

Supporting Information

Activation of Small Molecules by Cyclic Alkyl Amino Silylenes (CAASis) and Germylenes (CAAGes): A Theoretical Study

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Table S1 Calculated Mulliken spin density at the central atom (E =Si/Ge), α -nitrogen (N_α) and carbon (C_α) atom (with respect to the central atom) for **1Si-14Si** and **1Ge-14Ge**.

Molecules	Si	N_α	C_α	Molecules	Ge	N_α	C_α
1Si	1.446	0.125	0.281	1Ge	0.917	0.429	0.148
2Si	1.098	0.225	0.202	2Ge	1.029	0.284	0.145
3Si	1.477	0.083	0.319	3Ge	1.271	0.096	0.498
4Si	1.471	0.066	0.267	4Ge	1.248	0.036	0.449
5Si	1.558	0.088	0.215	5Ge	1.292	0.064	0.554
6Si	1.229	0.206	0.240	6Ge	1.024	0.329	0.176
7Si	1.566	0.105	0.019	7Ge	0.834	0.502	-0.105
8Si	0.847	0.078	0.718	8Ge	0.884	0.078	0.715
9Si	0.967	0.137	0.184	9Ge	0.951	0.167	0.205
10Si	1.045	0.115	0.273	10Ge	0.996	0.146	0.265
11Si	1.600	0.095	0.096	11Ge	0.828	0.506	0.036
12Si	0.890	0.052	0.656	12Ge	0.904	0.057	0.671
13Si	1.496	0.026	0.152	13Ge	0.924	0.103	0.667
14Si	1.407	0.032	0.103	14Ge	0.885	0.355	0.159

Table S2 Calculated natural charges (q) and occupancies of the formally vacant valence p-orbital (Occ) at the central atom (Si/Ge) for **1Si-14Si** and **1Ge-14Ge**.

Molecules	q_{Si}	Occ _{Si}	Molecules	q_{Ge}	Occ _{Ge}
1Si	1.105	0.256	1Ge	1.071	0.291
2Si	1.024	0.301	2Ge	1.000	0.310
3Si	1.145	0.388	3Ge	1.109	0.265
4Si	1.148	0.212	4Ge	1.099	0.286
5Si	1.155	0.182	5Ge	1.124	0.176
6Si	1.073	0.288	6Ge	1.043	0.288
7Si	0.996	0.240	7Ge	1.007	0.241
8Si	0.908	0.360	8Ge	0.908	0.353
9Si	0.755	0.531	9Ge	0.755	0.530
10Si	0.842	0.426	10Ge	0.841	0.442
11Si	0.965	0.294	11Ge	0.965	0.298
12Si	0.937	0.346	12Ge	0.938	0.348
13Si	1.005	0.276	13Ge	1.007	0.278
14Si	1.001	0.262	14Ge	1.005	0.262

Table S3 Calculated important geometrical parameters and natural charges at pseudo hydridic ($q_{H_{hy}}$) and positively polarized hydrogen atom (q_H) and occupancies of the formally vacant p-orbital ($Occ_{Si/Ge}$) of the transition states involved in the activation of hydrogen by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**) and CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**). Bond lengths (E – X, E = Si, Ge and X = N, C), bond angles ($\angle C-E-N$) are given in Å and in degree ($^\circ$) respectively.

Molecules	$H_{hy} - H$	E – H	E – H_{hy}	E - X	$\angle C-E-N$	$Occ_{Si/Ge}$	$q_{H_{hy}}$	q_H
1SiTS^{H-H}	1.174	1.514	1.764	1.746/1.879	96.8	0.791	-0.080	0.121
2SiTS^{H-H}	1.184	1.512	1.732	1.765/1.883	95.0	0.596	-0.055	0.029
3SiTS^{H-H}	1.151	1.520	1.756	1.751/1.880	98.9	0.484	-0.064	0.014
4SiTS^{H-H}	1.145	1.521	1.747	1.744/1.894	103.3	0.928	-0.062	0.012
5SiTS^{H-H}	1.180	1.510	1.732	1.770/1.873	95.8	0.671	-0.048	0.034
8SiTS^{H-H}	1.238	1.507	1.871	1.757/1.783	95.5	0.579	-0.171	-0.001
9SiTS^{H-H}	1.303	1.502	2.029	1.750/1.799	94.1	0.783	-0.282	-0.028
14SiTS^{H-H}	1.191	1.510	1.845	1.750/1.808	96.6	0.665	-0.133	-0.001
1GeTS^{H-H}	1.309	1.559	1.825	1.874/1.977	93.3	0.814	-0.108	0.037
2GeTS^{H-H}	1.316	1.557	1.804	1.885/1.975	91.6	0.603	-0.089	0.041
3GeTS^{H-H}	1.282	1.563	1.841	1.874/1.978	95.7	0.739	-0.177	0.028
4GeTS^{H-H}	1.287	1.565	1.819	1.866/1.984	98.7	0.535	-0.101	0.026
5GeTS^{H-H}	1.310	1.556	1.798	1.889/1.968	92.0	0.550	-0.079	0.044
8GeTS^{H-H}	1.351	1.548	1.898	1.877/1.887	92.3	0.625	-0.173	0.022
9GeTS^{H-H}	1.413	1.541	2.042	1.866/1.888	91.0	0.759	-0.294	-0.001
14GeTS^{H-H}	1.320	1.550	1.902	1.868/1.891	93.2	0.697	-0.171	0.017

Table S4 Calculated important geometrical parameters and natural charges at the nitrogen atom of NH₃ and Si/Ge center for the intermediate (**Int**) involved in the activation of N – H bond of NH₃ by CAASis (**1Si-5Si** and **14Si**), CAAGes (**1Ge-5Ge** and **14Ge**) and NacNacSi (**IIa**). Bond lengths are given in Å and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	H₃N – Si	q_{NH₃}	q_{Si}	Molecules	H₃N – Ge	q_{NH₃}	q_{Ge}
1SiInt^{N-H}	2.135 (0.344)	-1.013	1.021	1GeInt^{N-H}	2.267 (0.317)	-1.020	1.004
2SiInt^{N-H}	2.085 (0.366)	-1.026	0.985	2GeInt^{N-H}	2.304 (0.303)	-1.027	1.010
3SiInt^{N-H}	2.097 (0.356)	-1.024	1.016	3GeInt^{N-H}	2.349 (0.289)	-1.023	1.031
4SiInt^{N-H}	2.137 (0.335)	-1.031	1.040	4GeInt^{N-H}	2.369 (0.281)	-1.025	1.040
5SiInt^{N-H}	2.087 (0.371)	-1.029	1.009	5GeInt^{N-H}	2.317 (0.311)	-1.030	1.040
14SiInt^{N-H}	2.097 (0.360)	-1.013	0.935	14GeInt^{N-H}	2.310 (0.282)	-1.023	0.987
IIa-Int^{N-H}	2.141 (0.335)	-1.027	1.092				

Table S5 Calculated important geometrical parameters and natural charges at the nitrogen atom of the pseudo amide fragment (q_{NH_2}) and hydrogen atom (q_{H}) of the transition states involved in the activation of N-H bond of NH_3 by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and NacNacSi (**IIa**). Bond lengths (E – X, E = Si, Ge and X = N, C), bond angles ($\angle\text{C-E-N}$) are given in Å and in degree ($^\circ$) respectively.

Molecule	$\text{H}_2\text{N} - \text{H}$	E – H	E – NH_2	E - X	$\angle\text{C-E-N}$	q_{NH_2}	q_{H}
1SiTS^{N-H}	1.364	1.638	1.898	1.761/1.892	94.5	-1.250	0.226
2SiTS^{N-H}	1.371	1.636	1.881	1.781/1.889	92.7	-1.244	0.226
3SiTS^{N-H}	1.336	1.652	1.881	1.766/1.888	96.1	-1.238	0.231
4SiTS^{N-H}	1.356	1.641	1.913	1.739/1.905	100.2	-1.258	0.222
5SiTS^{N-H}	1.373	1.628	1.871	1.778/1.892	93.2	-1.203	0.231
8SiTS^{N-H}	1.368	1.640	1.896	1.776/1.811	93.2	-1.242	0.197
9SiTS^{N-H}	1.377	1.644	1.889	1.791/1.824	91.4	-1.238	0.189
14SiTS^{N-H}	1.369	1.638	1.890	1.772/1.821	94.3	-1.234	0.207
IIa-TS^{N-H}	1.382	1.632	1.865	1.740/1.758	101.9	-1.237	0.212
1GeTS^{N-H}	1.490	1.648	2.014	1.889/1.982	90.8	-1.242	0.166
2GeTS^{N-H}	1.520	1.632	2.015	1.891/1.985	90.3	-1.237	0.160
3GeTS^{N-H}	1.514	1.636	2.012	1.878/1.981	93.1	-1.234	0.160
4GeTS^{N-H}	1.518	1.634	2.032	1.867/1.998	98.1	-1.240	0.157
5GeTS^{N-H}	1.513	1.637	1.993	1.890/1.987	90.4	-1.229	0.165
8GeTS^{N-H}	1.511	1.634	2.062	1.887/1.883	90.0	-1.257	0.142
9GeTS^{N-H}	1.515	1.649	2.046	1.899/1.898	88.5	-1.254	0.136
14GeTS^{N-H}	1.494	1.647	2.014	1.886/1.899	91.8	-1.247	0.151

Table S6 Calculated important geometrical parameters and natural charges at the carbon atom of the PhCH₂ fragment (q_{PhCH_2}) and hydrogen atom (q_{H}) and occupancies of the formally vacant p-orbital ($\text{Occ}_{\text{Si/Ge}}$) of the transition states involved in the activation of toluene by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**) and CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**). Bond lengths (E – X, E = Si, Ge and X = N, C), bond angles ($\angle\text{C-E-N}$) are given in Å and in degree (°) respectively.

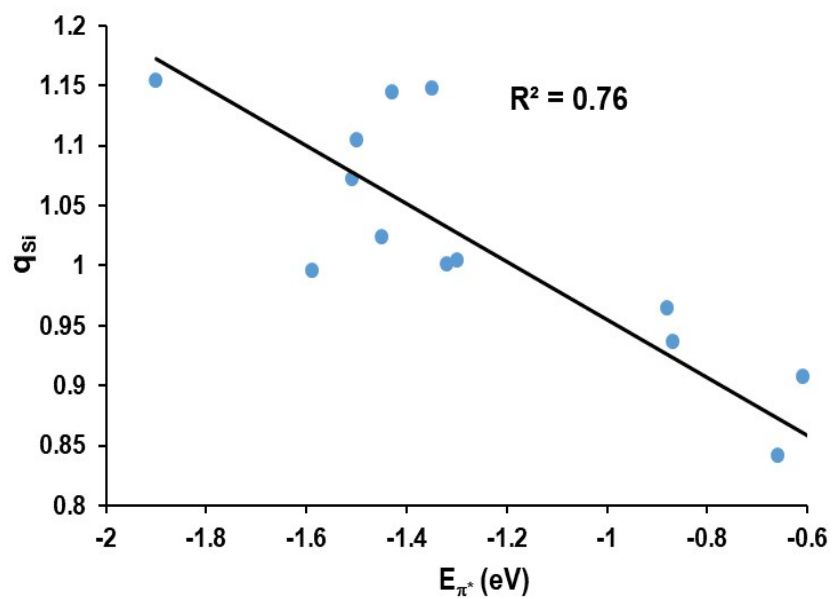
Molecule	PhCH ₂ – H	E – H	E – CH ₂ Ph	E - X	$\angle\text{C-E-N}$	$\text{Occ}_{\text{Si/Ge}}$	q_{PhCH_2}	q_{H}
1SiTS^{C-H}	1.652	1.595	2.156	1.772/1.932	92.4	0.475	-0.570	0.066
2SiTS^{C-H}	1.676	1.596	2.155	1.799/1.948	91.7	0.524	-0.565	0.075
3SiTS^{C-H}	1.609	1.609	2.136	1.790/1.937	95.1	0.359	-0.616	0.093
4SiTS^{C-H}	1.622	1.610	2.171	1.772/1.954	100.5	0.431	-0.573	0.056
5SiTS^{C-H}	1.654	1.600	2.156	1.803/1.933	92.6	0.461	-0.562	0.063
8SiTS^{C-H}	1.655	1.626	2.117	1.788/1.825	92.9	0.963	-0.604	0.073
9SiTS^{C-H}	1.723	1.608	2.135	1.800/1.858	90.9	0.957	-0.576	0.066
14SiTS^{C-H}	1.676	1.603	2.105	1.789/1.865	94.5	0.461	-0.606	0.087
1GeTS^{C-H}	1.807	1.668	2.239	1.908/2.047	88.1	0.503	-0.500	0.030
2GeTS^{C-H}	1.860	1.666	2.257	1.936/2.065	87.2	0.542	-0.481	0.029
3GeTS^{C-H}	1.781	1.689	2.220	1.924/2.058	90.9	0.373	-0.540	0.052
4GeTS^{C-H}	1.786	1.683	2.271	1.909/2.081	96.3	0.477	-0.491	0.020
5GeTS^{C-H}	1.811	1.672	2.242	1.937/2.049	88.5	0.491	-0.490	0.028
8GeTS^{C-H}	1.795	1.684	2.224	1.933/1.954	90.7	0.382	-0.496	0.043
9GeTS^{C-H}	1.854	1.669	2.189	1.936/1.986	88.6	0.450	-0.550	0.081
14GeTS^{C-H}	1.815	1.712	2.192	1.914/1.956	90.4	0.863	-0.545	0.037

Table S7 Calculated important geometrical parameters and natural charges at the silicon atom of the SiEt₃H and at the central atom (E = Si, Ge) of the van der Waals complexes involved in the activation of Si-H bond of SiEt₃H by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and **IX**. The E-X (E = Si, Ge and X = C, N), Si – E bond lengths and ∠C – E – N bond angles (∠C-E-N, E = Si, Ge) are given in Å and in degree (°) respectively.

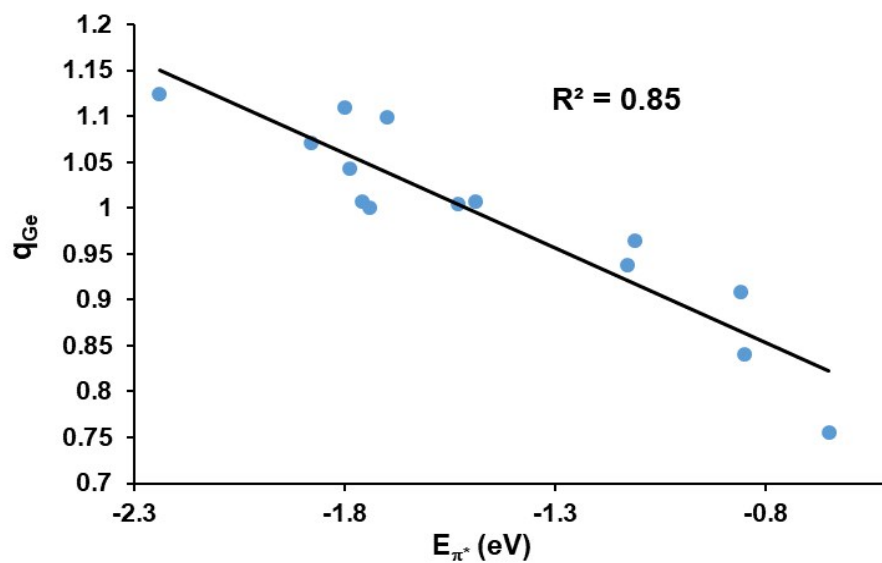
Molecule	Et ₃ HSi – E	E - X	∠C-E-N	q _{SiEt₃H}	q _E
1Si_v	4.198	1.749/1.903	91.3	1.498	1.155
2Si_v	3.852	1.775/1.904	89.0	1.516	1.103
3Si_v	4.039	1.759/1.898	93.2	1.515	1.192
4Si_v	4.071	1.738/1.912	97.0	1.494	1.211
5Si_v	3.822	1.773/1.895	90.6	1.514	1.210
8Si_v	3.880	1.787/1.796	89.9	1.477	0.947
9Si_v	4.264	1.803/1.823	87.2	1.458	0.777
14Si_v	3.807	1.787/1.825	92.2	1.512	1.035
IX_v	4.247	1.903/1.903	92.9	1.453	1.246
1Ge_v	4.259	1.873/2.013	87.5	1.463	1.079
2Ge_v	3.860	1.891/2.007	85.5	1.486	1.002
3Ge_v	3.924	1.880/2.009	90.1	1.509	1.097
4Ge_v	3.770	1.881/2.023	93.9	1.523	1.095
5Ge_v	3.844	1.899/2.003	87.2	1.514	1.118
8Ge_v	4.136	1.908/1.890	86.2	1.470	0.907
9Ge_v	4.205	1.932/1.914	83.9	1.453	0.764
14Ge_v	3.938	1.916/1.912	88.7	1.487	1.002

Table S8 Calculated important geometrical parameters and natural charges at the silicon atom of the SiEt₃ fragment (q_{SiEt_3}) and hydrogen atom (q_{H}) of the transition states involved in the activation of Si-H bond of SiEt₃H by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and **IX**. Bond lengths (E – X, E = Si, Ge and X = N, C), bond angles ($\angle\text{C-E-N}$) are given in Å and in degree (°) respectively.

Molecule	Et ₃ Si – H	E – H	E – SiEt ₃	E - X	$\angle\text{C-E-N}$	q_{SiEt_3}	q_{H}
1SiTS ^{Si-H}	1.845	1.659	2.425	1.761/1.917	93.4	1.522	-0.186
2SiTS ^{Si-H}	1.749	1.693	2.469	1.790/1.903	92.0	1.527	-0.178
3SiTS ^{Si-H}	1.704	1.768	2.444	1.769/1.905	96.1	1.348	-0.259
4SiTS ^{Si-H}	1.713	1.734	2.475	1.763/1.914	99.6	1.497	-0.189
5SiTS ^{Si-H}	1.785	1.669	2.440	1.787/1.915	92.7	1.545	-0.177
8SiTS ^{Si-H}	1.750	1.773	2.389	1.767/1.799	93.5	1.397	-0.184
9SiTS ^{Si-H}	1.735	1.810	2.390	1.774/1.807	92.1	1.381	-0.195
14SiTS ^{Si-H}	1.714	1.770	2.437	1.773/1.822	94.5	1.427	-0.171
IX-TS ^{Si-H}	1.624	1.783	2.582	1.942/1.950	96.0	1.536	-0.193
1GeTS ^{Si-H}	1.794	1.765	2.476	1.896/2.007	90.4	1.504	-0.164
2GeTS ^{Si-H}	1.929	1.733	2.451	1.909/2.001	89.8	1.540	-0.151
3GeTS ^{Si-H}	1.799	1.772	2.502	1.898/2.001	91.9	1.509	-0.159
4GeTS ^{Si-H}	1.831	1.771	2.485	1.891/2.012	97.0	1.527	-0.167
5GeTS ^{Si-H}	1.863	1.750	2.484	1.910/1.989	89.4	1.542	-0.154
8GeTS ^{Si-H}	1.839	1.815	2.416	1.893/1.892	89.7	1.412	-0.185
9GeTS ^{Si-H}	1.902	1.850	2.403	1.888/1.903	89.0	1.420	-0.215
14GeTS ^{Si-H}	1.814	1.813	2.446	1.896/1.908	90.9	1.453	-0.168

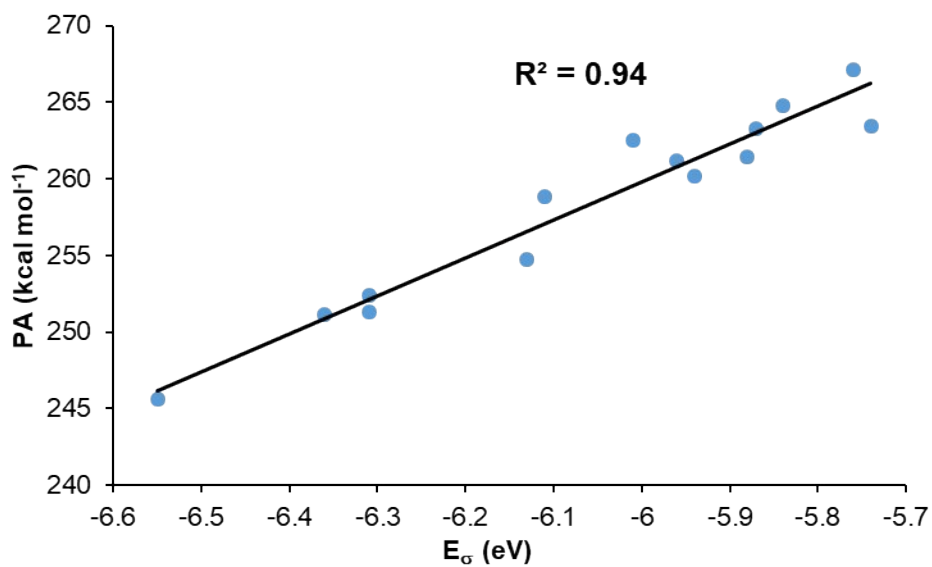


(a)

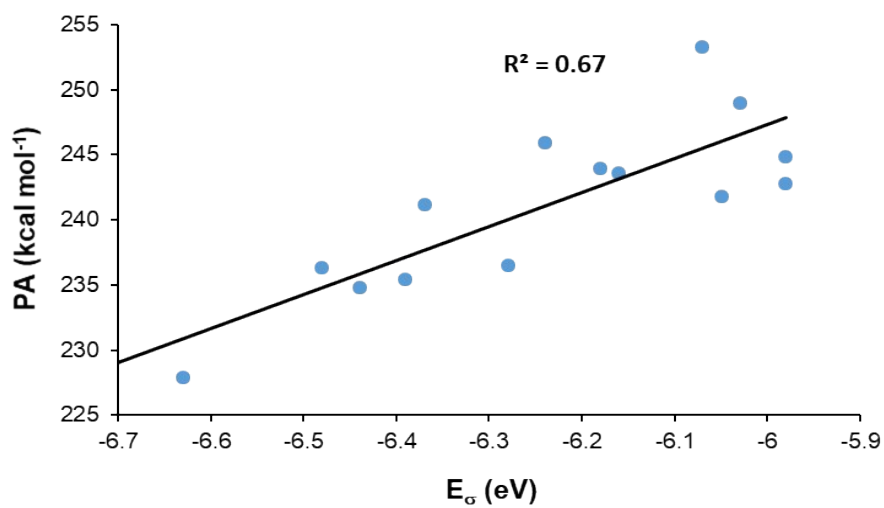


(b)

Fig. S1 Correlation plot between E_{π^*} (eV) and natural charge at the central atom ($E = \text{Si/Ge}$) for the (a) CAASis and (b) CAAGes.

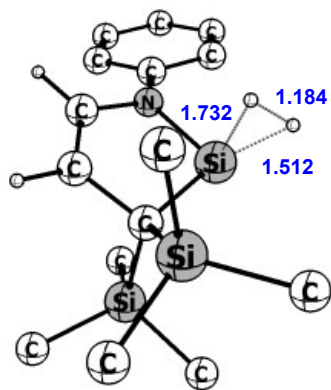


(a)

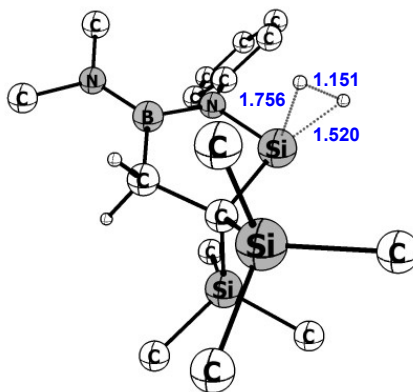


(b)

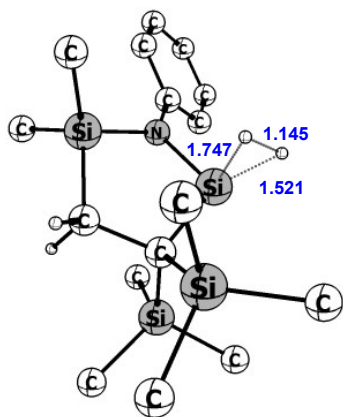
Fig. S2 Correlation plots between the E_σ (eV) and PA (kcal mol⁻¹) for (a) CAASis (1Si-14Si) and (b) CAAGes (1Ge-14Ge).



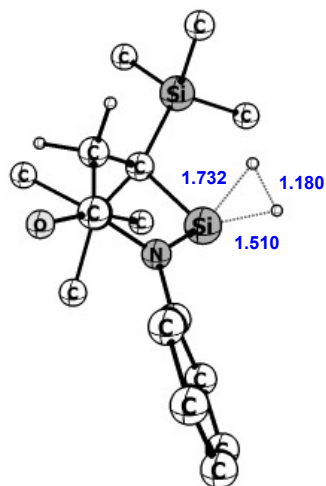
2SiTS^{H-H}



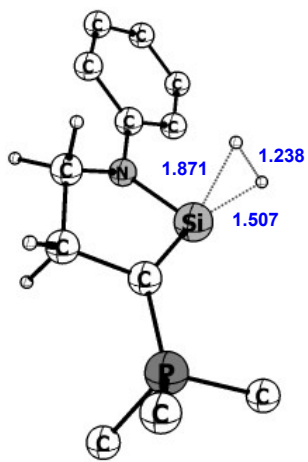
3SiTS^{H-H}



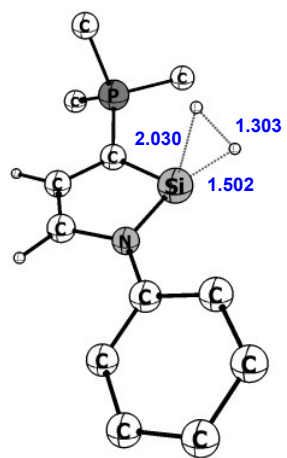
4SiTS^{H-H}



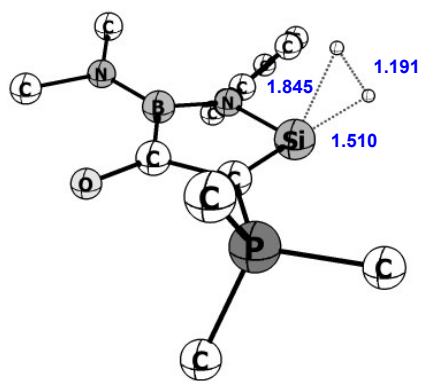
5SiTS^{H-H}



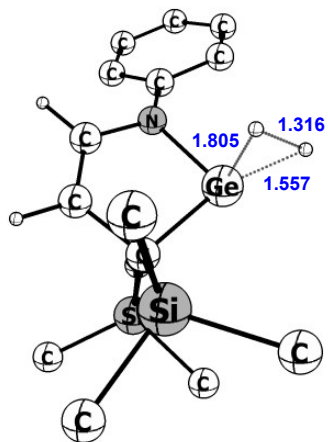
8SiTS^{H-H}



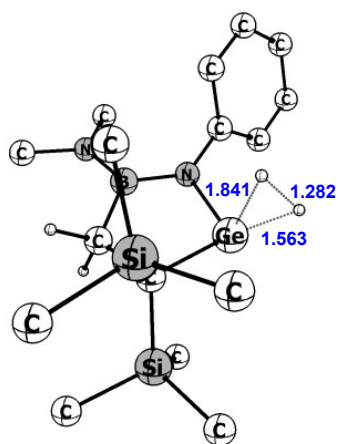
9SiTS^{H-H}



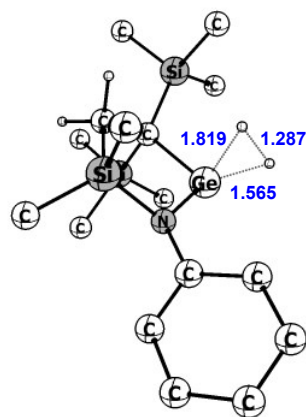
14SiTS^{H-H}



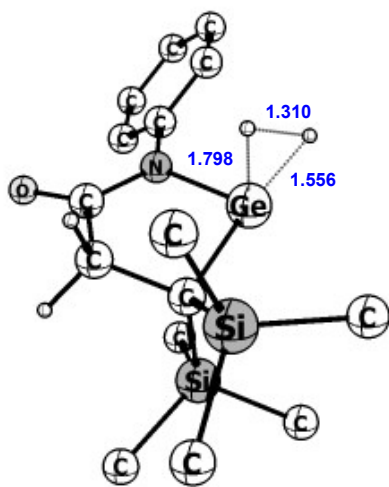
2GeTS^{H-H}



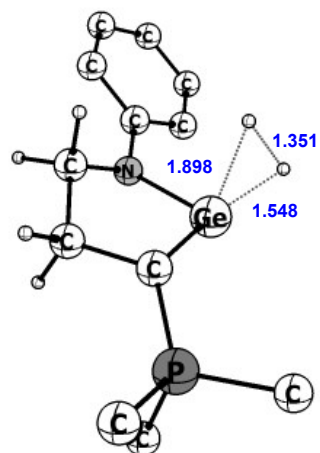
3GeTS^{H-H}



4GeTs^{H-H}



5GeTS^{H-H}



8GeTS^{H-H}

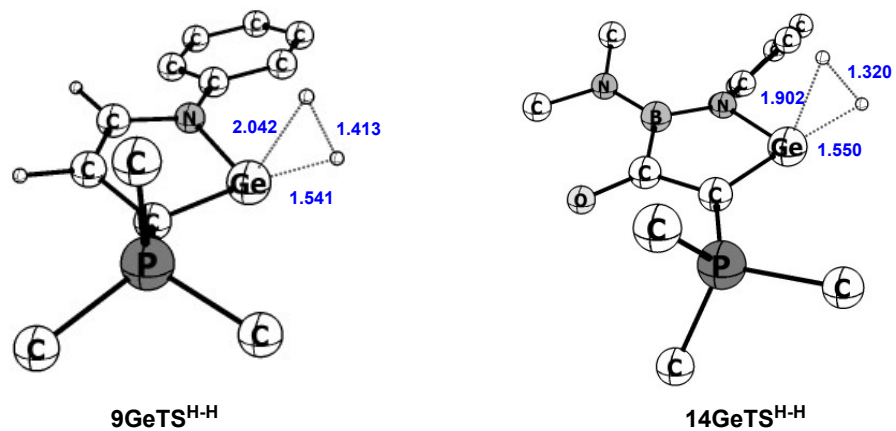
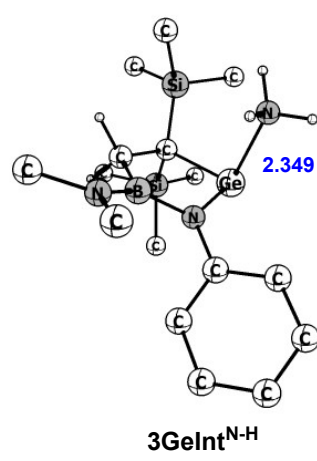
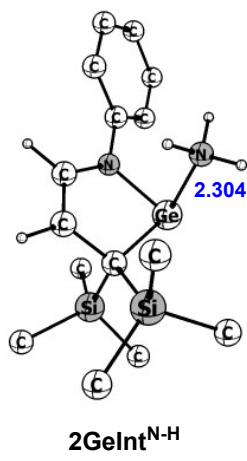
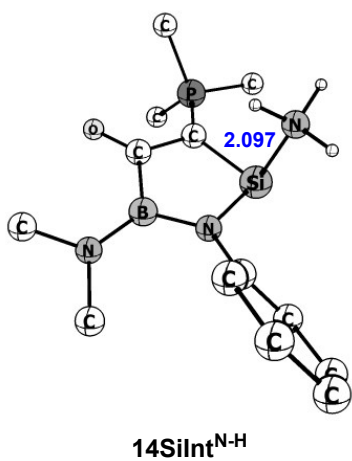
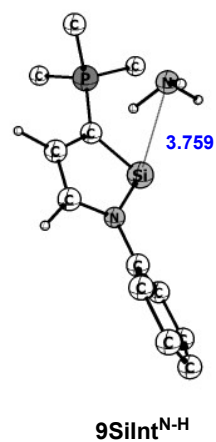
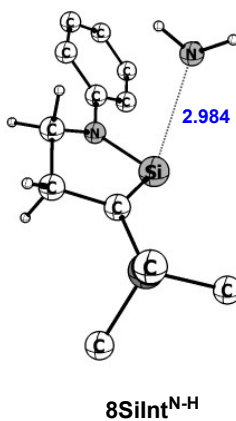
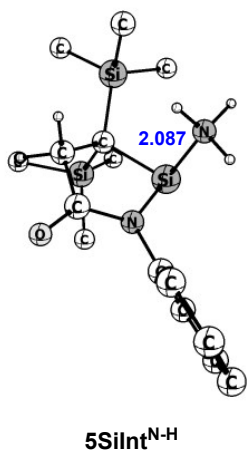
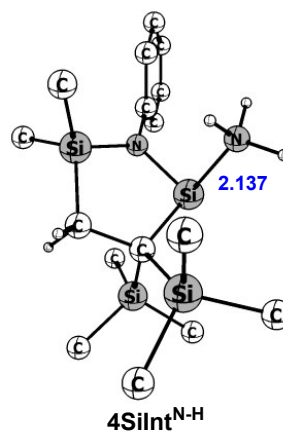
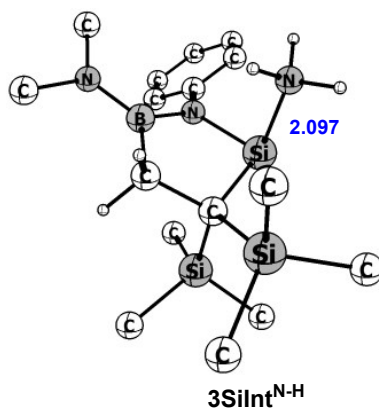
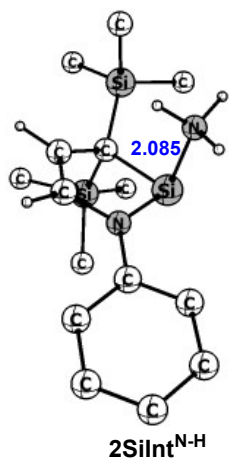


Fig. S3 Optimized geometries for the transition states involved in the activation of dihydrogen by CAASis (2Si-5Si, 8Si-9Si and 14Si) and CAAGes (2Ge-5Ge, 8Ge-9Ge and 14Ge). The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



