000	1.416813000	-0.251819000
7	-1.271191000	0.151584000	-0.073387000
1	2.152079000	2.075058000	-0.345600000
6	2.824406000	-0.281779000	0.012327000
6	3.258595000	-1.354289000	-0.756523000
6	3.699284000	0.319166000	0.908918000
6	4.562927000	-1.799548000	-0.646373000
1	2.567232000	-1.826891000	-1.445019000
6	5.004763000	-0.128595000	1.010532000
1	3.343993000	1.120235000	1.548650000
6	5.441022000	-1.186854000	0.232392000
1	4.895439000	-2.632381000	-1.254507000
1	5.679414000	0.344346000	1.714471000
1	6.461253000	-1.540848000	0.318017000
6	-2.602892000	-0.360158000	0.032975000
6	-3.080079000	-1.224746000	-0.940615000
6	-3.398632000	-0.065918000	1.132446000
6	-4.340881000	-1.786902000	-0.819581000
1	-2.455420000	-1.448399000	-1.798898000
6	-4.657182000	-0.623065000	1.248063000
1	-3.020487000	0.608742000	1.892012000
6	-5.133184000	-1.486271000	0.272741000
1	-4.702437000	-2.462008000	-1.586447000
1	-5.271558000	-0.385145000	2.108763000
1	-6.119532000	-1.924716000	0.368046000
6	-1.216284000	1.487151000	-0.215428000
13	0.017915000	-1.291768000	0.134841000
8	-2.129730000	2.275784000	-0.281127000
7	0.116497000	2.057512000	-0.319317000
6	0.127710000	3.500617000	-0.523625000
1	-0.404246000	3.757904000	-1.438215000
1	-0.370350000	4.004020000	0.303385000

1 1.159011000 3.841459000 -0.593135000

5AI-T (T.E = -1061.382420)

7 1.492440000 0.175630000 -0.146204000
6 1.311942000 1.528564000 -0.273532000
7 -1.323671000 0.221931000 -0.084926000
1 2.108267000 2.114281000 -0.718115000
6 2.806866000 -0.302594000 -0.008138000
6 3.099830000 -1.611131000 -0.395650000
6 3.834920000 0.481960000 0.512115000
6 4.369573000 -2.128854000 -0.240632000
1 2.318826000 -2.215562000 -0.853436000
6 5.109763000 -0.039239000 0.647668000
1 3.618422000 1.490952000 0.843059000
6 5.388129000 -1.343534000 0.278600000
1 4.570356000 -3.148885000 -0.547128000
1 5.894469000 0.585165000 1.059932000
1 6.388569000 -1.744013000 0.386650000
6 -2.610278000 -0.365119000 0.003529000
6 -2.845892000 -1.532279000 -0.718871000
6 -3.611244000 0.115160000 0.844383000
6 -4.041915000 -2.219624000 -0.594287000
1 -2.089046000 -1.881711000 -1.418015000
6 -4.808214000 -0.565629000 0.951492000
1 -3.444361000 1.024664000 1.404430000
6 -5.031103000 -1.735993000 0.240645000
1 -4.201998000 -3.125527000 -1.167130000
1 -5.578628000 -0.179125000 1.608969000
1 -5.973128000 -2.262551000 0.335479000
6 -1.220505000 1.605246000 -0.182157000
13 0.074904000 -0.922100000 0.079095000
8 -2.178914000 2.347710000 -0.204275000
7 0.059962000 2.140377000 -0.260623000
6 0.079172000 3.593161000 -0.356944000
1 -0.460186000 3.931962000 -1.241598000
1 -0.394680000 4.043746000 0.515529000
1 1.113297000 3.926067000 -0.409722000

6AI-S (T.E = -1274.218691)

6 -1.467983000 1.217407000 -0.101948000
6 -1.438935000 -0.184831000 -0.013029000
6 1.025247000 1.383795000 -0.206962000
1 1.828527000 2.121857000 -0.290235000
13 0.075159000 -1.485351000 -0.008489000
7 1.350190000 0.132441000 -0.118962000
15 -3.049368000 -0.765324000 0.110140000

6	-3.970230000	-0.210004000	1.562853000
1	-4.022483000	0.877715000	1.548826000
1	-4.977475000	-0.632015000	1.563483000
1	-3.440914000	-0.534664000	2.459743000
6	-4.120754000	-0.386128000	-1.295127000
1	-3.688132000	-0.824673000	-2.195400000
1	-5.120754000	-0.795357000	-1.136854000
1	-4.175190000	0.695385000	-1.410988000
6	-3.095662000	-2.562451000	0.223357000
1	-2.545765000	-2.903006000	1.101646000
1	-4.135891000	-2.887267000	0.295184000
1	-2.633460000	-3.011025000	-0.657029000
8	-2.447238000	1.967340000	-0.098152000
7	-0.193224000	1.921124000	-0.223552000
6	-0.303825000	3.365470000	-0.364337000
1	-0.879863000	3.617912000	-1.253776000
1	-0.820965000	3.792050000	0.493997000
1	0.693250000	3.795853000	-0.442756000
6	2.740883000	-0.138273000	-0.028517000
6	3.301381000	-1.109186000	-0.849848000
6	3.543893000	0.521217000	0.894517000
6	4.651528000	-1.393009000	-0.763911000
1	2.665141000	-1.633984000	-1.553370000
6	4.895863000	0.234347000	0.973815000
1	3.096791000	1.240006000	1.573210000
6	5.454765000	-0.721293000	0.143807000
1	5.079980000	-2.147096000	-1.413740000
1	5.511159000	0.752051000	1.700545000
1	6.511621000	-0.950377000	0.210571000

6Al-T (T.E = -1274.172866)

6	-1.479424000	1.255510000	-0.101103000
6	-1.476699000	-0.188078000	-0.009823000
6	1.030997000	1.495747000	-0.119216000
1	1.767984000	2.236278000	-0.411276000
13	0.135913000	-1.151290000	-0.082056000
7	1.392848000	0.171530000	-0.183337000
15	-3.051779000	-0.819414000	0.110558000
6	-3.999450000	-0.309832000	1.560631000
1	-4.099279000	0.774478000	1.542010000
1	-4.986607000	-0.776976000	1.558286000
1	-3.458248000	-0.605445000	2.460313000
6	-4.147610000	-0.508003000	-1.290990000
1	-3.697095000	-0.923928000	-2.193140000
1	-5.124373000	-0.967766000	-1.125637000
1	-4.256242000	0.569240000	-1.408561000
6	-2.976222000	-2.617445000	0.230485000
1	-2.396278000	-2.910193000	1.107235000

1	-3.984976000	-3.025024000	0.317414000
1	-2.499747000	-3.033200000	-0.658838000
8	-2.549460000	1.882173000	-0.104554000
7	-0.283849000	1.957369000	-0.185761000
6	-0.363915000	3.405184000	-0.260302000
1	-1.408813000	3.696589000	-0.284554000
1	0.121389000	3.857195000	0.609376000
1	0.137964000	3.765159000	-1.162692000
6	2.753678000	-0.132640000	-0.060767000
6	3.235718000	-1.337095000	-0.584477000
6	3.664208000	0.718037000	0.571665000
6	4.563269000	-1.688897000	-0.457627000
1	2.552019000	-1.988259000	-1.124281000
6	4.997038000	0.361807000	0.682497000
1	3.311104000	1.642820000	1.011997000
6	5.460028000	-0.839476000	0.175453000
1	4.906240000	-2.628705000	-0.875511000
1	5.682357000	1.036069000	1.184583000
1	6.505416000	-1.108955000	0.263196000

7AI-S (T.E = -1386.991787)

7	0.667446000	0.073181000	0.133932000
6	0.739990000	-1.294075000	0.533462000
6	-0.428595000	-2.016342000	0.796091000
6	-1.689679000	-1.486993000	0.644696000
1	-0.344246000	-3.041965000	1.131102000
1	-2.514694000	-2.160592000	0.889660000
15	2.317751000	0.016652000	0.002116000
6	2.099605000	-1.606700000	0.552915000
6	2.841394000	-2.854434000	0.840900000
1	3.672157000	-2.700889000	1.535201000
1	2.172725000	-3.583678000	1.304931000
1	3.258466000	-3.332309000	-0.054203000
7	2.972681000	0.204060000	-1.503884000
7	3.029645000	1.226876000	0.871385000
6	2.884166000	1.505186000	-2.154932000
1	1.929899000	1.614757000	-2.685883000
1	2.954806000	2.309984000	-1.425287000
1	3.700767000	1.608336000	-2.874808000
6	2.791578000	-0.893069000	-2.441090000
1	3.517623000	-0.791793000	-3.251313000
1	2.949932000	-1.850421000	-1.948061000
1	1.783667000	-0.887556000	-2.877539000
6	4.459937000	1.461288000	0.814621000
1	4.658817000	2.535019000	0.886762000
1	4.978386000	0.965079000	1.644448000
1	4.876471000	1.094645000	-0.121879000
6	2.438232000	1.616347000	2.139777000

1	1.359142000	1.475312000	2.114934000
1	2.854467000	1.036057000	2.972343000
1	2.643175000	2.674897000	2.319799000
13	-0.795216000	1.219679000	-0.292949000
6	-3.413943000	-0.011726000	0.084489000
6	-4.248820000	-0.918802000	-0.566002000
6	-3.959205000	1.187997000	0.537062000
6	-5.593725000	-0.643227000	-0.734141000
1	-3.828320000	-1.834860000	-0.966770000
6	-5.302034000	1.463313000	0.356213000
1	-3.316045000	1.898323000	1.045040000
6	-6.128788000	0.548501000	-0.274571000
1	-6.225690000	-1.361289000	-1.244677000
1	-5.707260000	2.400357000	0.720816000
1	-7.181220000	0.765565000	-0.413008000
7	-2.035795000	-0.258714000	0.255431000

7Al-T (T.E = -1386.927288)

7	0.731171000	-0.093771000	-0.318163000
6	0.719506000	1.389729000	-0.288139000
6	-0.421777000	2.142067000	-0.412882000
6	-1.735413000	1.676152000	-0.498277000
1	-0.279658000	3.217227000	-0.462309000
1	-2.533659000	2.372197000	-0.728600000
15	2.353493000	-0.008056000	-0.003917000
6	2.112128000	1.664686000	-0.138916000
6	2.837743000	2.948012000	-0.026408000
1	3.917759000	2.792188000	0.018110000
1	2.645395000	3.604412000	-0.882416000
1	2.555682000	3.512739000	0.872846000
7	2.827823000	-0.629436000	1.471945000
7	3.226006000	-0.961122000	-1.047429000
6	2.656030000	-2.049131000	1.729511000
1	1.642978000	-2.262106000	2.102538000
1	2.810712000	-2.631817000	0.822420000
1	3.372813000	-2.385055000	2.485135000
6	2.498431000	0.178497000	2.634016000
1	3.100563000	-0.152465000	3.484037000
1	2.710489000	1.229137000	2.442083000
1	1.437169000	0.084509000	2.908040000
6	4.614743000	-1.314566000	-0.830712000
1	4.800666000	-2.332415000	-1.189716000
1	5.285802000	-0.639397000	-1.376619000
1	4.866608000	-1.267090000	0.226693000
6	2.874982000	-0.877525000	-2.453723000
1	1.825548000	-0.608520000	-2.565923000
1	3.484206000	-0.129502000	-2.975732000
1	3.039790000	-1.848759000	-2.929325000

13	-0.839081000	-0.923017000	0.010113000
6	-3.448529000	0.018532000	-0.166931000
6	-4.376774000	0.902023000	0.389536000
6	-3.898137000	-1.249144000	-0.547993000
6	-5.693131000	0.518654000	0.565891000
1	-4.048042000	1.880841000	0.717675000
6	-5.210297000	-1.631941000	-0.348584000
1	-3.203200000	-1.924761000	-1.041931000
6	-6.122522000	-0.748416000	0.205640000
1	-6.392748000	1.220715000	1.006331000
1	-5.527832000	-2.622929000	-0.652982000
1	-7.156128000	-1.040303000	0.346209000
7	-2.098022000	0.347965000	-0.330847000

8A1-S (T.E = -1508.266511)

7	1.293164000	0.367239000	-0.966191000
6	1.032385000	1.447974000	-0.076330000
6	-0.117336000	2.307647000	-0.336229000
15	2.496020000	-0.052632000	0.089411000
6	1.959121000	1.389148000	0.927652000
6	2.228950000	2.204655000	2.131069000
1	3.227767000	2.650582000	2.123089000
1	1.509531000	3.024557000	2.196238000
1	2.145647000	1.628470000	3.058708000
7	2.365798000	-1.422692000	0.995035000
7	3.934602000	-0.211689000	-0.683912000
6	2.661465000	-2.728753000	0.420135000
1	1.761017000	-3.169644000	-0.025738000
1	3.416333000	-2.647152000	-0.359646000
1	3.034532000	-3.390407000	1.206858000
6	1.304302000	-1.489745000	1.990259000
1	1.589563000	-2.201002000	2.769207000
1	1.138843000	-0.515224000	2.446565000
1	0.359994000	-1.826375000	1.541016000
6	5.153684000	-0.492394000	0.046515000
1	5.721805000	-1.281149000	-0.457866000
1	5.789399000	0.398420000	0.106634000
1	4.929588000	-0.827863000	1.058863000
6	4.144630000	0.290596000	-2.029140000
1	3.189573000	0.416122000	-2.534921000
1	4.675274000	1.249625000	-2.018683000
1	4.748281000	-0.428797000	-2.590559000
13	-0.096691000	-0.886504000	-1.595416000
6	-2.530397000	-0.752729000	-0.265260000
6	-2.914515000	-0.809883000	1.077788000
6	-3.178038000	-1.610043000	-1.158742000
6	-3.921515000	-1.657076000	1.501253000
1	-2.406350000	-0.161921000	1.786532000

6	-4.177575000	-2.466005000	-0.729765000
1	-2.898075000	-1.578861000	-2.206677000
6	-4.562465000	-2.493174000	0.600118000
1	-4.204303000	-1.669368000	2.548478000
1	-4.666793000	-3.113784000	-1.448972000
1	-5.349252000	-3.160071000	0.931994000
7	-1.487640000	0.094728000	-0.672050000
5	-1.514396000	1.488486000	-0.371798000
7	-2.709289000	2.254123000	-0.191443000
6	-4.020363000	1.806840000	-0.605505000
1	-3.957255000	0.944372000	-1.263966000
1	-4.656430000	1.535418000	0.248132000
1	-4.526949000	2.610901000	-1.153158000
6	-2.788186000	3.573059000	0.382533000
1	-1.844546000	3.888930000	0.821540000
1	-3.085067000	4.324960000	-0.361885000
1	-3.543064000	3.598570000	1.179584000
1	-0.131774000	3.139790000	0.368169000
1	0.000056000	2.739829000	-1.339497000

8AI-T (T.E = -1508.201836)

7	1.322789000	0.962660000	-0.916494000
6	0.816703000	1.594379000	0.261625000
6	-0.367363000	2.455847000	0.185662000
15	2.262553000	0.057417000	0.119039000
6	1.521324000	1.089019000	1.322482000
6	1.506062000	1.356381000	2.777417000
1	2.451728000	1.768594000	3.141455000
1	0.724848000	2.081463000	3.017778000
1	1.302811000	0.457032000	3.367206000
7	1.977436000	-1.540072000	0.331529000
7	3.837732000	0.125866000	-0.352112000
6	2.326074000	-2.501732000	-0.706742000
1	1.442624000	-2.725755000	-1.318569000
1	3.099076000	-2.105775000	-1.363963000
1	2.691512000	-3.422272000	-0.239437000
6	0.853952000	-1.995023000	1.142783000
1	1.138128000	-2.917248000	1.657304000
1	0.576285000	-1.245732000	1.881440000
1	-0.021379000	-2.195524000	0.512601000
6	4.879505000	-0.649297000	0.291015000
1	5.544710000	-1.079268000	-0.465163000
1	5.483759000	-0.020044000	0.954819000
1	4.453406000	-1.461552000	0.877096000
6	4.333826000	1.287206000	-1.069024000
1	3.510051000	1.808171000	-1.552473000
1	4.850639000	1.978987000	-0.393555000
1	5.044215000	0.963848000	-1.835377000

13	-0.084976000	0.272355000	-2.013644000
6	-2.134897000	-0.874284000	-0.306261000
6	-2.716352000	-0.938925000	0.969497000
6	-2.193150000	-2.032940000	-1.095868000
6	-3.283633000	-2.106729000	1.440360000
1	-2.677761000	-0.058051000	1.604623000
6	-2.762978000	-3.198896000	-0.615810000
1	-1.776374000	-1.998156000	-2.099115000
6	-3.307720000	-3.252660000	0.656555000
1	-3.703216000	-2.126215000	2.440648000
1	-2.787515000	-4.076751000	-1.252754000
1	-3.755282000	-4.166426000	1.028130000
7	-1.453755000	0.244222000	-0.730600000
5	-1.670691000	1.597205000	-0.259543000
7	-2.944649000	2.205635000	-0.186106000
6	-4.138811000	1.588696000	-0.714410000
1	-3.895753000	0.680988000	-1.262313000
1	-4.845598000	1.329846000	0.084323000
1	-4.647570000	2.277796000	-1.398690000
6	-3.209463000	3.520263000	0.338260000
1	-2.312501000	3.976452000	0.752280000
1	-3.595745000	4.185997000	-0.444209000
1	-3.966730000	3.480929000	1.131805000
1	-0.522557000	2.952219000	1.148654000
1	-0.201308000	3.232554000	-0.573795000

9AI-S (T.E = -1677.694215)

7	0.889842000	-0.017389000	-0.108000000
6	1.095368000	1.409832000	-0.125317000
6	0.020897000	2.293281000	-0.219594000
1	0.222634000	3.357929000	-0.268150000
15	2.532891000	-0.149920000	0.024297000
6	2.480117000	1.570746000	-0.028010000
6	3.345020000	2.769441000	0.036392000
1	4.142612000	2.761349000	-0.712697000
1	2.745895000	3.665072000	-0.148059000
1	3.826679000	2.905638000	1.012302000
7	3.166150000	-0.843738000	1.384315000
7	3.176657000	-1.077336000	-1.191524000
6	3.115992000	-2.286687000	1.574068000
1	2.173007000	-2.589003000	2.046870000
1	3.192448000	-2.805128000	0.620463000
1	3.946439000	-2.596347000	2.215286000
6	2.989176000	-0.116416000	2.629992000
1	3.755180000	-0.431730000	3.342984000
1	3.083876000	0.955798000	2.463971000
1	2.003267000	-0.314282000	3.071545000
6	4.620764000	-1.212987000	-1.268676000

1	4.872432000	-2.143527000	-1.785095000
1	5.074450000	-0.381969000	-1.826337000
1	5.061871000	-1.241117000	-0.273324000
6	2.556230000	-0.993743000	-2.502887000
1	1.471685000	-0.988801000	-2.409853000
1	2.870848000	-0.092334000	-3.045844000
1	2.849543000	-1.868864000	-3.087660000
13	-0.529640000	-1.306242000	0.042074000
6	-3.268376000	-0.386877000	0.004353000
6	-4.089056000	-0.070241000	1.085816000
6	-3.781937000	-1.214075000	-0.993489000
6	-5.387865000	-0.541361000	1.154158000
1	-3.682851000	0.539878000	1.887206000
6	-5.078728000	-1.690738000	-0.918041000
1	-3.144613000	-1.473565000	-1.832019000
6	-5.891405000	-1.353140000	0.151224000
1	-6.007574000	-0.279947000	2.004606000
1	-5.457365000	-2.332475000	-1.705670000
1	-6.907124000	-1.726032000	0.206729000
7	-1.937035000	0.072567000	-0.066896000
14	-1.609152000	1.693440000	-0.206873000
6	-3.023647000	2.874882000	-0.366790000
1	-3.772894000	2.481588000	-1.056468000
1	-3.519544000	3.031743000	0.592536000
1	-2.665407000	3.837692000	-0.732985000

9Al-T (T.E = -1677.641632)

7	0.944557000	-0.067872000	-0.266185000
6	1.076239000	1.402210000	-0.231363000
6	0.017185000	2.242569000	-0.312787000
1	0.253649000	3.305124000	-0.274189000
15	2.579561000	-0.140563000	0.018555000
6	2.488730000	1.545862000	-0.068877000
6	3.315893000	2.765292000	0.055165000
1	4.381963000	2.535099000	-0.001517000
1	3.099442000	3.478055000	-0.747788000
1	3.150277000	3.297355000	1.001722000
7	3.032853000	-0.846563000	1.455609000
7	3.322855000	-1.135984000	-1.086562000
6	2.794185000	-2.262892000	1.674154000
1	1.789580000	-2.433498000	2.089062000
1	2.872164000	-2.819361000	0.741341000
1	3.525969000	-2.662717000	2.382681000
6	2.812691000	-0.059665000	2.656884000
1	3.439034000	-0.450446000	3.462847000
1	3.072163000	0.983469000	2.483649000
1	1.763940000	-0.105142000	2.985062000
6	4.708635000	-1.539691000	-0.943874000

1	4.849428000	-2.533335000	-1.380859000
1	5.382855000	-0.846384000	-1.463263000
1	4.997436000	-1.577685000	0.104643000
6	2.929745000	-0.970411000	-2.475623000
1	1.887012000	-0.663525000	-2.541012000
1	3.546215000	-0.216770000	-2.981027000
1	3.048097000	-1.922062000	-3.001027000
13	-0.593471000	-0.934373000	0.098697000
6	-3.294227000	-0.410988000	-0.055798000
6	-4.270058000	0.112653000	0.794540000
6	-3.624791000	-1.538567000	-0.810253000
6	-5.520885000	-0.469057000	0.881595000
1	-4.023742000	0.972744000	1.405800000
6	-4.872990000	-2.128180000	-0.708934000
1	-2.887257000	-1.934347000	-1.503318000
6	-5.831496000	-1.594505000	0.134199000
1	-6.259149000	-0.043980000	1.552538000
1	-5.099694000	-3.004857000	-1.305306000
1	-6.811744000	-2.049673000	0.209050000
7	-2.005997000	0.150654000	-0.130021000
14	-1.714172000	1.803602000	-0.687177000
6	-2.860314000	3.066523000	0.113536000
1	-3.905142000	2.931808000	-0.166135000
1	-2.777017000	3.038845000	1.204368000
1	-2.546487000	4.057587000	-0.223503000

10A1-S (T.E = -1599.762997)

7	-0.519943000	-0.066236000	0.117581000
6	-0.549523000	1.362871000	0.163255000
6	0.610284000	2.125481000	0.194165000
6	1.888809000	1.573989000	0.146454000
1	0.500765000	3.203037000	0.246834000
1	2.681031000	2.331299000	0.188649000
15	-2.171619000	0.006199000	0.024958000
6	-1.919479000	1.694572000	0.140698000
6	-2.632132000	2.989911000	0.059640000
1	-2.443368000	3.630189000	0.928417000
1	-2.350878000	3.570499000	-0.829070000
1	-3.713275000	2.837522000	0.010715000
6	2.240515000	0.233592000	0.044918000
15	3.882531000	-0.192459000	-0.011066000
6	5.090085000	1.153977000	0.076535000
1	6.100419000	0.743514000	0.030830000
1	4.947562000	1.841847000	-0.757775000
1	4.971546000	1.704554000	1.010549000
6	4.316610000	-1.105414000	-1.508711000
1	5.353689000	-1.447150000	-1.482500000
1	3.647797000	-1.966399000	-1.587133000

1	4.158390000	-0.466474000	-2.378289000
6	4.357724000	-1.325107000	1.314070000
1	4.226690000	-0.828779000	2.276334000
1	3.689105000	-2.189053000	1.277801000
1	5.392757000	-1.656693000	1.205016000
7	-2.902038000	-0.557243000	-1.350843000
7	-2.888193000	-0.919995000	1.207015000
6	-2.956912000	-1.987864000	-1.613659000
1	-2.048969000	-2.329455000	-2.127319000
1	-3.045513000	-2.545933000	-0.683543000
1	-3.821955000	-2.209643000	-2.245933000
6	-2.705277000	0.220599000	-2.561589000
1	-3.495469000	-0.022992000	-3.276705000
1	-2.746323000	1.286706000	-2.341918000
1	-1.736153000	-0.001191000	-3.029180000
6	-4.334856000	-0.859436000	1.320005000
1	-4.694765000	-1.740405000	1.858422000
1	-4.661126000	0.033371000	1.873260000
1	-4.799614000	-0.843558000	0.334876000
6	-2.235548000	-0.945253000	2.505506000
1	-1.161309000	-1.075912000	2.386406000
1	-2.421061000	-0.023022000	3.073287000
1	-2.626550000	-1.788902000	3.079393000
13	0.890947000	-1.326175000	-0.057985000

10Al-T (T.E = -1599.707421)

7	0.603207000	-0.127316000	-0.205043000
6	0.531734000	1.351172000	-0.102819000
6	-0.635201000	2.068845000	-0.065873000
6	-1.948514000	1.563180000	-0.082535000
1	-0.511008000	3.147458000	-0.014063000
1	-2.743342000	2.311937000	-0.080814000
15	2.232500000	0.024970000	-0.032595000
6	1.923805000	1.686729000	-0.044005000
6	2.591616000	2.987698000	0.179132000
1	2.359875000	3.714511000	-0.608134000
1	2.300909000	3.454037000	1.131725000
1	3.678723000	2.876290000	0.195193000
6	-2.305510000	0.171393000	-0.067912000
15	-3.932726000	-0.260389000	-0.029567000
6	-4.860828000	0.378983000	1.393598000
1	-5.923453000	0.135141000	1.330313000
1	-4.436642000	-0.041326000	2.306276000
1	-4.741978000	1.463288000	1.430212000
6	-4.204252000	-2.040646000	0.001386000
1	-5.275828000	-2.244740000	0.041518000
1	-3.782739000	-2.495787000	-0.895586000
1	-3.720730000	-2.473265000	0.878293000

6	-4.911775000	0.336827000	-1.436289000
1	-4.805022000	1.421025000	-1.502096000
1	-4.513526000	-0.101294000	-2.352225000
1	-5.969300000	0.084813000	-1.332233000
7	2.884440000	-0.667742000	1.345686000
7	3.056483000	-0.823775000	-1.216825000
6	2.846884000	-2.112405000	1.490937000
1	1.858622000	-2.451221000	1.838859000
1	3.058110000	-2.602275000	0.541860000
1	3.592332000	-2.433190000	2.225283000
6	2.554708000	0.009519000	2.587803000
1	3.244023000	-0.317118000	3.371093000
1	2.643217000	1.088479000	2.468138000
1	1.528799000	-0.217019000	2.914800000
6	4.507486000	-0.843402000	-1.185262000
1	4.874651000	-1.679811000	-1.787446000
1	4.934443000	0.081526000	-1.600368000
1	4.871981000	-0.962274000	-0.166291000
6	2.546020000	-0.654527000	-2.566452000
1	1.457021000	-0.634804000	-2.557952000
1	2.906134000	0.277046000	-3.023664000
1	2.877958000	-1.493982000	-3.183612000
13	-0.914291000	-1.112655000	-0.054895000

11A1-S (T.E = -1517.573309)

7	0.735650000	-0.238216000	-0.206633000
6	0.795299000	1.149025000	0.004731000
6	-1.691669000	1.425876000	0.030763000
15	2.384714000	-0.239699000	-0.053179000
6	2.152872000	1.462883000	0.142530000
6	2.999668000	2.642330000	0.463973000
1	3.092145000	3.357729000	-0.358830000
1	2.648559000	3.195964000	1.339673000
1	4.014541000	2.306021000	0.694443000
7	3.064749000	-1.017349000	1.228437000
7	3.095406000	-0.951812000	-1.358933000
6	3.125104000	-2.473863000	1.255255000
1	2.222055000	-2.892765000	1.715124000
1	3.206824000	-2.875972000	0.247474000
1	3.996060000	-2.790162000	1.835594000
6	2.869647000	-0.444922000	2.551555000
1	3.653329000	-0.813609000	3.217468000
1	2.925819000	0.641645000	2.514099000
1	1.896707000	-0.731368000	2.971307000
6	4.544824000	-0.999497000	-1.446514000
1	4.849032000	-1.898534000	-1.989701000
1	4.941175000	-0.127335000	-1.981716000
1	4.992440000	-1.029196000	-0.453916000

6	2.448800000	-0.849500000	-2.657614000
1	1.369691000	-0.944485000	-2.553984000
1	2.679828000	0.102419000	-3.152010000
1	2.807695000	-1.663076000	-3.292175000
7	-0.312477000	1.898838000	0.044035000
6	-0.138025000	3.337527000	0.181075000
1	0.030407000	3.621208000	1.222769000
1	0.708863000	3.660746000	-0.421669000
1	-1.043373000	3.825289000	-0.164634000
8	-2.542777000	2.285583000	0.072412000
7	-1.888225000	0.092168000	0.003011000
6	-3.265829000	-0.281672000	0.003941000
6	-4.094976000	0.011163000	-1.071939000
6	-3.770707000	-1.022467000	1.062664000
6	-5.406291000	-0.422814000	-1.081054000
1	-3.698199000	0.588557000	-1.899153000
6	-5.084695000	-1.462134000	1.049670000
1	-3.120396000	-1.249835000	1.900743000
6	-5.907488000	-1.162230000	-0.020313000
1	-6.043361000	-0.185567000	-1.925608000
1	-5.464278000	-2.041401000	1.883631000
1	-6.935622000	-1.504764000	-0.031736000
13	-0.729489000	-1.475716000	-0.144659000

11A1-T (T.E = -1517.497447)

6	1.678358000	-1.526220000	-0.330301000
6	-0.832300000	-1.223604000	-0.333086000
13	0.639140000	1.135093000	-0.028068000
7	-0.846127000	0.176154000	-0.150569000
7	1.901186000	-0.181052000	-0.111951000
6	3.247440000	0.233836000	0.081437000
6	3.723509000	1.315479000	-0.650177000
6	4.073460000	-0.347991000	1.037703000
6	4.994482000	1.819618000	-0.424820000
1	3.094390000	1.747923000	-1.423872000
6	5.344610000	0.148226000	1.249173000
1	3.712047000	-1.195051000	1.606265000
6	5.811047000	1.235436000	0.524532000
1	5.347208000	2.663718000	-1.005824000
1	5.979197000	-0.316581000	1.995027000
1	6.808663000	1.620373000	0.699015000
8	2.571177000	-2.337517000	-0.414210000
7	0.339333000	-1.946918000	-0.482581000
15	-2.596879000	0.201879000	-0.278917000
6	-2.133920000	-1.601939000	-0.358573000
6	-2.985772000	-2.801377000	-0.503488000
1	-2.795692000	-3.394039000	-1.403128000
1	-2.906747000	-3.476054000	0.355699000

1	-4.032814000	-2.482793000	-0.552646000
6	0.143095000	-3.357169000	-0.781272000
1	-0.403154000	-3.849370000	0.025787000
1	-0.422747000	-3.466805000	-1.707538000
1	1.114976000	-3.825426000	-0.891643000
7	-3.303449000	0.375247000	1.241106000
7	-2.780502000	1.900031000	-0.763585000
6	-2.989318000	-0.538045000	2.312502000
1	-1.979816000	-0.932502000	2.206142000
1	-3.047856000	-0.008552000	3.270254000
1	-3.687750000	-1.386349000	2.359126000
6	-4.546050000	1.085063000	1.444051000
1	-5.377608000	0.387057000	1.610797000
1	-4.479174000	1.736284000	2.324850000
1	-4.777953000	1.699526000	0.576639000
6	-2.163257000	2.928285000	0.023076000
1	-1.074189000	3.032959000	-0.191743000
1	-2.607601000	3.908342000	-0.191566000
1	-2.274269000	2.722838000	1.089461000
6	-2.622264000	2.118874000	-2.177669000
1	-3.105973000	3.053853000	-2.480023000
1	-1.560796000	2.184532000	-2.479980000
1	-3.079199000	1.296782000	-2.734246000

12Al-S (T.E = -1730.350088)

7	0.658662000	-0.302638000	-0.152061000
6	0.593833000	1.098277000	-0.050371000
6	-1.906962000	1.166810000	-0.081183000
15	2.298630000	-0.145758000	-0.017839000
6	1.925289000	1.537162000	0.057373000
6	2.674222000	2.798907000	0.302631000
1	2.554144000	3.544909000	-0.487635000
1	2.414051000	3.284701000	1.249678000
1	3.743466000	2.574156000	0.354655000
6	-2.043559000	-0.235948000	-0.000709000
15	-3.707487000	-0.625144000	0.020809000
6	-4.663631000	0.039212000	1.407110000
1	-5.708127000	-0.272773000	1.339961000
1	-4.234002000	-0.332521000	2.338428000
1	-4.598077000	1.125950000	1.388718000
6	-3.960326000	-2.405605000	0.146954000
1	-5.032129000	-2.614855000	0.163589000
1	-3.500795000	-2.915575000	-0.700720000
1	-3.498731000	-2.789067000	1.057872000
6	-4.659515000	-0.162086000	-1.448003000
1	-4.592666000	0.916645000	-1.581190000
1	-4.225423000	-0.659824000	-2.316407000
1	-5.704666000	-0.461482000	-1.343102000

7	3.068405000	-0.778699000	1.294701000
7	3.074399000	-0.857034000	-1.293961000
6	3.321590000	-2.210441000	1.391094000
1	2.472580000	-2.728247000	1.853229000
1	3.480351000	-2.639634000	0.404072000
1	4.214077000	-2.378175000	2.000694000
6	2.790950000	-0.173549000	2.587217000
1	3.614465000	-0.396455000	3.270096000
1	2.698114000	0.907495000	2.492678000
1	1.863491000	-0.568285000	3.022094000
6	4.501658000	-0.618336000	-1.425835000
1	4.957484000	-1.431656000	-1.996706000
1	4.705316000	0.324698000	-1.952005000
1	4.978315000	-0.577485000	-0.446436000
6	2.386127000	-0.894656000	-2.574510000
1	1.357771000	-1.226336000	-2.441700000
1	2.386656000	0.086616000	-3.068096000
1	2.899779000	-1.607191000	-3.223828000
13	-0.666935000	-1.691957000	-0.001821000
8	-2.822036000	1.992447000	-0.145195000
7	-0.564211000	1.763868000	-0.069068000
6	-0.479815000	3.215011000	-0.062535000
1	-0.063879000	3.581233000	0.878403000
1	0.144448000	3.562879000	-0.887131000
1	-1.486681000	3.602665000	-0.181212000

12AI-T (T.E = -1730.277384)

7	-0.693720000	-0.232062000	0.470346000
6	-0.568567000	1.118248000	-0.008233000
6	1.927449000	1.190133000	0.131608000
15	-2.298833000	-0.093547000	0.096700000
6	-1.879459000	1.537681000	-0.270727000
6	-2.553631000	2.731955000	-0.845032000
1	-2.420053000	3.637778000	-0.248302000
1	-2.221981000	2.962231000	-1.864026000
1	-3.630478000	2.552569000	-0.899473000
6	2.084010000	-0.185831000	-0.126953000
15	3.698403000	-0.692965000	0.051616000
6	4.900692000	0.145490000	-1.003998000
1	5.906678000	-0.241000000	-0.828030000
1	4.624694000	-0.015526000	-2.046950000
1	4.863819000	1.211780000	-0.784740000
6	3.853942000	-2.434358000	-0.379012000
1	4.893446000	-2.754483000	-0.284825000
1	3.219914000	-3.028763000	0.282779000
1	3.518887000	-2.584795000	-1.406968000
6	4.371639000	-0.562224000	1.723055000
1	4.315028000	0.481971000	2.031002000

1	3.756373000	-1.167688000	2.390668000
1	5.406892000	-0.907414000	1.761636000
7	-2.890651000	-0.961931000	-1.175962000
7	-3.216949000	-0.623727000	1.361291000
6	-2.905605000	-2.414071000	-1.104812000
1	-1.999808000	-2.823286000	-1.575857000
1	-2.932911000	-2.752848000	-0.069145000
1	-3.784672000	-2.806814000	-1.626313000
6	-2.688611000	-0.475872000	-2.532152000
1	-3.458948000	-0.906508000	-3.179404000
1	-2.769104000	0.608507000	-2.570908000
1	-1.694892000	-0.764618000	-2.905666000
6	-4.650290000	-0.808682000	1.265053000
1	-4.946976000	-1.701825000	1.824372000
1	-5.190538000	0.047766000	1.687241000
1	-4.955049000	-0.933708000	0.227492000
6	-2.754436000	-0.366915000	2.713491000
1	-1.669560000	-0.277394000	2.723951000
1	-3.194678000	0.552664000	3.117949000
1	-3.046075000	-1.200000000	3.359413000
13	0.577963000	-1.369626000	-0.379011000
8	2.832092000	1.976634000	0.445767000
7	0.600376000	1.774867000	-0.019473000
6	0.537923000	3.216976000	-0.188666000
1	0.173740000	3.481288000	-1.183653000
1	-0.116248000	3.663271000	0.562434000
1	1.544957000	3.601381000	-0.053558000

13AI-S (T.E = -1843.122347)

7	-1.318448000	-0.213983000	0.091939000
6	-1.214120000	1.221091000	0.032025000
6	-0.000487000	1.891569000	-0.018238000
6	1.213667000	1.221114000	-0.055757000
1	-0.000956000	2.976283000	-0.029286000
13	0.000724000	-1.593162000	0.015878000
15	-2.952183000	0.002889000	0.032827000
6	-2.545599000	1.667812000	0.026880000
6	-3.138064000	3.016902000	-0.120864000
1	-2.856645000	3.689696000	0.696464000
1	-2.835030000	3.507986000	-1.054778000
1	-4.229457000	2.967918000	-0.126520000
7	1.319025000	-0.214771000	-0.086648000
6	2.544738000	1.668878000	-0.061221000
15	2.952708000	0.004417000	-0.033447000
6	3.135624000	3.021474000	0.058016000
1	2.850598000	3.677310000	-0.771743000
1	2.834525000	3.530620000	0.982845000
1	4.227090000	2.974488000	0.061342000

7	3.765437000	-0.545139000	1.305084000
7	3.712997000	-0.815121000	-1.260559000
6	3.865042000	-1.979889000	1.531888000
1	2.974234000	-2.360122000	2.049353000
1	3.956626000	-2.515192000	0.588350000
1	4.744215000	-2.193899000	2.146703000
6	3.553566000	0.191233000	2.539592000
1	2.589345000	-0.062579000	3.001775000
1	4.349083000	-0.060049000	3.245796000
1	3.575471000	1.264351000	2.355578000
6	3.062518000	-0.831507000	-2.558867000
1	3.400378000	-1.709090000	-3.116274000
1	1.981930000	-0.893403000	-2.440400000
1	3.304646000	0.065296000	-3.144152000
6	5.159703000	-0.806348000	-1.362004000
1	5.516569000	0.043811000	-1.959105000
1	5.617001000	-0.750637000	-0.375586000
1	5.497834000	-1.725169000	-1.850653000
7	-3.713503000	-0.790588000	1.276752000
7	-3.764002000	-0.574770000	-1.294228000
6	-5.160188000	-0.767571000	1.378921000
1	-5.504688000	-1.668788000	1.894974000
1	-5.510092000	0.102834000	1.950582000
1	-5.617925000	-0.737969000	0.391537000
6	-3.062739000	-0.778075000	2.575101000
1	-1.982849000	-0.853520000	2.458221000
1	-3.296020000	0.136480000	3.136109000
1	-3.409026000	-1.637039000	3.155765000
6	-3.549272000	0.133805000	-2.544386000
1	-4.345168000	-0.130384000	-3.245421000
1	-3.568004000	1.210736000	-2.383662000
1	-2.585583000	-0.132958000	-3.000332000
6	-3.867665000	-2.013874000	-1.489305000
1	-3.962434000	-2.527628000	-0.534169000
1	-4.746550000	-2.238674000	-2.100667000
1	-2.977295000	-2.408274000	-1.996835000

13Al-T (T.E = -1843.038580)

7	-1.377194000	0.239496000	-0.554202000
6	-1.226858000	-1.194442000	-0.459004000
6	-0.000091000	-1.846301000	-0.443362000
6	1.226717000	-1.194487000	-0.458740000
1	-0.000110000	-2.924901000	-0.324926000
15	-2.950085000	-0.007485000	-0.118727000
6	-2.537208000	-1.664223000	-0.287817000
6	-3.068849000	-3.028312000	-0.070302000
1	-2.972234000	-3.663405000	-0.957221000
1	-2.552696000	-3.544809000	0.749439000

1	-4.130151000	-3.002204000	0.186126000
7	-3.389120000	0.471088000	1.405906000
7	-3.967538000	0.870347000	-1.079197000
6	-3.327264000	1.888878000	1.732287000
1	-2.325006000	2.148811000	2.106821000
1	-3.535207000	2.500132000	0.854477000
1	-4.062958000	2.125733000	2.507020000
6	-2.955105000	-0.359781000	2.520803000
1	-3.555563000	-0.109346000	3.400207000
1	-3.093254000	-1.415071000	2.291670000
1	-1.891782000	-0.185511000	2.750018000
6	-5.372488000	1.058027000	-0.787035000
1	-5.670870000	2.081587000	-1.037568000
1	-5.995715000	0.373134000	-1.375414000
1	-5.572956000	0.887681000	0.269212000
6	-3.644433000	0.988320000	-2.489298000
1	-2.572254000	0.868807000	-2.637288000
1	-4.174598000	0.235318000	-3.085118000
1	-3.937523000	1.979332000	-2.847451000
13	0.000023000	1.328418000	0.112275000
7	1.377212000	0.239502000	-0.554544000
15	2.949984000	-0.007465000	-0.118693000
6	2.536961000	-1.664250000	-0.287045000
6	3.068880000	-3.028192000	-0.069294000
1	2.550996000	-3.545494000	0.748828000
1	2.974926000	-3.662806000	-0.956850000
1	4.129514000	-3.001578000	0.189864000
7	3.388890000	0.471644000	1.405814000
7	3.967709000	0.869847000	-1.079349000
6	3.327048000	1.889549000	1.731657000
1	3.534484000	2.500485000	0.853494000
1	2.324935000	2.149524000	2.106546000
1	4.063093000	2.126847000	2.505933000
6	2.955145000	-0.358852000	2.521067000
1	1.891830000	-0.184643000	2.750368000
1	3.093396000	-1.414219000	2.292337000
1	3.555690000	-0.108001000	3.400301000
6	5.372593000	1.057701000	-0.786978000
1	5.671096000	2.080973000	-1.038520000
1	5.572741000	0.888452000	0.269505000
1	5.995961000	0.372155000	-1.374454000
6	3.644902000	0.987177000	-2.489575000
1	4.175439000	0.234099000	-3.084972000
1	2.572795000	0.867264000	-2.637775000
1	3.937779000	1.978135000	-2.848059000

1Ga-S (T.E = -2613.258555)

7	0.586602000	0.266836000	1.452935000
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7	0.586602000	0.266836000	-1.452935000
6	1.848855000	0.562935000	1.233987000
6	1.848855000	0.562935000	-1.233987000
6	2.464240000	0.713449000	0.000000000
1	3.508156000	0.995359000	0.000000000
6	0.166190000	0.087531000	2.784155000
6	0.904502000	-0.663925000	3.696058000
6	-1.047780000	0.635086000	3.191958000
6	0.448069000	-0.840787000	4.989277000
6	-1.501963000	0.449407000	4.484643000
6	-0.755691000	-0.285503000	5.390692000
1	1.032606000	-1.430966000	5.685827000
1	-2.444876000	0.889603000	4.787748000
1	-1.113326000	-0.430321000	6.402994000
6	0.166190000	0.087531000	-2.784155000
6	-1.047780000	0.635086000	-3.191958000
6	0.904502000	-0.663925000	-3.696058000
6	-1.501963000	0.449407000	-4.484643000
6	0.448069000	-0.840787000	-4.989277000
6	-0.755691000	-0.285503000	-5.390692000
1	-2.444876000	0.889603000	-4.787748000
1	1.032606000	-1.430966000	-5.685827000
1	-1.113326000	-0.430321000	-6.402994000
1	1.827507000	-1.133666000	-3.373858000
1	-1.619153000	1.230474000	-2.487798000
1	-1.619153000	1.230474000	2.487798000
1	1.827507000	-1.133666000	3.373858000
31	-0.889664000	-0.260066000	0.000000000
1	2.480929000	0.731560000	-2.111419000
1	2.480929000	0.731560000	2.111419000

1Ga-T (T.E = -2613.180916)

7	-0.635694000	-0.113475000	1.440590000
7	-0.611872000	0.063406000	-1.463973000
6	-1.978887000	-0.188627000	1.236117000
6	-1.968605000	0.081034000	-1.274758000
6	-2.557333000	-0.064631000	-0.025310000
1	-3.642262000	-0.095509000	-0.034532000
6	-0.095697000	-0.226233000	2.706093000
6	-0.833095000	-0.136787000	3.896360000
6	1.285684000	-0.456454000	2.806938000
6	-0.210057000	-0.285775000	5.119594000
6	1.898678000	-0.599472000	4.030500000
6	1.153791000	-0.517743000	5.200792000
1	-0.799114000	-0.210477000	6.026724000
1	2.965714000	-0.783602000	4.077081000
1	1.633972000	-0.631709000	6.164974000
6	-0.071920000	-0.101900000	-2.710875000

6	1.316334000	0.064877000	-2.880268000
6	-0.819201000	-0.491057000	-3.839539000
6	1.918811000	-0.134292000	-4.098953000
6	-0.202041000	-0.691232000	-5.057003000
6	1.164327000	-0.510500000	-5.205046000
1	2.989002000	0.008446000	-4.194799000
1	-0.799472000	-1.003154000	-5.906376000
1	1.638041000	-0.663819000	-6.166847000
1	-1.880386000	-0.680169000	-3.747714000
1	1.913866000	0.375793000	-2.027917000
1	1.865198000	-0.545341000	1.892335000
1	-1.894485000	0.072936000	3.865043000
31	0.371139000	1.082053000	0.069760000
1	-2.622925000	0.207860000	-2.131418000
1	-2.637342000	-0.376528000	2.077204000

2Ga-S (T.E = -2734.524165)

7	1.841461000	0.472945000	0.534455000
6	1.519504000	1.700620000	0.501169000
6	0.248733000	2.196181000	1.064548000
7	-1.127101000	0.151242000	0.332579000
1	0.256964000	3.283752000	1.081602000
1	2.174949000	2.418990000	-0.011213000
6	3.046524000	0.014475000	-0.017205000
6	3.014764000	-1.122787000	-0.817774000
6	4.262869000	0.635264000	0.244051000
6	4.180667000	-1.611389000	-1.374761000
1	2.060362000	-1.602210000	-1.012963000
6	5.427843000	0.135920000	-0.311344000
1	4.290584000	1.494332000	0.905632000
6	5.391196000	-0.984208000	-1.124086000
1	4.145313000	-2.490600000	-2.007299000
1	6.373146000	0.621835000	-0.098998000
1	6.305666000	-1.374660000	-1.554123000
6	-2.257488000	-0.594859000	0.010962000
6	-2.138314000	-1.762601000	-0.750419000
6	-3.528999000	-0.267972000	0.497858000
6	-3.239218000	-2.558613000	-1.023362000
1	-1.164184000	-2.014495000	-1.161706000
6	-4.625450000	-1.055932000	0.211952000
1	-3.635030000	0.623443000	1.108207000
6	-4.490535000	-2.208831000	-0.550126000
1	-3.115030000	-3.455300000	-1.620416000
1	-5.599383000	-0.774728000	0.597747000
1	-5.353264000	-2.826829000	-0.767707000
31	0.149053000	-1.049385000	1.345263000
5	-0.980481000	1.554380000	0.214040000
7	-1.745078000	2.405488000	-0.638946000

6	-2.596079000	1.919879000	-1.701970000
1	-2.411502000	0.868817000	-1.910958000
1	-3.662193000	2.036796000	-1.465944000
1	-2.398080000	2.487663000	-2.619250000
6	-1.792993000	3.844444000	-0.570023000
1	-2.831275000	4.189296000	-0.479338000
1	-1.248358000	4.231198000	0.288268000
1	-1.380607000	4.307607000	-1.476672000
1	0.150567000	1.848840000	2.098343000

2Ga-T (T.E = -2734.453350)

7	-1.793719000	0.355487000	-0.292407000
6	-1.454571000	1.673479000	-0.399797000
6	-0.177306000	2.066387000	-1.042196000
7	1.215605000	0.042005000	-0.259580000
1	-0.159509000	3.151499000	-1.141218000
1	-2.062109000	2.395614000	0.138519000
6	-3.101316000	-0.037686000	-0.003006000
6	-3.342635000	-1.292935000	0.558333000
6	-4.193653000	0.791491000	-0.262651000
6	-4.626785000	-1.708952000	0.841369000
1	-2.496977000	-1.938379000	0.788909000
6	-5.476834000	0.375383000	0.042697000
1	-4.028090000	1.753359000	-0.733571000
6	-5.706357000	-0.873593000	0.593585000
1	-4.786278000	-2.689868000	1.274301000
1	-6.311131000	1.035119000	-0.168387000
1	-6.713943000	-1.195174000	0.827066000
6	2.401719000	-0.682536000	-0.130844000
6	2.435746000	-1.894067000	0.561545000
6	3.586153000	-0.233479000	-0.719460000
6	3.604254000	-2.626295000	0.663722000
1	1.525881000	-2.248037000	1.040946000
6	4.756084000	-0.958938000	-0.599774000
1	3.571726000	0.698657000	-1.274391000
6	4.775444000	-2.161330000	0.089246000
1	3.600212000	-3.564774000	1.206503000
1	5.662440000	-0.585987000	-1.063663000
1	5.692498000	-2.731476000	0.174000000
31	-0.389392000	-0.893164000	-0.615889000
5	1.065567000	1.484559000	-0.216602000
7	1.895235000	2.310326000	0.581754000
6	2.758038000	1.824528000	1.634496000
1	2.557306000	0.780073000	1.862605000
1	3.819970000	1.917862000	1.372243000
1	2.590570000	2.408911000	2.546841000
6	1.965135000	3.747486000	0.476608000
1	3.004038000	4.071179000	0.336213000

1	1.387734000	4.117520000	-0.367235000
1	1.594616000	4.233802000	1.388063000
1	-0.144186000	1.646992000	-2.063793000

3Ga-S (T.E = -2903.955395)

7	1.706801000	0.595816000	-0.171335000
6	1.579694000	1.902632000	-0.273472000
6	0.400337000	2.631411000	-0.341646000
7	-1.395329000	0.319643000	-0.078487000
1	0.493834000	3.702896000	-0.476066000
1	2.512673000	2.476296000	-0.337844000
6	3.008993000	0.076607000	-0.054438000
6	3.371118000	-1.035798000	-0.811811000
6	3.941185000	0.610918000	0.833765000
6	4.634302000	-1.586147000	-0.695502000
1	2.654595000	-1.448192000	-1.514234000
6	5.205977000	0.061569000	0.940272000
1	3.655195000	1.448431000	1.461024000
6	5.559829000	-1.039036000	0.177574000
1	4.899592000	-2.446465000	-1.299205000
1	5.917131000	0.489702000	1.637729000
1	6.549007000	-1.471561000	0.267747000
6	-2.635438000	-0.324438000	0.025444000
6	-2.976194000	-1.333058000	-0.877522000
6	-3.536834000	-0.026052000	1.048772000
6	-4.181551000	-2.003357000	-0.768767000
1	-2.283305000	-1.569734000	-1.678376000
6	-4.743437000	-0.693647000	1.149168000
1	-3.264918000	0.729121000	1.780310000
6	-5.074552000	-1.685766000	0.240535000
1	-4.425307000	-2.780712000	-1.484113000
1	-5.427463000	-0.442247000	1.951968000
1	-6.018511000	-2.210798000	0.322650000
31	0.228644000	-1.013670000	0.172231000
14	-1.201174000	1.940302000	-0.269287000
6	-2.678930000	3.040010000	-0.435183000
1	-3.471460000	2.534138000	-0.989116000
1	-3.081600000	3.303257000	0.544729000
1	-2.408280000	3.962121000	-0.950739000

3Ga-T (T.E = -2903.882977)

7	1.711858000	0.549028000	-0.183182000
6	1.532419000	1.913810000	-0.126859000
6	0.363352000	2.583128000	-0.153511000
7	-1.394900000	0.272041000	-0.085958000
1	0.463798000	3.665882000	-0.140993000

1	2.466709000	2.474380000	-0.083962000
6	2.999704000	0.000323000	-0.068401000
6	3.310507000	-1.168175000	-0.763374000
6	3.980430000	0.567082000	0.744921000
6	4.555264000	-1.755932000	-0.643599000
1	2.565631000	-1.600546000	-1.426129000
6	5.231005000	-0.015665000	0.844647000
1	3.751439000	1.453122000	1.325290000
6	5.527986000	-1.179870000	0.156781000
1	4.771405000	-2.663281000	-1.195728000
1	5.977472000	0.440403000	1.485153000
1	6.507069000	-1.634629000	0.244137000
6	-2.599697000	-0.435663000	0.002661000
6	-2.730290000	-1.513454000	0.880696000
6	-3.706839000	-0.084397000	-0.772499000
6	-3.918416000	-2.211072000	0.978667000
1	-1.882163000	-1.787953000	1.502476000
6	-4.899735000	-0.773959000	-0.657696000
1	-3.612273000	0.732015000	-1.483226000
6	-5.014730000	-1.842844000	0.214806000
1	-3.991610000	-3.045226000	1.667201000
1	-5.744711000	-0.479522000	-1.269856000
1	-5.947975000	-2.386409000	0.297419000
31	0.232756000	-0.644758000	-0.149351000
14	-1.353223000	2.002992000	-0.405732000
6	-2.545274000	2.885300000	0.747509000
1	-3.588584000	2.710767000	0.485844000
1	-2.383424000	2.547716000	1.774959000
1	-2.355922000	3.959705000	0.703044000

4Ga-S (T.E = -2826.033818)

7	1.262213000	0.596711000	-0.204057000
6	0.993042000	1.882339000	-0.379957000
6	-0.249179000	2.482187000	-0.432524000
6	-1.473857000	1.822829000	-0.286312000
6	-1.660321000	0.474838000	-0.082439000
6	2.616599000	0.233146000	-0.091059000
6	3.086171000	-0.896209000	-0.759188000
6	3.505703000	0.951633000	0.707331000
6	4.407710000	-1.284270000	-0.642496000
1	2.399472000	-1.456791000	-1.383745000
6	4.828487000	0.562213000	0.815742000
1	3.141613000	1.805630000	1.268171000
6	5.288191000	-0.556624000	0.141678000
1	4.754620000	-2.161784000	-1.176414000
1	5.502766000	1.131948000	1.445486000
1	6.323589000	-0.863099000	0.231389000
1	1.851837000	2.545453000	-0.521246000

15	-3.241650000	-0.145708000	0.066192000
6	-4.617086000	1.023955000	-0.058765000
1	-5.565148000	0.494336000	0.051567000
1	-4.537266000	1.778840000	0.724467000
1	-4.597378000	1.521526000	-1.029161000
6	-3.581797000	-1.410047000	-1.174744000
1	-3.528515000	-0.963514000	-2.168201000
1	-2.811227000	-2.181013000	-1.101600000
1	-4.564825000	-1.860817000	-1.023658000
6	-3.487654000	-0.999315000	1.636301000
1	-3.377749000	-0.287478000	2.455093000
1	-4.473207000	-1.467278000	1.682732000
1	-2.714336000	-1.764168000	1.738923000
1	-2.340507000	2.492068000	-0.350583000
1	-0.261929000	3.550742000	-0.608762000
31	-0.108020000	-0.968581000	0.123860000

4Ga-T (T.E = -2825.971894)

7	1.324718000	0.570836000	-0.225909000
6	0.999061000	1.912316000	-0.352541000
6	-0.269055000	2.449231000	-0.307116000
6	-1.493627000	1.810481000	-0.132259000
6	-1.686910000	0.393445000	0.023656000
6	2.644306000	0.178467000	-0.065478000
6	3.022317000	-1.135866000	-0.373635000
6	3.638318000	1.037763000	0.421764000
6	4.318308000	-1.571357000	-0.194502000
1	2.276259000	-1.811968000	-0.785170000
6	4.937316000	0.593969000	0.586457000
1	3.379248000	2.048585000	0.711080000
6	5.294720000	-0.709167000	0.283249000
1	4.573467000	-2.594706000	-0.447273000
1	5.681556000	1.281262000	0.974503000
1	6.314929000	-1.048066000	0.415075000
1	1.828787000	2.582160000	-0.557723000
15	-3.237615000	-0.262599000	0.146843000
6	-4.180194000	0.382262000	1.553539000
1	-5.197150000	-0.014784000	1.570593000
1	-3.663293000	0.121018000	2.477349000
1	-4.221717000	1.470418000	1.480794000
6	-4.339009000	0.063901000	-1.257433000
1	-4.377574000	1.141498000	-1.427376000
1	-3.924789000	-0.407780000	-2.149309000
1	-5.349890000	-0.307693000	-1.076476000
6	-3.228323000	-2.049498000	0.343447000
1	-2.655657000	-2.320987000	1.230815000
1	-4.253568000	-2.408062000	0.450703000
1	-2.771951000	-2.518910000	-0.528601000

1	-2.375858000	2.453637000	-0.138913000
1	-0.305324000	3.524729000	-0.448178000
31	-0.116441000	-0.689771000	-0.178969000

5Ga-S (T.E = -2743.835892)

7	1.514479000	0.319326000	-0.125676000
6	1.298216000	1.581738000	-0.250394000
7	-1.311293000	0.332819000	-0.098993000
1	2.156284000	2.256490000	-0.338908000
6	2.854950000	-0.109328000	-0.025787000
6	3.266524000	-1.201416000	-0.782294000
6	3.757766000	0.496003000	0.842331000
6	4.567125000	-1.660484000	-0.690991000
1	2.558453000	-1.673159000	-1.454964000
6	5.059325000	0.033671000	0.926415000
1	3.426035000	1.313067000	1.474312000
6	5.469752000	-1.043229000	0.159663000
1	4.878406000	-2.507013000	-1.291649000
1	5.753142000	0.511281000	1.608473000
1	6.487433000	-1.407261000	0.231961000
6	-2.633649000	-0.178311000	-0.018324000
6	-3.027550000	-1.164696000	-0.914536000
6	-3.515928000	0.208779000	0.986108000
6	-4.277423000	-1.754756000	-0.811569000
1	-2.347604000	-1.451659000	-1.710537000
6	-4.762563000	-0.376790000	1.082351000
1	-3.214076000	0.978642000	1.685942000
6	-5.149929000	-1.362174000	0.185810000
1	-4.568238000	-2.521082000	-1.520864000
1	-5.440376000	-0.063581000	1.868345000
1	-6.128901000	-1.819520000	0.266949000
6	-1.222052000	1.664404000	-0.222178000
8	-2.119552000	2.474878000	-0.295049000
7	0.122421000	2.218262000	-0.302792000
6	0.141816000	3.665011000	-0.485149000
1	-0.381938000	3.941040000	-1.399131000
1	-0.358864000	4.160137000	0.345387000
1	1.175021000	4.002554000	-0.541863000
31	-0.008900000	-1.238785000	0.223885000

5Ga-T (T.E = -2743.743235)

7	1.503966000	0.255266000	-0.036379000
6	1.211133000	1.512703000	-0.465106000
7	-1.394794000	0.358361000	0.002598000
1	1.872504000	2.010094000	-1.167068000
6	2.811352000	-0.235677000	-0.087555000

6	3.020753000	-1.614476000	-0.119277000
6	3.921126000	0.608856000	-0.110732000
6	4.296781000	-2.134561000	-0.163974000
1	2.157292000	-2.277169000	-0.123260000
6	5.197493000	0.079726000	-0.175610000
1	3.776929000	1.681268000	-0.049061000
6	5.397087000	-1.289502000	-0.201525000
1	4.435473000	-3.209302000	-0.182807000
1	6.048691000	0.750987000	-0.192601000
1	6.399316000	-1.697290000	-0.248780000
6	-2.646552000	-0.281834000	-0.115021000
6	-2.651368000	-1.565211000	-0.659545000
6	-3.850246000	0.259750000	0.329966000
6	-3.819680000	-2.296474000	-0.754026000
1	-1.717540000	-1.977008000	-1.036984000
6	-5.018578000	-0.473447000	0.219293000
1	-3.863284000	1.255194000	0.748741000
6	-5.014654000	-1.750199000	-0.316409000
1	-3.796699000	-3.292024000	-1.181773000
1	-5.947972000	-0.037429000	0.567803000
1	-5.935606000	-2.315615000	-0.393053000
6	-1.264749000	1.728703000	-0.109142000
8	-2.186904000	2.503515000	-0.211021000
7	0.060780000	2.201115000	-0.082724000
6	0.206887000	3.647356000	-0.142782000
1	0.271887000	4.001735000	-1.177258000
1	-0.654867000	4.119342000	0.320413000
1	1.115941000	3.931970000	0.387458000
31	0.043961000	-0.640334000	0.756794000