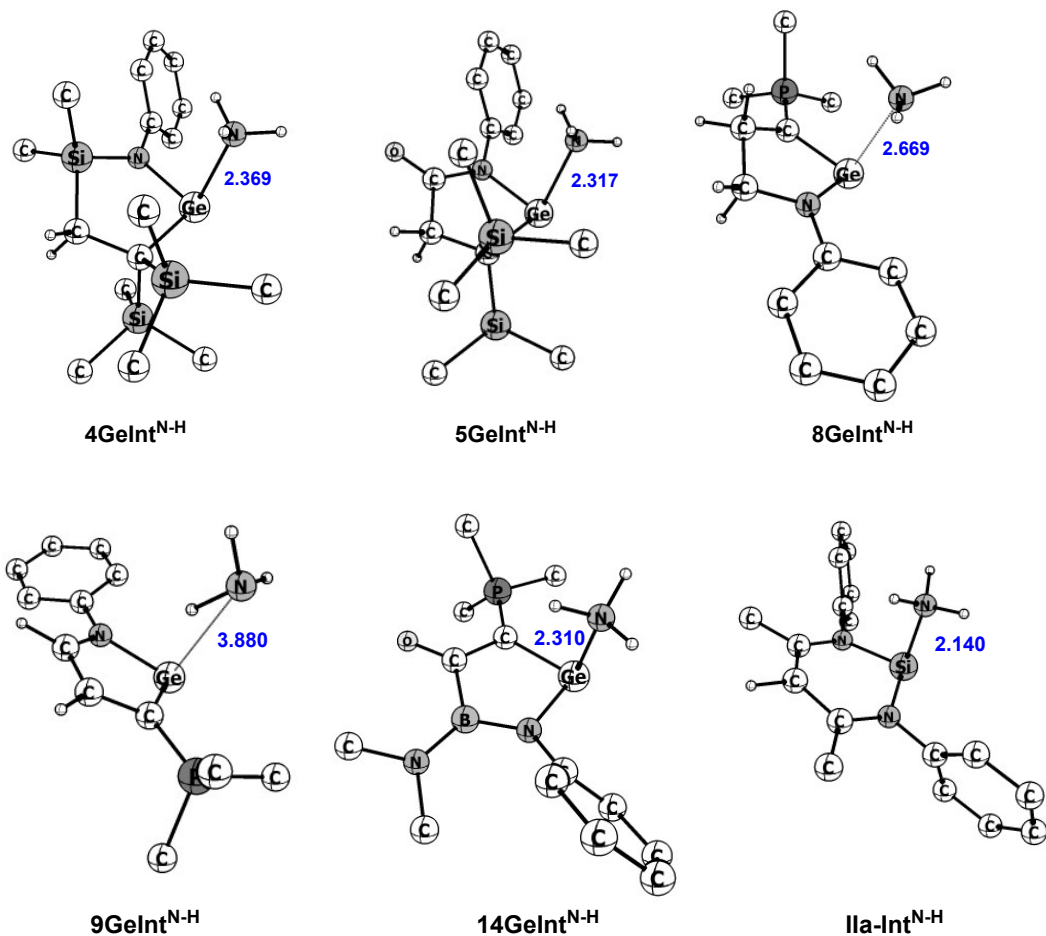
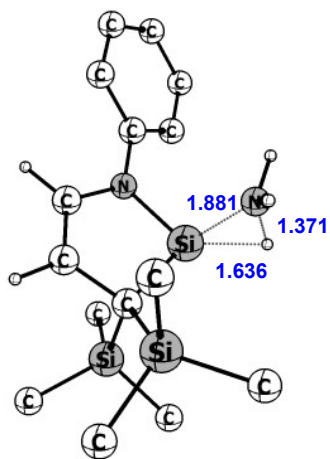
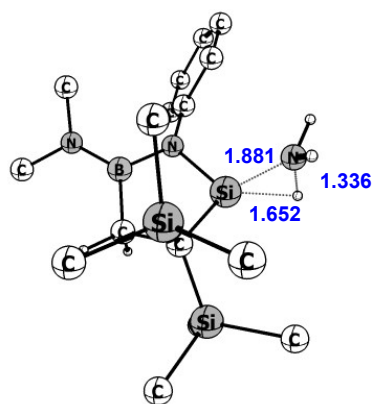


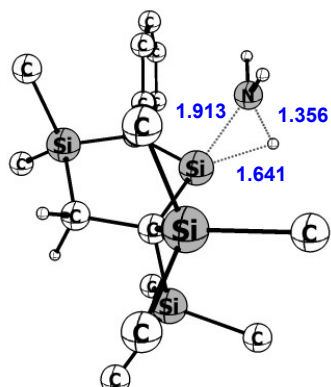
Fig. S4 Optimized geometries for the intermediate (Int^{N-H}) involved in the activation of N-H bond of NH₃ by CAASis (2Si-5Si, 8Si-9Si and 14Si), CAAGes (2Ge-5Ge, 8Ge-9Ge and 14Ge) and NacNacSi (**IIa**). The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



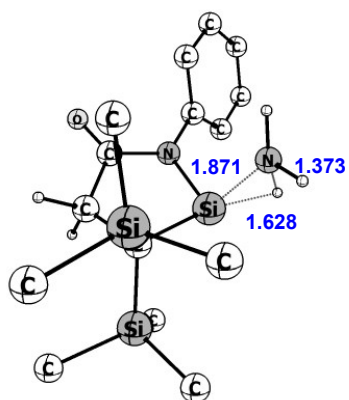
2SiTS^{N-H}



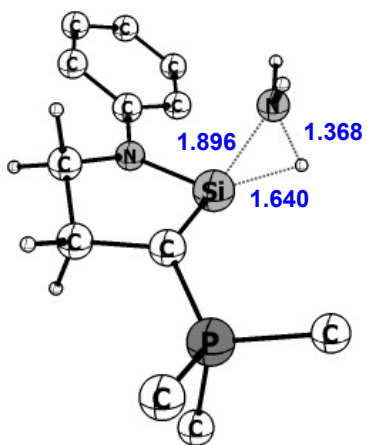
3SiTS^{N-H}



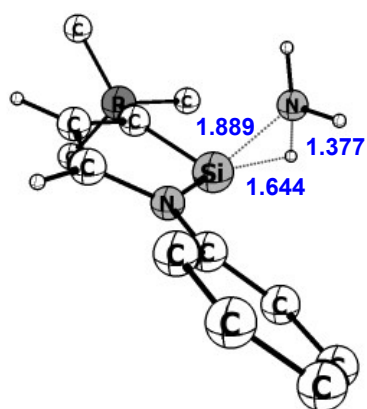
4SiTS^{N-H}



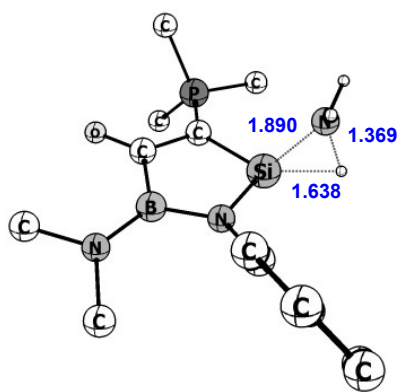
5SiTS^{N-H}



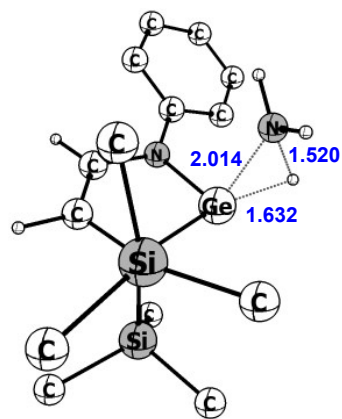
8SiTS^{N-H}



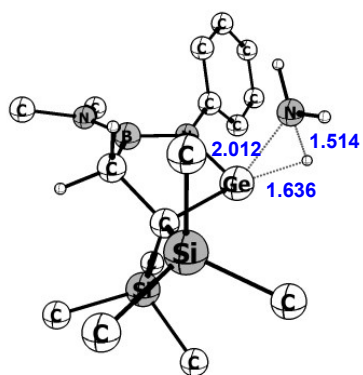
9SiTS^{N-H}



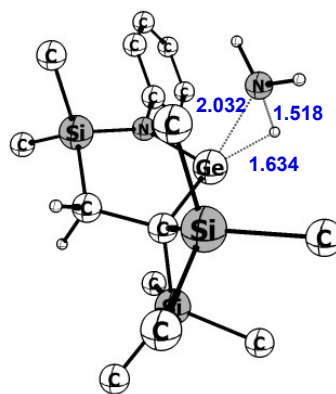
14SiTS^{N-H}



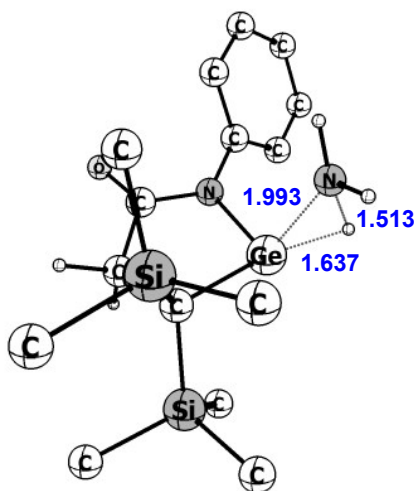
2GeTS^{N-H}



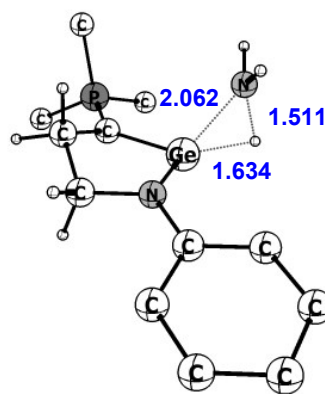
3GeTS^{N-H}



4GeTS^{N-H}



5GeTS^{N-H}



8GeTS^{N-H}

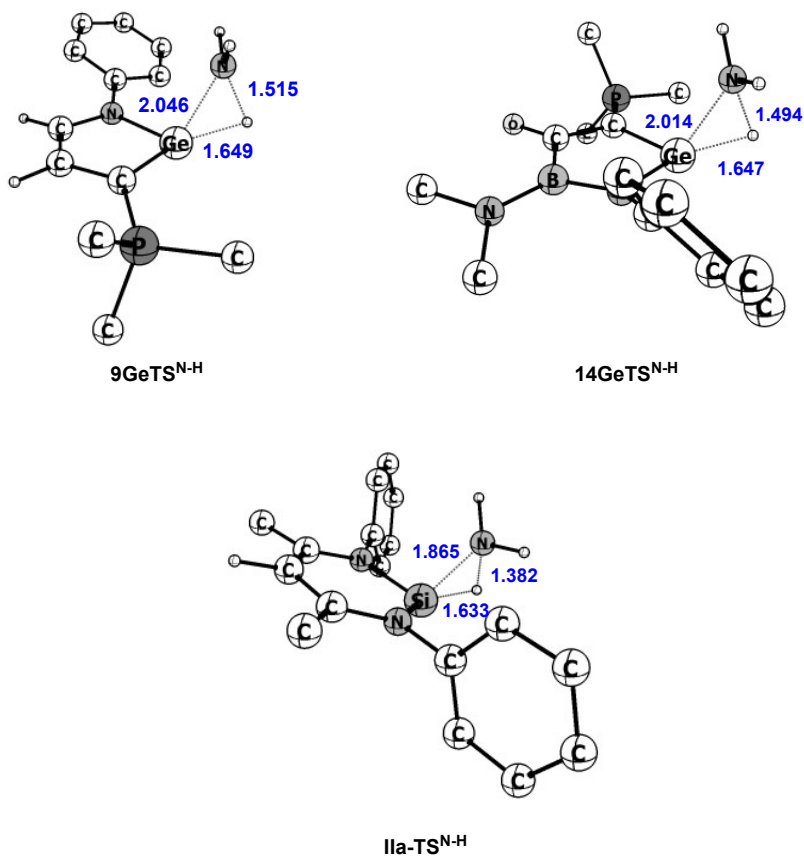
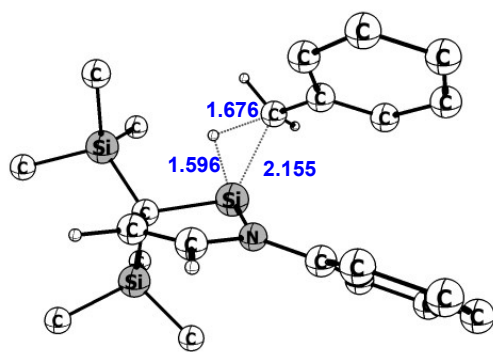
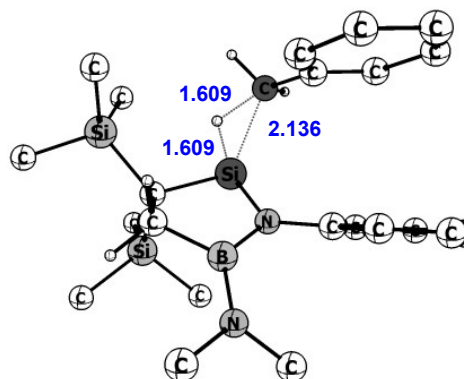


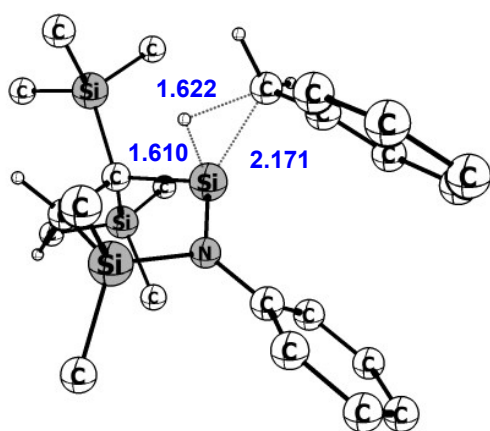
Fig. S5 Optimized geometries for the transition states involved in the activation of N–H bond of NH₃ by CAASis (2Si-5Si, 8Si-9Si and 14Si), CAAGes (2Ge-5Ge, 8Ge-9Ge and 14Ge) and NacNacSi (IIa). The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



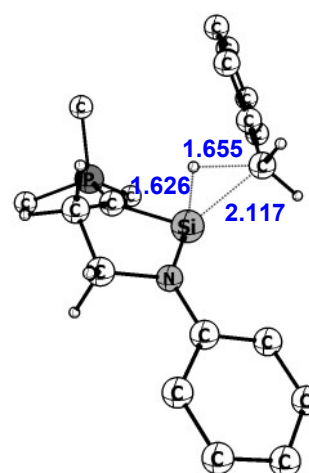
2SiTS^{C-H}



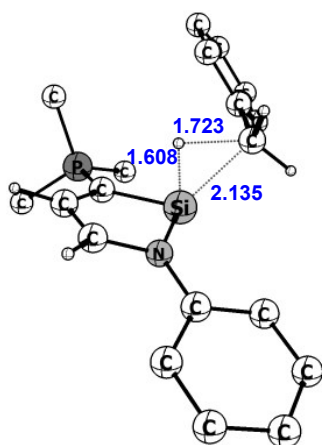
3SiTS^{C-H}



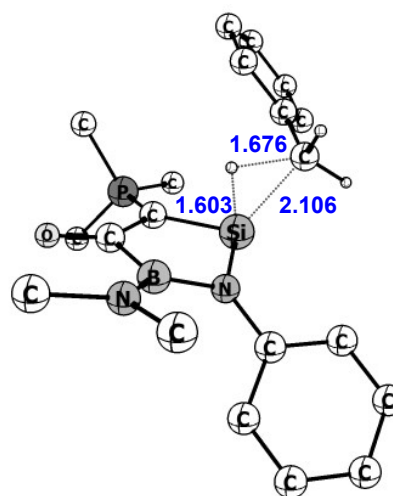
4SiTS^{C-H}



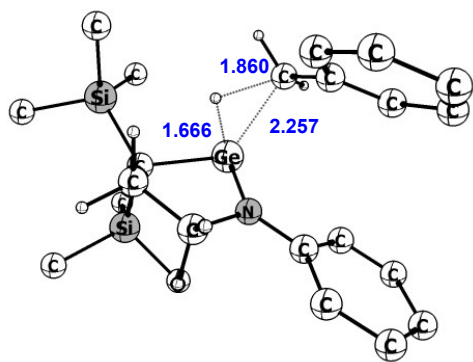
8SiTS^{C-H}



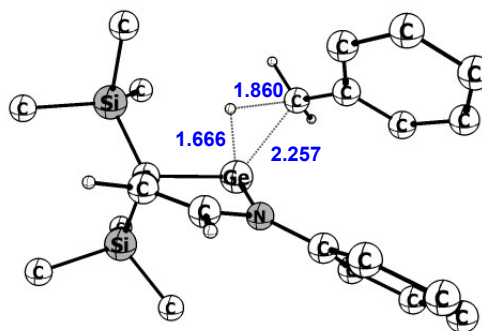
9SiTS^{C-H}



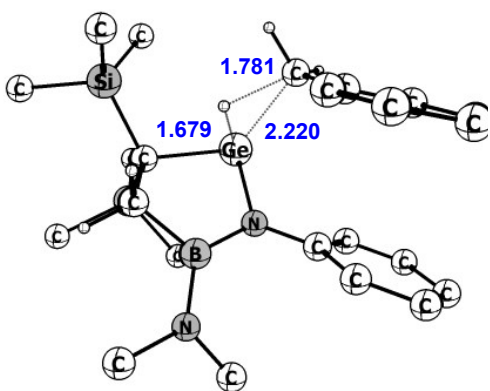
14SiTS^{C-H}



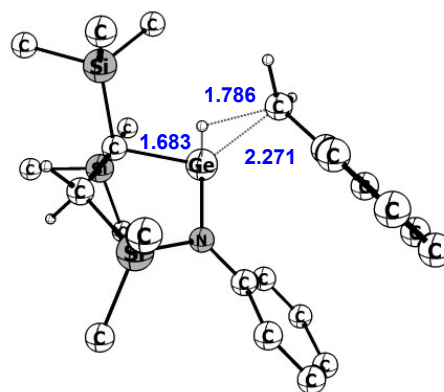
1GeTS^{C-H}



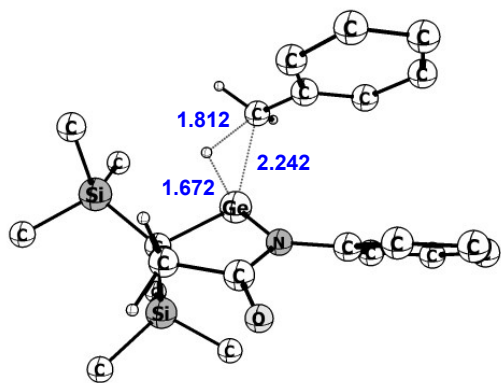
2GeTS^{C-H}



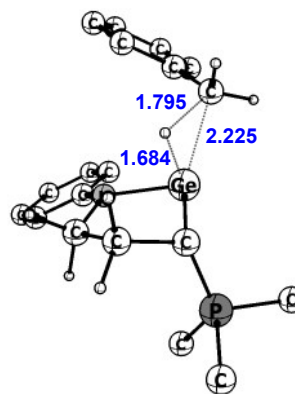
3GeTS^{C-H}



4GeTS^{C-H}



5GeTS^{C-H}



8GeTS^{C-H}

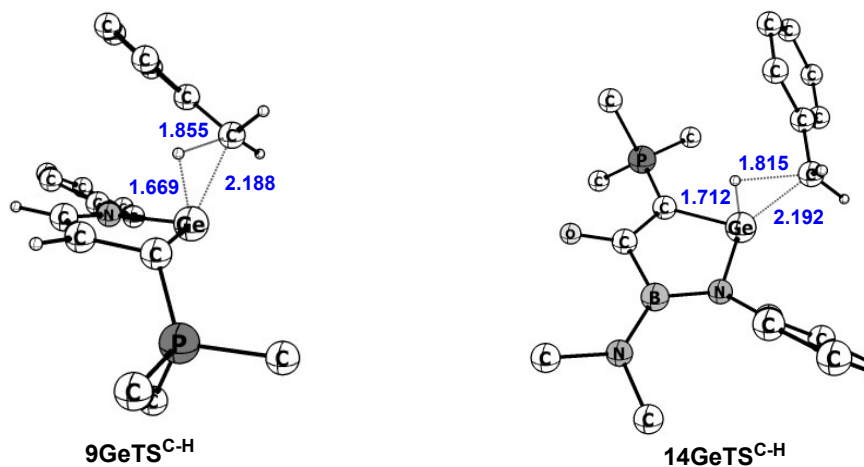
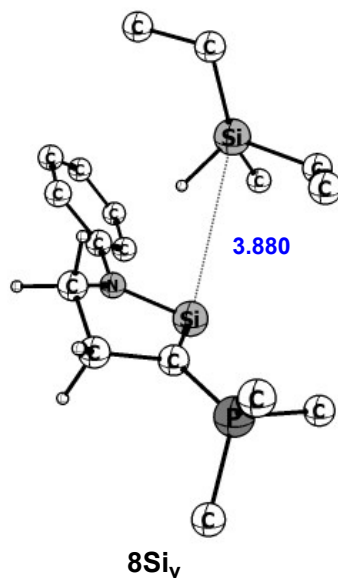
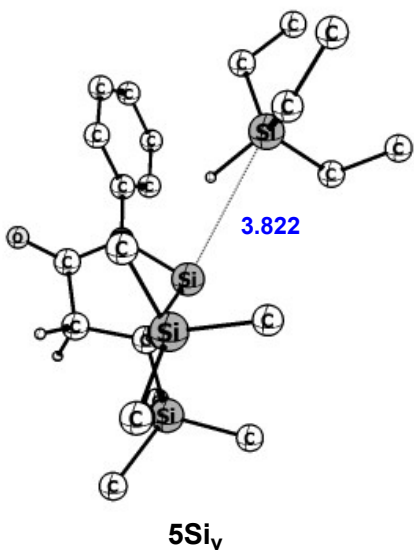
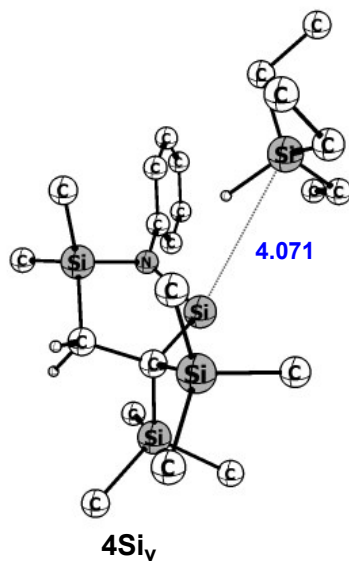
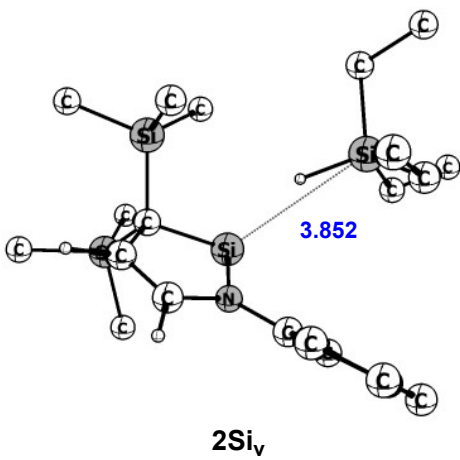
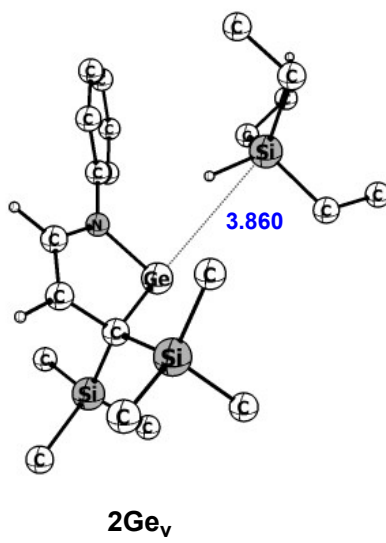
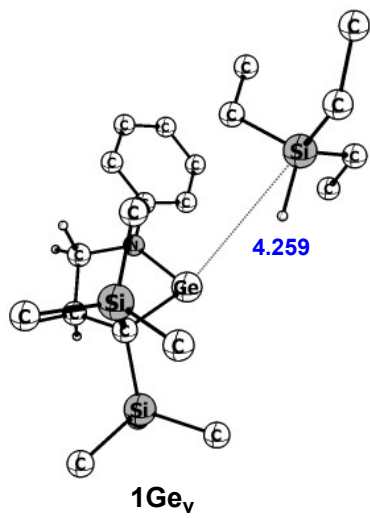
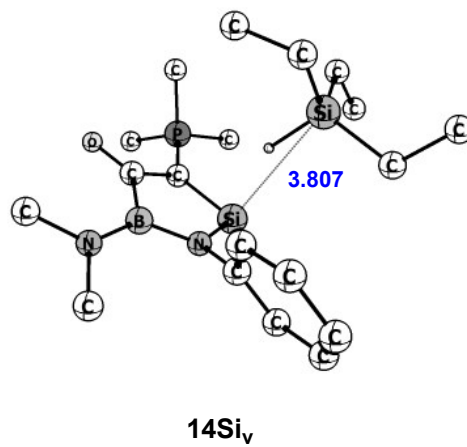
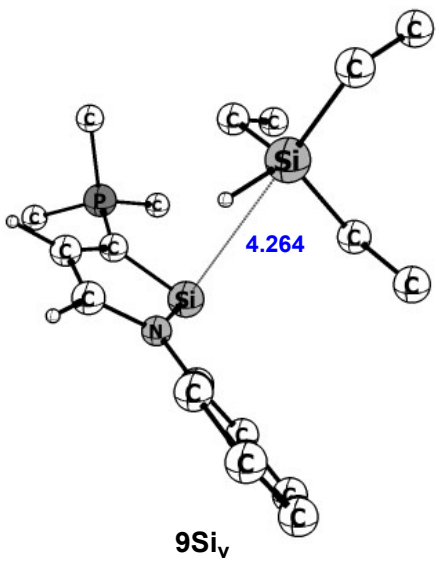
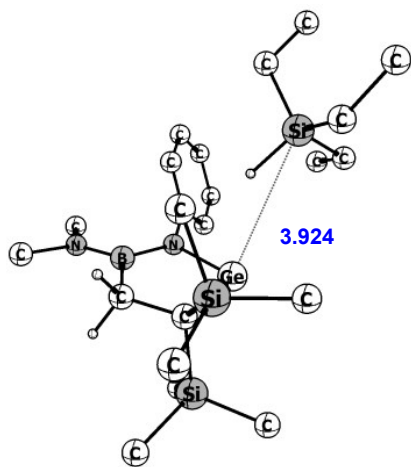


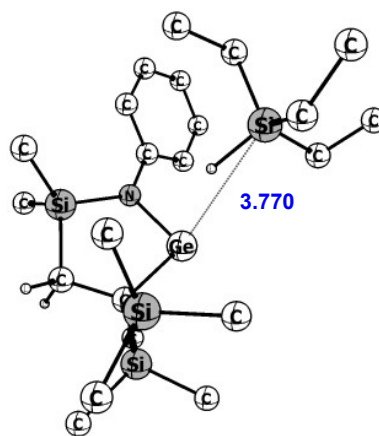
Fig. S6 Optimized geometries for the transition states involved in the activation of C – H bond of CH₃Ph by CAASis (2Si-4Si, 8Si-9Si and 14Si) and CAAGes (1Ge-5Ge, 8Ge-9Ge and 14Ge). The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



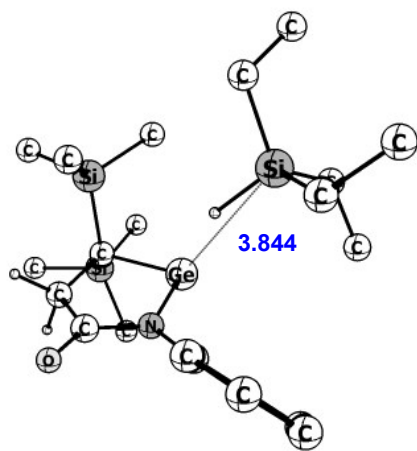




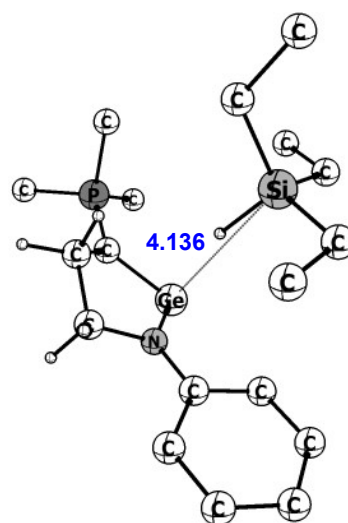
3Ge_v



4Ge_v



5Ge_v



8Ge_v

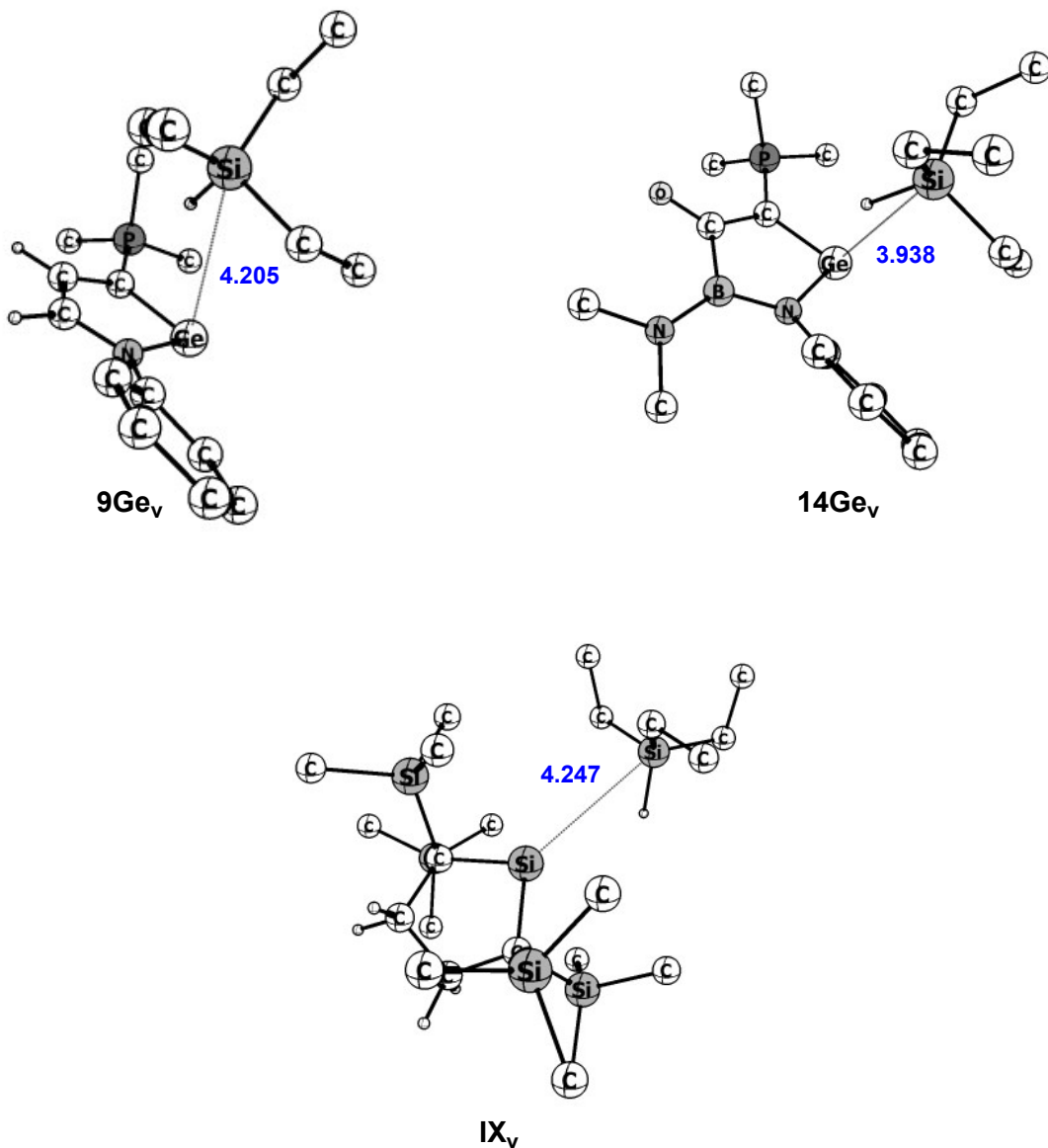
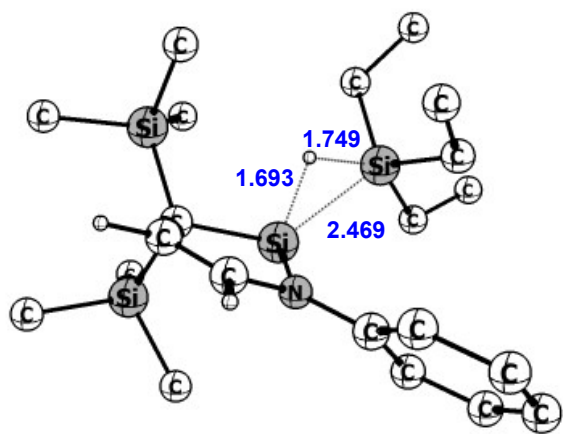
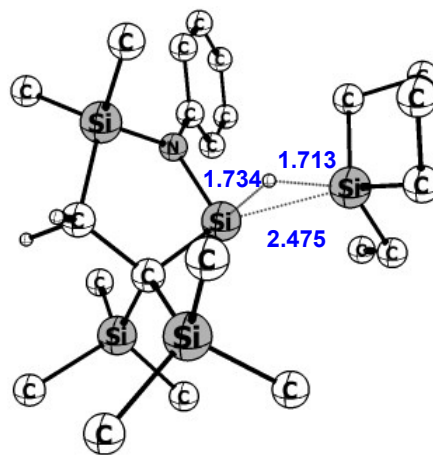


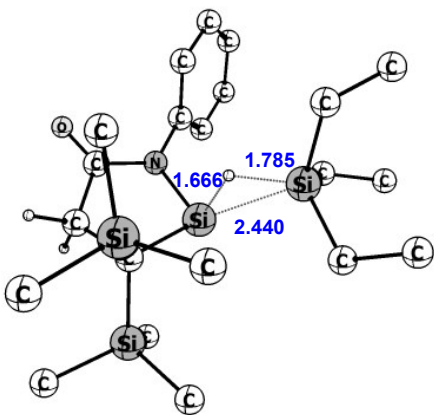
Fig. S7 Optimized geometries for the van der Waals complexes involved in the activation of Si – H bond of SiEt₃H by CAASiS (2Si-5Si, 8Si-9Si and 14Si), CAAGes (1Ge-5Ge, 8Ge-9Ge and 14Ge) and IX. The hydrogen atoms of the methyl and phenyl rings are omitted for clarity.



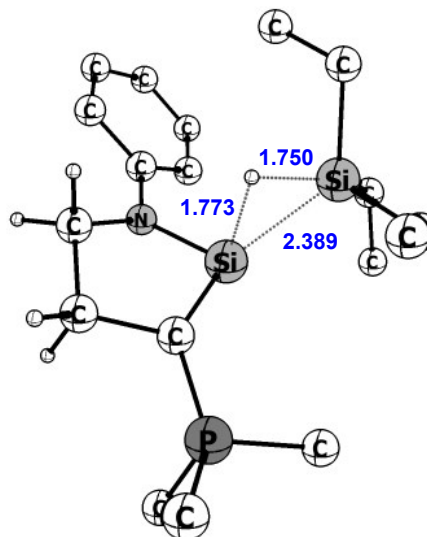
2SiTS^{Si-H}



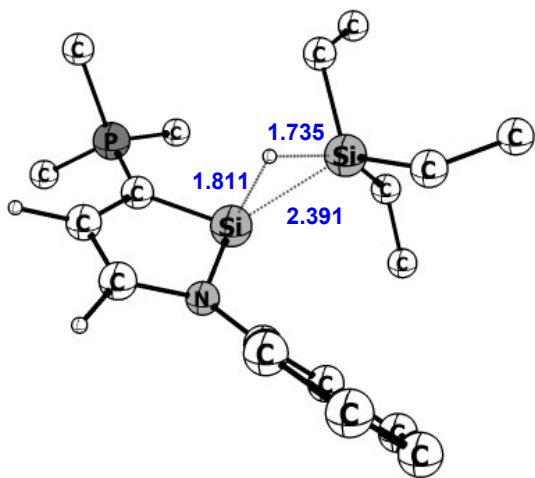
4SiTS^{Si-H}



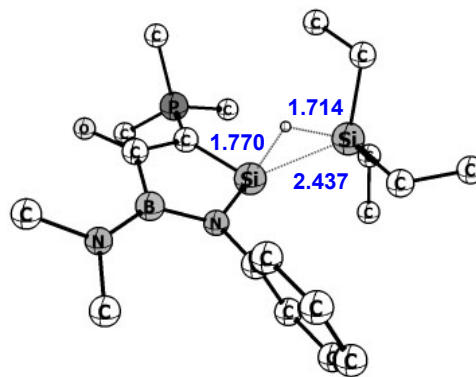
5SiTS^{Si-H}



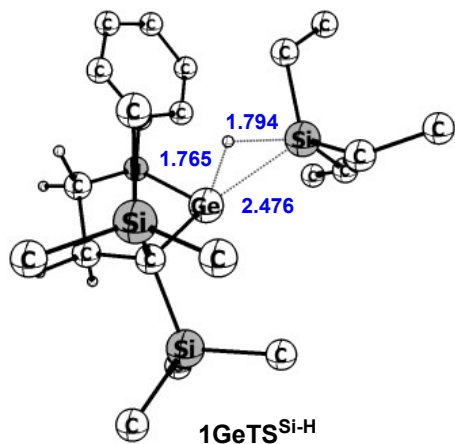
8SiTS^{Si-H}



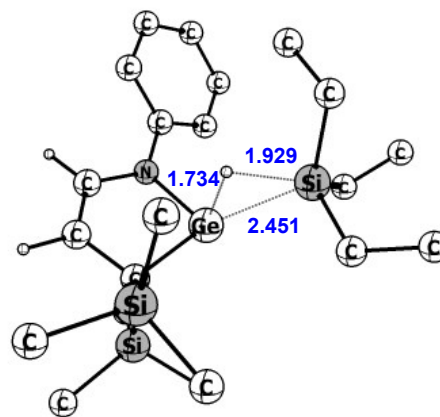
9SiTS^{Si-H}



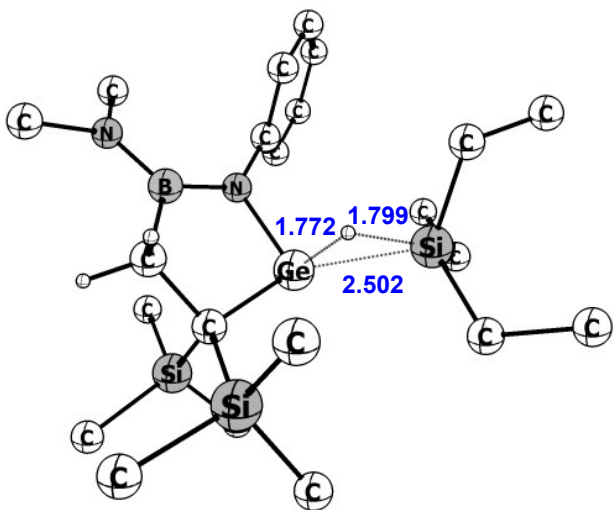
14SiTS^{Si-H}



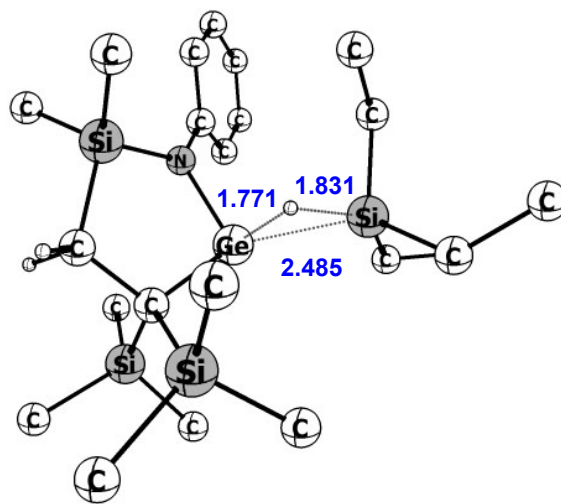
1GeTS^{Si-H}



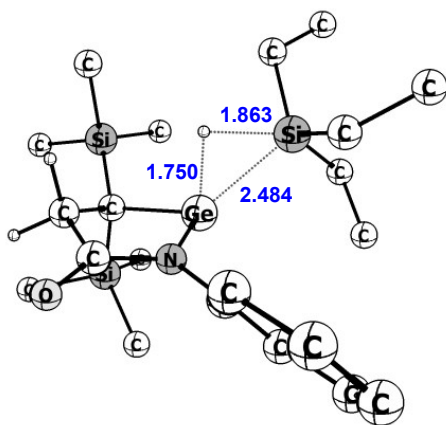
2GeTS^{Si-H}



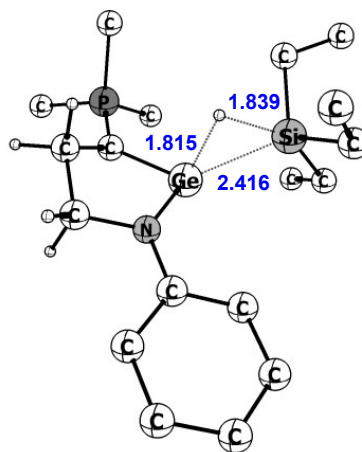
3GeTS^{Si-H}



4GeTS^{Si-H}



5GeTS^{Si-H}



8GeTS^{Si-H}

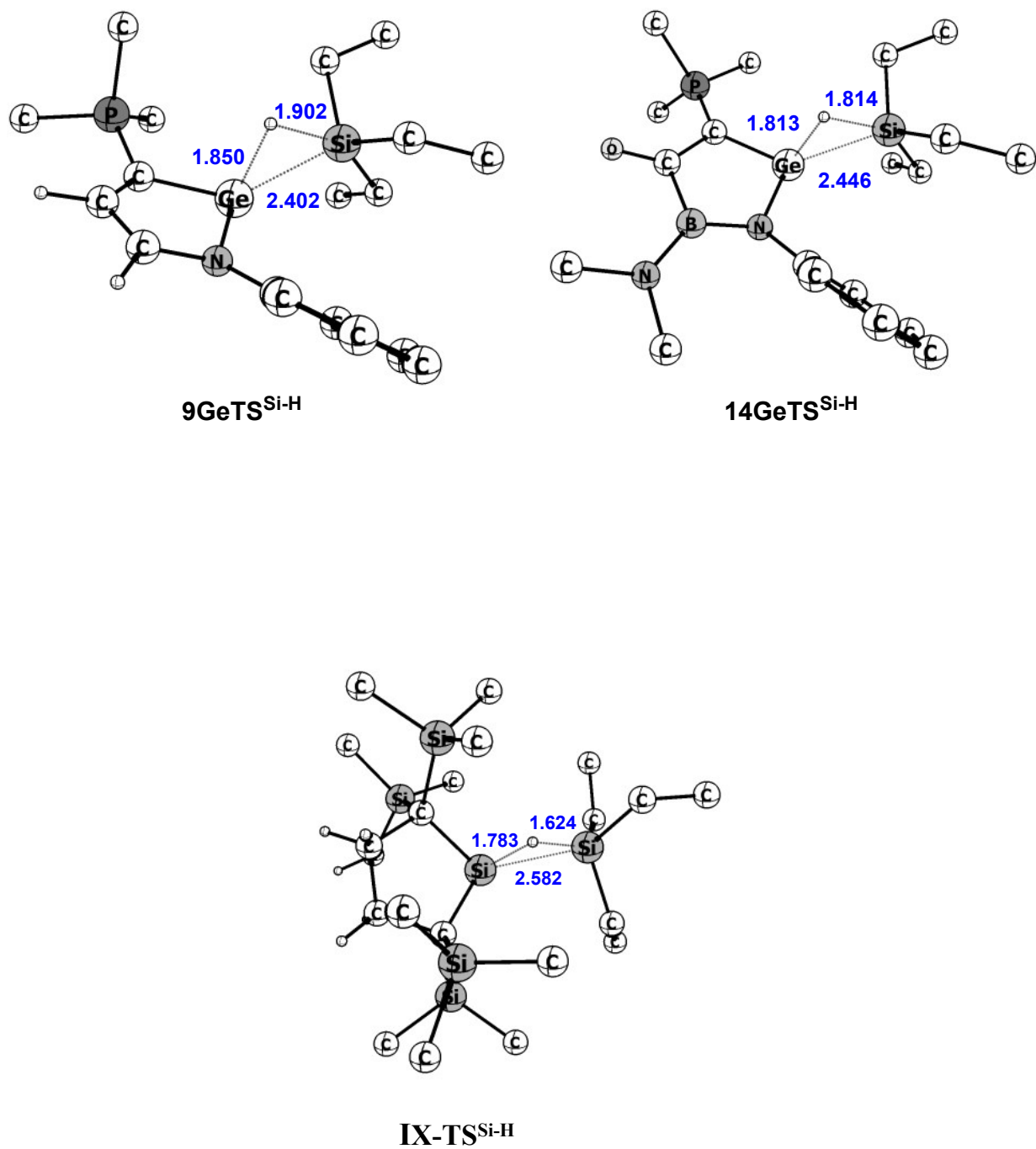
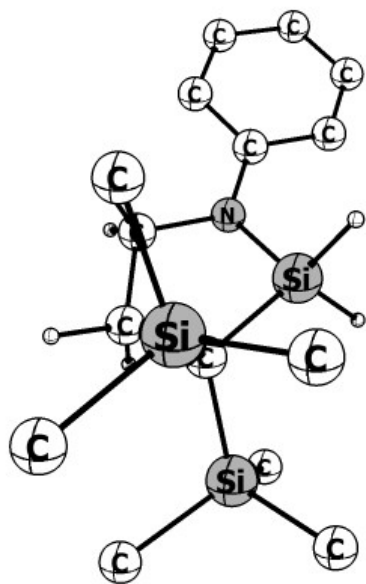
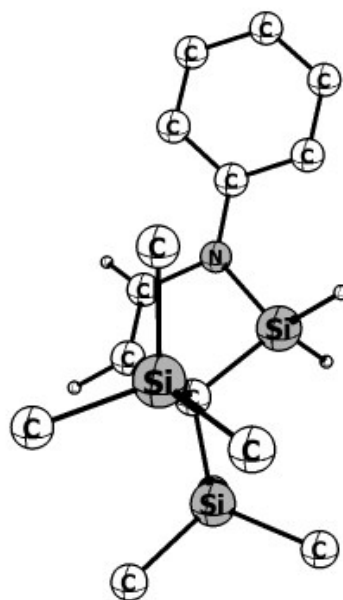


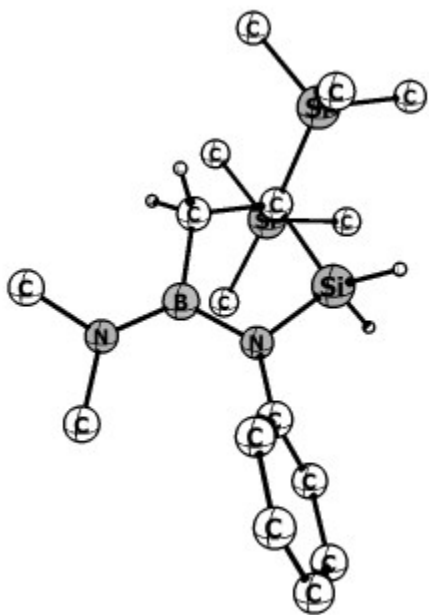
Fig. S8 Optimized geometries for the transition states involved in the activation of Si – H bond of SiEt₃H by CAASi (2Si-5Si, 8Si-9Si and 14Si), CAAGes (1Ge-5Ge, 8Ge-9Ge and 14Ge) and IX. The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



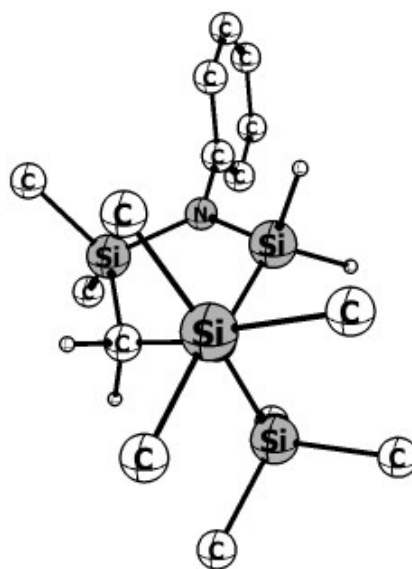
1Si^{PH-H}



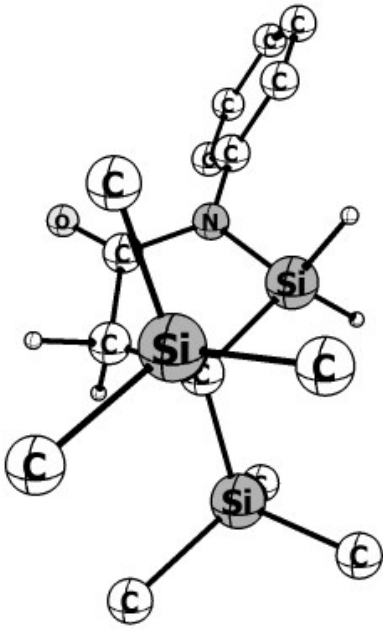
2Si^{PH-H}



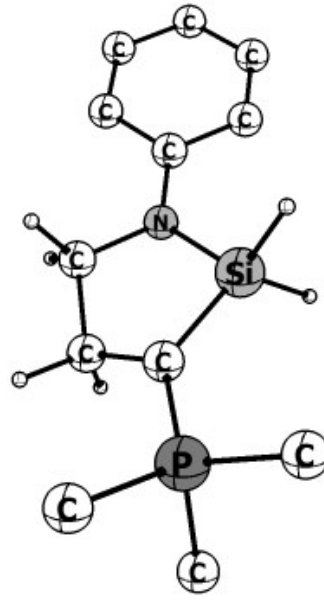
3Si^{PH-H}



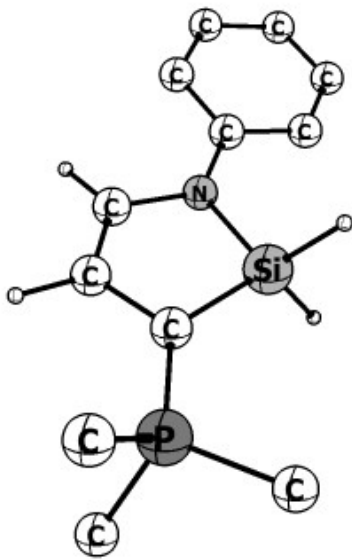
4Si^{PH-H}



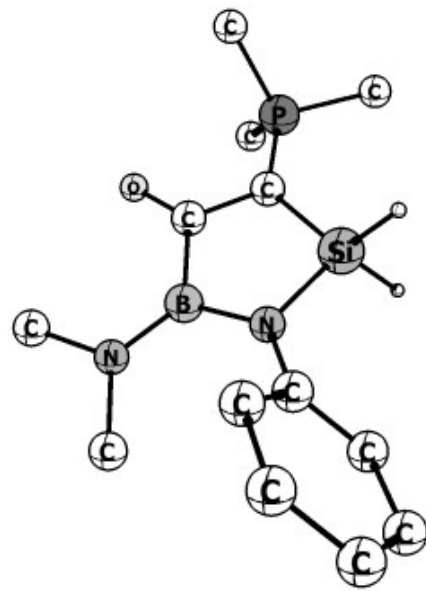
5Si^{H-H}



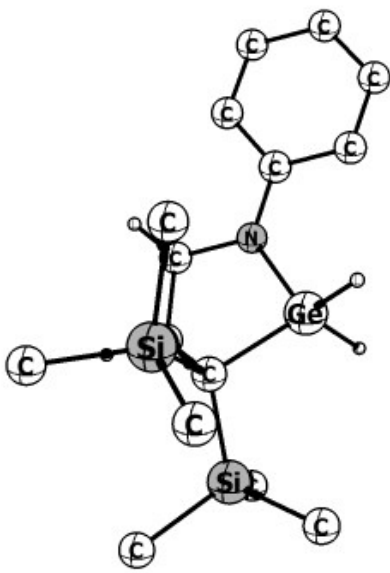
8Si^{H-H}



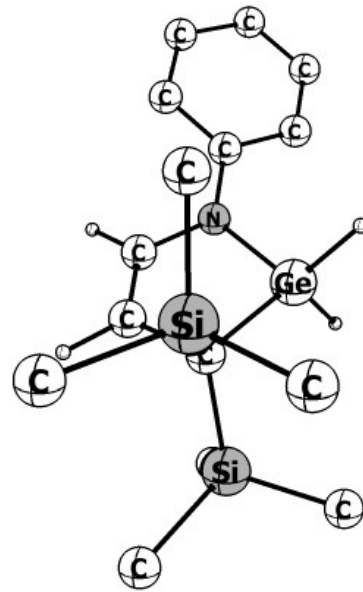
9Si^{H-H}



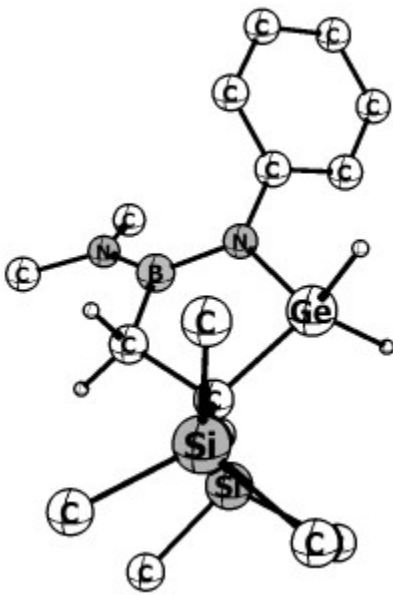
14Si^{H-H}



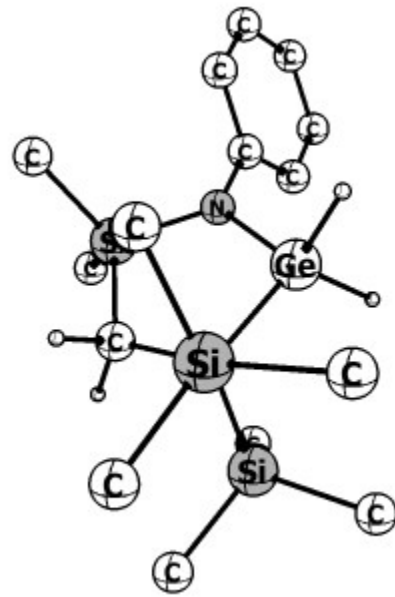
1Ge^{PH-H}



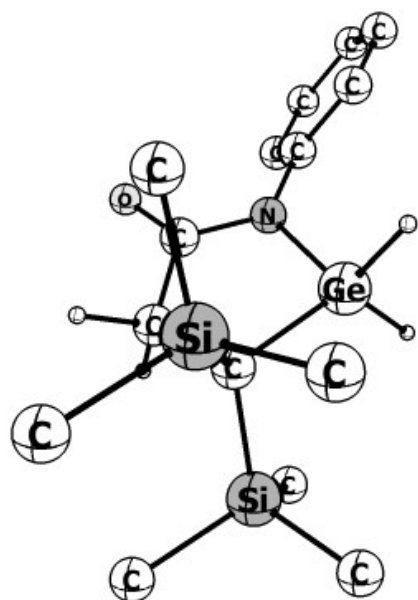
2Ge^{PH-H}



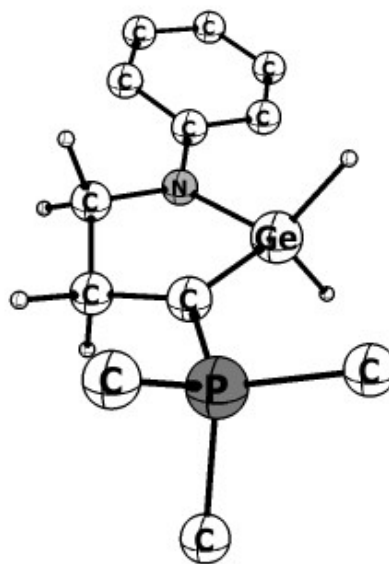
3Ge^{PH-H}



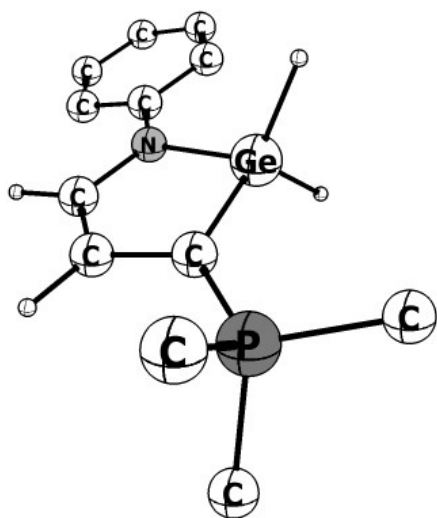
4Ge^{PH-H}



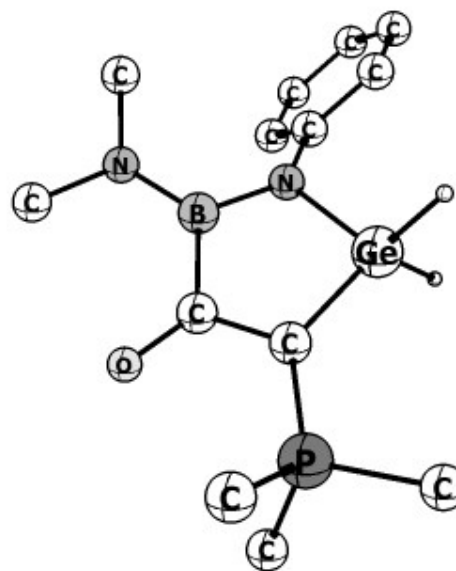
5Ge^{PH-H}



8Ge^{PH-H}

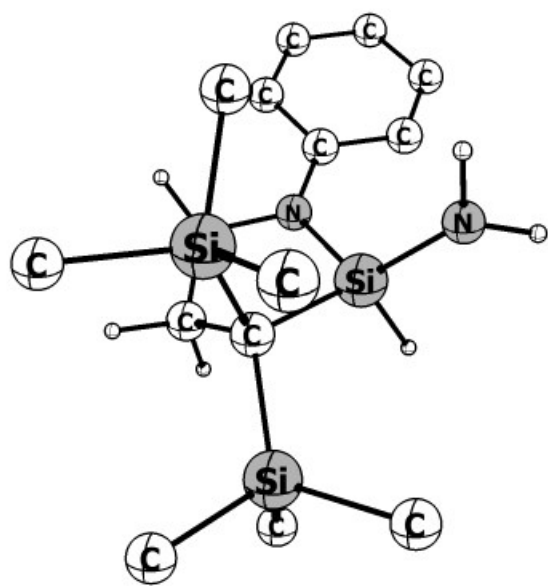


9Ge^{PH-H}

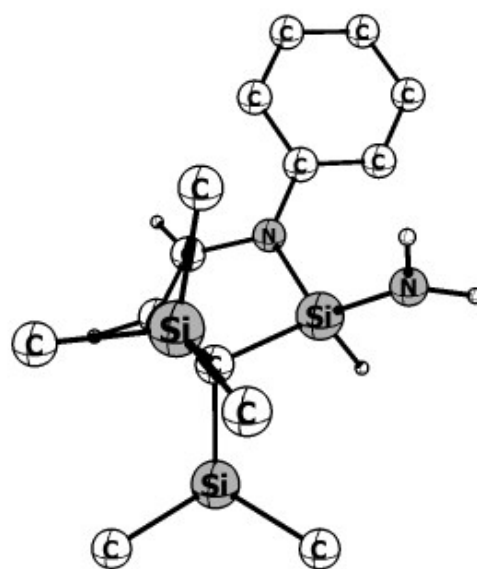


14Ge^{PH-H}

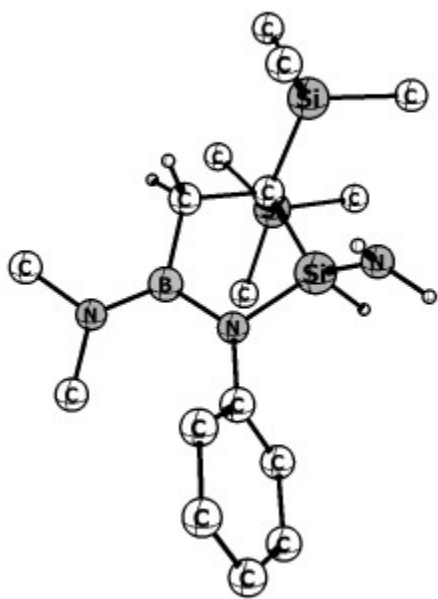
Fig. S9 Optimized geometries of the H-H splitting product obtained for CAASi (1Si-5Si, 8Si-9Si and 14Si) and CAAGes (1Ge-5Ge, 8Ge-9Ge and 14Ge). The hydrogen atoms of the methyl and phenyl groups are omitted for the sake of clarity.



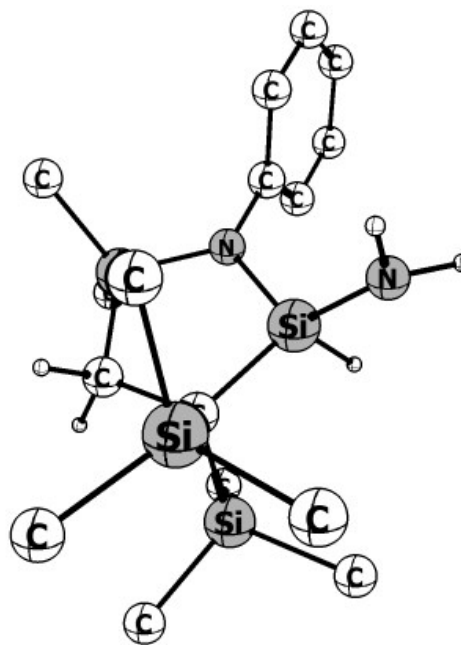
1SiP^{N-H}



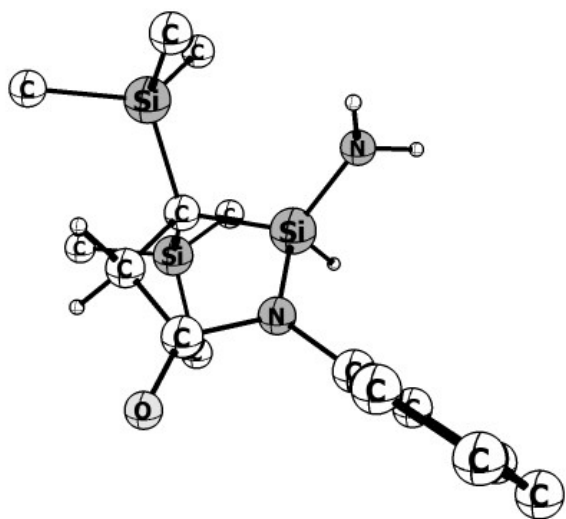
2SiP^{N-H}



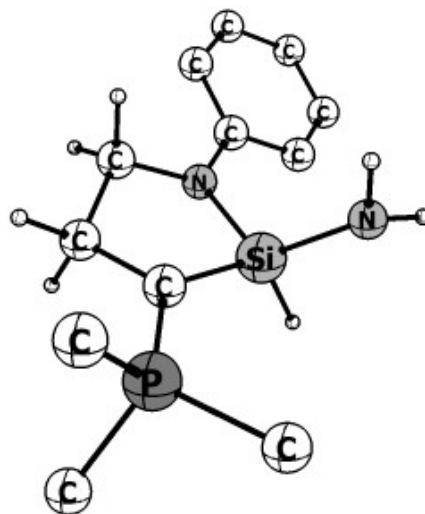
3SiP^{N-H}



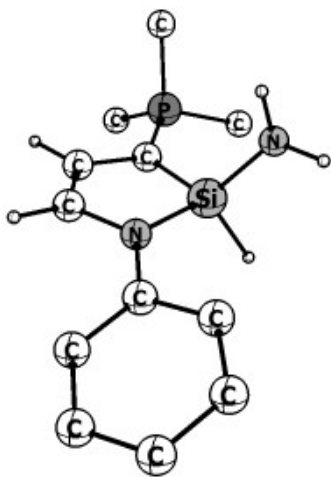
4SiP^{N-H}



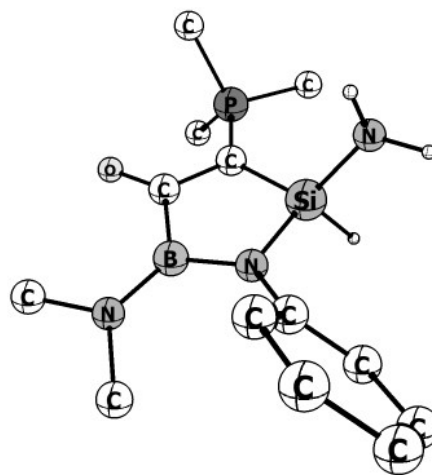
5SiP^{N-H}



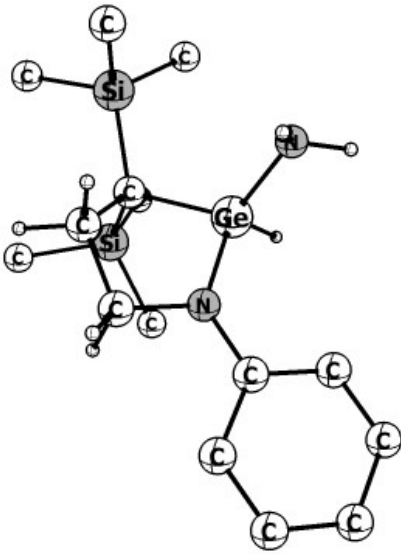
8SiP^{N-H}



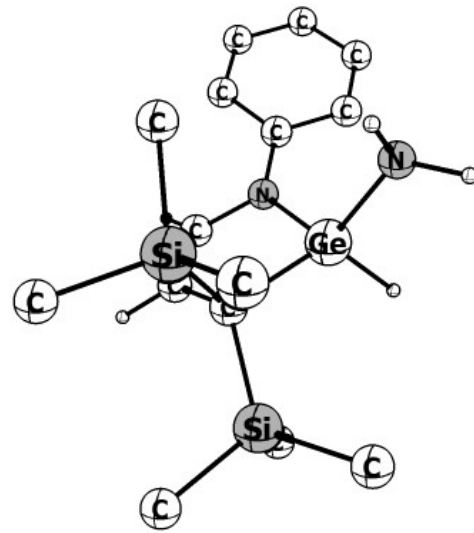
9SiP^{N-H}



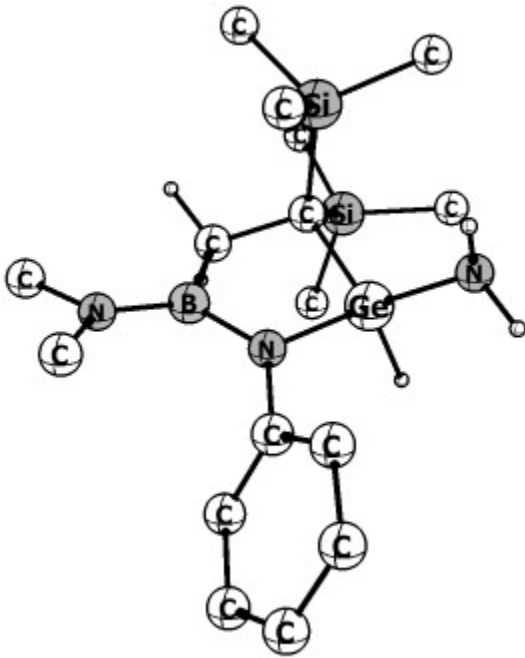
14SiP^{N-H}



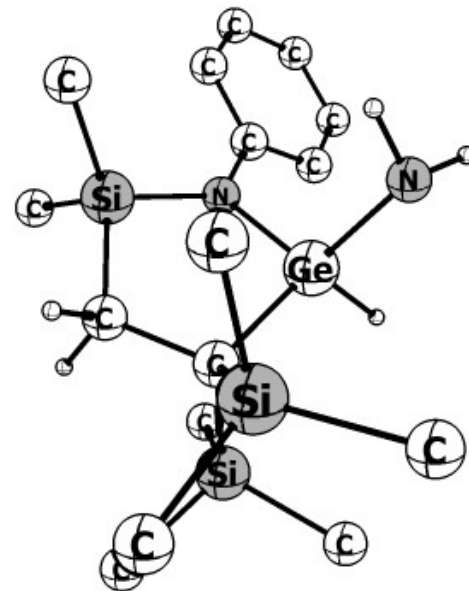
1Ge^{PN-H}



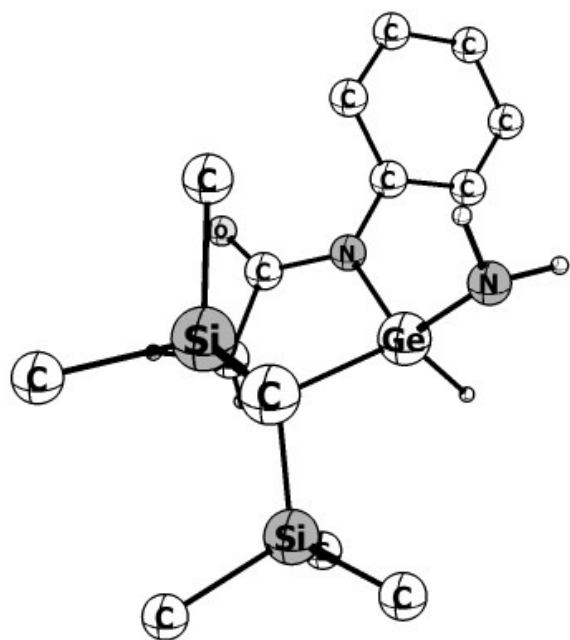
2Ge^{PN-H}



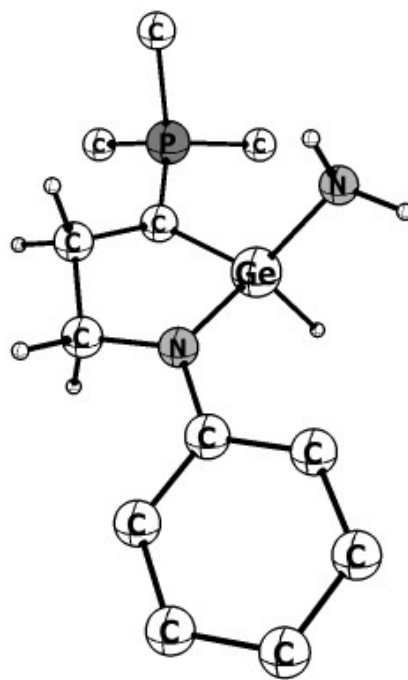
3Ge^{PN-H}



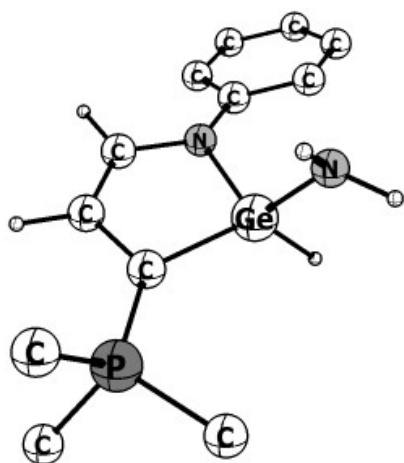
4Ge^{PN-H}



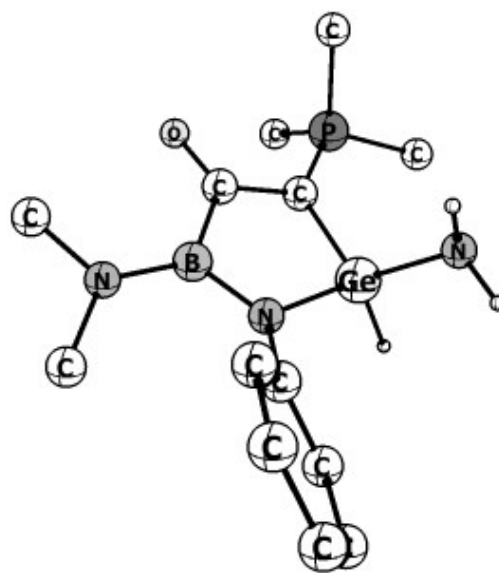
5GePN-H



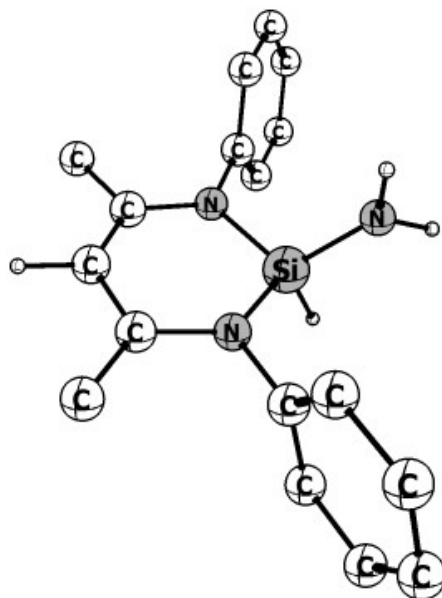
8GePN-H



9GePN-H

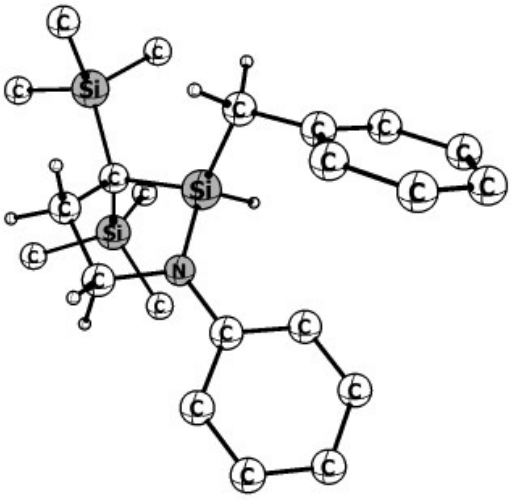


14GePN-H

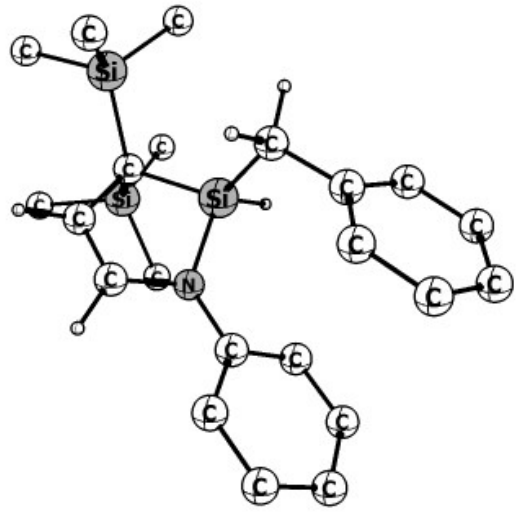


IIa-P^{N-H}

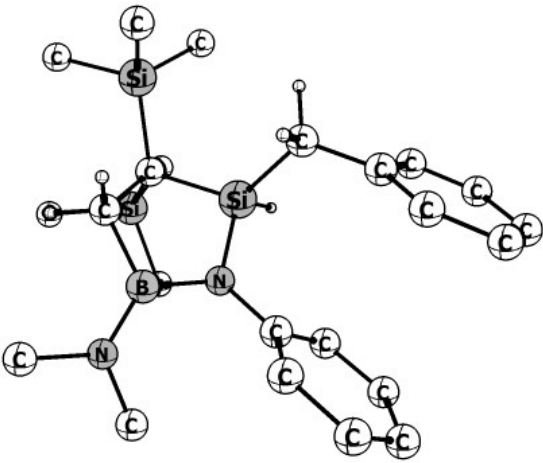
Fig. S10 Optimized geometries of the N-H splitting product obtained for CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and NacNacSi (**IIa**). The hydrogen atoms of the methyl and phenyl groups are omitted for the sake of clarity.