6Ga-S (T.E = -2956.616610)

6	-1.461689000	1.382630000	-0.109544000
6	-1.460961000	-0.021180000	-0.008435000
6	1.040163000	1.569449000	-0.195170000
1	1.826003000	2.329788000	-0.262096000
7	1.386205000	0.331056000	-0.124838000
15	-3.080240000	-0.565989000	0.105239000
6	-4.014717000	0.007535000	1.543897000
1	-4.060093000	1.095287000	1.518180000
1	-5.024557000	-0.408383000	1.537930000
1	-3.497159000	-0.310360000	2.449986000
6	-4.143699000	-0.199747000	-1.311289000
1	-3.707720000	-0.648798000	-2.204715000
1	-5.146390000	-0.603224000	-1.154605000
1	-4.192689000	0.880629000	-1.438939000
6	-3.146420000	-2.363630000	0.238727000
1	-2.606282000	-2.699742000	1.124942000
1	-4.188370000	-2.681260000	0.311051000

1	-2.690044000	-2.827417000	-0.636944000
8	-2.445404000	2.130667000	-0.123824000
7	-0.193970000	2.088876000	-0.215041000
6	-0.316662000	3.533405000	-0.348246000
1	-0.881095000	3.788732000	-1.244493000
1	-0.849442000	3.951622000	0.504759000
1	0.677592000	3.973054000	-0.409208000
6	2.767553000	0.059761000	-0.032876000
6	3.319301000	-0.930948000	-0.838740000
6	3.584655000	0.729042000	0.872993000
6	4.667495000	-1.222761000	-0.758019000
1	2.675577000	-1.461564000	-1.531148000
6	4.934784000	0.432987000	0.948163000
1	3.148428000	1.463082000	1.542264000
6	5.482542000	-0.540823000	0.131894000
1	5.086128000	-1.991434000	-1.397303000
1	5.558660000	0.959140000	1.661615000
1	6.538182000	-0.776133000	0.195720000
31	0.040012000	-1.423947000	0.013678000

6Ga-T (T.E = -2956.545740)

6	-1.480929000	1.385438000	-0.097793000
6	-1.515546000	-0.052293000	0.022247000
6	1.029635000	1.623916000	-0.067990000
1	1.763040000	2.377792000	-0.334262000
7	1.409680000	0.312007000	-0.152123000
15	-3.095959000	-0.678493000	0.124061000
6	-4.059147000	-0.139616000	1.552063000
1	-4.161975000	0.943702000	1.509713000
1	-5.044804000	-0.609965000	1.547955000
1	-3.527186000	-0.414558000	2.463584000
6	-4.167500000	-0.384033000	-1.299142000
1	-3.703787000	-0.814198000	-2.187776000
1	-5.147781000	-0.839344000	-1.142433000
1	-4.271734000	0.691551000	-1.434348000
6	-3.020560000	-2.472757000	0.273392000
1	-2.451846000	-2.750159000	1.161981000
1	-4.030958000	-2.877365000	0.353622000
1	-2.532566000	-2.902101000	-0.602753000
8	-2.555847000	2.006578000	-0.126699000
7	-0.287901000	2.078545000	-0.176600000
6	-0.368157000	3.525969000	-0.275879000
1	-1.412219000	3.818066000	-0.318806000
1	0.105144000	3.990552000	0.593609000
1	0.146745000	3.870355000	-1.176618000
6	2.764978000	0.005504000	-0.036290000
6	3.236657000	-1.219799000	-0.521801000
6	3.690532000	0.876212000	0.548245000

6	4.565913000	-1.566613000	-0.413487000
1	2.537962000	-1.893644000	-1.012465000
6	5.025590000	0.522048000	0.643103000
1	3.350709000	1.815038000	0.968126000
6	5.478278000	-0.695239000	0.167673000
1	4.898601000	-2.522730000	-0.801872000
1	5.720782000	1.212499000	1.108456000
1	6.525122000	-0.962838000	0.242585000
31	0.102968000	-1.070780000	-0.079052000

7Ga-S (T.E = -3069.382359)

7	0.785281000	0.024414000	-0.145057000
6	0.838022000	1.404203000	-0.488114000
6	-0.319384000	2.157861000	-0.694529000
6	-1.602926000	1.663472000	-0.578307000
7	-1.997894000	0.432564000	-0.284334000
1	-0.206396000	3.200573000	-0.963684000
1	-2.398337000	2.389364000	-0.775823000
15	2.433788000	0.097076000	-0.033685000
6	2.202026000	1.728612000	-0.531933000
6	2.921101000	3.001535000	-0.765823000
1	2.362809000	3.631465000	-1.464117000
1	3.074802000	3.597061000	0.143967000
1	3.905877000	2.838500000	-1.209825000
6	-3.373066000	0.207762000	-0.125294000
6	-3.940353000	-0.959708000	-0.636309000
6	-4.197166000	1.093966000	0.569777000
6	-5.287168000	-1.222568000	-0.470751000
1	-3.310104000	-1.650953000	-1.185632000
6	-5.546009000	0.830379000	0.723969000
1	-3.763516000	1.982567000	1.015626000
6	-6.100556000	-0.328008000	0.205652000
1	-5.707141000	-2.133106000	-0.883129000
1	-6.167141000	1.531949000	1.269811000
1	-7.156338000	-0.535054000	0.333161000
31	-0.757703000	-1.231181000	0.232799000
7	3.097381000	-0.141197000	1.467609000
7	3.146805000	-1.093998000	-0.934573000
6	2.928070000	-1.448162000	2.086963000
1	2.989645000	-2.240636000	1.342323000
1	3.712220000	-1.606091000	2.832376000
1	1.952390000	-1.525385000	2.585928000
6	2.945022000	0.942471000	2.424828000
1	3.170625000	1.900486000	1.960044000
1	1.925267000	0.984081000	2.831874000
1	3.639270000	0.783985000	3.253659000
6	4.569977000	-1.361675000	-0.867184000
1	4.748362000	-2.433763000	-0.996905000

1	5.114876000	-0.831633000	-1.658588000
1	4.975624000	-1.056966000	0.095782000
6	2.569215000	-1.406443000	-2.229893000
1	1.497950000	-1.211530000	-2.222646000
1	3.030804000	-0.813618000	-3.029078000
1	2.728569000	-2.465512000	-2.450437000

7Ga-T (T.E = -3069.302507)

7	0.827692000	0.028656000	-0.341377000
6	0.792443000	1.476602000	-0.442042000
6	-0.329261000	2.236024000	-0.552359000
6	-1.660370000	1.773325000	-0.548358000
7	-2.013464000	0.471981000	-0.335101000
1	-0.180991000	3.307006000	-0.657850000
1	-2.447088000	2.484359000	-0.782893000
15	2.423749000	0.072548000	-0.045716000
6	2.200428000	1.798072000	-0.299607000
6	2.927851000	3.073557000	-0.318589000
1	2.795063000	3.598929000	-1.271518000
1	2.553891000	3.752056000	0.459786000
1	3.998222000	2.937917000	-0.156289000
6	-3.362158000	0.194519000	-0.170495000
6	-3.867667000	-1.054918000	-0.562546000
6	-4.265652000	1.109098000	0.394657000
6	-5.197974000	-1.375471000	-0.385122000
1	-3.199582000	-1.759342000	-1.046735000
6	-5.595688000	0.780531000	0.562421000
1	-3.897932000	2.067096000	0.743003000
6	-6.077142000	-0.461456000	0.176516000
1	-5.557283000	-2.346815000	-0.706679000
1	-6.266930000	1.503434000	1.013848000
1	-7.123231000	-0.711388000	0.306577000
31	-0.796421000	-1.144310000	0.208906000
7	3.013568000	-0.316748000	1.458839000
7	3.291474000	-0.918016000	-1.035935000
6	2.963208000	-1.710039000	1.885053000
1	3.159947000	-2.380022000	1.049596000
1	3.717276000	-1.884005000	2.657396000
1	1.976855000	-1.961785000	2.296409000
6	2.651784000	0.591874000	2.537286000
1	2.787083000	1.629011000	2.231185000
1	1.607897000	0.454535000	2.851219000
1	3.298813000	0.399686000	3.396156000
6	4.710099000	-1.168388000	-0.878754000
1	4.917452000	-2.238395000	-0.987128000
1	5.286572000	-0.635492000	-1.643756000
1	5.053688000	-0.846424000	0.102441000
6	2.785334000	-1.238934000	-2.358713000

1	1.718493000	-1.030227000	-2.412893000
1	3.303780000	-0.660164000	-3.131750000
1	2.944530000	-2.302083000	-2.561562000

8Ga-S (T.E = -3190.659332)

7	1.481236000	0.408018000	-1.054030000
6	1.058279000	1.514652000	-0.281124000
6	-0.030784000	2.357978000	-0.764711000
15	2.396413000	0.016438000	0.266699000
6	1.734475000	1.493538000	0.916609000
6	1.686659000	2.352276000	2.120726000
1	2.637917000	2.848696000	2.334737000
1	0.935912000	3.136132000	1.983546000
1	1.406131000	1.800522000	3.024352000
7	2.036718000	-1.342187000	1.131176000
7	3.975497000	-0.203411000	-0.155292000
6	2.327241000	-2.654768000	0.573771000
1	1.464958000	-3.042989000	0.015600000
1	3.178714000	-2.608894000	-0.103529000
1	2.558833000	-3.352676000	1.383560000
6	0.845875000	-1.348457000	1.968115000
1	0.976353000	-2.081873000	2.768048000
1	0.682164000	-0.368756000	2.413363000
1	-0.053646000	-1.616734000	1.397513000
6	4.975100000	-0.591056000	0.819903000
1	5.693637000	-1.277125000	0.360358000
1	5.529290000	0.280040000	1.190451000
1	4.513038000	-1.093909000	1.668193000
6	4.516853000	0.540869000	-1.278449000
1	3.722663000	0.774973000	-1.984780000
1	4.990870000	1.473708000	-0.949036000
1	5.273151000	-0.066716000	-1.783436000
6	-2.396808000	-0.648471000	-0.104875000
6	-2.624677000	-0.615280000	1.278693000
6	-3.086752000	-1.620034000	-0.841025000
6	-3.509480000	-1.485897000	1.884748000
1	-2.093056000	0.127835000	1.867579000
6	-3.961226000	-2.500327000	-0.226900000
1	-2.946322000	-1.654780000	-1.916699000
6	-4.184131000	-2.440968000	1.138169000
1	-3.670843000	-1.422206000	2.955795000
1	-4.483902000	-3.235510000	-0.829322000
1	-4.874672000	-3.126336000	1.614725000
7	-1.471238000	0.201380000	-0.700229000
5	-1.436152000	1.601489000	-0.484808000
7	-2.566032000	2.399105000	-0.113934000
6	-3.932314000	1.953385000	-0.255498000
1	-3.993482000	1.051083000	-0.859909000

1	-4.403969000	1.743531000	0.714574000
1	-4.526987000	2.732274000	-0.749280000
6	-2.517859000	3.724683000	0.445369000
1	-1.501509000	4.028669000	0.689456000
1	-2.946070000	4.474274000	-0.234889000
1	-3.100694000	3.768282000	1.375309000
1	0.012640000	3.350471000	-0.317926000
1	0.063718000	2.476341000	-1.850477000
31	-0.109878000	-0.896949000	-1.802235000

8Ga-T (T.E = -3190.568204)

7	-1.399134000	-1.008292000	-0.709884000
6	-0.862048000	-1.553599000	0.493300000
6	0.317670000	-2.424103000	0.458900000
15	-2.296065000	-0.014324000	0.286626000
6	-1.546718000	-0.984642000	1.535258000
6	-1.517574000	-1.178438000	3.001500000
1	-2.468702000	-1.545915000	3.397724000
1	-0.752241000	-1.911077000	3.268489000
1	-1.282828000	-0.255954000	3.541920000
7	-1.978640000	1.586412000	0.403767000
7	-3.880629000	-0.077159000	-0.152212000
6	-2.312835000	2.490319000	-0.688845000
1	-1.422108000	2.676371000	-1.302653000
1	-3.080745000	2.060872000	-1.331160000
1	-2.680051000	3.436847000	-0.278132000
6	-0.863989000	2.079724000	1.203468000
1	-1.153491000	3.025151000	1.671089000
1	-0.593369000	1.366422000	1.979231000
1	0.017571000	2.250677000	0.573591000
6	-4.895642000	0.772207000	0.436643000
1	-5.548251000	1.172301000	-0.346603000
1	-5.518741000	0.208236000	1.140379000
1	-4.442241000	1.607421000	0.967415000
6	-4.413455000	-1.265531000	-0.794426000
1	-3.605150000	-1.844922000	-1.235896000
1	-4.957430000	-1.892004000	-0.077952000
1	-5.108617000	-0.970583000	-1.586010000
6	2.161493000	0.883464000	-0.092793000
6	2.809889000	0.964726000	1.151515000
6	2.216467000	2.016535000	-0.919890000
6	3.432489000	2.127433000	1.558191000
1	2.776486000	0.103239000	1.812480000
6	2.844883000	3.175949000	-0.502584000
1	1.746896000	1.964374000	-1.898851000
6	3.453262000	3.249191000	0.739522000
1	3.901893000	2.162115000	2.535688000
1	2.865284000	4.033798000	-1.166420000

1	3.947179000	4.158085000	1.060716000
7	1.428722000	-0.222315000	-0.434141000
5	1.627830000	-1.590795000	-0.007673000
7	2.889707000	-2.227502000	0.025601000
6	4.080794000	-1.641195000	-0.542710000
1	3.843425000	-0.727013000	-1.082516000
1	4.821131000	-1.401463000	0.231101000
1	4.547177000	-2.342866000	-1.244210000
6	3.132907000	-3.553636000	0.531060000
1	2.241016000	-3.979400000	0.986654000
1	3.458252000	-4.228666000	-0.271087000
1	3.927705000	-3.543954000	1.287723000
1	0.469211000	-2.875908000	1.444826000
1	0.151857000	-3.233929000	-0.263369000
31	0.082418000	-0.277802000	-1.852122000

9Ga-S (T.E = -3360.084922)

7	0.988181000	0.086189000	-0.105024000
6	1.177844000	1.506612000	-0.211731000
6	0.102286000	2.386934000	-0.303763000
1	0.310645000	3.447709000	-0.400778000
15	2.630833000	-0.020687000	-0.001525000
6	2.568693000	1.687443000	-0.191692000
6	3.413373000	2.901853000	-0.223604000
1	4.247704000	2.819009000	-0.925914000
1	2.813434000	3.757198000	-0.546262000
1	3.842870000	3.167199000	0.751116000
7	3.281303000	-0.592995000	1.415225000
7	3.242211000	-1.080318000	-1.120640000
6	3.054758000	-1.984811000	1.775214000
1	2.083776000	-2.112308000	2.273185000
1	3.064587000	-2.621541000	0.891947000
1	3.840421000	-2.319571000	2.458503000
6	3.191190000	0.289282000	2.566688000
1	3.890510000	-0.052795000	3.333733000
1	3.448470000	1.310052000	2.289700000
1	2.180199000	0.290731000	2.997473000
6	4.644495000	-1.446694000	-1.137122000
1	4.750288000	-2.482916000	-1.473806000
1	5.216793000	-0.809872000	-1.824052000
1	5.079423000	-1.359306000	-0.143180000
6	2.638477000	-1.097135000	-2.440669000
1	1.585421000	-0.827605000	-2.377202000
1	3.140955000	-0.398691000	-3.121706000
1	2.715660000	-2.103725000	-2.861193000
6	-3.275502000	-0.205920000	0.005709000
6	-4.126920000	0.192814000	1.038585000
6	-3.767801000	-1.119414000	-0.929452000

6	-5.423335000	-0.281935000	1.117995000
1	-3.744694000	0.872866000	1.794133000
6	-5.062267000	-1.598860000	-0.841703000
1	-3.115147000	-1.437428000	-1.735907000
6	-5.901025000	-1.180682000	0.178079000
1	-6.063443000	0.046710000	1.929349000
1	-5.420031000	-2.305420000	-1.582440000
1	-6.915379000	-1.555565000	0.243325000
7	-1.953485000	0.245009000	-0.077810000
14	-1.546307000	1.835457000	-0.247488000
6	-2.902160000	3.087693000	-0.411648000
1	-3.705908000	2.702950000	-1.041989000
1	-3.338957000	3.327646000	0.559347000
1	-2.509798000	4.007271000	-0.847652000
31	-0.519745000	-1.296031000	0.068400000

9Ga-T (T.E = -3360.013882)

7	1.043624000	0.143932000	-0.424794000
6	1.082153000	1.547183000	-0.056332000
6	0.031235000	2.395317000	-0.153243000
1	0.195726000	3.423978000	0.161592000
15	2.587841000	-0.019825000	0.049085000
6	2.431577000	1.711538000	0.384365000
6	3.203235000	2.887036000	0.810720000
1	3.888200000	3.238518000	0.030722000
1	2.531600000	3.714824000	1.050393000
1	3.815383000	2.677886000	1.693558000
7	2.988123000	-0.902224000	1.388631000
7	3.554341000	-0.641603000	-1.125261000
6	3.007904000	-2.357983000	1.325070000
1	2.019641000	-2.773849000	1.556411000
1	3.289770000	-2.699619000	0.330699000
1	3.732016000	-2.743763000	2.048115000
6	2.489228000	-0.415461000	2.666750000
1	3.080700000	-0.857396000	3.471825000
1	2.576442000	0.668690000	2.730490000
1	1.436562000	-0.688408000	2.817732000
6	4.965639000	-0.901663000	-0.925807000
1	5.223448000	-1.896257000	-1.304916000
1	5.575906000	-0.167351000	-1.463634000
1	5.222132000	-0.859179000	0.131666000
6	3.149433000	-0.610012000	-2.519846000
1	2.082966000	-0.407320000	-2.595394000
1	3.701064000	0.158613000	-3.072572000
1	3.356956000	-1.580238000	-2.980812000
6	-3.180518000	-0.237648000	-0.048143000
6	-3.852125000	-0.001936000	1.154513000
6	-3.843662000	-0.974020000	-1.032573000

6	-5.134731000	-0.475449000	1.358343000
1	-3.337199000	0.557783000	1.928598000
6	-5.127340000	-1.448846000	-0.823995000
1	-3.329165000	-1.157717000	-1.970511000
6	-5.782347000	-1.201349000	0.370182000
1	-5.632998000	-0.279899000	2.301747000
1	-5.620018000	-2.017476000	-1.605188000
1	-6.787139000	-1.573199000	0.532467000
7	-1.867601000	0.218998000	-0.242257000
14	-1.636184000	1.832752000	-0.793555000
6	-2.935720000	3.027300000	-0.133757000
1	-3.940094000	2.731399000	-0.440266000
1	-2.911993000	3.067804000	0.959771000
1	-2.744888000	4.031113000	-0.519448000
31	-0.528685000	-1.268641000	-0.221008000

10Ga-S (T.E = -3282.154071)

7	-0.644888000	0.055571000	0.137875000
6	-0.675652000	1.476300000	0.221998000
6	0.477023000	2.252597000	0.255908000
6	1.766032000	1.730837000	0.191032000
1	0.350374000	3.327100000	0.332395000
1	2.538814000	2.508408000	0.241253000
15	-2.293145000	0.128857000	0.045283000
6	-2.047964000	1.812504000	0.231308000
6	-2.752071000	3.114581000	0.187262000
1	-2.535311000	3.738484000	1.061585000
1	-2.488737000	3.709040000	-0.698384000
1	-3.835372000	2.973565000	0.164180000
6	2.163775000	0.406789000	0.068161000
15	3.810586000	0.025136000	-0.004532000
6	4.998495000	1.390048000	0.102241000
1	6.016496000	1.000525000	0.043401000
1	4.837448000	2.091090000	-0.717668000
1	4.873873000	1.920800000	1.046909000
6	4.259016000	-0.851397000	-1.521837000
1	5.304121000	-1.168629000	-1.508800000
1	3.613196000	-1.727652000	-1.615137000
1	4.080666000	-0.200457000	-2.378497000
6	4.319836000	-1.126349000	1.293531000
1	4.183622000	-0.653842000	2.266939000
1	3.673063000	-2.005547000	1.244386000
1	5.361350000	-1.432514000	1.172681000
31	0.855808000	-1.270906000	-0.060063000
7	-3.002329000	-0.378278000	-1.369766000
7	-3.004279000	-0.873543000	1.163993000
6	-2.923224000	-1.787944000	-1.723145000
1	-1.968334000	-2.020033000	-2.214128000

1	-3.003185000	-2.413103000	-0.835298000
1	-3.737849000	-2.040849000	-2.408185000
6	-2.825594000	0.485781000	-2.524020000
1	-3.557924000	0.214237000	-3.288928000
1	-2.976010000	1.528560000	-2.248551000
1	-1.820424000	0.383049000	-2.956772000
6	-4.447245000	-1.001203000	1.215863000
1	-4.713434000	-1.980718000	1.624868000
1	-4.898537000	-0.233711000	1.859820000
1	-4.879066000	-0.913394000	0.220121000
6	-2.389029000	-0.941801000	2.477358000
1	-1.305560000	-0.879791000	2.388927000
1	-2.737984000	-0.130929000	3.130518000
1	-2.646854000	-1.896211000	2.944375000

10Ga-T (T.E = -3282.078591)

7	0.688099000	0.045076000	-0.211781000
6	0.613999000	1.499353000	-0.252480000
6	-0.537879000	2.228827000	-0.312774000
6	-1.855109000	1.708733000	-0.300309000
1	-0.411588000	3.307722000	-0.373952000
1	-2.646675000	2.451112000	-0.425862000
15	2.295674000	0.136842000	-0.049670000
6	2.001416000	1.860614000	-0.193092000
6	2.690525000	3.160866000	-0.185793000
1	2.448669000	3.753280000	-1.075754000
1	2.394170000	3.768907000	0.679654000
1	3.775354000	3.045442000	-0.149827000
6	-2.153317000	0.329526000	-0.083361000
15	-3.813594000	-0.031857000	0.011499000
6	-4.784044000	0.392215000	-1.467765000
1	-5.847663000	0.189096000	-1.323256000
1	-4.645333000	1.450837000	-1.692586000
1	-4.409076000	-0.190115000	-2.310381000
6	-4.700032000	0.853659000	1.329578000
1	-5.768387000	0.626725000	1.317226000
1	-4.273343000	0.568113000	2.291789000
1	-4.556037000	1.926630000	1.194615000
6	-4.185933000	-1.769169000	0.305808000
1	-3.799134000	-2.383263000	-0.507375000
1	-3.722605000	-2.100424000	1.235391000
1	-5.269018000	-1.891513000	0.372943000
31	-0.847711000	-1.300630000	0.058626000
7	3.019457000	-0.317050000	1.381508000
7	3.116784000	-0.774975000	-1.154916000
6	3.013093000	-1.733406000	1.726795000
1	2.052380000	-2.028450000	2.169376000
1	3.174485000	-2.349321000	0.843493000

1	3.809794000	-1.937733000	2.447842000
6	2.701866000	0.515588000	2.531620000
1	3.394815000	0.280487000	3.343111000
1	2.806381000	1.571787000	2.284356000
1	1.676691000	0.341888000	2.887893000
6	4.548987000	-0.979856000	-1.123217000
1	4.783548000	-2.033424000	-1.312217000
1	5.047904000	-0.382119000	-1.895751000
1	4.957272000	-0.703442000	-0.152766000
6	2.516520000	-1.041716000	-2.448463000
1	1.442486000	-0.868212000	-2.405903000
1	2.953174000	-0.404929000	-3.227278000
1	2.688662000	-2.087105000	-2.722603000

11Ga-S (T.E = -3199.962225)

7	0.828430000	-0.155712000	-0.120853000
6	0.888149000	1.243033000	-0.174606000
6	-1.607934000	1.589625000	-0.223464000
7	-1.857506000	0.280588000	-0.068178000
15	2.477518000	-0.129461000	-0.029907000
6	2.255540000	1.576852000	-0.160940000
6	3.119008000	2.788106000	-0.120318000
1	2.950777000	3.471018000	-0.956334000
1	3.016319000	3.372075000	0.801590000
1	4.167386000	2.483363000	-0.177760000
6	-3.233169000	-0.062613000	-0.043537000
6	-3.714222000	-0.994899000	-0.955216000
6	-4.101863000	0.435044000	0.923699000
6	-5.031036000	-1.423458000	-0.903573000
1	-3.042917000	-1.372421000	-1.720002000
6	-5.415213000	0.011024000	0.970172000
1	-3.733626000	1.164050000	1.635718000
6	-5.887786000	-0.921575000	0.058128000
1	-5.386628000	-2.150596000	-1.624827000
1	-6.078899000	0.410245000	1.729101000
1	-6.918821000	-1.252784000	0.099620000
31	-0.729039000	-1.432121000	0.258922000
7	3.195354000	-0.665988000	1.356720000
7	3.140841000	-1.094832000	-1.193486000
6	3.138643000	-2.085168000	1.681252000
1	3.156228000	-2.689653000	0.775848000
1	3.998642000	-2.353953000	2.300491000
1	2.221386000	-2.325226000	2.234014000
6	3.091576000	0.177838000	2.536374000
1	3.248652000	1.223301000	2.276957000
1	2.109496000	0.080004000	3.018015000
1	3.857321000	-0.122270000	3.255595000
6	4.580004000	-1.264479000	-1.280662000

1	4.807789000	-2.262962000	-1.664899000
1	5.028981000	-0.529311000	-1.960611000
1	5.042500000	-1.157666000	-0.300755000
6	2.480549000	-1.170850000	-2.486590000
1	1.401207000	-1.101182000	-2.364852000
1	2.814939000	-0.369907000	-3.157534000
1	2.718569000	-2.130885000	-2.951326000
8	-2.423672000	2.474926000	-0.371363000
7	-0.206095000	2.013955000	-0.218734000
6	0.024364000	3.447745000	-0.330973000
1	0.639562000	3.800700000	0.497217000
1	0.521458000	3.686196000	-1.273259000
1	-0.940338000	3.942695000	-0.305812000

11Ga-T (T.E = -3199.865868)

7	0.900406000	-0.133537000	-0.647263000
6	0.648542000	0.927780000	0.382863000
6	-1.640633000	1.623690000	-0.127421000
7	-1.957023000	0.283291000	-0.064036000
15	2.462484000	-0.176384000	-0.067490000
6	1.970822000	1.124797000	0.920017000
6	2.517783000	1.993997000	1.984813000
1	2.620572000	3.043820000	1.687028000
1	1.880750000	1.980945000	2.877756000
1	3.510804000	1.651870000	2.289323000
6	-3.304020000	-0.118945000	-0.138173000
6	-3.621250000	-1.264063000	-0.864055000
6	-4.326218000	0.540717000	0.542310000
6	-4.916825000	-1.748418000	-0.902448000
1	-2.834710000	-1.767477000	-1.420083000
6	-5.620426000	0.060616000	0.490136000
1	-4.096911000	1.437148000	1.102406000
6	-5.925980000	-1.086226000	-0.226611000
1	-5.137345000	-2.642539000	-1.474404000
1	-6.402758000	0.588573000	1.023937000
1	-6.943416000	-1.457481000	-0.259468000
31	-0.600881000	-1.067192000	0.222674000
7	3.000000000	-1.531853000	0.715941000
7	3.529292000	-0.063824000	-1.340305000
6	3.285567000	-2.760570000	-0.004110000
1	3.579348000	-2.546156000	-1.029805000
1	4.098628000	-3.300987000	0.489973000
1	2.403077000	-3.413519000	-0.023950000
6	2.544574000	-1.768509000	2.073426000
1	2.324895000	-0.825174000	2.572967000
1	1.637344000	-2.388796000	2.088477000
1	3.323844000	-2.290291000	2.636034000
6	4.948599000	0.016289000	-1.033967000

1	5.526165000	-0.246653000	-1.923827000
1	5.239275000	1.031654000	-0.729116000
1	5.213757000	-0.673479000	-0.233964000
6	3.146090000	0.843189000	-2.412591000
1	2.081027000	0.751982000	-2.619366000
1	3.367391000	1.888319000	-2.154685000
1	3.705476000	0.583542000	-3.314422000
8	-2.430317000	2.506661000	-0.390473000
7	-0.293860000	1.912062000	0.106538000
6	0.136512000	3.292630000	0.025159000
1	0.346951000	3.713600000	1.013061000
1	1.041978000	3.362498000	-0.583868000
1	-0.664074000	3.869205000	-0.432979000

12Ga-S (T.E = -3412.741359)

7	0.754416000	-0.151684000	-0.241189000
6	0.695257000	1.238702000	-0.090723000
6	-1.806322000	1.348956000	-0.115715000
15	2.381456000	-0.011871000	-0.017318000
6	2.026638000	1.672369000	0.079422000
6	2.762797000	2.920623000	0.415724000
1	2.839240000	3.631861000	-0.413149000
1	2.332788000	3.459841000	1.266065000
1	3.789380000	2.666048000	0.696562000
6	-1.991925000	-0.048242000	-0.033562000
15	-3.665339000	-0.376816000	0.025438000
6	-4.571642000	0.308577000	1.436026000
1	-5.626531000	0.029012000	1.391316000
1	-4.132792000	-0.079212000	2.356417000
1	-4.473060000	1.392879000	1.419425000
6	-3.968305000	-2.150978000	0.154248000
1	-5.043920000	-2.331390000	0.204655000
1	-3.554693000	-2.670641000	-0.710989000
1	-3.491602000	-2.551256000	1.050061000
6	-4.645345000	0.113310000	-1.417287000
1	-4.558686000	1.191065000	-1.546492000
1	-4.244382000	-0.387931000	-2.299431000
1	-5.693698000	-0.164479000	-1.287113000
31	-0.668583000	-1.627219000	-0.063744000
7	3.068533000	-0.681041000	1.328336000
7	3.217436000	-0.724966000	-1.255724000
6	3.246964000	-2.124243000	1.414320000
1	2.342323000	-2.610687000	1.800241000
1	3.463006000	-2.543992000	0.433918000
1	4.079985000	-2.346302000	2.087233000
6	2.719530000	-0.090807000	2.610382000
1	3.476248000	-0.367452000	3.348694000
1	2.682937000	0.994964000	2.536047000

1	1.743579000	-0.449315000	2.964471000
6	4.657680000	-0.544932000	-1.298003000
1	5.113549000	-1.367074000	-1.856518000
1	4.931684000	0.397062000	-1.793216000
1	5.075477000	-0.539823000	-0.291465000
6	2.607221000	-0.716703000	-2.575257000
1	1.548923000	-0.959669000	-2.502075000
1	2.716008000	0.258684000	-3.068509000
1	3.098995000	-1.471477000	-3.193585000
7	-0.458232000	1.918177000	-0.125039000
6	-0.367488000	3.369358000	-0.099124000
1	-0.242348000	3.747105000	0.919226000
1	0.474508000	3.695305000	-0.707706000
1	-1.290937000	3.774031000	-0.500562000
8	-2.704637000	2.197198000	-0.159584000

12Ga-T (T.E = -3412.652663)

7	0.771432000	-0.049631000	-0.607776000
6	0.630488000	1.208797000	0.077410000
6	-1.847814000	1.354937000	-0.102866000
15	2.356930000	0.012986000	-0.132020000
6	1.932326000	1.577893000	0.450709000
6	2.565321000	2.662432000	1.245428000
1	2.470629000	3.651413000	0.789060000
1	2.159120000	2.735220000	2.261634000
1	3.636121000	2.468425000	1.347179000
6	-2.050664000	-0.028658000	0.074674000
15	-3.664612000	-0.513650000	-0.154998000
6	-4.878474000	0.283666000	0.918431000
1	-5.885164000	-0.080056000	0.702478000
1	-4.626194000	0.066645000	1.957158000
1	-4.823467000	1.359181000	0.754295000
6	-3.834030000	-2.272791000	0.184237000
1	-4.870929000	-2.584084000	0.043790000
1	-3.181610000	-2.834392000	-0.487638000
1	-3.529331000	-2.475132000	1.212354000
6	-4.301603000	-0.289647000	-1.830194000
1	-4.229055000	0.768884000	-2.080744000
1	-3.678022000	-0.864419000	-2.516662000
1	-5.338940000	-0.622021000	-1.906890000
31	-0.543334000	-1.261717000	0.301969000
7	2.879732000	-1.039954000	1.029944000
7	3.339415000	-0.342376000	-1.411352000
6	2.873294000	-2.466000000	0.752538000
1	1.934479000	-2.917694000	1.105214000
1	2.959870000	-2.653881000	-0.317545000
1	3.711282000	-2.951566000	1.263060000
6	2.640280000	-0.745265000	2.433191000

1	3.392464000	-1.262412000	3.037327000
1	2.718097000	0.323294000	2.622515000
1	1.636975000	-1.077214000	2.737506000
6	4.765206000	-0.550889000	-1.267593000
1	5.094281000	-1.340105000	-1.951226000
1	5.327892000	0.359599000	-1.509528000
1	5.010914000	-0.850256000	-0.250191000
6	2.952102000	0.125832000	-2.730012000
1	1.869807000	0.233299000	-2.781032000
1	3.420253000	1.089810000	-2.964892000
1	3.271165000	-0.602742000	-3.481007000
7	-0.528728000	1.897619000	0.101078000
6	-0.439484000	3.323102000	0.367703000
1	-0.140552000	3.516950000	1.400611000
1	0.281077000	3.790916000	-0.305442000
1	-1.423507000	3.747570000	0.188221000
8	-2.747962000	2.158490000	-0.393823000

¹³Ga-S (T.E = -3525.507336)

7	-1.358159000	-0.131253000	0.153981000
6	-1.219945000	1.272956000	0.415943000
6	0.000077000	1.923376000	0.532474000
6	1.220293000	1.273863000	0.411560000
1	0.000106000	2.993034000	0.714830000
15	-2.978229000	0.146894000	0.072783000
6	-2.542740000	1.753754000	0.473777000
6	-3.090533000	3.123657000	0.602740000
1	-2.796523000	3.602684000	1.542996000
1	-2.761602000	3.788430000	-0.207442000
1	-4.182759000	3.114271000	0.582966000
7	1.358664000	-0.129566000	0.146179000
6	2.542800000	1.754793000	0.471379000
15	2.979117000	0.147912000	0.070153000
6	3.088658000	3.123734000	0.615892000
1	2.856519000	3.771505000	-0.240653000
1	2.695662000	3.626237000	1.506103000
1	4.176047000	3.108151000	0.717938000
7	3.819794000	-0.899982000	1.047347000
7	3.727315000	-0.084942000	-1.398422000
6	3.241325000	-1.213657000	2.341229000
1	3.535664000	-0.481841000	3.104746000
1	2.154663000	-1.230653000	2.272603000
1	3.586758000	-2.201090000	2.659883000
6	5.268904000	-0.911093000	1.062397000
1	5.669603000	-0.222776000	1.818714000
1	5.626262000	-1.917347000	1.303065000
1	5.667612000	-0.625460000	0.090454000
6	3.778507000	-1.435563000	-1.937216000

1	4.594016000	-1.512379000	-2.662129000
1	3.946539000	-2.162183000	-1.143638000
1	2.838273000	-1.696893000	-2.442778000
6	3.436491000	0.900301000	-2.425837000
1	2.434619000	0.756223000	-2.855091000
1	3.493565000	1.908228000	-2.017913000
1	4.170939000	0.805003000	-3.229803000
7	-3.821639000	-0.902744000	1.045942000
7	-3.723605000	-0.082407000	-1.397737000
6	-5.270866000	-0.907578000	1.060630000
1	-5.632555000	-1.912445000	1.300498000
1	-5.668793000	-0.217979000	1.817249000
1	-5.668155000	-0.619620000	0.088774000
6	-3.245425000	-1.220589000	2.339872000
1	-2.158910000	-1.244332000	2.271514000
1	-3.535438000	-0.487391000	3.103766000
1	-3.597254000	-2.205971000	2.657807000
6	-3.429192000	0.903239000	-2.423788000
1	-4.163297000	0.810947000	-3.228423000
1	-3.483430000	1.910929000	-2.014772000
1	-2.427430000	0.756675000	-2.852461000
6	-3.780130000	-1.431980000	-1.938440000
1	-3.950725000	-2.159080000	-1.145887000
1	-4.596031000	-1.504696000	-2.663359000
1	-2.840996000	-1.696125000	-2.444566000
31	-0.000071000	-1.584360000	-0.236959000

¹³Ga-T (T.E = -3525.411802)

7	1.427783000	-0.044723000	-0.777947000
6	1.232884000	1.414119000	-0.809755000
6	0.025656000	2.015184000	-0.420786000
6	-1.176700000	1.351436000	-0.270292000
1	0.026926000	3.090924000	-0.263413000
15	2.871795000	0.150561000	-0.057041000
6	2.545522000	1.850439000	-0.289984000
6	3.149576000	3.177120000	-0.118952000
1	3.264126000	3.695647000	-1.079813000
1	2.519656000	3.825304000	0.504148000
1	4.131771000	3.120274000	0.354643000
7	-1.336318000	-0.082151000	-0.483831000
6	-2.486219000	1.780291000	0.068745000
15	-2.897331000	0.118177000	-0.026435000
6	-3.014759000	3.084716000	0.521554000
1	-2.519568000	3.445528000	1.434725000
1	-2.891686000	3.870796000	-0.232406000
1	-4.083635000	3.021569000	0.740049000
7	-3.961895000	-0.540770000	-1.128787000
7	-3.405525000	-0.602107000	1.390827000

6	-3.605051000	-0.392985000	-2.529744000
1	-3.849823000	0.609378000	-2.907836000
1	-2.538505000	-0.564291000	-2.663619000
1	-4.159974000	-1.128609000	-3.117921000
6	-5.382383000	-0.346709000	-0.901330000
1	-5.710386000	0.653027000	-1.222698000
1	-5.948800000	-1.086471000	-1.474105000
1	-5.625074000	-0.465922000	0.153835000
6	-3.540998000	-2.049473000	1.441044000
1	-4.208916000	-2.326496000	2.262069000
1	-3.954944000	-2.429661000	0.508789000
1	-2.568497000	-2.535519000	1.605818000
6	-2.817522000	-0.069608000	2.607215000
1	-1.791778000	-0.438499000	2.757591000
1	-2.788954000	1.018903000	2.573319000
1	-3.420435000	-0.379373000	3.464957000
7	4.088165000	-0.659121000	-0.831680000
7	3.131065000	-0.288346000	1.535733000
6	5.451623000	-0.684200000	-0.347029000
1	5.864730000	-1.695677000	-0.430884000
1	6.089141000	-0.012887000	-0.935461000
1	5.497033000	-0.378022000	0.696777000
6	3.967256000	-0.961549000	-2.244973000
1	2.923151000	-0.911451000	-2.548173000
1	4.550914000	-0.259816000	-2.853240000
1	4.341293000	-1.972235000	-2.435970000
6	2.365827000	0.460137000	2.520703000
1	2.807485000	0.306792000	3.508550000
1	2.380793000	1.526089000	2.290983000
1	1.315110000	0.132840000	2.551684000
6	3.223674000	-1.699175000	1.884544000
1	3.721645000	-2.262480000	1.096927000
1	3.794683000	-1.809612000	2.810878000
1	2.227776000	-2.138274000	2.034083000
31	0.056598000	-1.535831000	-0.404133000

Cartesian coordinates of the transition states involved in the dihydrogen activation by some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AITS^{H-H} (T.E = -931.965796)

7	1.426588000	0.464323000	-0.379623000
6	1.230276000	1.741670000	-0.632028000
6	0.000008000	2.369047000	-0.773016000
7	-1.426592000	0.464320000	-0.379605000
1	0.000004000	3.420223000	-1.022827000
1	2.123416000	2.356686000	-0.756249000
6	2.740998000	0.016678000	-0.101396000
6	3.204813000	-1.154097000	-0.689807000
6	3.553095000	0.708198000	0.789461000
6	4.480815000	-1.607062000	-0.413618000
1	2.558392000	-1.694581000	-1.373082000
6	4.831341000	0.250173000	1.058517000
1	3.162048000	1.585352000	1.293505000
6	5.299246000	-0.905347000	0.457850000
1	4.839863000	-2.514329000	-0.884882000
1	5.457769000	0.792400000	1.757092000
1	6.297374000	-1.265928000	0.675712000
6	-2.740999000	0.016679000	-0.101377000
6	-3.204720000	-1.154208000	-0.689643000
6	-3.553206000	0.708292000	0.789309000
6	-4.480720000	-1.607195000	-0.413486000
1	-2.558220000	-1.694776000	-1.372780000
6	-4.831452000	0.250249000	1.058328000
1	-3.162254000	1.585538000	1.293266000
6	-5.299257000	-0.905386000	0.457805000
1	-4.839684000	-2.514552000	-0.884642000
1	-5.457959000	0.792553000	1.756774000
1	-6.297384000	-1.265983000	0.675646000
6	-1.230254000	1.741690000	-0.631925000
1	-2.123386000	2.356745000	-0.756012000
13	-0.000004000	-0.736489000	0.043199000
1	0.000044000	-1.444737000	1.458860000
1	0.000155000	-0.237032000	1.902768000

4AITS^{H-H} (T.E = -1144.755857)

7	1.244653000	0.537855000	-0.017571000
6	0.938396000	1.812854000	0.278062000
6	-0.298483000	2.401161000	0.276065000
6	-1.528598000	1.728531000	0.080297000

6	-1.669833000	0.398467000	-0.211326000
6	2.586935000	0.132771000	0.019875000
6	2.878769000	-1.171731000	0.417319000
6	3.637130000	0.962396000	-0.374546000
6	4.184724000	-1.627993000	0.428668000
1	2.072148000	-1.815797000	0.754781000
6	4.939493000	0.501749000	-0.350329000
1	3.426308000	1.962573000	-0.735783000
6	5.223047000	-0.794843000	0.050709000
1	4.390494000	-2.643740000	0.746438000
1	5.741735000	1.158859000	-0.666957000
1	6.245480000	-1.152974000	0.061506000
1	1.774459000	2.440605000	0.586879000
15	-3.217213000	-0.321363000	-0.018537000
6	-4.602167000	0.683140000	-0.598691000
1	-5.544451000	0.160352000	-0.424767000
1	-4.625224000	1.633588000	-0.064409000
1	-4.487194000	0.882512000	-1.664410000
6	-3.331386000	-1.881918000	-0.894288000
1	-3.204072000	-1.718910000	-1.964563000
1	-2.536406000	-2.542519000	-0.541106000
1	-4.300610000	-2.346083000	-0.704728000
6	-3.588845000	-0.679445000	1.707078000
1	-3.637232000	0.261844000	2.257409000
1	-4.537241000	-1.211131000	1.804538000
1	-2.770953000	-1.284125000	2.105558000
1	-2.412656000	2.356220000	0.233411000
1	-0.331157000	3.450604000	0.540548000
13	-0.086847000	-0.704586000	-0.596620000
1	-0.176432000	-2.243168000	-0.109866000
1	-0.627445000	-1.924458000	0.969258000

6AITS^{H-H} (T.E = -1275.334086)

6	-1.505394000	1.242311000	-0.136654000
6	-1.489202000	-0.155822000	-0.200700000
6	1.002869000	1.458715000	-0.260613000
1	1.801249000	2.203420000	-0.255150000
13	0.099963000	-1.263004000	-0.345720000
7	1.347814000	0.209735000	-0.276839000
15	-3.038063000	-0.799294000	0.104002000
6	-3.710925000	-0.385714000	1.727397000
1	-3.818534000	0.696226000	1.796473000
1	-4.678667000	-0.866941000	1.882653000
1	-3.005109000	-0.725597000	2.487603000
6	-4.335955000	-0.364467000	-1.072891000
1	-4.052795000	-0.721224000	-2.063830000
1	-5.287203000	-0.814406000	-0.781324000
1	-4.429507000	0.720767000	-1.095629000

6	-2.960613000	-2.596554000	0.088940000
1	-2.274971000	-2.937996000	0.867860000
1	-3.951355000	-3.015059000	0.275149000
1	-2.591057000	-2.949115000	-0.875175000
8	-2.481797000	1.979175000	0.000838000
7	-0.230535000	1.971361000	-0.252275000
6	-0.364053000	3.420100000	-0.285696000
1	-0.960903000	3.728543000	-1.143550000
1	-0.865599000	3.779340000	0.611785000
1	0.625490000	3.869062000	-0.356813000
6	2.725022000	-0.087897000	-0.097581000
6	3.374795000	-0.905759000	-1.011153000
6	3.405682000	0.394420000	1.011842000
6	4.711053000	-1.212903000	-0.825963000
1	2.823595000	-1.288902000	-1.862686000
6	4.744135000	0.087822000	1.187063000
1	2.866480000	0.979392000	1.749332000
6	5.398840000	-0.715217000	0.268957000
1	5.219004000	-1.843895000	-1.545715000
1	5.271104000	0.463324000	2.056287000
1	6.444413000	-0.961489000	0.411111000
1	0.637653000	-2.444072000	0.594418000
1	0.554043000	-1.638185000	1.520945000

8AITS^{H-H} (T.E = -1509.381932)

7	1.305141000	0.167635000	-1.118627000
6	1.071997000	1.421900000	-0.498439000
6	-0.039299000	2.250124000	-0.963885000
15	2.381865000	-0.111025000	0.108623000
6	1.932681000	1.518044000	0.562831000
6	2.187672000	2.566410000	1.573913000
1	3.208522000	2.957958000	1.534870000
1	1.512458000	3.411157000	1.411969000
1	2.020509000	2.213374000	2.596768000
7	2.090712000	-1.229321000	1.265660000
7	3.844177000	-0.533777000	-0.512599000
6	2.405716000	-2.642135000	1.095786000
1	1.501293000	-3.196233000	0.824680000
1	3.140609000	-2.783720000	0.306002000
1	2.811719000	-3.034372000	2.033714000
6	0.988755000	-1.015784000	2.195315000
1	1.248959000	-1.449170000	3.165009000
1	0.793292000	0.048325000	2.324324000
1	0.077628000	-1.496120000	1.818110000
6	4.990521000	-0.722608000	0.355369000
1	5.561816000	-1.600055000	0.035924000
1	5.656474000	0.147619000	0.321298000
1	4.676097000	-0.876537000	1.387051000

6	4.196136000	-0.226964000	-1.887814000
1	3.300585000	-0.163315000	-2.501986000
1	4.745972000	0.719105000	-1.958889000
1	4.835581000	-1.023689000	-2.278103000
13	-0.212001000	-0.714090000	-1.877535000
6	-2.527654000	-0.707111000	-0.378012000
6	-2.725149000	-0.839012000	0.998742000
6	-3.284718000	-1.511101000	-1.228974000
6	-3.656449000	-1.726778000	1.501124000
1	-2.134536000	-0.219549000	1.667618000
6	-4.205334000	-2.412469000	-0.720558000
1	-3.143886000	-1.411264000	-2.300799000
6	-4.401630000	-2.524001000	0.644716000
1	-3.797217000	-1.804142000	2.573866000
1	-4.781770000	-3.027063000	-1.403185000
1	-5.127402000	-3.224672000	1.039989000
7	-1.554509000	0.165898000	-0.889552000
5	-1.441534000	1.536958000	-0.554368000
7	-2.463681000	2.341516000	0.036221000
6	-3.869165000	2.009958000	0.008646000
1	-4.068761000	1.178289000	-0.663552000
1	-4.252390000	1.740642000	1.002248000
1	-4.445530000	2.875163000	-0.342998000
6	-2.241224000	3.586517000	0.724115000
1	-1.181104000	3.778569000	0.883821000
1	-2.669953000	4.441007000	0.181687000
1	-2.716545000	3.565038000	1.713681000
1	0.051118000	3.274091000	-0.604752000
1	-0.022735000	2.280537000	-2.062273000
1	-0.095116000	-2.313302000	-1.863902000
1	0.040019000	-2.277496000	-0.656720000

10AITS^{H-H} (T.E = -1600.882768)

7	0.597294000	-0.049371000	-0.395313000
6	0.570912000	1.385326000	-0.300057000
6	-0.604684000	2.129737000	-0.293244000
6	-1.888479000	1.585796000	-0.261993000
1	-0.496883000	3.208794000	-0.307096000
1	-2.681771000	2.338010000	-0.323651000
15	2.212844000	0.060473000	-0.092041000
6	1.923308000	1.749396000	-0.201936000
6	2.573537000	3.058904000	0.031100000
1	2.525083000	3.718197000	-0.842420000
1	2.113717000	3.602671000	0.866443000
1	3.631851000	2.936348000	0.273388000
6	-2.251248000	0.252615000	-0.139146000
15	-3.875838000	-0.212789000	-0.039327000
6	-5.072870000	1.134363000	0.085918000

1	-6.079183000	0.723391000	0.181198000
1	-4.851457000	1.748070000	0.959615000
1	-5.029360000	1.760645000	-0.805862000
6	-4.165746000	-1.267374000	1.393427000
1	-5.199199000	-1.617270000	1.432442000
1	-3.493248000	-2.127102000	1.321219000
1	-3.917785000	-0.716386000	2.301015000
6	-4.451435000	-1.217237000	-1.428692000
1	-4.414052000	-0.623478000	-2.342709000
1	-3.776104000	-2.068356000	-1.538688000
1	-5.469062000	-1.577880000	-1.263919000
7	2.745751000	-0.475640000	1.382115000
7	3.067959000	-0.885709000	-1.145188000
6	2.622036000	-1.893676000	1.695356000
1	1.643800000	-2.105324000	2.146091000
1	2.721553000	-2.500353000	0.796309000
1	3.404180000	-2.185189000	2.402692000
6	2.466715000	0.363469000	2.539778000
1	3.121394000	0.058226000	3.360604000
1	2.660114000	1.410041000	2.311504000
1	1.422386000	0.260594000	2.864442000
6	4.480411000	-1.158412000	-0.989175000
1	4.691065000	-2.197294000	-1.264882000
1	5.085436000	-0.509904000	-1.635366000
1	4.790667000	-1.005153000	0.042951000
6	2.605171000	-0.988839000	-2.515873000
1	1.532255000	-0.808693000	-2.563283000
1	3.116253000	-0.269571000	-3.167793000
1	2.805707000	-1.996466000	-2.891759000
13	-0.856912000	-1.143854000	-0.012465000
1	-0.760223000	-2.117862000	1.275229000
1	-0.735162000	-1.113239000	1.960759000

11AITS^{H-H} (T.E = -1518.683993)

7	-0.762806000	-0.163930000	0.427947000
6	-0.804288000	1.191661000	0.047917000
6	1.694149000	1.483820000	0.002042000
15	-2.393886000	-0.199517000	0.130296000
6	-2.153471000	1.494851000	-0.138922000
6	-2.984238000	2.652894000	-0.563574000
1	-3.033790000	3.450290000	0.183119000
1	-2.648963000	3.102906000	-1.502386000
1	-4.012582000	2.320890000	-0.726708000
7	-2.952346000	-1.022701000	-1.172547000
7	-3.161475000	-0.904213000	1.401442000
6	-2.868145000	-2.477788000	-1.206546000
1	-1.980301000	-2.791921000	-1.766648000
1	-2.799128000	-2.887666000	-0.199834000

1	-3.756759000	-2.889175000	-1.693985000
6	-2.883531000	-0.427133000	-2.501720000
1	-3.667808000	-0.867875000	-3.122928000
1	-3.042611000	0.647929000	-2.451600000
1	-1.905462000	-0.616857000	-2.961025000
6	-4.569781000	-1.247144000	1.372925000
1	-4.719403000	-2.234872000	1.820233000
1	-5.162104000	-0.523197000	1.944216000
1	-4.942631000	-1.271056000	0.350616000
6	-2.623779000	-0.767674000	2.744290000
1	-1.556102000	-0.561946000	2.704317000
1	-3.124215000	0.038750000	3.292379000
1	-2.778488000	-1.702053000	3.290635000
7	0.309054000	1.931391000	-0.076431000
6	0.119709000	3.349587000	-0.351219000
1	-0.171637000	3.511494000	-1.391017000
1	-0.646933000	3.756726000	0.306678000
1	1.061850000	3.854626000	-0.165751000
8	2.538950000	2.347418000	0.017601000
7	1.913497000	0.151222000	0.011669000
6	3.277401000	-0.258758000	0.039810000
6	4.163956000	0.165664000	1.022017000
6	3.703581000	-1.179121000	-0.908660000
6	5.455476000	-0.324829000	1.046816000
1	3.834403000	0.884703000	1.761216000
6	4.997085000	-1.673250000	-0.875546000
1	3.014433000	-1.488898000	-1.689381000
6	5.878227000	-1.246579000	0.101089000
1	6.139516000	0.013537000	1.816844000
1	5.315446000	-2.390837000	-1.622862000
1	6.891895000	-1.628932000	0.127234000
13	0.675984000	-1.260587000	-0.022226000
1	0.457010000	-2.248678000	-1.255855000
1	0.207685000	-1.236424000	-1.982696000

13AITS^{H-H} (T.E = -1844.233287)

7	1.348573000	-0.172014000	0.151840000
6	1.215315000	1.187504000	-0.306843000
6	-0.002840000	1.838944000	-0.432465000
6	-1.224965000	1.247069000	-0.136464000
1	-0.004980000	2.853130000	-0.817253000
13	-0.039360000	-1.377506000	0.343651000
15	2.974281000	0.021352000	-0.017083000
6	2.536030000	1.589232000	-0.558063000
6	3.109748000	2.890177000	-0.969624000
1	4.172963000	2.799166000	-1.201929000
1	2.622987000	3.280352000	-1.869486000
1	3.015591000	3.664432000	-0.196737000

7	-1.364175000	-0.080219000	0.401951000
6	-2.546058000	1.684865000	-0.312939000
15	-2.978475000	0.076845000	0.103281000
6	-3.094472000	2.915453000	-0.927329000
1	-2.938832000	3.803621000	-0.305684000
1	-2.639862000	3.125886000	-1.903996000
1	-4.171496000	2.829550000	-1.088451000
7	-3.621001000	-0.833899000	-1.119051000
7	-3.853895000	-0.417422000	1.416519000
6	-3.616930000	-2.285688000	-0.985572000
1	-2.682756000	-2.703887000	-1.382632000
1	-3.710495000	-2.579955000	0.059012000
1	-4.455960000	-2.710397000	-1.544503000
6	-3.350132000	-0.413282000	-2.487825000
1	-2.342402000	-0.716415000	-2.802925000
1	-4.083628000	-0.881182000	-3.150178000
1	-3.436093000	0.667811000	-2.581264000
6	-3.348879000	-0.106379000	2.740443000
1	-3.594173000	-0.923898000	3.424696000
1	-2.266497000	0.008765000	2.711534000
1	-3.793814000	0.816477000	3.132528000
6	-5.286912000	-0.618705000	1.379668000
1	-5.820737000	0.244314000	1.796877000
1	-5.628204000	-0.775982000	0.358204000
1	-5.553757000	-1.498155000	1.975273000
7	3.614093000	-1.187213000	-0.943145000
7	3.897093000	-0.064493000	1.359341000
6	5.036079000	-1.437539000	-1.048525000
1	5.220756000	-2.516759000	-1.074189000
1	5.447451000	-1.005529000	-1.969255000
1	5.569794000	-1.014511000	-0.199530000
6	2.862568000	-1.654651000	-2.096769000
1	1.802044000	-1.403784000	-2.015485000
1	3.253620000	-1.214760000	-3.021734000
1	2.947576000	-2.743025000	-2.169561000
6	3.878494000	1.087166000	2.244091000
1	4.734936000	1.030011000	2.921102000
1	3.947073000	2.011730000	1.673330000
1	2.962349000	1.120832000	2.849265000
6	3.928899000	-1.322975000	2.089413000
1	3.851705000	-2.168950000	1.407434000
1	4.866469000	-1.406467000	2.646999000
1	3.094705000	-1.385687000	2.800418000
1	-0.196470000	-2.641985000	-0.628950000
1	-0.335757000	-1.850449000	-1.612727000

1GaTS^{H-H} (T.E = -2614.336421)

7	-1.460965000	0.565516000	-0.368719000
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7	1.460951000	0.565472000	-0.368673000
6	-1.236481000	1.836837000	-0.609883000
6	1.236470000	1.836800000	-0.609867000
6	0.000009000	2.453447000	-0.748671000
1	0.000029000	3.506582000	-0.991174000
6	-2.772362000	0.123367000	-0.092821000
6	-3.611532000	0.847524000	0.746912000
6	-3.216333000	-1.077358000	-0.635638000
6	-4.891928000	0.391802000	1.006996000
6	-4.494528000	-1.528259000	-0.367355000
6	-5.338830000	-0.794044000	0.450604000
1	-5.537436000	0.960369000	1.666254000
1	-4.835195000	-2.459894000	-0.803599000
1	-6.339009000	-1.152296000	0.662636000
6	2.772359000	0.123339000	-0.092791000
6	3.216266000	-1.077474000	-0.635465000
6	3.611613000	0.847598000	0.746772000
6	4.494472000	-1.528365000	-0.367219000
6	4.892017000	0.391883000	1.006825000
6	5.338854000	-0.794051000	0.450568000
1	4.835083000	-2.460072000	-0.803354000
1	5.537586000	0.960529000	1.665955000
1	6.339040000	-1.152296000	0.662578000
1	3.241340000	1.749452000	1.221421000
1	2.551192000	-1.643086000	-1.279512000
1	-2.551326000	-1.642881000	-1.279830000
1	-3.241197000	1.749300000	1.221662000
31	-0.000010000	-0.702543000	-0.000401000
1	2.119515000	2.467967000	-0.729021000
1	-2.119515000	2.468020000	-0.729038000
1	-0.000003000	-1.545346000	1.302386000
1	-0.000088000	-0.262715000	1.892996000

4GaTS^{H-H} (T.E = -2827.131640)

7	1.263865000	0.584724000	-0.396268000
6	0.959603000	1.871768000	-0.536790000
6	-0.288748000	2.442972000	-0.661347000
6	-1.514616000	1.776020000	-0.469517000
6	-1.694952000	0.427269000	-0.326543000
6	2.578393000	0.224587000	-0.060965000
6	3.118060000	-0.957019000	-0.566230000
6	3.359537000	1.003664000	0.791427000
6	4.409926000	-1.329972000	-0.251967000
1	2.509580000	-1.574152000	-1.219354000
6	4.655476000	0.627339000	1.096178000
1	2.933945000	1.892267000	1.243536000
6	5.190353000	-0.538239000	0.576003000
1	4.813578000	-2.248441000	-0.662897000

1	5.245642000	1.244713000	1.764188000
1	6.202633000	-0.834850000	0.823270000
1	1.808318000	2.558493000	-0.557752000
15	-3.159780000	-0.187218000	0.309958000
6	-4.641069000	0.724755000	-0.172539000
1	-5.524737000	0.262896000	0.271143000
1	-4.574349000	1.755975000	0.176044000
1	-4.735561000	0.725005000	-1.258728000
6	-3.412764000	-1.889262000	-0.199647000
1	-3.435068000	-1.951065000	-1.287990000
1	-2.579995000	-2.492639000	0.168378000
1	-4.346273000	-2.274093000	0.213834000
6	-3.171565000	-0.210453000	2.110410000
1	-3.174796000	0.817549000	2.476450000
1	-4.042583000	-0.742890000	2.496730000
1	-2.249141000	-0.702140000	2.435561000
1	-2.381370000	2.441332000	-0.401196000
1	-0.312212000	3.514522000	-0.813103000
31	-0.150777000	-0.809869000	-0.560294000
1	0.038718000	-2.140544000	0.266901000
1	-0.258411000	-1.471390000	1.387767000

6GaTS^{H-H} (T.E = -2957.713283)

6	-1.514493000	1.389386000	-0.184028000
6	-1.526726000	-0.004564000	-0.252760000
6	0.993823000	1.604910000	-0.289243000
1	1.781373000	2.362117000	-0.252535000
7	1.352184000	0.364772000	-0.268386000
15	-3.020079000	-0.656845000	0.247865000
6	-3.461216000	-0.249946000	1.949299000
1	-3.558205000	0.832039000	2.035229000
1	-4.397759000	-0.730925000	2.238213000
1	-2.653729000	-0.592916000	2.599196000
6	-4.462766000	-0.220190000	-0.743207000
1	-4.310460000	-0.564038000	-1.766873000
1	-5.363675000	-0.681275000	-0.333121000
1	-4.563881000	0.864574000	-0.741307000
6	-2.924779000	-2.451842000	0.210608000
1	-2.130089000	-2.779979000	0.885816000
1	-3.872284000	-2.885888000	0.533818000
1	-2.695324000	-2.794180000	-0.799436000
8	-2.478016000	2.129619000	0.021066000
7	-0.244106000	2.107595000	-0.363195000
6	-0.380413000	3.554658000	-0.445318000
1	-1.032389000	3.823875000	-1.275204000
1	-0.821906000	3.957388000	0.465756000
1	0.601635000	3.997114000	-0.605549000
6	2.711580000	0.066502000	-0.020709000