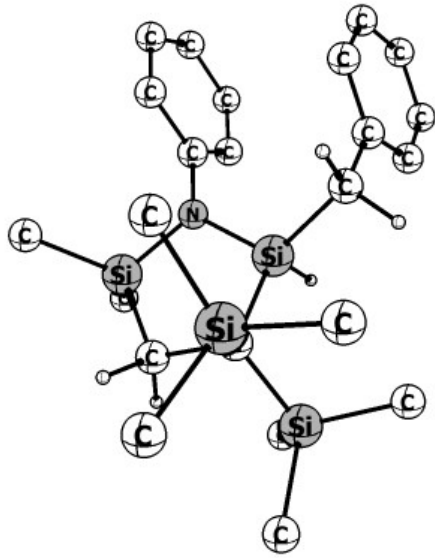
1SiPC-H



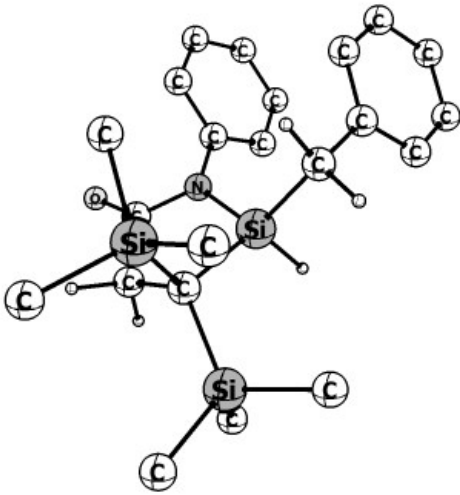
2SiPC-H



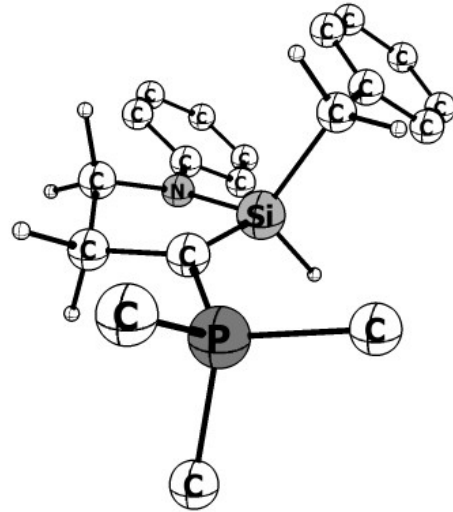
3SiPC-H



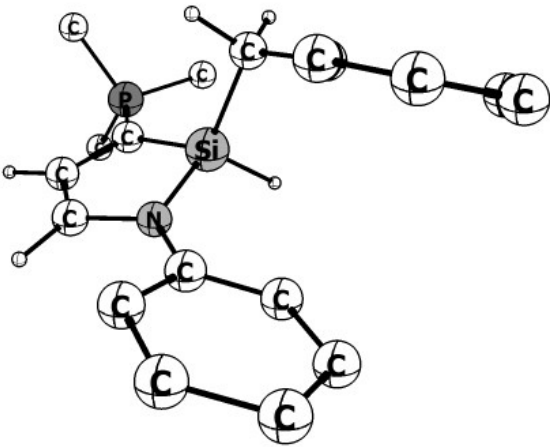
4SiPC-H



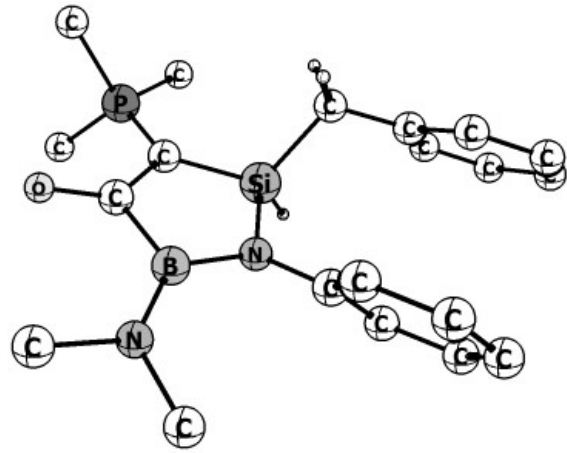
5SiP^C-H



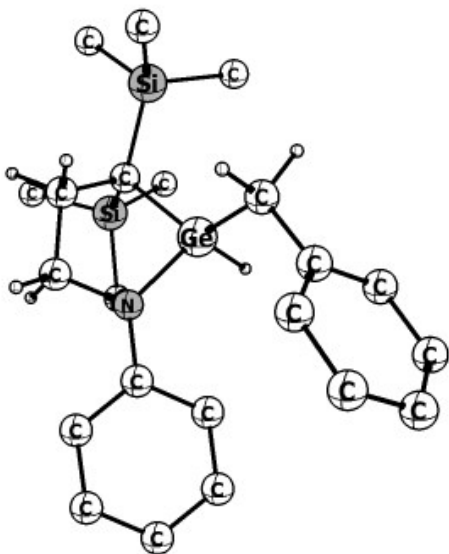
8SiP^C-H



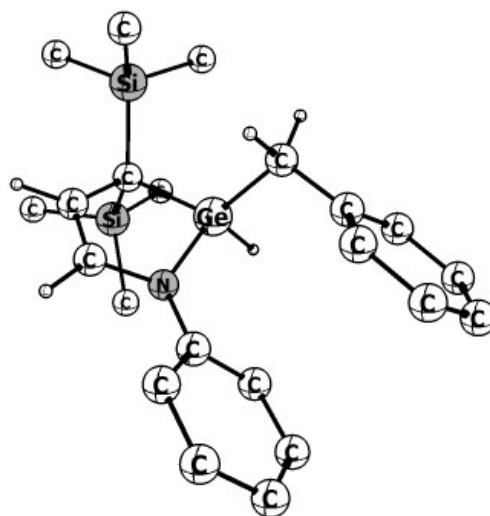
9SiP^C-H



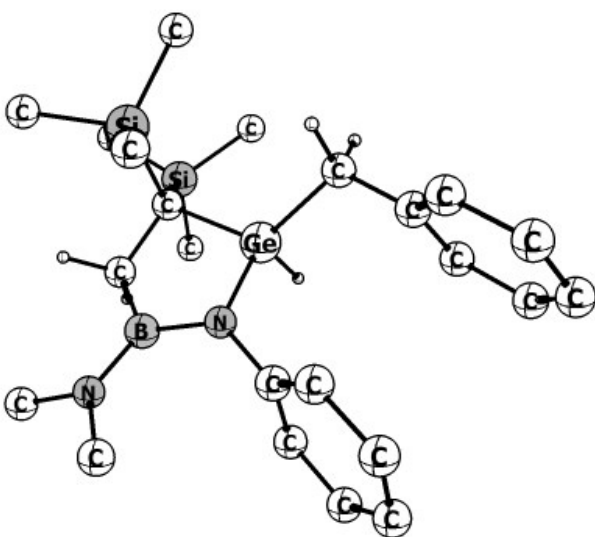
14SiP^C-H



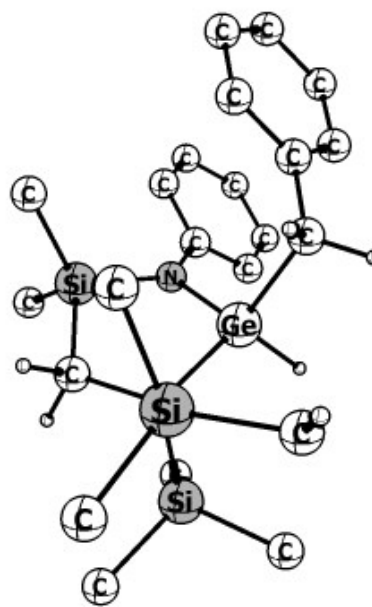
1GePC-H



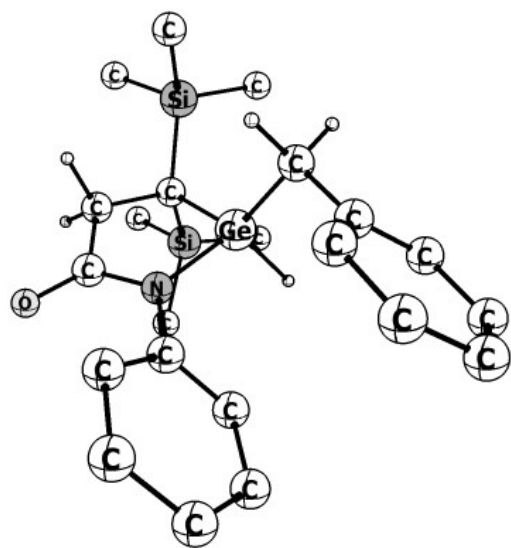
2GePC-H



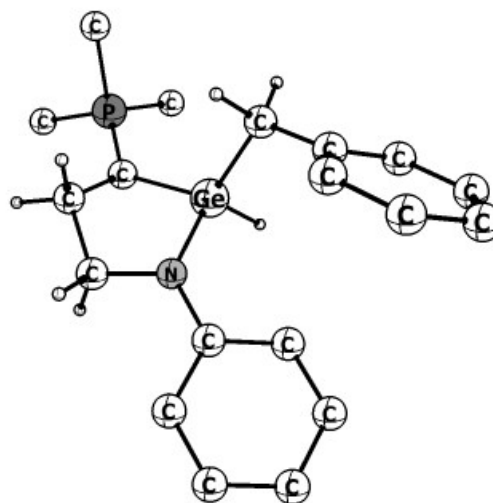
3GePC-H



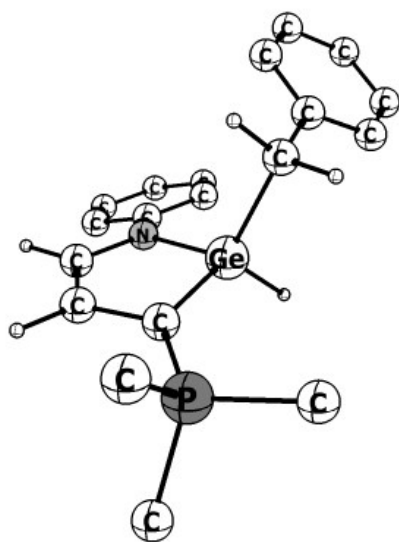
4GePC-H



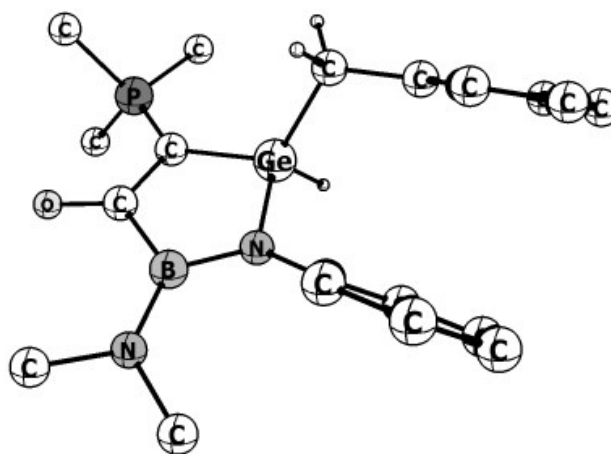
5GePC-H



8GePC-H

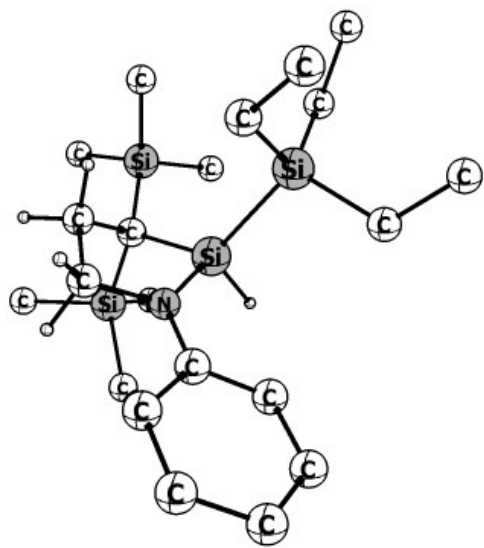


9GePC-H

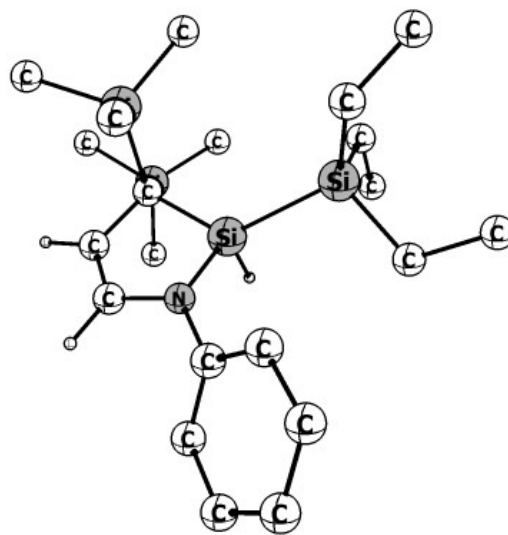


14GePC-H

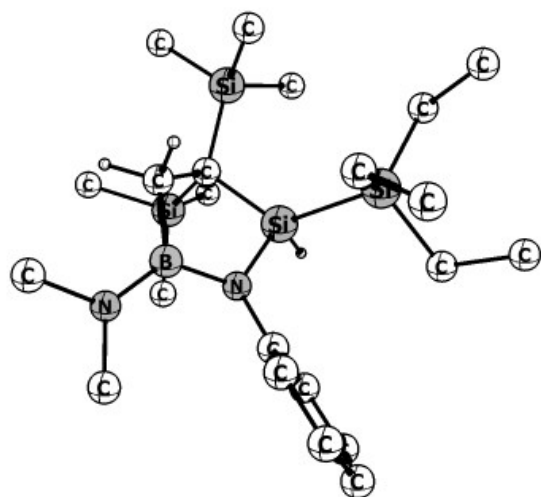
Fig. S11 Optimized geometries of the C-H splitting product obtained for CAASis (1Si-5Si, 8Si-9Si and 14Si) and CAAGes (1Ge-5Ge, 8Ge-9Ge and 14Ge). The hydrogen atoms of the phenyl and methyl groups are omitted for clarity.



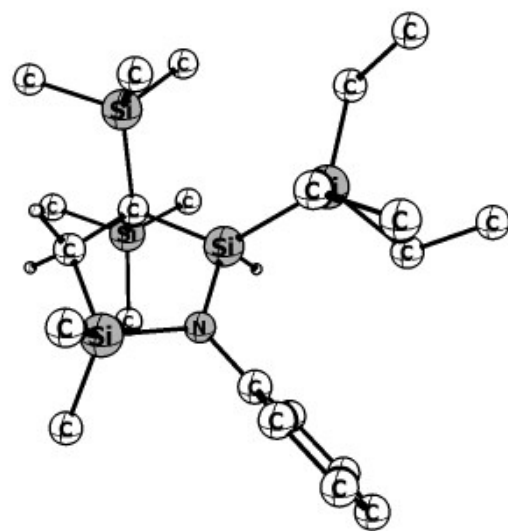
1SiP^{Si-H}



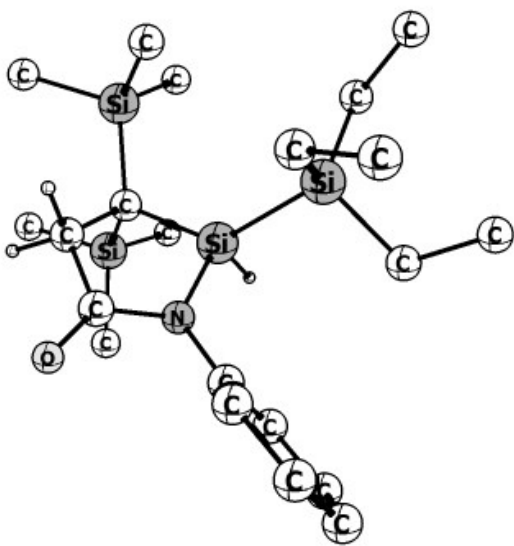
2SiP^{Si-H}



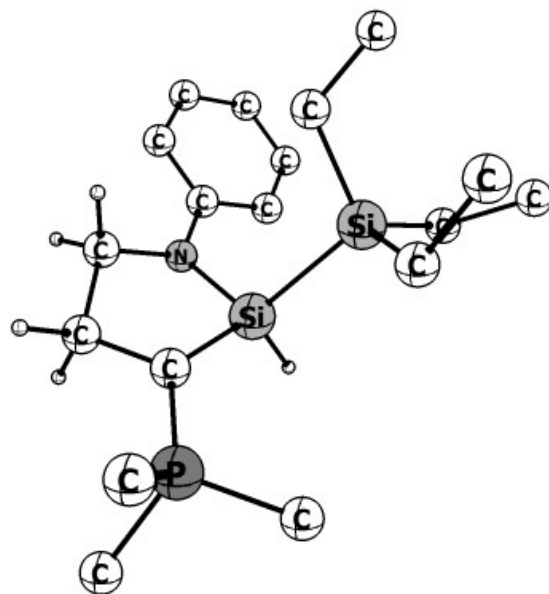
3SiP^{Si-H}



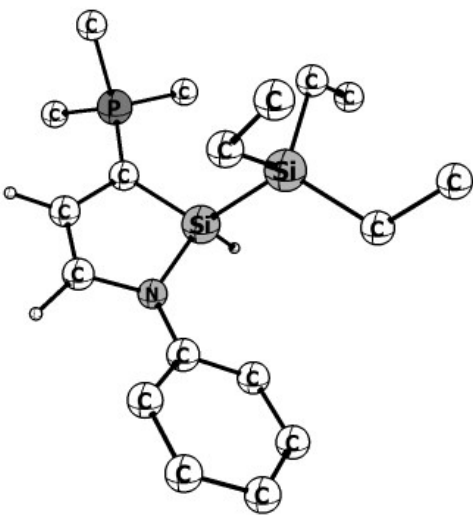
4SiP^{Si-H}



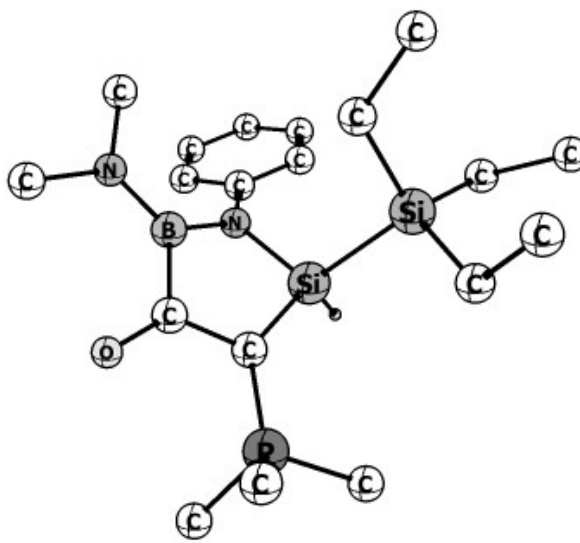
5SiP^{Si}-H



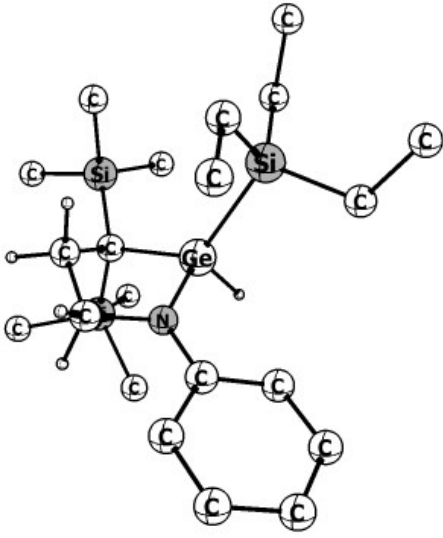
8SiP^{Si}-H



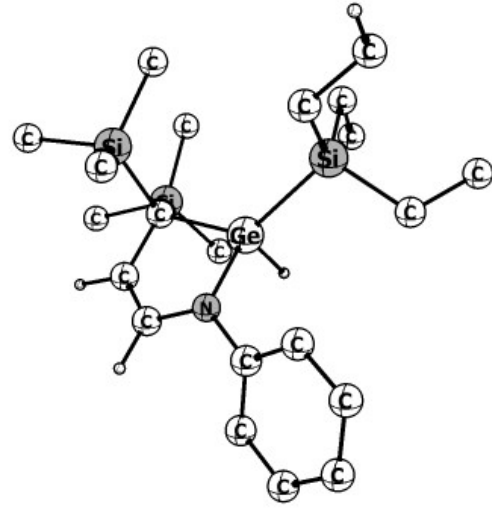
9SiP^{Si}-H



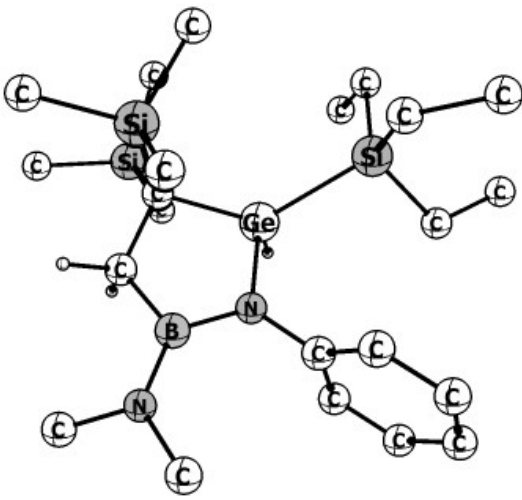
14SiP^{Si}-H



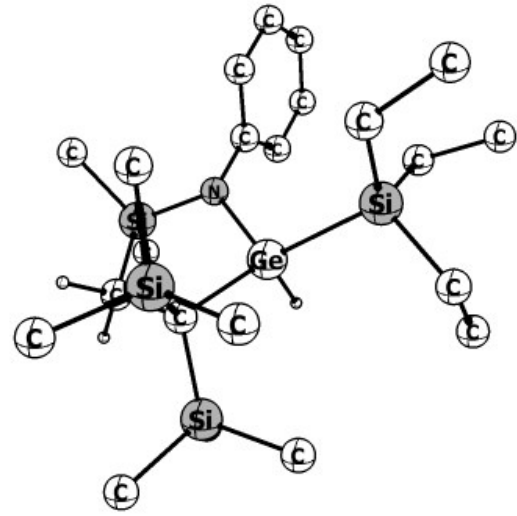
1GePSi-H



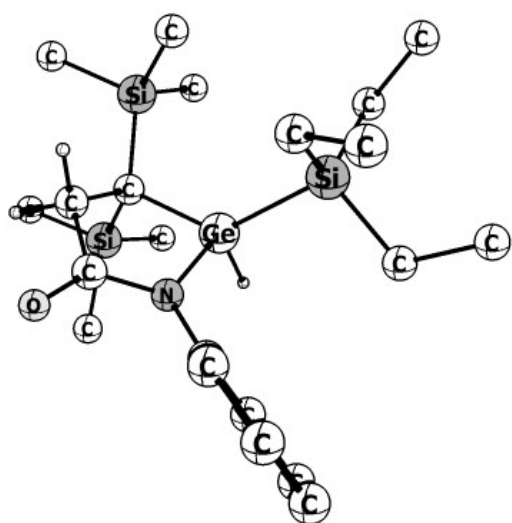
2GePSi-H



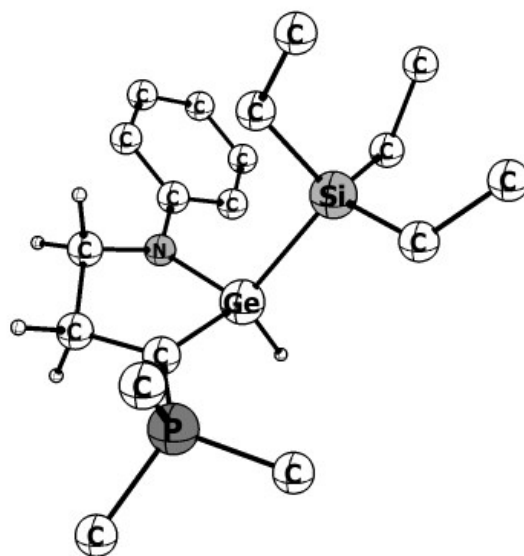
3GePSi-H



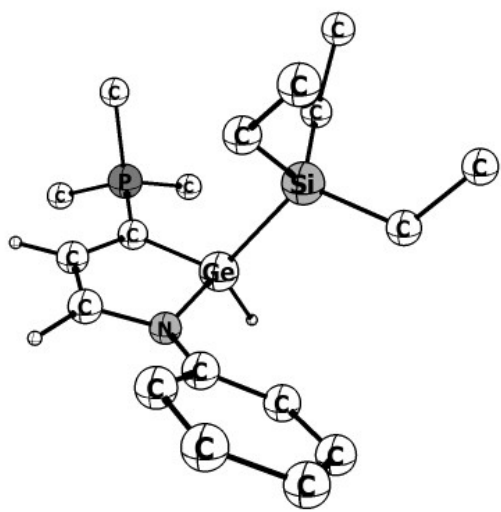
4GePSi-H



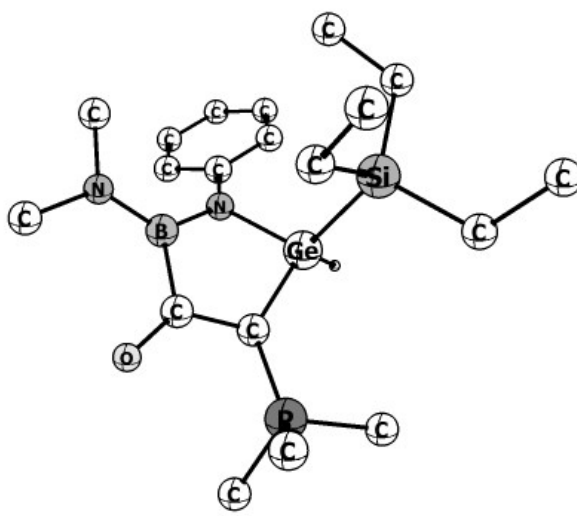
5GePSi-H



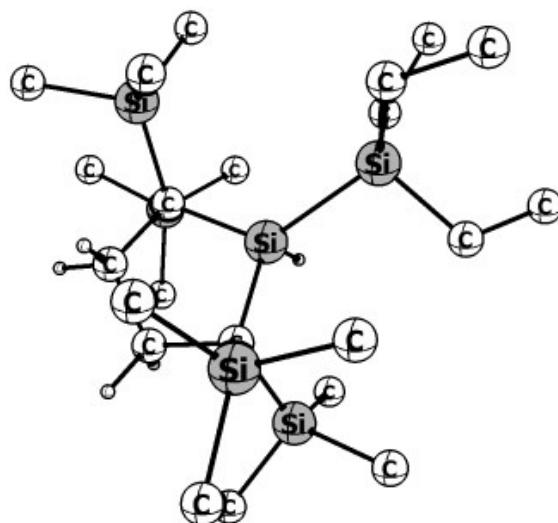
8GePSi-H



9GePSi-H



14GePSi-H



IX-PSi-H

Fig. S12 Optimized geometries of the Si-H splitting product obtained for CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and **IX**. The hydrogen atoms of the phenyl and methyl groups are omitted clarity.

Cartesian coordinates of CAASis (**1Si-14Si**) and CAAGes (**1Ge-14Ge**) in their optimized singlet (S) and triplet (T) state, along with their total energies (in hartrees) including zero point vibrational correction.