6	3.374703000	-0.832672000	-0.846263000
6	3.377187000	0.629890000	1.060713000
6	4.700402000	-1.140233000	-0.604278000
1	2.838799000	-1.279145000	-1.676547000
6	4.706142000	0.321185000	1.293031000
1	2.834544000	1.281294000	1.737201000
6	5.371809000	-0.562597000	0.461543000
1	5.214625000	-1.836223000	-1.256690000
1	5.217432000	0.761236000	2.141244000
1	6.409837000	-0.809816000	0.649382000
31	0.036063000	-1.159135000	-0.492709000
1	0.599674000	-2.403375000	0.281226000
1	0.361073000	-1.706445000	1.412385000

8GaTS^{H-H} (T.E = -3191.751259)

7	1.395188000	0.253505000	-1.040245000
6	1.079840000	1.478324000	-0.400172000
6	-0.023377000	2.294988000	-0.903899000
15	2.373807000	-0.042794000	0.269253000
6	1.854695000	1.563945000	0.725923000
6	2.001042000	2.588741000	1.782281000
1	1.298600000	3.408159000	1.605800000
1	1.787898000	2.193650000	2.780862000
1	3.003512000	3.025546000	1.820106000
7	2.028247000	-1.196186000	1.374684000
7	3.895733000	-0.411006000	-0.239918000
6	2.392992000	-2.596280000	1.201675000
1	1.516065000	-3.173140000	0.892389000
1	3.157589000	-2.706957000	0.435286000
1	2.778781000	-2.987235000	2.149045000
6	0.872267000	-1.026997000	2.245987000
1	1.089502000	-1.476737000	3.218886000
1	0.647328000	0.029754000	2.386250000
1	-0.008006000	-1.515095000	1.810412000
6	4.967204000	-0.625364000	0.713791000
1	5.597975000	-1.457988000	0.386499000
1	5.599740000	0.266161000	0.800642000
1	4.569894000	-0.863243000	1.699514000
6	4.362198000	0.024395000	-1.544379000
1	3.521997000	0.133358000	-2.226137000
1	4.894765000	0.981049000	-1.478838000
1	5.051800000	-0.723092000	-1.946578000
6	-2.456954000	-0.663412000	-0.136364000
6	-2.675897000	-0.669185000	1.243952000
6	-3.164972000	-1.581382000	-0.912733000
6	-3.572938000	-1.549287000	1.818600000
1	-2.126311000	0.038211000	1.858057000
6	-4.051600000	-2.470318000	-0.331730000

1	-3.009585000	-1.582450000	-1.987607000
6	-4.266201000	-2.460034000	1.036311000
1	-3.726995000	-1.529057000	2.892197000
1	-4.586408000	-3.175183000	-0.958818000
1	-4.964612000	-3.153770000	1.488775000
7	-1.519781000	0.200704000	-0.712256000
5	-1.421393000	1.592313000	-0.472611000
7	-2.467106000	2.414257000	0.049565000
6	-3.864192000	2.049693000	0.019949000
1	-4.032193000	1.172638000	-0.601383000
1	-4.259737000	1.834558000	1.021964000
1	-4.452721000	2.877684000	-0.395276000
6	-2.284856000	3.705298000	0.659895000
1	-1.231999000	3.939928000	0.808733000
1	-2.736791000	4.510064000	0.063258000
1	-2.763933000	3.732088000	1.647659000
1	0.060595000	3.326221000	-0.564133000
1	0.003380000	2.301213000	-2.001326000
31	-0.180898000	-0.691663000	-1.808947000
1	-0.040880000	-2.246055000	-1.939249000
1	0.126962000	-2.266039000	-0.602694000

10GaTS^{H-H} (T.E = -3283.257407)

7	0.700931000	0.065572000	-0.488458000
6	0.682559000	1.488563000	-0.340991000
6	-0.486532000	2.249540000	-0.333875000
6	-1.774485000	1.726472000	-0.297863000
1	-0.364974000	3.327111000	-0.325857000
1	-2.557765000	2.489895000	-0.342066000
15	2.297328000	0.144195000	-0.087145000
6	2.032205000	1.840736000	-0.182027000
6	2.683610000	3.138073000	0.110577000
1	2.181275000	3.675136000	0.925659000
1	3.723583000	2.996753000	0.414721000
1	2.697977000	3.812028000	-0.753021000
6	-2.170596000	0.403304000	-0.179248000
15	-3.794121000	-0.043012000	-0.025375000
6	-4.968486000	1.324263000	0.083629000
1	-5.979231000	0.931038000	0.203648000
1	-4.725331000	1.955803000	0.938579000
1	-4.927993000	1.927134000	-0.824242000
6	-4.066414000	-1.048963000	1.445980000
1	-5.104871000	-1.377621000	1.521700000
1	-3.411943000	-1.922480000	1.388080000
1	-3.784426000	-0.474987000	2.329114000
6	-4.409244000	-1.084491000	-1.369494000
1	-4.391504000	-0.518348000	-2.301364000
1	-3.741074000	-1.942029000	-1.472032000

1	-5.423844000	-1.435411000	-1.169040000
31	-0.818358000	-1.058132000	-0.070044000
7	2.757148000	-0.413580000	1.400322000
7	3.192896000	-0.798025000	-1.111486000
6	2.644875000	-1.835103000	1.697825000
1	1.682304000	-2.047610000	2.179362000
1	2.710778000	-2.428315000	0.786464000
1	3.451897000	-2.138998000	2.372264000
6	2.481941000	0.414385000	2.565883000
1	3.153372000	0.116072000	3.376350000
1	2.654298000	1.464959000	2.339624000
1	1.443946000	0.291528000	2.901469000
6	4.595217000	-1.080071000	-0.895151000
1	4.813482000	-2.117286000	-1.171494000
1	5.232058000	-0.428543000	-1.506971000
1	4.860215000	-0.938754000	0.151238000
6	2.793572000	-0.882591000	-2.503223000
1	1.725737000	-0.691313000	-2.596822000
1	3.340767000	-0.160937000	-3.122589000
1	3.004051000	-1.887545000	-2.881291000
1	-0.641572000	-2.072048000	1.136652000
1	-0.586355000	-1.023376000	1.946262000

$^{11}\text{GaTS}^{\text{H-H}}$ (T.E = -3201.049026)

7	0.821343000	-0.150681000	-0.394330000
6	0.862928000	1.248527000	-0.223976000
6	-1.631588000	1.552923000	-0.281579000
7	-1.890091000	0.260766000	-0.003062000
15	2.461365000	-0.130021000	-0.139300000
6	2.217359000	1.582252000	-0.141973000
6	3.055974000	2.800131000	0.016247000
1	2.817443000	3.578023000	-0.711936000
1	2.988163000	3.253443000	1.011827000
1	4.106698000	2.543368000	-0.138045000
6	-3.248749000	-0.151626000	-0.073432000
6	-3.579569000	-1.267290000	-0.831578000
6	-4.246369000	0.492450000	0.649082000
6	-4.882230000	-1.733671000	-0.869654000
1	-2.800860000	-1.765965000	-1.400412000
6	-5.546885000	0.026918000	0.605582000
1	-3.993271000	1.362621000	1.241000000
6	-5.872443000	-1.087422000	-0.151504000
1	-5.122207000	-2.604835000	-1.468441000
1	-6.314947000	0.538627000	1.174433000
1	-6.893530000	-1.449263000	-0.180224000
31	-0.614366000	-1.109966000	0.489122000
7	3.060659000	-0.748167000	1.256737000
7	3.204319000	-1.014192000	-1.311102000

6	2.940925000	-2.173163000	1.530647000
1	2.802627000	-2.735964000	0.607796000
1	3.845607000	-2.535041000	2.028328000
1	2.081386000	-2.366859000	2.182394000
6	3.101407000	0.063883000	2.465874000
1	3.302890000	1.104776000	2.220937000
1	2.148546000	0.010155000	3.006350000
1	3.906272000	-0.304958000	3.107517000
6	4.602937000	-1.389385000	-1.253542000
1	4.722662000	-2.423772000	-1.590935000
1	5.209888000	-0.749353000	-1.904512000
1	4.983897000	-1.310733000	-0.237181000
6	2.658569000	-1.011623000	-2.657896000
1	1.602010000	-0.752103000	-2.634141000
1	3.188994000	-0.298158000	-3.298812000
1	2.764197000	-2.008965000	-3.093591000
8	-2.440251000	2.395782000	-0.595820000
7	-0.248959000	1.996182000	-0.162034000
6	-0.063132000	3.439723000	-0.097254000
1	0.643534000	3.683872000	0.694617000
1	0.304434000	3.835004000	-1.046772000
1	-1.022491000	3.899553000	0.112534000
1	-0.403664000	-1.688915000	1.921561000
1	-0.067075000	-0.384646000	2.275251000

$^{13}\text{GaTS}^{\text{H-H}}$ (T.E = -3526.598350)

7	1.387696000	-0.129917000	-0.555503000
6	1.225167000	1.297924000	-0.540079000
6	0.000006000	1.949621000	-0.575395000
6	-1.225171000	1.297954000	-0.540093000
1	0.000024000	3.033408000	-0.524103000
15	2.956102000	0.143550000	-0.116748000
6	2.533946000	1.784295000	-0.384646000
6	3.045677000	3.161171000	-0.196234000
1	2.946077000	3.772885000	-1.098992000
1	2.520180000	3.692668000	0.608336000
1	4.106394000	3.155376000	0.064406000
7	-1.387702000	-0.129886000	-0.555531000
6	-2.533942000	1.784326000	-0.384659000
15	-2.956104000	0.143581000	-0.116761000
6	-3.045648000	3.161214000	-0.196234000
1	-4.106277000	3.155443000	0.064758000
1	-2.519877000	3.692797000	0.608098000
1	-2.946356000	3.772826000	-1.099094000
7	-3.977429000	-0.789471000	-1.023784000
7	-3.396629000	-0.243747000	1.430164000
6	-3.670079000	-0.968498000	-2.430616000
1	-4.213334000	-0.247511000	-3.053712000

1	-2.601340000	-0.844547000	-2.598294000
1	-3.958513000	-1.976959000	-2.741488000
6	-5.381121000	-0.959929000	-0.714750000
1	-6.006672000	-0.299318000	-1.328107000
1	-5.683783000	-1.992476000	-0.918761000
1	-5.574517000	-0.743145000	0.334112000
6	-3.355507000	-1.639127000	1.848050000
1	-4.123701000	-1.822747000	2.605436000
1	-3.536429000	-2.302612000	1.002929000
1	-2.374827000	-1.880669000	2.278144000
6	-2.991648000	0.659452000	2.499471000
1	-1.943063000	0.494731000	2.781173000
1	-3.114110000	1.696382000	2.191836000
1	-3.625180000	0.476507000	3.371919000
7	3.977437000	-0.789460000	-1.023805000
7	3.396629000	-0.243828000	1.430163000
6	5.381117000	-0.959963000	-0.714743000
1	5.683771000	-1.992501000	-0.918813000
1	6.006694000	-0.299321000	-1.328039000
1	5.574485000	-0.743251000	0.334139000
6	3.670117000	-0.968373000	-2.430659000
1	2.601396000	-0.844319000	-2.598373000
1	4.213462000	-0.247393000	-3.053685000
1	3.958475000	-1.976838000	-2.741590000
6	2.991823000	0.659416000	2.499491000
1	3.625422000	0.476436000	3.371884000
1	3.114342000	1.696331000	2.191825000
1	1.943253000	0.494781000	2.781294000
6	3.355352000	-1.639205000	1.848035000
1	3.536110000	-2.302701000	1.002887000
1	4.123584000	-1.822945000	2.605354000
1	2.374674000	-1.880612000	2.278209000
31	-0.000027000	-1.354344000	-0.054209000
1	-0.000053000	-2.173023000	1.281404000
1	0.000001000	-0.977494000	1.994432000

Cartesian coordinates of the loosely associated intermediates involved in the ammonia activation by some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AlInt^{N-H} (T.E = -987.381180)

7	1.429850000	0.432391000	-0.521589000
6	1.230627000	1.699490000	-0.805712000
6	-0.000001000	2.323971000	-0.965700000
7	-1.429859000	0.432396000	-0.521599000
1	0.000002000	3.366453000	-1.251588000
1	2.116071000	2.327014000	-0.943005000
6	2.749458000	0.023642000	-0.238896000
6	3.234465000	-1.163615000	-0.782184000
6	3.564469000	0.754453000	0.622485000
6	4.516582000	-1.589132000	-0.490067000
1	2.593471000	-1.737948000	-1.440862000
6	4.848536000	0.323324000	0.909431000
1	3.175661000	1.658302000	1.081793000
6	5.330360000	-0.848811000	0.353367000
1	4.885079000	-2.509220000	-0.928672000
1	5.471052000	0.903744000	1.580878000
1	6.333611000	-1.188637000	0.581110000
6	-2.749466000	0.023646000	-0.238896000
6	-3.234489000	-1.163589000	-0.782215000
6	-3.564457000	0.754435000	0.622522000
6	-4.516605000	-1.589105000	-0.490093000
1	-2.593508000	-1.737906000	-1.440921000
6	-4.848523000	0.323307000	0.909473000
1	-3.175634000	1.658266000	1.081854000
6	-5.330364000	-0.848807000	0.353378000
1	-4.885115000	-2.509177000	-0.928722000
1	-5.471024000	0.903709000	1.580949000
1	-6.333614000	-1.188632000	0.581126000
6	-1.230632000	1.699499000	-0.805698000
1	-2.116075000	2.327031000	-0.942962000
13	-0.000013000	-0.981382000	-0.102173000
7	0.000037000	-0.026635000	1.996581000
1	0.818380000	-0.354094000	2.499030000
1	-0.818298000	-0.353932000	2.499148000
1	0.000141000	0.989676000	2.018179000

4AlInt^{N-H} (T.E = -1200.155040)

7	1.200827000	0.429129000	-0.367031000
6	0.939254000	1.699262000	-0.657324000

6	-0.293064000	2.319966000	-0.692878000
6	-1.529235000	1.670079000	-0.508802000
6	-1.691161000	0.359037000	-0.147914000
6	2.554608000	0.054769000	-0.290655000
6	2.959808000	-1.178998000	-0.799392000
6	3.506856000	0.860069000	0.334990000
6	4.279071000	-1.577959000	-0.705898000
1	2.218068000	-1.813689000	-1.270574000
6	4.828186000	0.455399000	0.423885000
1	3.198904000	1.804715000	0.772900000
6	5.222831000	-0.764058000	-0.097494000
1	4.574814000	-2.536969000	-1.116109000
1	5.551140000	1.096216000	0.916535000
1	6.255980000	-1.082444000	-0.024665000
1	1.794038000	2.322374000	-0.934351000
15	-3.245610000	-0.339735000	-0.114295000
6	-4.641361000	0.734037000	-0.527473000
1	-5.572832000	0.168196000	-0.468233000
1	-4.688893000	1.572508000	0.168648000
1	-4.525295000	1.123467000	-1.539639000
6	-3.364218000	-1.742096000	-1.238433000
1	-3.239675000	-1.392995000	-2.264080000
1	-2.544761000	-2.426773000	-1.000798000
1	-4.322371000	-2.254987000	-1.133085000
6	-3.635803000	-1.038063000	1.502521000
1	-3.663180000	-0.240097000	2.246263000
1	-4.593218000	-1.563382000	1.489943000
1	-2.834167000	-1.737122000	1.761610000
1	-2.398101000	2.309145000	-0.710659000
1	-0.300714000	3.360244000	-0.994660000
13	-0.117304000	-0.908092000	0.403192000
7	0.186376000	0.350409000	2.269465000
1	1.147221000	0.217761000	2.568200000
1	-0.415458000	0.069949000	3.034734000
1	0.042546000	1.339670000	2.083118000

6AllInt^{N-H} (T.E = -1330.734135)

6	-1.531854000	1.301115000	-0.004037000
6	-1.476075000	-0.098645000	-0.023844000
6	0.960972000	1.548844000	-0.203972000
1	1.745673000	2.311670000	-0.218218000
13	0.061599000	-1.345398000	-0.500319000
7	1.311853000	0.307867000	-0.305150000
15	-3.075762000	-0.701725000	-0.039904000
6	-4.128110000	-0.260604000	1.365457000
1	-4.231540000	0.822582000	1.400691000
1	-5.109679000	-0.730199000	1.268293000
1	-3.652829000	-0.606585000	2.284665000

6	-4.050264000	-0.264483000	-1.499892000
1	-3.546046000	-0.666811000	-2.380402000
1	-5.060662000	-0.674024000	-1.438579000
1	-4.094401000	0.821591000	-1.574243000
6	-3.091287000	-2.504188000	-0.030472000
1	-2.664199000	-2.876918000	0.902299000
1	-4.119215000	-2.861721000	-0.121918000
1	-2.484744000	-2.887113000	-0.854257000
8	-2.523899000	2.034463000	0.069374000
7	-0.270800000	2.051992000	-0.096673000
6	-0.417724000	3.498259000	-0.079115000
1	-0.996322000	3.838300000	-0.937891000
1	-0.947330000	3.816066000	0.817974000
1	0.568860000	3.959521000	-0.103486000
6	2.696605000	0.039027000	-0.222678000
6	3.293912000	-0.800015000	-1.158827000
6	3.461862000	0.545775000	0.823650000
6	4.640261000	-1.099150000	-1.057612000
1	2.682956000	-1.208071000	-1.955893000
6	4.810351000	0.242124000	0.917756000
1	2.985172000	1.163265000	1.579171000
6	5.404191000	-0.580100000	-0.023644000
1	5.098292000	-1.744863000	-1.797927000
1	5.394259000	0.643184000	1.738239000
1	6.457837000	-0.821701000	0.050799000
7	0.652546000	-1.631151000	1.685211000
1	1.643127000	-1.828901000	1.787706000
1	0.421317000	-0.813233000	2.242206000
1	0.144079000	-2.424410000	2.058171000

8AllInt^{N-H} (T.E = -1564.787393)

7	-1.310953000	-0.992244000	-0.577909000
6	-0.853874000	-1.377799000	0.715499000
6	0.339202000	-2.218983000	0.827667000
15	-2.321677000	0.041221000	0.235338000
6	-1.610480000	-0.722140000	1.644853000
6	-1.621443000	-0.687119000	3.122952000
1	-2.558063000	-1.059758000	3.548522000
1	-0.815999000	-1.310734000	3.519776000
1	-1.472267000	0.321981000	3.520968000
7	-2.097926000	1.669396000	0.221625000
7	-3.874352000	-0.151130000	-0.269070000
6	-2.533461000	2.488446000	-0.901180000
1	-1.698188000	2.666608000	-1.588325000
1	-3.322872000	1.992090000	-1.462700000
1	-2.909955000	3.444434000	-0.523230000
6	-0.976069000	2.268298000	0.933382000
1	-1.276661000	3.249645000	1.310581000

1	-0.666958000	1.645866000	1.770508000
1	-0.110012000	2.398464000	0.272159000
6	-4.965134000	0.589493000	0.326992000
1	-5.583724000	1.049053000	-0.452021000
1	-5.605846000	-0.070307000	0.923244000
1	-4.587069000	1.381892000	0.972360000
6	-4.290921000	-1.253311000	-1.111441000
1	-3.420609000	-1.723510000	-1.564012000
1	-4.849417000	-2.003289000	-0.538902000
1	-4.941723000	-0.877114000	-1.907644000
13	-0.009000000	-0.170025000	-1.895996000
6	2.157199000	0.905949000	-0.267332000
6	2.572915000	1.209572000	1.039955000
6	2.484623000	1.836054000	-1.265103000
6	3.268117000	2.367733000	1.330754000
1	2.310292000	0.518809000	1.838775000
6	3.166479000	3.001168000	-0.964660000
1	2.180310000	1.627882000	-2.285853000
6	3.567334000	3.282166000	0.332182000
1	3.567730000	2.564978000	2.354870000
1	3.397137000	3.697852000	-1.763929000
1	4.105839000	4.194139000	0.560198000
7	1.402745000	-0.224244000	-0.526781000
5	1.609133000	-1.443514000	0.183612000
7	2.879105000	-2.087734000	0.275782000
6	4.068085000	-1.550969000	-0.345510000
1	3.805046000	-0.826067000	-1.114344000
1	4.721527000	-1.049606000	0.380668000
1	4.646976000	-2.358211000	-0.809832000
6	3.177418000	-3.226574000	1.105692000
1	2.275639000	-3.654240000	1.540144000
1	3.677523000	-4.013985000	0.527765000
1	3.853545000	-2.956752000	1.928775000
1	0.530478000	-2.462827000	1.877021000
1	0.170411000	-3.171415000	0.307168000
7	0.510539000	-2.239042000	-2.557885000
1	0.626815000	-2.190077000	-3.562629000
1	1.351861000	-2.653131000	-2.161907000
1	-0.274400000	-2.853415000	-2.364224000

10AllInt^{N-H} (T.E = -1656.279472)

7	-0.552527000	0.019514000	0.102827000
6	-0.585073000	1.127901000	-0.803893000
6	0.568557000	1.707628000	-1.316765000
6	1.864148000	1.325740000	-0.935179000
1	0.444638000	2.577490000	-1.953251000
1	2.637084000	2.013704000	-1.301665000
15	-2.192883000	0.115334000	0.125320000

6	-1.957399000	1.419687000	-0.960323000
6	-2.685649000	2.448566000	-1.737235000
1	-2.354468000	3.466578000	-1.501233000
1	-2.572330000	2.323730000	-2.822444000
1	-3.757633000	2.409866000	-1.526496000
6	2.232696000	0.226194000	-0.185123000
15	3.841582000	0.012989000	0.292508000
6	5.058111000	1.216636000	-0.303106000
1	6.050731000	0.954976000	0.067894000
1	5.075491000	1.223393000	-1.393810000
1	4.798745000	2.215532000	0.049851000
6	4.499719000	-1.597331000	-0.198492000
1	5.492143000	-1.772211000	0.222676000
1	3.806550000	-2.362640000	0.165033000
1	4.548895000	-1.652216000	-1.287380000
6	4.036113000	0.008298000	2.087975000
1	3.757575000	0.987049000	2.480499000
1	3.346843000	-0.737491000	2.493445000
1	5.060330000	-0.232649000	2.381242000
7	-3.108305000	-1.153027000	-0.432299000
7	-2.750420000	0.264373000	1.686845000
6	-3.226537000	-2.383674000	0.330637000
1	-2.444627000	-3.101127000	0.048199000
1	-3.124278000	-2.183908000	1.395519000
1	-4.204270000	-2.840268000	0.145151000
6	-3.201780000	-1.362644000	-1.860336000
1	-4.158031000	-1.837253000	-2.100936000
1	-3.133173000	-0.412957000	-2.389946000
1	-2.402685000	-2.022741000	-2.229617000
6	-4.160328000	0.546184000	1.876399000
1	-4.464219000	0.241243000	2.881876000
1	-4.379013000	1.618540000	1.766860000
1	-4.763783000	-0.003801000	1.154330000
6	-1.904985000	0.974852000	2.630990000
1	-0.872057000	0.645543000	2.532000000
1	-1.948396000	2.062794000	2.480677000
1	-2.248632000	0.754082000	3.644800000
13	0.866216000	-1.247559000	0.439668000
7	0.752074000	-1.770008000	-1.759571000
1	1.594145000	-2.236745000	-2.075902000
1	-0.034580000	-2.375647000	-1.963729000
1	0.646407000	-0.903648000	-2.284651000

11AllInt^{N-H} (T.E = -1574.090453)

7	-0.784396000	-0.211380000	0.094493000
6	-0.876446000	1.188579000	0.035343000
6	1.606692000	1.562940000	0.151150000
15	-2.433281000	-0.228094000	0.048590000

6	-2.245914000	1.485528000	-0.048772000
6	-3.138261000	2.665279000	-0.207688000
1	-3.029262000	3.410337000	0.584400000
1	-3.009098000	3.185718000	-1.163259000
1	-4.179336000	2.331754000	-0.176575000
7	-3.193571000	-0.952548000	-1.225311000
7	-3.073857000	-0.997455000	1.360998000
6	-3.246729000	-2.403932000	-1.311070000
1	-2.364466000	-2.800872000	-1.830041000
1	-3.278459000	-2.845942000	-0.317135000
1	-4.139794000	-2.705658000	-1.865177000
6	-3.090958000	-0.312366000	-2.523783000
1	-3.915399000	-0.648675000	-3.157263000
1	-3.146595000	0.770661000	-2.423020000
1	-2.147784000	-0.566846000	-3.027131000
6	-4.514082000	-0.914580000	1.545282000
1	-4.852625000	-1.760820000	2.148277000
1	-4.800985000	0.010819000	2.063215000
1	-5.029795000	-0.948498000	0.585574000
6	-2.334915000	-0.932535000	2.615308000
1	-1.293790000	-1.223067000	2.459755000
1	-2.375396000	0.069892000	3.061700000
1	-2.785029000	-1.639944000	3.314599000
7	0.202722000	1.978774000	0.081019000
6	-0.043878000	3.412932000	0.063882000
1	-0.573511000	3.705020000	-0.844272000
1	-0.634613000	3.708510000	0.932730000
1	0.918168000	3.913688000	0.092177000
8	2.422154000	2.459725000	0.082555000
7	1.849662000	0.253782000	0.296125000
6	3.222550000	-0.097859000	0.230443000
6	3.792046000	-0.837574000	1.260225000
6	3.995009000	0.184361000	-0.894599000
6	5.101356000	-1.281499000	1.169233000
1	3.191464000	-1.061447000	2.134395000
6	5.301260000	-0.259751000	-0.982714000
1	3.563352000	0.776335000	-1.695034000
6	5.861610000	-0.997355000	0.049148000
1	5.527757000	-1.854569000	1.984729000
1	5.888514000	-0.024184000	-1.863371000
1	6.885710000	-1.344867000	-0.020708000
13	0.716474000	-1.406982000	0.417122000
7	1.172928000	-1.560735000	-1.791813000
1	0.726128000	-2.357828000	-2.229479000
1	2.179001000	-1.691134000	-1.866952000
1	0.933221000	-0.720077000	-2.310920000

13AllInt^{N-H} (T.E = -1899.636331)

7	-1.393160000	0.386697000	0.046983000
6	-1.263445000	-0.211370000	-1.252623000
6	-0.036772000	-0.448578000	-1.868356000
6	1.170906000	-0.320467000	-1.192707000
1	-0.031077000	-0.875473000	-2.865882000
13	-0.041219000	1.071908000	1.265769000
15	-2.968490000	-0.066557000	-0.023593000
6	-2.577906000	-0.542542000	-1.627649000
6	-3.095280000	-1.380246000	-2.735201000
1	-3.173769000	-0.840739000	-3.685216000
1	-2.456346000	-2.254563000	-2.917445000
1	-4.096102000	-1.757302000	-2.507491000
7	1.265136000	0.148491000	0.160812000
6	2.497448000	-0.623802000	-1.555201000
15	2.874325000	-0.143621000	0.047059000
6	3.099783000	-1.171821000	-2.792396000
1	2.569394000	-2.061906000	-3.148966000
1	3.107105000	-0.454099000	-3.623220000
1	4.137774000	-1.470241000	-2.624781000
7	3.972691000	1.087993000	0.215138000
7	3.352877000	-1.184441000	1.255092000
6	4.258335000	1.680222000	1.508982000
1	3.662595000	2.588627000	1.667392000
1	4.021033000	0.981784000	2.309318000
1	5.318507000	1.947711000	1.571870000
6	4.208134000	1.987358000	-0.892589000
1	3.590201000	2.894518000	-0.822127000
1	5.255714000	2.304666000	-0.896236000
1	3.984379000	1.493281000	-1.837519000
6	2.389353000	-2.182495000	1.690320000
1	2.737874000	-2.619332000	2.629340000
1	1.417775000	-1.720359000	1.860125000
1	2.276354000	-2.990893000	0.954017000
6	4.707257000	-1.701990000	1.204423000
1	4.789162000	-2.560766000	0.522360000
1	5.402588000	-0.931237000	0.872153000
1	5.011822000	-2.032894000	2.201248000
7	-4.006264000	1.156586000	0.402475000
7	-3.442061000	-1.296517000	0.992744000
6	-5.436504000	0.920596000	0.427877000
1	-5.905490000	1.582783000	1.162148000
1	-5.895440000	1.120595000	-0.549992000
1	-5.651495000	-0.110309000	0.704978000
6	-3.663005000	2.500067000	-0.018379000
1	-2.586628000	2.646457000	0.054357000
1	-3.982904000	2.700395000	-1.050071000
1	-4.154496000	3.219748000	0.641809000
6	-2.839335000	-2.591460000	0.715834000

1	-3.366526000	-3.358034000	1.288818000
1	-2.912992000	-2.835098000	-0.342832000
1	-1.777620000	-2.613290000	1.004133000
6	-3.488237000	-1.024087000	2.424681000
1	-3.901826000	-0.036108000	2.618292000
1	-4.117101000	-1.772718000	2.914663000
1	-2.483491000	-1.059262000	2.867656000
7	0.303242000	2.794374000	-0.276723000
1	1.287435000	3.027104000	-0.196536000
1	0.145707000	2.424446000	-1.211474000
1	-0.225408000	3.651776000	-0.169626000

1GaInt^{N-H} (T.E = -2669.778246)

7	-1.477011000	0.533042000	-0.594486000
7	1.477058000	0.532995000	-0.594279000
6	-1.241112000	1.789104000	-0.884336000
6	1.241217000	1.789069000	-0.884157000
6	0.000072000	2.392997000	-1.059605000
1	0.000107000	3.434450000	-1.351879000
6	-2.782536000	0.156748000	-0.254879000
6	-3.571206000	0.926273000	0.601163000
6	-3.293570000	-1.052067000	-0.726809000
6	-4.845166000	0.512145000	0.947956000
6	-4.565242000	-1.461453000	-0.373900000
6	-5.349701000	-0.681984000	0.461856000
1	-5.443705000	1.123752000	1.613804000
1	-4.950090000	-2.398509000	-0.759795000
1	-6.345587000	-1.007363000	0.737590000
6	2.782620000	0.156713000	-0.254713000
6	3.293617000	-1.052102000	-0.726662000
6	3.571338000	0.926259000	0.601260000
6	4.565329000	-1.461469000	-0.373860000
6	4.845335000	0.512153000	0.947944000
6	5.349849000	-0.681972000	0.461808000
1	4.950151000	-2.398529000	-0.759770000
1	5.443926000	1.123775000	1.613731000
1	6.345769000	-1.007320000	0.737454000
1	3.166106000	1.846949000	1.009724000
1	2.683361000	-1.653108000	-1.391760000
1	-2.683375000	-1.653045000	-1.391988000
1	-3.165948000	1.846960000	1.009607000
31	-0.000030000	-1.017644000	-0.108323000
1	2.109995000	2.445356000	-1.009164000
1	-2.109863000	2.445405000	-1.009484000
7	-0.000525000	0.270089000	2.085514000
1	0.000016000	1.253728000	1.839052000
1	-0.822405000	0.084936000	2.647326000
1	0.820766000	0.084155000	2.647931000

4GaInt^{N-H} (T.E = -2882.550125)

7	1.253127000	0.565726000	-0.473781000
6	0.971613000	1.844362000	-0.669489000
6	-0.272831000	2.444581000	-0.695861000
6	-1.506254000	1.791946000	-0.527334000
6	-1.703028000	0.458911000	-0.278202000
6	2.598814000	0.209053000	-0.331041000
6	3.061766000	-0.981774000	-0.893743000
6	3.497239000	0.980644000	0.410578000
6	4.377659000	-1.371530000	-0.737605000
1	2.369242000	-1.587984000	-1.466750000
6	4.815679000	0.586545000	0.559765000
1	3.145515000	1.889186000	0.889796000
6	5.265537000	-0.590192000	-0.013717000
1	4.716107000	-2.296173000	-1.191672000
1	5.493889000	1.201593000	1.141134000
1	6.296755000	-0.899940000	0.107000000
1	1.820886000	2.510484000	-0.855295000
15	-3.272032000	-0.161520000	-0.084723000
6	-4.671740000	0.966031000	-0.308500000
1	-5.610813000	0.429132000	-0.161887000
1	-4.612309000	1.783061000	0.411695000
1	-4.652916000	1.384571000	-1.315597000
6	-3.589452000	-1.536788000	-1.207985000
1	-3.559079000	-1.175681000	-2.236506000
1	-2.795764000	-2.276444000	-1.078327000
1	-4.557947000	-1.999079000	-1.006532000
6	-3.501068000	-0.878798000	1.556924000
1	-3.410662000	-0.091698000	2.306932000
1	-4.472415000	-1.368872000	1.650782000
1	-2.704148000	-1.607832000	1.724485000
1	-2.367918000	2.465378000	-0.621916000
1	-0.287625000	3.505909000	-0.912844000
31	-0.134178000	-0.997792000	0.058547000
7	0.315707000	0.326445000	2.353527000
1	1.322541000	0.222078000	2.405757000
1	0.120489000	1.270392000	2.038311000
1	-0.059275000	0.213109000	3.286346000

6GaInt^{N-H} (T.E = -3013.131294)

6	-1.512558000	1.451790000	-0.122068000
6	-1.491562000	0.049971000	-0.150445000
6	0.988276000	1.689062000	-0.277238000
1	1.763325000	2.464211000	-0.249569000
7	1.351949000	0.455490000	-0.332996000
15	-3.076539000	-0.530006000	0.089047000
6	-3.837366000	-0.105617000	1.677660000

1	-3.885779000	0.979487000	1.759855000
1	-4.840178000	-0.530881000	1.758462000
1	-3.212568000	-0.500689000	2.481130000
6	-4.321134000	-0.075439000	-1.144215000
1	-3.997130000	-0.438096000	-2.120707000
1	-5.291253000	-0.512519000	-0.897906000
1	-4.397013000	1.010780000	-1.172181000
6	-3.095228000	-2.334374000	0.081915000
1	-2.432410000	-2.716314000	0.860918000
1	-4.110039000	-2.693673000	0.262794000
1	-2.743984000	-2.713948000	-0.878858000
8	-2.495140000	2.192234000	0.014442000
7	-0.254665000	2.188824000	-0.259605000
6	-0.401080000	3.635788000	-0.290965000
1	-1.011199000	3.939396000	-1.141246000
1	-0.896550000	3.993915000	0.610767000
1	0.583525000	4.093727000	-0.375553000
6	2.719649000	0.181028000	-0.165381000
6	3.350197000	-0.720158000	-1.019816000
6	3.451939000	0.746739000	0.876892000
6	4.687898000	-1.019933000	-0.850103000
1	2.772396000	-1.174591000	-1.816507000
6	4.793004000	0.441309000	1.041051000
1	2.953501000	1.413172000	1.574539000
6	5.417462000	-0.440465000	0.177279000
1	5.167551000	-1.715910000	-1.528740000
1	5.347862000	0.889406000	1.857521000
1	6.465049000	-0.683782000	0.308198000
31	0.008109000	-1.346323000	-0.615644000
7	0.529382000	-1.291866000	2.053873000
1	1.490686000	-0.989010000	2.159430000
1	-0.074560000	-0.483104000	2.150073000
1	0.322963000	-1.948689000	2.795015000

8GaInt^{N-H} (T.E = -3247.178266)

7	-1.407981000	1.071570000	0.443597000
6	-0.827430000	1.332731000	-0.820808000
6	0.333139000	2.218464000	-0.936940000
15	-2.305042000	-0.056577000	-0.372159000
6	-1.441601000	0.544330000	-1.764635000
6	-1.252699000	0.357574000	-3.220046000
1	-2.161924000	0.551335000	-3.797035000
1	-0.486134000	1.046012000	-3.586543000
1	-0.919886000	-0.653243000	-3.481170000
7	-2.108800000	-1.667006000	-0.096676000
7	-3.916690000	0.181298000	-0.092802000
6	-2.640338000	-2.306834000	1.094867000
1	-1.843029000	-2.476802000	1.827508000

1	-3.402377000	-1.684371000	1.561883000
1	-3.086820000	-3.270896000	0.828589000
6	-1.000174000	-2.402641000	-0.686519000
1	-1.338363000	-3.407964000	-0.954630000
1	-0.633464000	-1.902625000	-1.580215000
1	-0.159389000	-2.494306000	0.012616000
6	-4.922246000	-0.675611000	-0.686113000
1	-5.733643000	-0.848300000	0.028515000
1	-5.355211000	-0.218544000	-1.584653000
1	-4.495836000	-1.639335000	-0.960659000
6	-4.402620000	1.510835000	0.221978000
1	-3.609973000	2.090134000	0.691026000
1	-4.746197000	2.036443000	-0.678044000
1	-5.247011000	1.434826000	0.913724000
6	2.135826000	-0.911273000	0.097645000
6	2.408439000	-1.273959000	-1.235355000
6	2.509872000	-1.836757000	1.087223000
6	2.995655000	-2.481980000	-1.554072000
1	2.113856000	-0.585177000	-2.024812000
6	3.081439000	-3.052790000	0.758525000
1	2.345777000	-1.579571000	2.128878000
6	3.329747000	-3.393133000	-0.561720000
1	3.184003000	-2.722587000	-2.595467000
1	3.349773000	-3.741572000	1.552987000
1	3.783703000	-4.344028000	-0.812968000
7	1.473219000	0.255375000	0.393800000
5	1.636597000	1.459557000	-0.342629000
7	2.906293000	2.075894000	-0.554015000
6	4.131647000	1.518375000	-0.031496000
1	3.917695000	0.780417000	0.739490000
1	4.724499000	1.028019000	-0.815159000
1	4.752428000	2.310001000	0.405477000
6	3.154418000	3.217336000	-1.395178000
1	2.227557000	3.665046000	-1.749292000
1	3.713446000	3.990739000	-0.852706000
1	3.756615000	2.946807000	-2.273834000
1	0.505803000	2.467453000	-1.988503000
1	0.143395000	3.163088000	-0.412568000
31	0.071263000	0.123571000	1.928164000
7	0.471501000	2.514028000	2.396815000
1	0.497485000	2.720905000	3.386221000
1	1.277841000	2.941120000	1.954820000
1	-0.372365000	2.911013000	1.999803000

$^{11}\text{GaInt}^{\text{N-H}}$ (T.E = -3256.480287)

7	0.912894000	-0.100574000	-0.456533000
6	0.954965000	1.289378000	-0.315593000
6	-1.540684000	1.637341000	-0.426987000

7	-1.798309000	0.323725000	-0.393649000
15	2.517391000	-0.093219000	-0.074363000
6	2.298074000	1.620295000	-0.053164000
6	3.096134000	2.822860000	0.306726000
1	3.293266000	3.493239000	-0.536170000
1	2.635394000	3.423872000	1.097437000
1	4.074487000	2.510771000	0.682513000
6	-3.162345000	-0.020997000	-0.271393000
6	-3.703166000	-0.966492000	-1.138057000
6	-3.970480000	0.472214000	0.753960000
6	-5.006236000	-1.409783000	-0.985873000
1	-3.086879000	-1.343065000	-1.947623000
6	-5.270907000	0.028921000	0.902412000
1	-3.573237000	1.228179000	1.421992000
6	-5.797645000	-0.916523000	0.035503000
1	-5.404268000	-2.144688000	-1.676557000
1	-5.882313000	0.429593000	1.703545000
1	-6.818256000	-1.260704000	0.154439000
31	-0.634436000	-1.446417000	-0.236255000
7	2.997267000	-0.756784000	1.360453000
7	3.369173000	-0.963575000	-1.187033000
6	2.855866000	-2.194233000	1.552268000
1	2.992033000	-2.725258000	0.611381000
1	3.607384000	-2.545168000	2.265043000
1	1.858842000	-2.438800000	1.941154000
6	2.752733000	-0.012005000	2.583951000
1	2.939942000	1.049592000	2.435332000
1	1.718847000	-0.141641000	2.928059000
1	3.424892000	-0.379441000	3.363793000
6	4.791360000	-1.203333000	-1.041683000
1	5.035455000	-2.204255000	-1.410914000
1	5.379045000	-0.478083000	-1.617880000
1	5.089479000	-1.139123000	0.003518000
6	2.921775000	-0.973201000	-2.569242000
1	1.841487000	-0.849306000	-2.615450000
1	3.398531000	-0.175309000	-3.151489000
1	3.183778000	-1.932657000	-3.023330000
8	-2.344685000	2.548992000	-0.450180000
7	-0.140389000	2.057349000	-0.427856000
6	0.055074000	3.500084000	-0.461594000
1	-0.010442000	3.943335000	0.535324000
1	1.028365000	3.719795000	-0.893018000
1	-0.723838000	3.944293000	-1.073253000
7	-0.968203000	-0.468271000	2.465349000
1	-0.837678000	0.534336000	2.383536000
1	-1.951218000	-0.640225000	2.275335000
1	-0.803128000	-0.724241000	3.431546000

Cartesian coordinates of the transition states involved in the ammonia activation by some of the representative Al(I) and Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AITS^{N-H} (T.E = -987.334775)

7	1.400224000	0.589904000	-0.383278000
6	1.204875000	1.886824000	-0.487154000
6	-0.024889000	2.530895000	-0.546486000
7	-1.447847000	0.589853000	-0.379596000
1	-0.024510000	3.606060000	-0.654338000
1	2.096313000	2.515872000	-0.536017000
6	2.726304000	0.136356000	-0.177658000
6	3.220381000	-0.922213000	-0.932277000
6	3.528534000	0.709724000	0.803514000
6	4.506198000	-1.382805000	-0.716445000
1	2.584730000	-1.372944000	-1.685697000
6	4.816000000	0.246324000	1.009926000
1	3.125324000	1.505653000	1.420860000
6	5.309773000	-0.800332000	0.250278000
1	4.885073000	-2.203210000	-1.314731000
1	5.431298000	0.699258000	1.778723000
1	6.316156000	-1.166141000	0.415548000
6	-2.766845000	0.126768000	-0.158698000
6	-3.236007000	-0.964706000	-0.883469000
6	-3.590710000	0.713964000	0.795798000
6	-4.516728000	-1.439856000	-0.671887000
1	-2.585649000	-1.428100000	-1.617651000
6	-4.873855000	0.236677000	0.998066000
1	-3.209609000	1.530429000	1.399530000
6	-5.342637000	-0.839960000	0.265314000
1	-4.873909000	-2.284505000	-1.249431000
1	-5.505563000	0.702051000	1.745920000
1	-6.345149000	-1.216492000	0.429674000
6	-1.249131000	1.892531000	-0.446171000
1	-2.137722000	2.527377000	-0.434016000
13	-0.019062000	-0.749244000	-0.313284000
1	0.550635000	-2.192873000	0.404620000
7	0.235597000	-1.363079000	1.505428000
1	-0.503448000	-1.931565000	1.905633000
1	0.860443000	-1.048600000	2.250281000

4AITS^{N-H} (T.E = -1200.115016)

7	1.226307000	0.615320000	-0.199135000
6	0.954126000	1.916212000	-0.080851000

6	-0.282367000	2.511523000	0.008886000
6	-1.512872000	1.828285000	0.003328000
6	-1.672975000	0.466740000	-0.010858000
6	2.582271000	0.227708000	-0.196356000
6	3.006300000	-0.783011000	-1.057040000
6	3.508866000	0.794952000	0.675829000
6	4.324742000	-1.196802000	-1.058155000
1	2.282419000	-1.235224000	-1.726873000
6	4.829337000	0.380385000	0.665493000
1	3.180671000	1.545568000	1.386387000
6	5.245932000	-0.615411000	-0.200888000
1	4.636657000	-1.978915000	-1.741029000
1	5.535015000	0.831325000	1.354278000
1	6.278898000	-0.942520000	-0.203060000
1	1.814906000	2.588002000	-0.090928000
15	-3.237698000	-0.212936000	-0.141737000
6	-4.615056000	0.949369000	-0.023337000
1	-5.558605000	0.406350000	-0.098909000
1	-4.580747000	1.476354000	0.930877000
1	-4.561675000	1.679140000	-0.832021000
6	-3.474499000	-1.088975000	-1.697579000
1	-3.406059000	-0.380981000	-2.524367000
1	-2.667146000	-1.819984000	-1.793133000
1	-4.442123000	-1.594609000	-1.720457000
6	-3.531322000	-1.459970000	1.122787000
1	-3.444933000	-1.007020000	2.111390000
1	-4.519337000	-1.909358000	1.005318000
1	-2.762906000	-2.231375000	1.018673000
1	-2.387827000	2.487449000	-0.003429000
1	-0.297030000	3.593589000	0.043215000
13	-0.105536000	-0.792812000	-0.038768000
1	-0.420257000	-2.302582000	0.779022000
7	0.012159000	-1.490053000	1.791319000
1	0.866172000	-1.983451000	2.031006000
1	-0.452804000	-1.184060000	2.651235000

6AITS^{N-H} (T.E = -1330.694573)

6	-1.538200000	1.363897000	-0.022077000
6	-1.484952000	-0.033656000	-0.010787000
6	0.965555000	1.604331000	-0.123364000
1	1.755822000	2.358652000	-0.081110000
13	0.069550000	-1.174637000	-0.396349000
7	1.321569000	0.362977000	-0.245723000
15	-3.067620000	-0.681838000	-0.009163000
6	-4.138218000	-0.164880000	1.350641000
1	-4.282546000	0.912897000	1.297686000
1	-5.100236000	-0.678251000	1.287599000
1	-3.654764000	-0.416739000	2.295466000

6	-4.022628000	-0.358582000	-1.508293000
1	-3.491032000	-0.796632000	-2.354982000
1	-5.023479000	-0.789846000	-1.441229000
1	-4.092834000	0.720265000	-1.646684000
6	-3.004129000	-2.474827000	0.121744000
1	-2.605208000	-2.758362000	1.096968000
1	-4.004471000	-2.895441000	0.004767000
1	-2.335506000	-2.873574000	-0.647623000
8	-2.528016000	2.098052000	-0.001158000
7	-0.264454000	2.107824000	-0.061366000
6	-0.408169000	3.555237000	-0.020149000
1	-0.968869000	3.908413000	-0.884851000
1	-0.955280000	3.857268000	0.871770000
1	0.579565000	4.014065000	-0.016610000
6	2.708417000	0.082789000	-0.157808000
6	3.294201000	-0.752647000	-1.102355000
6	3.476410000	0.581323000	0.887163000
6	4.639977000	-1.056996000	-1.013173000
1	2.677588000	-1.156866000	-1.898019000
6	4.824794000	0.276307000	0.966628000
1	3.003879000	1.183626000	1.655805000
6	5.411170000	-0.541420000	0.016649000
1	5.090513000	-1.702371000	-1.758202000
1	5.414777000	0.668550000	1.786861000
1	6.464767000	-0.785249000	0.083430000
1	0.165178000	-2.866961000	-0.036303000
7	0.497370000	-2.285189000	1.169380000
1	0.019784000	-2.351357000	2.071925000
1	1.449863000	-2.623188000	1.267635000

8AITS^{N-H} (T.E = -1564.745933)

7	1.274680000	0.128771000	-1.054264000
6	1.114473000	1.469885000	-0.617103000
6	-0.002227000	2.248382000	-1.142111000
15	2.416039000	-0.001350000	0.128986000
6	2.051229000	1.694673000	0.356824000
6	2.375274000	2.856039000	1.212609000
1	3.403331000	3.206903000	1.084209000
1	1.716259000	3.693280000	0.966764000
1	2.241993000	2.644397000	2.279115000
7	2.141379000	-0.906156000	1.475542000
7	3.820411000	-0.597664000	-0.479632000
6	2.392624000	-2.336693000	1.521716000
1	1.457540000	-2.890864000	1.374945000
1	3.092072000	-2.635396000	0.742982000
1	2.812303000	-2.603142000	2.496612000
6	1.050470000	-0.517034000	2.357245000
1	1.288457000	-0.814165000	3.381902000

1	0.893483000	0.560671000	2.329428000
1	0.118660000	-1.012157000	2.054375000
6	5.013263000	-0.662384000	0.341832000
1	5.533008000	-1.611500000	0.175819000
1	5.705086000	0.151438000	0.095529000
1	4.760550000	-0.592163000	1.399805000
6	4.084015000	-0.600460000	-1.908976000
1	3.150729000	-0.646299000	-2.467633000
1	4.641233000	0.292267000	-2.215946000
1	4.684419000	-1.480551000	-2.155719000
13	-0.222985000	-0.867599000	-1.742392000
6	-2.568842000	-0.576442000	-0.303427000
6	-2.705205000	-0.671589000	1.083769000
6	-3.421109000	-1.348018000	-1.096565000
6	-3.658214000	-1.496400000	1.653691000
1	-2.049174000	-0.071028000	1.707416000
6	-4.366928000	-2.179954000	-0.523071000
1	-3.318978000	-1.285318000	-2.175109000
6	-4.495386000	-2.259647000	0.854120000
1	-3.745633000	-1.546860000	2.733758000
1	-5.014157000	-2.770454000	-1.162249000
1	-5.239301000	-2.908759000	1.300416000
7	-1.556123000	0.201882000	-0.879063000
5	-1.401381000	1.586667000	-0.644376000
7	-2.381976000	2.459591000	-0.072693000
6	-3.799091000	2.186552000	-0.048776000
1	-4.051562000	1.339702000	-0.683065000
1	-4.165635000	1.971170000	0.964696000
1	-4.350840000	3.060306000	-0.418749000
6	-2.087162000	3.720488000	0.555983000
1	-1.015851000	3.862767000	0.695646000
1	-2.478275000	4.573633000	-0.016915000
1	-2.548661000	3.766167000	1.551479000
1	0.096847000	3.305412000	-0.900051000
1	-0.011018000	2.152420000	-2.236031000
1	-0.606944000	-2.513843000	-2.056501000
7	-0.271426000	-2.559592000	-0.712986000
1	0.502205000	-3.212167000	-0.787566000
1	-0.933552000	-2.881618000	-0.001959000

10AITS^{N-H} (T.E = -1656.241180)

7	-0.597103000	0.110336000	0.230119000
6	-0.619643000	1.395225000	-0.410728000
6	0.532179000	2.091973000	-0.749307000
6	1.827359000	1.608295000	-0.552952000
1	0.401340000	3.083655000	-1.168590000
1	2.601797000	2.343634000	-0.799519000
15	-2.238684000	0.125239000	0.097220000

6	-1.989666000	1.679413000	-0.574253000
6	-2.706404000	2.783678000	-1.251320000
1	-3.777694000	2.573522000	-1.309999000
1	-2.601764000	3.743855000	-0.733703000
1	-2.354201000	2.937493000	-2.279670000
6	2.213962000	0.352561000	-0.108667000
15	3.850942000	0.030086000	0.196447000
6	5.030727000	1.276618000	-0.376414000
1	6.047366000	0.947026000	-0.155626000
1	4.926895000	1.424156000	-1.451987000
1	4.850217000	2.226300000	0.128427000
6	4.399500000	-1.521900000	-0.542384000
1	5.437279000	-1.736982000	-0.279494000
1	3.755026000	-2.321496000	-0.166236000
1	4.295744000	-1.466869000	-1.626941000
6	4.233214000	-0.188543000	1.949588000
1	4.025274000	0.741613000	2.480002000
1	3.574517000	-0.967760000	2.340660000
1	5.276687000	-0.475320000	2.098842000
7	-2.973729000	-0.985355000	-0.890773000
7	-2.958362000	-0.185301000	1.564082000
6	-3.100652000	-2.374622000	-0.486128000
1	-2.226365000	-2.959435000	-0.802781000
1	-3.185139000	-2.455054000	0.595879000
1	-3.991529000	-2.812246000	-0.947039000
6	-2.752372000	-0.842676000	-2.319785000
1	-3.550389000	-1.359334000	-2.859839000
1	-2.758213000	0.208829000	-2.603534000
1	-1.788747000	-1.277796000	-2.620501000
6	-4.398608000	-0.023380000	1.647211000
1	-4.783528000	-0.596356000	2.495358000
1	-4.680155000	1.029672000	1.792003000
1	-4.880804000	-0.386542000	0.739775000
6	-2.272148000	0.296819000	2.751570000
1	-1.213668000	0.046333000	2.703682000
1	-2.376236000	1.384138000	2.871308000
1	-2.707069000	-0.189517000	3.628143000
13	0.864353000	-1.058589000	0.368770000
1	1.426936000	-2.681632000	0.042625000
7	0.932241000	-2.304733000	-1.168010000
1	0.211247000	-3.013750000	-1.252246000
1	1.418703000	-2.203739000	-2.064529000

11AITS^{N-H} (T.E = -1574.048327)

7	-0.779575000	-0.140001000	0.252173000
6	-0.854615000	1.249755000	0.092558000
6	1.630330000	1.596079000	0.128284000
15	-2.417257000	-0.169692000	0.053444000

6	-2.214071000	1.541403000	-0.089366000
6	-3.072458000	2.713859000	-0.403044000
1	-3.216555000	3.397416000	0.439640000
1	-2.697214000	3.306589000	-1.242863000
1	-4.069224000	2.365109000	-0.688434000
7	-3.050904000	-0.923880000	-1.265644000
7	-3.146263000	-0.927155000	1.321076000
6	-3.115403000	-2.377970000	-1.326703000
1	-2.216783000	-2.789347000	-1.802332000
1	-3.190141000	-2.802030000	-0.327347000
1	-3.989429000	-2.681061000	-1.909527000
6	-2.857459000	-0.313368000	-2.569963000
1	-3.644359000	-0.656014000	-3.246224000
1	-2.904528000	0.771911000	-2.498481000
1	-1.887419000	-0.590612000	-3.003685000
6	-4.597802000	-0.919677000	1.390924000
1	-4.942583000	-1.811317000	1.921155000
1	-4.969064000	-0.037307000	1.928046000
1	-5.033358000	-0.924961000	0.391863000
6	-2.503846000	-0.877097000	2.627122000
1	-1.443447000	-1.114894000	2.539187000
1	-2.622014000	0.104866000	3.102903000
1	-2.969566000	-1.628912000	3.267505000
7	0.236649000	2.026471000	0.138065000
6	0.041173000	3.466457000	0.048568000
1	0.019200000	3.806563000	-0.989583000
1	-0.893147000	3.731860000	0.537920000
1	0.868255000	3.963163000	0.545475000
8	2.446778000	2.477048000	-0.022326000
7	1.878284000	0.284891000	0.298731000
6	3.248903000	-0.086697000	0.187858000
6	3.864996000	-0.741086000	1.245433000
6	3.954554000	0.102729000	-0.994842000
6	5.169839000	-1.192759000	1.126372000
1	3.308178000	-0.892228000	2.163866000
6	5.256753000	-0.343685000	-1.108908000
1	3.467972000	0.606749000	-1.821854000
6	5.870923000	-0.993971000	-0.048725000
1	5.638183000	-1.701452000	1.961185000
1	5.797498000	-0.186721000	-2.035432000
1	6.891767000	-1.345688000	-0.142166000
13	0.735730000	-1.245471000	0.435290000
1	0.281730000	-2.837957000	-0.079060000
7	0.703348000	-2.215283000	-1.250824000
1	0.200766000	-2.020352000	-2.124680000
1	1.513748000	-2.792379000	-1.457350000

13AITS^{N-H} (T.E = -1899.596853)

7	1.372282000	-0.150679000	0.011367000
6	1.246292000	1.131327000	-0.632555000
6	0.028733000	1.726820000	-0.927499000
6	-1.191952000	1.162766000	-0.580911000
1	0.030880000	2.687740000	-1.430871000
13	0.027049000	-1.264430000	0.699288000
15	2.996854000	0.102065000	-0.011432000
6	2.573978000	1.552635000	-0.819215000
6	3.151191000	2.816510000	-1.330801000
1	2.821737000	3.691672000	-0.755593000
1	4.242519000	2.796205000	-1.282013000
1	2.885864000	3.006303000	-2.376468000
7	-1.318557000	-0.078986000	0.129066000
6	-2.517817000	1.589090000	-0.772905000
15	-2.943587000	0.146165000	0.047314000
6	-3.099576000	2.750863000	-1.482630000
1	-2.981402000	2.693001000	-2.572852000
1	-4.170445000	2.837565000	-1.283716000
1	-2.643056000	3.694251000	-1.164754000
7	-3.865504000	-0.948215000	-0.788902000
7	-3.632267000	0.093489000	1.558794000
6	-4.132514000	-2.267202000	-0.240291000
1	-3.368325000	-2.990152000	-0.555647000
1	-4.136057000	-2.236274000	0.847775000
1	-5.106693000	-2.622768000	-0.589654000
6	-3.754272000	-0.952798000	-2.235142000
1	-2.901425000	-1.557636000	-2.574326000
1	-4.665203000	-1.376155000	-2.667157000
1	-3.624418000	0.061159000	-2.611104000
6	-2.842575000	0.616476000	2.662743000
1	-3.320189000	0.323744000	3.600579000
1	-1.837815000	0.194901000	2.643635000
1	-2.775448000	1.712896000	2.634986000
6	-5.038694000	0.439062000	1.665780000
1	-5.186856000	1.527975000	1.701586000
1	-5.599388000	0.042688000	0.819505000
1	-5.451414000	0.011554000	2.583604000
7	3.790051000	-1.174980000	-0.721576000
7	3.785594000	0.244091000	1.439194000
6	5.234703000	-1.118881000	-0.851723000
1	5.632112000	-2.133714000	-0.943577000
1	5.538021000	-0.555085000	-1.745226000
1	5.684962000	-0.648834000	0.021285000
6	3.153874000	-1.773352000	-1.883857000
1	2.076968000	-1.843758000	-1.733911000
1	3.347598000	-1.192433000	-2.795619000
1	3.553283000	-2.780951000	-2.026511000
6	3.505957000	1.445594000	2.208343000

1	4.296002000	1.586297000	2.950400000
1	3.476601000	2.318506000	1.557586000
1	2.544918000	1.371617000	2.735713000
6	3.940219000	-0.928557000	2.289462000
1	4.102211000	-1.821765000	1.688847000
1	4.799798000	-0.787246000	2.951188000
1	3.045254000	-1.091798000	2.903965000
1	-0.665467000	-2.841743000	0.926567000
7	-0.353746000	-2.826035000	-0.419893000
1	-0.988259000	-2.910395000	-1.223139000
1	0.308133000	-3.596637000	-0.428212000

1GaTS^{N-H} (T.E = -2669.697094)

7	1.506062000	-0.059261000	0.874647000
7	1.459956000	-0.021393000	-2.063781000
6	2.718166000	0.391036000	0.627954000
6	2.687921000	0.392745000	-1.843665000
6	3.271783000	0.664297000	-0.613250000
1	4.277032000	1.061707000	-0.624976000
6	1.171118000	-0.446811000	2.185802000
6	2.075191000	-1.124754000	2.999880000
6	-0.104460000	-0.178672000	2.675087000
6	1.718606000	-1.495582000	4.283578000
6	-0.457398000	-0.559536000	3.955599000
6	0.452987000	-1.213997000	4.769127000
1	2.432503000	-2.026308000	4.902957000
1	-1.452640000	-0.337369000	4.322532000
1	0.173702000	-1.512235000	5.772407000
6	1.089034000	-0.385599000	-3.375161000
6	-0.172897000	-0.039006000	-3.849359000
6	1.946990000	-1.109140000	-4.198426000
6	-0.553949000	-0.388407000	-5.131125000
6	1.560671000	-1.450384000	-5.481950000
6	0.310454000	-1.090531000	-5.955136000
1	-1.536453000	-0.105005000	-5.490160000
1	2.237620000	-2.017496000	-6.110457000
1	0.006695000	-1.364854000	-6.958208000
1	2.909119000	-1.431737000	-3.816019000
1	-0.845717000	0.523431000	-3.211410000
1	-0.815374000	0.345187000	2.045205000
1	3.051093000	-1.390918000	2.609417000
31	0.105039000	-0.158044000	-0.575431000
1	3.318298000	0.543191000	-2.723161000
1	3.360413000	0.566718000	1.494293000
1	-1.417036000	0.363901000	-0.920562000
7	-0.698420000	1.729832000	-0.742151000
1	-0.512370000	2.458720000	-1.427551000
1	-1.172487000	2.140141000	0.055015000

4GaTS^{N-H} (T.E = -2882.482988)