1Si-S (T.E.= -1510.522303)

6	0.968003000	0.558559000	-1.500008000
6	-0.480596000	0.123522000	-1.613044000
6	-1.112922000	-0.002647000	-0.202145000
1	1.553467000	0.217208000	-2.360776000
1	1.053434000	1.652647000	-1.471941000
1	-0.504880000	-0.846050000	-2.125038000
1	-1.035194000	0.812484000	-2.261998000
7	1.497928000	-0.024501000	-0.269155000
14	0.331276000	-0.352699000	0.982472000
14	-1.962663000	1.596272000	0.324789000
14	-2.222956000	-1.527912000	-0.157073000
6	-3.178063000	-1.700324000	1.444189000
1	-3.962558000	-0.947641000	1.549746000
1	-3.659826000	-2.681871000	1.461354000
1	-2.523778000	-1.636259000	2.317557000
6	-1.147269000	-3.060818000	-0.326468000
1	-0.543067000	-3.225741000	0.570843000
1	-1.779274000	-3.942941000	-0.460762000
1	-0.468305000	-3.007975000	-1.181075000
6	-3.438896000	-1.534088000	-1.585315000
1	-3.932126000	-2.509392000	-1.627411000
1	-4.213951000	-0.773609000	-1.473505000
1	-2.946949000	-1.373250000	-2.547415000
6	-2.304990000	1.661670000	2.165634000
1	-2.789858000	2.614841000	2.395634000
1	-2.962115000	0.862385000	2.510535000
1	-1.383342000	1.611979000	2.751524000
6	-0.861418000	3.066178000	-0.065140000
1	0.112080000	2.993186000	0.428551000
1	-0.692810000	3.186843000	-1.137637000
1	-1.346641000	3.977615000	0.295431000
6	-3.569684000	1.860979000	-0.603768000
1	-4.346838000	1.156052000	-0.300494000
1	-3.940422000	2.870387000	-0.405099000

1	-3.429952000	1.763824000	-1.683660000
6	2.889946000	-0.060135000	-0.098334000
6	3.736765000	0.804470000	-0.791377000
6	3.461780000	-0.981060000	0.782054000
6	5.106519000	0.757712000	-0.592812000
1	3.324175000	1.530084000	-1.481115000
6	4.827151000	-1.013724000	0.982064000
1	2.818684000	-1.685445000	1.299057000
6	5.662227000	-0.144934000	0.295566000
1	5.744051000	1.441043000	-1.142542000
1	5.245419000	-1.739413000	1.670387000
1	6.734570000	-0.180908000	0.444728000

1Si-T (T.E.= -1510.441248)

6	0.900768000	-0.478896000	-1.660937000
6	-0.630468000	-0.574693000	-1.569042000
6	-1.205002000	-0.134422000	-0.194950000
1	1.275137000	-1.221180000	-2.376709000
1	1.197573000	0.507868000	-2.037548000
1	-0.920788000	-1.611884000	-1.772712000
1	-1.070763000	0.033464000	-2.369066000
7	1.476373000	-0.668375000	-0.344718000
14	0.216139000	-0.829289000	0.867275000
14	-1.235052000	1.740704000	0.088967000
14	-2.814838000	-1.079147000	0.102730000
6	-3.641393000	-0.573079000	1.701611000
1	-4.034515000	0.445001000	1.672399000
1	-4.478779000	-1.247315000	1.899674000
1	-2.948259000	-0.647342000	2.544475000
6	-2.492177000	-2.922463000	0.202423000
1	-2.025212000	-3.186290000	1.154220000
1	-3.443036000	-3.458899000	0.129402000
1	-1.839459000	-3.285755000	-0.594731000
6	-3.980409000	-0.780768000	-1.334786000
1	-4.888861000	-1.371829000	-1.191696000
1	-4.273370000	0.266084000	-1.428244000
1	-3.531699000	-1.091701000	-2.281316000
6	-1.471425000	2.163101000	1.896369000
1	-1.435798000	3.250520000	2.008892000
1	-2.418643000	1.815421000	2.311062000

1	-0.658575000	1.740773000	2.494650000
6	0.367208000	2.548328000	-0.453849000
1	1.240606000	2.105887000	0.033946000
1	0.513760000	2.503484000	-1.535521000
1	0.328998000	3.604915000	-0.174063000
6	-2.621048000	2.519800000	-0.910836000
1	-3.606967000	2.250294000	-0.525276000
1	-2.532908000	3.608772000	-0.867930000
1	-2.577083000	2.223949000	-1.962409000
6	2.821089000	-0.488491000	-0.125458000
6	3.719659000	-0.200438000	-1.159524000
6	3.325394000	-0.572431000	1.181150000
6	5.057501000	0.018345000	-0.883421000
1	3.368969000	-0.139438000	-2.182078000
6	4.659920000	-0.344066000	1.442417000
1	2.649584000	-0.833787000	1.993162000
6	5.541243000	-0.045350000	0.412903000
1	5.732244000	0.245410000	-1.701489000
1	5.019605000	-0.410530000	2.463116000
1	6.590978000	0.124108000	0.618783000

2Si-S (T.E.= -1509.336249)

6	-1.103647000	-0.014175000	-0.171096000
6	-0.461759000	0.134093000	-1.503327000
6	0.874507000	0.069311000	-1.504397000
1	-1.027691000	0.268207000	-2.420387000
1	1.510826000	0.135670000	-2.379991000
14	0.311636000	-0.278628000	1.071234000
7	1.463993000	-0.151833000	-0.261237000
14	-2.241959000	-1.519443000	-0.140095000
14	-1.897967000	1.653483000	0.255593000
6	-3.793039000	-1.249511000	-1.156879000
1	-4.330366000	-2.197517000	-1.250027000
1	-4.472126000	-0.529509000	-0.693678000
1	-3.562500000	-0.898372000	-2.165917000
6	-2.741834000	-1.990059000	1.602111000
1	-3.392564000	-2.868042000	1.556527000
1	-1.874694000	-2.251120000	2.213905000
1	-3.288538000	-1.198298000	2.116161000
6	-1.306715000	-2.963171000	-0.882029000

1	-1.906661000	-3.874428000	-0.812254000
1	-1.072876000	-2.794081000	-1.935060000
1	-0.364936000	-3.142843000	-0.355064000
6	-2.952062000	1.563533000	1.799103000
1	-3.265523000	2.574094000	2.075049000
1	-3.854939000	0.966795000	1.652079000
1	-2.400021000	1.143450000	2.643939000
6	-0.547105000	2.924701000	0.538829000
1	-0.032829000	2.772292000	1.491307000
1	0.199034000	2.898285000	-0.260396000
1	-0.980527000	3.928605000	0.554072000
6	-2.940550000	2.269688000	-1.172028000
1	-3.717339000	1.562319000	-1.466785000
1	-3.428129000	3.203760000	-0.879343000
1	-2.320682000	2.480643000	-2.046211000
6	2.867566000	-0.124580000	-0.122089000
6	3.496748000	-1.027167000	0.729105000
6	3.636951000	0.814624000	-0.802507000
6	4.868033000	-0.983706000	0.902379000
1	2.898293000	-1.771833000	1.242921000
6	5.009795000	0.842583000	-0.636193000
1	3.149221000	1.539798000	-1.444664000
6	5.632378000	-0.053097000	0.217715000
1	5.344016000	-1.693626000	1.568832000
1	5.596532000	1.580897000	-1.170662000
1	6.707529000	-0.026479000	0.347889000

2Si-T (T.E.= -1509.261800)

6	-1.192324000	-0.145496000	-0.217618000
6	-0.556751000	-0.408957000	-1.503332000
6	0.808140000	-0.532049000	-1.541223000
1	-1.128186000	-0.588727000	-2.412934000
1	1.371178000	-0.676689000	-2.459039000
14	0.159858000	-0.962548000	0.992067000
7	1.427192000	-0.556380000	-0.345611000
14	-2.851445000	-1.043661000	-0.053680000
14	-1.160410000	1.709752000	0.206722000
6	-4.225054000	-0.120696000	-0.932101000
1	-5.121622000	-0.744861000	-0.971856000
1	-4.488686000	0.810450000	-0.425976000

1	-3.941275000	0.122701000	-1.959994000
6	-3.304949000	-1.289450000	1.743427000
1	-4.246644000	-1.841648000	1.805192000
1	-2.541659000	-1.874268000	2.263538000
1	-3.432652000	-0.346938000	2.277823000
6	-2.664825000	-2.723239000	-0.858915000
1	-3.534606000	-3.348615000	-0.642350000
1	-2.572220000	-2.646255000	-1.944888000
1	-1.773707000	-3.231104000	-0.478290000
6	-1.990784000	2.009379000	1.855427000
1	-1.825327000	3.049914000	2.147781000
1	-3.070109000	1.845835000	1.819067000
1	-1.569849000	1.371986000	2.637473000
6	0.573177000	2.412333000	0.279235000
1	1.182930000	1.950393000	1.059553000
1	1.099156000	2.323015000	-0.674118000
1	0.488561000	3.479565000	0.506057000
6	-2.053260000	2.670345000	-1.136173000
1	-3.116281000	2.432375000	-1.194054000
1	-1.957525000	3.743270000	-0.948003000
1	-1.606665000	2.464465000	-2.113026000
6	2.796096000	-0.439754000	-0.181968000
6	3.375087000	-0.861870000	1.018722000
6	3.611921000	0.140969000	-1.158666000
6	4.730859000	-0.707133000	1.231429000
1	2.750259000	-1.335441000	1.769040000
6	4.966089000	0.282580000	-0.936938000
1	3.172355000	0.521056000	-2.073676000
6	5.535413000	-0.139364000	0.256642000
1	5.164527000	-1.043435000	2.165896000
1	5.583633000	0.744778000	-1.698271000
1	6.599015000	-0.022361000	0.425114000

3Si-S (T.E.= -1630.623646)

6	-0.710193000	0.782798000	-1.148750000
6	-1.384737000	-0.139117000	-0.088643000
1	-0.801809000	0.338409000	-2.152178000
1	-1.215005000	1.753319000	-1.234113000
14	-0.025847000	-1.231286000	0.654247000
7	1.268812000	-0.263090000	-0.018409000

5	0.827063000	0.891375000	-0.798300000
7	1.632500000	1.992521000	-1.151539000
6	1.158886000	3.023582000	-2.046085000
1	0.959616000	3.960412000	-1.508111000
1	1.913330000	3.240966000	-2.810843000
1	0.247229000	2.718764000	-2.556346000
6	2.922279000	2.332520000	-0.593751000
1	2.903417000	3.367405000	-0.232213000
1	3.182094000	1.692851000	0.246867000
1	3.722836000	2.257590000	-1.340364000
14	-2.676337000	-1.238736000	-0.900391000
14	-2.027676000	0.941355000	1.317118000
6	-1.776837000	-2.454571000	-2.017406000
1	-1.226894000	-3.192707000	-1.425773000
1	-2.482549000	-2.999766000	-2.649610000
1	-1.059849000	-1.956556000	-2.675756000
6	-3.854857000	-0.237533000	-1.961447000
1	-4.478979000	-0.915597000	-2.550236000
1	-4.516459000	0.388187000	-1.358817000
1	-3.323392000	0.412497000	-2.660414000
6	-3.567878000	1.886214000	0.817197000
1	-4.442540000	1.235204000	0.751932000
1	-3.781053000	2.654029000	1.566127000
1	-3.445366000	2.382802000	-0.148193000
6	-2.404388000	-0.026913000	2.878461000
1	-2.789158000	0.662070000	3.636009000
1	-3.151129000	-0.808355000	2.730197000
1	-1.506687000	-0.497898000	3.288156000
6	-3.672085000	-2.236698000	0.332268000
1	-4.332525000	-1.609930000	0.935477000
1	-4.297557000	-2.955682000	-0.203631000
1	-3.023667000	-2.799409000	1.009141000
6	-0.719690000	2.209629000	1.784273000
1	0.206873000	1.739036000	2.128573000
1	-0.466692000	2.881048000	0.959695000
1	-1.102980000	2.822590000	2.604935000
6	2.613813000	-0.649557000	0.174992000
6	3.438201000	-0.895318000	-0.919118000
6	3.134145000	-0.799372000	1.456195000
6	4.759575000	-1.257007000	-0.733841000

1	3.027150000	-0.786705000	-1.917631000
6	4.455994000	-1.170307000	1.638292000
1	2.494750000	-0.595685000	2.309522000
6	5.276040000	-1.394413000	0.545624000
1	5.390694000	-1.438978000	-1.596248000
1	4.848475000	-1.276381000	2.643157000
1	6.311750000	-1.678685000	0.688622000

3Si-T (T.E.= -1630.544869)

6	-0.725562000	0.735537000	-1.211773000
6	-1.460184000	-0.131781000	-0.150773000
1	-0.807730000	0.275999000	-2.206450000
1	-1.221128000	1.711283000	-1.278979000
14	-0.015842000	-1.303608000	0.284720000
7	1.351372000	-0.299644000	-0.213468000
5	0.826879000	0.883651000	-0.848413000
7	1.530577000	2.093147000	-1.040639000
6	0.970718000	3.202137000	-1.776710000
1	0.583813000	3.980281000	-1.102151000
1	1.736931000	3.667499000	-2.406388000
1	0.162040000	2.879542000	-2.430303000
6	2.746603000	2.465374000	-0.355293000
1	2.602671000	3.429006000	0.149105000
1	3.017244000	1.732923000	0.402713000
1	3.593245000	2.577465000	-1.044017000
14	-2.852775000	-1.178767000	-0.868893000
14	-1.822824000	0.890873000	1.400504000
6	-2.357655000	-1.835115000	-2.551961000
1	-1.381931000	-2.327322000	-2.513485000
1	-3.096249000	-2.571665000	-2.879756000
1	-2.316786000	-1.049398000	-3.309592000
6	-4.399613000	-0.143605000	-1.097788000
1	-5.143302000	-0.705763000	-1.668487000
1	-4.854636000	0.144252000	-0.147502000
1	-4.171489000	0.770199000	-1.654060000
6	-2.920907000	2.356353000	0.977669000
1	-3.896008000	2.065893000	0.584349000
1	-3.086599000	2.945085000	1.884485000
1	-2.440906000	3.013608000	0.247500000
6	-2.663139000	-0.141307000	2.715156000

1	-2.727228000	0.435519000	3.641516000
1	-3.679537000	-0.423188000	2.430507000
1	-2.099224000	-1.054229000	2.926479000
6	-3.230073000	-2.642783000	0.235933000
1	-3.589514000	-2.346560000	1.222428000
1	-4.000250000	-3.264336000	-0.228462000
1	-2.342465000	-3.268707000	0.372668000
6	-0.263614000	1.643746000	2.127901000
1	0.480901000	0.897125000	2.416831000
1	0.207803000	2.351345000	1.438785000
1	-0.545242000	2.201690000	3.025953000
6	2.677478000	-0.686802000	0.014154000
6	3.640128000	-0.571810000	-0.987850000
6	3.052527000	-1.235124000	1.239522000
6	4.944341000	-0.966462000	-0.756375000
1	3.347944000	-0.168673000	-1.951694000
6	4.357773000	-1.636500000	1.463069000
1	2.302937000	-1.325242000	2.022645000
6	5.313088000	-1.500217000	0.469200000
1	5.679682000	-0.866346000	-1.546913000
1	4.630738000	-2.054240000	2.425577000
1	6.334954000	-1.814637000	0.644402000

4Si-S (T.E.= -1840.535173)

6	0.907781000	-0.070592000	1.538512000
6	1.351725000	-0.027397000	0.040769000
1	1.224897000	-1.002649000	2.022762000
1	1.379371000	0.721686000	2.132923000
14	-0.102906000	-0.124675000	-1.194192000
7	-1.374691000	-0.042568000	-0.027370000
14	2.418245000	-1.548427000	-0.299291000
14	2.212194000	1.612305000	-0.315539000
6	1.304674000	-3.056883000	-0.153945000
1	0.546205000	-3.074163000	-0.943181000
1	1.887818000	-3.977643000	-0.237768000
1	0.784518000	-3.082185000	0.807688000
6	3.798409000	-1.736988000	0.956309000
1	4.247647000	-2.727775000	0.842750000
1	4.585057000	-0.995404000	0.806832000
1	3.446137000	-1.649719000	1.986189000

6	3.879526000	1.730057000	0.535530000
1	4.624820000	1.109405000	0.032011000
1	4.231500000	2.764737000	0.499691000
1	3.839562000	1.424086000	1.583776000
6	2.470794000	1.940820000	-2.143158000
1	3.035032000	2.871994000	-2.250636000
1	3.030338000	1.151533000	-2.647144000
1	1.522821000	2.065787000	-2.672171000
6	3.194618000	-1.548225000	-2.004420000
1	3.983135000	-0.795706000	-2.086418000
1	3.650432000	-2.524406000	-2.191463000
1	2.463725000	-1.362201000	-2.795020000
6	1.132724000	3.010866000	0.323231000
1	0.163165000	3.026097000	-0.185286000
1	0.948460000	2.949833000	1.398306000
1	1.622500000	3.968282000	0.125353000
14	-0.964066000	0.011607000	1.677718000
6	-1.621433000	1.556759000	2.490971000
1	-1.306735000	2.459271000	1.963303000
1	-2.713699000	1.543260000	2.524871000
1	-1.260803000	1.622827000	3.520897000
6	-1.683295000	-1.470240000	2.555634000
1	-1.315987000	-2.403749000	2.121435000
1	-1.417046000	-1.461254000	3.615473000
1	-2.774239000	-1.471033000	2.487176000
6	-2.733685000	-0.048136000	-0.432721000
6	-3.409618000	1.149000000	-0.644692000
6	-3.404773000	-1.249079000	-0.636747000
6	-4.733317000	1.143566000	-1.048363000
1	-2.876450000	2.083319000	-0.497646000
6	-4.728271000	-1.251088000	-1.041927000
1	-2.867215000	-2.179171000	-0.477206000
6	-5.397995000	-0.055721000	-1.247139000
1	-5.246414000	2.083872000	-1.215309000
1	-5.238072000	-2.194109000	-1.203172000
1	-6.433369000	-0.058502000	-1.566240000

4Si-T (T.E.= -1840.459688)

6	-0.920729000	1.053855000	1.120107000
6	-1.428534000	0.022866000	0.075043000

1	-1.527089000	1.967221000	1.113392000
1	-1.009590000	0.645351000	2.135460000
14	0.025971000	-0.118312000	-1.168687000
7	1.444933000	0.394230000	-0.272019000
14	-2.884375000	0.701584000	-0.915101000
14	-1.607696000	-1.687398000	0.858800000
6	-2.571304000	2.496295000	-1.359287000
1	-1.620868000	2.611948000	-1.887726000
1	-3.370128000	2.843501000	-2.020528000
1	-2.560342000	3.153526000	-0.486558000
6	-4.459416000	0.632244000	0.099190000
1	-5.244301000	1.210939000	-0.394710000
1	-4.823622000	-0.390375000	0.220591000
1	-4.306580000	1.056817000	1.095515000
6	-2.881848000	-1.659506000	2.239508000
1	-3.899024000	-1.563954000	1.856776000
1	-2.820761000	-2.595033000	2.802406000
1	-2.708620000	-0.840298000	2.941424000
6	-2.120040000	-2.980416000	-0.393430000
1	-2.048112000	-3.971250000	0.063038000
1	-3.152470000	-2.845353000	-0.724126000
1	-1.470771000	-2.969033000	-1.273677000
6	-3.130700000	-0.249238000	-2.509539000
1	-3.388179000	-1.296139000	-2.341196000
1	-3.945970000	0.206634000	-3.078015000
1	-2.235841000	-0.215875000	-3.138596000
6	0.014275000	-2.211228000	1.641362000
1	0.836925000	-2.258481000	0.923096000
1	0.308857000	-1.544061000	2.455504000
1	-0.112618000	-3.208839000	2.071554000
14	0.902215000	1.565372000	0.916784000
6	1.788228000	1.357782000	2.546744000
1	2.016042000	0.304654000	2.727844000
1	2.721105000	1.919935000	2.603946000
1	1.137605000	1.706263000	3.353178000
6	1.016507000	3.310818000	0.276947000
1	0.516762000	3.378679000	-0.693249000
1	0.524041000	4.007910000	0.959669000
1	2.051950000	3.633993000	0.149713000
6	2.735586000	-0.088710000	-0.468406000

6	3.852884000	0.614019000	-0.006528000
6	2.960821000	-1.292005000	-1.146149000
6	5.130530000	0.118989000	-0.188661000
1	3.715910000	1.567632000	0.492212000
6	4.240461000	-1.777657000	-1.329473000
1	2.106173000	-1.850367000	-1.523575000
6	5.338536000	-1.080299000	-0.849818000
1	5.975605000	0.686998000	0.184196000
1	4.380760000	-2.715457000	-1.855732000
1	6.341484000	-1.461396000	-0.998482000

5Si-S (T.E.= -1584.588707)

6	0.558245000	-0.368212000	1.494022000
6	1.185909000	-0.088364000	0.119996000
1	0.750284000	-1.395486000	1.831161000
1	0.940390000	0.258650000	2.307189000
14	-0.228085000	-0.093798000	-1.134005000
7	-1.420989000	-0.177210000	0.161744000
14	2.396791000	-1.468866000	-0.326166000
14	1.903221000	1.666317000	0.084765000
6	1.394834000	-3.034438000	-0.597404000
1	0.802152000	-2.970608000	-1.515186000
1	2.054675000	-3.900452000	-0.694470000
1	0.708755000	-3.235840000	0.230135000
6	3.601161000	-1.784160000	1.072098000
1	4.161543000	-2.699278000	0.861834000
1	4.320482000	-0.971492000	1.184557000
1	3.096221000	-1.921845000	2.031150000
6	3.444807000	1.780712000	1.138519000
1	4.284821000	1.252407000	0.681978000
1	3.731975000	2.829466000	1.251674000
1	3.286758000	1.367186000	2.137527000
6	2.302726000	2.252263000	-1.648290000
1	2.675755000	3.278670000	-1.587655000
1	3.068303000	1.649910000	-2.138677000
1	1.420398000	2.262322000	-2.293380000
6	3.351205000	-1.105770000	-1.892719000
1	4.094210000	-0.318335000	-1.746334000
1	3.883323000	-2.007719000	-2.206178000
1	2.693078000	-0.805706000	-2.712366000

6	0.618182000	2.845199000	0.775421000
1	-0.282605000	2.868686000	0.154410000
1	0.312131000	2.602182000	1.795206000
1	1.031659000	3.857275000	0.789276000
6	-2.823641000	-0.114177000	-0.063817000
6	-3.658942000	-1.129193000	0.382397000
6	-3.357607000	0.959563000	-0.761121000
6	-5.015936000	-1.067031000	0.127742000
1	-3.236565000	-1.965422000	0.926793000
6	-4.716467000	1.013160000	-1.022174000
1	-2.700030000	1.758423000	-1.089160000
6	-5.548833000	0.001560000	-0.576882000
1	-5.663037000	-1.862201000	0.479204000
1	-5.124687000	1.854629000	-1.569464000
1	-6.612976000	0.045130000	-0.776246000
6	-0.944707000	-0.235238000	1.473686000
8	-1.637835000	-0.199558000	2.457706000

5Si-T (T.E.= -1584.506604)

6	0.598037000	-0.678554000	1.377614000
6	1.272119000	-0.144078000	0.089801000
1	0.779514000	-1.753703000	1.514666000
1	1.011517000	-0.187539000	2.266572000
14	-0.209013000	-0.391211000	-1.076644000
7	-1.469547000	-0.436536000	0.182675000
14	2.737001000	-1.244039000	-0.377294000
14	1.550438000	1.737103000	0.167287000
6	2.128183000	-2.970697000	-0.768955000
1	1.628105000	-2.993890000	-1.740219000
1	2.974614000	-3.662330000	-0.804055000
1	1.419980000	-3.346748000	-0.026315000
6	3.914998000	-1.352204000	1.074384000
1	4.701693000	-2.076048000	0.846536000
1	4.392749000	-0.396770000	1.295688000
1	3.406279000	-1.693772000	1.979089000
6	3.028284000	2.111110000	1.260231000
1	3.966355000	1.787149000	0.803921000
1	3.091659000	3.190454000	1.422456000
1	2.944472000	1.632918000	2.239512000
6	1.838617000	2.466944000	-1.528531000

1	1.967902000	3.548365000	-1.430597000
1	2.725209000	2.069426000	-2.024723000
1	0.974655000	2.292615000	-2.176298000
6	3.626389000	-0.579591000	-1.880405000
1	4.152745000	0.355212000	-1.675249000
1	4.365965000	-1.309683000	-2.218652000
1	2.930522000	-0.405009000	-2.706266000
6	0.049793000	2.562779000	0.921515000
1	-0.857455000	2.384607000	0.337315000
1	-0.137045000	2.235126000	1.947076000
1	0.222157000	3.642114000	0.947009000
6	-2.849108000	-0.283071000	-0.063990000
6	-3.818293000	-0.886603000	0.731785000
6	-3.245778000	0.461483000	-1.171313000
6	-5.156549000	-0.731317000	0.419766000
1	-3.519960000	-1.470300000	1.590605000
6	-4.586123000	0.606039000	-1.478712000
1	-2.486697000	0.945121000	-1.784003000
6	-5.549500000	0.011676000	-0.681845000
1	-5.903084000	-1.205552000	1.046465000
1	-4.876436000	1.191251000	-2.343520000
1	-6.600632000	0.123548000	-0.919583000
6	-0.913509000	-0.512456000	1.438688000
8	-1.513910000	-0.469441000	2.488347000

6Si-S (T.E.= -1662.881811)

6	0.893797000	1.061413000	-0.293215000
6	-0.509224000	1.098148000	-0.258907000
6	-1.162484000	-0.212067000	0.047126000
7	1.417877000	-0.204736000	-0.021176000
14	0.254054000	-1.472954000	0.283546000
14	-2.021709000	-0.124994000	1.734020000
14	-2.195625000	-0.823625000	-1.417244000
6	-2.527881000	-2.665678000	-1.315028000
1	-3.038535000	-2.951998000	-0.393911000
1	-3.171035000	-2.949067000	-2.153321000
1	-1.611515000	-3.256599000	-1.385503000
6	-1.205888000	-0.497266000	-2.974109000
1	-0.231024000	-0.993917000	-2.935431000
1	-1.738809000	-0.881986000	-3.847518000

1	-1.030522000	0.570065000	-3.127137000
6	-3.858768000	0.026295000	-1.568299000
1	-4.353210000	-0.331130000	-2.476106000
1	-4.510806000	-0.209433000	-0.723490000
1	-3.773956000	1.112351000	-1.641708000
6	-2.872907000	-1.741046000	2.143022000
1	-3.246077000	-1.698868000	3.169785000
1	-3.729123000	-1.923846000	1.488880000
1	-2.198077000	-2.597158000	2.066486000
6	-0.709841000	0.239367000	3.025407000
1	-0.022878000	-0.599291000	3.171195000
1	-0.119762000	1.113578000	2.734423000
1	-1.175772000	0.458036000	3.989790000
6	-3.288569000	1.248743000	1.843746000
1	-4.049367000	1.190082000	1.063857000
1	-3.792878000	1.172839000	2.811611000
1	-2.818516000	2.232581000	1.791969000
6	1.636443000	2.191272000	-0.611663000
6	0.977107000	3.375662000	-0.890838000
6	-0.407299000	3.436023000	-0.852310000
6	-1.142262000	2.303741000	-0.537588000
1	2.718381000	2.140224000	-0.647562000
1	1.551708000	4.259467000	-1.142819000
1	-0.917656000	4.366570000	-1.071125000
1	-2.225239000	2.355709000	-0.513730000
6	2.821247000	-0.406450000	0.041575000
6	3.559809000	0.126245000	1.091346000
6	3.454446000	-1.167025000	-0.929930000
6	4.921947000	-0.099208000	1.162158000
1	3.047701000	0.710017000	1.850177000
6	4.818169000	-1.398260000	-0.850408000
1	2.864602000	-1.571001000	-1.746222000
6	5.554243000	-0.862819000	0.191884000
1	5.493008000	0.314538000	1.985087000
1	5.306457000	-1.997179000	-1.610206000
1	6.621160000	-1.041931000	0.252421000

6Si-T (T.E.= -1662.799844)

6	0.795339000	1.316522000	-0.132262000
6	-0.605048000	1.185411000	0.065529000

6	-1.185609000	-0.171568000	-0.095224000
7	1.409638000	0.152847000	-0.531425000
14	0.165847000	-0.966386000	-1.271434000
14	-1.100839000	-1.143448000	1.535434000
14	-2.839838000	-0.227285000	-1.028283000
6	-3.024829000	-1.872602000	-1.905499000
1	-2.961978000	-2.731857000	-1.236104000
1	-4.003472000	-1.900279000	-2.393439000
1	-2.264736000	-1.989080000	-2.682994000
6	-2.851835000	1.107589000	-2.340721000
1	-1.922054000	1.075309000	-2.916507000
1	-3.683101000	0.930553000	-3.028313000
1	-2.960845000	2.112792000	-1.930748000
6	-4.334053000	-0.010628000	0.086705000
1	-5.234706000	-0.008533000	-0.533849000
1	-4.432229000	-0.829200000	0.803627000
1	-4.316040000	0.927377000	0.646078000
6	-1.879013000	-2.832152000	1.334165000
1	-1.757423000	-3.388319000	2.267693000
1	-2.947269000	-2.787491000	1.112757000
1	-1.384044000	-3.400332000	0.541697000
6	0.651155000	-1.386828000	2.143576000
1	1.252398000	-1.978937000	1.448192000
1	1.164230000	-0.439316000	2.321961000
1	0.608997000	-1.924181000	3.095611000
6	-2.004574000	-0.171256000	2.860590000
1	-3.056675000	-0.003587000	2.622917000
1	-1.955760000	-0.709599000	3.811050000
1	-1.530379000	0.803168000	3.004723000
6	1.414607000	2.566692000	-0.009313000
6	0.667288000	3.665955000	0.339703000
6	-0.706492000	3.549491000	0.551467000
6	-1.331839000	2.331165000	0.390988000
1	2.473880000	2.665183000	-0.210540000
1	1.148013000	4.632232000	0.436678000
1	-1.284840000	4.418633000	0.841240000
1	-2.399839000	2.248108000	0.563432000
6	2.764416000	-0.124904000	-0.449815000
6	3.319695000	-1.035728000	-1.354014000
6	3.578435000	0.391642000	0.565077000

6	4.643405000	-1.418790000	-1.244020000
1	2.706431000	-1.407591000	-2.169036000
6	4.898810000	0.005118000	0.661271000
1	3.156646000	1.063363000	1.303031000
6	5.443160000	-0.898355000	-0.241685000
1	5.054787000	-2.120790000	-1.959918000
1	5.509541000	0.403916000	1.463082000
1	6.482527000	-1.192455000	-0.161512000

7Si-S (T.E.= -924.355305)

6	-0.399829000	-0.901968000	0.000096000
6	-1.828218000	-0.419494000	0.000022000
6	-2.011723000	0.964146000	-0.000427000
7	0.421214000	0.333684000	-0.000342000
14	-0.359466000	1.872645000	-0.000508000
6	1.837724000	0.214946000	-0.000022000
6	2.543924000	0.182293000	-1.197721000
6	2.543853000	0.183788000	1.197681000
6	3.925427000	0.098058000	-1.197143000
1	1.993376000	0.237641000	-2.130606000
6	3.925394000	0.099538000	1.197218000
1	1.993327000	0.240143000	2.130498000
6	4.620204000	0.050766000	0.000104000
1	4.462024000	0.078792000	-2.138739000
1	4.461947000	0.081445000	2.138861000
1	5.701931000	-0.011535000	0.000184000
6	-2.922513000	-1.271845000	0.000449000
6	-3.305964000	1.479496000	-0.000458000
6	-4.201847000	-0.742823000	0.000426000
6	-4.398597000	0.632074000	-0.000037000
1	-2.787684000	-2.349595000	0.000788000
1	-5.057183000	-1.409121000	0.000761000
1	-5.405341000	1.034355000	-0.000075000
1	-3.458936000	2.555354000	-0.000844000
6	-0.121409000	-1.730179000	1.249125000
1	0.920751000	-2.055613000	1.276839000
1	-0.333462000	-1.148633000	2.149324000
1	-0.751407000	-2.621769000	1.261426000
6	-0.121556000	-1.731205000	-1.248338000
1	-0.751704000	-2.622677000	-1.260050000

1	-0.333371000	-1.150311000	-2.149019000
1	0.920541000	-2.056835000	-1.275682000

7Si-T (T.E.= -924.269379)

6	-0.432403000	-0.948205000	0.000054000
6	-1.850730000	-0.371727000	-0.000005000
6	-2.031218000	1.020222000	-0.000016000
7	0.505624000	0.200202000	0.000105000
14	-0.350771000	1.721103000	0.000195000
6	1.889017000	0.123452000	0.000025000
6	2.640078000	-1.058271000	0.000036000
6	2.611506000	1.327867000	-0.000016000
6	4.023623000	-1.022863000	-0.000045000
1	2.156367000	-2.022935000	0.000106000
6	3.989291000	1.354650000	-0.000096000
1	2.068204000	2.273964000	0.000027000
6	4.716468000	0.174431000	-0.000125000
1	4.565691000	-1.962136000	-0.000044000
1	4.499458000	2.311342000	-0.000138000
1	5.799087000	0.190434000	-0.000181000
6	-2.972447000	-1.184557000	-0.000024000
6	-3.311304000	1.573257000	-0.000084000
6	-4.246525000	-0.636780000	-0.000085000
6	-4.412692000	0.742070000	-0.000127000
1	-2.860659000	-2.264283000	0.000009000
1	-5.111517000	-1.289055000	-0.000097000
1	-5.409460000	1.168322000	-0.000189000
1	-3.441578000	2.649348000	-0.000108000
6	-0.264660000	-1.771689000	1.275888000
1	0.733199000	-2.196407000	1.371132000
1	-0.448571000	-1.136972000	2.145644000
1	-0.982134000	-2.593598000	1.296747000
6	-0.264577000	-1.771584000	-1.275864000
1	-0.982088000	-2.593453000	-1.296838000
1	-0.448407000	-1.136761000	-2.145559000
1	0.733277000	-2.196316000	-1.371071000

8Si-S (T.E.= -1153.213590)

6	0.507748000	-1.586780000	0.088004000
6	-0.950784000	-1.514398000	0.509058000

6	-1.474192000	-0.173075000	0.034526000
1	1.078749000	-2.250610000	0.747331000
1	0.582327000	-2.002126000	-0.929752000
1	-1.021830000	-1.601737000	1.603014000
1	-1.494598000	-2.374582000	0.096893000
14	-0.164118000	1.036155000	-0.185829000
7	1.050362000	-0.233947000	0.122704000
15	-3.129037000	0.133053000	-0.047366000
6	-4.026483000	-0.922261000	-1.210941000
1	-3.845632000	-1.968731000	-0.958322000
1	-5.100304000	-0.728749000	-1.174151000
1	-3.653285000	-0.739234000	-2.219094000
6	-4.023036000	-0.123456000	1.505729000
1	-3.631613000	0.557902000	2.262034000
1	-5.094670000	0.042556000	1.379473000
1	-3.861538000	-1.148579000	1.845224000
6	-3.491173000	1.820236000	-0.547802000
1	-3.070524000	2.520529000	0.174049000
1	-3.053437000	2.017839000	-1.526541000
1	-4.572111000	1.959671000	-0.601189000
6	2.425929000	-0.067419000	0.052079000
6	3.296711000	-1.116591000	-0.264550000
6	2.997018000	1.187714000	0.310720000
6	4.666094000	-0.912481000	-0.322791000
1	2.903989000	-2.101910000	-0.481043000
6	4.359927000	1.381705000	0.239290000
1	2.346783000	2.012937000	0.581282000
6	5.213448000	0.332875000	-0.076428000
1	5.311310000	-1.748391000	-0.571531000
1	4.764913000	2.366432000	0.446477000
1	6.284889000	0.486034000	-0.122345000

8Si-T (T.E.= -1153.123659)

6	-0.152890000	1.751506000	0.445430000
6	1.275525000	1.797965000	0.999773000
6	1.741279000	0.385200000	0.937318000
1	-0.765782000	2.569246000	0.849144000
1	-0.108647000	1.908107000	-0.645342000
1	1.248417000	2.109728000	2.050669000
1	1.875722000	2.529850000	0.446194000

14	0.334542000	-0.715304000	1.725798000
7	-0.720302000	0.449022000	0.748205000
15	2.561828000	-0.255407000	-0.449155000
6	3.707850000	0.888318000	-1.239097000
1	4.422985000	1.259059000	-0.503992000
1	4.246202000	0.389646000	-2.046640000
1	3.152611000	1.732299000	-1.651589000
6	3.495830000	-1.709645000	0.024198000
1	2.800235000	-2.423557000	0.470780000
1	3.970547000	-2.152454000	-0.852918000
1	4.255146000	-1.441318000	0.759002000
6	1.410674000	-0.789257000	-1.729718000
1	0.693747000	-1.479252000	-1.277379000
1	0.872912000	0.070952000	-2.131864000
1	1.955716000	-1.288600000	-2.533174000
6	-1.965601000	0.166930000	0.239009000
6	-2.536051000	-1.106968000	0.426701000
6	-2.722704000	1.103608000	-0.486205000
6	-3.783295000	-1.413548000	-0.071923000
1	-1.969252000	-1.856059000	0.970108000
6	-3.975222000	0.780070000	-0.979529000
1	-2.337200000	2.099672000	-0.661298000
6	-4.522254000	-0.475658000	-0.782054000
1	-4.187704000	-2.406179000	0.096251000
1	-4.530662000	1.531476000	-1.531149000
1	-5.502731000	-0.721535000	-1.171505000

9Si-S (T.E.= -1152.036609)

6	0.451976000	-1.430098000	0.486395000
6	-0.899352000	-1.434510000	0.454340000
6	-1.463450000	-0.170190000	0.060845000
14	-0.158163000	1.063668000	-0.270212000
7	1.030211000	-0.215605000	0.159512000
15	-3.140081000	0.077660000	-0.051997000
6	-3.969679000	-1.065306000	-1.174676000
1	-3.777061000	-2.087851000	-0.845232000
1	-5.046960000	-0.890442000	-1.190760000
1	-3.559599000	-0.941133000	-2.177287000
6	-3.534087000	1.729824000	-0.632995000
1	-4.616995000	1.857175000	-0.668761000