7	1.245634000	0.715678000	-0.242015000
6	0.958938000	2.004671000	-0.156735000
6	-0.288145000	2.593460000	-0.059673000
6	-1.512619000	1.915847000	-0.026478000
6	-1.709579000	0.559496000	-0.104567000
6	2.596625000	0.326836000	-0.203789000
6	3.049203000	-0.681467000	-1.051725000
6	3.494331000	0.899850000	0.694960000
6	4.368698000	-1.088664000	-1.013035000
1	2.347074000	-1.137983000	-1.740204000
6	4.815989000	0.490697000	0.724895000
1	3.138935000	1.648805000	1.394448000
6	5.261684000	-0.503155000	-0.129155000
1	4.704615000	-1.870558000	-1.684728000
1	5.498763000	0.943788000	1.434991000
1	6.295379000	-0.826692000	-0.100329000
1	1.811703000	2.687786000	-0.188609000
15	-3.268814000	-0.120458000	-0.077293000
6	-4.636452000	1.038950000	0.132392000
1	-5.582646000	0.495231000	0.130620000
1	-4.532261000	1.572513000	1.077756000
1	-4.641060000	1.762841000	-0.683326000
6	-3.635645000	-1.040668000	-1.583803000
1	-3.662956000	-0.353692000	-2.430203000
1	-2.830870000	-1.761253000	-1.747296000
1	-4.588300000	-1.568100000	-1.503637000
6	-3.445378000	-1.343444000	1.234529000
1	-3.229648000	-0.877711000	2.196588000
1	-4.448516000	-1.774882000	1.238867000
1	-2.710150000	-2.134112000	1.065928000
1	-2.381364000	2.577005000	0.063481000
1	-0.305420000	3.675138000	-0.017845000
31	-0.150713000	-0.735156000	-0.136235000
1	0.550481000	-2.096425000	0.475399000
7	0.382243000	-1.344416000	1.803800000
1	1.142819000	-0.995379000	2.382922000
1	-0.173292000	-2.002888000	2.338474000

6GaTS^{N-H} (T.E = -3013.065274)

6	-1.545399000	1.472217000	-0.052906000
6	-1.538328000	0.078333000	-0.178186000
6	0.955392000	1.705352000	-0.189071000
1	1.736385000	2.470925000	-0.171606000
7	1.323612000	0.470407000	-0.253435000
15	-3.109583000	-0.554101000	0.028914000
6	-3.845026000	-0.259161000	1.652175000

1	-3.915797000	0.816064000	1.812528000
1	-4.836370000	-0.712240000	1.720260000
1	-3.190009000	-0.693172000	2.409518000
6	-4.353477000	-0.004569000	-1.159875000
1	-4.035511000	-0.290595000	-2.163219000
1	-5.321774000	-0.459492000	-0.941022000
1	-4.429842000	1.080415000	-1.102572000
6	-3.084758000	-2.347528000	-0.132284000
1	-2.447548000	-2.780419000	0.640795000
1	-4.097586000	-2.740580000	-0.026236000
1	-2.683565000	-2.631096000	-1.106487000
8	-2.528238000	2.196120000	0.129975000
7	-0.284412000	2.206212000	-0.148110000
6	-0.427380000	3.654642000	-0.114220000
1	0.557541000	4.112807000	-0.189858000
1	-1.047350000	3.995662000	-0.942562000
1	-0.909206000	3.971518000	0.809856000
6	2.707201000	0.201131000	-0.141666000
6	3.320993000	-0.632968000	-1.068474000
6	3.452349000	0.725169000	0.908129000
6	4.668680000	-0.916144000	-0.954295000
1	2.725295000	-1.055141000	-1.869391000
6	4.802758000	0.438844000	1.014535000
1	2.957635000	1.331973000	1.659418000
6	5.415888000	-0.380004000	0.082973000
1	5.140936000	-1.563065000	-1.684453000
1	5.373562000	0.848316000	1.839951000
1	6.471258000	-0.609310000	0.169711000
31	0.017828000	-1.130267000	-0.369869000
1	1.006134000	-2.401599000	0.004007000
7	0.735537000	-1.952463000	1.430601000
1	0.285821000	-2.790914000	1.782262000
1	1.380452000	-1.600206000	2.137145000

8GaTS^{N-H} (T.E = -3247.109727)

7	-1.372580000	-0.999914000	-0.449956000
6	-0.828324000	-1.402897000	0.800789000
6	0.338264000	-2.285410000	0.839652000
15	-2.262484000	0.083852000	0.435084000
6	-1.489387000	-0.715888000	1.785475000
6	-1.397685000	-0.714246000	3.261737000
1	-0.675505000	-1.466221000	3.589487000
1	-1.063064000	0.246698000	3.666709000
1	-2.350237000	-0.949007000	3.745093000
7	-1.951931000	1.691479000	0.335658000
7	-3.852792000	-0.037670000	0.027651000
6	-2.303256000	2.445347000	-0.858713000
1	-1.414857000	2.615234000	-1.477857000

1	-3.034047000	1.905220000	-1.459266000
1	-2.726086000	3.414120000	-0.573375000
6	-0.889875000	2.321065000	1.106828000
1	-1.228829000	3.302567000	1.451120000
1	-0.625613000	1.715452000	1.970949000
1	0.013404000	2.456871000	0.501581000
6	-4.862029000	0.864488000	0.542308000
1	-5.542485000	1.160526000	-0.262818000
1	-5.457058000	0.384332000	1.327940000
1	-4.405240000	1.762845000	0.954154000
6	-4.387585000	-1.295881000	-0.461075000
1	-3.583238000	-1.911318000	-0.858695000
1	-4.901855000	-1.844448000	0.336783000
1	-5.108709000	-1.098394000	-1.259606000
6	2.088051000	0.933187000	-0.183307000
6	2.546783000	1.280732000	1.098781000
6	2.246401000	1.895036000	-1.192363000
6	3.115992000	2.513289000	1.352913000
1	2.420091000	0.564361000	1.906710000
6	2.805147000	3.131755000	-0.926977000
1	1.912709000	1.653684000	-2.197042000
6	3.245438000	3.458466000	0.346044000
1	3.451542000	2.744117000	2.358659000
1	2.904914000	3.849472000	-1.734479000
1	3.685902000	4.427000000	0.548808000
7	1.446301000	-0.265745000	-0.413297000
5	1.646638000	-1.466927000	0.343085000
7	2.927774000	-1.998887000	0.637442000
6	4.147438000	-1.435773000	0.106946000
1	3.931123000	-0.702280000	-0.666660000
1	4.741469000	-0.943219000	0.888080000
1	4.766898000	-2.227100000	-0.331219000
6	3.194716000	-3.145015000	1.467374000
1	2.279562000	-3.580986000	1.861953000
1	3.719620000	-3.925020000	0.901552000
1	3.836821000	-2.877390000	2.317226000
1	0.479948000	-2.673887000	1.850563000
1	0.186084000	-3.134105000	0.162427000
31	0.040208000	-0.403978000	-1.781758000
1	-0.209590000	-0.896786000	-3.327252000
7	0.273919000	-2.233245000	-2.692271000
1	-0.372129000	-3.013371000	-2.630555000
1	1.121493000	-2.512318000	-3.171313000

10GaTS^{N-H} (T.E = -3338.605606)

7	-0.725495000	0.193265000	0.299005000
6	-0.756575000	1.573500000	-0.055714000
6	0.385695000	2.364641000	-0.121371000

6	1.682148000	1.879608000	0.032845000
1	0.247434000	3.407511000	-0.384495000
1	2.446605000	2.639342000	-0.170158000
15	-2.340476000	0.166701000	-0.017003000
6	-2.114394000	1.837733000	-0.327778000
6	-2.806905000	3.025090000	-0.878749000
1	-2.386265000	3.347769000	-1.840455000
1	-3.865540000	2.814211000	-1.049212000
1	-2.763051000	3.889691000	-0.207474000
6	2.115231000	0.606240000	0.377627000
15	3.717730000	0.163815000	0.023424000
6	4.973576000	1.426735000	0.348187000
1	5.959956000	1.054840000	0.064204000
1	4.759732000	2.324198000	-0.233546000
1	4.970245000	1.685506000	1.407387000
6	3.948549000	-0.307360000	-1.700693000
1	4.951041000	-0.698067000	-1.890696000
1	3.176656000	-1.056536000	-1.923665000
1	3.769322000	0.569193000	-2.326689000
6	4.227658000	-1.277581000	0.970623000
1	4.153115000	-1.064011000	2.037362000
1	3.563877000	-2.112449000	0.737702000
1	5.253400000	-1.550858000	0.716810000
31	0.832013000	-0.886557000	0.724973000
7	-2.858093000	-0.774681000	-1.280756000
7	-3.197289000	-0.457579000	1.262138000
6	-2.800739000	-2.223491000	-1.144019000
1	-1.791159000	-2.603419000	-1.352719000
1	-3.070551000	-2.525389000	-0.133693000
1	-3.497694000	-2.684040000	-1.849471000
6	-2.463204000	-0.332255000	-2.608933000
1	-3.084930000	-0.837259000	-3.352313000
1	-2.600082000	0.743544000	-2.709767000
1	-1.410252000	-0.568368000	-2.817846000
6	-4.646085000	-0.479368000	1.172830000
1	-5.042031000	-1.239702000	1.851875000
1	-5.083539000	0.488758000	1.455241000
1	-4.966607000	-0.720446000	0.159978000
6	-2.725667000	-0.121815000	2.595280000
1	-1.641333000	-0.206262000	2.644859000
1	-3.016892000	0.896500000	2.886599000
1	-3.162155000	-0.823519000	3.310233000
1	0.703663000	-2.433954000	0.277047000
7	1.188197000	-2.195069000	-1.242913000
1	1.639752000	-3.109355000	-1.256828000
1	0.369079000	-2.293517000	-1.843885000

11GaTS^{N-H} (T.E = -3256.405916)

7	-0.760824000	-0.130369000	0.382857000
6	-0.841856000	1.263481000	0.199131000
6	1.642505000	1.596227000	0.270931000
7	1.919378000	0.305911000	0.021115000
15	-2.414100000	-0.137363000	0.301743000
6	-2.207294000	1.574846000	0.165436000
6	-3.074244000	2.782651000	0.116831000
1	-2.777629000	3.550337000	0.835504000
1	-3.112574000	3.258326000	-0.870090000
1	-4.101792000	2.505664000	0.365980000
6	3.250663000	-0.138405000	0.199648000
6	3.461541000	-1.360949000	0.830146000
6	4.352062000	0.558325000	-0.290431000
6	4.737256000	-1.878966000	0.967464000
1	2.606292000	-1.902368000	1.222658000
6	5.625059000	0.039393000	-0.145820000
1	4.202497000	1.511327000	-0.779364000
6	5.827592000	-1.179587000	0.481764000
1	4.876888000	-2.833021000	1.463033000
1	6.471490000	0.595364000	-0.533462000
1	6.828643000	-1.580064000	0.590787000
31	0.637085000	-1.009414000	-0.714727000
7	-3.174055000	-0.871029000	-0.953833000
7	-3.009691000	-0.927627000	1.621072000
6	-3.147363000	-2.316874000	-1.106022000
1	-2.829105000	-2.796501000	-0.181175000
1	-4.144432000	-2.686162000	-1.368468000
1	-2.444769000	-2.602450000	-1.896670000
6	-3.513691000	-0.167810000	-2.175320000
1	-3.488022000	0.909296000	-2.017339000
1	-2.813530000	-0.422222000	-2.978787000
1	-4.521012000	-0.453446000	-2.494737000
6	-4.420302000	-1.222076000	1.773075000
1	-4.544478000	-2.206472000	2.234996000
1	-4.914111000	-0.483242000	2.415931000
1	-4.922097000	-1.229854000	0.806965000
6	-2.301139000	-0.834967000	2.886427000
1	-1.242345000	-0.657960000	2.709858000
1	-2.701458000	-0.025924000	3.508960000
1	-2.414596000	-1.775352000	3.432682000
8	2.409599000	2.467296000	0.616291000
7	0.258107000	2.018721000	0.072945000
6	0.079247000	3.455920000	-0.068936000
1	-0.777948000	3.647641000	-0.711483000
1	-0.071175000	3.943111000	0.897168000
1	0.971187000	3.879447000	-0.519454000
1	-0.017654000	-1.779708000	-2.032034000
7	-0.038000000	-0.351375000	-2.557568000

1	-0.754775000	0.328128000	-2.820776000
1	0.636941000	-0.416863000	-3.312649000

¹³GaTS^{N-H} (T.E = -3581.951525)

7	1.378501000	-0.045669000	-0.188793000
6	1.240174000	1.345810000	-0.515672000
6	0.023541000	2.002721000	-0.634918000
6	-1.207247000	1.373864000	-0.487596000
1	0.037259000	3.067573000	-0.840808000
15	2.997840000	0.224571000	-0.108888000
6	2.566740000	1.804436000	-0.617430000
6	3.128256000	3.147593000	-0.886008000
1	2.666546000	3.606552000	-1.766406000
1	2.988548000	3.850408000	-0.053057000
1	4.201294000	3.098634000	-1.083665000
7	-1.359473000	-0.018671000	-0.186888000
6	-2.526404000	1.859096000	-0.552537000
15	-2.974163000	0.267709000	-0.088410000
6	-3.076813000	3.208368000	-0.811550000
1	-2.443827000	3.750541000	-1.520430000
1	-4.075080000	3.164058000	-1.253795000
1	-3.153884000	3.835418000	0.087254000
7	-3.813179000	-0.810906000	-1.026575000
7	-3.699660000	0.081597000	1.392837000
6	-3.236253000	-1.179295000	-2.306336000
1	-3.616940000	-0.544692000	-3.116452000
1	-2.151080000	-1.088107000	-2.267593000
1	-3.493432000	-2.218302000	-2.535074000
6	-5.257301000	-0.907030000	-0.999511000
1	-5.713695000	-0.312316000	-1.801387000
1	-5.561953000	-1.949323000	-1.141045000
1	-5.649884000	-0.558855000	-0.045656000
6	-3.755927000	-1.251578000	1.978778000
1	-4.598068000	-1.311760000	2.674544000
1	-3.885782000	-2.008725000	1.206430000
1	-2.830492000	-1.482194000	2.522915000
6	-3.411006000	1.102872000	2.385849000
1	-2.413322000	0.968025000	2.826854000
1	-3.459604000	2.095077000	1.940243000
1	-4.151809000	1.040395000	3.187312000
7	3.817932000	-0.906126000	-1.001864000
7	3.736170000	0.098651000	1.373534000
6	5.265860000	-0.937442000	-1.031620000
1	5.610842000	-1.969967000	-1.147541000
1	5.663426000	-0.354306000	-1.872672000
1	5.680054000	-0.536945000	-0.107489000
6	3.209520000	-1.362582000	-2.239708000
1	2.124525000	-1.372313000	-2.143673000

1	3.489243000	-0.722988000	-3.086613000
1	3.550499000	-2.380196000	-2.450836000
6	3.451207000	1.155589000	2.329793000
1	4.198408000	1.126055000	3.127109000
1	3.492389000	2.130552000	1.846965000
1	2.457468000	1.034019000	2.783510000
6	3.826507000	-1.207076000	2.011034000
1	3.972829000	-1.989582000	1.267994000
1	4.672400000	-1.219647000	2.704747000
1	2.910717000	-1.437807000	2.571685000
31	0.002947000	-1.180628000	0.593755000
1	-0.493779000	-2.728451000	0.952898000
7	-0.265599000	-2.900190000	-0.537863000
1	-0.912910000	-3.129486000	-1.293222000
1	0.487301000	-3.581890000	-0.526622000

Cartesian coordinates of the transition states involved in the hexa-fluorobenzene activation by some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AITS^{C-F} (T.E = -1758.421085)

7	1.499688000	0.524026000	-0.341513000
6	1.303905000	1.828620000	-0.295124000
6	0.075993000	2.465519000	-0.231660000
7	-1.319975000	0.501626000	-0.275292000
1	0.067553000	3.545898000	-0.226952000
1	2.192222000	2.461456000	-0.335968000
6	2.838696000	0.052336000	-0.353069000
6	3.191859000	-0.963550000	-1.231963000
6	3.782892000	0.548693000	0.536884000
6	4.479036000	-1.468679000	-1.226451000
1	2.450069000	-1.347279000	-1.924545000

6	5.069908000	0.043122000	0.533833000
1	3.490869000	1.300488000	1.261959000
6	5.422391000	-0.966366000	-0.345979000
1	4.746154000	-2.259472000	-1.917280000
1	5.796873000	0.427639000	1.239416000
1	6.428525000	-1.367662000	-0.338826000
6	-2.650160000	0.008064000	-0.224092000
6	-3.027293000	-1.013884000	-1.085915000
6	-3.559100000	0.487733000	0.710606000
6	-4.303317000	-1.542267000	-1.018302000
1	-2.313218000	-1.384217000	-1.813999000
6	-4.835416000	-0.041026000	0.769547000
1	-3.245938000	1.244769000	1.421252000
6	-5.211684000	-1.057209000	-0.092505000
1	-4.589276000	-2.337859000	-1.695949000
1	-5.534161000	0.330437000	1.509784000
1	-6.208705000	-1.476964000	-0.036560000
6	-1.143240000	1.809233000	-0.237282000
1	-2.042551000	2.427718000	-0.235614000
13	0.104967000	-0.806561000	-0.114231000
9	0.160595000	-0.642544000	2.093798000
6	0.164756000	-2.081761000	1.859429000
6	-1.013978000	-2.745192000	2.227575000
6	1.370532000	-2.728268000	2.165122000
6	-0.995446000	-4.043169000	2.684057000
6	1.394393000	-4.026181000	2.621573000
6	0.210523000	-4.695459000	2.896337000
9	-2.178921000	-2.156893000	1.977505000
9	-2.131163000	-4.673809000	2.929422000
9	0.231972000	-5.925995000	3.382768000
9	2.550151000	-4.640577000	2.807417000
9	2.512174000	-2.123256000	1.854504000

4AITS^{C-F} (T.E = -1971.216050)

7	0.064836000	1.860670000	-0.340596000
6	-0.414385000	2.797989000	0.479551000
6	-1.696561000	2.891630000	0.968616000
1	-1.909092000	3.729234000	1.620605000
1	0.286175000	3.577325000	0.783976000
6	1.458770000	1.851117000	-0.572451000
6	1.942918000	1.546151000	-1.842327000
6	2.369306000	2.078861000	0.457067000
6	3.304263000	1.475663000	-2.075243000
1	1.236146000	1.372026000	-2.647310000
6	3.729571000	2.017949000	0.214714000
1	2.005251000	2.261583000	1.462652000
6	4.204540000	1.713600000	-1.050230000
1	3.662764000	1.233525000	-3.068859000

1	4.423485000	2.181529000	1.031067000
1	5.270401000	1.652533000	-1.233190000
6	-2.725408000	1.980004000	0.695913000
1	-3.653971000	2.191078000	1.239213000
13	-0.950853000	0.404016000	-1.124450000
9	-0.992325000	-2.380006000	-0.330010000
6	0.121758000	-1.620075000	-0.077968000
6	1.300642000	-1.951423000	-0.776219000
6	0.285375000	-1.184358000	1.250488000
6	2.542774000	-1.701295000	-0.247215000
6	1.531943000	-0.921564000	1.778065000
6	2.672198000	-1.194291000	1.042343000
9	1.193683000	-2.388054000	-2.018047000
9	3.628906000	-1.947809000	-0.958515000
9	3.869885000	-1.001237000	1.568371000
9	1.642056000	-0.425540000	2.999906000
9	-0.797416000	-0.939273000	1.985421000
6	-2.647764000	0.905662000	-0.162902000
15	-4.008500000	-0.143694000	-0.251874000
6	-4.014099000	-1.421610000	1.018824000
1	-4.891180000	-2.065340000	0.924965000
1	-3.104588000	-2.015966000	0.923964000
1	-4.010103000	-0.942794000	1.999735000
6	-4.054253000	-1.021323000	-1.817358000
1	-4.901450000	-1.709217000	-1.836521000
1	-4.139869000	-0.306130000	-2.636489000
1	-3.123742000	-1.578994000	-1.945133000
6	-5.611089000	0.674634000	-0.095811000
1	-5.706094000	1.441185000	-0.865473000
1	-6.414101000	-0.056189000	-0.207567000
1	-5.701372000	1.146464000	0.883204000

6AITS^{C-F} (T.E = -2101.787959)

7	1.098398000	2.027374000	0.193274000
6	2.265631000	2.286365000	-0.311363000
1	2.470786000	3.315930000	-0.615137000
6	0.164714000	3.102831000	0.231303000
6	-0.435812000	3.432278000	1.437319000
6	-0.193567000	3.773348000	-0.928745000
6	-1.379381000	4.441638000	1.482629000
1	-0.158939000	2.887334000	2.333186000
6	-1.138263000	4.783281000	-0.876628000
1	0.240323000	3.469525000	-1.875496000
6	-1.732241000	5.119703000	0.327531000
1	-1.846619000	4.695594000	2.426547000
1	-1.424116000	5.296722000	-1.786964000
1	-2.479616000	5.903038000	0.364309000
6	3.330056000	0.019824000	-0.185365000

13	0.447060000	0.235065000	0.677191000
9	-0.748601000	0.447854000	-1.489254000
6	-1.477171000	-0.383869000	-0.616205000
6	-1.477640000	-1.747486000	-0.967762000
6	-2.707496000	0.121792000	-0.147807000
6	-2.502771000	-2.589951000	-0.606373000
6	-3.738223000	-0.712924000	0.202929000
6	-3.652492000	-2.083557000	-0.021129000
9	-0.347519000	-2.274316000	-1.461440000
9	-2.393452000	-3.892677000	-0.828384000
9	-4.679806000	-2.877205000	0.250201000
9	-4.827420000	-0.218646000	0.769407000
9	-2.765560000	1.407675000	0.183623000
6	2.179573000	-0.579833000	0.357246000
15	2.475518000	-2.244359000	0.676083000
8	4.411530000	-0.506288000	-0.438973000
7	3.280847000	1.450280000	-0.504701000
6	4.511391000	1.986077000	-1.071787000
1	5.338676000	1.857727000	-0.375186000
1	4.765145000	1.455781000	-1.988164000
1	4.375388000	3.044446000	-1.287170000
6	3.810523000	-2.545481000	1.853013000
1	3.556431000	-2.077352000	2.804944000
1	3.950417000	-3.617952000	2.002238000
1	4.726614000	-2.102219000	1.465329000
6	2.867300000	-3.255902000	-0.763395000
1	2.035782000	-3.206414000	-1.466671000
1	3.767190000	-2.861459000	-1.233493000
1	3.029226000	-4.293071000	-0.462830000
6	1.037574000	-3.031828000	1.420702000
1	1.307635000	-4.044923000	1.724872000
1	0.708600000	-2.469802000	2.296474000
1	0.216584000	-3.088648000	0.706206000

8AITS^{C-F} (T.E = -2335.835216)

7	1.902443000	0.280215000	-0.409717000
6	2.675214000	1.390878000	0.022453000
6	2.208249000	2.776543000	-0.174881000
7	-0.319471000	2.006619000	-0.386954000
1	2.787354000	3.181238000	-1.017199000
6	-1.681367000	2.249808000	-0.115852000
6	-2.689612000	1.647374000	-0.870616000
6	-2.065212000	3.033762000	0.973105000
6	-4.024606000	1.811631000	-0.541225000
1	-2.413780000	1.045379000	-1.732439000
6	-3.398690000	3.213510000	1.285958000
1	-1.292788000	3.490943000	1.583052000
6	-4.389941000	2.599309000	0.535753000

1	-4.784061000	1.315646000	-1.135783000
1	-3.667338000	3.826105000	2.139523000
1	-5.434124000	2.727311000	0.793566000
13	0.033186000	0.190719000	-0.664505000
9	-0.037070000	-1.574923000	1.391040000
6	-1.137711000	-1.662766000	0.541686000
6	-2.353858000	-1.215122000	1.088209000
6	-1.203677000	-2.786240000	-0.299537000
6	-3.557792000	-1.647787000	0.583360000
6	-2.402632000	-3.208227000	-0.817552000
6	-3.595674000	-2.645649000	-0.381488000
9	-2.321811000	-0.218296000	1.966342000
9	-4.690220000	-1.131325000	1.029359000
9	-4.758105000	-3.125589000	-0.804430000
9	-2.429759000	-4.154454000	-1.744192000
9	-0.062422000	-3.211268000	-0.854453000
5	0.647760000	3.059514000	-0.459249000
7	0.332779000	4.400648000	-0.832165000
6	-0.900897000	4.813197000	-1.462453000
1	-1.484836000	3.959065000	-1.796048000
1	-1.530185000	5.410240000	-0.789335000
1	-0.675581000	5.431115000	-2.340127000
6	1.227297000	5.522077000	-0.688295000
1	2.113273000	5.270479000	-0.108940000
1	1.556507000	5.906699000	-1.663591000
1	0.724053000	6.349556000	-0.172035000
1	2.546313000	3.366020000	0.685948000
15	3.166863000	-0.668129000	0.100199000
6	3.836155000	0.888607000	0.537903000
6	5.064928000	1.493418000	1.093348000
1	5.942318000	1.314196000	0.464131000
1	4.945817000	2.576204000	1.178429000
1	5.304739000	1.112893000	2.091335000
7	3.040496000	-1.715555000	1.350315000
7	3.757213000	-1.529883000	-1.157474000
6	2.635746000	-3.101759000	1.173826000
1	3.320730000	-3.755667000	1.722053000
1	1.619158000	-3.254780000	1.544503000
1	2.647930000	-3.379802000	0.120806000
6	2.894970000	-1.234414000	2.714061000
1	3.251238000	-0.208296000	2.795676000
1	1.848538000	-1.265973000	3.030675000
1	3.482726000	-1.866458000	3.385606000
6	3.022043000	-1.839317000	-2.368796000
1	2.817954000	-2.915508000	-2.425995000
1	2.069590000	-1.311498000	-2.385521000
1	3.603400000	-1.548621000	-3.248974000
6	5.024979000	-2.215018000	-1.017940000
1	5.662046000	-1.999245000	-1.880816000

1	5.548420000	-1.884708000	-0.118666000
1	4.890210000	-3.301983000	-0.955186000

10AITS^{C-F} (T.E = -2427.336982)

7	-1.664604000	0.605944000	0.059141000
6	-2.691601000	1.596130000	0.183817000
6	-2.401085000	2.956854000	0.256908000
13	0.180546000	0.799940000	0.210416000
9	1.526311000	-0.115818000	-2.062325000
6	1.816975000	-0.872427000	-0.947571000
6	3.102420000	-0.734866000	-0.398881000
6	1.267641000	-2.163726000	-0.895623000
6	3.640126000	-1.700169000	0.415512000
6	1.798986000	-3.133952000	-0.082271000
6	2.992386000	-2.915512000	0.591412000
9	3.663277000	0.483030000	-0.415854000
9	4.782122000	-1.472764000	1.047834000
9	3.563501000	-3.891562000	1.287382000
9	1.163441000	-4.289439000	0.068250000
9	0.052542000	-2.355064000	-1.421716000
15	-2.884159000	-0.527593000	0.097960000
6	-3.886751000	0.864934000	0.206425000
6	-5.304315000	1.271510000	0.329685000
1	-5.658772000	1.324091000	1.367395000
1	-5.456870000	2.262602000	-0.107061000
1	-5.972186000	0.588106000	-0.200251000
7	-2.831435000	-1.522483000	-1.208256000
7	-2.864116000	-1.571051000	1.382153000
6	-3.455659000	-2.825074000	-1.284967000
1	-4.316198000	-2.804533000	-1.963727000
1	-2.738248000	-3.560221000	-1.667095000
1	-3.798836000	-3.150350000	-0.304900000
6	-2.500133000	-0.952000000	-2.501032000
1	-1.934395000	-0.029300000	-2.376413000
1	-1.877355000	-1.655868000	-3.058966000
1	-3.403420000	-0.740987000	-3.085013000
6	-1.746894000	-2.501823000	1.499102000
1	-2.051124000	-3.365506000	2.096437000
1	-1.422382000	-2.853103000	0.521005000
1	-0.886775000	-2.023484000	1.988115000
6	-3.263817000	-1.027640000	2.669724000
1	-2.463224000	-0.424837000	3.120675000
1	-4.149635000	-0.403179000	2.565652000
1	-3.493965000	-1.853504000	3.347236000
6	-1.114369000	3.476761000	0.219118000
1	-1.099072000	4.571429000	0.255826000
1	-3.237367000	3.640632000	0.345800000
6	0.103301000	2.797893000	0.162311000

15	1.552448000	3.689755000	0.079719000
6	2.445107000	3.457346000	-1.470851000
1	1.831471000	3.829892000	-2.292129000
1	3.403252000	3.981389000	-1.457594000
1	2.619783000	2.391142000	-1.623592000
6	2.737742000	3.215632000	1.352587000
1	2.315547000	3.434133000	2.334142000
1	2.923799000	2.142406000	1.281963000
1	3.681178000	3.750764000	1.226337000
6	1.380530000	5.481786000	0.243393000
1	2.368089000	5.943561000	0.193421000
1	0.763870000	5.879777000	-0.563182000
1	0.918202000	5.731061000	1.199137000

11AITS^{C-F} (T.E = -2345.136033)

7	-0.231374000	-1.393589000	-0.280016000
6	0.186938000	-2.737911000	-0.379574000
13	0.847846000	0.109774000	-0.594388000
9	1.181127000	1.780049000	1.373925000
6	0.091015000	2.089787000	0.571861000
6	0.189694000	3.251495000	-0.224929000
6	-1.170032000	1.858858000	1.155886000
6	-0.924549000	3.947984000	-0.616490000
6	-2.289430000	2.560797000	0.768262000
6	-2.183957000	3.614592000	-0.123175000
9	1.354896000	3.502848000	-0.804104000
9	-0.815502000	4.945014000	-1.478783000
9	-3.245984000	4.348813000	-0.429819000
9	-3.480952000	2.240590000	1.263782000
9	-1.307081000	0.790937000	1.955603000
15	-1.790280000	-1.994482000	-0.212102000
6	-0.975904000	-3.505097000	-0.362476000
6	-1.372768000	-4.931569000	-0.240458000
1	-1.428270000	-5.458620000	-1.198483000
1	-0.703852000	-5.501377000	0.408278000
1	-2.368801000	-4.991770000	0.209762000
7	-2.670701000	-1.866747000	1.163426000
7	-2.697481000	-1.373517000	-1.425797000
6	-3.779249000	-0.950460000	1.361005000
1	-4.654528000	-1.502993000	1.715958000
1	-3.522319000	-0.187411000	2.098505000
1	-4.040616000	-0.443069000	0.435180000
6	-2.158442000	-2.429450000	2.401788000
1	-2.972149000	-2.914302000	2.948172000
1	-1.387792000	-3.171193000	2.193115000
1	-1.730293000	-1.644908000	3.033591000
6	-2.629426000	0.008464000	-1.860480000
1	-3.494064000	0.586524000	-1.507386000

1	-1.723099000	0.494495000	-1.489071000
1	-2.609455000	0.053795000	-2.952932000
6	-3.862590000	-2.109998000	-1.870439000
1	-3.915455000	-2.092806000	-2.962731000
1	-3.798698000	-3.153396000	-1.553563000
1	-4.793857000	-1.685175000	-1.474756000
6	2.634341000	-2.221078000	-0.245104000
8	3.688929000	-2.782249000	-0.071385000
6	3.567664000	-0.069158000	-0.061570000
6	3.936774000	0.860096000	-1.022527000
6	4.256826000	-0.114093000	1.143563000
6	4.977339000	1.742470000	-0.780617000
1	3.400082000	0.888285000	-1.965261000
6	5.300999000	0.758807000	1.376796000
1	3.962911000	-0.837393000	1.894740000
6	5.663440000	1.693337000	0.418093000
1	5.250133000	2.468677000	-1.537272000
1	5.832479000	0.716260000	2.320547000
1	6.477857000	2.382036000	0.609398000
7	2.420920000	-0.888112000	-0.292793000
7	1.483146000	-3.076340000	-0.471554000
6	1.801646000	-4.486987000	-0.647545000
1	1.882469000	-5.006038000	0.309977000
1	1.027207000	-4.953108000	-1.252855000
1	2.758803000	-4.569787000	-1.152774000

13AITS^{C-F} (T.E = -2670.691503)

7	-0.510759000	-1.688743000	-0.169840000
6	0.208108000	-2.934840000	-0.281160000
6	1.592992000	-2.999726000	-0.354915000
7	1.896311000	-0.523816000	-0.278890000
1	2.067165000	-3.972597000	-0.422641000
6	2.405204000	-1.874256000	-0.316805000
13	0.127668000	0.038905000	-0.404529000
9	-0.150630000	1.464434000	1.849258000
6	-0.882572000	2.004276000	0.802735000
6	-0.409405000	3.197189000	0.231234000
6	-2.277695000	1.866237000	0.881052000
6	-1.246593000	4.030173000	-0.469246000
6	-3.118316000	2.695802000	0.178958000
6	-2.614606000	3.792744000	-0.504402000
9	0.911429000	3.346224000	0.101212000
9	-0.750166000	5.065681000	-1.128374000
9	-3.433823000	4.653572000	-1.094126000
9	-4.420950000	2.448979000	0.154851000
9	-2.772640000	0.744530000	1.417648000
15	3.466149000	-0.035238000	-0.091358000
6	3.795184000	-1.711165000	-0.276770000

6	4.896495000	-2.694723000	-0.164175000
1	5.060797000	-3.256355000	-1.089850000
1	5.841544000	-2.202602000	0.077136000
1	4.707164000	-3.431389000	0.626656000
7	3.844486000	1.174637000	-1.146223000
7	3.893956000	0.612514000	1.370433000
6	5.049760000	1.971886000	-1.046318000
1	5.786640000	1.662825000	-1.797124000
1	4.813834000	3.027341000	-1.219170000
1	5.500140000	1.874761000	-0.060561000
6	3.264808000	1.178289000	-2.475935000
1	3.986456000	0.826409000	-3.222278000
1	2.384501000	0.538995000	-2.511850000
1	2.959377000	2.195612000	-2.739329000
6	3.374573000	1.917271000	1.761881000
1	2.411868000	1.816199000	2.277015000
1	4.083293000	2.406345000	2.436301000
1	3.217900000	2.554610000	0.894611000
6	3.970117000	-0.301720000	2.498498000
1	2.971113000	-0.548188000	2.884164000
1	4.469962000	-1.226566000	2.216302000
1	4.539359000	0.173176000	3.301329000
15	-1.899478000	-2.590700000	-0.126795000
6	-0.801064000	-3.905864000	-0.267452000
6	-0.763209000	-5.383321000	-0.342212000
1	-0.869462000	-5.773844000	-1.362208000
1	0.188590000	-5.759606000	0.043268000
1	-1.551261000	-5.843817000	0.258854000
7	-2.777622000	-2.283856000	1.229346000
7	-2.983302000	-2.321122000	-1.350679000
6	-2.624530000	-2.850315000	-2.656459000
1	-3.515321000	-2.870508000	-3.288921000
1	-1.864686000	-2.228821000	-3.150796000
1	-2.236397000	-3.863776000	-2.566895000
6	-3.590280000	-0.997317000	-1.442478000
1	-4.527138000	-1.062284000	-2.002012000
1	-3.803328000	-0.590308000	-0.454759000
1	-2.923030000	-0.292445000	-1.959117000
6	-4.194070000	-2.527712000	1.387051000
1	-4.686236000	-1.630979000	1.781474000
1	-4.652497000	-2.787131000	0.434953000
1	-4.370463000	-3.349372000	2.090807000
6	-2.067906000	-2.106439000	2.482644000
1	-2.533486000	-1.299065000	3.054121000
1	-2.091561000	-3.022312000	3.084300000
1	-1.029760000	-1.831459000	2.296959000

1GaTS^{C-F} (T.E = -3440.794017)

7	1.347540000	-2.220528000	-0.018215000
6	1.095966000	-3.344742000	-0.657612000
6	-0.151276000	-3.841333000	-0.999987000
7	-1.544680000	-2.120313000	-0.033622000
1	-0.181963000	-4.793171000	-1.510655000
1	1.960669000	-3.958485000	-0.918854000
6	2.690578000	-1.850992000	0.230260000
6	3.033703000	-1.360351000	1.483710000
6	3.653753000	-1.914542000	-0.768797000
6	4.327828000	-0.945751000	1.737063000
1	2.276836000	-1.316448000	2.260481000
6	4.947792000	-1.503146000	-0.507510000
1	3.372450000	-2.243934000	-1.762841000
6	5.289608000	-1.017428000	0.743440000
1	4.586068000	-0.565404000	2.718165000
1	5.690114000	-1.543044000	-1.295920000
1	6.301796000	-0.685948000	0.940540000
6	-2.862043000	-1.648979000	0.179508000
6	-3.218492000	-1.184602000	1.438731000
6	-3.781258000	-1.592530000	-0.860566000
6	-4.485946000	-0.678370000	1.657666000
1	-2.493793000	-1.232505000	2.245187000
6	-5.048935000	-1.088404000	-0.633927000
1	-3.481438000	-1.904386000	-1.854971000
6	-5.405513000	-0.630314000	0.623305000
1	-4.756541000	-0.319028000	2.643332000
1	-5.756996000	-1.035104000	-1.452481000
1	-6.396028000	-0.226620000	0.794266000
6	-1.365093000	-3.254029000	-0.678660000
1	-2.268429000	-3.797836000	-0.963705000
9	-0.087548000	0.110247000	-1.556783000
6	0.038721000	1.192650000	-0.401106000
6	-1.096912000	1.997144000	-0.285977000
6	1.271135000	1.849530000	-0.430660000
6	-1.005038000	3.359705000	-0.099526000
6	1.371978000	3.211629000	-0.244627000
6	0.232234000	3.984418000	-0.087666000
9	-2.292913000	1.414455000	-0.243340000
9	-2.102513000	4.077839000	0.069454000
9	0.322879000	5.297791000	0.057712000
9	2.562068000	3.787609000	-0.220890000
9	2.382198000	1.124948000	-0.542622000
31	-0.055712000	-0.862760000	0.381490000

6GaTS^{C-F} (T.E = -3784.170554)

7	1.151094000	1.983720000	0.082339000
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6	2.350990000	2.214105000	-0.336135000
1	2.606036000	3.242562000	-0.605523000
6	0.244345000	3.078391000	0.112297000
6	-0.360169000	3.418388000	1.312575000
6	-0.081930000	3.759944000	-1.050272000
6	-1.272774000	4.455558000	1.352421000
1	-0.112190000	2.858154000	2.207620000
6	-0.998409000	4.795756000	-1.004071000
1	0.354213000	3.444081000	-1.991835000
6	-1.593132000	5.146832000	0.195633000
1	-1.744516000	4.718536000	2.291569000
1	-1.261430000	5.319040000	-1.915667000
1	-2.317640000	5.951574000	0.227239000
6	3.371661000	-0.076029000	-0.187093000
9	-0.854428000	0.461359000	-1.532353000
6	-1.514143000	-0.375644000	-0.487953000
6	-1.653248000	-1.715358000	-0.904605000
6	-2.686609000	0.183371000	0.061647000
6	-2.779887000	-2.466945000	-0.661973000
6	-3.819524000	-0.555960000	0.299928000
6	-3.891742000	-1.894201000	-0.067224000
9	-0.565592000	-2.327631000	-1.418327000
9	-2.803579000	-3.746616000	-1.012089000
9	-5.014431000	-2.587910000	0.096783000
9	-4.859804000	0.008094000	0.896602000
9	-2.613841000	1.430597000	0.537548000
6	2.199653000	-0.690486000	0.294264000
15	2.445180000	-2.365621000	0.601998000
8	4.450505000	-0.625188000	-0.398006000
7	3.359609000	1.351041000	-0.483635000
6	4.629763000	1.870525000	-0.977311000
1	5.419192000	1.704337000	-0.245825000
1	4.915368000	1.360093000	-1.895688000
1	4.528362000	2.936999000	-1.169477000
6	3.761298000	-2.717832000	1.783307000
1	3.524956000	-2.235776000	2.732795000
1	3.849254000	-3.795269000	1.936231000
1	4.698224000	-2.318049000	1.398879000
6	2.806982000	-3.365965000	-0.851241000
1	1.971403000	-3.288318000	-1.547753000
1	3.711465000	-2.983091000	-1.322929000
1	2.950772000	-4.410690000	-0.568563000
6	0.972156000	-3.096293000	1.332477000
1	1.184708000	-4.132468000	1.601580000
1	0.688939000	-2.546299000	2.231422000
1	0.143935000	-3.081134000	0.624127000
31	0.429861000	0.111233000	0.437466000

8GaTS^{C-F} (T.E = -4018.210894)

7	0.957417000	-1.425861000	-0.825717000
6	2.380281000	-1.470765000	-0.852426000
6	3.111145000	-0.467866000	-1.620068000
7	1.615175000	1.438739000	-0.718640000
1	2.652525000	-0.387935000	-2.613743000
6	1.289811000	2.635920000	-0.048155000
6	0.653785000	3.679586000	-0.714683000
6	1.559619000	2.782300000	1.310751000
6	0.336370000	4.851818000	-0.052249000
1	0.423805000	3.557867000	-1.768630000
6	1.244946000	3.955843000	1.970897000
1	2.034578000	1.957870000	1.834599000
6	0.637029000	4.999747000	1.291359000
1	-0.155735000	5.654419000	-0.589657000
1	1.469404000	4.054344000	3.027145000
1	0.386441000	5.917315000	1.809965000
9	-0.987368000	0.155793000	1.191772000
6	-1.992379000	0.340318000	0.125495000
6	-2.703866000	1.549782000	0.237042000
6	-2.784459000	-0.791466000	-0.130662000
6	-4.048201000	1.638304000	-0.039375000
6	-4.129243000	-0.711164000	-0.413455000
6	-4.786317000	0.505860000	-0.357054000
9	-2.019195000	2.663150000	0.480943000
9	-4.654170000	2.813841000	0.012243000
9	-6.096296000	0.582755000	-0.557205000
9	-4.798836000	-1.807215000	-0.741668000
9	-2.161615000	-1.970138000	-0.317836000
5	2.945402000	0.998298000	-0.951796000
7	4.134257000	1.752089000	-0.709132000
6	4.209402000	3.191416000	-0.590942000
1	3.289110000	3.672064000	-0.912425000
1	4.415868000	3.510826000	0.439312000
1	5.023698000	3.568376000	-1.222151000
6	5.439015000	1.162866000	-0.533642000
1	5.385901000	0.081483000	-0.415310000
1	6.113459000	1.389229000	-1.371338000
1	5.910504000	1.560269000	0.373956000
1	4.149998000	-0.762156000	-1.760614000
15	1.047235000	-2.671578000	0.270438000
6	2.766486000	-2.485000000	-0.026330000
6	4.075179000	-3.050888000	0.364524000
1	4.278129000	-2.938992000	1.434913000
1	4.158647000	-4.116902000	0.134364000
1	4.879848000	-2.540575000	-0.171377000
7	0.629555000	-2.464042000	1.839719000
7	0.187455000	-3.970003000	-0.233230000
6	-0.701461000	-2.716487000	2.371033000

1	-0.619081000	-3.289618000	3.299681000
1	-1.210318000	-1.772227000	2.579737000
1	-1.307201000	-3.272137000	1.659689000
6	1.404182000	-1.543644000	2.658810000
1	2.402388000	-1.404634000	2.243933000
1	0.910941000	-0.567112000	2.711333000
1	1.495847000	-1.944895000	3.671765000
6	-0.323858000	-4.091606000	-1.586068000
1	-1.344526000	-4.483305000	-1.552804000
1	-0.341624000	-3.119114000	-2.071487000
1	0.293447000	-4.776845000	-2.177866000
6	0.241668000	-5.223598000	0.492867000
1	0.829920000	-5.966518000	-0.057612000
1	0.692791000	-5.086912000	1.475578000
1	-0.768116000	-5.623307000	0.632015000
31	0.024352000	0.335210000	-0.957921000

10GaTS^{C-F} (T.E = -4109.721909)

7	-0.133363000	-1.697098000	0.015035000
6	0.309357000	-3.002463000	-0.333836000
6	1.656635000	-3.308670000	-0.534943000
9	0.789790000	2.138653000	2.090848000
6	-0.008478000	2.138517000	0.962602000
6	0.368236000	3.037657000	-0.056276000
6	-1.398080000	2.049339000	1.186190000
6	-0.541830000	3.605343000	-0.914318000
6	-2.313877000	2.631523000	0.342870000
6	-1.904409000	3.420904000	-0.721678000
9	1.676699000	3.133935000	-0.340500000
9	-0.120813000	4.348401000	-1.928175000
9	-2.793356000	4.059862000	-1.477248000
9	-3.612962000	2.428334000	0.541990000
9	-1.831589000	1.186436000	2.113404000
15	-1.684128000	-2.283233000	-0.120556000
6	-0.865324000	-3.767599000	-0.418634000
6	-1.107700000	-5.173459000	-0.814569000
1	-1.055609000	-5.340315000	-1.898973000
1	-0.371615000	-5.841231000	-0.356537000
1	-2.090327000	-5.517999000	-0.485521000
7	-2.586428000	-1.925827000	1.203290000
7	-2.564231000	-1.648619000	-1.374001000
6	-4.020780000	-1.739858000	1.237474000
1	-4.493672000	-2.519140000	1.845198000
1	-4.263714000	-0.766488000	1.679650000
1	-4.440911000	-1.782544000	0.234926000
6	-1.974153000	-2.057323000	2.512876000
1	-0.896463000	-2.186735000	2.418596000
1	-2.157609000	-1.153329000	3.099796000

1	-2.386358000	-2.918937000	3.049190000
6	-2.765585000	-0.205856000	-1.357656000
1	-3.642516000	0.058801000	-1.954194000
1	-2.924656000	0.148349000	-0.340724000
1	-1.892040000	0.320875000	-1.767683000
6	-2.258530000	-2.145502000	-2.705293000
1	-1.300773000	-1.754326000	-3.076243000
1	-2.213544000	-3.233087000	-2.710898000
1	-3.047593000	-1.825270000	-3.389830000
6	2.692765000	-2.397720000	-0.399213000
1	3.674733000	-2.839526000	-0.602173000
1	1.895381000	-4.328978000	-0.812847000
6	2.647272000	-1.050498000	-0.042343000
15	4.068265000	-0.113642000	-0.016102000
6	4.134961000	0.971819000	1.417948000
1	4.137976000	0.371020000	2.327982000
1	5.028754000	1.597837000	1.383401000
1	3.249381000	1.611230000	1.429633000
6	4.229746000	1.009208000	-1.422065000
1	4.262202000	0.426728000	-2.343687000
1	3.353900000	1.660189000	-1.449827000
1	5.130705000	1.621395000	-1.340929000
6	5.616170000	-1.047454000	0.000774000
1	6.459613000	-0.357264000	0.058246000
1	5.637379000	-1.716245000	0.861880000
1	5.710221000	-1.640931000	-0.909398000
31	0.906751000	-0.101984000	0.387349000

$^{11}\text{GaTS}^{\text{C-F}}$ (T.E = -4027.513195)

7	-0.017014000	-1.305803000	0.054353000
6	0.608711000	-2.534520000	-0.199410000
9	0.844876000	2.867504000	0.748719000
6	-0.383798000	1.888332000	0.337127000
6	-0.905870000	2.210381000	-0.935373000
6	-1.373550000	1.833248000	1.342492000
6	-2.213298000	2.575088000	-1.155494000
6	-2.679617000	2.217160000	1.147917000
6	-3.124443000	2.603268000	-0.108819000
9	-0.089588000	2.046595000	-2.002202000
9	-2.621978000	2.878675000	-2.383766000
9	-4.366393000	3.053403000	-0.291493000
9	-3.543762000	2.170175000	2.157993000
9	-1.028654000	1.288503000	2.529720000
15	-1.485180000	-2.082624000	-0.157300000
6	-0.423758000	-3.429590000	-0.458791000
6	-0.584723000	-4.857121000	-0.839145000
1	0.088552000	-5.156212000	-1.644971000
1	-0.430107000	-5.553924000	-0.007339000

1	-1.600333000	-5.027372000	-1.203149000
7	-2.478068000	-2.239818000	1.128517000
7	-2.365310000	-1.323158000	-1.301365000
6	-3.171002000	-1.084564000	1.691118000
1	-4.195722000	-1.358155000	1.955997000
1	-2.655445000	-0.730614000	2.588747000
1	-3.200455000	-0.261018000	0.978648000
6	-2.269803000	-3.307747000	2.092760000
1	-3.233978000	-3.584419000	2.526167000
1	-1.839905000	-4.185578000	1.614298000
1	-1.607321000	-2.988762000	2.904907000
6	-1.707280000	-0.765063000	-2.474753000
1	-2.053585000	0.257805000	-2.641453000
1	-0.627179000	-0.739490000	-2.343879000
1	-1.937817000	-1.365019000	-3.360303000
6	-3.811058000	-1.377326000	-1.427650000
1	-4.087994000	-1.866609000	-2.366388000
1	-4.257980000	-1.931635000	-0.606101000
1	-4.220337000	-0.361257000	-1.433976000
6	2.965070000	-1.640847000	-0.144839000
8	4.097514000	-2.010466000	-0.319827000
6	3.637995000	0.634927000	0.045619000
6	3.513539000	1.732401000	-0.790540000
6	4.719926000	0.545572000	0.910268000
6	4.464243000	2.737942000	-0.765261000
1	2.659278000	1.806670000	-1.456789000
6	5.672417000	1.545763000	0.923181000
1	4.811882000	-0.310512000	1.566687000
6	5.548664000	2.644528000	0.086869000
1	4.349518000	3.597327000	-1.414503000
1	6.516033000	1.470399000	1.599335000
1	6.294905000	3.429837000	0.106760000
7	2.590787000	-0.344082000	0.051439000
7	1.948844000	-2.672748000	-0.150540000
6	2.482658000	-4.024238000	-0.294782000
1	1.767961000	-4.731306000	0.117447000
1	2.681560000	-4.267495000	-1.340350000
1	3.418235000	-4.096094000	0.250391000
31	0.856856000	0.349888000	0.300820000

Cartesian coordinates of the van der Waals complexes involved in the pinacolborane activation by some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1Alv^{B-H} (T.E = -1342.445710)

7	-0.270045000	-2.047008000	0.461422000
6	0.003896000	-2.254866000	1.734579000
6	1.205316000	-1.977859000	2.365371000
7	2.382702000	-1.106414000	0.456666000
1	1.295264000	-2.227332000	3.412997000
1	-0.781720000	-2.702131000	2.347627000
6	-1.592397000	-2.303910000	0.031055000
6	-1.799920000	-2.919991000	-1.199399000
6	-2.694735000	-1.902475000	0.781253000
6	-3.084584000	-3.141972000	-1.662543000
1	-0.942337000	-3.233932000	-1.784068000
6	-3.976385000	-2.141389000	0.319535000
1	-2.539153000	-1.356468000	1.704671000
6	-4.178313000	-2.758682000	-0.904555000
1	-3.229793000	-3.626377000	-2.620992000
1	-4.825558000	-1.823023000	0.914048000
1	-5.183622000	-2.935521000	-1.267665000
6	3.562876000	-0.459008000	0.017437000
6	4.177067000	-0.884037000	-1.155573000
6	4.089576000	0.628636000	0.706424000
6	5.313978000	-0.245739000	-1.616006000
1	3.761493000	-1.729586000	-1.692416000
6	5.229739000	1.260067000	0.243001000
1	3.580115000	0.994496000	1.591701000
6	5.847087000	0.824930000	-0.917628000
1	5.788724000	-0.591067000	-2.526933000
1	5.628584000	2.109309000	0.785644000
1	6.736559000	1.324880000	-1.281895000
6	2.306993000	-1.426279000	1.733087000
1	3.195900000	-1.254469000	2.344759000
13	0.898004000	-1.118110000	-0.885149000
1	0.714976000	1.081544000	1.243487000
6	-1.545429000	3.205544000	-0.124766000
6	-2.335359000	1.866660000	-0.015238000
5	-0.236606000	1.605244000	0.762238000
8	-0.182308000	2.785649000	0.093899000
8	-1.492168000	1.088040000	0.864926000
6	-1.876392000	4.188926000	0.981886000
1	-1.148189000	5.001277000	0.956919000
1	-2.872731000	4.617146000	0.854255000

1	-1.822563000	3.717206000	1.965358000
6	-1.637667000	3.887322000	-1.467390000
1	-2.676172000	4.141354000	-1.697250000
1	-1.058764000	4.812400000	-1.448091000
1	-1.245220000	3.258919000	-2.265779000
6	-3.706487000	1.986453000	0.604001000
1	-4.339536000	2.646301000	0.004422000
1	-4.178396000	1.002149000	0.632175000
1	-3.662930000	2.373391000	1.621610000
6	-2.427156000	1.112539000	-1.327391000
1	-2.834432000	0.117318000	-1.135214000
1	-3.088644000	1.621089000	-2.031597000
1	-1.445884000	0.985555000	-1.792087000

4Alv^{B-H} (T.E = -1555.222802)

7	-1.680043000	-1.219837000	0.642986000
6	-1.308771000	-0.685153000	1.803377000
6	-0.053861000	-0.720392000	2.371820000
6	1.084902000	-1.228502000	1.731722000
6	1.109576000	-1.800119000	0.481652000
6	-2.992664000	-0.913698000	0.209623000
6	-3.819791000	-1.925708000	-0.269239000
6	-3.465677000	0.396169000	0.219560000
6	-5.098341000	-1.634620000	-0.707301000
1	-3.447272000	-2.943978000	-0.286045000
6	-4.748497000	0.679595000	-0.215379000
1	-2.799224000	1.192961000	0.532749000
6	-5.571481000	-0.332504000	-0.679049000
1	-5.733037000	-2.435222000	-1.069816000
1	-5.101369000	1.704946000	-0.205879000
1	-6.573714000	-0.107569000	-1.024437000
1	-2.088268000	-0.172050000	2.371994000
15	2.620250000	-2.219068000	-0.211833000
6	4.089297000	-1.843231000	0.772079000
1	4.983966000	-2.143595000	0.223909000
1	4.135868000	-0.771063000	0.970735000
1	4.057375000	-2.377880000	1.722105000
6	2.728882000	-3.975463000	-0.599268000
1	2.673970000	-4.555403000	0.322655000
1	1.872526000	-4.238782000	-1.225467000
1	3.656650000	-4.204659000	-1.127429000
6	2.872881000	-1.387757000	-1.787722000
1	2.849854000	-0.304443000	-1.642736000
1	3.820303000	-1.689056000	-2.239331000
1	2.048155000	-1.659560000	-2.452172000
1	2.009790000	-1.107806000	2.309034000
1	0.052120000	-0.288379000	3.359545000
13	-0.567728000	-2.249233000	-0.644588000

1	-0.001504000	0.303253000	-1.954595000
6	1.719986000	2.702781000	-0.273243000
6	0.233013000	2.995805000	0.095954000
5	0.352189000	1.209149000	-1.276174000
8	1.592513000	1.773000000	-1.370134000
8	-0.441219000	1.805191000	-0.350261000
6	2.478964000	1.978583000	0.821195000
1	3.434898000	1.640244000	0.411930000
1	2.685613000	2.632458000	1.670788000
1	1.925534000	1.106144000	1.175387000
6	2.507005000	3.904270000	-0.736466000
1	2.550304000	4.659541000	0.053081000
1	3.529631000	3.603617000	-0.972177000
1	2.074028000	4.355783000	-1.628158000
6	-0.034293000	3.177025000	1.570176000
1	0.527471000	4.028041000	1.965159000
1	-1.097703000	3.373680000	1.723887000
1	0.225018000	2.282376000	2.135810000
6	-0.365736000	4.147792000	-0.688114000
1	-1.445045000	4.153628000	-0.525535000
1	0.036046000	5.109645000	-0.363033000
1	-0.188612000	4.037530000	-1.759959000

6Alv^{B-H} (T.E = -1685.805279)

6	-1.461328000	1.288507000	1.302115000
6	-1.445426000	1.368878000	-0.101373000
6	1.031784000	1.213823000	1.453302000
1	1.835712000	1.085330000	2.182726000
13	0.081099000	1.467046000	-1.390915000
7	1.352722000	1.431798000	0.219089000
15	-3.057734000	1.498518000	-0.672336000
6	-4.173920000	0.146969000	-0.224347000
1	-4.191784000	0.052926000	0.860613000
1	-5.180113000	0.346613000	-0.598598000
1	-3.805895000	-0.780970000	-0.664532000
6	-3.930902000	2.999664000	-0.172067000
1	-3.377967000	3.865252000	-0.539593000
1	-4.943630000	3.014312000	-0.580377000
1	-3.968848000	3.032724000	0.916230000
6	-3.114552000	1.524680000	-2.472456000
1	-2.681879000	0.607611000	-2.876181000
1	-4.154060000	1.609725000	-2.796146000
1	-2.539880000	2.366158000	-2.861569000
8	-2.436875000	1.299907000	2.059091000
7	-0.186010000	1.147208000	1.992058000
6	-0.287184000	0.965850000	3.431883000
1	-0.743080000	1.837973000	3.899873000
1	-0.917159000	0.106268000	3.658674000

1	0.708135000	0.807295000	3.843956000
6	2.744063000	1.433570000	-0.068903000
6	3.255873000	2.430048000	-0.890542000
6	3.592138000	0.445846000	0.418417000
6	4.603949000	2.452410000	-1.196304000
1	2.583877000	3.185173000	-1.282670000
6	4.941280000	0.476260000	0.110910000
1	3.178274000	-0.369288000	1.002248000
6	5.452592000	1.479232000	-0.694279000
1	4.993889000	3.237774000	-1.833195000
1	5.592959000	-0.302471000	0.490137000
1	6.507739000	1.496400000	-0.939981000
6	-0.392451000	-3.246268000	-0.774204000
6	0.118583000	-2.783729000	0.621066000
5	1.430431000	-1.945708000	-1.016021000
8	0.717730000	-2.925459000	-1.632951000
8	1.038819000	-1.726581000	0.276440000
6	-1.577005000	-2.438808000	-1.269954000
1	-1.726646000	-2.652497000	-2.329957000
1	-2.489195000	-2.705425000	-0.730130000
1	-1.401482000	-1.364476000	-1.157056000
6	-0.691688000	-4.721409000	-0.883268000
1	-1.471525000	-5.006842000	-0.171723000
1	-1.051480000	-4.947447000	-1.888560000
1	0.192163000	-5.330379000	-0.696523000
6	-0.948510000	-2.237715000	1.537699000
1	-1.709999000	-2.997347000	1.734082000
1	-0.501080000	-1.958390000	2.494508000
1	-1.432331000	-1.354267000	1.119566000
6	0.930119000	-3.843362000	1.342000000
1	1.422692000	-3.382238000	2.200054000
1	0.297767000	-4.655198000	1.707125000
1	1.701932000	-4.265430000	0.695048000
1	2.323608000	-1.362364000	-1.527850000

8Alv^{B-H} (T.E = -1919.853489)

7	-1.318717000	0.378955000	0.047979000
6	-1.316948000	1.096316000	1.280364000
6	-0.139891000	1.034307000	2.155665000
15	-2.908144000	0.854640000	-0.071135000
6	-2.534089000	1.711089000	1.410985000
6	-3.177643000	2.487622000	2.493235000
1	-4.039897000	1.970666000	2.926387000
1	-2.465712000	2.661790000	3.303769000
1	-3.529651000	3.467454000	2.155946000
7	-3.445363000	1.747118000	-1.335839000
7	-3.895204000	-0.466208000	-0.057864000
6	-3.593895000	1.149621000	-2.656713000

1	-2.692804000	1.324961000	-3.255998000
1	-3.746061000	0.073808000	-2.578029000
1	-4.458891000	1.593280000	-3.159245000
6	-3.156545000	3.171662000	-1.386454000
1	-3.973665000	3.681535000	-1.904786000
1	-3.068363000	3.580779000	-0.380700000
1	-2.218211000	3.360918000	-1.922656000
6	-5.333401000	-0.320509000	-0.180187000
1	-5.741762000	-1.182932000	-0.714996000
1	-5.815550000	-0.273959000	0.804704000
1	-5.588614000	0.581460000	-0.733530000
6	-3.507900000	-1.626781000	0.727343000
1	-2.424607000	-1.699538000	0.796137000
1	-3.932268000	-1.577197000	1.738243000
1	-3.874462000	-2.534490000	0.240817000
13	0.008545000	1.021669000	-1.321696000
6	2.563893000	1.746246000	-0.559066000
6	3.208147000	2.874982000	-0.043910000
6	3.112706000	1.154337000	-1.700701000
6	4.366619000	3.361961000	-0.617231000
1	2.780749000	3.361536000	0.827298000
6	4.267158000	1.652863000	-2.280878000
1	2.629103000	0.275915000	-2.117712000
6	4.908703000	2.753011000	-1.739871000
1	4.848240000	4.234181000	-0.188365000
1	4.671264000	1.167816000	-3.162710000
1	5.815798000	3.138247000	-2.190166000
7	1.381846000	1.256109000	0.015995000
5	1.292986000	0.998708000	1.417622000
7	2.396772000	0.655974000	2.265683000
6	3.718962000	0.271330000	1.829791000
1	3.798290000	0.228159000	0.747139000
1	4.483461000	0.971167000	2.192335000
1	3.969218000	-0.722896000	2.227021000
6	2.292065000	0.519622000	3.697373000
1	1.381454000	0.967139000	4.089570000
1	2.313334000	-0.536147000	4.008240000
1	3.137433000	1.014450000	4.191355000
1	-0.184217000	1.855041000	2.880580000
1	-0.245310000	0.114047000	2.749173000
6	0.486939000	-3.492832000	0.353088000
6	1.392365000	-3.080538000	-0.844280000
5	-0.757032000	-2.554120000	-1.276010000
8	0.518264000	-2.227406000	-1.614509000
8	-0.837657000	-3.410553000	-0.218049000
6	0.526173000	-2.497184000	1.495937000
1	-0.264634000	-2.746097000	2.208047000
1	1.482900000	-2.514789000	2.023521000
1	0.349522000	-1.483875000	1.131870000

6	0.716605000	-4.890722000	0.870940000
1	1.743222000	-4.997675000	1.231881000
1	0.042446000	-5.087417000	1.706616000
1	0.535625000	-5.644174000	0.105178000
6	2.624394000	-2.300282000	-0.461347000
1	3.247687000	-2.875338000	0.229584000
1	3.218918000	-2.083372000	-1.351090000
1	2.361882000	-1.350482000	0.004527000
6	1.763679000	-4.242771000	-1.744474000
1	2.208608000	-3.845573000	-2.658124000
1	2.491698000	-4.902126000	-1.267245000
1	0.887417000	-4.831970000	-2.023447000
1	-1.711047000	-2.158596000	-1.858974000

10Alv^{B-H} (T.E = -2011.352129)

7	1.529648000	0.672356000	0.005961000
6	1.326445000	0.276608000	-1.351433000
6	0.234512000	0.711539000	-2.091448000
6	-0.794652000	1.483777000	-1.547615000
1	0.164527000	0.388726000	-3.124856000
1	-1.602195000	1.675941000	-2.265897000
15	2.940611000	-0.196784000	-0.057270000
6	2.405844000	-0.578680000	-1.641980000
6	2.785342000	-1.299573000	-2.877326000
1	3.551555000	-2.052896000	-2.681589000
1	1.925701000	-1.828614000	-3.305248000
1	3.177041000	-0.642742000	-3.666188000
6	-0.901238000	1.981761000	-0.258025000
15	-2.304229000	2.849193000	0.165509000
6	-2.023049000	4.630624000	0.316825000
1	-2.920258000	5.154314000	0.654405000
1	-1.217006000	4.783584000	1.038277000
1	-1.702328000	5.028538000	-0.646751000
6	-2.947216000	2.380064000	1.780136000
1	-3.751839000	3.053438000	2.082852000
1	-3.316690000	1.355157000	1.725321000
1	-2.134014000	2.425374000	2.509483000
6	-3.720490000	2.685596000	-0.948446000
1	-3.471808000	3.033509000	-1.951395000
1	-4.006362000	1.632679000	-0.994275000
1	-4.559109000	3.271204000	-0.567475000
7	4.357088000	0.660661000	0.058300000
7	3.063251000	-1.246291000	1.213911000
6	4.664614000	1.342621000	1.307756000
1	4.210408000	2.341535000	1.332621000
1	4.279443000	0.784986000	2.160020000
1	5.748891000	1.446240000	1.413649000
6	4.750715000	1.439816000	-1.102394000

1	5.809993000	1.696430000	-1.016681000
1	4.601248000	0.868412000	-2.017059000
1	4.175207000	2.372942000	-1.177860000
6	4.286202000	-1.940257000	1.553998000
1	4.419253000	-1.949587000	2.641466000
1	4.258420000	-2.982039000	1.210807000
1	5.148361000	-1.451000000	1.104518000
6	1.871219000	-1.899591000	1.720350000
1	0.975784000	-1.370250000	1.400854000
1	1.806387000	-2.937066000	1.369518000
1	1.889095000	-1.906544000	2.814436000
13	0.566804000	1.817881000	1.184766000
1	-1.862618000	-0.585981000	2.631789000
6	-1.978255000	-2.780383000	0.047858000
6	-3.208188000	-1.858215000	-0.214730000
5	-2.126254000	-1.210190000	1.659429000
8	-2.979988000	-0.761218000	0.695937000
8	-1.624293000	-2.447651000	1.408244000
6	-3.297789000	-1.318225000	-1.621362000
1	-3.384694000	-2.137168000	-2.340638000
1	-4.190245000	-0.694943000	-1.718552000
1	-2.425442000	-0.716035000	-1.879148000
6	-4.528887000	-2.483112000	0.190997000
1	-5.303286000	-1.714248000	0.162462000
1	-4.819410000	-3.286849000	-0.488555000
1	-4.486940000	-2.882123000	1.206620000
6	-2.267722000	-4.259009000	-0.035555000
1	-2.609127000	-4.524136000	-1.040037000
1	-1.353520000	-4.819157000	0.168221000
1	-3.023423000	-4.571006000	0.684666000
6	-0.776791000	-2.433635000	-0.806954000
1	0.086853000	-2.999363000	-0.452404000
1	-0.937344000	-2.684520000	-1.858104000
1	-0.532776000	-1.370868000	-0.746520000

11Alv^{B-H} (T.E = -1929.156912)

7	-0.764098000	1.097332000	-0.074531000
6	-1.808913000	2.019561000	-0.235997000
6	-3.585020000	0.260623000	-0.325427000
15	0.248750000	2.410493000	0.068483000
6	-1.216200000	3.287241000	-0.220752000
6	-1.632798000	4.713760000	-0.274381000
1	-2.175080000	5.047437000	0.617979000
1	-0.746919000	5.348246000	-0.354739000
1	-2.257992000	4.946540000	-1.139041000
7	0.964377000	2.631844000	1.535833000
7	1.498975000	2.340190000	-0.984541000
6	1.914268000	1.620844000	1.986312000

1	1.411639000	0.869739000	2.609503000
1	2.354247000	1.097325000	1.137375000
1	2.713161000	2.090636000	2.569357000
6	0.157709000	3.172304000	2.616585000
1	0.822449000	3.531950000	3.405700000
1	-0.448771000	4.006738000	2.268199000
1	-0.505545000	2.409784000	3.047036000
6	2.793513000	2.961811000	-0.808344000
1	3.579406000	2.204425000	-0.910040000
1	2.952488000	3.734047000	-1.568759000
1	2.873948000	3.425105000	0.172658000
6	1.245493000	1.882348000	-2.338416000
1	0.303600000	1.336870000	-2.387359000
1	1.207428000	2.726259000	-3.036049000
1	2.045465000	1.204197000	-2.646399000
7	-3.084063000	1.628717000	-0.361153000
6	-4.068069000	2.670164000	-0.615533000
1	-4.027894000	3.428910000	0.166558000
1	-3.889661000	3.143640000	-1.583113000
1	-5.048973000	2.206915000	-0.626957000
8	-4.750254000	0.110594000	-0.617231000
7	-2.721056000	-0.696933000	0.068409000
6	-3.292998000	-2.003680000	0.111559000
6	-3.704018000	-2.652116000	-1.046496000
6	-3.368787000	-2.674335000	1.323765000
6	-4.189877000	-3.943914000	-0.988047000
1	-3.642302000	-2.127087000	-1.992831000
6	-3.851076000	-3.971981000	1.380111000
1	-3.045296000	-2.164856000	2.225237000
6	-4.265177000	-4.610512000	0.225595000
1	-4.509450000	-4.437773000	-1.898755000
1	-3.903532000	-4.483324000	2.334578000
1	-4.643312000	-5.625297000	0.268008000
13	-0.816373000	-0.737059000	0.487191000
1	1.385822000	-1.020121000	-1.965609000
6	4.200633000	-1.128441000	-0.088160000
6	3.670845000	-2.588898000	-0.015472000
5	2.273008000	-1.327653000	-1.244766000
8	2.690357000	-2.606815000	-1.071984000
8	3.051970000	-0.408659000	-0.586946000
6	4.708872000	-3.649469000	-0.288499000
1	5.515521000	-3.592427000	0.447801000
1	4.250143000	-4.636444000	-0.210930000
1	5.137338000	-3.553802000	-1.285815000
6	2.933437000	-2.895287000	1.273212000
1	2.419312000	-3.851125000	1.159523000
1	3.619718000	-2.971816000	2.119495000
1	2.170113000	-2.142889000	1.491296000
6	4.626998000	-0.543559000	1.235909000

1	5.472038000	-1.105134000	1.642888000
1	4.947173000	0.492492000	1.096078000
1	3.820709000	-0.558617000	1.968650000
6	5.302399000	-0.937311000	-1.113640000
1	5.470518000	0.133083000	-1.252836000
1	6.240944000	-1.390371000	-0.788341000
1	5.025170000	-1.364546000	-2.079409000

13Alv^{B-H} (T.E = -2254.708666)

7	1.699821000	-0.543208000	-0.123095000
6	1.766864000	-1.351175000	1.066622000
6	0.657657000	-1.959456000	1.633295000
6	-0.601254000	-1.902945000	1.052282000
1	0.786922000	-2.543500000	2.538288000
13	0.281512000	-0.255539000	-1.364160000
15	3.340013000	-0.419526000	-0.007375000
6	3.130514000	-1.363855000	1.405107000
6	3.886408000	-2.082207000	2.456379000
1	4.951954000	-1.846349000	2.403619000
1	3.553681000	-1.814785000	3.465098000
1	3.795388000	-3.173065000	2.370665000
7	-0.879111000	-1.209415000	-0.176885000
6	-1.829910000	-2.474349000	1.419681000
15	-2.424086000	-1.780605000	-0.026614000
6	-2.238997000	-3.306737000	2.574361000
1	-1.632957000	-4.214573000	2.670678000
1	-2.162872000	-2.770658000	3.528540000
1	-3.278340000	-3.630061000	2.473846000
7	-3.719511000	-0.775357000	0.112089000
7	-2.820053000	-2.656434000	-1.392076000
6	-4.297320000	-0.066282000	-1.011553000
1	-4.236374000	1.011542000	-0.833249000
1	-3.762266000	-0.297880000	-1.932384000
1	-5.353256000	-0.334330000	-1.142103000
6	-4.215940000	-0.332082000	1.400045000
1	-4.025311000	0.737029000	1.541947000
1	-5.296905000	-0.503541000	1.459343000
1	-3.727443000	-0.881395000	2.203641000
6	-1.766820000	-3.433546000	-2.024229000
1	-2.124908000	-3.784563000	-2.994984000
1	-0.881714000	-2.820261000	-2.187049000
1	-1.486809000	-4.309585000	-1.422325000
6	-4.080226000	-3.378062000	-1.370009000
1	-3.984227000	-4.343064000	-0.851106000
1	-4.853487000	-2.796874000	-0.868878000
1	-4.408282000	-3.576708000	-2.393964000
7	3.853891000	1.163197000	0.015609000
7	4.241117000	-1.063879000	-1.243289000

6	5.279375000	1.429028000	0.093875000
1	5.473397000	2.454431000	-0.232945000
1	5.654062000	1.327083000	1.122906000
1	5.839977000	0.749071000	-0.545200000
6	3.086900000	2.053632000	0.873344000
1	2.020411000	1.843049000	0.796939000
1	3.391322000	1.959355000	1.924727000
1	3.263697000	3.086509000	0.558497000
6	4.243229000	-2.512982000	-1.346644000
1	5.088796000	-2.826030000	-1.964584000
1	4.342540000	-2.966575000	-0.361214000
1	3.319674000	-2.887191000	-1.810632000
6	4.213409000	-0.419176000	-2.548690000
1	4.140167000	0.662024000	-2.443168000
1	5.129837000	-0.660396000	-3.095556000
1	3.351719000	-0.758719000	-3.138998000
1	-1.523559000	0.843118000	1.816299000
6	-0.521877000	3.611974000	0.128192000
6	-2.031341000	3.500596000	-0.250728000
8	-0.248244000	2.325150000	0.719955000
8	-2.515422000	2.500973000	0.674871000
5	-1.436415000	1.795248000	1.118539000
6	0.404239000	3.828213000	-1.044657000
1	0.134811000	4.743128000	-1.579759000
1	1.430260000	3.938993000	-0.688654000
1	0.379294000	2.985978000	-1.738645000
6	-0.242586000	4.639239000	1.209051000
1	0.786676000	4.511504000	1.550664000
1	-0.355726000	5.658965000	0.835308000
1	-0.900877000	4.505773000	2.070190000
6	-2.826823000	4.768310000	-0.050302000
1	-2.433607000	5.569382000	-0.682144000
1	-3.866093000	4.594203000	-0.335115000
1	-2.812312000	5.101543000	0.986825000
6	-2.260532000	2.967048000	-1.650482000
1	-3.327676000	2.780921000	-1.786676000
1	-1.948402000	3.689857000	-2.406719000
1	-1.721233000	2.029963000	-1.825445000

1Gav^{B-H} (T.E = -3024.843240)

7	-0.374923000	-1.971605000	0.601117000
6	-0.093033000	-2.092119000	1.879361000
6	1.106738000	-1.775485000	2.499759000
7	2.358315000	-0.982783000	0.594383000
1	1.180261000	-1.972562000	3.560384000
1	-0.874557000	-2.502388000	2.525942000
6	-1.687398000	-2.236830000	0.178079000
6	-1.889036000	-2.889397000	-1.036586000

6	-2.799752000	-1.809123000	0.902323000
6	-3.168843000	-3.121344000	-1.507003000
1	-1.026194000	-3.230655000	-1.598579000
6	-4.076807000	-2.057358000	0.433331000
1	-2.652433000	-1.236582000	1.811133000
6	-4.269840000	-2.711262000	-0.773326000
1	-3.305798000	-3.635264000	-2.451365000
1	-4.931253000	-1.717961000	1.008849000
1	-5.272006000	-2.895926000	-1.141001000
6	3.532139000	-0.341976000	0.159323000
6	4.144127000	-0.771798000	-1.015494000
6	4.066988000	0.751305000	0.837409000
6	5.278545000	-0.137421000	-1.486556000
1	3.730577000	-1.626355000	-1.540421000
6	5.204859000	1.378390000	0.363591000
1	3.562926000	1.124783000	1.722496000
6	5.816892000	0.937198000	-0.797955000
1	5.748805000	-0.489598000	-2.397387000
1	5.607171000	2.230742000	0.899090000
1	6.704869000	1.434285000	-1.169601000
6	2.228097000	-1.249940000	1.874141000
1	3.093148000	-1.054473000	2.515473000
1	0.716377000	1.281962000	1.207497000
6	-1.675737000	3.279866000	-0.126336000
6	-2.383851000	1.897051000	-0.020363000
5	-0.269892000	1.756129000	0.746596000
8	-0.288241000	2.935723000	0.073546000
8	-1.492839000	1.167140000	0.853588000
6	-2.050726000	4.231519000	0.993794000
1	-1.368679000	5.083062000	0.972121000
1	-3.070165000	4.605289000	0.878615000
1	-1.962999000	3.752967000	1.971445000
6	-1.824504000	3.967805000	-1.460575000
1	-2.879311000	4.160361000	-1.675220000
1	-1.302781000	4.926196000	-1.438748000
1	-1.405542000	3.372840000	-2.270992000
6	-3.759404000	1.933285000	0.599222000
1	-4.426856000	2.566570000	0.008393000
1	-4.177683000	0.924914000	0.614173000
1	-3.735667000	2.308460000	1.621851000
6	-2.430820000	1.143588000	-1.335787000
1	-2.758294000	0.118872000	-1.145848000
1	-3.134642000	1.603769000	-2.032212000
1	-1.447685000	1.097650000	-1.811139000
31	0.822289000	-1.003533000	-0.875020000

4Gav^{B-H} (T.E = -3237.620310)

7	-1.688162000	-0.952157000	0.765328000
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6	-1.275773000	-0.402340000	1.893737000
6	-0.008823000	-0.466438000	2.446053000
6	1.112409000	-1.023787000	1.823178000
6	1.153816000	-1.624241000	0.585553000
6	-2.986828000	-0.629351000	0.330116000
6	-3.824747000	-1.633574000	-0.150555000
6	-3.449073000	0.685795000	0.331341000
6	-5.098253000	-1.331799000	-0.594481000
1	-3.464306000	-2.656360000	-0.157703000
6	-4.726858000	0.980211000	-0.110256000
1	-2.776421000	1.477109000	0.644066000
6	-5.559113000	-0.024807000	-0.573199000
1	-5.739746000	-2.127431000	-0.956361000
1	-5.069151000	2.009285000	-0.106446000
1	-6.557666000	0.208926000	-0.923259000
1	-2.022356000	0.156572000	2.467195000
15	2.655907000	-2.096377000	-0.071363000
6	4.135287000	-1.738432000	0.908120000
1	5.024953000	-2.074623000	0.372615000
1	4.208062000	-0.663385000	1.082218000
1	4.084306000	-2.248393000	1.870847000
6	2.727939000	-3.865792000	-0.417832000
1	2.642577000	-4.422321000	0.516067000
1	1.879277000	-4.126961000	-1.054119000
1	3.658243000	-4.132166000	-0.923774000
6	2.949194000	-1.318554000	-1.669179000
1	2.960105000	-0.232458000	-1.550601000
1	3.889645000	-1.660264000	-2.106373000
1	2.123193000	-1.576524000	-2.336633000
1	2.033906000	-0.917169000	2.409997000
1	0.118399000	-0.015240000	3.423020000
1	-0.000358000	0.440831000	-1.932785000
6	1.812874000	2.825473000	-0.328837000
6	0.340342000	3.165318000	0.059602000
5	0.389357000	1.348446000	-1.276082000
8	1.642736000	1.875604000	-1.402452000
8	-0.374040000	1.986695000	-0.353736000
6	2.572643000	2.106739000	0.768661000
1	3.515892000	1.740977000	0.353389000
1	2.804941000	2.772786000	1.601992000
1	2.006643000	1.252852000	1.147393000
6	2.621612000	3.995944000	-0.832487000
1	2.699215000	4.766316000	-0.060301000
1	3.631498000	3.663583000	-1.080297000
1	2.183803000	4.439811000	-1.725692000
6	0.104371000	3.379286000	1.534933000
1	0.699642000	4.218382000	1.905746000
1	-0.949327000	3.612588000	1.703313000
1	0.344719000	2.485601000	2.110843000

6	-0.240869000	4.319375000	-0.734601000
1	-1.316629000	4.356932000	-0.553672000
1	0.191982000	5.275661000	-0.433796000
1	-0.085734000	4.185551000	-1.807200000
31	-0.548324000	-2.068854000	-0.625027000

6Gav^{B-H} (T.E = -3368.203594)

6	1.459204000	-1.115489000	1.470731000
6	1.469780000	-1.244064000	0.068908000
6	-1.041368000	-1.036949000	1.640480000
1	-1.827552000	-0.863926000	2.382222000
7	-1.383435000	-1.320742000	0.433695000
15	3.089471000	-1.389029000	-0.463953000
6	4.199020000	-0.012016000	-0.074507000
1	4.202726000	0.136856000	1.004474000
1	5.210668000	-0.226418000	-0.425324000
1	3.833899000	0.891297000	-0.565373000
6	3.976563000	-2.859661000	0.103010000
1	3.431618000	-3.746591000	-0.222956000
1	4.989098000	-2.883691000	-0.305556000
1	4.015369000	-2.842068000	1.191473000
6	3.163264000	-1.496954000	-2.262851000
1	2.721976000	-0.605713000	-2.712768000
1	4.205099000	-1.579854000	-2.578146000
1	2.610187000	-2.368032000	-2.616818000
8	2.439222000	-1.099777000	2.225936000
7	0.192277000	-0.946597000	2.157330000
6	0.307188000	-0.701871000	3.587047000
1	0.764806000	-1.552738000	4.091452000
1	0.939679000	0.165953000	3.772491000
1	-0.684414000	-0.523386000	3.999973000
6	-2.765111000	-1.321238000	0.143898000
6	-3.278946000	-2.337758000	-0.653805000
6	-3.615041000	-0.315669000	0.594628000
6	-4.624664000	-2.364577000	-0.967425000
1	-2.607704000	-3.108323000	-1.016328000
6	-4.961896000	-0.349787000	0.278386000
1	-3.202134000	0.516091000	1.155198000
6	-5.473331000	-1.374039000	-0.499680000
1	-5.013694000	-3.166576000	-1.584056000
1	-5.612739000	0.442888000	0.629490000
1	-6.526909000	-1.394167000	-0.751727000
6	0.381992000	3.291667000	-0.841875000
6	-0.116813000	2.914955000	0.584539000
5	-1.443591000	1.978993000	-0.986414000
8	-0.731565000	2.912432000	-1.672485000
8	-1.048106000	1.846262000	0.314169000
6	1.567329000	2.461188000	-1.295477000

1	1.706683000	2.607689000	-2.368304000
1	2.482426000	2.767338000	-0.782282000
1	1.401022000	1.395833000	-1.109280000
6	0.673134000	4.758366000	-1.046473000
1	1.456146000	5.092285000	-0.360042000
1	1.025298000	4.921352000	-2.066622000
1	-0.212354000	5.374185000	-0.893167000
6	0.956457000	2.413135000	1.519721000
1	1.728753000	3.174221000	1.661235000
1	0.517689000	2.196976000	2.496640000
1	1.424299000	1.499311000	1.150526000
6	-0.912898000	4.020534000	1.251213000
1	-1.395552000	3.614555000	2.142052000
1	-0.271554000	4.849379000	1.557678000
1	-1.692052000	4.406983000	0.590877000
1	-2.334664000	1.358731000	-1.458161000
31	-0.049409000	-1.386728000	-1.316079000

8Gav^{B-H} (T.E = -3602.243197)

7	-1.856025000	-1.122189000	-0.346309000
6	-1.641342000	-1.077455000	1.050944000
6	-0.283232000	-1.142610000	1.581292000
15	-3.420732000	-0.742561000	0.024279000
6	-2.849499000	-0.844012000	1.668140000
6	-3.248022000	-0.656059000	3.080511000
1	-3.693182000	0.326919000	3.269765000
1	-3.968957000	-1.402517000	3.427169000
1	-2.367542000	-0.734372000	3.724894000
7	-4.017490000	0.737884000	-0.400574000
7	-4.474267000	-1.799023000	-0.677606000
6	-4.353549000	1.023655000	-1.787630000
1	-3.497465000	1.463530000	-2.315473000
1	-4.645101000	0.114910000	-2.311544000
1	-5.185724000	1.732918000	-1.822617000
6	-3.517085000	1.913351000	0.296445000
1	-4.270276000	2.704363000	0.250884000
1	-3.308672000	1.684359000	1.340339000
1	-2.592327000	2.290590000	-0.161733000
6	-5.907077000	-1.661928000	-0.509392000
1	-6.417395000	-1.937207000	-1.437887000
1	-6.279043000	-2.317303000	0.287768000
1	-6.171001000	-0.634234000	-0.263425000
6	-4.044628000	-3.163707000	-0.926793000
1	-2.965576000	-3.192740000	-1.065829000
1	-4.316923000	-3.826616000	-0.096273000
1	-4.530015000	-3.534986000	-1.833831000
6	0.660681000	2.216517000	-0.178242000
6	0.104685000	3.300799000	0.510310000

6	1.568899000	2.497348000	-1.205558000
6	0.474804000	4.600140000	0.217663000
1	-0.606289000	3.093591000	1.305677000
6	1.929999000	3.800837000	-1.499864000
1	2.012913000	1.662984000	-1.740397000
6	1.393164000	4.861403000	-0.788383000
1	0.039615000	5.419816000	0.779631000
1	2.646042000	3.988535000	-2.292904000
1	1.681363000	5.880306000	-1.018097000
7	0.283211000	0.905093000	0.104514000
5	0.435354000	0.295929000	1.368278000
7	1.241143000	0.794821000	2.453119000
6	2.302864000	1.764640000	2.317291000
1	2.486946000	2.022778000	1.276832000
1	2.082779000	2.694818000	2.858086000
1	3.235681000	1.357711000	2.734747000
6	1.205110000	0.291826000	3.803104000
1	0.284958000	-0.248276000	4.017717000
1	2.055022000	-0.375034000	4.019180000
1	1.262757000	1.123366000	4.516040000
1	-0.287326000	-1.473090000	2.618979000
1	0.292845000	-1.876789000	1.003638000
31	-0.617540000	0.159492000	-1.612162000
1	1.033977000	-2.115936000	-1.532948000
6	3.968323000	-2.134512000	0.165545000
6	4.210504000	-1.071534000	-0.951457000
5	2.136433000	-1.932913000	-1.129559000
8	2.766172000	-2.794260000	-0.286347000
8	2.883826000	-0.852259000	-1.471068000
6	3.644715000	-1.531107000	1.518408000
1	3.290430000	-2.327330000	2.177235000
1	4.524436000	-1.073524000	1.976947000
1	2.855741000	-0.778315000	1.450367000
6	5.066167000	-3.159968000	0.310973000
1	6.008790000	-2.673604000	0.576891000
1	4.809235000	-3.858186000	1.109553000
1	5.214463000	-3.732443000	-0.603885000
6	5.043117000	-1.593325000	-2.106867000
1	4.995642000	-0.871202000	-2.923578000
1	6.089594000	-1.722783000	-1.823178000
1	4.660357000	-2.546579000	-2.477418000
6	4.765638000	0.245082000	-0.465845000
1	5.735346000	0.099273000	0.018134000
1	4.907494000	0.918016000	-1.313799000
1	4.090753000	0.733116000	0.237323000

10Gav^{B-H} (T.E = -3693.743658)

7	1.496128000	0.533483000	-0.103855000
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6	1.273134000	0.079556000	-1.433461000
6	0.176806000	0.478566000	-2.189495000
6	-0.855788000	1.276614000	-1.693598000
1	0.104992000	0.099548000	-3.203857000
1	-1.659341000	1.423432000	-2.427762000
15	2.901528000	-0.337437000	-0.151025000
6	2.344154000	-0.798406000	-1.705308000
6	2.701283000	-1.569309000	-2.917261000
1	3.494272000	-2.291664000	-2.711293000
1	1.843613000	-2.142004000	-3.290747000
1	3.048924000	-0.942049000	-3.750031000
6	-0.983229000	1.853006000	-0.441210000
15	-2.387170000	2.735915000	-0.079347000
6	-2.092689000	4.517827000	0.050174000
1	-2.991969000	5.055731000	0.358727000
1	-1.302356000	4.677084000	0.787185000
1	-1.746300000	4.897142000	-0.911947000
6	-3.081019000	2.309731000	1.528265000
1	-3.904104000	2.980548000	1.783288000
1	-3.432891000	1.277628000	1.495799000
1	-2.296717000	2.390921000	2.284710000
6	-3.777959000	2.573754000	-1.228123000
1	-3.497352000	2.915219000	-2.225000000
1	-4.069824000	1.523031000	-1.281158000
1	-4.623932000	3.165907000	-0.874447000
7	4.319524000	0.531496000	-0.097070000
7	3.054189000	-1.321941000	1.172007000
6	4.606943000	1.295402000	1.108251000
1	4.097443000	2.268326000	1.090571000
1	4.270878000	0.760370000	1.995331000
1	5.684569000	1.466843000	1.187713000
6	4.679103000	1.258873000	-1.301636000
1	5.730278000	1.553042000	-1.239839000
1	4.540796000	0.633985000	-2.182491000
1	4.073334000	2.167970000	-1.423516000
6	4.280566000	-2.023306000	1.484875000
1	4.428718000	-2.044392000	2.569962000
1	4.247752000	-3.062059000	1.131350000
1	5.136386000	-1.529317000	1.028226000
6	1.870663000	-1.977701000	1.694748000
1	0.973356000	-1.422164000	1.429260000
1	1.772951000	-3.000476000	1.308287000
1	1.931098000	-2.029055000	2.785866000
1	-1.712450000	-0.510387000	2.490034000
6	-1.952277000	-2.924879000	0.118325000
6	-3.211881000	-2.041716000	-0.147797000
5	-2.029779000	-1.222126000	1.595898000
8	-2.958626000	-0.874639000	0.662210000
8	-1.518841000	-2.468251000	1.418564000

6	-3.381952000	-1.605951000	-1.583299000
1	-3.490136000	-2.474293000	-2.238823000
1	-4.288612000	-1.002967000	-1.676424000
1	-2.534513000	-1.009671000	-1.925366000
6	-4.498704000	-2.652507000	0.371477000
1	-5.288747000	-1.900879000	0.321581000
1	-4.806272000	-3.512606000	-0.226725000
1	-4.398766000	-2.968301000	1.412026000
6	-2.221699000	-4.408166000	0.186967000
1	-2.616959000	-4.768103000	-0.767000000
1	-1.287047000	-4.935904000	0.384872000
1	-2.927790000	-4.662500000	0.976872000
6	-0.812253000	-2.645202000	-0.838271000
1	0.083537000	-3.161385000	-0.487512000
1	-1.033495000	-2.998181000	-1.848257000
1	-0.585263000	-1.578450000	-0.892047000
31	0.477971000	1.786719000	1.110102000

11Gav^{B-H} (T.E = -3611.552092)

7	-0.868641000	-1.243602000	-0.007078000
6	-0.916148000	-0.909495000	1.347700000
6	1.563063000	-0.705413000	1.610954000
7	1.844416000	-1.310806000	0.454741000
15	-2.508761000	-1.044819000	-0.018078000
6	-2.274862000	-0.707660000	1.660993000
6	-3.080408000	-0.244075000	2.823580000
1	-3.064814000	-0.933401000	3.672823000
1	-2.773686000	0.739466000	3.198599000
1	-4.128743000	-0.152689000	2.528920000
6	3.195961000	-1.229867000	0.033746000
6	3.870534000	-2.408481000	-0.262685000
6	3.839668000	-0.014828000	-0.183196000
6	5.165467000	-2.378519000	-0.753264000
1	3.364264000	-3.353594000	-0.094527000
6	5.133139000	0.010819000	-0.668541000
1	3.305426000	0.903832000	0.025086000
6	5.804511000	-1.168496000	-0.954778000
1	5.676185000	-3.308634000	-0.976063000
1	5.622912000	0.964707000	-0.831507000
1	6.818408000	-1.141933000	-1.336883000
31	0.695382000	-1.934252000	-1.171770000
7	-3.152954000	0.165816000	-0.915812000
7	-3.214298000	-2.405884000	-0.639195000
6	-3.131250000	0.127740000	-2.366355000
1	-2.627242000	-0.771999000	-2.721228000
1	-4.148234000	0.142630000	-2.776826000
1	-2.589823000	0.997568000	-2.750330000
6	-3.669445000	1.398066000	-0.356535000

1	-3.537664000	1.412938000	0.724684000
1	-3.135171000	2.252996000	-0.780738000
1	-4.737469000	1.503590000	-0.582879000
6	-4.626827000	-2.451950000	-0.958644000
1	-4.781853000	-3.034696000	-1.871946000
1	-5.201944000	-2.926160000	-0.153803000
1	-5.023672000	-1.450371000	-1.118226000
6	-2.666618000	-3.710705000	-0.314250000
1	-1.601495000	-3.635178000	-0.104118000
1	-3.168940000	-4.147947000	0.557153000
1	-2.803693000	-4.384486000	-1.164462000
8	2.320602000	-0.110266000	2.354049000
7	0.188523000	-0.815738000	2.098075000
6	0.017688000	-0.542906000	3.516315000
1	-0.157748000	0.517633000	3.716658000
1	-0.823602000	-1.122955000	3.890494000
1	0.922548000	-0.833994000	4.040356000
1	-0.098339000	0.785809000	-2.167324000
6	0.675625000	2.986533000	0.301273000
6	-0.268589000	3.800819000	-0.630021000
5	-0.000536000	1.709913000	-1.430830000
8	0.989740000	1.837307000	-0.513708000
8	-0.863615000	2.767588000	-1.449340000
6	1.965225000	3.674365000	0.677882000
1	1.763364000	4.595597000	1.231285000
1	2.548665000	3.011894000	1.321304000
1	2.567692000	3.915790000	-0.197461000
6	-0.007078000	2.470834000	1.552749000
1	0.682147000	1.792888000	2.059542000
1	-0.250540000	3.285924000	2.237528000
1	-0.924880000	1.919627000	1.319171000
6	-1.363108000	4.558605000	0.079711000
1	-0.934109000	5.312320000	0.745308000
1	-1.988497000	5.072000000	-0.653641000
1	-1.999316000	3.900094000	0.670683000
6	0.473677000	4.725763000	-1.574634000
1	-0.227095000	5.104984000	-2.320437000
1	0.904629000	5.576697000	-1.043466000
1	1.275090000	4.201145000	-2.098670000

13Gav^{B-H} (T.E = -3937.098992)

7	-1.358031000	-1.108971000	0.027997000
6	-1.224234000	-0.524975000	1.324990000
6	0.000152000	-0.281337000	1.938201000
6	1.217143000	-0.566925000	1.331109000
15	2.972412000	-0.990446000	0.221993000
1	0.006090000	0.131462000	2.942740000
31	-0.018182000	-1.754748000	-1.349136000

1	0.279661000	0.979419000	-2.250089000
6	0.768643000	3.551996000	-0.075146000
6	-0.789053000	3.434311000	-0.159988000
5	0.181948000	1.864672000	-1.467107000
8	1.211136000	2.698067000	-1.152417000
8	-0.984287000	2.181433000	-0.845417000
6	1.345769000	2.993231000	1.209415000
1	2.434086000	2.981685000	1.131353000
1	1.077644000	3.613346000	2.067318000
1	1.007652000	1.971514000	1.394843000
6	1.315489000	4.939837000	-0.313031000
1	0.956766000	5.630276000	0.455247000
1	2.405757000	4.909934000	-0.256708000
1	1.039149000	5.330057000	-1.291909000
6	-1.482399000	3.368907000	1.180699000
1	-1.251190000	4.255494000	1.777261000
1	-2.564212000	3.334769000	1.036944000
1	-1.189604000	2.475434000	1.735387000
6	-1.426247000	4.501125000	-1.029898000
1	-2.477898000	4.251192000	-1.182702000
1	-1.375638000	5.486302000	-0.561714000
1	-0.948388000	4.553991000	-2.010377000
7	1.343749000	-1.076686000	0.001208000
6	2.543258000	-0.423504000	1.785091000
6	3.096935000	0.096419000	3.056293000
1	2.986949000	1.184969000	3.165501000
1	2.607441000	-0.357418000	3.924785000
1	4.163148000	-0.123995000	3.147003000
7	3.857569000	0.017565000	-0.739911000
7	3.648205000	-2.470347000	-0.119392000
6	3.841625000	-0.155417000	-2.178809000
1	4.856292000	-0.088742000	-2.589047000
1	3.424951000	-1.127647000	-2.445489000
1	3.226814000	0.619814000	-2.651406000
6	4.273526000	1.333536000	-0.307105000
1	4.247987000	1.399050000	0.780392000
1	5.299462000	1.523913000	-0.642010000
1	3.621744000	2.112962000	-0.719516000
6	2.966711000	-3.662923000	0.344802000
1	3.023704000	-4.444565000	-0.419466000
1	3.422287000	-4.047473000	1.265747000
1	1.916731000	-3.447712000	0.538197000
6	5.059181000	-2.679211000	-0.351191000
1	5.542483000	-1.752950000	-0.655697000
1	5.563987000	-3.054476000	0.548674000
1	5.199387000	-3.420896000	-1.145067000
15	-2.983308000	-0.966937000	0.232246000
6	-2.546545000	-0.316624000	1.761425000
7	-3.691609000	-2.449214000	-0.022632000

7	-3.848245000	-0.002155000	-0.793303000
6	-3.773226000	-0.246054000	-2.220666000
1	-3.027702000	0.411671000	-2.685769000
1	-3.484275000	-1.278616000	-2.420582000
1	-4.745181000	-0.060715000	-2.691327000
6	-4.174510000	1.364312000	-0.452163000
1	-3.451608000	2.062510000	-0.888369000
1	-5.173292000	1.608452000	-0.830143000
1	-4.170745000	1.496467000	0.629447000
6	-5.105840000	-2.642684000	-0.247993000
1	-5.257316000	-3.435123000	-0.988996000
1	-5.624260000	-2.943765000	0.671910000
1	-5.565715000	-1.729600000	-0.620837000
6	-3.034667000	-3.626543000	0.510691000
1	-1.978071000	-3.424742000	0.680789000
1	-3.490698000	-3.942228000	1.457291000
1	-3.118365000	-4.452286000	-0.203071000
6	-3.094331000	0.289602000	2.996183000
1	-3.036693000	1.387971000	3.006992000
1	-4.144915000	0.026969000	3.141340000
1	-2.557638000	-0.061909000	3.883734000

Cartesian coordinates of the transition states involved in the pinacolborane activation by some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AITS^{B-H} (T.E = -1342.418129)

7	1.241326000	-2.226238000	0.387795000
6	0.957092000	-3.512038000	0.463438000
6	-0.313299000	-4.062009000	0.564988000
7	-1.601902000	-2.030969000	0.351651000
1	-0.388313000	-5.134494000	0.672505000
1	1.800983000	-4.202501000	0.441924000
6	2.572809000	-1.830376000	0.097757000
6	3.083627000	-0.685445000	0.695232000
6	3.354815000	-2.537694000	-0.809968000
6	4.366085000	-0.264273000	0.400281000
1	2.465881000	-0.110153000	1.376691000
6	4.642945000	-2.118703000	-1.087358000

1	2.939292000	-3.394331000	-1.328848000
6	5.154258000	-0.982192000	-0.483215000
1	4.745776000	0.637863000	0.865299000
1	5.242415000	-2.672990000	-1.800065000
1	6.158768000	-0.648403000	-0.714230000
6	-2.863654000	-1.462816000	0.040319000
6	-3.193607000	-0.220413000	0.568074000
6	-3.755190000	-2.099103000	-0.818326000
6	-4.407168000	0.363571000	0.260017000
1	-2.488045000	0.299978000	1.207982000
6	-4.973858000	-1.514753000	-1.109085000
1	-3.479132000	-3.034733000	-1.291298000
6	-5.306989000	-0.283534000	-0.569586000
1	-4.644016000	1.337531000	0.671691000
1	-5.658340000	-2.016796000	-1.782913000
1	-6.256930000	0.177915000	-0.811321000
6	-1.493415000	-3.343989000	0.443163000
1	-2.421901000	-3.914879000	0.416734000
13	-0.098274000	-0.887458000	0.631737000
6	1.024768000	3.074592000	-0.266036000
6	-0.452805000	3.310371000	0.152894000
8	1.287764000	1.790646000	0.300500000
8	-1.000937000	1.994565000	0.102624000
5	0.068343000	1.095877000	0.278214000
6	-0.582043000	3.808059000	1.583256000
1	-0.253826000	4.844983000	1.688784000
1	-1.632660000	3.751002000	1.875924000
1	-0.005489000	3.183367000	2.268805000
6	-1.239202000	4.206715000	-0.775190000
1	-2.259273000	4.317261000	-0.400314000
1	-0.788285000	5.202117000	-0.828895000
1	-1.294642000	3.791146000	-1.780934000
6	1.201659000	2.968629000	-1.771487000
1	1.100118000	3.938648000	-2.263724000
1	2.203305000	2.582398000	-1.974031000
1	0.479860000	2.276263000	-2.209875000
6	2.014667000	4.066200000	0.297475000
1	3.018721000	3.820469000	-0.056366000
1	1.778552000	5.082145000	-0.032245000
1	2.026503000	4.044794000	1.387048000
1	0.026991000	0.132947000	-0.862969000

4AITS^{B-H} (T.E = -1555.214881)

7	-2.240457000	-1.270981000	-0.279079000
6	-2.589587000	-2.566200000	-0.237825000
6	-1.762421000	-3.658346000	-0.175488000
1	-2.245791000	-4.627045000	-0.174807000
1	-3.659438000	-2.769945000	-0.267257000

6	-3.240363000	-0.285583000	-0.134125000
6	-3.023603000	0.977719000	-0.680077000
6	-4.415489000	-0.510010000	0.581877000
6	-3.965686000	1.977283000	-0.537305000
1	-2.100618000	1.178881000	-1.217423000
6	-5.360027000	0.492312000	0.708757000
1	-4.578970000	-1.460765000	1.075258000
6	-5.145352000	1.740002000	0.148806000
1	-3.769602000	2.952160000	-0.968267000
1	-6.265572000	0.298717000	1.272755000
1	-5.883376000	2.525203000	0.260984000
6	-0.352743000	-3.622373000	-0.065762000
1	0.110634000	-4.604061000	0.070406000
6	1.129644000	3.130413000	0.240059000
6	2.412341000	2.335804000	-0.130706000
8	0.104978000	2.323144000	-0.330527000
8	1.968586000	0.985944000	-0.056445000
5	0.543081000	0.989978000	-0.247665000
6	2.865335000	2.590644000	-1.559736000
1	3.292667000	3.588180000	-1.687439000
1	3.633859000	1.856913000	-1.817155000
1	2.033763000	2.469643000	-2.257066000
6	3.576129000	2.520661000	0.816708000
1	4.423635000	1.919357000	0.476206000
1	3.896582000	3.566122000	0.848584000
1	3.321792000	2.202949000	1.828611000
6	0.902602000	3.203845000	1.741681000
1	1.612064000	3.875970000	2.230475000
1	-0.106847000	3.580303000	1.919308000
1	0.975394000	2.216907000	2.204954000
6	1.050245000	4.516511000	-0.355928000
1	0.129322000	5.002840000	-0.027368000
1	1.893815000	5.131619000	-0.028455000
1	1.041585000	4.482391000	-1.445251000
1	0.001845000	0.321730000	0.962863000
6	0.422904000	-2.497724000	-0.114846000
15	2.128946000	-2.578214000	0.115883000
6	2.774770000	-4.254562000	0.280029000
1	3.857160000	-4.211910000	0.410462000
1	2.333254000	-4.747303000	1.146953000
1	2.546437000	-4.835719000	-0.614112000
6	3.021435000	-1.810035000	-1.239826000
1	2.751953000	-2.291189000	-2.180358000
1	2.743804000	-0.751163000	-1.268047000
1	4.097413000	-1.895008000	-1.073788000
6	2.647880000	-1.687391000	1.587619000
1	2.135818000	-2.093001000	2.460670000
1	3.729128000	-1.772523000	1.716130000
1	2.381836000	-0.633171000	1.458547000

13 -0.428965000 -0.760571000 -0.462341000

6AITS^{B-H} (T.E = -1685.790688)

7	-0.634034000	1.934768000	-0.309099000
6	-1.710722000	2.590165000	-0.006941000
1	-1.619839000	3.667836000	0.147449000
6	0.614903000	2.617732000	-0.259645000
6	1.443965000	2.594955000	-1.369829000
6	1.043529000	3.206641000	0.920938000
6	2.694252000	3.179458000	-1.302726000
1	1.110107000	2.094005000	-2.271403000
6	2.296230000	3.792286000	0.980659000
1	0.407445000	3.161898000	1.798726000
6	3.123180000	3.777905000	-0.129499000
1	3.343622000	3.153483000	-2.169419000
1	2.633923000	4.243248000	1.906312000
1	4.109098000	4.224288000	-0.076819000
6	-3.382267000	0.697489000	0.100246000
13	-0.562029000	0.031037000	-0.523392000
6	3.422500000	-1.038408000	0.303701000
6	2.834697000	-2.459560000	0.075297000
8	2.471514000	-0.215242000	-0.364845000
8	1.428973000	-2.222372000	0.092433000
5	1.228672000	-0.857516000	-0.229803000
6	3.186562000	-3.023247000	-1.292046000
1	4.239009000	-3.309659000	-1.361738000
1	2.577966000	-3.913162000	-1.466553000
1	2.963203000	-2.300560000	-2.079536000
6	3.182753000	-3.465940000	1.148009000
1	2.738351000	-4.433395000	0.902966000
1	4.266413000	-3.600225000	1.218577000
1	2.804173000	-3.157813000	2.122476000
6	3.447213000	-0.637131000	1.770020000
1	4.216610000	-1.174329000	2.329827000
1	3.661372000	0.432936000	1.827699000
1	2.479482000	-0.809672000	2.246013000
6	4.782905000	-0.802964000	-0.310197000
1	5.105112000	0.218796000	-0.094847000
1	5.525852000	-1.489208000	0.107237000
1	4.759476000	-0.926163000	-1.392882000
1	0.471180000	-0.264177000	0.944560000
6	-2.433285000	-0.279726000	-0.226907000
15	-3.052535000	-1.868853000	-0.106721000
6	-3.598902000	-2.322939000	1.551415000
1	-4.383484000	-1.633051000	1.861942000
1	-3.977152000	-3.346927000	1.569219000
1	-2.751111000	-2.235149000	2.232537000
6	-4.449990000	-2.246002000	-1.183830000

1	-4.148272000	-2.101878000	-2.221893000
1	-4.776527000	-3.277874000	-1.040060000
1	-5.264464000	-1.561495000	-0.949026000
6	-1.773664000	-3.055678000	-0.534219000
1	-2.163228000	-4.069181000	-0.420685000
1	-1.459160000	-2.904699000	-1.568508000
1	-0.890687000	-2.933613000	0.100825000
8	-4.570421000	0.543935000	0.369143000
7	-2.945999000	2.110864000	0.140109000
6	-4.012517000	3.058582000	0.431281000
1	-4.790313000	3.000117000	-0.329100000
1	-4.472419000	2.832524000	1.392175000
1	-3.600975000	4.066510000	0.449996000

8AITS^{B-H} (T.E = -1919.843861)

7	-0.433845000	1.529557000	-0.873543000
6	-1.717781000	2.112327000	-0.694180000
6	-2.867970000	1.503349000	-1.368369000
7	-1.993931000	-0.862800000	-0.691979000
1	-2.638754000	1.462207000	-2.443088000
6	-2.015848000	-2.055360000	0.058343000
6	-1.319684000	-3.181578000	-0.376523000
6	-2.646885000	-2.111620000	1.302906000
6	-1.251917000	-4.320521000	0.407127000
1	-0.811121000	-3.148848000	-1.335800000
6	-2.595997000	-3.258412000	2.071664000
1	-3.174178000	-1.231988000	1.659968000
6	-1.895060000	-4.371152000	1.631317000
1	-0.688910000	-5.175863000	0.051274000
1	-3.096731000	-3.278646000	3.033597000
1	-1.845818000	-5.265077000	2.241489000
6	3.434856000	-2.248194000	-0.118836000
6	3.891091000	-0.823888000	-0.544591000
5	-3.130336000	-0.039501000	-0.936787000
7	-4.476676000	-0.509475000	-0.936578000
6	-4.834274000	-1.905016000	-1.057607000
1	-3.973428000	-2.513994000	-1.324137000
1	-5.257769000	-2.306218000	-0.127330000
1	-5.590507000	-2.023942000	-1.843317000
6	-5.656751000	0.312971000	-0.854958000
1	-5.417804000	1.350133000	-0.628884000
1	-6.237516000	0.288915000	-1.787196000
1	-6.317863000	-0.048811000	-0.056837000
1	-3.749579000	2.134478000	-1.261991000
15	0.095428000	2.602805000	0.270867000
6	-1.568146000	3.148352000	0.183452000
6	-2.481924000	4.148849000	0.772438000
1	-2.500810000	4.100729000	1.866273000

1	-2.213044000	5.174537000	0.502524000
1	-3.503567000	3.979693000	0.423409000
7	0.513176000	2.075982000	1.766020000
7	1.347888000	3.480994000	-0.297944000
6	1.872150000	1.649655000	2.073498000
1	2.129683000	1.975261000	3.085358000
1	1.954713000	0.560811000	2.003748000
1	2.584628000	2.071256000	1.366665000
6	-0.485068000	1.421721000	2.601142000
1	-1.481064000	1.804792000	2.380578000
1	-0.479815000	0.337862000	2.430571000
1	-0.256674000	1.616449000	3.652299000
6	2.227762000	3.031120000	-1.362150000
1	3.225704000	2.811245000	-0.963672000
1	1.848921000	2.115726000	-1.813272000
1	2.313754000	3.807800000	-2.127955000
6	1.792844000	4.649954000	0.428043000
1	1.951242000	5.480842000	-0.265922000
1	1.044880000	4.958287000	1.161574000
1	2.734563000	4.462245000	0.959058000
5	1.611928000	-1.021462000	-0.691312000
8	2.129449000	-2.322902000	-0.680769000
8	2.676854000	-0.085564000	-0.500353000
6	3.309757000	-2.406340000	1.387985000
1	2.793358000	-3.346759000	1.592424000
1	4.283653000	-2.431878000	1.883049000
1	2.711922000	-1.603425000	1.824743000
6	4.275197000	-3.372987000	-0.677867000
1	5.316054000	-3.281652000	-0.352768000
1	3.890894000	-4.329887000	-0.318371000
1	4.247039000	-3.388290000	-1.767134000
6	4.898675000	-0.177123000	0.379108000
1	5.827107000	-0.754695000	0.413189000
1	5.139969000	0.824819000	0.012761000
1	4.512679000	-0.082588000	1.394448000
6	4.404989000	-0.776412000	-1.975402000
1	4.506710000	0.270900000	-2.271714000
1	5.379882000	-1.258132000	-2.083694000
1	3.697035000	-1.251585000	-2.657515000
1	0.698717000	-0.747220000	0.499046000
13	-0.248730000	-0.331240000	-1.031598000

10AITS^{B-H} (T.E = -2011.344478)

7	-1.634846000	0.394562000	0.192429000
6	-2.686248000	1.251020000	-0.241546000
6	-2.511609000	2.628202000	-0.390065000
1	-3.381897000	3.209628000	-0.672317000
6	-1.290606000	3.289820000	-0.250265000

1	-1.362693000	4.366907000	-0.434681000
6	2.467000000	-2.570399000	-0.316435000
6	3.602482000	-1.641615000	0.199220000
8	1.302681000	-1.922738000	0.190439000
8	3.002362000	-0.353278000	0.156478000
5	1.594968000	-0.530115000	0.220264000
6	3.972473000	-1.926713000	1.646941000
1	4.515323000	-2.868914000	1.757949000
1	4.613852000	-1.118357000	2.004282000
1	3.081321000	-1.953781000	2.277535000
6	4.851123000	-1.639049000	-0.653541000
1	5.594607000	-0.972246000	-0.210849000
1	5.288232000	-2.640541000	-0.711887000
1	4.643475000	-1.287780000	-1.664296000
6	2.380167000	-2.600177000	-1.834317000
1	3.221313000	-3.133523000	-2.283056000
1	1.459938000	-3.116398000	-2.121490000
1	2.341841000	-1.589513000	-2.247600000
6	2.509192000	-3.983569000	0.218008000
1	1.684945000	-4.561974000	-0.207435000
1	3.444480000	-4.480119000	-0.057001000
1	2.408019000	-4.002699000	1.303106000
1	1.031822000	0.095846000	-1.058667000
6	-0.041486000	2.764445000	0.064081000
15	1.381997000	3.684419000	0.081673000
6	1.197324000	5.420426000	-0.380593000
1	2.166940000	5.919131000	-0.341630000
1	0.797505000	5.494506000	-1.392533000
1	0.512653000	5.919500000	0.306336000
6	2.196696000	3.693306000	1.693558000
1	1.542010000	4.152355000	2.434829000
1	2.383412000	2.655965000	1.982831000
1	3.146421000	4.230683000	1.652424000
6	2.642908000	3.000780000	-1.009796000
1	2.259566000	2.968803000	-2.030236000
1	3.555259000	3.600001000	-0.971120000
1	2.873467000	1.975903000	-0.697496000
15	-2.676486000	-0.877598000	-0.022046000
6	-3.763353000	0.376852000	-0.475882000
7	-2.151266000	-1.976267000	-1.126967000
7	-2.939484000	-1.769579000	1.349350000
6	-1.527136000	-1.432613000	-2.323356000
1	-1.887751000	-0.420282000	-2.513655000
1	-0.436306000	-1.393896000	-2.218940000
1	-1.788205000	-2.056033000	-3.183053000
6	-1.838063000	-3.367400000	-0.880634000
1	-2.423603000	-3.749549000	-0.046905000
1	-2.087055000	-3.951657000	-1.771423000
1	-0.769602000	-3.499703000	-0.662728000

6	-4.004912000	-1.334248000	2.233389000
1	-4.241172000	-2.143736000	2.929231000
1	-3.717641000	-0.449583000	2.818432000
1	-4.903072000	-1.094699000	1.665233000
6	-1.738496000	-2.180648000	2.072632000
1	-0.884319000	-2.312193000	1.403103000
1	-1.455650000	-1.421400000	2.812529000
1	-1.921779000	-3.126326000	2.591309000
6	-5.146813000	0.590427000	-0.954395000
1	-5.877709000	0.729552000	-0.147648000
1	-5.198342000	1.481973000	-1.586410000
1	-5.497552000	-0.247833000	-1.562132000
13	0.129978000	0.842431000	0.362387000

11AITS^{B-H} (T.E = -1929.142772)

7	0.596145000	-2.404579000	-0.287038000
7	1.444681000	0.165697000	-0.184223000
6	-0.397482000	-3.424970000	-0.223374000
6	-1.388128000	-3.442033000	-1.196711000
6	-0.470040000	-4.328036000	0.832269000
6	-2.438038000	-4.341864000	-1.118268000
1	-1.334633000	-2.739103000	-2.023119000
6	-1.511092000	-5.232808000	0.897493000
1	0.295229000	-4.318108000	1.597204000
6	-2.501044000	-5.244408000	-0.073764000
1	-3.205213000	-4.334585000	-1.883408000
1	-1.555064000	-5.933126000	1.723860000
1	-3.318335000	-5.953146000	-0.011695000
6	2.687724000	-0.397615000	0.103280000
13	-0.135287000	-0.705566000	-0.509691000
6	-3.898716000	1.100116000	0.209586000
6	-2.978235000	2.325896000	-0.042507000
8	-3.168850000	0.046561000	-0.413913000
8	-1.675460000	1.753523000	0.039550000
5	-1.815240000	0.361692000	-0.282044000
6	-3.138274000	2.902676000	-1.440515000
1	-4.093358000	3.417410000	-1.569667000
1	-2.338789000	3.629120000	-1.610977000
1	-3.053146000	2.118985000	-2.196556000
6	-3.101975000	3.431567000	0.981378000
1	-2.444728000	4.262682000	0.709831000
1	-4.124798000	3.817374000	1.019979000
1	-2.821369000	3.088843000	1.978134000
6	-4.042571000	0.772663000	1.686944000
1	-4.662160000	1.504928000	2.210125000
1	-4.516365000	-0.206633000	1.777981000
1	-3.069126000	0.717165000	2.179989000
6	-5.264322000	1.191941000	-0.429757000

1	-5.841623000	0.297723000	-0.186426000
1	-5.813303000	2.061841000	-0.056981000
1	-5.192581000	1.259276000	-1.515180000
1	-1.191765000	-0.357099000	0.926700000
15	2.122639000	1.656285000	0.097992000
6	3.521609000	0.675811000	0.427908000
7	1.318431000	2.486885000	1.246734000
7	2.183941000	2.657194000	-1.200946000
6	0.704399000	1.752051000	2.343631000
1	1.095574000	0.736554000	2.398364000
1	0.924987000	2.257275000	3.287626000
1	-0.379310000	1.694576000	2.194703000
6	0.959623000	3.887923000	1.202108000
1	1.506020000	4.403400000	0.415548000
1	-0.116955000	3.996906000	1.023580000
1	1.202623000	4.358622000	2.159067000
6	3.309339000	2.587847000	-2.114043000
1	3.197351000	1.770940000	-2.838171000
1	3.375178000	3.528183000	-2.667218000
1	4.241111000	2.443945000	-1.568741000
6	0.911563000	2.963427000	-1.852537000
1	0.068996000	2.784272000	-1.178548000
1	0.896008000	4.008088000	-2.176924000
1	0.769264000	2.319209000	-2.727865000
6	4.926233000	0.893850000	0.858114000
1	5.023983000	1.885883000	1.305137000
1	5.247117000	0.179153000	1.619034000
1	5.652948000	0.845718000	0.038202000
7	2.888681000	-1.726010000	0.015390000
6	4.251063000	-2.214101000	0.182901000
1	4.475300000	-2.433555000	1.229268000
1	4.369751000	-3.132076000	-0.384231000
1	4.944832000	-1.463755000	-0.188701000
6	1.879848000	-2.774124000	-0.070317000
8	2.286710000	-3.904366000	0.054807000

13AITS^{B-H} (T.E = -2254.692097)

7	0.570271000	-1.598749000	0.240312000
6	-0.075650000	-2.781957000	-0.237054000
6	-1.446838000	-2.857581000	-0.469665000
1	-1.859591000	-3.796423000	-0.821429000
6	-2.308678000	-1.775246000	-0.335379000
6	2.770372000	2.939531000	-0.269262000
6	1.638810000	3.922206000	0.144970000
8	2.301090000	1.706487000	0.272962000
8	0.473009000	3.109926000	0.082160000
5	0.880418000	1.767614000	0.230005000
6	1.784917000	4.404124000	1.580212000

1	2.613727000	5.106789000	1.698826000
1	0.861914000	4.911329000	1.868382000
1	1.932888000	3.562280000	2.259838000
6	1.466888000	5.109719000	-0.775118000
1	0.663100000	5.747697000	-0.400921000
1	2.381792000	5.708585000	-0.817803000
1	1.204587000	4.797010000	-1.785852000
6	2.891146000	2.788493000	-1.777329000
1	3.298812000	3.686102000	-2.247727000
1	3.567912000	1.956754000	-1.992641000
1	1.923219000	2.561451000	-2.230496000
6	4.127429000	3.245038000	0.321479000
1	4.856287000	2.510960000	-0.032034000
1	4.474130000	4.236570000	0.015615000
1	4.107595000	3.201145000	1.410311000
1	0.430268000	1.019841000	-1.048914000
15	-3.460929000	0.005443000	-0.048955000
15	2.011627000	-2.390251000	0.037355000
6	0.983721000	-3.684121000	-0.434504000
7	3.007980000	-1.689622000	-1.067176000
7	2.930378000	-2.477883000	1.413529000
6	2.380702000	-1.211349000	-2.289285000
1	1.443898000	-1.741931000	-2.468619000
1	2.159219000	-0.139536000	-2.228830000
1	3.047301000	-1.397975000	-3.136080000
6	4.325019000	-1.142877000	-0.825371000
1	4.792983000	-1.634124000	0.025263000
1	4.949776000	-1.313851000	-1.707092000
1	4.278202000	-0.062098000	-0.636194000
6	2.681507000	-3.594536000	2.306784000
1	3.514286000	-3.678381000	3.010016000
1	1.755445000	-3.460868000	2.883053000
1	2.607298000	-4.526432000	1.747136000
6	3.112876000	-1.215612000	2.126171000
1	3.094317000	-0.357271000	1.448812000
1	2.309759000	-1.067193000	2.859182000
1	4.071733000	-1.220651000	2.652702000
6	1.042379000	-5.069318000	-0.950785000
1	0.183520000	-5.273671000	-1.596853000
1	1.938401000	-5.237353000	-1.554457000
1	1.038139000	-5.833569000	-0.163758000
7	-1.897668000	-0.477085000	0.139048000
6	-3.677790000	-1.609009000	-0.599336000
6	-4.714265000	-2.551084000	-1.076764000
1	-4.291784000	-3.255141000	-1.800007000
1	-5.166173000	-3.151661000	-0.276404000
1	-5.529697000	-2.031178000	-1.584757000
7	-3.532166000	1.371952000	-0.965575000
7	-4.266830000	0.455766000	1.326814000

6	-4.631604000	2.311045000	-0.978393000
1	-5.178841000	2.257824000	-1.926713000
1	-5.325741000	2.106048000	-0.165834000
1	-4.253030000	3.333088000	-0.865529000
6	-3.720198000	1.569496000	2.090207000
1	-4.523729000	2.100542000	2.608969000
1	-2.999045000	1.212633000	2.836472000
1	-3.200888000	2.272820000	1.438481000
6	-4.796202000	-0.596431000	2.175489000
1	-5.544615000	-0.168939000	2.847996000
1	-5.270708000	-1.371622000	1.576247000
1	-4.010609000	-1.062010000	2.785794000
6	-2.603727000	1.539531000	-2.071812000
1	-2.050842000	2.478163000	-1.962200000
1	-1.874493000	0.730303000	-2.096202000
1	-3.143845000	1.553349000	-3.024489000
13	-0.169063000	0.065109000	0.406599000

1GaTS^{B-H} (T.E = -3024.789056)