1	-3.104089000	2.469977000	0.042482000
1	-3.119083000	1.879380000	-1.630028000
6	-4.019755000	-0.126792000	1.510805000
1	-3.645107000	0.602809000	2.229319000
1	-5.095489000	0.003238000	1.378485000
1	-3.823750000	-1.127688000	1.899613000
6	2.424840000	-0.084754000	0.070162000
6	3.229875000	-1.127356000	-0.386903000
6	3.034617000	1.117030000	0.427647000
6	4.601760000	-0.970557000	-0.475130000
1	2.770601000	-2.058348000	-0.698901000
6	4.404035000	1.272185000	0.321463000
1	2.416447000	1.925272000	0.803397000
6	5.199378000	0.228645000	-0.124952000
1	5.208245000	-1.794445000	-0.834806000
1	4.855781000	2.215914000	0.606174000
1	6.273637000	0.348938000	-0.197956000
1	1.079474000	-2.261251000	0.785250000
1	-1.472976000	-2.317296000	0.723344000

9Si-T (T.E.= -1151.955778)

6	-0.473241000	1.469862000	-0.314561000
6	0.922884000	1.472572000	-0.267275000
6	1.518748000	0.245274000	-0.071470000
14	0.167158000	-1.176100000	-0.188285000
7	-1.083879000	0.283046000	-0.131568000
15	3.190857000	-0.036259000	0.081822000
6	3.763014000	-1.246525000	-1.122070000
1	3.630279000	-0.849834000	-2.128872000
1	4.812596000	-1.494182000	-0.954657000
1	3.155687000	-2.148750000	-1.023688000
6	3.591206000	-0.764534000	1.679790000
1	4.631750000	-1.091718000	1.713813000
1	3.406062000	-0.035478000	2.468946000
1	2.931792000	-1.621101000	1.836520000
6	4.216588000	1.427701000	-0.107488000
1	3.958442000	2.162526000	0.655589000
1	5.268418000	1.158025000	-0.001782000
1	4.056984000	1.864228000	-1.094073000
6	-2.452196000	0.134399000	-0.036874000

6	-3.002025000	-1.155780000	-0.107311000
6	-3.331804000	1.212940000	0.149794000
6	-4.365818000	-1.350351000	-0.009045000
1	-2.341021000	-2.002253000	-0.258425000
6	-4.691441000	1.002537000	0.243960000
1	-2.947235000	2.220408000	0.252268000
6	-5.226402000	-0.277852000	0.162712000
1	-4.761463000	-2.358163000	-0.072563000
1	-5.346946000	1.853207000	0.395928000
1	-6.295674000	-0.433464000	0.239112000
1	-1.048118000	2.369138000	-0.508736000
1	1.455445000	2.413911000	-0.390710000

10Si-S (T.E.= -1305.580320)

6	0.493348000	1.017467000	-0.096632000
6	-0.921866000	0.967969000	-0.056293000
6	-1.423109000	-0.385727000	0.020837000
14	-0.067629000	-1.604403000	0.037217000
7	1.077696000	-0.242329000	-0.054807000
6	1.157607000	2.232384000	-0.216517000
6	0.432797000	3.410507000	-0.271353000
6	-0.953997000	3.384061000	-0.211706000
6	-1.621385000	2.176231000	-0.109801000
1	2.239784000	2.255245000	-0.273325000
1	0.954546000	4.356086000	-0.364513000
1	-1.517461000	4.309341000	-0.251872000
1	-2.707546000	2.180507000	-0.077325000
15	-3.071550000	-0.794224000	0.079231000
6	-3.964633000	-0.128913000	1.500837000
1	-3.869639000	0.956886000	1.523912000
1	-5.021597000	-0.397282000	1.454046000
1	-3.523757000	-0.532374000	2.413036000
6	-3.300280000	-2.574072000	0.167131000
1	-4.367781000	-2.793289000	0.224882000
1	-2.883510000	-3.048183000	-0.721838000
1	-2.799179000	-2.974842000	1.048485000
6	-4.037391000	-0.273270000	-1.355353000
1	-3.623224000	-0.745975000	-2.246728000
1	-5.083547000	-0.562926000	-1.239041000
1	-3.973800000	0.808199000	-1.477399000

6	2.478076000	-0.414948000	-0.005921000
6	3.241726000	0.146459000	1.014634000
6	3.107792000	-1.205775000	-0.960165000
6	4.605474000	-0.072649000	1.068605000
1	2.749850000	0.746398000	1.772490000
6	4.472126000	-1.434826000	-0.894393000
1	2.510686000	-1.636307000	-1.756710000
6	5.227481000	-0.865435000	0.115500000
1	5.186542000	0.368997000	1.870267000
1	4.947216000	-2.056772000	-1.644465000
1	6.296002000	-1.039181000	0.163777000

10Si-T (T.E.= -1305.485019)

6	-0.497933000	1.019111000	-0.166651000
6	0.939157000	0.946491000	-0.016863000
6	1.425491000	-0.359223000	0.122095000
14	0.045688000	-1.602079000	-0.520643000
7	-1.122142000	-0.188368000	-0.136048000
6	-1.107347000	2.261046000	-0.387343000
6	-0.354365000	3.412921000	-0.396322000
6	1.036161000	3.366732000	-0.216583000
6	1.667244000	2.163390000	-0.052995000
1	-2.175459000	2.309152000	-0.557268000
1	-0.841067000	4.367249000	-0.561901000
1	1.611752000	4.284729000	-0.231685000
1	2.747339000	2.143685000	0.050871000
15	3.076965000	-0.804100000	0.194544000
6	4.023744000	-0.465896000	-1.305511000
1	4.044146000	0.606013000	-1.503424000
1	5.045073000	-0.839498000	-1.210429000
1	3.526171000	-0.963787000	-2.140140000
6	3.192499000	-2.576641000	0.438537000
1	4.236528000	-2.870848000	0.555783000
1	2.624091000	-2.859124000	1.325643000
1	2.767499000	-3.090515000	-0.425785000
6	3.993982000	-0.051258000	1.550586000
1	3.513776000	-0.312286000	2.493872000
1	5.020523000	-0.423074000	1.548291000
1	4.006123000	1.033403000	1.452165000
6	-2.496389000	-0.362450000	-0.005636000

6	-3.118469000	-1.415582000	-0.681783000
6	-3.270528000	0.421859000	0.854767000
6	-4.469742000	-1.661591000	-0.514364000
1	-2.529540000	-2.022251000	-1.362178000
6	-4.618759000	0.169696000	1.013175000
1	-2.796431000	1.211816000	1.425532000
6	-5.231685000	-0.869894000	0.326729000
1	-4.931300000	-2.479789000	-1.055877000
1	-5.196522000	0.784808000	1.694219000
1	-6.290187000	-1.062765000	0.454463000

11Si-S (T.E.= -1305.827806)

6	0.468082000	1.252670000	-0.000112000
6	-1.061164000	1.111829000	-0.000108000
6	-1.497432000	-0.246844000	-0.000117000
7	1.012510000	-0.114949000	-0.000201000
6	2.416942000	-0.296623000	-0.000073000
6	3.118616000	-0.408380000	-1.196885000
6	4.488414000	-0.608453000	-1.196895000
6	5.178669000	-0.703909000	0.000220000
6	4.488163000	-0.608424000	1.197188000
6	3.118366000	-0.408349000	1.196886000
1	5.018049000	-0.697716000	-2.138648000
1	6.250654000	-0.863058000	0.000334000
1	5.017602000	-0.697654000	2.139055000
6	0.876144000	2.018638000	-1.248681000
1	1.957544000	2.173238000	-1.275162000
1	0.580933000	1.473067000	-2.149220000
1	0.383628000	2.992411000	-1.254948000
6	0.876212000	2.018438000	1.248553000
1	0.383701000	2.992212000	1.254999000
1	0.581051000	1.472726000	2.149024000
1	1.957616000	2.173026000	1.274999000
15	-3.186014000	-0.509898000	0.000040000
6	-4.030579000	0.181112000	-1.430935000
1	-5.105123000	0.000013000	-1.366605000
1	-3.836989000	1.253493000	-1.459555000
1	-3.634891000	-0.278710000	-2.337038000
6	-3.552991000	-2.267775000	-0.000229000
1	-3.122638000	-2.735577000	0.886128000

1	-4.633579000	-2.418687000	-0.000135000
1	-3.122840000	-2.735242000	-0.886862000
6	-4.030255000	0.180606000	1.431452000
1	-3.836755000	1.252996000	1.460363000
1	-5.104801000	-0.000560000	1.367350000
1	-3.634291000	-0.279465000	2.337307000
1	2.568721000	-0.344625000	-2.129824000
1	2.568275000	-0.344534000	2.129709000
8	-1.772114000	2.117481000	0.000210000
14	-0.107102000	-1.440094000	-0.000267000

11Si-T (T.E.= -1305.728575)

6	-0.446753000	1.333126000	0.000107000
6	1.084317000	1.110572000	0.000087000
6	1.525524000	-0.235050000	-0.000225000
7	-1.102820000	0.005953000	0.000102000
6	-2.463433000	-0.220911000	0.000175000
6	-2.903670000	-1.556908000	0.000374000
6	-4.242935000	-1.884232000	0.000426000
6	-5.211433000	-0.892282000	0.000251000
6	-4.798376000	0.429295000	0.000014000
6	-3.456664000	0.767815000	-0.000028000
1	-4.532289000	-2.929304000	0.000604000
1	-6.264323000	-1.145553000	0.000280000
1	-5.534395000	1.225987000	-0.000153000
6	-0.760346000	2.113966000	1.272043000
1	-1.812737000	2.382310000	1.350171000
1	-0.498047000	1.514286000	2.147786000
1	-0.166902000	3.028754000	1.287354000
6	-0.760401000	2.113940000	-1.271834000
1	-0.167064000	3.028800000	-1.287158000
1	-0.498044000	1.514277000	-2.147574000
1	-1.812830000	2.382160000	-1.349958000
15	3.202589000	-0.549625000	-0.000204000
6	4.057073000	0.112539000	1.434994000
1	5.125620000	-0.101439000	1.373263000
1	3.895670000	1.190197000	1.463612000
1	3.642484000	-0.336625000	2.337900000
6	3.473913000	-2.322687000	-0.001163000
1	3.014545000	-2.758542000	-0.889809000

1	4.542485000	-2.541081000	-0.001191000
1	3.014414000	-2.759472000	0.886963000
6	4.057387000	0.114302000	-1.434400000
1	3.895798000	1.191967000	-1.461781000
1	5.125953000	-0.099571000	-1.372602000
1	3.643125000	-0.333861000	-2.337950000
1	-2.162213000	-2.357940000	0.000557000
1	-3.191060000	1.814130000	-0.000265000
8	1.838312000	2.089995000	0.000243000
14	0.056357000	-1.309117000	-0.000327000

12Si-S (T.E.= -1305.824553)

6	0.626872000	1.280217000	-0.130567000
6	-0.904771000	1.279185000	-0.240659000
6	-1.377799000	-0.147817000	-0.036060000
7	1.146519000	0.009132000	-0.030825000
6	2.547956000	-0.189718000	0.016418000
6	3.133110000	-1.107006000	-0.847333000
6	4.493897000	-1.354988000	-0.790914000
6	5.285997000	-0.680887000	0.122376000
6	4.705619000	0.238031000	0.982588000
6	3.345448000	0.482330000	0.936017000
1	4.936114000	-2.075171000	-1.469697000
1	6.352205000	-0.870259000	0.164882000
1	5.318363000	0.768555000	1.702553000
15	-2.992800000	-0.630816000	0.131141000
6	-4.134968000	-0.079294000	-1.159791000
1	-5.117264000	-0.529820000	-1.003614000
1	-4.240504000	1.005911000	-1.131233000
1	-3.749420000	-0.369928000	-2.137610000
6	-3.140386000	-2.424992000	0.128798000
1	-2.566934000	-2.857318000	0.948945000
1	-4.192164000	-2.688567000	0.252614000
1	-2.773795000	-2.832885000	-0.812957000
6	-3.839698000	-0.133508000	1.654531000
1	-3.913968000	0.952262000	1.713370000
1	-4.844710000	-0.559988000	1.682944000
1	-3.266843000	-0.491297000	2.511012000
1	2.508127000	-1.621790000	-1.569583000
1	2.891337000	1.194907000	1.612624000

8	1.276924000	2.301629000	-0.176210000
6	-1.446999000	2.268759000	0.785427000
1	-0.958900000	3.238741000	0.669834000
1	-2.522760000	2.417143000	0.650143000
1	-1.275329000	1.912301000	1.804458000
6	-1.208930000	1.794375000	-1.651241000
1	-0.825480000	1.101403000	-2.404243000
1	-2.285021000	1.900947000	-1.803662000
1	-0.744854000	2.771367000	-1.806220000
14	-0.042093000	-1.337811000	0.104731000

12Si-T (T.E.= -1305.735428)

6	0.355761000	1.293878000	-0.292047000
6	-1.093099000	1.551847000	0.216901000
6	-1.555933000	0.203372000	0.662621000
7	0.920423000	0.206084000	0.304041000
6	2.273715000	-0.119748000	0.056903000
6	2.619905000	-1.453810000	-0.130199000
6	3.939850000	-1.818002000	-0.330523000
6	4.933528000	-0.854368000	-0.349063000
6	4.593310000	0.476073000	-0.159775000
6	3.276910000	0.845819000	0.044381000
1	4.190715000	-2.862676000	-0.476108000
1	5.967766000	-1.136948000	-0.507090000
1	5.364199000	1.238466000	-0.166267000
15	-2.636450000	-0.848832000	-0.201137000
6	-1.784939000	-1.644946000	-1.575192000
1	-2.403373000	-2.438349000	-1.998620000
1	-1.556328000	-0.906893000	-2.345709000
1	-0.852955000	-2.067597000	-1.190673000
6	-3.174470000	-2.154426000	0.906178000
1	-3.698901000	-1.719342000	1.757943000
1	-3.843474000	-2.831600000	0.372131000
1	-2.299738000	-2.699505000	1.265502000
6	-4.164696000	-0.155590000	-0.865435000
1	-3.961807000	0.524911000	-1.690249000
1	-4.794757000	-0.973100000	-1.220815000
1	-4.693592000	0.383781000	-0.078671000
1	1.833627000	-2.202456000	-0.112987000
1	3.015866000	1.885084000	0.194596000

8	0.869150000	2.021692000	-1.117750000
6	-0.968536000	2.511963000	1.409094000
1	-0.471938000	3.430223000	1.086659000
1	-1.961225000	2.768783000	1.786380000
1	-0.396366000	2.065892000	2.225791000
6	-1.898787000	2.233635000	-0.874767000
1	-1.961110000	1.623161000	-1.780204000
1	-2.909150000	2.456370000	-0.522903000
1	-1.422628000	3.172549000	-1.158415000
14	-0.079240000	-0.720613000	1.576859000

13Si-S (T.E.= -1347.354555)

6	0.734374000	1.235795000	0.036571000
6	-1.298790000	-0.378076000	-0.068497000
7	1.316194000	-0.030729000	-0.051132000
6	2.720058000	-0.196913000	-0.028784000
6	3.330814000	-0.973054000	-1.007411000
6	4.697756000	-1.190584000	-0.982868000
6	5.474384000	-0.623852000	0.012560000
6	4.870604000	0.155778000	0.987259000
6	3.504257000	0.366770000	0.973085000
1	5.157050000	-1.800966000	-1.752080000
1	6.545539000	-0.787564000	0.030440000
1	5.470410000	0.601686000	1.772655000
15	-2.773230000	-1.182890000	0.140440000
6	-3.835274000	-1.355566000	-1.318625000
1	-4.742937000	-1.907578000	-1.065526000
1	-4.110898000	-0.388617000	-1.736625000
1	-3.278073000	-1.908704000	-2.076808000
6	-2.572435000	-2.903234000	0.651697000
1	-2.039554000	-2.955116000	1.601608000
1	-3.560058000	-3.354071000	0.766145000
1	-2.008509000	-3.464314000	-0.094127000
6	-3.836434000	-0.495080000	1.429444000
1	-4.106713000	0.535324000	1.204289000
1	-4.744432000	-1.093221000	1.527981000
1	-3.288258000	-0.511742000	2.372417000
1	2.719956000	-1.401775000	-1.795045000
1	3.033680000	0.968277000	1.740073000
8	1.406036000	2.244745000	0.146423000

5	-0.888383000	1.098250000	-0.083720000
7	-1.675357000	2.260593000	-0.235158000
6	-1.191847000	3.621482000	-0.094162000
1	-0.141515000	3.631784000	0.177868000
1	-1.321750000	4.172469000	-1.033342000
1	-1.773175000	4.147018000	0.673365000
6	-3.075667000	2.265505000	-0.567278000
1	-3.417612000	1.277968000	-0.863604000
1	-3.692906000	2.619524000	0.269836000
1	-3.262461000	2.942196000	-1.409325000
14	0.195546000	-1.415093000	-0.093108000

¹³Si-T (T.E.= -1347.264565)

6	0.703790000	1.251960000	-0.191065000
6	-1.325651000	-0.373342000	0.179636000
7	1.361337000	0.027422000	0.008552000
6	2.756308000	-0.152801000	0.004358000
6	3.257913000	-1.417077000	-0.306398000
6	4.615207000	-1.675203000	-0.266562000
6	5.504007000	-0.669767000	0.073350000
6	5.012587000	0.589001000	0.380282000
6	3.655272000	0.854284000	0.352125000
1	4.978372000	-2.666569000	-0.512668000
1	6.569697000	-0.864474000	0.097833000
1	5.697565000	1.383937000	0.653665000
15	-2.780321000	-1.211789000	-0.030986000
6	-3.845998000	-0.513099000	-1.306315000
1	-4.730237000	-1.140890000	-1.431692000
1	-4.158687000	0.494790000	-1.036963000
1	-3.291303000	-0.470414000	-2.244013000
6	-2.495899000	-2.914136000	-0.550731000
1	-1.930054000	-3.445106000	0.217821000
1	-3.451291000	-3.420364000	-0.699913000
1	-1.922190000	-2.922103000	-1.478202000
6	-3.842021000	-1.409789000	1.420957000
1	-4.181278000	-0.443153000	1.791961000
1	-4.711451000	-2.023022000	1.174536000
1	-3.264818000	-1.899583000	2.206828000
1	2.562114000	-2.196846000	-0.612086000
1	3.282315000	1.837835000	0.594127000

8	1.321843000	2.273036000	-0.464717000
5	-0.888829000	1.088049000	0.018453000
7	-1.729701000	2.233316000	0.067620000
6	-1.366644000	3.541721000	-0.435033000
1	-0.359607000	3.529284000	-0.840954000
1	-2.071387000	3.860064000	-1.214628000
1	-1.411960000	4.289595000	0.366849000
6	-3.046657000	2.246340000	0.639777000
1	-3.833965000	2.393817000	-0.114408000
1	-3.244690000	1.323727000	1.183642000
1	-3.140726000	3.074142000	1.353856000
14	0.233789000	-1.294006000	0.295369000

14Si-S (T.E.= -1347.372554)

6	1.194731000	1.032195000	0.103260000
6	1.645395000	-0.332384000	-0.027699000
7	-0.948504000	-0.267052000	-0.120462000
6	-2.297465000	-0.644724000	0.018656000
6	-3.045659000	-0.209258000	1.111106000
6	-4.369072000	-0.581157000	1.253984000
6	-4.969184000	-1.412995000	0.320528000
6	-4.227983000	-1.867409000	-0.756819000
6	-2.905197000	-1.486500000	-0.909237000
1	-2.570267000	0.436182000	1.842669000
1	-4.935627000	-0.225437000	2.107280000
1	-6.005891000	-1.706565000	0.434857000
1	-4.683841000	-2.519663000	-1.493279000
1	-2.329501000	-1.826028000	-1.764004000
5	-0.418187000	1.081972000	-0.073384000
7	-1.141224000	2.270592000	-0.270783000
6	-0.573659000	3.582108000	-0.031648000
1	-0.586540000	4.181502000	-0.950062000
1	-1.169301000	4.120202000	0.716153000
1	0.452734000	3.494133000	0.316397000
6	-2.502031000	2.366153000	-0.747941000
1	-3.184858000	2.710868000	0.039372000
1	-2.551118000	3.094655000	-1.564917000
1	-2.869496000	1.414029000	-1.123191000
15	3.330591000	-0.615164000	0.046257000
6	4.093145000	-0.105765000	1.595514000

1	5.170682000	-0.279038000	1.569435000
1	3.890908000	0.955057000	1.741985000
1	3.651083000	-0.671243000	2.416356000
6	4.264211000	0.225229000	-1.243431000
1	5.331069000	0.017446000	-1.141408000
1	3.916111000	-0.117267000	-2.218451000
1	4.085654000	1.296630000	-1.155699000
6	3.703105000	-2.364011000	-0.136090000
1	3.232789000	-2.931066000	0.668128000
1	3.322318000	-2.728309000	-1.091010000
1	4.783378000	-2.513453000	-0.096954000
8	1.956558000	1.992598000	0.285906000
14	0.292529000	-1.539964000	-0.173587000

14Si-T (T.E.= -1347.284273)

6	1.166565000	1.007422000	0.111393000
6	1.645488000	-0.350616000	-0.020862000
7	-0.987785000	-0.230848000	-0.231956000
6	-2.320674000	-0.614265000	-0.025064000
6	-3.114957000	0.007546000	0.938762000
6	-4.409940000	-0.418503000	1.163234000
6	-4.940332000	-1.481721000	0.447362000
6	-4.154949000	-2.114664000	-0.500214000
6	-2.861207000	-1.683482000	-0.738800000
1	-2.694625000	0.822301000	1.517942000
1	-5.008934000	0.078373000	1.918254000
1	-5.955202000	-1.813924000	0.630175000
1	-4.552560000	-2.947953000	-1.068541000
1	-2.254229000	-2.157714000	-1.505825000
5	-0.406630000	1.104097000	-0.123177000
7	-1.110504000	2.313571000	-0.310765000
6	-0.573291000	3.594201000	0.091052000
1	-0.529186000	4.280337000	-0.763940000
1	-1.214396000	4.061445000	0.850117000
1	0.430401000	3.473262000	0.494440000
6	-2.405924000	2.433381000	-0.930980000
1	-3.178778000	2.743225000	-0.214203000
1	-2.368809000	3.193709000	-1.720260000
1	-2.722676000	1.492579000	-1.378459000
15	3.332841000	-0.632732000	0.083314000

6	4.035082000	-0.177852000	1.673444000
1	5.113225000	-0.348284000	1.678659000
1	3.822161000	0.876401000	1.848882000
1	3.564208000	-0.774850000	2.454892000
6	4.285578000	0.247809000	-1.160339000
1	5.350832000	0.042934000	-1.038977000
1	3.959567000	-0.070960000	-2.150871000
1	4.091926000	1.313872000	-1.043668000
6	3.678023000	-2.379632000	-0.149184000
1	3.166249000	-2.959209000	0.620208000
1	3.319665000	-2.695279000	-1.130129000
1	4.752244000	-2.557701000	-0.081605000
8	1.986326000	1.934662000	0.312680000
14	0.255007000	-1.468298000	-0.332295000

1Ge-S (T.E.= -3298.002081)

6	-0.906280000	0.472034000	1.600402000
6	0.538151000	0.038241000	1.712647000
6	1.201131000	-0.014576000	0.316597000
1	-1.464118000	0.218343000	2.509581000
1	-0.977392000	1.565218000	1.485770000
1	0.551389000	-0.959869000	2.165430000
1	1.074838000	0.694974000	2.407263000
32	-0.265479000	-0.676917000	-0.890797000
7	-1.480569000	-0.208821000	0.450822000
14	1.608676000	1.720383000	-0.322744000
14	2.631388000	-1.233371000	0.299608000
6	2.075921000	-2.838633000	1.105500000
1	1.140791000	-3.207196000	0.671617000
1	2.838551000	-3.604967000	0.942105000
1	1.930240000	-2.745905000	2.183427000
6	3.184143000	-1.691279000	-1.432611000
1	3.653817000	-0.866539000	-1.968515000
1	3.915449000	-2.501385000	-1.361930000
1	2.350075000	-2.056335000	-2.038470000
6	4.100976000	-0.588848000	1.270846000
1	3.800678000	-0.284878000	2.277649000
1	4.860104000	-1.369058000	1.372543000
1	4.570851000	0.270275000	0.785626000
6	2.857745000	1.713657000	-1.719021000

1	2.502312000	1.116983000	-2.563677000
1	2.979862000	2.742066000	-2.071039000
1	3.841805000	1.341915000	-1.428113000
6	0.103517000	2.590318000	-1.053073000
1	-0.752508000	2.637036000	-0.376304000
1	0.385559000	3.617582000	-1.303438000
1	-0.231196000	2.119135000	-1.982726000
6	2.251295000	2.795389000	1.072162000
1	1.469677000	3.026558000	1.799648000
1	3.081803000	2.330562000	1.607643000
1	2.605670000	3.743437000	0.658090000
6	-2.864772000	-0.178401000	0.277740000
6	-3.485045000	-1.096734000	-0.576454000
6	-3.671887000	0.753699000	0.933988000
6	-4.847857000	-1.063502000	-0.784770000
1	-2.879573000	-1.852081000	-1.067067000
6	-5.041130000	0.774258000	0.724132000
1	-3.227393000	1.478278000	1.604670000
6	-5.640473000	-0.126229000	-0.136928000
1	-5.300202000	-1.788613000	-1.451986000
1	-5.643398000	1.510891000	1.244286000
1	-6.711869000	-0.107891000	-0.295372000

1Ge-T (T.E.= -3297.925808)

6	-0.637830000	-1.468691000	1.441408000
6	1.041728000	0.023315000	0.282622000
6	0.327600000	-0.307980000	1.621563000
1	-1.275059000	-1.628268000	2.313976000
1	-0.078445000	-2.394933000	1.260460000
1	1.029876000	-0.534859000	2.434744000
1	-0.263054000	0.546735000	1.981420000
32	0.062803000	-0.962669000	-1.286279000
7	-1.377000000	-1.187259000	0.231571000
14	2.764700000	-0.705494000	0.257683000
14	0.903108000	1.859072000	-0.044158000
6	1.834272000	2.393941000	-1.581339000
1	1.544599000	1.798263000	-2.451733000
1	1.605073000	3.440320000	-1.800751000
1	2.916688000	2.312394000	-1.454868000
6	1.550861000	2.875270000	1.404072000

1	2.634474000	2.793653000	1.507317000
1	1.307433000	3.930896000	1.252785000
1	1.102431000	2.568992000	2.353028000
6	-0.894731000	2.373403000	-0.271468000
1	-1.532199000	2.083333000	0.569083000
1	-0.947303000	3.462427000	-0.360942000
1	-1.318171000	1.937646000	-1.180543000
6	2.742378000	-2.473254000	0.898210000
1	2.092718000	-3.102576000	0.283072000
1	3.754360000	-2.885539000	0.851509000
1	2.409276000	-2.542882000	1.936834000
6	3.952581000	0.253933000	1.356866000
1	4.893054000	-0.294414000	1.461215000
1	4.184008000	1.235674000	0.936496000
1	3.542002000	0.407555000	2.358819000
6	3.499371000	-0.762797000	-1.467801000
1	3.594278000	0.224966000	-1.921656000
1	4.499953000	-1.201301000	-1.411301000
1	2.905338000	-1.389920000	-2.138692000
6	-2.621941000	-0.717431000	0.225935000
6	-3.230511000	-0.449923000	-1.034409000
6	-3.367273000	-0.417200000	1.400569000
6	-4.480147000	0.107431000	-1.106341000
1	-2.671298000	-0.696843000	-1.930329000
6	-4.613231000	0.145351000	1.304350000
1	-2.935305000	-0.595597000	2.376095000
6	-5.180175000	0.413980000	0.058040000
1	-4.925239000	0.306825000	-2.073542000
1	-5.160283000	0.390399000	2.206855000
1	-6.166917000	0.857091000	-0.002450000

2Ge-S (T.E.= -3296.819575)

6	1.160636000	0.020105000	0.272281000
6	0.479656000	0.201119000	1.576070000
6	-0.859238000	0.133402000	1.582194000
1	1.030867000	0.360060000	2.499051000
1	-1.471265000	0.224684000	2.473819000
32	-0.283273000	-0.298991000	-1.079470000
7	-1.483373000	-0.123347000	0.373988000
14	2.299409000	-1.481276000	0.316765000

14	1.961209000	1.673230000	-0.183479000
6	2.816705000	-2.014395000	-1.403778000
1	3.494102000	-2.869438000	-1.325894000
1	1.956290000	-2.329499000	-2.000354000
1	3.336058000	-1.228385000	-1.954278000
6	2.988122000	2.333532000	1.236161000
1	3.780935000	1.647154000	1.538109000
1	3.455123000	3.273987000	0.930442000
1	2.365778000	2.542229000	2.109082000
6	3.039964000	1.538912000	-1.708826000
1	2.500717000	1.098493000	-2.552074000
1	3.362352000	2.540149000	-2.007789000
1	3.938519000	0.943155000	-1.532790000
6	0.615960000	2.935726000	-0.530362000
1	0.129261000	2.761092000	-1.493905000
1	-0.152137000	2.920994000	0.247897000
1	1.043428000	3.941867000	-0.555980000
6	3.839425000	-1.167763000	1.338466000
1	4.372762000	-2.110481000	1.489851000
1	4.526760000	-0.474180000	0.848025000
1	3.595943000	-0.761738000	2.323693000
6	1.364672000	-2.901151000	1.103774000
1	1.971950000	-3.809990000	1.082685000
1	1.114203000	-2.686689000	2.144689000
1	0.431571000	-3.110586000	0.572357000
6	-2.882575000	-0.084359000	0.262051000
6	-3.532013000	-0.959725000	-0.605641000
6	-3.643702000	0.835507000	0.981072000
6	-4.904995000	-0.909357000	-0.756093000
1	-2.945492000	-1.693346000	-1.149134000
6	-5.018929000	0.869519000	0.837020000
1	-3.148360000	1.544445000	1.635004000
6	-5.658237000	0.001164000	-0.032188000
1	-5.392153000	-1.599507000	-1.435249000
1	-5.595006000	1.593126000	1.402609000
1	-6.735246000	0.032759000	-0.143969000

2Ge-T (T.E.= -3296.757434)

6	1.234983000	0.007376000	0.323765000
6	0.548269000	-0.038596000	1.599072000

6	-0.829557000	-0.108314000	1.643283000
1	1.088910000	-0.072228000	2.545772000
1	-1.379027000	-0.045551000	2.580748000
32	-0.125883000	-1.035198000	-0.916028000
7	-1.469828000	-0.329373000	0.497098000
14	2.873769000	-0.928525000	0.363908000
14	1.237154000	1.770565000	-0.377435000
6	3.344544000	-1.512104000	-1.351836000
1	4.284228000	-2.068635000	-1.296595000
1	2.586297000	-2.190403000	-1.754001000
1	3.481307000	-0.696380000	-2.062732000
6	2.100586000	2.916631000	0.833803000
1	3.161112000	2.690087000	0.952269000
1	2.013394000	3.952766000	0.495448000
1	1.629256000	2.847989000	1.818540000
6	2.117906000	1.812915000	-2.026918000
1	1.640505000	1.138670000	-2.743229000
1	2.066880000	2.826226000	-2.434217000
1	3.172285000	1.540402000	-1.945861000
6	-0.485688000	2.469726000	-0.605331000
1	-1.077510000	1.903909000	-1.329230000
1	-1.038917000	2.511403000	0.336193000
1	-0.386579000	3.494757000	-0.975122000
6	4.266733000	0.094558000	1.089072000
1	5.149417000	-0.532900000	1.237988000
1	4.552291000	0.925373000	0.440060000
1	3.983050000	0.508936000	2.060700000
6	2.634489000	-2.447793000	1.434592000
1	3.493637000	-3.117065000	1.342526000
1	2.519875000	-2.194651000	2.491221000
1	1.739917000	-2.993446000	1.118600000
6	-2.839668000	-0.242937000	0.350875000
6	-3.444766000	-0.896461000	-0.727814000
6	-3.639056000	0.516279000	1.213642000
6	-4.808062000	-0.807372000	-0.924617000
1	-2.830765000	-1.496102000	-1.391938000
6	-5.000979000	0.595988000	1.007821000
1	-3.180367000	1.075302000	2.021293000
6	-5.595173000	-0.066195000	-0.057552000
1	-5.261615000	-1.326558000	-1.760740000

1	-5.606057000	1.195817000	1.677824000
1	-6.664748000	0.003455000	-0.214074000

3Ge-S (T.E.= -3418.104528)

6	0.712845000	1.068008000	-1.025784000
6	1.420703000	0.002193000	-0.142157000
1	1.195287000	2.050431000	-0.934012000
1	0.823706000	0.812278000	-2.091842000
7	-1.317868000	-0.139695000	-0.136991000
5	-0.834858000	1.110698000	-0.696095000
7	-1.619936000	2.270069000	-0.893346000
6	-1.108401000	3.421567000	-1.599014000
1	-1.864635000	3.812341000	-2.289591000
1	-0.845438000	4.235741000	-0.908969000
1	-0.226347000	3.168675000	-2.184603000
6	-2.904185000	2.547420000	-0.292467000
1	-3.701383000	2.622499000	-1.043000000
1	-3.187195000	1.781227000	0.426163000
1	-2.861889000	3.505306000	0.240328000
14	1.984524000	0.814782000	1.458184000
14	2.751890000	-0.879005000	-1.122455000
6	0.617935000	1.919107000	2.127368000
1	-0.297573000	1.359230000	2.342842000
1	0.954180000	2.379184000	3.060771000
1	0.359370000	2.725475000	1.435538000
6	3.490484000	1.901995000	1.198505000
1	3.685843000	2.477501000	2.107541000
1	4.385909000	1.318185000	0.974256000
1	3.335342000	2.609733000	0.380225000
6	3.880650000	0.335289000	-1.998833000
1	4.541896000	-0.205366000	-2.681565000
1	3.311033000	1.055838000	-2.590345000
1	4.506091000	0.895635000	-1.301595000
6	3.789520000	-2.037736000	-0.074810000
1	4.446479000	-2.624955000	-0.722172000
1	4.420371000	-1.505400000	0.640916000
1	3.164414000	-2.739730000	0.484798000
6	2.372058000	-0.440000000	2.799987000
1	3.147301000	-1.150709000	2.507352000
1	2.720619000	0.085137000	3.693841000

1	1.486481000	-1.015609000	3.086863000
6	1.910807000	-1.929379000	-2.438490000
1	1.420618000	-2.800634000	-1.992320000
1	1.152696000	-1.366894000	-2.990488000
1	2.639843000	-2.301803000	-3.163048000
32	0.028204000	-1.339822000	0.380640000
6	-2.661740000	-0.529495000	0.001444000
6	-3.504635000	-0.587879000	-1.106930000
6	-3.173328000	-0.883260000	1.247777000
6	-4.825834000	-0.968375000	-0.965639000
1	-3.105967000	-0.322844000	-2.080756000
6	-4.495256000	-1.271428000	1.384595000
1	-2.523037000	-0.822606000	2.115534000
6	-5.329471000	-1.311338000	0.280432000
1	-5.468421000	-1.003413000	-1.838182000
1	-4.876531000	-1.537152000	2.364020000
1	-6.365388000	-1.610121000	0.387750000