7	-1.271011000	-2.161131000	-0.346780000
6	-0.960023000	-3.434116000	-0.459882000
6	0.315385000	-3.968006000	-0.585056000
7	1.625942000	-1.954917000	-0.306972000
1	0.393376000	-5.036890000	-0.723749000
1	-1.792420000	-4.139613000	-0.449251000
6	-2.597448000	-1.789498000	-0.028662000
6	-3.127261000	-0.626047000	-0.572681000
6	-3.366968000	-2.541626000	0.854259000
6	-4.411624000	-0.231594000	-0.251655000
1	-2.524407000	-0.019819000	-1.239239000
6	-4.657347000	-2.148366000	1.158687000
1	-2.939056000	-3.414356000	1.334548000
6	-5.186163000	-0.993579000	0.607331000
1	-4.805784000	0.683311000	-0.678634000
1	-5.244799000	-2.738713000	1.852317000
1	-6.192375000	-0.680728000	0.859270000
6	2.882872000	-1.403292000	0.029700000
6	3.231060000	-0.151465000	-0.464049000
6	3.762822000	-2.068259000	0.879354000
6	4.448019000	0.412190000	-0.133328000
1	2.539309000	0.388082000	-1.101675000
6	4.984603000	-1.503131000	1.194757000
1	3.473586000	-3.012493000	1.326432000
6	5.334944000	-0.262859000	0.688567000
1	4.699818000	1.391936000	-0.522041000
1	5.658097000	-2.028520000	1.861938000
1	6.287434000	0.183064000	0.948661000
6	1.498478000	-3.258904000	-0.435798000

1	2.421379000	-3.840365000	-0.417627000
6	-1.046891000	3.170727000	0.268170000
6	0.436692000	3.419157000	-0.125188000
8	-1.294914000	1.885988000	-0.319380000
8	0.985218000	2.094833000	-0.118879000
5	-0.079412000	1.219012000	-0.292478000
6	0.588903000	3.963364000	-1.534476000
1	0.264102000	5.003914000	-1.606838000
1	1.643198000	3.914257000	-1.813856000
1	0.020667000	3.366217000	-2.250638000
6	1.213075000	4.275648000	0.846314000
1	2.237560000	4.399019000	0.488706000
1	0.761650000	5.268431000	0.931598000
1	1.254526000	3.822236000	1.836078000
6	-1.251186000	3.035519000	1.766428000
1	-1.160094000	3.996921000	2.276674000
1	-2.255584000	2.643869000	1.942834000
1	-0.538061000	2.334750000	2.205684000
6	-2.032421000	4.162584000	-0.299803000
1	-3.040497000	3.906624000	0.033856000
1	-1.806680000	5.174211000	0.049339000
1	-2.025824000	4.158097000	-1.389475000
1	-0.036232000	0.158961000	0.985919000
31	0.088390000	-0.753625000	-0.568195000

4GaTS^{B-H} (T.E = -3237.590367)

7	-2.181149000	-1.259627000	-0.232421000
6	-2.493525000	-2.556191000	-0.198448000
6	-1.645699000	-3.638115000	-0.144349000
1	-2.117219000	-4.612643000	-0.147907000
1	-3.559417000	-2.784377000	-0.225732000
6	-3.196263000	-0.295898000	-0.089444000
6	-3.020679000	0.965770000	-0.653378000
6	-4.359431000	-0.543036000	0.639895000
6	-3.990667000	1.939041000	-0.516766000
1	-2.109389000	1.182215000	-1.201351000
6	-5.331103000	0.433415000	0.762672000
1	-4.489804000	-1.491592000	1.147307000
6	-5.157304000	1.678678000	0.183603000
1	-3.827788000	2.912812000	-0.964148000
1	-6.225276000	0.222077000	1.338454000
1	-5.916225000	2.444336000	0.291718000
6	-0.240283000	-3.589043000	-0.035266000
1	0.235425000	-4.565286000	0.096088000
6	1.043685000	3.234130000	0.248276000
6	2.368886000	2.499065000	-0.098571000
8	0.061991000	2.369196000	-0.329023000
8	1.978065000	1.125554000	-0.061583000

5	0.574320000	1.080188000	-0.250503000
6	2.853839000	2.790092000	-1.508669000
1	3.246923000	3.804573000	-1.608040000
1	3.656171000	2.088993000	-1.752235000
1	2.049968000	2.650184000	-2.234248000
6	3.493765000	2.712734000	0.887650000
1	4.376618000	2.156755000	0.561531000
1	3.765386000	3.770479000	0.949677000
1	3.222858000	2.363141000	1.884451000
6	0.782709000	3.303714000	1.743021000
1	1.457243000	4.003229000	2.242137000
1	-0.243218000	3.643135000	1.898451000
1	0.879808000	2.320855000	2.210502000
6	0.904671000	4.608279000	-0.362089000
1	-0.045876000	5.049035000	-0.055146000
1	1.709348000	5.266847000	-0.021992000
1	0.920583000	4.567486000	-1.451010000
1	0.014853000	0.311644000	1.101678000
31	-0.315183000	-0.698182000	-0.390017000
6	0.531119000	-2.463087000	-0.078135000
15	2.231793000	-2.501973000	0.157204000
6	2.915916000	-4.161719000	0.332020000
1	3.996748000	-4.096180000	0.465710000
1	2.481046000	-4.658694000	1.199847000
1	2.701905000	-4.751843000	-0.559770000
6	3.116209000	-1.718019000	-1.197000000
1	2.861098000	-2.207001000	-2.137412000
1	2.819059000	-0.665406000	-1.233881000
1	4.192953000	-1.780048000	-1.026012000
6	2.730744000	-1.587807000	1.622667000
1	2.237011000	-2.006073000	2.500294000
1	3.814950000	-1.634146000	1.745382000
1	2.424495000	-0.544840000	1.496306000

6GaTS^{B-H} (T.E = -3368.168344)

7	-0.524761000	1.920865000	-0.253003000
6	-1.573897000	2.609127000	0.042576000
1	-1.447420000	3.682707000	0.206331000
6	0.746611000	2.550547000	-0.209423000
6	1.543831000	2.550264000	-1.343348000
6	1.229522000	3.069253000	0.982918000
6	2.816177000	3.084839000	-1.287076000
1	1.164673000	2.101679000	-2.254622000
6	2.506475000	3.601979000	1.033358000
1	0.614162000	3.008436000	1.874371000
6	3.301455000	3.609666000	-0.099860000
1	3.439631000	3.077755000	-2.173216000
1	2.886178000	3.997494000	1.968211000

1	4.304601000	4.017149000	-0.056102000
6	-3.333931000	0.798375000	0.115743000
6	3.455338000	-1.024475000	0.328901000
6	2.917461000	-2.461548000	0.072982000
8	2.463616000	-0.219876000	-0.313442000
8	1.498827000	-2.270916000	0.070788000
5	1.267354000	-0.919864000	-0.204250000
6	3.301572000	-2.997428000	-1.295472000
1	4.363948000	-3.246280000	-1.354445000
1	2.726221000	-3.905526000	-1.486635000
1	3.064111000	-2.274971000	-2.079001000
6	3.280306000	-3.468187000	1.139323000
1	2.872344000	-4.446556000	0.876057000
1	4.366639000	-3.566417000	1.224801000
1	2.877123000	-3.183884000	2.110978000
6	3.473111000	-0.646068000	1.799972000
1	4.261483000	-1.168226000	2.346984000
1	3.653059000	0.429339000	1.873073000
1	2.512146000	-0.854507000	2.275587000
6	4.797615000	-0.722667000	-0.293645000
1	5.077281000	0.308383000	-0.064964000
1	5.571488000	-1.383694000	0.107516000
1	4.770593000	-0.830237000	-1.377839000
1	0.402551000	-0.336613000	1.117266000
31	-0.529356000	-0.075830000	-0.432641000
6	-2.441539000	-0.239868000	-0.171582000
15	-3.154963000	-1.785759000	-0.040263000
6	-4.516011000	-2.124058000	-1.175359000
1	-4.907544000	-3.131008000	-1.017401000
1	-5.300583000	-1.388149000	-1.001964000
1	-4.156339000	-2.029731000	-2.200564000
6	-1.916117000	-3.045468000	-0.370175000
1	-1.526474000	-2.930162000	-1.382974000
1	-1.077512000	-2.949167000	0.324820000
1	-2.359451000	-4.037218000	-0.264457000
6	-3.801276000	-2.170794000	1.599728000
1	-4.564054000	-1.435788000	1.855586000
1	-4.229925000	-3.174671000	1.622921000
1	-2.982780000	-2.105843000	2.318363000
8	-4.539231000	0.695451000	0.342462000
7	-2.834686000	2.179448000	0.171607000
6	-3.861391000	3.173667000	0.451484000
1	-4.630073000	3.155183000	-0.320103000
1	-4.345715000	2.967292000	1.404956000
1	-3.403451000	4.161114000	0.480798000

8GaTS^{B-H} (T.E = -3602.209562)

7	-0.354855000	1.569641000	-0.901361000
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6	-1.673329000	2.073879000	-0.784492000
6	-2.740953000	1.432627000	-1.554462000
15	0.021800000	2.569287000	0.363888000
6	-1.649840000	3.059840000	0.163872000
6	-2.670131000	3.972086000	0.722455000
1	-2.472425000	5.023655000	0.493481000
1	-3.654005000	3.730621000	0.310867000
1	-2.748654000	3.892347000	1.811682000
7	0.327414000	1.968420000	1.858695000
7	1.314025000	3.495660000	-0.020228000
6	1.662497000	1.536044000	2.247040000
1	1.702321000	0.443054000	2.280564000
1	2.408142000	1.861416000	1.522144000
1	1.909391000	1.941226000	3.233542000
6	-0.724498000	1.306716000	2.616984000
1	-0.556650000	1.473116000	3.684659000
1	-1.701735000	1.705144000	2.347222000
1	-0.721080000	0.227444000	2.419678000
6	1.744190000	4.559580000	0.858685000
1	2.692827000	4.311531000	1.351646000
1	1.887747000	5.482810000	0.288755000
1	0.999243000	4.749228000	1.633240000
6	2.215371000	3.200471000	-1.118641000
1	1.838349000	2.367668000	-1.708444000
1	2.327534000	4.080031000	-1.760206000
1	3.202005000	2.915902000	-0.731859000
6	-2.010603000	-2.001651000	0.191236000
6	-2.748198000	-1.966577000	1.377108000
6	-1.267701000	-3.150127000	-0.081579000
6	-2.753606000	-3.044277000	2.242779000
1	-3.313714000	-1.069908000	1.612786000
6	-1.261867000	-4.219322000	0.795752000
1	-0.676452000	-3.189346000	-0.992257000
6	-2.009430000	-4.179104000	1.960878000
1	-3.335827000	-2.990651000	3.156446000
1	-0.665184000	-5.093880000	0.561683000
1	-2.006618000	-5.018563000	2.645780000
7	-1.945193000	-0.883679000	-0.655255000
5	-3.049776000	-0.066971000	-1.022060000
7	-4.404193000	-0.517096000	-1.037343000
6	-4.779804000	-1.911276000	-1.081642000
1	-3.921996000	-2.544564000	-1.298115000
1	-5.222603000	-2.253531000	-0.136537000
1	-5.525219000	-2.066719000	-1.871461000
6	-5.569153000	0.329641000	-1.018107000
1	-5.311496000	1.373147000	-0.844542000
1	-6.138764000	0.266146000	-1.955474000
1	-6.247436000	0.025577000	-0.210003000
1	-3.629738000	2.061190000	-1.589874000

1	-2.388962000	1.312514000	-2.588064000
31	-0.130226000	-0.380714000	-1.013741000
1	0.708536000	-0.703791000	0.574349000
6	3.996054000	-0.696807000	-0.497818000
6	3.575652000	-2.145707000	-0.115004000
5	1.750094000	-0.982009000	-0.746398000
8	2.744187000	-0.009610000	-0.540708000
8	2.286076000	-2.256771000	-0.725580000
6	4.606527000	-0.602140000	-1.885577000
1	4.676579000	0.453367000	-2.160028000
1	5.608954000	-1.034766000	-1.926336000
1	3.976104000	-1.100591000	-2.624599000
6	4.897592000	-0.015255000	0.505782000
1	5.840231000	-0.559045000	0.616038000
1	5.131563000	0.995439000	0.160873000
1	4.424560000	0.061463000	1.485137000
6	3.391032000	-2.340150000	1.379794000
1	2.907354000	-3.305222000	1.544203000
1	4.343308000	-2.334327000	1.915072000
1	2.739997000	-1.572213000	1.803014000
6	4.473850000	-3.227990000	-0.664592000
1	5.496412000	-3.106399000	-0.295143000
1	4.110297000	-4.204870000	-0.339920000
1	4.491122000	-3.220486000	-1.754023000

10GaTS^{B-H} (T.E = -3693.716577)

7	-1.637342000	0.335161000	0.159260000
6	-2.688902000	1.199342000	-0.236684000
6	-2.524508000	2.581772000	-0.356880000
1	-3.404166000	3.164028000	-0.606482000
6	-1.308384000	3.248989000	-0.227403000
1	-1.390160000	4.329778000	-0.380793000
6	2.422179000	-2.671178000	-0.311766000
6	3.577750000	-1.758768000	0.189123000
8	1.268185000	-1.982749000	0.177656000
8	2.993229000	-0.457256000	0.149184000
5	1.601048000	-0.617796000	0.205305000
6	3.959252000	-2.038216000	1.633614000
1	4.488729000	-2.987902000	1.743051000
1	4.617210000	-1.238018000	1.978427000
1	3.076217000	-2.049101000	2.275975000
6	4.814931000	-1.774712000	-0.678470000
1	5.573430000	-1.118468000	-0.246113000
1	5.235310000	-2.783041000	-0.739314000
1	4.600041000	-1.422993000	-1.687362000
6	2.330007000	-2.725970000	-1.827261000
1	3.162004000	-3.279897000	-2.267518000
1	1.401381000	-3.232835000	-2.102865000

1	2.303693000	-1.721748000	-2.257189000
6	2.426267000	-4.072524000	0.252350000
1	1.583121000	-4.634388000	-0.157475000
1	3.345520000	-4.600229000	-0.018187000
1	2.331191000	-4.068159000	1.338086000
1	0.995947000	0.088903000	-1.212156000
31	0.204470000	0.800043000	0.296547000
6	-0.046806000	2.737785000	0.046049000
15	1.370981000	3.662913000	0.031693000
6	1.145508000	5.423706000	-0.297535000
1	2.111919000	5.929775000	-0.280139000
1	0.687857000	5.562861000	-1.277567000
1	0.497565000	5.865126000	0.460619000
6	2.291107000	3.563044000	1.581927000
1	1.685056000	3.962738000	2.395349000
1	2.500746000	2.509764000	1.784828000
1	3.233675000	4.110362000	1.515753000
6	2.561458000	3.073146000	-1.188024000
1	2.116660000	3.127667000	-2.182244000
1	3.481556000	3.660561000	-1.154977000
1	2.793021000	2.024896000	-0.975578000
15	-2.681852000	-0.928734000	-0.046896000
6	-3.775279000	0.333820000	-0.467994000
7	-2.176321000	-2.027593000	-1.161559000
7	-2.936302000	-1.833284000	1.321142000
6	-1.563142000	-1.488998000	-2.364641000
1	-1.881582000	-0.457562000	-2.524238000
1	-0.469392000	-1.496862000	-2.291212000
1	-1.875521000	-2.082209000	-3.229054000
6	-1.930369000	-3.434757000	-0.947170000
1	-2.509660000	-3.800318000	-0.101659000
1	-2.231615000	-3.993692000	-1.838568000
1	-0.864749000	-3.627781000	-0.761225000
6	-3.970793000	-1.375904000	2.230465000
1	-4.199797000	-2.177005000	2.938485000
1	-3.654591000	-0.491356000	2.800955000
1	-4.880239000	-1.126781000	1.684934000
6	-1.726356000	-2.260540000	2.018618000
1	-0.891771000	-2.408933000	1.328714000
1	-1.412342000	-1.501802000	2.746675000
1	-1.913162000	-3.200051000	2.547399000
6	-5.175396000	0.563575000	-0.887582000
1	-5.246075000	1.465823000	-1.502500000
1	-5.555428000	-0.261537000	-1.495836000
1	-5.875054000	0.693745000	-0.051475000

11GaTS^{B-H} (T.E = -3611.504198)

7	-0.533110000	2.402479000	-0.239146000
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7	-1.459275000	-0.202364000	-0.102568000
6	0.462857000	3.413059000	-0.138129000
6	1.532380000	3.378781000	-1.024889000
6	0.457790000	4.370453000	0.871760000
6	2.577592000	4.278556000	-0.908237000
1	1.543979000	2.633866000	-1.815252000
6	1.498725000	5.272426000	0.977164000
1	-0.367526000	4.406097000	1.570003000
6	2.564224000	5.233555000	0.091118000
1	3.403406000	4.229555000	-1.608307000
1	1.479975000	6.012408000	1.769378000
1	3.378982000	5.941915000	0.183730000
6	-2.691593000	0.409349000	0.101787000
6	3.892595000	-1.261002000	0.193058000
6	2.941438000	-2.458661000	-0.081907000
8	3.179817000	-0.171340000	-0.407116000
8	1.650584000	-1.845796000	-0.007608000
5	1.839407000	-0.478556000	-0.292224000
6	3.094229000	-3.022851000	-1.484588000
1	4.032554000	-3.568357000	-1.607893000
1	2.272047000	-3.717520000	-1.674220000
1	3.047092000	-2.228942000	-2.233013000
6	3.009366000	-3.576940000	0.931119000
1	2.301017000	-4.363090000	0.653947000
1	4.008621000	-4.020666000	0.958491000
1	2.755264000	-3.229119000	1.932788000
6	4.043127000	-0.958494000	1.673198000
1	4.642263000	-1.716329000	2.183201000
1	4.543502000	0.005633000	1.779933000
1	3.070741000	-0.882849000	2.165842000
6	5.251891000	-1.370084000	-0.453928000
1	5.850566000	-0.494591000	-0.195748000
1	5.779752000	-2.259323000	-0.097026000
1	5.177066000	-1.417715000	-1.540040000
1	1.151946000	0.318508000	1.065468000
15	-2.193493000	-1.657279000	0.170916000
6	-3.576200000	-0.628431000	0.419897000
7	-1.416513000	-2.496877000	1.335667000
7	-2.270186000	-2.692386000	-1.104057000
6	-0.732472000	-1.787273000	2.405297000
1	-0.907562000	-0.714937000	2.336829000
1	-1.088115000	-2.144274000	3.376151000
1	0.347725000	-1.950760000	2.325668000
6	-1.289380000	-3.934894000	1.410720000
1	-1.874288000	-4.420038000	0.632390000
1	-0.237245000	-4.224789000	1.296459000
1	-1.639037000	-4.293112000	2.383979000
6	-3.334899000	-2.548702000	-2.079858000
1	-3.118861000	-1.752851000	-2.803995000

1	-3.442474000	-3.488701000	-2.627122000
1	-4.280895000	-2.324740000	-1.589491000
6	-1.002856000	-3.127078000	-1.685148000
1	-0.187739000	-3.034771000	-0.964073000
1	-1.078073000	-4.167253000	-2.015495000
1	-0.742883000	-2.500906000	-2.547241000
6	-5.007906000	-0.791033000	0.780531000
1	-5.164642000	-1.774527000	1.229670000
1	-5.340269000	-0.058788000	1.519869000
1	-5.692996000	-0.724897000	-0.073888000
7	-2.851177000	1.738118000	-0.047877000
6	-4.211294000	2.258230000	0.017590000
1	-4.488909000	2.538010000	1.036290000
1	-4.282420000	3.145968000	-0.603040000
1	-4.897034000	1.500184000	-0.352583000
6	-1.823748000	2.771942000	-0.095274000
8	-2.229756000	3.907940000	-0.007461000
31	0.214322000	0.645448000	-0.448955000

$^{13}\text{GaTS}^{\text{B-H}}$ (T.E = -3937.052055)

7	-1.735702000	0.413545000	0.275853000
6	-2.764886000	1.271601000	-0.207892000
6	-2.584584000	2.631090000	-0.447445000
1	-3.431436000	3.210045000	-0.799181000
6	-1.363422000	3.281466000	-0.323495000
6	2.326831000	-2.610267000	-0.461894000
6	3.520586000	-1.683342000	-0.093681000
8	1.222813000	-1.922623000	0.139206000
8	2.922955000	-0.385123000	-0.081303000
5	1.556403000	-0.560855000	0.113153000
6	4.056850000	-1.945172000	1.303685000
1	4.606103000	-2.887974000	1.362814000
1	4.737933000	-1.134631000	1.569820000
1	3.248147000	-1.960333000	2.037229000
6	4.657112000	-1.694544000	-1.089149000
1	5.451716000	-1.029801000	-0.743848000
1	5.076699000	-2.699993000	-1.189483000
1	4.332566000	-1.349767000	-2.070703000
6	2.075131000	-2.682374000	-1.958143000
1	2.860653000	-3.235455000	-2.477488000
1	1.126895000	-3.199120000	-2.128938000
1	1.996133000	-1.683522000	-2.394142000
6	2.404031000	-4.004416000	0.113547000
1	1.532494000	-4.582327000	-0.203459000
1	3.298748000	-4.522674000	-0.243378000
1	2.419845000	-3.988603000	1.203057000
1	0.771889000	0.118394000	-1.261151000
31	0.122589000	0.795993000	0.325304000

15	0.591008000	4.112549000	-0.063311000
15	-2.781285000	-0.850923000	0.059251000
6	-3.856740000	0.404216000	-0.405045000
7	-2.305334000	-1.963116000	-1.056715000
7	-3.026287000	-1.746763000	1.437116000
6	-1.792951000	-1.437539000	-2.312624000
1	-2.155402000	-0.420674000	-2.473132000
1	-0.697526000	-1.409562000	-2.316895000
1	-2.144910000	-2.063114000	-3.138241000
6	-1.956599000	-3.344304000	-0.806648000
1	-2.502069000	-3.726104000	0.054178000
1	-2.231429000	-3.943465000	-1.679857000
1	-0.878160000	-3.459902000	-0.630289000
6	-4.068189000	-1.281515000	2.335029000
1	-4.287897000	-2.068920000	3.060894000
1	-3.764668000	-0.379323000	2.884633000
1	-4.980089000	-1.057184000	1.782444000
6	-1.808112000	-2.125766000	2.147346000
1	-0.974267000	-2.293723000	1.460836000
1	-1.502432000	-1.334601000	2.844129000
1	-1.979180000	-3.046218000	2.713155000
6	-5.233244000	0.614494000	-0.905269000
1	-5.579761000	-0.234725000	-1.500701000
1	-5.973585000	0.772039000	-0.110758000
1	-5.273985000	1.493017000	-1.556111000
7	-0.150947000	2.657636000	0.127836000
6	-0.970072000	4.606852000	-0.582838000
6	-1.739475000	5.801135000	-0.998707000
1	-2.395267000	5.579469000	-1.847049000
1	-2.377370000	6.206208000	-0.201819000
1	-1.077319000	6.608869000	-1.317934000
7	1.938238000	3.957952000	-1.003431000
7	1.198356000	4.824874000	1.306905000
6	2.994933000	4.943050000	-1.080810000
1	2.926871000	5.522024000	-2.009860000
1	2.946380000	5.631573000	-0.239511000
1	3.969681000	4.443474000	-1.067925000
6	2.231047000	4.102854000	2.037112000
1	2.851833000	4.806418000	2.599302000
1	1.785214000	3.390155000	2.743312000
1	2.870267000	3.541969000	1.355338000
6	0.246900000	5.473521000	2.192225000
1	0.789952000	6.125729000	2.881211000
1	-0.457104000	6.078284000	1.623037000
1	-0.322331000	4.743659000	2.783902000
6	1.897465000	3.062189000	-2.147395000
1	2.813212000	2.464092000	-2.180306000
1	1.057277000	2.371740000	-2.075023000
1	1.812297000	3.628031000	-3.082293000

Cartesian coordinates of the H–H splitting products obtained for some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AIP^{H-H} (T.E = -932.079238)

7	1.430642000	0.494458000	-0.303244000
6	1.229907000	1.768847000	-0.570368000
6	0.000001000	2.386576000	-0.745866000
7	-1.430642000	0.494458000	-0.303242000
1	0.000000000	3.436287000	-1.002445000
1	2.116279000	2.397852000	-0.668122000
6	2.742667000	0.050848000	-0.025257000
6	3.132903000	-1.209033000	-0.468596000
6	3.639632000	0.818443000	0.711751000
6	4.404691000	-1.679347000	-0.200749000
1	2.437618000	-1.807801000	-1.049362000
6	4.912557000	0.344011000	0.969801000
1	3.325609000	1.775100000	1.113884000
6	5.302465000	-0.904024000	0.513850000
1	4.696862000	-2.659515000	-0.558792000
1	5.599670000	0.949426000	1.549584000
1	6.297903000	-1.275472000	0.725055000
6	-2.742668000	0.050849000	-0.025256000
6	-3.132897000	-1.209040000	-0.468581000
6	-3.639640000	0.818449000	0.711739000
6	-4.404685000	-1.679355000	-0.200736000
1	-2.437608000	-1.807811000	-1.049338000
6	-4.912564000	0.344014000	0.969787000
1	-3.325623000	1.775110000	1.113864000
6	-5.302466000	-0.904027000	0.513849000
1	-4.696850000	-2.659529000	-0.558769000
1	-5.599682000	0.949434000	1.549560000
1	-6.297903000	-1.275476000	0.725053000
6	-1.229905000	1.768847000	-0.570369000
1	-2.116277000	2.397852000	-0.668127000
13	0.000000000	-0.806205000	-0.248641000
1	0.000004000	-1.555906000	1.143427000
1	-0.000001000	-1.677657000	-1.577723000

4AIP^{H-H} (T.E = -1144.858171)

7	1.233783000	0.501094000	-0.268516000
6	0.951336000	1.796743000	-0.427310000
6	-0.288598000	2.387983000	-0.487056000
6	-1.519160000	1.723662000	-0.308249000
6	-1.687098000	0.373942000	-0.156113000

6	2.574753000	0.126417000	-0.072916000
6	3.011679000	-1.102589000	-0.565168000
6	3.479401000	0.919938000	0.632024000
6	4.317554000	-1.513165000	-0.377871000
1	2.318178000	-1.725792000	-1.122388000
6	4.787101000	0.506241000	0.808464000
1	3.145191000	1.851299000	1.074718000
6	5.216646000	-0.709738000	0.304118000
1	4.636680000	-2.469659000	-0.775930000
1	5.473241000	1.135713000	1.364126000
1	6.240131000	-1.033252000	0.450972000
1	1.809312000	2.462786000	-0.529919000
15	-3.221631000	-0.296965000	0.161060000
6	-4.635464000	0.815081000	0.014645000
1	-5.557358000	0.270436000	0.224796000
1	-4.540300000	1.636431000	0.725862000
1	-4.682795000	1.225595000	-0.994622000
6	-3.555694000	-1.684414000	-0.936344000
1	-3.553180000	-1.338572000	-1.970558000
1	-2.756770000	-2.421117000	-0.825968000
1	-4.514001000	-2.150080000	-0.699638000
6	-3.318050000	-0.998361000	1.818549000
1	-3.243544000	-0.195686000	2.553122000
1	-4.250215000	-1.547654000	1.964378000
1	-2.466446000	-1.668782000	1.954424000
1	-2.387565000	2.390641000	-0.288360000
1	-0.305178000	3.459101000	-0.643793000
13	-0.119333000	-0.867485000	-0.292113000
1	-0.008940000	-1.823379000	0.991377000
1	-0.123555000	-1.684339000	-1.672039000

6AIP^{H-H} (T.E = -1275.439206)

6	-1.502812000	1.248032000	-0.105410000
6	-1.480924000	-0.144756000	-0.025450000
6	1.011275000	1.430136000	-0.218159000
1	1.811573000	2.171397000	-0.277761000
13	0.084220000	-1.313501000	-0.122450000
7	1.357887000	0.180990000	-0.146543000
15	-3.059712000	-0.765792000	0.133502000
6	-3.958391000	-0.257307000	1.615573000
1	-4.040523000	0.829303000	1.612272000
1	-4.953984000	-0.705174000	1.639259000
1	-3.395556000	-0.572038000	2.495181000
6	-4.186310000	-0.408952000	-1.232744000
1	-3.766509000	-0.818177000	-2.152513000
1	-5.168609000	-0.850104000	-1.051490000
1	-4.276769000	0.672567000	-1.330128000
6	-2.986624000	-2.562326000	0.221692000

1	-2.378516000	-2.863852000	1.076736000
1	-3.989324000	-2.979781000	0.325888000
1	-2.526784000	-2.955104000	-0.687555000
8	-2.472445000	2.007710000	-0.079256000
7	-0.210287000	1.954976000	-0.241854000
6	-0.327423000	3.399367000	-0.380665000
1	-0.905275000	3.650033000	-1.269431000
1	-0.844776000	3.823572000	0.478545000
1	0.667479000	3.834730000	-0.461901000
6	2.743571000	-0.100460000	-0.028839000
6	3.279495000	-1.150480000	-0.764768000
6	3.562561000	0.619299000	0.833524000
6	4.624023000	-1.452598000	-0.659140000
1	2.629084000	-1.716898000	-1.423335000
6	4.909094000	0.314802000	0.928536000
1	3.134881000	1.395805000	1.458515000
6	5.445776000	-0.718788000	0.181017000
1	5.033510000	-2.269546000	-1.241691000
1	5.537782000	0.879132000	1.607493000
1	6.498519000	-0.961101000	0.263109000
1	0.422700000	-2.177965000	1.178311000
1	0.258399000	-2.133644000	-1.488347000

8AIP^{H-H} (T.E = -1509.492255)

7	1.408846000	0.431620000	-1.131783000
6	1.057702000	1.528259000	-0.298764000
6	-0.059236000	2.383951000	-0.690206000
15	2.349455000	-0.068656000	0.134374000
6	1.802736000	1.432751000	0.846598000
6	1.870601000	2.243946000	2.081386000
1	2.848788000	2.708698000	2.235416000
1	1.132770000	3.049997000	2.036870000
1	1.651342000	1.658989000	2.980414000
7	1.937072000	-1.409896000	0.983782000
7	3.886007000	-0.366488000	-0.371268000
6	2.201148000	-2.746956000	0.466125000
1	1.301338000	-3.157519000	-0.002269000
1	2.989924000	-2.724474000	-0.283660000
1	2.511349000	-3.399287000	1.288068000
6	0.769071000	-1.375692000	1.853771000
1	0.921940000	-2.071347000	2.683102000
1	0.615342000	-0.375936000	2.256955000
1	-0.138269000	-1.670670000	1.312688000
6	4.906439000	-0.847034000	0.539595000
1	5.521504000	-1.603945000	0.042712000
1	5.565288000	-0.031122000	0.859317000
1	4.457168000	-1.295775000	1.424270000
6	4.419302000	0.334757000	-1.526348000

1	3.609206000	0.643568000	-2.183582000
1	4.993146000	1.219056000	-1.224696000
1	5.086074000	-0.334170000	-2.077535000
13	-0.069652000	-0.464860000	-1.978255000
6	-2.353914000	-0.744836000	-0.337534000
6	-2.696897000	-0.788228000	1.018860000
6	-2.919185000	-1.712330000	-1.172707000
6	-3.574094000	-1.738254000	1.507651000
1	-2.260540000	-0.051003000	1.687123000
6	-3.788675000	-2.667965000	-0.679127000
1	-2.676384000	-1.694759000	-2.231326000
6	-4.127617000	-2.688349000	0.663737000
1	-3.822127000	-1.740761000	2.563791000
1	-4.210763000	-3.402578000	-1.356095000
1	-4.811883000	-3.435017000	1.048339000
7	-1.437719000	0.186505000	-0.830797000
5	-1.448644000	1.564259000	-0.476077000
7	-2.591382000	2.291723000	-0.027111000
6	-3.950128000	1.852002000	-0.245790000
1	-3.987492000	1.007311000	-0.930138000
1	-4.445288000	1.554167000	0.688399000
1	-4.536143000	2.669487000	-0.683946000
6	-2.566796000	3.555284000	0.663417000
1	-1.558867000	3.836199000	0.964357000
1	-2.982116000	4.367250000	0.050629000
1	-3.173600000	3.501242000	1.576843000
1	-0.036703000	3.333567000	-0.158110000
1	0.011375000	2.599883000	-1.763947000
1	0.188580000	-2.027237000	-1.750713000
1	-0.220581000	0.055818000	-3.474923000

10AIP^{H-H} (T.E = -1600.982747)

7	0.577962000	-0.068589000	-0.156208000
6	0.569116000	1.360169000	-0.261880000
6	-0.594264000	2.120735000	-0.270779000
6	-1.883046000	1.592912000	-0.170107000
1	-0.475984000	3.193211000	-0.380460000
1	-2.666852000	2.353693000	-0.260109000
15	2.215482000	0.043362000	-0.073322000
6	1.930561000	1.715899000	-0.317873000
6	2.607960000	3.031853000	-0.331745000
1	2.370970000	3.615604000	-1.227991000
1	2.337171000	3.653576000	0.532124000
1	3.693954000	2.915369000	-0.311298000
6	-2.258738000	0.274683000	0.034729000
15	-3.885836000	-0.178656000	-0.001717000
6	-5.106537000	1.151667000	0.107653000
1	-6.114116000	0.732538000	0.100687000

1	-4.956755000	1.717431000	1.027841000
1	-5.000760000	1.827448000	-0.741829000
6	-4.285012000	-1.321057000	1.336170000
1	-5.324270000	-1.650330000	1.278239000
1	-3.627710000	-2.190597000	1.263882000
1	-4.098014000	-0.836419000	2.294874000
6	-4.347399000	-1.101571000	-1.488203000
1	-4.255343000	-0.448154000	-2.356742000
1	-3.642968000	-1.928066000	-1.604293000
1	-5.366370000	-1.489771000	-1.424638000
7	2.931813000	-0.385278000	1.361984000
7	2.926504000	-1.003010000	-1.144637000
6	2.845120000	-1.778100000	1.784213000
1	1.884695000	-1.981339000	2.276329000
1	2.936977000	-2.445707000	0.928691000
1	3.653717000	-1.998318000	2.486971000
6	2.744472000	0.532287000	2.474778000
1	3.467569000	0.291930000	3.258475000
1	2.904518000	1.560709000	2.154743000
1	1.734366000	0.452357000	2.899562000
6	4.365403000	-1.162984000	-1.194762000
1	4.611941000	-2.188026000	-1.489277000
1	4.821044000	-0.483761000	-1.927415000
1	4.808941000	-0.967603000	-0.219566000
6	2.284418000	-1.188453000	-2.434154000
1	1.202161000	-1.133356000	-2.327169000
1	2.610776000	-0.433453000	-3.161061000
1	2.545230000	-2.176303000	-2.823427000
13	-0.880747000	-1.156698000	0.290551000
1	-1.068308000	-2.380759000	-0.745471000
1	-0.767847000	-1.685515000	1.810535000

11AIP^{H-H} (T.E = -1518.791166)

7	-0.749195000	-0.199775000	0.276328000
6	-0.819953000	1.179819000	0.017828000
6	1.676170000	1.510390000	-0.029126000
15	-2.393893000	-0.219411000	0.120955000
6	-2.183601000	1.487423000	-0.067134000
6	-3.051052000	2.666501000	-0.329064000
1	-3.037196000	3.408633000	0.473987000
1	-2.805370000	3.187062000	-1.259424000
1	-4.088503000	2.335675000	-0.424590000
7	-3.043943000	-0.991302000	-1.179105000
7	-3.063791000	-0.992655000	1.407984000
6	-2.951182000	-2.445137000	-1.262443000
1	-2.027477000	-2.743787000	-1.772897000
1	-2.954736000	-2.890362000	-0.268590000
1	-3.805290000	-2.834722000	-1.822623000

6	-2.944848000	-0.354069000	-2.485084000
1	-3.700090000	-0.786865000	-3.145527000
1	-3.124358000	0.716542000	-2.405889000
1	-1.956334000	-0.514631000	-2.932729000
6	-4.491446000	-1.233517000	1.492610000
1	-4.673750000	-2.222446000	1.924248000
1	-4.981868000	-0.489282000	2.131062000
1	-4.948452000	-1.199449000	0.504688000
6	-2.398983000	-0.952953000	2.700614000
1	-1.321520000	-0.875907000	2.568558000
1	-2.749624000	-0.109633000	3.307042000
1	-2.618016000	-1.878300000	3.239437000
7	0.277606000	1.939596000	-0.111880000
6	0.060227000	3.366751000	-0.302566000
1	-0.392825000	3.561348000	-1.276262000
1	-0.586550000	3.762880000	0.480816000
1	1.025859000	3.858690000	-0.249081000
8	2.499354000	2.390574000	0.070271000
7	1.909668000	0.189456000	-0.114789000
6	3.266868000	-0.222916000	-0.022520000
6	4.098478000	0.167088000	1.022124000
6	3.748706000	-1.119311000	-0.968733000
6	5.384764000	-0.328534000	1.106775000
1	3.729419000	0.864777000	1.762762000
6	5.036410000	-1.620863000	-0.874083000
1	3.105374000	-1.412134000	-1.793617000
6	5.861442000	-1.225211000	0.162079000
1	6.023077000	-0.014620000	1.925046000
1	5.394719000	-2.319374000	-1.621552000
1	6.870945000	-1.612055000	0.236507000
13	0.697447000	-1.259269000	-0.292874000
1	0.438101000	-1.696043000	-1.814471000
1	0.966816000	-2.428926000	0.746538000

13AIP^{H-H} (T.E = -1844.338563)

7	-1.361382000	-0.220381000	0.096947000
6	-1.221411000	1.208045000	0.059431000
6	0.000003000	1.865691000	0.001111000
6	1.221403000	1.208105000	-0.058158000
1	0.000020000	2.950446000	0.001993000
13	0.000016000	-1.503062000	-0.000666000
15	-2.982578000	0.030653000	0.037967000
6	-2.543684000	1.686703000	0.075951000
6	-3.101216000	3.052001000	-0.053104000
1	-2.807294000	3.705212000	0.775622000
1	-2.782446000	3.549638000	-0.978376000
1	-4.193332000	3.030752000	-0.063717000
7	1.361342000	-0.220268000	-0.097893000

6	2.543694000	1.686755000	-0.073730000
15	2.982527000	0.030642000	-0.038040000
6	3.101252000	3.051834000	0.057509000
1	2.806859000	3.706492000	-0.769904000
1	2.782974000	3.547841000	0.983829000
1	4.193374000	3.030600000	0.067481000
7	3.786412000	-0.504505000	1.312642000
7	3.748077000	-0.799704000	-1.252475000
6	3.838406000	-1.941160000	1.552817000
1	2.908843000	-2.298318000	2.015972000
1	3.983495000	-2.482991000	0.619485000
1	4.672043000	-2.169773000	2.222417000
6	3.546423000	0.242134000	2.537453000
1	2.562332000	0.008941000	2.967360000
1	4.313257000	-0.021405000	3.270232000
1	3.595901000	1.313629000	2.349832000
6	3.092638000	-0.839863000	-2.549356000
1	3.444140000	-1.717683000	-3.097610000
1	2.013464000	-0.919839000	-2.427559000
1	3.320145000	0.053894000	-3.144741000
6	5.194668000	-0.799408000	-1.351628000
1	5.555754000	0.032100000	-1.971470000
1	5.649319000	-0.717907000	-0.365621000
1	5.530566000	-1.732710000	-1.813752000
7	-3.747766000	-0.801438000	1.251419000
7	-3.786818000	-0.502558000	-1.313288000
6	-5.194339000	-0.802076000	1.350768000
1	-5.529700000	-1.736397000	1.811229000
1	-5.555752000	0.028103000	1.972192000
1	-5.649174000	-0.718985000	0.364983000
6	-3.092114000	-0.843205000	2.548138000
1	-2.012917000	-0.922506000	2.426077000
1	-3.319958000	0.049563000	3.144872000
1	-3.443107000	-1.722002000	3.095154000
6	-3.547227000	0.245987000	-2.537018000
1	-4.314031000	-0.016771000	-3.270107000
1	-3.597106000	1.317186000	-2.347820000
1	-2.563087000	0.013814000	-2.967368000
6	-3.838374000	-1.938869000	-1.555647000
1	-3.983189000	-2.482180000	-0.623134000
1	-4.672008000	-2.166732000	-2.225505000
1	-2.908741000	-2.295029000	-2.019430000
1	0.098525000	-2.375519000	1.343221000
1	-0.098411000	-2.375148000	-1.344772000

1GaP^{H-H} (T.E = -2614.436783)

7	-0.581606000	-0.294446000	1.464712000
7	-0.581606000	-0.294446000	-1.464712000

6	-1.843111000	-0.583587000	1.236477000
6	-1.843111000	-0.583587000	-1.236477000
6	-2.443652000	-0.779527000	0.000000000
1	-3.488155000	-1.057730000	0.000000000
6	-0.160180000	0.012682000	2.772210000
6	-0.966828000	0.716360000	3.663192000
6	1.116621000	-0.368180000	3.175513000
6	-0.514254000	0.999901000	4.938720000
6	1.564266000	-0.076284000	4.449721000
6	0.750212000	0.603805000	5.340303000
1	-1.151296000	1.553538000	5.618865000
1	2.558026000	-0.387476000	4.749815000
1	1.104004000	0.834914000	6.337719000
6	-0.160180000	0.012682000	-2.772210000
6	1.116621000	-0.368180000	-3.175513000
6	-0.966828000	0.716360000	-3.663192000
6	1.564266000	-0.076284000	-4.449721000
6	-0.514254000	0.999901000	-4.938720000
6	0.750212000	0.603805000	-5.340303000
1	2.558026000	-0.387476000	-4.749815000
1	-1.151296000	1.553538000	-5.618865000
1	1.104004000	0.834914000	-6.337719000
1	-1.938674000	1.073863000	-3.342262000
1	1.749062000	-0.920708000	-2.487834000
1	1.749062000	-0.920708000	2.487834000
1	-1.938674000	1.073863000	3.342262000
31	0.781016000	-0.265587000	0.000000000
1	-2.488607000	-0.683747000	-2.111381000
1	-2.488607000	-0.683747000	2.111381000
1	1.558935000	-1.634851000	0.000000000
1	1.496374000	1.128062000	0.000000000

4GaP^{H-H} (T.E = -2827.221870)

7	1.280790000	0.602179000	-0.251887000
6	0.987140000	1.883453000	-0.442464000
6	-0.257743000	2.471853000	-0.517337000
6	-1.490306000	1.824351000	-0.316920000
6	-1.685798000	0.483169000	-0.131484000
6	2.615929000	0.229019000	-0.043520000
6	3.046651000	-1.024670000	-0.476421000
6	3.529777000	1.052583000	0.615554000
6	4.353442000	-1.427903000	-0.282226000
1	2.344968000	-1.674135000	-0.989883000
6	4.837816000	0.644225000	0.801465000
1	3.202592000	2.004954000	1.016650000
6	5.261053000	-0.595191000	0.352196000
1	4.666582000	-2.403947000	-0.635319000
1	5.529310000	1.297678000	1.321803000

1	6.284861000	-0.914306000	0.506320000
1	1.839600000	2.555207000	-0.560786000
15	-3.222557000	-0.165591000	0.203038000
6	-4.617992000	0.968451000	0.052256000
1	-5.547505000	0.442663000	0.276356000
1	-4.502743000	1.797112000	0.751864000
1	-4.665750000	1.366392000	-0.961961000
6	-3.587650000	-1.561521000	-0.874624000
1	-3.587895000	-1.228544000	-1.913039000
1	-2.800558000	-2.309889000	-0.759695000
1	-4.551515000	-2.008636000	-0.624997000
6	-3.324088000	-0.849330000	1.868433000
1	-3.235201000	-0.040649000	2.594715000
1	-4.263613000	-1.383562000	2.022860000
1	-2.483439000	-1.531946000	2.010109000
1	-2.351887000	2.499885000	-0.308547000
1	-0.271178000	3.538795000	-0.700810000
31	-0.134695000	-0.807327000	-0.239156000
1	0.042445000	-1.692904000	1.070816000
1	-0.110093000	-1.609354000	-1.614437000

6GaP^{H-H} (T.E = -2957.802878)

6	-1.498682000	1.384558000	-0.106376000
6	-1.501739000	-0.006163000	-0.013706000
6	1.018014000	1.570880000	-0.230066000
1	1.808224000	2.323843000	-0.289805000
7	1.379136000	0.332064000	-0.144465000
15	-3.085499000	-0.602783000	0.176708000
6	-3.955642000	-0.070249000	1.667555000
1	-4.023174000	1.017200000	1.655580000
1	-4.956706000	-0.504503000	1.708880000
1	-3.384709000	-0.384990000	2.541863000
6	-4.230714000	-0.245206000	-1.174248000
1	-3.832592000	-0.669907000	-2.096624000
1	-5.215684000	-0.670757000	-0.971263000
1	-4.307790000	0.836319000	-1.281618000
6	-3.033374000	-2.399303000	0.279980000
1	-2.418935000	-2.700992000	1.130064000
1	-4.039985000	-2.803001000	0.399677000
1	-2.589712000	-2.805646000	-0.631218000
8	-2.469634000	2.145246000	-0.067024000
7	-0.212484000	2.084787000	-0.270728000
6	-0.335660000	3.526442000	-0.435401000
1	-0.933045000	3.758286000	-1.316249000
1	-0.833529000	3.969970000	0.425773000
1	0.656664000	3.960293000	-0.549216000
6	2.758420000	0.055103000	-0.005008000
6	3.302961000	-1.014915000	-0.706067000

6	3.571841000	0.799767000	0.842398000
6	4.647067000	-1.310553000	-0.584415000
1	2.658837000	-1.601290000	-1.352640000
6	4.918158000	0.499814000	0.955863000
1	3.139321000	1.592757000	1.442803000
6	5.462356000	-0.552513000	0.240994000
1	5.061861000	-2.142652000	-1.141308000
1	5.540740000	1.083613000	1.624003000
1	6.514769000	-0.790925000	0.337462000
31	0.052058000	-1.222554000	-0.155043000
1	0.432316000	-2.075508000	1.126680000
1	0.244292000	-1.957117000	-1.553616000

8GaP^{H-H} (T.E = -3191.847799)

7	1.464331000	0.528372000	-0.997028000
6	1.029666000	1.580138000	-0.151967000
6	-0.081593000	2.429429000	-0.574848000
15	2.325727000	0.000881000	0.316609000
6	1.698334000	1.462505000	1.039993000
6	1.664129000	2.240418000	2.297923000
1	2.603501000	2.759790000	2.509859000
1	0.879231000	3.000393000	2.241511000
1	1.441832000	1.617246000	3.169961000
7	1.895726000	-1.379598000	1.091697000
7	3.898502000	-0.252049000	-0.100567000
6	2.213387000	-2.690638000	0.543314000
1	1.332165000	-3.123558000	0.059371000
1	3.006527000	-2.620150000	-0.199175000
1	2.540720000	-3.355576000	1.348836000
6	0.717498000	-1.404966000	1.946443000
1	0.887520000	-2.103363000	2.770598000
1	0.516296000	-0.416783000	2.356500000
1	-0.170260000	-1.729449000	1.390942000
6	4.869747000	-0.754424000	0.850627000
1	5.528017000	-1.480148000	0.362336000
1	5.493314000	0.057227000	1.243832000
1	4.375972000	-1.246753000	1.687021000
6	4.489309000	0.506615000	-1.189151000
1	3.714734000	0.830047000	-1.881363000
1	5.026820000	1.386316000	-0.815341000
1	5.201877000	-0.126597000	-1.725327000
6	-2.296846000	-0.729670000	-0.127079000
6	-2.659044000	-0.692017000	1.226743000
6	-2.788952000	-1.795679000	-0.887275000
6	-3.477209000	-1.658031000	1.780590000
1	-2.275650000	0.116798000	1.842762000
6	-3.599381000	-2.766475000	-0.327113000
1	-2.533478000	-1.846887000	-1.941198000

6	-3.954248000	-2.707523000	1.010398000
1	-3.736862000	-1.595508000	2.832152000
1	-3.962979000	-3.577195000	-0.949123000
1	-4.591604000	-3.467123000	1.446669000
7	-1.438000000	0.215991000	-0.676516000
5	-1.464981000	1.603479000	-0.366014000
7	-2.626161000	2.323720000	0.046008000
6	-3.970519000	1.839422000	-0.164239000
1	-3.978205000	0.971387000	-0.820051000
1	-4.462312000	1.558031000	0.776887000
1	-4.577192000	2.624868000	-0.631782000
6	-2.638375000	3.608643000	0.695649000
1	-1.638082000	3.931700000	0.978793000
1	-3.083156000	4.385763000	0.059060000
1	-3.237898000	3.565949000	1.614695000
1	-0.073213000	3.381311000	-0.045763000
1	0.009352000	2.639826000	-1.647446000
31	-0.047618000	-0.427821000	-1.912094000
1	0.221889000	-1.971834000	-1.697931000
1	-0.199899000	0.204561000	-3.346606000

10GaP^{H-H} (T.E = -3283.343597)

7	0.680151000	0.052316000	-0.297821000
6	0.680539000	1.479366000	-0.215047000
6	-0.475843000	2.252581000	-0.154592000
6	-1.772792000	1.742023000	-0.112937000
1	-0.341389000	3.328833000	-0.159982000
1	-2.544921000	2.517722000	-0.162464000
15	2.308320000	0.135488000	-0.104622000
6	2.043899000	1.829307000	-0.187595000
6	2.729049000	3.132002000	-0.029341000
1	2.620699000	3.780840000	-0.905730000
1	2.349744000	3.696738000	0.832503000
1	3.801567000	2.994584000	0.128277000
6	-2.180800000	0.424339000	0.000555000
15	-3.808675000	-0.013456000	-0.073916000
6	-5.010960000	1.332293000	0.039349000
1	-6.024073000	0.928187000	0.005505000
1	-4.870931000	1.877445000	0.973374000
1	-4.878694000	2.022615000	-0.794528000
6	-4.247831000	-1.176433000	1.234596000
1	-5.290291000	-1.490246000	1.152620000
1	-3.601552000	-2.053373000	1.154965000
1	-4.071495000	-0.712698000	2.205611000
6	-4.255441000	-0.904670000	-1.584092000
1	-4.143526000	-0.237051000	-2.439262000
1	-3.558838000	-1.737006000	-1.704512000
1	-5.278949000	-1.283810000	-1.542717000

31	-0.831624000	-1.061419000	0.231426000
7	2.947700000	-0.427771000	1.321095000
7	3.076780000	-0.812316000	-1.226330000
6	2.863501000	-1.853546000	1.609384000
1	1.900240000	-2.104470000	2.072247000
1	2.963921000	-2.437397000	0.695453000
1	3.667118000	-2.137820000	2.295286000
6	2.717905000	0.382715000	2.506512000
1	3.413156000	0.070193000	3.290330000
1	2.886166000	1.436263000	2.289090000
1	1.693360000	0.264455000	2.884444000
6	4.512526000	-0.996025000	-1.213114000
1	4.759922000	-2.007136000	-1.553056000
1	5.015202000	-0.284693000	-1.881480000
1	4.908491000	-0.863956000	-0.207237000
6	2.495271000	-0.905420000	-2.552871000
1	1.411159000	-0.822969000	-2.491160000
1	2.876055000	-0.119473000	-3.217810000
1	2.749220000	-1.875962000	-2.988644000
1	-1.006910000	-2.266672000	-0.804826000
1	-0.645353000	-1.526407000	1.754128000

$^{11}\text{Ga}^{\text{H-H}}$ (T.E = -3201.143583)

7	0.800297000	-0.165064000	-0.325732000
6	0.865137000	1.238813000	-0.199727000
6	-1.628691000	1.547196000	-0.250053000
7	-1.892923000	0.270116000	0.058102000
15	2.449836000	-0.144968000	-0.184662000
6	2.226502000	1.568146000	-0.195227000
6	3.076848000	2.787103000	-0.164308000
1	2.758791000	3.542608000	-0.886085000
1	3.117465000	3.272377000	0.818193000
1	4.105382000	2.524975000	-0.423624000
6	-3.236065000	-0.163752000	-0.090334000
6	-3.501121000	-1.308406000	-0.831806000
6	-4.290611000	0.493395000	0.534619000
6	-4.794209000	-1.788507000	-0.947394000
1	-2.678335000	-1.817691000	-1.321089000
6	-5.580785000	0.013005000	0.413909000
1	-4.089085000	1.388872000	1.108776000
6	-5.840314000	-1.130034000	-0.325667000
1	-4.983060000	-2.682149000	-1.531479000
1	-6.392985000	0.536411000	0.905782000
1	-6.853439000	-1.504019000	-0.416510000
31	-0.588204000	-0.987545000	0.808908000
7	3.115110000	-0.766454000	1.187251000
7	3.130351000	-1.040965000	-1.385074000
6	2.984306000	-2.191097000	1.460479000

1	2.853368000	-2.752159000	0.535594000
1	3.882523000	-2.557362000	1.966109000
1	2.118629000	-2.384030000	2.105658000
6	3.152446000	0.040799000	2.397083000
1	3.346004000	1.084170000	2.155058000
1	2.206758000	-0.021269000	2.949379000
1	3.958161000	-0.323867000	3.039818000
6	4.537251000	-1.387165000	-1.409742000
1	4.658120000	-2.415746000	-1.763877000
1	5.095464000	-0.729521000	-2.086638000
1	4.972200000	-1.310681000	-0.414853000
6	2.504185000	-1.046182000	-2.696793000
1	1.444416000	-0.815391000	-2.605709000
1	2.975331000	-0.316253000	-3.365162000
1	2.608926000	-2.038816000	-3.143054000
8	-2.403340000	2.396205000	-0.629591000
7	-0.241138000	1.986420000	-0.076084000
6	-0.073307000	3.430757000	-0.003672000
1	0.777892000	3.662323000	0.633439000
1	0.079433000	3.869824000	-0.992271000
1	-0.972251000	3.868033000	0.418603000
1	-0.220183000	-0.601151000	2.305036000
1	-0.847347000	-2.473521000	0.381949000

$^{13}\text{GaP}^{\text{H-H}}$ (T.E = -3526.689165)

7	1.387133000	-0.085015000	-0.480897000
6	1.227823000	1.328548000	-0.271950000
6	0.000000000	1.973384000	-0.186521000
6	-1.227834000	1.328573000	-0.272034000
1	0.000003000	3.041717000	0.004292000
15	2.978525000	0.152305000	-0.127835000
6	2.540209000	1.808483000	-0.113751000
6	3.062020000	3.160512000	0.188817000
1	2.820039000	3.884030000	-0.596927000
1	2.661311000	3.566198000	1.127602000
1	4.149984000	3.151877000	0.284246000
7	-1.387120000	-0.084997000	-0.480780000
6	-2.540226000	1.808523000	-0.113974000
15	-2.978548000	0.152345000	-0.127921000
6	-3.062167000	3.160588000	0.188203000
1	-2.659232000	3.567536000	1.125476000
1	-2.822825000	3.883440000	-0.598967000
1	-4.149867000	3.151266000	0.286593000
7	-3.944149000	-0.608729000	-1.237055000
7	-3.538783000	-0.469425000	1.307179000
6	-3.527335000	-0.574290000	-2.627010000
1	-3.984534000	0.267494000	-3.161942000
1	-2.443678000	-0.485726000	-2.687616000

1	-3.831968000	-1.501542000	-3.121048000
6	-5.374792000	-0.747423000	-1.068135000
1	-5.919525000	0.043314000	-1.599842000
1	-5.704047000	-1.710274000	-1.472833000
1	-5.644872000	-0.704385000	-0.014433000
6	-3.531374000	-1.914179000	1.487534000
1	-4.317588000	-2.204829000	2.190797000
1	-3.708718000	-2.422310000	0.540097000
1	-2.566387000	-2.255283000	1.885835000
6	-3.173385000	0.238866000	2.523947000
1	-2.134193000	0.034750000	2.815564000
1	-3.290404000	1.313134000	2.391063000
1	-3.830998000	-0.087375000	3.334301000
7	3.944258000	-0.608484000	-1.237070000
7	3.538700000	-0.469749000	1.307164000
6	5.374932000	-0.746859000	-1.068109000
1	5.704457000	-1.709522000	-1.473037000
1	5.919489000	0.044154000	-1.599586000
1	5.644949000	-0.704025000	-0.014382000
6	3.527546000	-0.573701000	-2.627046000
1	2.443893000	-0.485137000	-2.687711000
1	3.984770000	0.268235000	-3.161719000
1	3.832232000	-1.500817000	-3.121307000
6	3.173040000	0.238192000	2.524060000
1	3.830765000	-0.087945000	3.334364000
1	3.289679000	1.312522000	2.391354000
1	2.133918000	0.033648000	2.815623000
6	3.531508000	-1.914546000	1.487184000
1	3.709363000	-2.422421000	0.539709000
1	4.317494000	-2.205165000	2.190711000
1	2.566439000	-2.255953000	1.885031000
31	0.000011000	-1.307546000	0.140473000
1	-0.000128000	-2.671162000	-0.650452000
1	0.000122000	-1.348520000	1.743762000

Cartesian coordinates of the N–H splitting products obtained for some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AIP^{N-H} (T.E = -987.452668)

7	1.423137000	0.600510000	-0.315420000
6	1.227311000	1.895467000	-0.461276000
6	-0.000009000	2.532488000	-0.564378000
7	-1.423112000	0.600452000	-0.315362000
1	-0.000068000	3.601934000	-0.718966000
1	2.117381000	2.524892000	-0.514719000
6	2.749008000	0.142810000	-0.119075000
6	3.166520000	-1.019303000	-0.758694000
6	3.631712000	0.809599000	0.723602000
6	4.452984000	-1.489464000	-0.575353000
1	2.474665000	-1.541029000	-1.411602000
6	4.919664000	0.336154000	0.898607000
1	3.294681000	1.684806000	1.268117000
6	5.337078000	-0.812727000	0.249108000
1	4.768440000	-2.391977000	-1.085752000
1	5.596532000	0.862287000	1.561861000
1	6.344099000	-1.185477000	0.392880000
6	-2.748993000	0.142749000	-0.119034000
6	-3.166657000	-1.019146000	-0.758950000
6	-3.631542000	0.809398000	0.723892000
6	-4.453156000	-1.489207000	-0.575646000
1	-2.474865000	-1.540769000	-1.412005000
6	-4.919538000	0.336041000	0.898875000
1	-3.294363000	1.684435000	1.268595000
6	-5.337114000	-0.812614000	0.249093000
1	-4.768763000	-2.391538000	-1.086275000
1	-5.596289000	0.862064000	1.562335000
1	-6.344160000	-1.185313000	0.392824000
6	-1.227334000	1.895372000	-0.461282000
1	-2.117409000	2.524795000	-0.514748000
13	0.000086000	-0.707478000	-0.226295000
1	0.000007000	-1.658092000	-1.494622000
7	-0.000171000	-1.557543000	1.339168000
1	-0.000262000	-1.143370000	2.255855000
1	0.000672000	-2.560069000	1.422424000

4AIP^{N-H} (T.E = -1200.233684)

7	1.232481000	0.644920000	-0.262627000
6	0.956039000	1.952092000	-0.238994000
6	-0.281061000	2.550785000	-0.217468000

6	-1.512829000	1.869892000	-0.141019000
6	-1.676745000	0.510943000	-0.156892000
6	2.578827000	0.253051000	-0.131735000
6	3.037440000	-0.855082000	-0.842545000
6	3.465810000	0.912439000	0.717760000
6	4.348071000	-1.275193000	-0.721909000
1	2.352630000	-1.371315000	-1.508181000
6	4.778929000	0.491227000	0.827790000
1	3.112691000	1.742652000	1.319193000
6	5.229854000	-0.602674000	0.109138000
1	4.686037000	-2.134231000	-1.290529000
1	5.451890000	1.015830000	1.496926000
1	6.257136000	-0.934117000	0.202351000
1	1.817705000	2.621618000	-0.250412000
15	-3.224292000	-0.190772000	0.033908000
6	-4.624616000	0.946876000	-0.041944000
1	-5.556576000	0.391003000	0.072903000
1	-4.552492000	1.683225000	0.759386000
1	-4.632341000	1.467446000	-1.000261000
6	-3.522784000	-1.436481000	-1.230023000
1	-3.483582000	-0.972521000	-2.216099000
1	-2.730260000	-2.185780000	-1.173865000
1	-4.490869000	-1.918025000	-1.081223000
6	-3.382822000	-1.078214000	1.591256000
1	-3.323269000	-0.369443000	2.418318000
1	-4.326534000	-1.625297000	1.640240000
1	-2.532628000	-1.766429000	1.653073000
1	-2.383312000	2.529035000	-0.056014000
1	-0.294599000	3.633340000	-0.230148000
13	-0.122114000	-0.724997000	-0.360512000
1	-0.084858000	-1.516479000	-1.752030000
7	-0.107974000	-1.929482000	1.006215000
1	0.357953000	-2.815816000	0.872447000
1	0.070912000	-1.634186000	1.956357000

6AIP^{N-H} (T.E = -1330.814146)

6	-1.522878000	1.382385000	-0.064597000
6	-1.497491000	-0.007588000	-0.186021000
6	0.989032000	1.577960000	-0.178390000
1	1.789376000	2.321949000	-0.164402000
13	0.058202000	-1.175519000	-0.286976000
7	1.334367000	0.327431000	-0.228620000
15	-3.062497000	-0.670910000	-0.023500000
6	-3.806296000	-0.457818000	1.608905000
1	-3.854876000	0.608566000	1.829815000
1	-4.807958000	-0.890735000	1.648076000
1	-3.166333000	-0.950110000	2.343321000
6	-4.303890000	-0.064323000	-1.186397000

1	-3.963870000	-0.266421000	-2.202849000
1	-5.260583000	-0.562797000	-1.017199000
1	-4.412214000	1.011062000	-1.051967000
6	-3.005290000	-2.449035000	-0.283641000
1	-2.289548000	-2.890043000	0.415554000
1	-3.995341000	-2.883392000	-0.135198000
1	-2.666852000	-2.657136000	-1.300452000
8	-2.486964000	2.129738000	0.105904000
7	-0.232855000	2.102022000	-0.146849000
6	-0.351505000	3.552408000	-0.127950000
1	-0.955240000	3.893901000	-0.967960000
1	-0.843009000	3.883504000	0.785814000
1	0.641228000	3.995516000	-0.193255000
6	2.720806000	0.041591000	-0.130237000
6	3.286164000	-0.877221000	-1.006354000
6	3.511927000	0.629042000	0.849997000
6	4.632321000	-1.178091000	-0.916981000
1	2.655089000	-1.344934000	-1.753843000
6	4.860273000	0.326986000	0.929472000
1	3.058956000	1.300387000	1.571766000
6	5.426150000	-0.574608000	0.045325000
1	5.065853000	-1.890472000	-1.609247000
1	5.467353000	0.788496000	1.699694000
1	6.480248000	-0.815736000	0.112849000
1	0.352885000	-1.991600000	-1.627802000
7	0.214811000	-2.253727000	1.157284000
1	0.794913000	-3.078671000	1.157582000
1	0.136270000	-1.914056000	2.104162000

8AIP^{N-H} (T.E = -1564.865496)

7	1.343363000	0.240722000	-1.068128000
6	1.081211000	1.490561000	-0.446065000
6	-0.018872000	2.310075000	-0.948093000
15	2.396628000	-0.027072000	0.175953000
6	1.901386000	1.585270000	0.646023000
6	2.095143000	2.612042000	1.692146000
1	3.113521000	3.011203000	1.715292000
1	1.421908000	3.455442000	1.515934000
1	1.878767000	2.233372000	2.696667000
7	2.110891000	-1.188264000	1.297315000
7	3.901450000	-0.372679000	-0.397677000
6	2.441915000	-2.588500000	1.052658000
1	1.597297000	-3.094494000	0.573461000
1	3.303482000	-2.670834000	0.393118000
1	2.680697000	-3.065092000	2.007622000
6	0.932336000	-1.041320000	2.140267000
1	1.111694000	-1.538822000	3.096733000
1	0.718876000	0.011161000	2.326155000

1	0.052295000	-1.494815000	1.667997000
6	5.013699000	-0.518875000	0.522418000
1	5.695895000	-1.293827000	0.159815000
1	5.579261000	0.417010000	0.611837000
1	4.663327000	-0.806423000	1.512964000
6	4.297923000	0.105103000	-1.710946000
1	3.433541000	0.155795000	-2.369309000
1	4.759956000	1.098711000	-1.653473000
1	5.028825000	-0.587610000	-2.136741000
13	-0.158184000	-0.719593000	-1.781288000
6	-2.500441000	-0.615742000	-0.245920000
6	-2.709957000	-0.637203000	1.135572000
6	-3.270772000	-1.477764000	-1.030346000
6	-3.661960000	-1.465077000	1.703043000
1	-2.112119000	0.022204000	1.758402000
6	-4.216075000	-2.311127000	-0.460111000
1	-3.118977000	-1.472556000	-2.105698000
6	-4.422928000	-2.309283000	0.910286000
1	-3.806559000	-1.454413000	2.778070000
1	-4.801838000	-2.966120000	-1.095748000
1	-5.166290000	-2.959815000	1.355254000
7	-1.513735000	0.196115000	-0.818543000
5	-1.429060000	1.592443000	-0.576832000
7	-2.495312000	2.418718000	-0.103367000
6	-3.892506000	2.064919000	-0.198982000
1	-4.039866000	1.195295000	-0.835327000
1	-4.334702000	1.845519000	0.782629000
1	-4.455374000	2.900233000	-0.634401000
6	-2.336662000	3.710319000	0.513237000
1	-1.293289000	3.932221000	0.731568000
1	-2.738117000	4.519390000	-0.113102000
1	-2.879498000	3.745376000	1.467092000
1	0.052441000	3.335553000	-0.589217000
1	0.028471000	2.334507000	-2.044316000
1	-0.181197000	-0.494442000	-3.358316000
7	-0.025108000	-2.442318000	-1.193889000
1	0.174553000	-3.164329000	-1.871886000
1	-0.766178000	-2.797284000	-0.602559000

10AIP^{N-H} (T.E = -1656.358193)

7	-0.625469000	0.074928000	0.205119000
6	-0.652023000	1.477031000	-0.077870000
6	0.495020000	2.249393000	-0.204780000
6	1.795118000	1.745394000	-0.116676000
1	0.355765000	3.306139000	-0.405165000
1	2.563071000	2.512464000	-0.268448000
15	-2.260844000	0.108853000	0.045324000
6	-2.023887000	1.784601000	-0.206303000

6	-2.730683000	3.018867000	-0.616209000
1	-2.577498000	3.845950000	0.085799000
1	-2.411712000	3.378425000	-1.603845000
1	-3.809051000	2.850834000	-0.672114000
6	2.195483000	0.440962000	0.124464000
15	3.837351000	0.023442000	0.092298000
6	5.018818000	1.393760000	0.096814000
1	6.037702000	1.002836000	0.101231000
1	4.882184000	2.009637000	-0.792913000
1	4.866514000	2.014020000	0.980818000
6	4.296597000	-0.987476000	-1.332959000
1	5.327165000	-1.342201000	-1.260929000
1	3.602794000	-1.833363000	-1.363424000
1	4.171264000	-0.400321000	-2.243892000
6	4.288722000	-1.010199000	1.499654000
1	4.118494000	-0.458292000	2.424577000
1	3.641280000	-1.889901000	1.505454000
1	5.331883000	-1.326441000	1.438499000
7	-2.927761000	-0.756742000	-1.206058000
7	-3.000986000	-0.569155000	1.370577000
6	-2.870587000	-2.211295000	-1.150055000
1	-1.875343000	-2.578532000	-1.437621000
1	-3.085637000	-2.564432000	-0.143027000
1	-3.612325000	-2.629986000	-1.835621000
6	-2.656407000	-0.252459000	-2.541863000
1	-3.365775000	-0.698256000	-3.243849000
1	-2.766509000	0.830728000	-2.571234000
1	-1.638580000	-0.506723000	-2.870187000
6	-4.450400000	-0.524726000	1.435289000
1	-4.809897000	-1.303182000	2.114012000
1	-4.809999000	0.444358000	1.810116000
1	-4.885149000	-0.697111000	0.451111000
6	-2.374630000	-0.329874000	2.661814000
1	-1.299899000	-0.494336000	2.598929000
1	-2.561202000	0.690828000	3.022755000
1	-2.791070000	-1.033042000	3.387109000
13	0.873222000	-1.032254000	0.402997000
1	0.876188000	-1.733726000	1.850745000
7	1.080079000	-2.351072000	-0.842155000
1	1.017430000	-2.200395000	-1.838641000
1	0.840535000	-3.310693000	-0.643835000

11AIP^{N-H} (T.E = -1574.166981)

7	-0.768064000	-0.089935000	0.304112000
6	-0.838342000	1.252893000	-0.087711000
6	1.654610000	1.570752000	-0.184119000
15	-2.415774000	-0.124725000	0.182690000
6	-2.202542000	1.549223000	-0.205624000

6	-3.070706000	2.690333000	-0.599817000
1	-3.066796000	3.515894000	0.117647000
1	-2.819332000	3.108449000	-1.579248000
1	-4.106367000	2.346451000	-0.667090000
7	-3.118821000	-1.037498000	-0.988120000
7	-3.056423000	-0.720475000	1.577075000
6	-3.089215000	-2.494702000	-0.885533000
1	-2.170454000	-2.884469000	-1.340351000
1	-3.114611000	-2.806629000	0.157326000
1	-3.961984000	-2.909052000	-1.397232000
6	-3.040442000	-0.581931000	-2.367149000
1	-3.861427000	-1.027116000	-2.934732000
1	-3.125538000	0.501979000	-2.421603000
1	-2.094434000	-0.887334000	-2.830398000
6	-4.491289000	-0.868878000	1.731983000
1	-4.708009000	-1.771767000	2.310723000
1	-4.924424000	-0.012811000	2.263430000
1	-4.977832000	-0.957521000	0.761572000
6	-2.353772000	-0.523857000	2.834902000
1	-1.277512000	-0.552323000	2.677454000
1	-2.624409000	0.429943000	3.303893000
1	-2.625528000	-1.331772000	3.518711000
7	0.259818000	1.997120000	-0.288220000
6	0.042344000	3.397374000	-0.622264000
1	-0.391169000	3.496363000	-1.619317000
1	-0.623333000	3.861546000	0.105774000
1	1.005262000	3.896966000	-0.599141000
8	2.487124000	2.446779000	-0.241555000
7	1.883554000	0.249833000	-0.071668000
6	3.252117000	-0.121127000	0.070070000
6	4.030968000	0.348413000	1.122037000
6	3.798486000	-1.038804000	-0.816985000
6	5.332641000	-0.086721000	1.272645000
1	3.605380000	1.062381000	1.816652000
6	5.102683000	-1.479545000	-0.657534000
1	3.186962000	-1.403865000	-1.635221000
6	5.875795000	-1.003590000	0.384719000
1	5.929772000	0.289705000	2.095578000
1	5.515042000	-2.195817000	-1.359129000
1	6.896977000	-1.344547000	0.508824000
13	0.698234000	-1.229573000	0.063740000
1	0.964765000	-2.129574000	1.343209000
7	0.421717000	-2.213277000	-1.436866000
1	0.484640000	-1.815164000	-2.363143000
1	0.774453000	-3.158203000	-1.482636000

$^{13}\text{AIP}^{\text{N-H}}$ (T.E = -1899.714015)

7	1.358052000	-0.124382000	-0.057056000
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6	1.224643000	1.247311000	-0.460127000
6	0.003593000	1.889238000	-0.617066000
6	-1.214694000	1.275158000	-0.356292000
1	0.000894000	2.916541000	-0.965082000
13	0.020317000	-1.278457000	0.567251000
15	2.980095000	0.136469000	-0.042284000
6	2.549614000	1.694890000	-0.611540000
6	3.110850000	3.032020000	-0.909308000
1	2.815142000	3.398558000	-1.898319000
1	2.796135000	3.792079000	-0.182025000
1	4.202889000	3.012181000	-0.895854000
7	-1.334831000	-0.054425000	0.170857000
6	-2.543830000	1.701544000	-0.527075000
15	-2.958896000	0.132932000	0.026590000
6	-3.127097000	2.916168000	-1.140648000
1	-2.996182000	3.814492000	-0.527163000
1	-2.684559000	3.133125000	-2.121031000
1	-4.202356000	2.796390000	-1.296536000
7	-3.765028000	-0.854611000	-1.034178000
7	-3.725514000	-0.194693000	1.464175000
6	-3.905084000	-2.269042000	-0.704550000
1	-2.967672000	-2.812284000	-0.886457000
1	-4.168066000	-2.393543000	0.344201000
1	-4.698103000	-2.702686000	-1.319547000
6	-3.466697000	-0.650116000	-2.442020000
1	-2.507943000	-1.108722000	-2.722029000
1	-4.255192000	-1.106718000	-3.045495000
1	-3.419405000	0.413482000	-2.672558000
6	-3.039947000	0.209016000	2.681660000
1	-3.498107000	-0.307295000	3.528701000
1	-1.987781000	-0.067806000	2.636708000
1	-3.117519000	1.291375000	2.853377000
6	-5.159829000	0.017980000	1.536608000
1	-5.402546000	1.070681000	1.740094000
1	-5.640496000	-0.272296000	0.603001000
1	-5.578945000	-0.587374000	2.345250000
7	3.774942000	-1.032405000	-0.907850000
7	3.741496000	0.056653000	1.431973000
6	5.221107000	-1.112349000	-0.928941000
1	5.530601000	-2.158141000	-1.023731000
1	5.641999000	-0.559023000	-1.778724000
1	5.643457000	-0.708304000	-0.010425000
6	3.159532000	-1.489751000	-2.140287000
1	2.075026000	-1.447936000	-2.053487000
1	3.475309000	-0.882401000	-2.998224000
1	3.451745000	-2.527263000	-2.324830000
6	3.474922000	1.154970000	2.347480000
1	4.210031000	1.129677000	3.155857000
1	3.554035000	2.111497000	1.833043000

1	2.471700000	1.078555000	2.789785000
6	3.758177000	-1.229730000	2.118475000
1	3.897505000	-2.043870000	1.408377000
1	4.580480000	-1.249663000	2.839130000
1	2.815193000	-1.402524000	2.654296000
1	0.168131000	-1.592177000	2.132727000
7	-0.170859000	-2.816851000	-0.360247000
1	-0.182553000	-2.903995000	-1.364441000
1	-0.024336000	-3.724537000	0.050634000

1GaP^{N-H} (T.E = -2669.791340)

7	-0.607318000	-0.323797000	1.456863000
7	-0.605473000	-0.331524000	-1.459990000
6	-1.795893000	-0.835937000	1.234681000
6	-1.795154000	-0.848670000	-1.234565000
6	-2.356471000	-1.137794000	-0.000585000
1	-3.332439000	-1.602356000	0.001253000
6	-0.253951000	0.049771000	2.772680000
6	-1.162428000	0.689471000	3.610952000
6	1.038557000	-0.197586000	3.226154000
6	-0.790841000	1.049462000	4.893567000
6	1.401563000	0.171830000	4.507937000
6	0.490926000	0.790962000	5.348709000
1	-1.505114000	1.552294000	5.535386000
1	2.407578000	-0.033321000	4.855377000
1	0.781748000	1.079592000	6.351709000
6	-0.258355000	0.046166000	-2.772255000
6	1.046450000	-0.149982000	-3.216275000
6	-1.179301000	0.646568000	-3.627086000
6	1.412763000	0.225620000	-4.494724000
6	-0.807168000	1.013154000	-4.907488000
6	0.488188000	0.803522000	-5.349128000
1	2.430421000	0.058939000	-4.828321000
1	-1.533721000	1.484542000	-5.559316000
1	0.778451000	1.098346000	-6.350302000
1	-2.181517000	0.858086000	-3.271511000
1	1.761283000	-0.625135000	-2.552086000
1	1.735765000	-0.706138000	2.566116000
1	-2.152035000	0.934975000	3.241502000
31	0.720749000	-0.002950000	0.003662000
1	-2.401640000	-1.078812000	-2.113263000
1	-2.405849000	-1.052533000	2.114462000
1	1.222393000	1.474538000	-0.016032000
7	1.970884000	-1.379788000	0.146917000
1	1.676021000	-2.308146000	-0.121275000
1	2.885199000	-1.208415000	-0.246192000

4GaP^{N-H} (T.E = -2882.579751)

7	1.279791000	0.735549000	-0.278996000
6	0.988555000	2.033609000	-0.291329000
6	-0.254923000	2.627349000	-0.292779000
6	-1.488534000	1.959085000	-0.173400000
6	-1.680873000	0.605456000	-0.166152000
6	2.611799000	0.338197000	-0.093418000
6	3.069214000	-0.825233000	-0.712563000
6	3.494698000	1.044869000	0.723639000
6	4.371849000	-1.250544000	-0.540226000
1	2.390252000	-1.381441000	-1.350729000
6	4.799922000	0.616510000	0.886464000
1	3.143931000	1.918776000	1.260816000
6	5.249211000	-0.530975000	0.255868000
1	4.707328000	-2.152749000	-1.039271000
1	5.467677000	1.178872000	1.529704000
1	6.269945000	-0.867833000	0.391490000
1	1.843033000	2.713523000	-0.307546000
15	-3.209842000	-0.093809000	0.135960000
6	-4.610209000	1.044158000	0.084774000
1	-5.535744000	0.496991000	0.270838000
1	-4.495490000	1.811859000	0.850899000
1	-4.666063000	1.525223000	-0.892361000
6	-3.566733000	-1.393107000	-1.056852000
1	-3.557393000	-0.979926000	-2.065870000
1	-2.784415000	-2.151764000	-0.985861000
1	-4.534275000	-1.853820000	-0.850037000
6	-3.280272000	-0.919950000	1.731886000
1	-3.176595000	-0.180133000	2.526777000
1	-4.218950000	-1.464712000	1.853169000
1	-2.425376000	-1.606309000	1.770738000
1	-2.349266000	2.627291000	-0.066355000
1	-0.267561000	3.709294000	-0.332678000
31	-0.147176000	-0.664094000	-0.423201000
1	-0.068889000	-1.430875000	-1.808327000
7	-0.124305000	-1.866285000	1.046235000
1	0.477058000	-2.669409000	0.908377000
1	0.180245000	-1.430209000	1.909902000

6GaP^{N-H} (T.E = -3013.160003)

6	-1.516673000	1.506096000	-0.079478000
6	-1.523089000	0.116937000	-0.193272000
6	0.999139000	1.710423000	-0.217161000
1	1.787210000	2.468593000	-0.196017000
7	1.361954000	0.468831000	-0.240714000
15	-3.074624000	-0.538193000	0.090105000
6	-3.696840000	-0.294492000	1.767901000

1	-3.720394000	0.774987000	1.977261000
1	-4.696886000	-0.717087000	1.884453000
1	-3.009872000	-0.784551000	2.460176000
6	-4.392174000	0.056998000	-0.991663000
1	-4.128025000	-0.166331000	-2.026042000
1	-5.337761000	-0.429975000	-0.7444440000
1	-4.482190000	1.135607000	-0.870014000
6	-3.033670000	-2.319751000	-0.141802000
1	-2.267856000	-2.746412000	0.513281000
1	-4.010376000	-2.750627000	0.084556000
1	-2.770769000	-2.546417000	-1.177006000
8	-2.472345000	2.254624000	0.134453000
7	-0.233090000	2.221422000	-0.223124000
6	-0.360734000	3.671626000	-0.250741000
1	-1.000056000	3.977987000	-1.077695000
1	-0.815094000	4.037337000	0.669217000
1	0.625518000	4.115960000	-0.376831000
6	2.735366000	0.180809000	-0.081110000
6	3.320244000	-0.792419000	-0.884388000
6	3.504107000	0.814580000	0.889425000
6	4.659449000	-1.098905000	-0.737481000
1	2.710601000	-1.294785000	-1.627202000
6	4.846223000	0.505225000	1.027721000
1	3.037526000	1.528378000	1.559855000
6	5.430260000	-0.449130000	0.213941000
1	5.106371000	-1.853064000	-1.374853000
1	5.433646000	1.003523000	1.790287000
1	6.478945000	-0.695865000	0.328352000
31	0.017049000	-1.087088000	-0.391525000
1	0.342080000	-1.838390000	-1.742733000
7	0.172025000	-2.197055000	1.123120000
1	0.913001000	-2.885274000	1.107330000
1	0.238125000	-1.698320000	2.001830000

8GaP^{N-H} (T.E = -3247.203287)

7	1.407642000	0.268406000	-0.994374000
6	1.085187000	1.523325000	-0.419904000
6	-0.005655000	2.313622000	-0.987907000
15	2.391828000	0.052800000	0.321044000
6	1.842872000	1.667555000	0.712619000
6	1.960682000	2.736349000	1.728004000
1	2.962172000	3.174526000	1.776408000
1	1.264520000	3.547274000	1.495493000
1	1.717611000	2.385786000	2.736569000
7	2.075029000	-1.077170000	1.464450000
7	3.931896000	-0.281597000	-0.162442000
6	2.438750000	-2.479268000	1.283813000
1	1.612885000	-3.018795000	0.807887000

1	3.315898000	-2.569525000	0.645957000
1	2.667715000	-2.911512000	2.262238000
6	0.874881000	-0.918965000	2.273609000
1	1.039004000	-1.381161000	3.250504000
1	0.644115000	0.136205000	2.418051000
1	0.012251000	-1.400606000	1.797833000
6	4.996464000	-0.395261000	0.816154000
1	5.703425000	-1.171683000	0.507755000
1	5.548702000	0.548004000	0.911591000
1	4.598495000	-0.662588000	1.794140000
6	4.391943000	0.171458000	-1.463097000
1	3.560205000	0.205988000	-2.163131000
1	4.847205000	1.168105000	-1.402362000
1	5.145885000	-0.525672000	-1.839066000
6	-2.466709000	-0.554287000	-0.040151000
6	-2.664275000	-0.457205000	1.340944000
6	-3.218855000	-1.507700000	-0.732799000
6	-3.583053000	-1.260022000	1.992175000
1	-2.081867000	0.273577000	1.894631000
6	-4.129944000	-2.316465000	-0.077538000
1	-3.082320000	-1.593339000	-1.806907000
6	-4.322692000	-2.198073000	1.289591000
1	-3.716877000	-1.156478000	3.063673000
1	-4.701068000	-3.043561000	-0.644462000
1	-5.038696000	-2.829863000	1.801269000
7	-1.517414000	0.231425000	-0.695115000
5	-1.414880000	1.638001000	-0.551247000
7	-2.471035000	2.496958000	-0.113387000
6	-3.867786000	2.132469000	-0.150776000
1	-4.025225000	1.224370000	-0.728742000
1	-4.284095000	1.971157000	0.853291000
1	-4.446642000	2.936993000	-0.621695000
6	-2.301757000	3.824647000	0.417023000
1	-1.252716000	4.068347000	0.577106000
1	-2.736939000	4.589597000	-0.241249000
1	-2.805865000	3.914789000	1.388584000
1	0.073496000	3.361242000	-0.701332000
1	0.043356000	2.259748000	-2.082366000
31	-0.154662000	-0.765301000	-1.692854000
1	-0.189678000	-0.581289000	-3.256082000
7	0.015715000	-2.483404000	-0.920805000
1	0.143860000	-3.213520000	-1.610797000
1	-0.820474000	-2.739198000	-0.404593000

10GaP^{N-H} (T.E = -3338.699707)

7	-0.697194000	0.238936000	0.376197000
6	-0.706569000	1.557520000	-0.171222000
6	0.451916000	2.288791000	-0.442860000

6	1.746566000	1.796939000	-0.321084000
1	0.314373000	3.313061000	-0.772032000
1	2.517311000	2.552008000	-0.510997000
15	-2.323785000	0.221719000	0.110468000
6	-2.065683000	1.853914000	-0.365540000
6	-2.754634000	3.018321000	-0.966734000
1	-2.771445000	3.897427000	-0.312391000
1	-2.282626000	3.330597000	-1.906979000
1	-3.795851000	2.780186000	-1.198898000
6	2.159335000	0.503580000	-0.027699000
15	3.787337000	0.115912000	0.175829000
6	4.983216000	1.392196000	-0.284141000
1	5.998053000	1.020473000	-0.133158000
1	4.851642000	1.664124000	-1.332011000
1	4.837424000	2.280811000	0.331036000
6	4.262954000	-1.353529000	-0.760819000
1	5.301556000	-1.628861000	-0.566642000
1	3.609785000	-2.178781000	-0.468958000
1	4.118004000	-1.167551000	-1.825492000
6	4.223219000	-0.330396000	1.875048000
1	4.081041000	0.537525000	2.520006000
1	3.542545000	-1.118025000	2.204705000
1	5.254631000	-0.682052000	1.950308000
31	0.805473000	-0.978927000	0.152979000
7	-2.942160000	-0.780654000	-1.049512000
7	-3.114985000	-0.290674000	1.475633000
6	-2.906504000	-2.224877000	-0.843122000
1	-1.956192000	-2.631486000	-1.211747000
1	-3.002379000	-2.464282000	0.215187000
1	-3.737826000	-2.688937000	-1.382893000
6	-2.700978000	-0.431367000	-2.441314000
1	-3.457371000	-0.916854000	-3.064693000
1	-2.768335000	0.646354000	-2.582771000
1	-1.708728000	-0.774048000	-2.762041000
6	-4.552093000	-0.462843000	1.495073000
1	-4.816777000	-1.295496000	2.155231000
1	-5.059619000	0.436440000	1.868588000
1	-4.927808000	-0.681883000	0.496744000
6	-2.565067000	0.078493000	2.766187000
1	-1.480069000	0.143250000	2.703935000
1	-2.959918000	1.042224000	3.113786000
1	-2.831128000	-0.685478000	3.502596000
1	0.944977000	-1.980650000	1.381184000
7	0.483304000	-1.919936000	-1.478660000
1	0.869166000	-1.452656000	-2.291732000
1	0.835785000	-2.869329000	-1.492928000

11GaP^{N-H} (T.E = -3256.501293)

7	-0.817571000	-0.083428000	0.358410000
6	-0.882409000	1.287218000	0.040379000
6	1.609402000	1.626104000	0.110698000
7	1.882924000	0.315959000	0.024808000
15	-2.465901000	-0.097670000	0.174932000
6	-2.242076000	1.604549000	-0.044562000
6	-3.095359000	2.801357000	-0.266897000
1	-2.802022000	3.651742000	0.352573000
1	-3.110079000	3.146074000	-1.307786000
1	-4.129929000	2.568749000	-0.003357000
6	3.226768000	-0.078419000	0.249873000
6	3.490167000	-1.085318000	1.170563000
6	4.284044000	0.468450000	-0.469940000
6	4.782986000	-1.538210000	1.369504000
1	2.665633000	-1.507953000	1.734106000
6	5.574040000	0.016649000	-0.265610000
1	4.084721000	1.257250000	-1.184337000
6	5.831395000	-0.988760000	0.653201000
1	4.969797000	-2.323098000	2.093668000
1	6.388251000	0.453798000	-0.832669000
1	6.844583000	-1.340293000	0.809301000
31	0.616631000	-1.077219000	-0.535797000
7	-3.122936000	-0.899244000	-1.096073000
7	-3.153579000	-0.816213000	1.487035000
6	-2.951097000	-2.343038000	-1.191953000
1	-2.775690000	-2.778724000	-0.208010000
1	-3.851618000	-2.796607000	-1.616899000
1	-2.094841000	-2.575039000	-1.835505000
6	-3.216377000	-0.257767000	-2.399871000
1	-3.411549000	0.807388000	-2.288225000
1	-2.287006000	-0.398084000	-2.963030000
1	-4.046606000	-0.707151000	-2.951906000
6	-4.546818000	-1.209566000	1.538000000
1	-4.638179000	-2.181829000	2.032644000
1	-5.142523000	-0.485079000	2.106016000
1	-4.962338000	-1.291090000	0.535502000
6	-2.557584000	-0.613084000	2.796214000
1	-1.505334000	-0.355083000	2.692737000
1	-3.070826000	0.184225000	3.346224000
1	-2.635377000	-1.536001000	3.377659000
8	2.379576000	2.528452000	0.352143000
7	0.225998000	2.022884000	-0.153116000
6	0.047071000	3.442486000	-0.422310000
1	-0.782936000	3.575776000	-1.113327000
1	-0.147227000	4.005867000	0.493372000
1	0.957299000	3.832925000	-0.865651000
1	0.861025000	-2.496504000	0.070453000
7	0.182907000	-0.965064000	-2.370636000

1	0.410406000	-0.062368000	-2.773590000
1	0.652824000	-1.654559000	-2.944048000

$^{13}\text{GaP}^{\text{N-H}}$ (T.E = -3582.043684)

7	1.376899000	-0.051323000	-0.349159000
6	1.234229000	1.372521000	-0.484315000
6	0.015995000	2.036963000	-0.532269000
6	-1.218136000	1.397980000	-0.464519000
1	0.031321000	3.119167000	-0.606545000
15	2.982035000	0.230844000	-0.133125000
6	2.558147000	1.852900000	-0.485298000
6	3.104867000	3.228083000	-0.527408000
1	2.845774000	3.750790000	-1.454455000
1	2.741101000	3.851923000	0.300277000
1	4.195313000	3.221183000	-0.464816000
7	-1.369267000	-0.020767000	-0.319960000
6	-2.535599000	1.886521000	-0.470143000
15	-2.977327000	0.260034000	-0.129041000
6	-3.083205000	3.256856000	-0.580655000
1	-3.138383000	3.791743000	0.377462000
1	-2.460463000	3.864037000	-1.244447000
1	-4.090004000	3.261033000	-1.005176000
7	-3.871526000	-0.743335000	-1.088285000
7	-3.614917000	-0.033774000	1.376689000
6	-3.353365000	-1.108761000	-2.392149000
1	-3.831476000	-0.525431000	-3.188339000
1	-2.277657000	-0.942767000	-2.424862000
1	-3.544128000	-2.170318000	-2.577415000
6	-5.297549000	-0.933721000	-0.949314000
1	-5.848977000	-0.386596000	-1.724100000
1	-5.544358000	-1.996582000	-1.050050000
1	-5.638863000	-0.591281000	0.026040000
6	-3.573890000	-1.403593000	1.872877000
1	-4.397467000	-1.570329000	2.573568000
1	-3.660246000	-2.115761000	1.052756000
1	-2.627043000	-1.603059000	2.391875000
6	-3.313892000	0.935380000	2.417022000
1	-2.281086000	0.835104000	2.778971000
1	-3.453595000	1.950239000	2.048742000
1	-3.990716000	0.772822000	3.260101000
7	3.884143000	-0.793846000	-1.072928000
7	3.609781000	-0.051749000	1.380263000
6	5.323556000	-0.891923000	-0.958210000
1	5.639396000	-1.926751000	-1.127901000
1	5.829168000	-0.261268000	-1.700768000
1	5.652699000	-0.588622000	0.034260000
6	3.388261000	-1.113534000	-2.398517000
1	2.301454000	-1.043824000	-2.415118000

1	3.800008000	-0.436201000	-3.157243000
1	3.679173000	-2.135959000	-2.657692000
6	3.289071000	0.919044000	2.414067000
1	3.969189000	0.776288000	3.258077000
1	3.408409000	1.933597000	2.037504000
1	2.258532000	0.801625000	2.776793000
6	3.606248000	-1.416069000	1.888719000
1	3.748709000	-2.129967000	1.078007000
1	4.416065000	-1.544582000	2.613122000
1	2.654709000	-1.647520000	2.385995000
31	-0.010055000	-1.170086000	0.445247000
1	0.037645000	-1.177961000	2.034536000
7	-0.206136000	-2.851085000	-0.352212000
1	0.040890000	-2.889809000	-1.332643000
1	0.244726000	-3.626177000	0.113128000

Cartesian coordinates of the C–F splitting products obtained for some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AIP^{C-F} (T.E = -1758.613174)

7	1.430519000	-1.674669000	0.553968000
6	1.228947000	-2.317395000	1.691068000
6	-0.000027000	-2.583323000	2.274108000
7	-1.430548000	-1.674638000	0.553964000
1	-0.000034000	-3.079822000	3.233717000
1	2.115463000	-2.672830000	2.216849000
6	2.737307000	-1.646667000	0.005821000
6	3.170431000	-0.507330000	-0.663425000
6	3.582507000	-2.747948000	0.088363000
6	4.436348000	-0.462321000	-1.215058000
1	2.515822000	0.355503000	-0.736632000
6	4.851297000	-2.693262000	-0.459007000
1	3.230941000	-3.663669000	0.550025000
6	5.285420000	-1.551179000	-1.109538000
1	4.761145000	0.434015000	-1.729736000
1	5.498180000	-3.560170000	-0.392441000
1	6.276549000	-1.514550000	-1.544944000
6	-2.737332000	-1.646621000	0.005808000

6	-3.170445000	-0.507280000	-0.663440000
6	-3.582542000	-2.747894000	0.088350000
6	-4.436359000	-0.462262000	-1.215078000
1	-2.515829000	0.355547000	-0.736645000
6	-4.851330000	-2.693197000	-0.459025000
1	-3.230986000	-3.663615000	0.550018000
6	-5.285440000	-1.551113000	-1.109561000
1	-4.761147000	0.434076000	-1.729758000
1	-5.498221000	-3.560100000	-0.392459000
1	-6.276567000	-1.514476000	-1.544971000
6	-1.228995000	-2.317368000	1.691064000
1	-2.115521000	-2.672787000	2.216840000
13	-0.000003000	-0.837305000	-0.373241000
9	-0.000005000	-1.286514000	-1.961612000
6	0.000015000	1.124418000	-0.075723000
6	0.000036000	2.071622000	-1.084736000
6	0.000002000	1.622810000	1.213427000
6	0.000041000	3.434557000	-0.839702000
6	0.000013000	2.972663000	1.512518000
6	0.000032000	3.883693000	0.470100000
9	0.000039000	1.689696000	-2.356696000
9	0.000058000	4.309772000	-1.829285000
9	0.000037000	5.176191000	0.724067000
9	-0.000002000	3.403400000	2.761666000
9	-0.000026000	0.774719000	2.246165000

4AIP^{C-F} (T.E = -1971.399920)

7	-2.137354000	-0.720973000	-0.433962000
6	-2.376229000	-1.483982000	-1.506764000
6	-1.564182000	-2.450945000	-2.049324000
6	-0.330344000	-2.877327000	-1.520963000
6	0.314675000	-2.337629000	-0.437476000
6	-3.183136000	0.095720000	0.048529000
6	-2.883011000	1.341534000	0.593014000
6	-4.511899000	-0.321553000	0.029042000
6	-3.885997000	2.156128000	1.081896000
1	-1.851677000	1.678779000	0.618212000
6	-5.512629000	0.502292000	0.511167000
1	-4.757720000	-1.312243000	-0.335950000
6	-5.208025000	1.745863000	1.037497000
1	-3.630183000	3.124296000	1.496439000
1	-6.540517000	0.158297000	0.490975000
1	-5.993503000	2.385819000	1.420890000
1	-3.327630000	-1.309751000	-2.009277000
15	1.799759000	-2.982739000	0.120240000
6	2.281910000	-4.559381000	-0.608813000
1	3.221051000	-4.895351000	-0.166496000
1	1.509682000	-5.306657000	-0.423434000

1	2.418295000	-4.450367000	-1.685422000
6	3.187341000	-1.870485000	-0.174354000
1	3.289187000	-1.694854000	-1.246017000
1	2.987593000	-0.914638000	0.313375000
1	4.113653000	-2.290114000	0.222609000
6	1.762997000	-3.217114000	1.900422000
1	0.996192000	-3.950192000	2.153180000
1	2.734892000	-3.549718000	2.269204000
1	1.488790000	-2.271068000	2.374024000
1	0.110339000	-3.728140000	-2.049610000
1	-1.935440000	-2.947644000	-2.936427000
13	-0.471082000	-0.770617000	0.456150000
9	-0.667234000	-0.977628000	2.102396000
6	0.665508000	0.856981000	0.136948000
6	1.594997000	1.335381000	1.039755000
6	0.610052000	1.529097000	-1.069479000
6	2.410295000	2.426409000	0.789782000
6	1.397757000	2.626100000	-1.371586000
6	2.303734000	3.077574000	-0.427063000
9	1.769134000	0.719785000	2.213108000
9	3.291344000	2.848653000	1.682506000
9	3.070991000	4.118042000	-0.690005000
9	1.306899000	3.242820000	-2.537908000
9	-0.236325000	1.118493000	-2.016261000

6AIP^{C-F} (T.E = -2101.983725)

6	3.014717000	0.792652000	-0.639762000
6	2.298723000	-0.116142000	0.146117000
6	1.242597000	2.583898000	-0.458093000
1	1.009227000	3.593607000	-0.801376000
13	0.584688000	0.196526000	0.945419000
7	0.364487000	1.993502000	0.297595000
15	3.110984000	-1.609912000	0.297283000
6	3.373594000	-2.495007000	-1.252276000
1	3.979699000	-1.872639000	-1.910212000
1	3.875136000	-3.448682000	-1.076507000
1	2.404063000	-2.672268000	-1.720893000
6	4.730776000	-1.535993000	1.086409000
1	4.615989000	-1.129505000	2.091875000
1	5.177779000	-2.530453000	1.143070000
1	5.370052000	-0.874335000	0.502412000
6	2.124639000	-2.716731000	1.316315000
1	1.169302000	-2.913534000	0.824750000
1	2.648146000	-3.662096000	1.466204000
1	1.926889000	-2.253821000	2.285484000
8	4.106259000	0.640510000	-1.181774000
7	2.417766000	2.126457000	-0.875546000
6	3.245836000	3.015013000	-1.680710000

1	4.203410000	3.187147000	-1.191316000
1	3.446395000	2.566633000	-2.652287000
1	2.729732000	3.964300000	-1.813945000
6	-0.884974000	2.642867000	0.491272000
6	-1.449797000	2.639899000	1.760880000
6	-1.572426000	3.216031000	-0.571578000
6	-2.680018000	3.236964000	1.964844000
1	-0.914012000	2.166645000	2.576730000
6	-2.799839000	3.817297000	-0.355368000
1	-1.163634000	3.151762000	-1.574262000
6	-3.355362000	3.833124000	0.912282000
1	-3.114032000	3.235428000	2.957668000
1	-3.333260000	4.257712000	-1.189512000
1	-4.320728000	4.296306000	1.077089000
6	-0.953351000	-0.836111000	0.188713000
6	-1.707962000	-1.761816000	0.884317000
6	-1.322500000	-0.641444000	-1.129114000
6	-2.773340000	-2.448146000	0.325377000
6	-2.379503000	-1.295181000	-1.735540000
6	-3.110809000	-2.207429000	-0.994865000
9	0.512350000	0.203899000	2.615091000
9	-1.418926000	-2.045407000	2.152999000
9	-3.468523000	-3.328576000	1.026580000
9	-4.121930000	-2.849607000	-1.547846000
9	-2.699851000	-1.068501000	-2.999469000
9	-0.641754000	0.224345000	-1.891816000

8AIP^{C-F} (T.E = -2336.032890)

7	-1.033752000	-1.140069000	0.338715000
6	-1.988409000	-0.705543000	1.305511000
6	-1.622525000	0.334393000	2.265899000
15	-2.252200000	-2.062789000	-0.293051000
6	-3.146965000	-1.384276000	1.053365000
6	-4.479241000	-1.415697000	1.692634000
1	-4.745517000	-2.410070000	2.061851000
1	-4.501296000	-0.737121000	2.548587000
1	-5.278519000	-1.103686000	1.012600000
7	-2.878240000	-1.718137000	-1.765170000
7	-1.776381000	-3.630461000	-0.388446000
6	-2.219686000	-2.140592000	-2.997564000
1	-1.608537000	-1.327411000	-3.395517000
1	-1.571125000	-2.995383000	-2.815657000
1	-2.979740000	-2.424016000	-3.731022000
6	-3.605712000	-0.464599000	-1.925682000
1	-4.316092000	-0.569842000	-2.749013000
1	-4.156243000	-0.218766000	-1.018910000
1	-2.918259000	0.357488000	-2.156398000
6	-2.672132000	-4.659843000	-0.881068000

1	-2.126242000	-5.345880000	-1.536067000
1	-3.093575000	-5.242186000	-0.053683000
1	-3.491665000	-4.222030000	-1.449523000
6	-0.710338000	-4.137152000	0.460934000
1	-0.052196000	-3.326200000	0.767604000
1	-1.113501000	-4.625539000	1.355440000
1	-0.127472000	-4.873794000	-0.098554000
13	0.114373000	0.112344000	-0.451968000
6	-0.370434000	2.802109000	-0.522439000
6	-1.481946000	3.562166000	-0.886639000
6	0.866432000	3.149287000	-1.063610000
6	-1.353390000	4.645335000	-1.735622000
1	-2.452622000	3.286764000	-0.485485000
6	0.990518000	4.225533000	-1.924322000
1	1.742000000	2.570119000	-0.783664000
6	-0.116318000	4.986066000	-2.260331000
1	-2.231586000	5.224800000	-1.998964000
1	1.964596000	4.473262000	-2.330671000
1	-0.018569000	5.831642000	-2.930465000
7	-0.502899000	1.679682000	0.319077000
5	-1.155283000	1.730677000	1.586105000
7	-1.335805000	2.920012000	2.353519000
6	-0.559430000	4.126019000	2.167260000
1	0.288737000	3.958096000	1.508156000
1	-1.158943000	4.944648000	1.747369000
1	-0.170299000	4.464066000	3.135454000
6	-2.256675000	3.079544000	3.450793000
1	-2.959309000	2.251958000	3.521077000
1	-1.735570000	3.170359000	4.413730000
1	-2.847409000	3.995089000	3.318958000
1	-2.423318000	0.466100000	2.992910000
1	-0.742379000	-0.014020000	2.822951000
9	-0.213843000	0.018347000	-2.094120000
6	2.018587000	-0.368722000	-0.091752000
6	3.042073000	-0.252875000	-1.014082000
6	2.387069000	-0.875791000	1.138377000
6	4.349911000	-0.623053000	-0.746602000
6	3.675234000	-1.263393000	1.458469000
6	4.664974000	-1.134183000	0.500132000
9	2.801347000	0.240825000	-2.225374000
9	5.300368000	-0.495941000	-1.658066000
9	5.904522000	-1.493388000	0.775704000
9	3.975368000	-1.748799000	2.653202000
9	1.467477000	-1.011719000	2.104421000

10AIP^{C-F} (T.E = -2427.529196)

7	1.464060000	0.456010000	-0.162849000
6	2.209197000	1.311223000	-1.037335000

6	1.739670000	2.553496000	-1.452606000
6	0.529707000	3.117892000	-1.049310000
1	2.375038000	3.119383000	-2.124303000
1	0.359563000	4.110673000	-1.479383000
15	2.732961000	-0.594635000	-0.245562000
6	3.386059000	0.589669000	-1.305155000
6	4.591591000	0.911866000	-2.100144000
1	4.326254000	1.520673000	-2.969424000
1	5.351877000	1.472344000	-1.540187000
1	5.077973000	0.012255000	-2.484373000
6	-0.438443000	2.596734000	-0.199173000
15	-1.748421000	3.544641000	0.307111000
6	-2.105279000	5.007619000	-0.690227000
1	-2.981197000	5.521979000	-0.291595000
1	-1.256681000	5.692333000	-0.669249000
1	-2.296328000	4.713545000	-1.722802000
6	-1.573991000	4.157593000	1.998180000
1	-2.478347000	4.665700000	2.339974000
1	-1.356165000	3.304952000	2.645244000
1	-0.726721000	4.843351000	2.042168000
6	-3.277547000	2.592273000	0.357015000
1	-3.526503000	2.245505000	-0.646236000
1	-3.125321000	1.717259000	0.994286000
1	-4.096959000	3.188839000	0.761758000
7	3.511084000	-0.890670000	1.187202000
7	2.220044000	-2.096253000	-0.707640000
6	2.709578000	-1.488181000	2.253122000
1	2.065905000	-0.738265000	2.732580000
1	2.071740000	-2.280280000	1.863512000
1	3.373591000	-1.916493000	3.007905000
6	4.350469000	0.189438000	1.684436000
1	4.989773000	-0.198221000	2.481105000
1	4.982413000	0.581985000	0.889283000
1	3.749124000	1.013480000	2.092891000
6	3.029010000	-3.290107000	-0.571017000
1	2.392339000	-4.136082000	-0.292741000
1	3.530771000	-3.541272000	-1.513789000
1	3.786377000	-3.156995000	0.198994000
6	1.262091000	-2.168965000	-1.797188000
1	0.668640000	-1.255991000	-1.844061000
1	1.764135000	-2.313076000	-2.761352000
1	0.585170000	-3.012492000	-1.631462000
13	-0.134009000	0.855796000	0.655257000
9	-0.083949000	1.021319000	2.330830000
6	-1.378996000	-0.689507000	0.273239000
6	-1.459114000	-1.791681000	1.103519000
6	-2.124167000	-0.774304000	-0.886560000
6	-2.235859000	-2.904460000	0.825153000
6	-2.921827000	-1.857207000	-1.213057000

6	-2.976762000	-2.932063000	-0.343144000
9	-0.746567000	-1.838388000	2.229898000
9	-2.277788000	-3.940037000	1.649494000
9	-3.726865000	-3.980280000	-0.629912000
9	-3.623262000	-1.885958000	-2.336296000
9	-2.085021000	0.220888000	-1.781326000

11AIP^{C-F} (T.E = -2345.335075)

7	1.555791000	0.073955000	-0.221020000
6	2.515343000	1.085631000	-0.425372000
6	0.830402000	2.956397000	-0.420247000
15	2.826667000	-0.982540000	-0.088236000
6	3.750779000	0.436515000	-0.467844000
6	5.187335000	0.790957000	-0.611447000
1	5.394824000	1.383424000	-1.504826000
1	5.588355000	1.341763000	0.246540000
1	5.781502000	-0.121238000	-0.700383000
7	3.095745000	-1.651478000	1.386485000
7	2.582310000	-2.267551000	-1.078253000
6	2.093414000	-2.567952000	1.930490000
1	1.339010000	-2.016374000	2.504146000
1	1.591705000	-3.111927000	1.130729000
1	2.581850000	-3.291390000	2.587997000
6	3.707485000	-0.823043000	2.419697000
1	4.116727000	-1.476826000	3.193104000
1	4.520117000	-0.229696000	2.004094000
1	2.970226000	-0.153856000	2.878565000
6	3.388166000	-3.471763000	-1.022411000
1	2.743037000	-4.351445000	-1.110536000
1	4.111842000	-3.498372000	-1.844840000
1	3.929316000	-3.532834000	-0.079975000
6	1.891457000	-2.080522000	-2.344415000
1	1.294580000	-1.170798000	-2.321961000
1	2.601811000	-2.023278000	-3.176310000
1	1.222493000	-2.927810000	-2.519281000
7	2.169064000	2.379524000	-0.531065000
6	3.233674000	3.310261000	-0.880809000
1	4.045202000	3.243767000	-0.156092000
1	3.622417000	3.098090000	-1.878540000
1	2.819166000	4.312663000	-0.876083000
8	0.691629000	4.084115000	-0.825818000
7	-0.106767000	2.191432000	0.177688000
6	-1.421523000	2.722569000	0.292065000
6	-2.105683000	3.272457000	-0.786376000
6	-2.077455000	2.575925000	1.509122000
6	-3.420537000	3.670149000	-0.638863000
1	-1.601936000	3.380319000	-1.738098000
6	-3.398907000	2.967011000	1.647141000

1	-1.538193000	2.158827000	2.355548000
6	-4.074841000	3.518683000	0.574518000
1	-3.944614000	4.096847000	-1.486463000
1	-3.895822000	2.843376000	2.602282000
1	-5.107566000	3.829069000	0.680069000
13	0.037150000	0.433425000	0.766473000
9	0.422800000	0.278931000	2.388498000
6	-1.447895000	-0.747782000	0.210084000
6	-2.157448000	-1.558470000	1.076214000
6	-1.836484000	-0.802196000	-1.115788000
6	-3.194462000	-2.378921000	0.665743000
6	-2.864053000	-1.604365000	-1.577176000
6	-3.547468000	-2.398348000	-0.672254000
9	-1.856527000	-1.578282000	2.371829000
9	-3.848522000	-3.142301000	1.525029000
9	-4.530434000	-3.174133000	-1.085226000
9	-3.200811000	-1.627950000	-2.856091000
9	-1.206821000	-0.053154000	-2.025489000

13AIP^{C-F} (T.E = -2670.885961)

7	0.624718000	-1.555606000	0.290280000
6	0.154085000	-2.468779000	-0.715436000
6	-1.145009000	-2.475418000	-1.207525000
6	-2.101549000	-1.526740000	-0.871028000
1	-1.418512000	-3.253458000	-1.911593000
13	-0.296496000	-0.105718000	0.937260000
15	2.113440000	-2.227986000	0.080314000
6	1.282537000	-3.244867000	-1.023306000
6	1.507457000	-4.309008000	-2.027634000
1	1.006047000	-5.249560000	-1.774895000
1	1.150358000	-4.013393000	-3.021654000
1	2.571550000	-4.537071000	-2.126379000
7	-1.842776000	-0.407529000	-0.003511000
6	-3.449998000	-1.368928000	-1.230400000
15	-3.430958000	-0.010120000	-0.181437000
6	-4.356529000	-2.197739000	-2.055505000
1	-3.814374000	-2.637999000	-2.897502000
1	-4.816427000	-3.028815000	-1.504832000
1	-5.170816000	-1.607498000	-2.481657000
7	-4.348384000	-0.070699000	1.198070000
7	-3.593192000	1.563094000	-0.659025000
6	-3.956848000	0.817814000	2.289681000
1	-3.126798000	0.390804000	2.866850000
1	-3.636961000	1.786215000	1.905844000
1	-4.808842000	0.974434000	2.956403000
6	-4.682583000	-1.402214000	1.680866000
1	-3.815438000	-1.894276000	2.142738000
1	-5.471109000	-1.317915000	2.432490000

1	-5.043771000	-2.027494000	0.865982000
6	-2.695550000	2.049352000	-1.692177000
1	-2.363150000	3.062743000	-1.446832000
1	-1.818184000	1.408433000	-1.769480000
1	-3.195055000	2.075114000	-2.667493000
6	-4.826432000	2.315292000	-0.562670000
1	-5.338443000	2.361681000	-1.531586000
1	-5.499804000	1.862811000	0.162424000
1	-4.611543000	3.341779000	-0.247428000
7	2.723876000	-2.662287000	1.559618000
7	3.341079000	-1.320400000	-0.545722000
6	4.031740000	-3.282410000	1.654796000
1	4.501663000	-3.007494000	2.603897000
1	3.959028000	-4.377081000	1.618348000
1	4.679018000	-2.954261000	0.842879000
6	1.803551000	-3.141040000	2.579186000
1	0.871198000	-2.581734000	2.548164000
1	1.584598000	-4.209331000	2.454489000
1	2.260314000	-2.996770000	3.561459000
6	3.448754000	-1.111428000	-1.977991000
1	4.501599000	-1.142153000	-2.275066000
1	2.905116000	-1.884451000	-2.518402000
1	3.037980000	-0.137669000	-2.268704000
6	4.020082000	-0.298002000	0.230105000
1	3.815498000	-0.417163000	1.292994000
1	5.102213000	-0.356898000	0.071790000
1	3.684755000	0.700796000	-0.075156000
9	-0.539647000	-0.141020000	2.589415000
6	0.679197000	1.556773000	0.392116000
6	1.126877000	2.561588000	1.228760000
6	1.056658000	1.679043000	-0.932594000
6	1.909332000	3.619980000	0.791860000
6	1.837539000	2.710725000	-1.420775000
6	2.267825000	3.691204000	-0.542699000
9	0.820617000	2.550316000	2.521285000
9	2.318408000	4.561726000	1.626221000
9	3.011267000	4.690497000	-0.978200000
9	2.180324000	2.773799000	-2.698965000
9	0.668082000	0.757614000	-1.824133000

1GaP^{C-F} (T.E = -3440.933475)

7	1.468222000	-1.920937000	0.188441000
7	-1.454610000	-1.950887000	0.197420000
6	1.255966000	-2.948818000	0.984844000
6	-1.218206000	-2.965044000	1.001817000
6	0.025526000	-3.470710000	1.356141000
1	0.035853000	-4.343520000	1.993321000
6	2.768317000	-1.401157000	0.005209000

6	3.694738000	-1.358926000	1.041704000
6	3.101769000	-0.867590000	-1.236284000
6	4.948881000	-0.817178000	0.825645000
6	4.354057000	-0.319217000	-1.438993000
6	5.284531000	-0.297155000	-0.412896000
1	5.662304000	-0.783051000	1.640752000
1	4.604979000	0.088857000	-2.410796000
1	6.264791000	0.134501000	-0.574622000
6	-2.764408000	-1.445483000	0.041427000
6	-3.162013000	-0.997353000	-1.214170000
6	-3.633050000	-1.333380000	1.121409000
6	-4.427420000	-0.469219000	-1.387530000
6	-4.899903000	-0.810067000	0.935591000
6	-5.302821000	-0.379729000	-0.317306000
1	-4.732690000	-0.129072000	-2.369940000
1	-5.569562000	-0.719431000	1.782794000
1	-6.293018000	0.036865000	-0.456767000
1	-3.297360000	-1.618444000	2.112549000
1	-2.476111000	-1.088375000	-2.051529000
1	2.379205000	-0.910336000	-2.046845000
1	3.419334000	-1.715791000	2.027747000
31	-0.006743000	-0.965340000	-0.647850000
1	-2.092703000	-3.461844000	1.425037000
1	2.141875000	-3.442031000	1.387394000
9	-0.026344000	-1.346607000	-2.382377000
6	-0.016221000	0.939359000	-0.152683000
6	0.187983000	1.986570000	-1.028486000
6	-0.221116000	1.263205000	1.173694000
6	0.178153000	3.307336000	-0.612529000
6	-0.241077000	2.566888000	1.632172000
6	-0.040052000	3.593622000	0.724714000
9	0.410212000	1.751801000	-2.313240000
9	0.376014000	4.294235000	-1.467040000
9	-0.051459000	4.844803000	1.135655000
9	-0.441762000	2.845633000	2.907594000
9	-0.402329000	0.290854000	2.069751000

4GaP^{C-F} (T.E = -3653.724408)

7	1.223031000	0.467112000	-0.345315000
6	0.932428000	1.715590000	-0.710937000
6	-0.309329000	2.286518000	-0.888911000
6	-1.547276000	1.686049000	-0.595226000
6	-1.754334000	0.374108000	-0.263458000
6	2.551624000	0.131534000	-0.026270000
6	3.007283000	-1.162591000	-0.265469000
6	3.425705000	1.048896000	0.553882000
6	4.307109000	-1.518367000	0.035933000
1	2.333981000	-1.893678000	-0.700623000

6	4.728356000	0.688331000	0.846387000
1	3.073115000	2.041137000	0.810239000
6	5.179804000	-0.593926000	0.586189000
1	4.640876000	-2.529992000	-0.163747000
1	5.391286000	1.415560000	1.301388000
1	6.198506000	-0.875380000	0.823827000
1	1.789087000	2.366318000	-0.888415000
15	-3.241808000	-0.227732000	0.328487000
6	-4.648316000	0.878721000	0.119789000
1	-5.549012000	0.407370000	0.515959000
1	-4.472829000	1.810728000	0.658192000
1	-4.794038000	1.101774000	-0.937750000
6	-3.673073000	-1.781826000	-0.465036000
1	-3.719262000	-1.647139000	-1.546206000
1	-2.901027000	-2.519898000	-0.234884000
1	-4.631545000	-2.148734000	-0.093987000
6	-3.134168000	-0.621076000	2.078848000
1	-2.993215000	0.298576000	2.647951000
1	-4.031954000	-1.137529000	2.424119000
1	-2.252431000	-1.254131000	2.218066000
1	-2.399735000	2.370870000	-0.630638000
1	-0.314073000	3.320517000	-1.208881000
31	-0.209863000	-0.854203000	-0.269708000
6	-0.114289000	-2.193553000	-1.763700000
6	-0.487701000	-3.517847000	-1.654818000
6	0.316063000	-1.782679000	-3.010187000
6	-0.422931000	-4.406029000	-2.715516000
6	0.401314000	-2.632155000	-4.098963000
6	0.029304000	-3.956683000	-3.943971000
9	-0.140091000	-1.725858000	1.305073000
9	-0.953833000	-3.996014000	-0.501787000
9	-0.791761000	-5.668612000	-2.576366000
9	0.096404000	-4.786132000	-4.967111000
9	0.822696000	-2.203489000	-5.276245000
9	0.668632000	-0.512323000	-3.202425000

6GaP^{C-F} (T.E = -3784.304418)

6	2.835584000	-0.422939000	1.019827000
6	1.984500000	-0.901279000	0.021157000
6	1.780036000	1.873353000	1.107545000
1	1.900768000	2.837757000	1.605560000
7	0.891513000	1.800054000	0.164994000
15	2.444669000	-2.427805000	-0.588865000
6	4.066212000	-2.466840000	-1.375017000
1	4.812547000	-2.156082000	-0.643909000
1	4.297696000	-3.470846000	-1.735912000
1	4.068607000	-1.767214000	-2.211574000
6	2.471257000	-3.766993000	0.618508000

1	1.476421000	-3.870923000	1.053589000
1	2.763090000	-4.706942000	0.145943000
1	3.180154000	-3.510231000	1.405342000
6	1.266465000	-2.927690000	-1.849845000
1	1.194285000	-2.153755000	-2.617558000
1	1.573499000	-3.870760000	-2.304251000
1	0.281038000	-3.056167000	-1.396999000
8	3.806583000	-0.991950000	1.512051000
7	2.582395000	0.919199000	1.578458000
6	3.430297000	1.254742000	2.716119000
1	3.273869000	0.539761000	3.522477000
1	4.481904000	1.215618000	2.436408000
1	3.177113000	2.252863000	3.069132000
6	0.272449000	3.002330000	-0.257933000
6	-1.090448000	3.007015000	-0.525613000
6	1.009381000	4.166374000	-0.440301000
6	-1.710585000	4.170749000	-0.936819000
1	-1.660709000	2.092992000	-0.403870000
6	0.380382000	5.330027000	-0.846708000
1	2.084801000	4.149450000	-0.301037000
6	-0.981061000	5.338358000	-1.092267000
1	-2.775140000	4.164013000	-1.138445000
1	0.965476000	6.230735000	-0.991029000
1	-1.470450000	6.247679000	-1.419470000
31	0.441751000	0.039460000	-0.664777000
6	-1.392118000	-0.539730000	-0.098810000
6	-2.309913000	-1.164763000	-0.919305000
6	-1.767349000	-0.367421000	1.218545000
6	-3.550280000	-1.585511000	-0.466703000
6	-2.994067000	-0.766933000	1.716262000
6	-3.891747000	-1.380833000	0.858931000
9	0.450965000	0.371927000	-2.422251000
9	-2.022493000	-1.404564000	-2.193860000
9	-4.407723000	-2.183408000	-1.275995000
9	-5.067229000	-1.775955000	1.307010000
9	-3.320328000	-0.577861000	2.983480000
9	-0.923556000	0.215928000	2.075020000

8GaP^{C-F} (T.E = -4018.346988)

7	-0.920291000	-1.333530000	0.468617000
6	-1.865655000	-0.851224000	1.422550000
6	-1.468209000	0.173638000	2.385058000
15	-2.204470000	-2.128205000	-0.229182000
6	-3.063050000	-1.440347000	1.133743000
6	-4.406918000	-1.373137000	1.746383000
1	-4.743166000	-2.336269000	2.140902000
1	-4.404037000	-0.664737000	2.579038000
1	-5.170269000	-1.034639000	1.038599000

7	-2.795369000	-1.681945000	-1.685690000
7	-1.855155000	-3.725479000	-0.384641000
6	-2.200335000	-2.135184000	-2.939173000
1	-1.550208000	-1.357348000	-3.343606000
1	-1.602378000	-3.030756000	-2.782752000
1	-2.998113000	-2.362394000	-3.652334000
6	-3.416380000	-0.367213000	-1.811734000
1	-4.154306000	-0.400750000	-2.616837000
1	-3.920036000	-0.087708000	-0.887213000
1	-2.662573000	0.391938000	-2.049313000
6	-2.829925000	-4.657235000	-0.920002000
1	-2.338758000	-5.362767000	-1.597353000
1	-3.305080000	-5.231492000	-0.116260000
1	-3.605953000	-4.132310000	-1.475359000
6	-0.852388000	-4.351581000	0.460451000
1	-0.138421000	-3.608950000	0.810730000
1	-1.312401000	-4.840259000	1.327289000
1	-0.319473000	-5.111405000	-0.117824000
6	-0.601401000	2.672376000	-0.513496000
6	-1.804661000	3.279517000	-0.873368000
6	0.567751000	3.121826000	-1.124825000
6	-1.830256000	4.316071000	-1.788255000
1	-2.723473000	2.924588000	-0.415947000
6	0.538232000	4.150229000	-2.048669000
1	1.511435000	2.656380000	-0.854218000
6	-0.659678000	4.759940000	-2.382275000
1	-2.777767000	4.775665000	-2.047810000
1	1.462567000	4.479387000	-2.509762000
1	-0.682364000	5.567470000	-3.104078000
7	-0.573383000	1.601661000	0.397032000
5	-1.218556000	1.604604000	1.664721000
7	-1.583736000	2.783709000	2.379501000
6	-0.994283000	4.081670000	2.140776000
1	-0.123356000	4.009390000	1.493141000
1	-1.703343000	4.781183000	1.678095000
1	-0.671680000	4.519385000	3.093442000
6	-2.555917000	2.850669000	3.440872000
1	-3.123182000	1.925987000	3.533965000
1	-2.091112000	3.069742000	4.411911000
1	-3.278090000	3.653198000	3.242765000
1	-2.192892000	0.236550000	3.195538000
1	-0.507035000	-0.111014000	2.829464000
31	0.230379000	0.023332000	-0.324464000
6	2.171837000	-0.302605000	-0.037646000
6	3.123639000	-0.180432000	-1.032111000
6	2.634762000	-0.665845000	1.210059000
6	4.470010000	-0.418282000	-0.806842000
6	3.967548000	-0.914635000	1.481863000
6	4.890609000	-0.789277000	0.458244000