3Ge-T (T.E.= -3418.024983)

6	-0.725276000	0.863865000	-1.203141000
6	-1.518214000	0.048968000	-0.197154000
1	-0.796629000	0.437792000	-2.213285000
1	-1.163265000	1.870034000	-1.250341000
7	1.393273000	-0.168820000	-0.223633000
5	0.839140000	0.998031000	-0.817963000
7	1.507223000	2.238398000	-0.986339000
6	0.937906000	3.349477000	-1.709596000
1	0.498517000	4.096211000	-1.030657000
1	1.712130000	3.858265000	-2.294420000
1	0.168231000	3.023209000	-2.407386000
6	2.701595000	2.625093000	-0.271855000
1	2.521559000	3.566231000	0.263674000
1	2.986005000	1.875520000	0.464043000
1	3.553630000	2.786391000	-0.944282000
14	-2.871670000	-1.034109000	-0.952480000
14	-1.843375000	1.012832000	1.402258000
6	-2.337787000	-1.690775000	-2.620723000
1	-1.372135000	-2.199172000	-2.559463000
1	-3.080173000	-2.412982000	-2.971214000
1	-2.265399000	-0.901418000	-3.372024000

6	-4.376348000	0.057206000	-1.218958000
1	-5.120984000	-0.478050000	-1.813927000
1	-4.846680000	0.353774000	-0.278850000
1	-4.099017000	0.964787000	-1.762498000
6	-2.883774000	2.519932000	0.977676000
1	-3.087592000	3.078859000	1.895415000
1	-2.347848000	3.189497000	0.299322000
1	-3.840744000	2.264944000	0.519957000
6	-2.758609000	-0.018432000	2.664541000
1	-2.820446000	0.539568000	3.602632000
1	-3.780008000	-0.241817000	2.347440000
1	-2.246592000	-0.962186000	2.869120000
6	-3.332734000	-2.475832000	0.144223000
1	-3.680313000	-2.158905000	1.128394000
1	-4.140615000	-3.040235000	-0.329517000
1	-2.492109000	-3.161046000	0.283525000
6	-0.271351000	1.689822000	2.167268000
1	0.444703000	0.910130000	2.438591000
1	0.227829000	2.399598000	1.500565000
1	-0.545252000	2.232183000	3.077177000
32	-0.007451000	-1.370991000	0.307329000
6	2.723713000	-0.536125000	-0.035147000
6	3.674293000	-0.353495000	-1.041924000
6	3.132463000	-1.137130000	1.156901000
6	4.988602000	-0.733860000	-0.849188000
1	3.361027000	0.091679000	-1.980536000
6	4.447969000	-1.524335000	1.341079000
1	2.399332000	-1.278170000	1.948150000
6	5.386448000	-1.321660000	0.342233000
1	5.710070000	-0.579815000	-1.644034000
1	4.742993000	-1.983356000	2.278152000
1	6.416287000	-1.625446000	0.487056000

4Ge-S (T.E.= -3628.014139)

6	0.882131000	0.522121000	1.530503000
6	1.399307000	0.034347000	0.143079000
1	1.096970000	-0.212515000	2.317974000
1	1.398235000	1.432121000	1.862521000
7	-1.429084000	0.138905000	0.002051000
14	2.309491000	-1.592388000	0.405121000

14	2.419501000	1.382634000	-0.676812000
6	1.039295000	-2.886893000	0.911570000
1	0.374725000	-3.146553000	0.080404000
1	1.533091000	-3.808658000	1.230497000
1	0.414871000	-2.541639000	1.740479000
6	3.589880000	-1.485014000	1.772318000
1	4.006861000	-2.481861000	1.942617000
1	4.413689000	-0.819081000	1.507360000
1	3.169536000	-1.138284000	2.718406000
6	4.047214000	1.659053000	0.212094000
1	4.741079000	0.834652000	0.028462000
1	4.518438000	2.577321000	-0.148696000
1	3.912906000	1.751179000	1.292742000
6	2.793800000	1.040576000	-2.483566000
1	3.374191000	1.879482000	-2.878796000
1	3.377570000	0.132158000	-2.638507000
1	1.885701000	0.961043000	-3.087264000
6	3.178500000	-2.213205000	-1.135282000
1	4.057809000	-1.607911000	-1.369772000
1	3.520367000	-3.238071000	-0.966449000
1	2.526471000	-2.218958000	-2.012605000
6	1.448546000	2.990720000	-0.648788000
1	0.520622000	2.895703000	-1.222233000
1	1.187970000	3.319376000	0.359952000
1	2.041011000	3.784044000	-1.112818000
14	-0.977565000	0.792556000	1.559455000
6	-1.453443000	2.588870000	1.759125000
1	-1.129349000	3.184896000	0.903157000
1	-2.534509000	2.703368000	1.868118000
1	-0.984543000	3.003156000	2.656003000
6	-1.813180000	-0.200421000	2.902206000
1	-1.573127000	-1.262622000	2.802926000
1	-1.496227000	0.129512000	3.894503000
1	-2.899748000	-0.095305000	2.845947000
32	-0.088846000	-0.435553000	-1.145742000
6	-2.783665000	-0.086186000	-0.315151000
6	-3.271072000	-1.385909000	-0.441428000
6	-3.667250000	0.977291000	-0.492393000
6	-4.602021000	-1.614888000	-0.744105000
1	-2.587513000	-2.214706000	-0.280169000

6	-4.998778000	0.743987000	-0.786864000
1	-3.288304000	1.990630000	-0.410540000
6	-5.473216000	-0.551910000	-0.915183000
1	-4.961670000	-2.633232000	-0.839029000
1	-5.670814000	1.583431000	-0.925031000
1	-6.515933000	-0.731765000	-1.148275000

4Ge-T (T.E.= -3627.937085)

6	-0.968673000	0.939357000	1.327547000
6	-1.482268000	-0.031868000	0.296466000
1	-1.639694000	1.794857000	1.477518000
1	-0.845892000	0.457291000	2.307720000
7	1.465463000	0.528805000	-0.101716000
14	-2.958223000	0.623901000	-0.685704000
14	-1.425925000	-1.825023000	0.900670000
6	-2.759560000	2.451427000	-1.034225000
1	-1.882746000	2.627173000	-1.663206000
1	-3.640745000	2.808336000	-1.574408000
1	-2.659771000	3.056007000	-0.130461000
6	-4.472899000	0.365801000	0.392085000
1	-5.334497000	0.878681000	-0.043007000
1	-4.721143000	-0.694856000	0.478166000
1	-4.315951000	0.759200000	1.399923000
6	-2.556046000	-1.954039000	2.398104000
1	-3.606656000	-1.823034000	2.133295000
1	-2.444718000	-2.946724000	2.843529000
1	-2.306129000	-1.217280000	3.164840000
6	-2.037217000	-3.035440000	-0.384493000
1	-1.932492000	-4.050196000	0.008894000
1	-3.095257000	-2.877496000	-0.608207000
1	-1.470574000	-2.977914000	-1.316850000
6	-3.220171000	-0.245565000	-2.319986000
1	-3.284435000	-1.330223000	-2.223867000
1	-4.161229000	0.106547000	-2.752379000
1	-2.424594000	-0.011652000	-3.031834000
6	0.294310000	-2.298513000	1.464402000
1	1.011022000	-2.311870000	0.639655000
1	0.673760000	-1.619246000	2.232496000
1	0.257858000	-3.299998000	1.902476000
14	0.775690000	1.669837000	0.997177000

6	1.589849000	1.836579000	2.669645000
1	1.678351000	0.880067000	3.188632000
1	2.579331000	2.292238000	2.600130000
1	0.963847000	2.493297000	3.281159000
6	0.643836000	3.361612000	0.222816000
1	0.179525000	3.300553000	-0.764468000
1	0.044670000	4.033891000	0.843062000
1	1.635858000	3.804534000	0.104412000
32	0.073730000	-0.066567000	-1.279424000
6	2.755008000	0.055266000	-0.278939000
6	3.177812000	-0.390781000	-1.539108000
6	3.673847000	-0.041155000	0.774319000
6	4.438736000	-0.925645000	-1.729238000
1	2.509216000	-0.280115000	-2.389152000
6	4.937289000	-0.562984000	0.573552000
1	3.378405000	0.269397000	1.768412000
6	5.333211000	-1.014389000	-0.676398000
1	4.728496000	-1.260694000	-2.719114000
1	5.619724000	-0.628960000	1.413981000
1	6.324885000	-1.423312000	-0.827083000

5Ge-S (T.E.= -3372.070081)

6	0.571932000	-0.347550000	1.582036000
6	1.243359000	-0.074576000	0.229212000
1	0.738045000	-1.381195000	1.916430000
1	0.958052000	0.263820000	2.405506000
7	-1.444482000	-0.180562000	0.281005000
14	2.472820000	-1.446247000	-0.167004000
14	1.923642000	1.687991000	0.184427000
6	1.489908000	-3.022819000	-0.455171000
1	0.937845000	-2.976155000	-1.399772000
1	2.154048000	-3.889099000	-0.512185000
1	0.768090000	-3.214066000	0.343808000
6	3.648890000	-1.739306000	1.260233000
1	4.225732000	-2.649100000	1.072872000
1	4.355019000	-0.916254000	1.382699000
1	3.122016000	-1.873680000	2.207901000
6	3.458087000	1.844049000	1.244522000
1	4.306875000	1.314006000	0.806413000
1	3.735087000	2.897019000	1.342005000

1	3.294548000	1.446626000	2.249391000
6	2.316807000	2.253224000	-1.559053000
1	2.692147000	3.279631000	-1.518970000
1	3.075744000	1.641326000	-2.048257000
1	1.429061000	2.258726000	-2.198239000
6	3.460006000	-1.099431000	-1.718800000
1	4.183658000	-0.293366000	-1.577214000
1	4.017315000	-1.997782000	-1.997207000
1	2.816711000	-0.834754000	-2.562533000
6	0.619434000	2.861460000	0.848760000
1	-0.276900000	2.870661000	0.220707000
1	0.307100000	2.626104000	1.868405000
1	1.023230000	3.877623000	0.855707000
6	-2.845151000	-0.115483000	0.080097000
6	-3.690989000	-1.077951000	0.618258000
6	-3.378797000	0.904559000	-0.696458000
6	-5.050197000	-1.017245000	0.375933000
1	-3.274312000	-1.874095000	1.223322000
6	-4.740039000	0.956269000	-0.944382000
1	-2.716709000	1.667509000	-1.094784000
6	-5.580087000	-0.003103000	-0.407229000
1	-5.702511000	-1.771957000	0.799723000
1	-5.144133000	1.756789000	-1.552978000
1	-6.646289000	0.039304000	-0.595469000
6	-0.931255000	-0.190346000	1.569532000
8	-1.595326000	-0.105303000	2.574865000
32	-0.206481000	-0.135506000	-1.144128000

5Ge-T (T.E.= -3371.986298)

6	0.630649000	-0.601076000	1.496635000
6	1.358983000	-0.077817000	0.267061000
1	0.809488000	-1.673798000	1.655394000
1	1.022859000	-0.094407000	2.390120000
7	-1.455317000	-0.445335000	0.308402000
14	2.896893000	-1.114552000	-0.122357000
14	1.415912000	1.824181000	0.137927000
6	2.424613000	-2.899953000	-0.416476000
1	1.945623000	-3.024302000	-1.390160000
1	3.326341000	-3.518664000	-0.396325000
1	1.738271000	-3.284783000	0.341319000

6	4.007344000	-1.034485000	1.384341000
1	4.870642000	-1.686911000	1.230184000
1	4.376488000	-0.025837000	1.576004000
1	3.484734000	-1.381363000	2.278724000
6	2.803149000	2.365240000	1.283700000
1	3.783908000	2.085087000	0.893382000
1	2.778266000	3.454202000	1.377795000
1	2.696812000	1.939292000	2.284198000
6	1.782366000	2.436648000	-1.587382000
1	1.874121000	3.526093000	-1.551514000
1	2.710399000	2.038749000	-2.000589000
1	0.966664000	2.192966000	-2.272848000
6	3.792353000	-0.477553000	-1.631245000
1	4.244023000	0.503009000	-1.466456000
1	4.593745000	-1.172525000	-1.894226000
1	3.121108000	-0.404901000	-2.491661000
6	-0.176315000	2.599150000	0.728775000
1	-1.007485000	2.396761000	0.049166000
1	-0.465407000	2.268969000	1.729053000
1	-0.033239000	3.682721000	0.766933000
6	-2.834469000	-0.284192000	0.087717000
6	-3.795287000	-0.832081000	0.934513000
6	-3.251022000	0.413622000	-1.043871000
6	-5.138731000	-0.670925000	0.649561000
1	-3.482598000	-1.378332000	1.813024000
6	-4.596794000	0.564269000	-1.324765000
1	-2.501159000	0.855535000	-1.697189000
6	-5.548825000	0.024629000	-0.476712000
1	-5.876177000	-1.101465000	1.317506000
1	-4.900753000	1.113601000	-2.208371000
1	-6.604031000	0.142923000	-0.692655000
6	-0.885743000	-0.416369000	1.541656000
8	-1.458458000	-0.268815000	2.603466000
32	-0.169708000	-0.586694000	-1.131449000

6Ge-S (T.E.= -3450.363067)

6	-0.876320000	1.210654000	-0.251222000
6	0.530951000	1.225508000	-0.226738000
6	1.207686000	-0.079020000	0.037666000
7	-1.445900000	-0.035855000	-0.020730000

14	2.110655000	-0.669702000	-1.517044000
14	2.202878000	-0.037402000	1.642835000
6	2.470598000	-1.761428000	2.334200000
1	2.935255000	-2.440408000	1.616309000
1	3.132801000	-1.693215000	3.202132000
1	1.536814000	-2.220379000	2.670478000
6	1.209031000	0.943728000	2.891852000
1	0.180604000	0.573625000	2.952858000
1	1.655888000	0.862230000	3.885920000
1	1.163620000	2.002050000	2.625999000
6	3.892738000	0.753897000	1.469284000
1	4.368744000	0.786000000	2.453629000
1	4.546618000	0.183643000	0.805356000
1	3.837851000	1.778072000	1.094891000
6	2.955030000	-2.315918000	-1.218025000
1	3.332207000	-2.700566000	-2.169625000
1	3.808536000	-2.223446000	-0.542254000
1	2.275776000	-3.065211000	-0.802810000
6	0.840535000	-0.880451000	-2.883487000
1	0.181110000	-1.736137000	-2.708104000
1	0.216116000	0.012773000	-2.975011000
1	1.337737000	-1.040943000	-3.843704000
6	3.395622000	0.536808000	-2.147675000
1	4.163405000	0.771921000	-1.408197000
1	3.890920000	0.084866000	-3.012404000
1	2.939760000	1.471691000	-2.479227000
6	-1.593622000	2.374653000	-0.520347000
6	-0.919568000	3.561743000	-0.735728000
6	0.465679000	3.600899000	-0.687102000
6	1.177592000	2.439276000	-0.440341000
1	-2.675984000	2.344693000	-0.561850000
1	-1.482270000	4.464649000	-0.943417000
1	0.992196000	4.534097000	-0.848584000
1	2.261414000	2.472203000	-0.411806000
32	-0.252207000	-1.442907000	0.292353000
6	-2.846784000	-0.213560000	0.034611000
6	-3.604129000	0.386144000	1.036447000
6	-3.470939000	-1.042392000	-0.888577000
6	-4.965791000	0.160307000	1.106415000
1	-3.105899000	1.022125000	1.761170000

6	-4.834347000	-1.274493000	-0.808302000
1	-2.872078000	-1.496218000	-1.672020000
6	-5.585364000	-0.672130000	0.185498000
1	-5.547081000	0.627928000	1.892695000
1	-5.310959000	-1.926632000	-1.530874000
1	-6.652223000	-0.851296000	0.246617000

6Ge-T (T.E.= -3450.291848)

6	0.823179000	1.338706000	-0.256701000
6	-0.598170000	1.266873000	-0.091971000
6	-1.222504000	-0.060264000	0.026705000
7	1.440749000	0.147258000	-0.415444000
14	-1.159641000	-0.674993000	1.815479000
14	-2.881155000	-0.252640000	-0.863570000
6	-3.139447000	-2.048985000	-1.343226000
1	-3.102720000	-2.735504000	-0.495689000
1	-4.126039000	-2.142231000	-1.806922000
1	-2.401278000	-2.377103000	-2.080584000
6	-2.849116000	0.734176000	-2.457264000
1	-1.891447000	0.590659000	-2.967113000
1	-3.641208000	0.375050000	-3.119977000
1	-2.997731000	1.805128000	-2.310277000
6	-4.380705000	0.260326000	0.143943000
1	-5.271849000	0.160458000	-0.482488000
1	-4.521668000	-0.378829000	1.018837000
1	-4.332328000	1.295401000	0.488883000
6	-1.946663000	-2.364940000	1.979991000
1	-1.822103000	-2.707379000	3.011018000
1	-3.016142000	-2.362570000	1.758168000
1	-1.457620000	-3.090892000	1.324856000
6	0.586557000	-0.781643000	2.480711000
1	1.202986000	-1.491040000	1.922442000
1	1.081978000	0.192278000	2.473541000
1	0.539928000	-1.118504000	3.520466000
6	-2.063275000	0.545320000	2.920137000
1	-3.113269000	0.668285000	2.648036000
1	-2.021912000	0.205871000	3.958872000
1	-1.584920000	1.527367000	2.872414000
6	1.464364000	2.594451000	-0.335267000
6	0.732938000	3.746450000	-0.246473000

6	-0.656111000	3.689318000	-0.080067000
6	-1.301032000	2.474449000	-0.027081000
1	2.531666000	2.635699000	-0.510381000
1	1.227734000	4.707135000	-0.325376000
1	-1.226614000	4.606529000	0.006305000
1	-2.375724000	2.446317000	0.115807000
32	0.117714000	-1.283770000	-1.036227000
6	2.793589000	-0.087535000	-0.285059000
6	3.376774000	-1.105280000	-1.050710000
6	3.588967000	0.578152000	0.659457000
6	4.709364000	-1.429703000	-0.891037000
1	2.773874000	-1.607801000	-1.799734000
6	4.916155000	0.239994000	0.814300000
1	3.142589000	1.325487000	1.303834000
6	5.487749000	-0.759253000	0.038222000
1	5.144581000	-2.211138000	-1.502651000
1	5.510291000	0.751511000	1.562614000
1	6.532306000	-1.017161000	0.164085000

7Ge-S (T.E.= -2711.833155)

6	0.335167000	1.139365000	0.000531000
6	1.775762000	0.684578000	0.000145000
6	2.022616000	-0.688126000	-0.000173000
7	-0.486095000	-0.087519000	0.000350000
6	-1.898952000	0.021390000	0.000181000
6	-2.609110000	0.044971000	-1.197081000
6	-2.609710000	0.043367000	1.197134000
6	-3.991601000	0.110306000	-1.196997000
1	-2.058299000	-0.002540000	-2.130351000
6	-3.992203000	0.108693000	1.196435000
1	-2.059407000	-0.005506000	2.130630000
6	-4.688150000	0.148044000	-0.000430000
1	-4.527745000	0.122294000	-2.139100000
1	-4.528825000	0.119379000	2.138282000
1	-5.770641000	0.195390000	-0.000671000
6	2.839264000	1.578852000	0.000151000
6	3.336557000	-1.149146000	-0.000499000
6	4.139661000	1.106616000	-0.000164000
6	4.394189000	-0.258447000	-0.000491000
1	2.661696000	2.650336000	0.000412000

1	4.965016000	1.809713000	-0.000156000
1	5.416601000	-0.619303000	-0.000746000
1	3.536411000	-2.217308000	-0.000772000
6	0.051817000	1.970382000	1.249283000
1	-0.993830000	2.284398000	1.276945000
1	0.269672000	1.391423000	2.149885000
1	0.671718000	2.868858000	1.260795000
6	0.051186000	1.970863000	-1.247745000
1	0.670992000	2.869403000	-1.259202000
1	0.268635000	1.392272000	-2.148683000
1	-0.994514000	2.284779000	-1.274780000
32	0.341757000	-1.735037000	-0.000207000

7Ge-T (T.E.= -2711.749302)

6	-0.317304000	1.224921000	-0.000133000
6	-1.751799000	0.707239000	0.000034000
6	-1.982440000	-0.671150000	0.000168000
7	0.585691000	0.053605000	-0.000064000
6	1.913684000	0.126537000	0.000003000
6	2.645042000	-1.107914000	0.000055000
6	2.701748000	1.324206000	-0.000001000
6	4.014787000	-1.135935000	0.000205000
1	2.082499000	-2.033439000	-0.000058000
6	4.066737000	1.272167000	0.000133000
1	2.227114000	2.291444000	-0.000089000
6	4.743392000	0.047839000	0.000263000
1	4.528412000	-2.089729000	0.000263000
1	4.631174000	2.196912000	0.000146000
1	5.826352000	0.025231000	0.000378000
6	-2.821206000	1.591565000	-0.000001000
6	-3.307802000	-1.124432000	0.000331000
6	-4.126474000	1.124990000	0.000121000
6	-4.369147000	-0.242488000	0.000305000
1	-2.652607000	2.664912000	-0.000128000
1	-4.951013000	1.828328000	0.000092000
1	-5.388507000	-0.613293000	0.000409000
1	-3.505652000	-2.193849000	0.000477000
6	-0.116734000	2.037290000	-1.282979000
1	0.874544000	2.477066000	-1.372968000
1	-0.285222000	1.391668000	-2.147948000

1	-0.846870000	2.845847000	-1.322694000
6	-0.116668000	2.037577000	1.282543000
1	-0.847287000	2.845682000	1.322395000
1	-0.284493000	1.391953000	2.147639000
1	0.874360000	2.477979000	1.372096000
32	-0.419923000	-1.848638000	-0.000182000

8Ge-S (T.E.= -2940.691306)

6	-0.537798000	1.692658000	0.054137000
6	0.914360000	1.632889000	0.492775000
6	1.479432000	0.300697000	0.048520000
1	-1.092921000	2.419830000	0.659626000
1	-0.593342000	2.039060000	-0.992190000
1	0.965804000	1.734572000	1.587201000
1	1.452227000	2.497415000	0.080128000
32	0.154211000	-1.031407000	-0.136777000
7	-1.113320000	0.366744000	0.186823000
15	3.143387000	0.048360000	-0.025924000
6	4.004731000	1.070419000	-1.246575000
1	3.780169000	2.120938000	-1.052642000
1	5.085315000	0.922751000	-1.196773000
1	3.642948000	0.817329000	-2.243636000
6	3.561522000	-1.649053000	-0.442802000
1	3.166346000	-2.327752000	0.313593000
1	3.132299000	-1.908218000	-1.411171000
1	4.646264000	-1.755781000	-0.491458000
6	4.035383000	0.416127000	1.506669000
1	5.110957000	0.274792000	1.383989000
1	3.844868000	1.454043000	1.787655000
1	3.666447000	-0.231771000	2.302541000
6	-2.481735000	0.218182000	0.091166000
6	-3.075880000	-1.023342000	0.375675000
6	-3.339003000	1.266618000	-0.272638000
6	-4.438810000	-1.204555000	0.286209000
1	-2.441562000	-1.848258000	0.684496000
6	-4.709195000	1.074482000	-0.348686000
1	-2.932751000	2.241556000	-0.510660000
6	-5.276102000	-0.156689000	-0.075722000
1	-4.858165000	-2.178671000	0.514741000
1	-5.340496000	1.909822000	-0.633390000

1 -6.348134000 -0.299836000 -0.136451000

8Ge-T (T.E.= -2940.613120)

6 0.154242000 -0.706470000 1.717566000
6 -1.277262000 -0.260090000 2.034808000
6 -1.787051000 0.357554000 0.779412000
1 0.750027000 -0.808037000 2.636784000
1 0.104224000 -1.719314000 1.277507000
1 -1.254545000 0.503574000 2.820801000
1 -1.857035000 -1.111330000 2.413033000
32 -0.378250000 1.774510000 0.220983000
7 0.746783000 0.228585000 0.787471000
15 -2.428865000 -0.608583000 -0.505926000
6 -1.140570000 -1.337546000 -1.534902000
1 -0.548893000 -2.039892000 -0.945447000
1 -1.591533000 -1.857606000 -2.382214000
1 -0.487498000 -0.534808000 -1.886745000
6 -3.415121000 0.425519000 -1.587780000
1 -4.244854000 0.858337000 -1.028531000
1 -2.774999000 1.229554000 -1.958337000
1 -3.799616000 -0.156647000 -2.426676000
6 -3.471101000 -1.975947000 0.034593000
1 -3.902171000 -2.490090000 -0.825935000
1 -2.868262000 -2.684107000 0.605739000
1 -4.273589000 -1.600040000 0.670133000
6 1.977081000 -0.079055000 0.276605000
6 2.574270000 0.755918000 -0.690781000
6 2.704395000 -1.222293000 0.660636000
6 3.808208000 0.465024000 -1.228211000
1 2.038289000 1.641472000 -1.018071000
6 3.946113000 -1.497969000 0.113157000
1 2.302358000 -1.899108000 1.403762000
6 4.514428000 -0.665842000 -0.835101000
1 4.229835000 1.135037000 -1.970311000
1 4.476452000 -2.386685000 0.439768000
1 5.485523000 -0.888815000 -1.260144000

9Ge-S (T.E.= -2939.518274)

6 0.488292000 1.571363000 0.420337000
6 -0.866050000 1.578366000 0.382279000

6	-1.468027000	0.311750000	0.080789000
7	1.092432000	0.358236000	0.191006000
15	-3.150920000	0.109671000	-0.015733000
6	-4.033581000	0.508156000	1.508801000
1	-3.806877000	1.537499000	1.792504000
1	-5.112003000	0.401890000	1.376580000
1	-3.690927000	-0.153602000	2.304742000
6	-3.599207000	-1.581484000	-0.419751000
1	-4.685655000	-1.677151000	-0.443763000
1	-3.192521000	-1.847906000	-1.395765000
1	-3.194501000	-2.260993000	0.331095000
6	-3.948047000	1.148534000	-1.258822000
1	-3.560870000	0.888927000	-2.244509000
1	-5.032174000	1.022533000	-1.240710000
1	-3.704309000	2.192728000	-1.054930000
32	-0.154434000	-1.060543000	-0.185540000
6	2.482250000	0.242491000	0.100206000
6	3.106536000	-0.945217000	0.486074000
6	3.281584000	1.278483000	-0.386762000
6	4.476023000	-1.092893000	0.380075000
1	2.497197000	-1.748509000	0.887166000
6	4.654258000	1.128888000	-0.474957000
1	2.816697000	2.197918000	-0.723342000
6	5.263337000	-0.055709000	-0.096207000
1	4.935183000	-2.025858000	0.687840000
1	5.253020000	1.947888000	-0.858354000
1	6.338188000	-0.169836000	-0.169619000
1	1.097777000	2.434349000	0.665514000
1	-1.423775000	2.488400000	0.589438000

9Ge-T (T.E.= -2939.449841)

6	0.515215000	1.620147000	0.088673000
6	-0.881727000	1.617977000	0.052578000
6	-1.530814000	0.405408000	-0.041498000
7	1.155936000	0.445893000	0.041192000
15	-3.211559000	0.172122000	0.004125000
6	-3.734248000	-0.706201000	1.490168000
1	-3.545656000	-0.081510000	2.363601000
1	-4.793514000	-0.964509000	1.441565000
1	-3.138344000	-1.617036000	1.581334000

6	-3.752685000	-0.884679000	-1.349762000
1	-4.814306000	-1.121130000	-1.259701000
1	-3.562821000	-0.385847000	-2.300535000
1	-3.171628000	-1.809132000	-1.323406000
6	-4.202740000	1.672408000	-0.072632000
1	-3.966178000	2.227334000	-0.980986000
1	-5.262676000	1.412923000	-0.075355000
1	-3.993422000	2.299554000	0.794669000
32	-0.162599000	-1.157857000	-0.074578000
6	2.524853000	0.309879000	0.027279000
6	3.074443000	-0.978228000	0.134573000
6	3.416721000	1.388693000	-0.102822000
6	4.440725000	-1.173929000	0.125586000
1	2.406583000	-1.826620000	0.241977000
6	4.779636000	1.178143000	-0.110360000
1	3.041830000	2.398395000	-0.215946000
6	5.309966000	-0.100766000	0.005433000
1	4.831714000	-2.181584000	0.214961000
1	5.443261000	2.029726000	-0.215688000
1	6.382074000	-0.255345000	-0.003941000
1	1.065892000	2.551883000	0.180615000
1	-1.393869000	2.578124000	0.109802000

10Ge-S (T.E.= -3093.060391)

6	-0.514637000	1.181644000	-0.113243000
6	0.903969000	1.132668000	-0.062484000
6	1.440471000	-0.203944000	0.010918000
7	-1.124091000	-0.056946000	-0.087094000
6	-1.168704000	2.406706000	-0.236249000
6	-0.444411000	3.582983000	-0.280754000
6	0.942619000	3.554926000	-0.208068000
6	1.602086000	2.344815000	-0.105572000
1	-2.249949000	2.433132000	-0.305739000
1	-0.965110000	4.528968000	-0.376986000
1	1.509638000	4.478298000	-0.239673000
1	2.687917000	2.346492000	-0.064688000
15	3.097469000	-0.572126000	0.082261000
6	4.071443000	-0.034276000	-1.342030000
1	3.994700000	1.046206000	-1.464144000
1	5.120057000	-0.310368000	-1.214997000

1	3.672889000	-0.511740000	-2.238039000
6	3.365280000	-2.347830000	0.168623000
1	4.437099000	-2.543280000	0.230233000
1	2.872763000	-2.760730000	1.049456000
1	2.964880000	-2.831349000	-0.723010000
6	3.968524000	0.099532000	1.515925000
1	3.519758000	-0.310882000	2.421243000
1	5.028019000	-0.160779000	1.480977000
1	3.864775000	1.184292000	1.541913000
32	0.069793000	-1.541079000	0.014210000
6	-2.519267000	-0.217485000	-0.019874000
6	-3.160160000	-1.045448000	-0.937164000
6	-3.278963000	0.380577000	0.985242000
6	-4.523179000	-1.273546000	-0.851188000
1	-2.570807000	-1.503502000	-1.724477000
6	-4.641618000	0.161500000	1.058712000
1	-2.783594000	1.008761000	1.717450000
6	-5.271905000	-0.667477000	0.142392000
1	-5.003233000	-1.923614000	-1.573890000
1	-5.216014000	0.632815000	1.848387000
1	-6.339842000	-0.839752000	0.205900000

10Ge-T (T.E.= -3092.976697)

6	-0.521178000	1.171655000	-0.160814000
6	0.924193000	1.110936000	-0.024362000
6	1.458051000	-0.165168000	0.160752000
7	-1.163542000	-0.010653000	-0.082730000
6	-1.130985000	2.415103000	-0.408769000
6	-0.385290000	3.566829000	-0.469020000
6	1.008557000	3.532200000	-0.301708000
6	1.640269000	2.336711000	-0.101217000
1	-2.201335000	2.455126000	-0.566545000
1	-0.878239000	4.512452000	-0.664450000
1	1.582250000	4.449995000	-0.353600000
1	2.721022000	2.323530000	-0.002477000
15	3.122772000	-0.542449000	0.244579000
6	4.057553000	-0.210524000	-1.265742000
1	4.042863000	0.855466000	-1.492639000
1	5.090604000	-0.548261000	-1.163017000
1	3.576718000	-0.746792000	-2.086070000

6	3.301750000	-2.306205000	0.522404000
1	4.355268000	-2.564472000	0.639222000
1	2.749320000	-2.592251000	1.418656000
1	2.891321000	-2.851267000	-0.330421000
6	4.034084000	0.253102000	1.583314000
1	3.563041000	-0.001928000	2.533015000
1	5.067750000	-0.098677000	1.583142000
1	4.024580000	1.336109000	1.468259000
32	0.042744000	-1.625276000	-0.322079000
6	-2.537987000	-0.158839000	0.045986000
6	-3.176529000	-1.205550000	-0.625391000
6	-3.305185000	0.641241000	0.900029000
6	-4.532377000	-1.427250000	-0.466825000
1	-2.593327000	-1.828782000	-1.296360000
6	-4.658394000	0.412299000	1.052566000
1	-2.820703000	1.427571000	1.467280000
6	-5.285499000	-0.618843000	0.367312000
1	-5.004738000	-2.240475000	-1.006598000
1	-5.229545000	1.040162000	1.727661000
1	-6.347630000	-0.793556000	0.490805000

11Ge-S (T.E.= -3093.303644)

6	0.487580000	1.395369000	0.000345000
6	-1.043463000	1.255520000	0.000233000
6	-1.514357000	-0.088825000	0.000069000
7	1.060704000	0.046754000	0.000303000
6	2.462776000	-0.117727000	0.000105000
6	3.168693000	-0.225324000	-1.196430000
6	4.539532000	-0.417990000	-1.196954000
6	5.231362000	-0.510422000	-0.000447000
6	4.539903000	-0.418765000	1.196335000
6	3.169064000	-0.226105000	1.196361000
1	5.069175000	-0.503695000	-2.139165000
1	6.304188000	-0.663854000	-0.000661000
1	5.069833000	-0.505110000	2.138326000
6	0.885985000	2.171047000	-1.247886000
1	1.966216000	2.334009000	-1.274658000
1	0.595106000	1.623683000	-2.148868000
1	0.385303000	3.140630000	-1.252097000
6	0.885771000	2.171154000	1.248593000

1	0.385082000	3.140735000	1.252637000
1	0.594734000	1.623879000	2.149577000
1	1.965990000	2.334144000	1.275542000
15	-3.209352000	-0.301160000	-0.000139000
6	-4.041776000	0.405252000	-1.431803000
1	-5.119975000	0.247944000	-1.365058000
1	-3.824027000	1.472737000	-1.463555000
1	-3.658203000	-0.065853000	-2.337335000
6	-3.618856000	-2.050376000	-0.000393000
1	-3.199700000	-2.527534000	0.886536000
1	-4.702294000	-2.178641000	-0.000540000
1	-3.199487000	-2.527314000	-0.887340000
6	-4.042085000	0.404921000	1.431508000
1	-3.824406000	1.472413000	1.463510000
1	-5.120261000	0.247559000	1.364529000
1	-3.658654000	-0.066338000	2.337020000
1	2.618950000	-0.163743000	-2.129735000
1	2.619617000	-0.165222000	2.129879000
8	-1.745545000	2.270121000	0.000110000
32	-0.101508000	-1.397739000	0.000085000

11Ge-T (T.E.= -3093.213532)

6	0.505171000	1.473022000	0.000074000
6	-1.030415000	1.265556000	0.000670000
6	-1.475766000	-0.064088000	0.000291000
7	1.153048000	0.154602000	0.000087000
6	2.475606000	-0.029698000	0.000030000
6	2.959434000	-1.376943000	0.000084000
6	4.302249000	-1.658030000	0.000031000
6	5.237318000	-0.630171000	-0.000068000
6	4.801024000	0.697142000	-0.000097000
6	3.465923000	0.999296000	-0.000043000
1	4.631030000	-2.690340000	0.000074000
1	6.297329000	-0.854297000	-0.000106000
1	5.526493000	1.501825000	-0.000160000
6	0.820927000	2.250597000	-1.276633000
1	1.855203000	2.585017000	-1.340049000
1	0.607757000	1.627569000	-2.149315000
1	0.170339000	3.124406000	-1.310055000
6	0.821931000	2.251035000	1.276247000