9	-0.189857000	-0.086781000	-2.069682000
9	2.776010000	0.183325000	-2.258081000
9	5.357351000	-0.294441000	-1.778805000
9	6.168342000	-1.018711000	0.689619000
9	4.370457000	-1.264120000	2.692219000
9	1.778481000	-0.786586000	2.228613000

10GaP^{C-F} (T.E = -4109.852349)

7	1.469666000	-0.195551000	-0.394645000
6	2.564081000	0.395604000	-1.090311000
6	2.595232000	1.742065000	-1.456830000
6	1.640756000	2.689828000	-1.100087000
1	3.455650000	2.070143000	-2.029345000
1	1.868418000	3.690963000	-1.479078000
15	2.398980000	-1.548696000	-0.242129000
6	3.491308000	-0.650521000	-1.227003000
6	4.868471000	-0.685745000	-1.769513000
1	4.900664000	-0.436188000	-2.835234000
1	5.541707000	0.014855000	-1.257989000
1	5.306791000	-1.680611000	-1.667255000
6	0.490187000	2.547448000	-0.334159000
15	-0.455457000	3.863531000	0.153987000
6	-0.050624000	5.443881000	-0.616682000
1	-0.723192000	6.217436000	-0.242744000
1	0.976160000	5.723544000	-0.378537000
1	-0.155686000	5.369006000	-1.699552000
6	-0.376826000	4.143925000	1.934391000
1	-1.110909000	4.883213000	2.261538000
1	-0.548844000	3.188579000	2.437890000
1	0.628389000	4.477034000	2.196243000
6	-2.210300000	3.592363000	-0.164583000
1	-2.371518000	3.470807000	-1.236180000
1	-2.517471000	2.670114000	0.334694000
1	-2.813109000	4.420053000	0.213838000
31	0.096686000	0.793283000	0.474127000
7	2.902612000	-1.916358000	1.291844000
7	1.540327000	-2.887091000	-0.681619000
6	1.860535000	-2.208672000	2.277548000
1	1.400376000	-1.283225000	2.649232000
1	1.079189000	-2.830420000	1.842028000
1	2.302915000	-2.750620000	3.117201000
6	3.936435000	-1.055053000	1.849511000
1	4.346440000	-1.531708000	2.743074000
1	4.742142000	-0.906776000	1.132236000
1	3.531408000	-0.074696000	2.135056000
6	1.948860000	-4.241897000	-0.379837000
1	1.082258000	-4.828994000	-0.057089000
1	2.377509000	-4.731795000	-1.262438000

1	2.689899000	-4.251983000	0.417289000
6	0.612365000	-2.786891000	-1.792614000
1	0.372323000	-1.742969000	-1.991470000
1	1.031647000	-3.233098000	-2.701682000
1	-0.315574000	-3.313528000	-1.545585000
6	-1.608932000	-0.237336000	0.202769000
6	-2.191820000	-1.057333000	1.149607000
6	-2.193909000	-0.244824000	-1.048447000
6	-3.302476000	-1.841696000	0.878640000
6	-3.304148000	-1.007212000	-1.365294000
6	-3.860793000	-1.812760000	-0.386958000
9	0.401058000	0.869952000	2.265664000
9	-1.694228000	-1.138817000	2.377181000
9	-3.835052000	-2.618677000	1.808065000
9	-4.919671000	-2.551274000	-0.661108000
9	-3.835881000	-0.982621000	-2.577208000
9	-1.679153000	0.502384000	-2.028360000

11GaP^{C-F} (T.E = -4027.647336)

7	1.606055000	0.036643000	-0.409172000
6	2.575796000	1.062040000	-0.388627000
6	0.899669000	2.948154000	-0.357033000
7	-0.095289000	2.176519000	0.123578000
15	2.864896000	-1.029035000	-0.205274000
6	3.811989000	0.414127000	-0.377398000
6	5.254927000	0.772103000	-0.363365000
1	5.533083000	1.451705000	-1.171381000
1	5.582741000	1.229622000	0.576661000
1	5.856454000	-0.129861000	-0.496491000
6	-1.412041000	2.701356000	0.164673000
6	-1.998905000	3.355499000	-0.912577000
6	-2.171449000	2.454129000	1.303401000
6	-3.321403000	3.751795000	-0.841636000
1	-1.414557000	3.547297000	-1.802689000
6	-3.497217000	2.846264000	1.364739000
1	-1.706980000	1.955806000	2.151420000
6	-4.077896000	3.499320000	0.292083000
1	-3.769161000	4.259056000	-1.688654000
1	-4.073739000	2.644182000	2.259949000
1	-5.114729000	3.810601000	0.337322000
31	0.041277000	0.340458000	0.647884000
7	3.003257000	-1.795937000	1.235910000
7	2.720237000	-2.245357000	-1.297829000
6	1.962742000	-2.736914000	1.642399000
1	1.445347000	-3.142736000	0.772726000
1	2.410482000	-3.565714000	2.197580000
1	1.229643000	-2.232727000	2.282255000
6	3.596059000	-1.094999000	2.370089000

1	4.439416000	-0.487943000	2.046199000
1	2.855705000	-0.455725000	2.862661000
1	3.959424000	-1.837742000	3.084419000
6	3.488911000	-3.472383000	-1.231455000
1	2.835320000	-4.329236000	-1.423503000
1	4.284478000	-3.477933000	-1.984896000
1	3.939353000	-3.594528000	-0.248299000
6	2.153323000	-1.977036000	-2.609666000
1	1.574023000	-1.055980000	-2.591527000
1	2.938911000	-1.893823000	-3.368551000
1	1.488189000	-2.798296000	-2.891626000
8	0.807162000	4.095484000	-0.720802000
7	2.238619000	2.363394000	-0.370430000
6	3.332548000	3.318977000	-0.491889000
1	4.090892000	3.112243000	0.262421000
1	3.786212000	3.272595000	-1.484004000
1	2.932026000	4.316171000	-0.345730000
6	-1.492027000	-0.803085000	0.180587000
6	-2.223358000	-1.530219000	1.098488000
6	-1.907172000	-0.862757000	-1.135521000
6	-3.319864000	-2.293183000	0.734573000
6	-2.996109000	-1.611982000	-1.542861000
6	-3.704250000	-2.331293000	-0.595058000
9	0.614023000	0.187256000	2.344441000
9	-1.893003000	-1.512739000	2.383065000
9	-4.002285000	-2.981989000	1.631969000
9	-4.743904000	-3.054149000	-0.959168000
9	-3.367322000	-1.652628000	-2.810196000
9	-1.253384000	-0.175472000	-2.069798000

$^{13}\text{GaP}^{\text{C-F}}$ (T.E = -4353.195342)

7	-1.397315000	-1.005418000	-0.563482000
6	-1.231515000	-2.408325000	-0.850864000
6	-0.001011000	-3.033939000	-1.017690000
6	1.229953000	-2.409223000	-0.851160000
1	-0.001426000	-4.104428000	-1.195299000
15	-2.966504000	-1.369200000	-0.190817000
6	-2.538612000	-2.916809000	-0.799726000
6	-3.052640000	-4.300439000	-0.916510000
1	-2.955237000	-4.699453000	-1.931345000
1	-2.525980000	-4.994695000	-0.248625000
1	-4.112494000	-4.350829000	-0.658247000
7	1.396736000	-1.006620000	-0.562803000
6	2.536798000	-2.918499000	-0.800779000
15	2.965820000	-1.371562000	-0.190963000
6	3.050005000	-4.302382000	-0.918175000
1	2.522783000	-4.996650000	-0.250739000
1	2.952617000	-4.700849000	-1.933227000

1	4.109765000	-4.353514000	-0.659678000
7	3.984794000	-0.268912000	-0.877906000
7	3.380322000	-1.305646000	1.409939000
6	3.668692000	0.232770000	-2.203327000
1	4.236355000	-0.298223000	-2.976557000
1	2.604487000	0.119586000	-2.404844000
1	3.922340000	1.295769000	-2.260452000
6	5.384689000	-0.151331000	-0.529026000
1	6.021914000	-0.637314000	-1.277818000
1	5.668977000	0.905278000	-0.481442000
1	5.580140000	-0.606309000	0.440318000
6	3.318293000	-0.014496000	2.089015000
1	4.032828000	0.000030000	2.916878000
1	3.568591000	0.796056000	1.404684000
1	2.311950000	0.161979000	2.491110000
6	2.902286000	-2.387667000	2.263414000
1	1.839208000	-2.261522000	2.505812000
1	3.045461000	-3.350725000	1.776241000
1	3.476982000	-2.379145000	3.193017000
7	-3.984696000	-0.266103000	-0.878332000
7	-3.381001000	-1.301970000	1.409953000
6	-5.385062000	-0.149586000	-0.530940000
1	-5.670423000	0.906789000	-0.484867000
1	-6.021094000	-0.637086000	-1.279774000
1	-5.580985000	-0.603609000	0.438760000
6	-3.667706000	0.235816000	-2.203461000
1	-2.603277000	0.123177000	-2.404085000
1	-4.234456000	-0.295371000	-2.977240000
1	-3.921838000	1.298692000	-2.260695000
6	-2.905326000	-2.384031000	2.264613000
1	-3.482655000	-2.375827000	3.192606000
1	-3.046896000	-3.347007000	1.776816000
1	-1.842949000	-2.257777000	2.509962000
6	-3.318785000	-0.010502000	2.088328000
1	-3.568857000	0.799706000	1.403514000
1	-4.033434000	0.004590000	2.916089000
1	-2.312453000	0.165956000	2.490478000
31	-0.000098000	-0.081727000	0.326350000
6	0.000848000	1.889971000	0.145567000
6	0.001632000	2.779229000	1.202371000
6	0.000539000	2.437574000	-1.122858000
6	0.002096000	4.152229000	1.018504000
6	0.000957000	3.801756000	-1.352994000
6	0.001748000	4.662130000	-0.268378000
9	-0.001394000	-0.601875000	2.066924000
9	0.002098000	2.339925000	2.454335000
9	0.002874000	4.980625000	2.048836000
9	0.002173000	5.966337000	-0.461246000
9	-0.000321000	1.641356000	-2.190293000

9 0.000592000 4.293064000 -2.580626000

Cartesian coordinates of the B–H splitting products obtained for some of the representative Al(I)/Ga(I) carbenoids and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

1AIP^{B-H} (T.E = -1342.474048)

7	-1.408979000	-1.723141000	-0.510022000
6	-1.191212000	-2.358236000	-1.642728000
6	0.045939000	-2.597973000	-2.225324000
7	1.451768000	-1.694952000	-0.483304000
1	0.059793000	-3.095897000	-3.184313000
1	-2.068737000	-2.736472000	-2.170793000
6	-2.718249000	-1.721661000	0.024013000
6	-3.221081000	-0.554734000	0.590429000
6	-3.498213000	-2.873842000	0.027567000
6	-4.493096000	-0.542814000	1.132283000
1	-2.627167000	0.354219000	0.568490000
6	-4.771917000	-2.850570000	0.565974000
1	-3.087952000	-3.798332000	-0.363753000
6	-5.275323000	-1.685842000	1.120020000
1	-4.878570000	0.374396000	1.562304000
1	-5.367918000	-3.755930000	0.567970000
1	-6.270383000	-1.671557000	1.548380000
6	2.750988000	-1.668603000	0.073844000
6	3.216386000	-0.497028000	0.662607000
6	3.558212000	-2.801982000	0.078069000
6	4.478750000	-0.461508000	1.225843000
1	2.602396000	0.398590000	0.642622000
6	4.821950000	-2.754968000	0.637846000
1	3.176751000	-3.731680000	-0.329626000
6	5.288371000	-1.585227000	1.213295000
1	4.834345000	0.459354000	1.673309000
1	5.439059000	-3.646093000	0.639757000
1	6.275613000	-1.552335000	1.658388000
6	1.266987000	-2.332285000	-1.620856000
1	2.161266000	-2.690668000	-2.134410000
13	0.003335000	-0.838480000	0.483688000
1	-0.005852000	-1.366682000	1.978988000
6	0.721742000	3.378675000	-0.393987000
6	-0.786118000	3.423616000	-0.031705000

5	-0.014709000	1.275330000	0.122916000
8	1.107931000	2.076332000	0.081366000
8	-1.150355000	2.031950000	-0.081587000
6	1.571042000	4.427478000	0.282169000
1	2.609806000	4.318775000	-0.035589000
1	1.235842000	5.430823000	0.004012000
1	1.538786000	4.337196000	1.367405000
6	0.979018000	3.392231000	-1.889907000
1	0.783429000	4.374696000	-2.325299000
1	2.026732000	3.141956000	-2.065443000
1	0.364527000	2.651367000	-2.405478000
6	-1.047238000	3.894315000	1.387493000
1	-0.866721000	4.965816000	1.498157000
1	-2.092140000	3.696908000	1.633874000
1	-0.424571000	3.357279000	2.105852000
6	-1.649728000	4.198982000	-0.996811000
1	-2.687567000	4.178145000	-0.658930000
1	-1.330083000	5.244036000	-1.043224000
1	-1.613885000	3.777929000	-2.000930000

4AIP^{B-H} (T.E = -1555.255910)

7	0.187430000	-2.344202000	0.047179000
6	-0.437848000	-3.234267000	-0.723255000
6	-1.762907000	-3.230857000	-1.094446000
6	-2.689184000	-2.206817000	-0.805197000
6	-2.458863000	-1.099461000	-0.033005000
6	1.588336000	-2.381720000	0.141420000
6	2.193277000	-2.031293000	1.347335000
6	2.398999000	-2.674676000	-0.953168000
6	3.569574000	-1.973275000	1.452926000
1	1.566413000	-1.811439000	2.206628000
6	3.775838000	-2.620864000	-0.839129000
1	1.942240000	-2.893749000	-1.911730000
6	4.370565000	-2.266988000	0.361001000
1	4.020672000	-1.698344000	2.399783000
1	4.390888000	-2.838267000	-1.705330000
1	5.449823000	-2.216836000	0.443247000
1	0.172987000	-4.059499000	-1.094962000
15	-3.641002000	0.117316000	0.145326000
6	-5.291105000	-0.279206000	-0.470769000
1	-5.968230000	0.553967000	-0.276125000
1	-5.254675000	-0.460990000	-1.545566000
1	-5.668680000	-1.173855000	0.025515000
6	-3.836794000	0.570757000	1.876230000
1	-4.140734000	-0.302573000	2.453955000
1	-2.870768000	0.910739000	2.257778000
1	-4.570417000	1.370971000	1.989198000
6	-3.173069000	1.661889000	-0.656991000

1	-3.036633000	1.490139000	-1.725677000
1	-3.935986000	2.427440000	-0.499881000
1	-2.222830000	2.001028000	-0.232656000
1	-3.668056000	-2.350001000	-1.275341000
1	-2.098367000	-4.063974000	-1.699057000
13	-0.704376000	-0.874070000	0.912508000
1	-0.873869000	-1.090013000	2.496130000
6	0.899945000	3.074741000	-0.153282000
6	2.140451000	2.161915000	-0.338266000
5	0.363240000	0.900314000	0.343372000
8	0.000870000	2.220877000	0.577699000
8	1.552806000	0.855580000	-0.352354000
6	0.214142000	3.418988000	-1.463706000
1	-0.748593000	3.886700000	-1.244090000
1	0.802461000	4.120835000	-2.058902000
1	0.030095000	2.522257000	-2.060538000
6	1.148572000	4.334020000	0.641081000
1	1.899859000	4.957699000	0.147707000
1	0.225352000	4.912683000	0.715444000
1	1.489422000	4.111724000	1.651606000
6	2.908443000	2.374679000	-1.620817000
1	3.303761000	3.393587000	-1.672433000
1	3.750851000	1.680856000	-1.656505000
1	2.288813000	2.193664000	-2.498667000
6	3.094694000	2.196367000	0.843144000
1	3.801960000	1.371426000	0.735783000
1	3.656130000	3.132566000	0.889029000
1	2.562023000	2.057031000	1.786675000

6AIP^{B-H} (T.E = -1685.836942)

6	-2.686001000	1.404570000	0.547378000
6	-2.182793000	0.470121000	-0.357544000
6	-0.587846000	2.809323000	0.503963000
1	-0.153613000	3.709220000	0.946848000
13	-0.428695000	0.492769000	-1.230961000
7	0.170728000	2.098298000	-0.272601000
15	-3.228370000	-0.867884000	-0.513557000
6	-3.450424000	-1.842118000	0.991791000
1	-3.840863000	-1.191617000	1.774268000
1	-4.136165000	-2.675348000	0.824851000
1	-2.475083000	-2.228388000	1.295459000
6	-4.901424000	-0.497062000	-1.083712000
1	-4.843069000	-0.021876000	-2.063717000
1	-5.494656000	-1.410923000	-1.156613000
1	-5.361899000	0.193241000	-0.377787000
6	-2.563961000	-2.029256000	-1.715418000
1	-1.596181000	-2.409097000	-1.373692000
1	-3.254264000	-2.864473000	-1.846491000

1	-2.424962000	-1.526054000	-2.674512000
8	-3.752213000	1.391516000	1.164119000
7	-1.856291000	2.597686000	0.843291000
6	-2.506932000	3.585036000	1.691534000
1	-3.419653000	3.945653000	1.218711000
1	-2.783956000	3.146002000	2.649026000
1	-1.830325000	4.423226000	1.852141000
6	1.541366000	2.450229000	-0.353457000
6	2.169702000	2.419999000	-1.592581000
6	2.282080000	2.751094000	0.783142000
6	3.516936000	2.712989000	-1.691518000
1	1.586518000	2.166820000	-2.471977000
6	3.628487000	3.049921000	0.675259000
1	1.810997000	2.700580000	1.758685000
6	4.250739000	3.034416000	-0.561105000
1	3.997195000	2.690871000	-2.662817000
1	4.198954000	3.275422000	1.568851000
1	5.307554000	3.259094000	-0.642156000
1	-0.403389000	0.808471000	-2.801794000
6	1.399831000	-3.152421000	0.279607000
6	2.513030000	-2.135639000	0.641933000
5	0.835165000	-1.072642000	-0.494691000
8	0.641506000	-2.431478000	-0.704342000
8	1.861306000	-0.879296000	0.408364000
6	0.452339000	-3.436580000	1.432703000
1	-0.411339000	-3.982327000	1.044095000
1	0.919633000	-4.046896000	2.208794000
1	0.093491000	-2.508112000	1.884743000
6	1.889416000	-4.450944000	-0.314086000
1	2.543986000	-4.973376000	0.389754000
1	1.039245000	-5.101163000	-0.530630000
1	2.434609000	-4.289195000	-1.243296000
6	2.985436000	-2.191227000	2.075098000
1	3.408770000	-3.173413000	2.305457000
1	3.764021000	-1.441786000	2.231176000
1	2.176388000	-1.985930000	2.775648000
6	3.705672000	-2.194573000	-0.295878000
1	4.330277000	-1.317364000	-0.116006000
1	4.311536000	-3.088450000	-0.129629000
1	3.389253000	-2.172446000	-1.340688000

8AIP^{B-H} (T.E = -1919.889483)

7	-1.300553000	-1.331173000	0.027205000
6	-1.360046000	-0.903675000	1.385743000
6	-0.129945000	-0.499802000	2.065229000
15	-2.950102000	-1.198093000	0.045860000
6	-2.680799000	-0.819823000	1.732542000
6	-3.389684000	-0.435532000	2.971902000

1	-4.020593000	-1.238199000	3.364345000
1	-2.667982000	-0.181617000	3.752225000
1	-4.035224000	0.438107000	2.834418000
7	-3.693553000	-0.002043000	-0.795007000
7	-3.642427000	-2.580357000	-0.515670000
6	-3.894238000	-0.090821000	-2.235441000
1	-3.135540000	0.497629000	-2.760732000
1	-3.814272000	-1.121271000	-2.577155000
1	-4.887869000	0.291747000	-2.489032000
6	-3.614692000	1.377591000	-0.331756000
1	-4.541607000	1.895244000	-0.593217000
1	-3.479201000	1.418407000	0.747413000
1	-2.774927000	1.905630000	-0.798788000
6	-5.079777000	-2.720454000	-0.637494000
1	-5.326402000	-3.234103000	-1.572259000
1	-5.489321000	-3.309762000	0.191326000
1	-5.566248000	-1.746178000	-0.642331000
6	-2.939336000	-3.846531000	-0.402941000
1	-1.867383000	-3.674012000	-0.332913000
1	-3.270571000	-4.406975000	0.479248000
1	-3.143450000	-4.453212000	-1.289802000
13	-0.084058000	-0.326972000	-1.072910000
6	-0.113133000	2.493536000	-0.397488000
6	-0.641033000	3.512206000	0.408494000
6	0.223802000	2.830899000	-1.714036000
6	-0.818303000	4.793960000	-0.075516000
1	-0.923437000	3.268891000	1.429317000
6	0.035444000	4.113562000	-2.196014000
1	0.654594000	2.069944000	-2.358226000
6	-0.486220000	5.108138000	-1.384759000
1	-1.231625000	5.556218000	0.576630000
1	0.310176000	4.339128000	-3.220793000
1	-0.630196000	6.112216000	-1.765061000
7	0.006264000	1.195754000	0.075419000
5	0.457775000	0.858157000	1.388622000
7	1.471851000	1.564616000	2.094230000
6	2.318976000	2.553505000	1.465861000
1	2.233098000	2.510301000	0.381184000
1	2.078591000	3.574536000	1.789245000
1	3.367130000	2.361033000	1.729161000
6	1.847589000	1.348081000	3.467259000
1	1.186925000	0.639571000	3.962352000
1	2.873207000	0.960325000	3.542677000
1	1.816164000	2.287409000	4.034408000
1	-0.315187000	-0.368256000	3.132930000
1	0.630565000	-1.283900000	1.946912000
1	-0.861628000	-0.059689000	-2.444716000
6	3.740334000	-1.900905000	0.140884000
6	4.189048000	-1.112099000	-1.118250000

5	1.905193000	-1.090526000	-0.952017000
8	2.986901000	-0.422024000	-1.489294000
8	2.338104000	-2.094938000	-0.101829000
6	3.850322000	-1.090212000	1.421563000
1	3.341147000	-1.632074000	2.222646000
1	4.889415000	-0.936312000	1.721582000
1	3.361791000	-0.117549000	1.314191000
6	4.408143000	-3.242281000	0.325776000
1	5.490362000	-3.122606000	0.432905000
1	4.029317000	-3.718276000	1.232483000
1	4.212387000	-3.910462000	-0.512231000
6	5.282706000	-0.098382000	-0.877018000
1	6.186860000	-0.585266000	-0.499526000
1	5.533113000	0.399738000	-1.815622000
1	4.972092000	0.666165000	-0.164492000
6	4.564905000	-2.009218000	-2.283575000
1	4.658437000	-1.393803000	-3.180100000
1	5.517252000	-2.517363000	-2.114388000
1	3.794001000	-2.759825000	-2.469344000

10AIP^{B-H} (T.E = -2011.382726)

7	1.532834000	0.509796000	-0.019459000
6	2.303320000	1.537715000	-0.651889000
6	1.780810000	2.794941000	-0.943003000
6	0.463872000	3.179294000	-0.681385000
1	2.434290000	3.494515000	-1.452329000
1	0.214860000	4.161318000	-1.101113000
15	2.892574000	-0.410240000	-0.051935000
6	3.560097000	0.944815000	-0.873547000
6	4.811927000	1.456188000	-1.473528000
1	4.589796000	2.174930000	-2.268133000
1	5.469122000	1.969236000	-0.758149000
1	5.401938000	0.657372000	-1.929708000
6	-0.512224000	2.494691000	0.029898000
15	-2.107356000	3.057798000	0.057752000
6	-2.330279000	4.836023000	-0.202251000
1	-3.387611000	5.096253000	-0.129357000
1	-1.765312000	5.390487000	0.547664000
1	-1.968326000	5.117217000	-1.192032000
6	-2.908356000	2.669149000	1.622988000
1	-3.925918000	3.063889000	1.644702000
1	-2.949921000	1.581346000	1.726885000
1	-2.327706000	3.082911000	2.447797000
6	-3.204140000	2.293036000	-1.165097000
1	-2.821687000	2.495290000	-2.166510000
1	-3.199949000	1.214383000	-0.987988000
1	-4.225951000	2.670251000	-1.077301000
7	3.546479000	-0.805454000	1.423815000

7	2.585772000	-1.895320000	-0.708782000
6	2.725454000	-1.615827000	2.317059000
1	2.010668000	-0.989816000	2.868513000
1	2.160825000	-2.359970000	1.755697000
1	3.366350000	-2.133470000	3.036603000
6	4.220690000	0.269280000	2.135542000
1	4.814838000	-0.160346000	2.946382000
1	4.884922000	0.813734000	1.466318000
1	3.503035000	0.978951000	2.569590000
6	3.488352000	-3.019993000	-0.614538000
1	2.923359000	-3.934369000	-0.400727000
1	4.031664000	-3.173954000	-1.555395000
1	4.213619000	-2.867330000	0.182802000
6	1.643309000	-1.992070000	-1.806177000
1	0.994113000	-1.117284000	-1.822158000
1	2.162274000	-2.076913000	-2.768839000
1	1.010012000	-2.873801000	-1.664072000
13	-0.041944000	0.785361000	0.958449000
1	0.255385000	0.979942000	2.534730000
6	-2.262744000	-2.673651000	-0.513483000
6	-3.399654000	-1.958420000	0.259148000
5	-1.425637000	-0.803056000	0.508424000
8	-2.812089000	-0.675487000	0.529611000
8	-1.089031000	-2.062012000	0.039177000
6	-4.678909000	-1.763118000	-0.519455000
1	-5.104351000	-2.727114000	-0.813401000
1	-5.412244000	-1.247355000	0.104218000
1	-4.521103000	-1.166554000	-1.418120000
6	-3.706381000	-2.600750000	1.599798000
1	-4.348383000	-1.927752000	2.171205000
1	-4.227498000	-3.553896000	1.483120000
1	-2.794472000	-2.766414000	2.176635000
6	-2.190713000	-4.167724000	-0.308710000
1	-3.110822000	-4.651364000	-0.649923000
1	-1.359809000	-4.576393000	-0.888427000
1	-2.028222000	-4.424049000	0.737646000
6	-2.265531000	-2.357539000	-2.000148000
1	-1.337693000	-2.729400000	-2.439159000
1	-3.101742000	-2.832483000	-2.518352000
1	-2.307196000	-1.279186000	-2.175193000

11AIP^{B-H} (T.E = -1929.191930)

7	1.560599000	0.193184000	0.143738000
6	2.412567000	1.255284000	-0.195510000
6	0.589651000	2.969454000	-0.122774000
15	2.851991000	-0.804233000	-0.078872000
6	3.642533000	0.674665000	-0.523218000
6	4.974574000	1.108452000	-1.017272000

1	4.906354000	1.830182000	-1.834261000
1	5.608674000	1.554319000	-0.241313000
1	5.522328000	0.248488000	-1.409618000
7	3.449525000	-1.568670000	1.254487000
7	2.448155000	-2.033492000	-1.088288000
6	2.584468000	-2.532875000	1.926662000
1	1.924648000	-2.030192000	2.645849000
1	1.964307000	-3.064401000	1.205169000
1	3.195862000	-3.261689000	2.464670000
6	4.236726000	-0.780810000	2.192562000
1	4.792509000	-1.460496000	2.842731000
1	4.947090000	-0.149896000	1.661109000
1	3.599113000	-0.143642000	2.818715000
6	3.320889000	-3.165244000	-1.327299000
1	2.729932000	-4.086237000	-1.354454000
1	3.839839000	-3.068988000	-2.288158000
1	4.064253000	-3.255330000	-0.536715000
6	1.461771000	-1.815827000	-2.136926000
1	0.776471000	-1.017374000	-1.858825000
1	1.944985000	-1.578338000	-3.091431000
1	0.869810000	-2.726761000	-2.261544000
7	1.984179000	2.527682000	-0.145535000
6	2.941925000	3.578492000	-0.454549000
1	3.916490000	3.296328000	-0.061511000
1	3.016782000	3.757775000	-1.529488000
1	2.616309000	4.502303000	0.014227000
8	0.385245000	4.070560000	-0.580087000
7	-0.298186000	2.125259000	0.430353000
6	-1.672325000	2.436124000	0.313000000
6	-2.248495000	2.905062000	-0.866235000
6	-2.505041000	2.146343000	1.390515000
6	-3.617503000	3.067717000	-0.956002000
1	-1.615284000	3.138118000	-1.711743000
6	-3.877574000	2.297912000	1.290990000
1	-2.066503000	1.800013000	2.322663000
6	-4.442589000	2.760994000	0.116103000
1	-4.048053000	3.430536000	-1.882716000
1	-4.503668000	2.055437000	2.141983000
1	-5.515851000	2.886492000	0.035375000
13	0.065541000	0.437904000	1.258762000
1	0.540271000	0.573896000	2.781852000
6	-2.805773000	-1.844396000	-0.955326000
6	-3.214208000	-2.356091000	0.452906000
5	-1.436386000	-0.934473000	0.628851000
8	-2.491920000	-1.472717000	1.324742000
8	-1.501794000	-1.291524000	-0.707863000
6	-4.688735000	-2.251608000	0.761299000
1	-5.276642000	-2.836776000	0.048041000
1	-4.882626000	-2.642590000	1.762045000

1	-5.029613000	-1.216496000	0.732074000
6	-2.719750000	-3.761368000	0.745746000
1	-2.856494000	-3.963924000	1.809461000
1	-3.272138000	-4.514276000	0.178588000
1	-1.655367000	-3.860357000	0.518040000
6	-2.695386000	-2.911946000	-2.017532000
1	-3.660385000	-3.401790000	-2.176528000
1	-2.389728000	-2.455397000	-2.961601000
1	-1.959840000	-3.672597000	-1.754723000
6	-3.675395000	-0.705395000	-1.455595000
1	-3.198781000	-0.261484000	-2.331981000
1	-4.670865000	-1.051579000	-1.743180000
1	-3.780281000	0.081901000	-0.704781000

13AIP^{B-H} (T.E = -2254.735357)

7	-1.579539000	-0.785902000	0.083180000
6	-1.637720000	-1.936787000	-0.771453000
6	-0.518981000	-2.668672000	-1.151049000
6	0.764921000	-2.392098000	-0.703565000
1	-0.651699000	-3.496984000	-1.838362000
13	-0.108508000	-0.164535000	1.065934000
15	-3.218121000	-0.740895000	-0.015799000
6	-3.003441000	-2.075848000	-1.073496000
6	-3.747900000	-3.085391000	-1.858537000
1	-3.156614000	-3.416484000	-2.717515000
1	-4.007692000	-3.986839000	-1.287140000
1	-4.681340000	-2.682233000	-2.258435000
7	1.077844000	-1.380587000	0.268614000
6	2.015399000	-2.941300000	-1.044813000
15	2.653863000	-1.758609000	0.014264000
6	2.419763000	-3.919321000	-2.079882000
1	2.122437000	-4.946527000	-1.841489000
1	1.987231000	-3.681942000	-3.060174000
1	3.505762000	-3.927541000	-2.204233000
7	3.618820000	-0.585975000	-0.660050000
7	3.434536000	-2.083915000	1.444620000
6	4.001549000	0.557652000	0.160291000
1	3.160606000	1.245162000	0.327809000
1	4.362744000	0.230938000	1.133196000
1	4.802318000	1.105734000	-0.343806000
6	3.240677000	-0.197202000	-2.012091000
1	2.309211000	0.387059000	-2.023792000
1	4.037611000	0.414410000	-2.442143000
1	3.099517000	-1.078404000	-2.636786000
6	2.661989000	-2.776646000	2.464778000
1	3.180253000	-2.679476000	3.421756000
1	1.671659000	-2.333747000	2.560396000
1	2.553476000	-3.845831000	2.236498000

6	4.804373000	-2.560271000	1.367022000
1	4.844726000	-3.640724000	1.167776000
1	5.348673000	-2.044280000	0.576477000
1	5.311766000	-2.372293000	2.317279000
7	-3.755327000	0.758922000	-0.464730000
7	-4.043911000	-1.005100000	1.402706000
6	-5.152532000	1.134404000	-0.400984000
1	-5.236772000	2.196274000	-0.147661000
1	-5.652764000	0.980007000	-1.365891000
1	-5.676524000	0.553748000	0.356056000
6	-3.029630000	1.433562000	-1.528584000
1	-1.981879000	1.138316000	-1.526934000
1	-3.469389000	1.213875000	-2.509610000
1	-3.066937000	2.514016000	-1.362995000
6	-4.013141000	-2.370558000	1.903783000
1	-4.770674000	-2.479263000	2.684046000
1	-4.231246000	-3.077190000	1.104660000
1	-3.033578000	-2.621667000	2.334291000
6	-3.853652000	-0.033731000	2.474090000
1	-3.812060000	0.979203000	2.074887000
1	-4.688683000	-0.095970000	3.177407000
1	-2.919552000	-0.225720000	3.019452000
1	-0.283723000	-0.461228000	2.637494000
6	0.633533000	3.709967000	-0.824003000
6	1.110344000	4.035816000	0.616784000
8	-0.061897000	2.468395000	-0.640413000
8	1.216647000	2.732717000	1.207762000
5	0.388911000	1.862670000	0.521655000
6	-0.313859000	4.719107000	-1.429588000
1	0.165381000	5.698540000	-1.517508000
1	-0.602213000	4.392536000	-2.431260000
1	-1.221316000	4.828943000	-0.836163000
6	1.774986000	3.445231000	-1.789700000
1	1.365654000	3.003036000	-2.700477000
1	2.300464000	4.364360000	-2.058952000
1	2.497850000	2.741324000	-1.371489000
6	2.447558000	4.733078000	0.704122000
1	2.416695000	5.696284000	0.186344000
1	2.694667000	4.919519000	1.750967000
1	3.247911000	4.131736000	0.272356000
6	0.079880000	4.802136000	1.427518000
1	0.393519000	4.806811000	2.472791000
1	-0.014835000	5.837442000	1.091524000
1	-0.900371000	4.323472000	1.373946000

1GaP^{B-H} (T.E = -3024.841936)

7	1.306690000	-2.079171000	-0.035983000
7	-1.583705000	-1.911340000	-0.069283000

6	1.021504000	-3.133267000	0.693938000
6	-1.437395000	-2.992252000	0.662034000
6	-0.244873000	-3.657694000	0.925526000
1	-0.304950000	-4.570731000	1.501144000
6	2.561301000	-1.460342000	0.063855000
6	3.239115000	-1.357926000	1.276660000
6	3.109528000	-0.857888000	-1.067107000
6	4.450277000	-0.692800000	1.345453000
6	4.315763000	-0.188801000	-0.989595000
6	4.995034000	-0.105633000	0.215607000
1	4.962485000	-0.615519000	2.297689000
1	4.728304000	0.271448000	-1.879815000
1	5.938159000	0.423860000	0.275857000
6	-2.768709000	-1.164305000	-0.004977000
6	-3.220267000	-0.512016000	-1.150431000
6	-3.467594000	-0.993052000	1.187503000
6	-4.354868000	0.275844000	-1.106683000
6	-4.606657000	-0.209327000	1.222522000
6	-5.056332000	0.428916000	0.078527000
1	-4.695693000	0.771125000	-2.008402000
1	-5.135914000	-0.079517000	2.159641000
1	-5.943129000	1.050172000	0.112271000
1	-3.086172000	-1.441012000	2.098102000
1	-2.683256000	-0.646830000	-2.084401000
1	2.586202000	-0.932933000	-2.015358000
1	2.789260000	-1.764601000	2.175365000
31	-0.079943000	-1.176134000	-1.189235000
1	-2.337243000	-3.393665000	1.135224000
1	1.857660000	-3.630750000	1.192199000
1	-0.107643000	-1.903725000	-2.585009000
6	0.635299000	2.988360000	-0.333701000
6	-0.190435000	2.507789000	0.889596000
5	0.057273000	0.818786000	-0.600664000
8	0.382542000	1.947186000	-1.300378000
8	-0.152691000	1.077354000	0.730703000
6	-1.652715000	2.910018000	0.825290000
1	-2.203266000	2.342954000	1.578866000
1	-1.790154000	3.975447000	1.023210000
1	-2.088746000	2.673042000	-0.148242000
6	0.392873000	2.871346000	2.232740000
1	0.472974000	3.957303000	2.336244000
1	-0.259147000	2.502805000	3.026935000
1	1.380081000	2.431650000	2.374592000
6	0.205608000	4.315131000	-0.908610000
1	0.301622000	5.105278000	-0.158321000
1	0.843986000	4.573316000	-1.755565000
1	-0.825987000	4.289283000	-1.258120000
6	2.132008000	2.987443000	-0.080165000
1	2.646864000	3.113388000	-1.034666000

1	2.430528000	3.803215000	0.581929000
1	2.464541000	2.041216000	0.354616000

4GaP^{B-H} (T.E = -3237.624762)

7	0.214539000	-2.235724000	-0.083806000
6	-0.402713000	-3.053228000	-0.924919000
6	-1.717681000	-3.004813000	-1.341403000
6	-2.647478000	-1.995887000	-1.027492000
6	-2.458282000	-0.934541000	-0.184638000
6	1.605967000	-2.300494000	0.056488000
6	2.177150000	-2.014929000	1.296200000
6	2.450824000	-2.559728000	-1.022017000
6	3.549552000	-1.992477000	1.451364000
1	1.524297000	-1.815373000	2.140069000
6	3.823741000	-2.538089000	-0.859466000
1	2.024635000	-2.723326000	-2.005298000
6	4.383765000	-2.252939000	0.375313000
1	3.972363000	-1.769509000	2.424714000
1	4.463901000	-2.727436000	-1.714121000
1	5.460249000	-2.229241000	0.496790000
1	0.202695000	-3.866808000	-1.332343000
15	-3.645104000	0.262472000	0.044994000
6	-5.231689000	-0.024199000	-0.767228000
1	-5.917808000	0.792007000	-0.535576000
1	-5.093224000	-0.075505000	-1.847796000
1	-5.663011000	-0.964258000	-0.421512000
6	-4.010844000	0.495856000	1.793439000
1	-4.405846000	-0.431128000	2.210261000
1	-3.080672000	0.732782000	2.314690000
1	-4.726062000	1.307256000	1.940144000
6	-3.098209000	1.890104000	-0.506326000
1	-2.904541000	1.859497000	-1.579661000
1	-3.853216000	2.648752000	-0.289549000
1	-2.165548000	2.147536000	0.005089000
1	-3.607537000	-2.104395000	-1.542961000
1	-2.037526000	-3.794157000	-2.009951000
31	-0.724622000	-0.723684000	0.845022000
1	-0.939975000	-1.084913000	2.385356000
6	1.138345000	3.080537000	-0.131920000
6	2.269849000	2.063547000	-0.438004000
5	0.431058000	0.955544000	0.310586000
8	0.208083000	2.281893000	0.626827000
8	1.554628000	0.820551000	-0.466711000
6	0.404320000	3.545603000	-1.376518000
1	-0.494241000	4.087566000	-1.072583000
1	1.017220000	4.217550000	-1.981406000
1	0.100326000	2.698161000	-1.995775000
6	1.558857000	4.272143000	0.693046000

1	2.333855000	4.843416000	0.173709000
1	0.703229000	4.931397000	0.853364000
1	1.941425000	3.972458000	1.668012000
6	2.972211000	2.257736000	-1.759934000
1	3.471266000	3.230610000	-1.795262000
1	3.729662000	1.480327000	-1.880073000
1	2.282508000	2.186012000	-2.600426000
6	3.294807000	1.948594000	0.676578000
1	3.906577000	1.063404000	0.489678000
1	3.948954000	2.822443000	0.721229000
1	2.812186000	1.817997000	1.647989000

6GaP^{B-H} (T.E = -3368.206266)

6	-2.758087000	1.267348000	0.604238000
6	-2.236447000	0.285017000	-0.235394000
6	-0.698896000	2.729810000	0.516509000
1	-0.295077000	3.645447000	0.958637000
7	0.088233000	2.023399000	-0.224857000
15	-3.226055000	-1.099689000	-0.272761000
6	-3.423156000	-1.953556000	1.308351000
1	-3.837264000	-1.252264000	2.032433000
1	-4.082862000	-2.818072000	1.209263000
1	-2.439291000	-2.283604000	1.647232000
6	-4.910461000	-0.853674000	-0.878348000
1	-4.866399000	-0.466406000	-1.897011000
1	-5.467328000	-1.792955000	-0.868672000
1	-5.401208000	-0.121116000	-0.238293000
6	-2.507271000	-2.332683000	-1.369612000
1	-1.519308000	-2.631049000	-1.007978000
1	-3.154255000	-3.210243000	-1.419615000
1	-2.396204000	-1.913323000	-2.371685000
8	-3.823756000	1.245637000	1.226042000
7	-1.978116000	2.502112000	0.824324000
6	-2.671559000	3.512789000	1.609354000
1	-3.592717000	3.811164000	1.110177000
1	-2.940575000	3.124360000	2.590915000
1	-2.027965000	4.384281000	1.720630000
6	1.457807000	2.359455000	-0.267293000
6	2.128964000	2.289426000	-1.482810000
6	2.167371000	2.671558000	0.886674000
6	3.485267000	2.547414000	-1.541844000
1	1.571132000	2.028945000	-2.376121000
6	3.524556000	2.932533000	0.819969000
1	1.662406000	2.650744000	1.846210000
6	4.189440000	2.872374000	-0.392879000
1	3.997681000	2.492754000	-2.495349000
1	4.069359000	3.164091000	1.728077000
1	5.254183000	3.067022000	-0.441666000

31	-0.511408000	0.332247000	-1.222189000
1	-0.594806000	0.739437000	-2.757220000
6	1.795219000	-2.984568000	0.303382000
6	2.665729000	-1.777832000	0.741357000
8	0.963496000	-2.402804000	-0.717949000
8	1.782406000	-0.672886000	0.499286000
6	2.562062000	-4.147328000	-0.276064000
1	3.267535000	-4.545608000	0.459008000
1	1.870629000	-4.946967000	-0.549188000
1	3.114785000	-3.859569000	-1.169659000
6	0.858089000	-3.469478000	1.395731000
1	0.132904000	-4.156238000	0.952484000
1	1.391033000	-4.000057000	2.187883000
1	0.309305000	-2.635215000	1.840934000
6	3.883672000	-1.562082000	-0.139037000
1	4.296970000	-0.575438000	0.082314000
1	4.657000000	-2.312020000	0.042746000
1	3.615894000	-1.580754000	-1.197791000
6	3.074323000	-1.773174000	2.194407000
1	3.686403000	-2.649273000	2.427772000
1	3.667440000	-0.879205000	2.399451000
1	2.210335000	-1.762391000	2.858336000
5	0.883410000	-1.047813000	-0.472085000

8GaP^{B-H} (T.E = -3602.251425)

7	-1.247044000	-1.400551000	0.126442000
6	-1.287144000	-0.905141000	1.457988000
6	-0.051381000	-0.484504000	2.116794000
15	-2.895186000	-1.229152000	0.152188000
6	-2.604147000	-0.781401000	1.815760000
6	-3.289963000	-0.335580000	3.047889000
1	-3.926782000	-1.110960000	3.483768000
1	-2.553079000	-0.059821000	3.806513000
1	-3.924372000	0.541716000	2.883739000
7	-3.632997000	-0.063382000	-0.735526000
7	-3.616942000	-2.623955000	-0.344524000
6	-3.858417000	-0.212544000	-2.165562000
1	-3.130344000	0.381051000	-2.727511000
1	-3.752570000	-1.252292000	-2.470676000
1	-4.867885000	0.129543000	-2.416178000
6	-3.583513000	1.332916000	-0.323155000
1	-4.535429000	1.813081000	-0.567374000
1	-3.408075000	1.416577000	0.747571000
1	-2.778329000	1.869469000	-0.838301000
6	-5.057160000	-2.745760000	-0.444655000
1	-5.323194000	-3.299539000	-1.350911000
1	-5.467634000	-3.287577000	0.415721000
1	-5.527869000	-1.764843000	-0.491091000

6	-2.934864000	-3.894853000	-0.175285000
1	-1.859581000	-3.736380000	-0.125009000
1	-3.265235000	-4.404667000	0.737673000
1	-3.159398000	-4.542378000	-1.027869000
6	-0.203045000	2.498929000	-0.340795000
6	-0.751242000	3.497886000	0.479623000
6	0.053574000	2.842664000	-1.674746000
6	-1.031587000	4.758693000	-0.009326000
1	-0.973741000	3.250979000	1.514423000
6	-0.238004000	4.104456000	-2.160397000
1	0.498815000	2.100671000	-2.330403000
6	-0.784475000	5.075565000	-1.337059000
1	-1.461238000	5.502146000	0.654030000
1	-0.025956000	4.332787000	-3.199504000
1	-1.011048000	6.062799000	-1.721037000
7	0.004913000	1.220729000	0.136927000
5	0.481374000	0.893261000	1.439061000
7	1.475330000	1.638854000	2.136788000
6	2.270640000	2.662710000	1.498510000
1	2.167314000	2.617141000	0.415226000
1	1.993951000	3.672687000	1.827834000
1	3.330326000	2.513727000	1.744636000
6	1.871023000	1.441502000	3.506495000
1	1.254410000	0.695244000	4.003150000
1	2.917491000	1.111804000	3.575085000
1	1.791112000	2.375983000	4.077264000
1	-0.220426000	-0.360652000	3.188266000
1	0.722521000	-1.251754000	1.980474000
31	-0.019605000	-0.357154000	-1.076031000
1	-0.867782000	-0.079816000	-2.382141000
6	3.783087000	-1.796871000	0.216664000
6	4.226172000	-1.000350000	-1.040863000
5	1.952344000	-1.037756000	-0.897137000
8	2.385420000	-2.025852000	-0.041414000
8	3.009272000	-0.338922000	-1.427139000
6	3.857571000	-0.980560000	1.495337000
1	3.346111000	-1.528823000	2.290540000
1	4.889349000	-0.807679000	1.809395000
1	3.353527000	-0.016877000	1.379156000
6	4.478475000	-3.122113000	0.410772000
1	5.556391000	-2.976647000	0.527322000
1	4.102599000	-3.603959000	1.315436000
1	4.305914000	-3.796716000	-0.427121000
6	4.633211000	-1.890282000	-2.200515000
1	4.722212000	-1.274770000	-3.097327000
1	5.595119000	-2.375552000	-2.019824000
1	3.882572000	-2.659604000	-2.392806000
6	5.291198000	0.040479000	-0.791011000
1	6.202242000	-0.423931000	-0.402372000

1	5.539898000	0.541683000	-1.728287000
1	4.954664000	0.798956000	-0.084069000

10GaP^{B-H} (T.E = -3693.748745)

7	-1.405008000	0.805906000	0.114470000
6	-1.810209000	1.653068000	-0.958646000
6	-1.013168000	2.658880000	-1.497693000
6	0.298240000	2.933666000	-1.111555000
1	-1.453801000	3.252524000	-2.291372000
1	0.747982000	3.753221000	-1.683446000
15	-2.849532000	0.047638000	-0.048290000
6	-3.103111000	1.202546000	-1.290298000
6	-4.051409000	1.564042000	-2.367911000
1	-4.545308000	2.530265000	-2.211420000
1	-3.558617000	1.614426000	-3.347029000
1	-4.844839000	0.815558000	-2.450921000
6	1.069356000	2.322532000	-0.136859000
15	2.700411000	2.725754000	0.050847000
6	3.193520000	4.351857000	-0.571413000
1	4.251394000	4.524039000	-0.365890000
1	3.033466000	4.403542000	-1.649037000
1	2.597256000	5.127761000	-0.090573000
6	3.860047000	1.574932000	-0.729724000
1	4.897789000	1.861062000	-0.542231000
1	3.673261000	0.577206000	-0.322244000
1	3.671700000	1.553486000	-1.804599000
6	3.193318000	2.681594000	1.783753000
1	2.578681000	3.373911000	2.359469000
1	3.023655000	1.673392000	2.169067000
1	4.249849000	2.932840000	1.894386000
31	0.348261000	0.787328000	0.974214000
7	-2.916746000	-1.546380000	-0.482977000
7	-3.681490000	0.051223000	1.397132000
6	-2.734219000	-2.626081000	0.472814000
1	-1.684018000	-2.938260000	0.506012000
1	-3.031922000	-2.308305000	1.469972000
1	-3.349735000	-3.482088000	0.176797000
6	-2.447190000	-1.892780000	-1.813728000
1	-2.969100000	-2.790107000	-2.159745000
1	-2.649480000	-1.077956000	-2.508898000
1	-1.368338000	-2.093300000	-1.808832000
6	-5.084075000	-0.319804000	1.329465000
1	-5.439049000	-0.600092000	2.325054000
1	-5.704952000	0.513192000	0.967368000
1	-5.228502000	-1.169351000	0.661631000
6	-3.457454000	1.197763000	2.264990000
1	-2.391277000	1.379365000	2.391989000
1	-3.926777000	2.108727000	1.866814000

1	-3.896506000	0.984950000	3.242855000
1	0.166584000	1.171136000	2.518080000
6	2.821275000	-2.564821000	-0.237802000
6	1.443649000	-3.263896000	-0.108109000
5	1.256920000	-1.061298000	0.491607000
8	2.611732000	-1.347607000	0.499731000
8	0.549465000	-2.145009000	0.007345000
6	3.152505000	-2.163730000	-1.664885000
1	4.036852000	-1.523051000	-1.653807000
1	3.372682000	-3.031372000	-2.290715000
1	2.333037000	-1.599967000	-2.117998000
6	3.980260000	-3.320976000	0.364720000
1	4.104691000	-4.290449000	-0.126603000
1	4.901710000	-2.751851000	0.225540000
1	3.844518000	-3.485601000	1.433001000
6	1.035695000	-4.100990000	-1.296984000
1	1.746204000	-4.916845000	-1.458510000
1	0.052532000	-4.541757000	-1.114916000
1	0.973641000	-3.507063000	-2.208793000
6	1.305083000	-4.076788000	1.166698000
1	0.257475000	-4.358539000	1.291021000
1	1.901636000	-4.991219000	1.131841000
1	1.602199000	-3.495386000	2.041695000

11GaP^{B-H} (T.E = -3611.550431)

7	-1.565162000	-0.431591000	-0.418383000
6	-2.116005000	-1.477884000	0.325061000
6	-0.073731000	-2.939588000	0.375974000
7	0.690187000	-2.048993000	-0.273897000
15	-2.885541000	0.456746000	0.006191000
6	-3.337463000	-0.998708000	0.821284000
6	-4.357176000	-1.407264000	1.822304000
1	-5.082790000	-2.136547000	1.447907000
1	-3.917252000	-1.824918000	2.733198000
1	-4.932622000	-0.528352000	2.128372000
6	2.091566000	-2.208303000	-0.180000000
6	2.865322000	-2.028368000	-1.321417000
6	2.738954000	-2.436860000	1.033366000
6	4.247611000	-2.060619000	-1.255789000
1	2.370915000	-1.863074000	-2.274287000
6	4.118321000	-2.478220000	1.092914000
1	2.149877000	-2.586015000	1.929146000
6	4.883318000	-2.287749000	-0.048556000
1	4.827859000	-1.911242000	-2.159086000
1	4.603564000	-2.657232000	2.046103000
1	5.965222000	-2.320473000	0.004818000
31	0.143031000	-0.488143000	-1.377250000
7	-2.708271000	1.789893000	0.948058000

7	-3.670235000	1.019429000	-1.338227000
6	-2.367850000	3.092619000	0.392810000
1	-2.723795000	3.181372000	-0.631216000
1	-2.834122000	3.874594000	0.998977000
1	-1.281996000	3.233601000	0.396145000
6	-2.153337000	1.592836000	2.280873000
1	-2.476968000	0.637212000	2.692109000
1	-1.057238000	1.614367000	2.250077000
1	-2.505554000	2.392954000	2.936765000
6	-4.993412000	1.587572000	-1.126385000
1	-5.245537000	2.247082000	-1.960576000
1	-5.759640000	0.802286000	-1.065125000
1	-5.024533000	2.170262000	-0.205865000
6	-3.610447000	0.193460000	-2.537186000
1	-2.591292000	-0.136226000	-2.732028000
1	-4.257264000	-0.690272000	-2.452759000
1	-3.952692000	0.789536000	-3.385856000
8	0.287815000	-3.962932000	0.915483000
7	-1.504152000	-2.667969000	0.460015000
6	-2.277864000	-3.751229000	1.050967000
1	-2.165929000	-3.792405000	2.136423000
1	-3.325730000	-3.614395000	0.792894000
1	-1.926305000	-4.696361000	0.647113000
1	-0.149855000	-0.917953000	-2.871788000
6	3.112924000	2.206245000	0.114796000
6	1.834036000	2.940518000	0.596323000
5	1.283900000	1.120565000	-0.666739000
8	2.599550000	1.375278000	-0.941584000
8	0.804550000	1.969805000	0.312057000
6	4.195323000	3.100810000	-0.437331000
1	4.538672000	3.805106000	0.326029000
1	5.047533000	2.491457000	-0.743138000
1	3.854436000	3.663752000	-1.305773000
6	3.694906000	1.269057000	1.157543000
1	4.422178000	0.614614000	0.671934000
1	4.196495000	1.815769000	1.959443000
1	2.925889000	0.626521000	1.593258000
6	1.797234000	3.267817000	2.069147000
1	2.621437000	3.934327000	2.338214000
1	0.860107000	3.776890000	2.309365000
1	1.861563000	2.369235000	2.682399000
6	1.520426000	4.180637000	-0.220343000
1	0.522202000	4.539114000	0.039611000
1	2.229186000	4.985833000	-0.015529000
1	1.535799000	3.964731000	-1.290435000

$^{13}\text{GaP}^{\text{B-H}}$ (T.E = -3937.096532)

7	-1.421632000	-1.258577000	-0.128975000
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6	-1.251761000	-1.326873000	1.293589000
6	-0.017415000	-1.330592000	1.932970000
6	1.203379000	-1.346718000	1.265621000
1	-0.005963000	-1.376875000	3.017212000
15	-3.035604000	-1.150531000	0.163544000
6	-2.564027000	-1.367449000	1.798866000
6	-3.086846000	-1.439523000	3.181820000
1	-2.674465000	-2.291937000	3.732735000
1	-2.858854000	-0.541559000	3.772340000
1	-4.173008000	-1.556031000	3.189271000
7	1.341516000	-1.276472000	-0.158005000
6	2.523900000	-1.420631000	1.742928000
15	2.963260000	-1.222105000	0.095016000
6	3.071529000	-1.516719000	3.114855000
1	2.919033000	-0.601006000	3.703102000
1	2.612359000	-2.334532000	3.680851000
1	4.146870000	-1.709054000	3.101611000
7	3.679177000	-2.337192000	-0.906036000
7	3.831235000	0.138595000	-0.252888000
6	2.981572000	-3.575281000	-1.197999000
1	3.285473000	-4.378676000	-0.514988000
1	1.906827000	-3.424725000	-1.114076000
1	3.214599000	-3.890628000	-2.219647000
6	5.112257000	-2.439910000	-1.066899000
1	5.529902000	-3.243371000	-0.446366000
1	5.354715000	-2.665359000	-2.111120000
1	5.599915000	-1.505318000	-0.794791000
6	3.912657000	0.638804000	-1.611260000
1	4.942832000	0.921634000	-1.857702000
1	3.586386000	-0.122024000	-2.321463000
1	3.270539000	1.520213000	-1.727845000
6	4.106154000	1.143447000	0.751380000
1	3.404490000	1.979273000	0.665268000
1	4.017693000	0.718922000	1.750015000
1	5.125197000	1.524179000	0.620222000
7	-3.833733000	-2.233848000	-0.806745000
7	-3.839558000	0.256199000	-0.171074000
6	-5.275051000	-2.272123000	-0.919259000
1	-5.561119000	-2.504487000	-1.950771000
1	-5.708282000	-3.044295000	-0.270338000
1	-5.708799000	-1.310675000	-0.649773000
6	-3.201473000	-3.508059000	-1.092387000
1	-2.118898000	-3.405586000	-1.039451000
1	-3.522491000	-4.283896000	-0.385752000
1	-3.475632000	-3.830749000	-2.101325000
6	-3.836326000	1.329484000	0.806018000
1	-4.722438000	1.953774000	0.653049000
1	-3.865481000	0.926038000	1.816787000
1	-2.945934000	1.960293000	0.700763000

6	-3.919782000	0.735029000	-1.542433000
1	-3.793497000	-0.090391000	-2.243531000
1	-4.897033000	1.195401000	-1.723989000
1	-3.138998000	1.480542000	-1.735403000
31	-0.045386000	-0.452585000	-1.267829000
1	-0.069433000	-1.105280000	-2.708473000
6	0.728681000	3.384154000	0.439521000
6	-0.543911000	3.772025000	-0.353799000
5	0.015150000	1.597737000	-0.780724000
8	1.139812000	2.179654000	-0.230663000
8	-1.041412000	2.484631000	-0.764596000
6	1.839998000	4.404794000	0.381228000
1	1.491307000	5.372863000	0.752289000
1	2.673857000	4.089616000	1.011650000
1	2.213703000	4.534470000	-0.634949000
6	0.444422000	2.996831000	1.880581000
1	1.334418000	2.516371000	2.293789000
1	0.202921000	3.866351000	2.496428000
1	-0.372683000	2.273146000	1.945629000
6	-0.245188000	4.552240000	-1.621030000
1	-1.152716000	4.595697000	-2.225958000
1	0.069877000	5.575009000	-1.403204000
1	0.531181000	4.063817000	-2.213316000
6	-1.601649000	4.488342000	0.450316000
1	-2.476446000	4.673458000	-0.177536000
1	-1.922628000	3.909775000	1.315930000
1	-1.225883000	5.453752000	0.801150000

Cartesian coordinates of the different substrates which undergo activation by some of the representative Al(I)/Ga(I) carbenoids considered in this study and also their total energies (in hartrees) including the zero point vibrational correction that have been calculated at **M06-D3/Def2-TZVP** level of theory.

Hydrogen (T.E = -1.160821)

1	0.000000000	0.000000000	0.373371000
1	0.000000000	0.000000000	-0.373371000

Ammonia (T.E = -56.506612)

7	0.000000000	0.000000000	0.112148000
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1	0.000000000	0.940203000	-0.261679000
1	-0.814240000	-0.470102000	-0.261679000
1	0.814240000	-0.470102000	-0.261679000

Hexa-fluorobenzene (T.E = -827.571894)

6	0.373080000	1.333631000	0.000008000
6	1.341568000	0.343679000	0.000031000
6	0.968494000	-0.989852000	0.000004000
6	-0.373139000	-1.333614000	0.000012000
6	-1.341554000	-0.343737000	0.000013000
6	-0.968449000	0.989894000	-0.000011000
9	-1.888748000	1.930625000	-0.000023000
9	-2.616491000	-0.670147000	0.000015000
9	-0.727678000	-2.600976000	-0.000009000
9	1.888645000	-1.930724000	-0.000023000
9	2.616457000	0.670284000	0.000004000
9	0.727815000	2.600939000	-0.000002000

Pinacolborane (T.E = -411.568530)

6	-0.776031000	-0.184705000	0.057389000
6	0.776115000	-0.184425000	-0.057541000
5	-0.000365000	1.927358000	0.000312000
1	-0.000772000	3.111447000	0.000099000
8	-1.058120000	1.182319000	0.421228000
8	1.057832000	1.182904000	-0.420565000
6	-1.334596000	-1.104214000	1.115395000
1	-2.424103000	-1.039902000	1.118541000
1	-1.057103000	-2.140905000	0.905426000
1	-0.978254000	-0.842044000	2.110875000
6	-1.473963000	-0.434394000	-1.266213000
1	-1.375241000	-1.474748000	-1.582719000
1	-2.535561000	-0.210882000	-1.148822000
1	-1.078528000	0.209295000	-2.054688000
6	1.473828000	-0.434642000	1.266054000
1	1.375639000	-1.475286000	1.581778000
1	2.535321000	-0.210383000	1.149136000
1	1.077735000	0.208229000	2.054873000
6	1.335196000	-1.103267000	-1.115885000
1	2.424691000	-1.038757000	-1.118623000
1	1.057838000	-2.140132000	-0.906584000
1	0.979167000	-0.840621000	-2.111344000