1	0.171461000	3.124921000	1.309823000
1	0.609350000	1.628356000	2.149321000
1	1.856294000	2.585363000	1.338752000
15	-3.176053000	-0.253587000	-0.000059000
6	-4.009753000	0.448033000	-1.434681000
1	-5.087044000	0.282409000	-1.370291000
1	-3.798470000	1.516370000	-1.468230000
1	-3.620010000	-0.024369000	-2.337083000
6	-3.593714000	-2.001904000	-0.000615000
1	-3.174531000	-2.479053000	0.886999000
1	-4.677198000	-2.130240000	-0.000857000
1	-3.174191000	-2.478567000	-0.888329000
6	-4.010288000	0.447231000	1.434644000
1	-3.799048000	1.515555000	1.468843000
1	-5.087550000	0.281602000	1.369777000
1	-3.620855000	-0.025645000	2.336931000
1	2.235851000	-2.182831000	0.000193000
1	3.171829000	2.035819000	-0.000052000
8	-1.742651000	2.284467000	-0.000173000
32	-0.162540000	-1.528890000	0.000184000

12Ge-S (T.E.= -3093.303455)

6	-0.644019000	1.415193000	0.133007000
6	0.889834000	1.409082000	0.254054000
6	1.401221000	-0.005636000	0.077197000
7	-1.192829000	0.164179000	0.070551000
6	-2.590165000	-0.017915000	0.003235000
6	-3.185279000	-0.989618000	0.801348000
6	-4.545641000	-1.232156000	0.722943000
6	-5.334210000	-0.499517000	-0.147547000
6	-4.747051000	0.472844000	-0.941820000
6	-3.387074000	0.713057000	-0.874103000
1	-4.990913000	-1.993837000	1.352866000
1	-6.400512000	-0.683702000	-0.206753000
1	-5.355381000	1.050802000	-1.628546000
15	3.026911000	-0.435414000	-0.129205000
6	4.205607000	0.255028000	1.058659000
1	5.199964000	-0.158393000	0.877323000
1	4.253391000	1.339606000	0.950704000
1	3.888390000	0.014885000	2.073916000

6	3.247307000	-2.218742000	-0.003447000
1	2.666340000	-2.731888000	-0.770582000
1	4.303130000	-2.453410000	-0.147598000
1	2.929648000	-2.569535000	0.978370000
6	3.787418000	-0.027815000	-1.724858000
1	3.814348000	1.052342000	-1.867841000
1	4.806231000	-0.418705000	-1.769559000
1	3.190858000	-0.470288000	-2.523804000
1	-2.567065000	-1.550513000	1.495146000
1	-2.931936000	1.469645000	-1.499520000
8	-1.269135000	2.457755000	0.149026000
6	1.437973000	2.391160000	-0.776853000
1	0.954908000	3.363764000	-0.665960000
1	2.515123000	2.531991000	-0.642353000
1	1.262135000	2.031254000	-1.794130000
6	1.179827000	1.943486000	1.662053000
1	0.786781000	1.260237000	2.418963000
1	2.254267000	2.049596000	1.825940000
1	0.714978000	2.922701000	1.798863000
32	0.047189000	-1.312105000	-0.045833000

12Ge-T (T.E.= -3093.225654)

6	0.340760000	1.423962000	-0.250223000
6	-1.110215000	1.609435000	0.296952000
6	-1.611532000	0.225214000	0.542954000
7	0.932247000	0.287747000	0.187547000
6	2.275147000	0.002552000	-0.125272000
6	2.625995000	-1.309578000	-0.433949000
6	3.940004000	-1.645905000	-0.707369000
6	4.928525000	-0.677139000	-0.678513000
6	4.586944000	0.629898000	-0.367031000
6	3.276326000	0.972145000	-0.090511000
1	4.190382000	-2.673101000	-0.947934000
1	5.958179000	-0.937745000	-0.893694000
1	5.353404000	1.396255000	-0.334077000
15	-2.591679000	-0.696388000	-0.551876000
6	-4.109512000	0.048773000	-1.186775000
1	-4.688839000	-0.721070000	-1.700061000
1	-4.697400000	0.440922000	-0.356004000
1	-3.892475000	0.856041000	-1.883159000

6	-1.627632000	-1.218515000	-1.982571000
1	-0.739535000	-1.739435000	-1.615287000
1	-2.213693000	-1.883610000	-2.619211000
1	-1.315262000	-0.342070000	-2.552594000
6	-3.141056000	-2.191681000	0.274886000
1	-3.720633000	-1.927220000	1.160243000
1	-3.760985000	-2.779147000	-0.404671000
1	-2.267501000	-2.772245000	0.577619000
1	1.845336000	-2.064572000	-0.456378000
1	3.016084000	1.993834000	0.152153000
8	0.822688000	2.263305000	-0.989257000
6	-0.983872000	2.385665000	1.615456000
1	-0.474743000	3.335279000	1.433991000
1	-1.976732000	2.597330000	2.019973000
1	-0.423277000	1.820103000	2.363098000
6	-1.907200000	2.455841000	-0.682987000
1	-1.937418000	2.011223000	-1.681358000
1	-2.929527000	2.593457000	-0.321494000
1	-1.447043000	3.438137000	-0.792075000
32	-0.093952000	-0.893163000	1.449375000

¹³Ge-S (T.E.= -3134.833994)

6	0.712141000	1.367966000	0.133378000
6	-1.353908000	-0.236248000	-0.063035000
7	1.335732000	0.145406000	-0.063442000
6	2.735264000	-0.005907000	-0.022144000
6	3.356266000	-0.795090000	-0.987466000
6	4.722224000	-1.012797000	-0.954354000
6	5.495296000	-0.434962000	0.037997000
6	4.885097000	0.356772000	0.998548000
6	3.518828000	0.569884000	0.976309000
1	5.184393000	-1.631899000	-1.714996000
1	6.566343000	-0.598334000	0.063220000
1	5.480674000	0.812885000	1.781557000
15	-2.843455000	-0.990333000	0.207300000
6	-3.928055000	-1.260823000	-1.222922000
1	-4.835307000	-1.787532000	-0.919648000
1	-4.204637000	-0.323694000	-1.703927000
1	-3.383979000	-1.870019000	-1.947126000
6	-2.665247000	-2.672314000	0.842929000

1	-2.123725000	-2.658887000	1.789430000
1	-3.653819000	-3.107972000	0.998538000
1	-2.115371000	-3.291700000	0.132569000
6	-3.880985000	-0.182787000	1.445960000
1	-4.136859000	0.829659000	1.136758000
1	-4.798063000	-0.754586000	1.600597000
1	-3.324087000	-0.130235000	2.382445000
1	2.751403000	-1.231226000	-1.776224000
1	3.046621000	1.185620000	1.729600000
8	1.340989000	2.384749000	0.384418000
5	-0.901540000	1.227569000	-0.069614000
7	-1.674739000	2.388821000	-0.297977000
6	-1.201296000	3.753952000	-0.167708000
1	-0.180042000	3.772444000	0.199000000
1	-1.245760000	4.268486000	-1.135382000
1	-1.846820000	4.308631000	0.524302000
6	-3.038930000	2.378466000	-0.755593000
1	-3.353470000	1.375582000	-1.031067000
1	-3.729536000	2.774960000	0.001595000
1	-3.144736000	3.011845000	-1.644435000
32	0.178477000	-1.375348000	-0.167033000

¹³Ge-T (T.E.= -3134.758936)

6	0.078873000	1.383094000	-0.404271000
6	-1.551754000	-0.368341000	0.410927000
7	0.929687000	0.530443000	0.254644000
6	2.288973000	0.396640000	-0.035052000
6	3.144969000	-0.074796000	0.964976000
6	4.483833000	-0.304724000	0.709727000
6	5.007962000	-0.066971000	-0.549927000
6	4.170026000	0.404322000	-1.548578000
6	2.829534000	0.637589000	-1.303577000
1	5.123052000	-0.668195000	1.506593000
1	6.058373000	-0.242610000	-0.750305000
1	4.565836000	0.596124000	-2.539996000
15	-1.741111000	-1.681508000	-0.667505000
6	-3.036176000	-1.417049000	-1.888777000
1	-3.120492000	-2.273618000	-2.559671000
1	-3.989165000	-1.259109000	-1.381865000
1	-2.794523000	-0.523514000	-2.467669000

6	-0.227721000	-2.020349000	-1.582304000
1	0.577035000	-2.196753000	-0.863428000
1	-0.362481000	-2.900480000	-2.213496000
1	0.029543000	-1.157542000	-2.198919000
6	-2.143479000	-3.191815000	0.212654000
1	-3.078123000	-3.061268000	0.759158000
1	-2.239952000	-4.024035000	-0.486179000
1	-1.339220000	-3.395691000	0.923349000
1	2.748119000	-0.251395000	1.959681000
1	2.189305000	1.016283000	-2.086864000
8	0.398733000	2.175800000	-1.283219000
5	-1.443317000	1.110404000	0.055123000
7	-2.446276000	2.078016000	0.107087000
6	-2.231143000	3.487969000	-0.132706000
1	-1.212773000	3.661083000	-0.473521000
1	-2.921354000	3.853238000	-0.901638000
1	-2.414829000	4.068636000	0.778638000
6	-3.804000000	1.771820000	0.486898000
1	-4.504788000	2.043783000	-0.311781000
1	-3.905483000	0.706289000	0.699091000
1	-4.096699000	2.329260000	1.384274000
32	0.043398000	-0.504370000	1.770475000

14Ge-S (T.E.= -3134.851339)

6	1.149472000	1.184147000	0.104867000
6	1.644758000	-0.165194000	-0.001051000
7	-1.023500000	-0.100298000	-0.112122000
6	-2.365697000	-0.469232000	0.041946000
6	-3.118790000	0.004205000	1.117838000
6	-4.440484000	-0.367633000	1.275757000
6	-5.039553000	-1.236913000	0.376053000
6	-4.296893000	-1.728403000	-0.684147000
6	-2.976127000	-1.348584000	-0.852032000
1	-2.645434000	0.676171000	1.826530000
1	-5.007243000	0.018220000	2.115904000
1	-6.074888000	-1.530074000	0.503050000
1	-4.750835000	-2.409280000	-1.395643000
1	-2.401943000	-1.716431000	-1.696575000
5	-0.465568000	1.227790000	-0.079840000
7	-1.176981000	2.424591000	-0.301724000

6	-0.620287000	3.739330000	-0.061346000
1	-0.618020000	4.333667000	-0.983536000
1	-1.232132000	4.280958000	0.671290000
1	0.399553000	3.658660000	0.306281000
6	-2.532183000	2.509495000	-0.794982000
1	-3.234621000	2.820418000	-0.010385000
1	-2.582900000	3.256219000	-1.595275000
1	-2.877053000	1.559947000	-1.198322000
15	3.338741000	-0.386518000	0.082762000
6	4.089881000	0.174811000	1.620395000
1	5.170887000	0.023780000	1.597117000
1	3.864339000	1.233880000	1.742648000
1	3.660334000	-0.381378000	2.454149000
6	4.252926000	0.447254000	-1.226091000
1	5.325041000	0.273101000	-1.116416000
1	3.917654000	0.069597000	-2.192631000
1	4.043309000	1.514882000	-1.167119000
6	3.759848000	-2.128783000	-0.061336000
1	3.304933000	-2.690178000	0.755914000
1	3.389565000	-2.523359000	-1.008559000
1	4.843235000	-2.251917000	-0.019856000
8	1.896510000	2.159920000	0.278458000
32	0.279469000	-1.493577000	-0.153024000

¹⁴Ge-T (T.E.= -3134.764111)

6	1.009754000	1.148624000	0.372503000
6	1.543594000	-0.092109000	-0.064884000
7	-1.070924000	-0.050546000	-0.315480000
6	-2.293190000	-0.456172000	0.110265000
6	-3.076350000	0.325926000	0.988355000
6	-4.300011000	-0.119642000	1.430100000
6	-4.796763000	-1.350088000	1.011490000
6	-4.044980000	-2.133875000	0.146367000
6	-2.813331000	-1.705147000	-0.295617000
1	-2.682528000	1.276361000	1.331214000
1	-4.876747000	0.492238000	2.114007000
1	-5.764166000	-1.693808000	1.357785000
1	-4.430236000	-3.089202000	-0.190898000
1	-2.237063000	-2.306190000	-0.990030000
5	-0.494419000	1.272966000	-0.158256000

7	-1.107642000	2.471234000	-0.542115000
6	-0.514938000	3.771435000	-0.309007000
1	-0.327193000	4.283426000	-1.259901000
1	-1.197797000	4.400918000	0.273539000
1	0.419924000	3.664633000	0.238262000
6	-2.345860000	2.553475000	-1.281650000
1	-3.127175000	3.050366000	-0.693320000
1	-2.198173000	3.140093000	-2.194813000
1	-2.704203000	1.565468000	-1.564655000
15	3.196054000	-0.392601000	0.342682000
6	3.508175000	-0.393159000	2.115157000
1	4.562110000	-0.590999000	2.319381000
1	3.224495000	0.580513000	2.513786000
1	2.893270000	-1.164650000	2.580173000
6	4.360826000	0.775807000	-0.376600000
1	5.382471000	0.507875000	-0.099629000
1	4.260108000	0.757503000	-1.462171000
1	4.123505000	1.774249000	-0.010775000
6	3.691474000	-2.013023000	-0.253854000
1	3.047168000	-2.776849000	0.184868000
1	3.591901000	-2.050501000	-1.339836000
1	4.728965000	-2.209223000	0.021279000
8	1.655955000	2.015339000	1.000608000
32	0.321080000	-1.407121000	-0.969834000

Cartesian coordinates of **IIa**, **IX**, diammino silylene/germylene (**I**), H₂, NH₃, CH₃Ph and SiEt₃H in their optimized state, along with their total energies (in hartrees) including zero point vibrational correction.

IIa-S (T.E.= -1055.849000)

6	0.013883000	2.338432000	-0.080898000
6	1.203747000	1.714547000	-0.077208000
1	0.024670000	3.420818000	-0.122223000
14	-0.028244000	-0.812426000	-0.009541000
6	-2.410002000	2.500163000	-0.046537000
6	-1.302133000	1.737995000	-0.045929000
1	-3.408301000	2.087144000	-0.025365000
1	-2.310167000	3.576872000	-0.069573000
6	2.605351000	-0.286060000	-0.001832000
6	3.305054000	-0.376908000	1.194319000

6	3.146321000	-0.835725000	-1.155081000
6	4.542360000	-0.994738000	1.230419000
1	2.863738000	0.039546000	2.094055000
6	4.382166000	-1.460109000	-1.115576000
1	2.585518000	-0.766659000	-2.081321000
6	5.083818000	-1.536825000	0.075292000
1	5.082123000	-1.062394000	2.167782000
1	4.796407000	-1.889296000	-2.020384000
1	6.050423000	-2.025447000	0.106269000
7	1.310687000	0.319580000	-0.039776000
6	-2.637170000	-0.274076000	0.013969000
6	-3.278568000	-0.605764000	-1.169664000
6	-3.251636000	-0.532992000	1.230077000
6	-4.530504000	-1.196537000	-1.136348000
1	-2.784630000	-0.391384000	-2.111699000
6	-4.503634000	-1.123245000	1.261130000
1	-2.736284000	-0.261733000	2.145593000
6	-5.145240000	-1.453184000	0.078377000
1	-5.026409000	-1.459868000	-2.063319000
1	-4.978451000	-1.328680000	2.213451000
1	-6.124758000	-1.916020000	0.103571000
7	-1.340688000	0.329494000	-0.018378000
6	2.469446000	2.500858000	-0.140940000
1	3.084187000	2.351536000	0.749941000
1	3.080010000	2.198257000	-0.996317000
1	2.247789000	3.562748000	-0.231226000

IX-S (T.E.= -2080.604836)

6	-0.695317000	-0.354106000	-1.563809000
6	0.689913000	0.280966000	-1.571296000
6	1.380858000	0.032404000	-0.205987000
6	-1.381913000	-0.066416000	-0.205727000
1	-1.290307000	0.000084000	-2.416461000
1	-0.590636000	-1.436368000	-1.714568000
1	0.578976000	1.357496000	-1.748274000
1	1.285659000	-0.090958000	-2.416003000
14	0.002844000	-0.038303000	1.103618000
14	-2.397244000	1.531523000	-0.261151000
14	-2.464565000	-1.522445000	0.339054000
14	2.415595000	1.531612000	0.329610000

14	2.456848000	-1.521327000	-0.248549000
6	3.353611000	2.239479000	-1.130968000
1	2.667514000	2.594185000	-1.903768000
1	3.934365000	3.101337000	-0.789727000
1	4.042103000	1.529884000	-1.590869000
6	3.588711000	1.156301000	1.741741000
1	4.108657000	2.081223000	2.007605000
1	3.033704000	0.825847000	2.623875000
1	4.343418000	0.402883000	1.513278000
6	1.340907000	2.936986000	0.973419000
1	1.981991000	3.808753000	1.136491000
1	0.553366000	3.240473000	0.281563000
1	0.880082000	2.689844000	1.933956000
6	2.699227000	-2.272091000	1.451024000
1	3.379991000	-3.124470000	1.370789000
1	3.119550000	-1.574425000	2.176675000
1	1.754428000	-2.642867000	1.858685000
6	1.704436000	-2.854354000	-1.334472000
1	2.415091000	-3.685075000	-1.377534000
1	0.764251000	-3.245225000	-0.945323000
1	1.538924000	-2.512127000	-2.358575000
6	4.136351000	-1.221477000	-1.038587000
1	4.020770000	-0.838014000	-2.056301000
1	4.785791000	-0.538311000	-0.490051000
1	4.650558000	-2.184654000	-1.108674000
6	-1.698684000	2.760398000	-1.500471000
1	-0.691258000	3.114584000	-1.282433000
1	-1.698662000	2.347865000	-2.512459000
1	-2.360770000	3.631545000	-1.504803000
6	-4.148980000	1.268362000	-0.888994000
1	-4.771846000	0.656872000	-0.234777000
1	-4.623248000	2.250485000	-0.977011000
1	-4.147953000	0.813301000	-1.883183000
6	-2.504576000	2.378137000	1.407570000
1	-3.210017000	3.211166000	1.337286000
1	-2.855250000	1.708516000	2.195443000
1	-1.541654000	2.788697000	1.722571000
6	-1.426712000	-3.047523000	0.723514000
1	-1.093847000	-3.543089000	-0.190866000
1	-0.551385000	-2.863308000	1.353450000

1	-2.063122000	-3.758786000	1.258563000
6	-3.615557000	-2.087489000	-1.030960000
1	-3.993037000	-3.083158000	-0.780375000
1	-4.472197000	-1.430744000	-1.180826000
1	-3.080925000	-2.169956000	-1.981054000
6	-3.435628000	-1.138328000	1.894007000
1	-4.129678000	-0.303900000	1.781467000
1	-4.019132000	-2.020808000	2.171051000
1	-2.762841000	-0.911110000	2.725002000

Ia-S (T.E.= -939.250417)

14	-0.000004000	-0.946749000	-0.366643000
7	1.217053000	0.216585000	0.179341000
6	0.670945000	1.388317000	0.680784000
6	-0.670939000	1.388324000	0.680784000
7	-1.217051000	0.216588000	0.179342000
1	1.303539000	2.169474000	1.077646000
1	-1.303528000	2.169476000	1.077657000
6	2.611141000	0.058083000	0.050135000
6	3.183794000	-1.192907000	0.259598000
6	4.546997000	-1.372333000	0.111984000
6	5.362494000	-0.304826000	-0.224977000
6	4.797072000	0.943365000	-0.426292000
6	3.431761000	1.126243000	-0.299278000
1	2.550677000	-2.021078000	0.560374000
1	4.976399000	-2.353330000	0.279483000
1	6.431899000	-0.443834000	-0.327741000
1	5.423201000	1.785604000	-0.697654000
1	2.993449000	2.098630000	-0.492730000
6	-2.611141000	0.058086000	0.050137000
6	-3.431765000	1.126249000	-0.299252000
6	-4.797076000	0.943368000	-0.426268000
6	-5.362494000	-0.304828000	-0.224978000
6	-4.546992000	-1.372339000	0.111959000
6	-3.183789000	-1.192911000	0.259574000
1	-2.993463000	2.098643000	-0.492688000
1	-5.423208000	1.785612000	-0.697612000
1	-6.431899000	-0.443838000	-0.327745000
1	-4.976388000	-2.353342000	0.279439000
1	-2.550672000	-2.021088000	0.560334000

Ib-S (T.E.= -2726.727271)

7	1.255496000	0.338080000	0.225692000
6	0.673155000	1.517254000	0.634186000
6	-0.673155000	1.517254000	0.634186000
7	-1.255496000	0.338080000	0.225692000
1	1.283681000	2.338872000	0.984416000
1	-1.283681000	2.338872000	0.984415000
6	2.647400000	0.210901000	0.100321000
6	3.251862000	-1.018214000	0.356220000
6	4.617674000	-1.173835000	0.211172000
6	5.409734000	-0.103105000	-0.170267000
6	4.815626000	1.123253000	-0.417547000
6	3.447093000	1.281794000	-0.293050000
1	2.639676000	-1.847432000	0.696526000
1	5.068556000	-2.138049000	0.416215000
1	6.481568000	-0.222925000	-0.271151000
1	5.422124000	1.968029000	-0.723845000
1	2.988813000	2.236333000	-0.525001000
6	-2.647400000	0.210901000	0.100321000
6	-3.447093000	1.281794000	-0.293049000
6	-4.815626000	1.123253000	-0.417547000
6	-5.409734000	-0.103105000	-0.170267000
6	-4.617674000	-1.173835000	0.211171000
6	-3.251862000	-1.018214000	0.356220000
1	-2.988813000	2.236334000	-0.525001000
1	-5.422124000	1.968029000	-0.723844000
1	-6.481568000	-0.222925000	-0.271151000
1	-5.068556000	-2.138049000	0.416214000
1	-2.639676000	-1.847433000	0.696525000
32	0.000000000	-0.983105000	-0.292701000

H₂ (T.E.= -1.160757)

1	0.000000000	0.000000000	0.373348000
1	0.000000000	0.000000000	-0.373348000

NH₃ (T.E.= -56.509164)

7	0.000000000	0.000000000	0.114387000
1	0.000000000	0.937860000	-0.266904000
1	-0.812210000	-0.468930000	-0.266904000
1	0.812210000	-0.468930000	-0.266904000

CH₃Ph (T.E.= -271.312590)

6	-1.190970000	1.195862000	0.002055000
6	0.193341000	1.192933000	-0.009159000
6	0.907633000	0.000323000	-0.011804000
6	0.193730000	-1.192699000	-0.009155000
6	-1.190430000	-1.196162000	0.002050000
6	-1.889262000	-0.000226000	0.008923000
1	-1.727620000	2.137968000	0.001651000
1	0.735070000	2.134048000	-0.019241000
1	0.735885000	-2.133590000	-0.019221000
1	-1.726777000	-2.138442000	0.001636000
1	-2.972936000	-0.000478000	0.014623000
6	2.402332000	0.000128000	0.009202000
1	2.780169000	-0.014336000	1.035724000
1	2.809036000	-0.877697000	-0.496150000
1	2.808928000	0.891574000	-0.471693000

SiEt₃H (T.E.= -527.468352)

14	0.596999000	0.082557000	-0.042389000
1	1.916492000	-0.607467000	0.026270000
6	-0.239009000	-0.391123000	-1.655928000
1	-1.159239000	0.197369000	-1.748271000
1	0.405786000	-0.069738000	-2.481385000
6	-0.431926000	-0.483277000	1.430181000
1	-0.250920000	0.213138000	2.257162000
1	-1.491466000	-0.365454000	1.171225000
6	0.850480000	1.941164000	0.033495000
1	1.434588000	2.165682000	0.932706000
1	1.470506000	2.252618000	-0.813760000
6	-0.458532000	2.719672000	0.049195000
1	-1.092288000	2.421045000	0.889418000
1	-0.297324000	3.796907000	0.134155000
1	-1.036206000	2.552275000	-0.863562000
6	-0.557517000	-1.874624000	-1.772014000
1	-1.271428000	-2.185030000	-1.004269000
1	-0.993069000	-2.131080000	-2.740660000
1	0.338756000	-2.488768000	-1.643819000
6	-0.147710000	-1.909891000	1.880072000
1	-0.765658000	-2.206356000	2.731261000
1	-0.329563000	-2.631788000	1.079644000

1 0.897576000 -2.025741000 2.176982000

Cartesian coordinates of the transition states involved in the activation of hydrogen by CAASis (1Si-5Si, 8Si-9Si and 14Si) and CAAGes (1Ge-5Ge, 8Ge-9Ge and 14Ge), along with their total energies (in hartrees) including zero point vibrational correction.

1SiTS^{H-H} (T.E.= -1511.632841)

6 -0.974082000 -0.707404000 -1.444993000
6 0.471457000 -0.239741000 -1.570468000
6 1.148641000 -0.039667000 -0.177028000
1 -1.521162000 -0.468978000 -2.363050000
1 -1.023892000 -1.799600000 -1.305299000
1 0.463061000 0.707807000 -2.120604000
1 1.038299000 -0.940713000 -2.193139000
7 -1.560996000 -0.018055000 -0.308586000
14 -0.351049000 0.148946000 0.939558000
14 2.242172000 -1.506091000 0.285412000
14 2.008956000 1.647903000 -0.169815000
6 2.988790000 1.928259000 1.399831000
1 3.881671000 1.301680000 1.456638000
1 3.316305000 2.970655000 1.437290000
1 2.382186000 1.740669000 2.289965000
6 0.709723000 3.000402000 -0.281999000
1 0.097405000 3.059421000 0.622396000
1 1.209156000 3.965998000 -0.401536000
1 0.037441000 2.867029000 -1.132733000
6 3.137861000 1.840407000 -1.653113000
1 3.476268000 2.878375000 -1.711050000
1 4.020941000 1.204584000 -1.583907000
1 2.628100000 1.609810000 -2.591435000
6 2.574945000 -1.576145000 2.127368000
1 3.198785000 -2.449016000 2.339057000
1 3.109412000 -0.694386000 2.485240000
1 1.659783000 -1.681395000 2.714155000
6 1.483016000 -3.130258000 -0.264801000
1 0.519393000 -3.335375000 0.203846000
1 1.353457000 -3.173148000 -1.349370000
1 2.169617000 -3.935709000 0.012298000
6 3.894817000 -1.406669000 -0.600527000
1 4.523232000 -0.587561000 -0.243445000

1	4.443155000	-2.338586000	-0.436292000
1	3.763916000	-1.287600000	-1.679659000
6	-2.936649000	-0.016178000	-0.119127000
6	-3.803512000	-0.732308000	-0.947761000
6	-3.495919000	0.729203000	0.926354000
6	-5.172733000	-0.693631000	-0.737066000
1	-3.409957000	-1.332108000	-1.758642000
6	-4.859195000	0.755579000	1.129166000
1	-2.839608000	1.302274000	1.574776000
6	-5.714470000	0.044335000	0.298514000
1	-5.821492000	-1.259909000	-1.396317000
1	-5.261147000	1.346206000	1.944901000
1	-6.785384000	0.068579000	0.458758000
1	-0.607402000	-0.673542000	2.184813000
1	-0.411813000	-1.546801000	1.424168000

2SiTS^{H-H} (T.E.= -1510.439678)

6	-0.814529000	-0.428569000	-1.570821000
6	0.500194000	-0.192436000	-1.533137000
6	1.165187000	-0.099355000	-0.181195000
7	-1.469877000	-0.626397000	-0.349791000
14	-0.239149000	-0.714640000	0.912486000
14	2.732685000	-1.145284000	-0.079685000
14	1.346798000	1.749100000	0.232690000
6	2.269365000	1.986221000	1.844078000
1	3.305926000	1.646652000	1.792764000
1	2.280557000	3.048201000	2.102961000
1	1.775005000	1.452774000	2.660844000
6	-0.353254000	2.518663000	0.428562000
1	-0.902025000	2.128379000	1.290915000
1	-0.236112000	3.595356000	0.581489000
1	-0.971864000	2.376953000	-0.461016000
6	2.207280000	2.663468000	-1.154731000
1	2.194230000	3.734718000	-0.936625000
1	3.247066000	2.361092000	-1.285579000
1	1.684941000	2.514471000	-2.102708000
6	3.112286000	-1.590200000	1.699478000
1	4.066393000	-2.122362000	1.743454000
1	3.195000000	-0.705536000	2.334105000
1	2.354400000	-2.247985000	2.132469000

6	2.537721000	-2.701935000	-1.099109000
1	1.660605000	-3.286801000	-0.817016000
1	2.452878000	-2.459019000	-2.160946000
1	3.423511000	-3.329615000	-0.968550000
6	4.205419000	-0.240187000	-0.807048000
1	4.518324000	0.629457000	-0.225287000
1	5.053807000	-0.929018000	-0.852081000
1	3.997855000	0.089977000	-1.828847000
6	-2.837556000	-0.429313000	-0.184491000
6	-3.613567000	0.241068000	-1.132283000
6	-3.462822000	-0.894693000	0.974518000
6	-4.969076000	0.423203000	-0.924578000
1	-3.151155000	0.645463000	-2.024710000
6	-4.813490000	-0.691806000	1.179296000
1	-2.874748000	-1.427856000	1.715110000
6	-5.581276000	-0.036886000	0.229135000
1	-5.550834000	0.948292000	-1.673977000
1	-5.272870000	-1.061248000	2.089234000
1	-6.642158000	0.114006000	0.387013000
1	-0.211400000	-1.997159000	1.712465000
1	0.132409000	-2.386252000	0.648149000
1	-1.392743000	-0.501134000	-2.484390000
1	1.076185000	-0.058928000	-2.443622000

3SiTS^{H-H} (T.E.= -1631.735980)

6	0.729064000	1.308607000	0.509445000
6	1.418358000	0.021246000	-0.045835000
1	0.955574000	1.439357000	1.575729000
1	1.139564000	2.207264000	0.030620000
7	-1.318480000	0.114525000	-0.405857000
14	0.039294000	-0.803740000	-1.022583000
14	2.915861000	0.411779000	-1.119512000
14	1.752608000	-1.178700000	1.378305000
6	2.638769000	-2.723931000	0.797358000
1	3.673142000	-2.527514000	0.505452000
1	2.661031000	-3.450944000	1.613778000
1	2.128036000	-3.192114000	-0.048267000
6	0.128047000	-1.712685000	2.160636000
1	-0.534370000	-2.231674000	1.461140000
1	0.345515000	-2.406121000	2.978309000

1	-0.424796000	-0.869291000	2.583778000
6	2.761561000	-0.390766000	2.749031000
1	2.798292000	-1.087139000	3.591586000
1	3.787511000	-0.178245000	2.446291000
1	2.316533000	0.537518000	3.114011000
6	3.282442000	-0.976763000	-2.324762000
1	4.213577000	-0.750590000	-2.852011000
1	3.407777000	-1.940289000	-1.827837000
1	2.500904000	-1.085442000	-3.080406000
6	2.654969000	1.994378000	-2.094446000
1	1.689876000	2.031875000	-2.603418000
1	2.739054000	2.876798000	-1.455434000
1	3.439699000	2.064625000	-2.853252000
6	4.455554000	0.718936000	-0.091261000
1	4.834548000	-0.180055000	0.398948000
1	5.247143000	1.099827000	-0.742883000
1	4.267089000	1.474659000	0.676586000
6	-2.620324000	-0.415709000	-0.429098000
6	-3.354932000	-0.545325000	0.748780000
6	-3.187298000	-0.858137000	-1.620753000
6	-4.629520000	-1.078953000	0.726533000
1	-2.906957000	-0.221389000	1.682954000
6	-4.460168000	-1.403395000	-1.636949000
1	-2.625344000	-0.751366000	-2.543299000
6	-5.190298000	-1.511429000	-0.466015000
1	-5.186781000	-1.169192000	1.652189000
1	-4.885142000	-1.740072000	-2.575750000
1	-6.188084000	-1.933370000	-0.479898000
1	0.084420000	-0.965210000	-2.533659000
1	0.329592000	0.156991000	-2.464105000
5	-0.849325000	1.300530000	0.277453000
7	-1.658695000	2.394939000	0.652647000
6	-3.016163000	2.628827000	0.217831000
1	-3.315085000	1.925812000	-0.556295000
1	-3.731602000	2.549126000	1.046501000
1	-3.103436000	3.640783000	-0.194595000
6	-1.168261000	3.484962000	1.462229000
1	-1.812781000	3.638032000	2.336431000
1	-0.159215000	3.292816000	1.821400000
1	-1.157913000	4.425712000	0.897320000

4SiTS^{H-H} (T.E.= -1841.647014)

6	0.864400000	0.863790000	1.243251000
6	1.376277000	-0.000938000	0.041239000
1	0.938543000	0.310316000	2.187822000
1	1.484842000	1.755202000	1.391885000
7	-1.457685000	0.267112000	-0.183575000
14	-0.096321000	-0.307769000	-1.109876000
14	2.781791000	0.888123000	-0.849886000
14	1.810217000	-1.724823000	0.694450000
6	2.543067000	-2.823280000	-0.633155000
1	3.539321000	-2.495300000	-0.938840000
1	2.634997000	-3.841478000	-0.245362000
1	1.908318000	-2.861629000	-1.522176000
6	0.241911000	-2.552225000	1.321221000
1	-0.444084000	-2.813892000	0.510940000
1	0.510779000	-3.481923000	1.830470000
1	-0.307720000	-1.931570000	2.033957000
6	3.004292000	-1.659696000	2.140203000
1	3.030925000	-2.645963000	2.611755000
1	4.019490000	-1.411644000	1.828179000
1	2.703200000	-0.939561000	2.903868000
6	3.083888000	0.195555000	-2.565008000
1	3.908919000	0.746618000	-3.025138000
1	3.360065000	-0.859961000	-2.547416000
1	2.215939000	0.304966000	-3.219304000
6	2.437533000	2.726162000	-1.019846000
1	1.567311000	2.939100000	-1.643322000
1	2.291207000	3.218939000	-0.055749000
1	3.309040000	3.187626000	-1.493813000
6	4.379990000	0.768666000	0.127688000
1	4.826001000	-0.227404000	0.094545000
1	5.106848000	1.469461000	-0.292149000
1	4.229228000	1.035173000	1.177362000
6	-2.781772000	-0.131719000	-0.417157000
6	-3.843645000	0.742661000	-0.183345000
6	-3.085514000	-1.415564000	-0.875394000
6	-5.154010000	0.343225000	-0.378934000
1	-3.635071000	1.757102000	0.139588000
6	-4.394638000	-1.806914000	-1.079528000
1	-2.277172000	-2.112788000	-1.073004000

6	-5.441567000	-0.933837000	-0.828333000
1	-5.956773000	1.046475000	-0.187270000
1	-4.598443000	-2.811760000	-1.432436000
1	-6.467260000	-1.244517000	-0.985986000
1	-0.081356000	0.205822000	-2.541349000
1	0.160758000	1.179713000	-1.989375000
14	-0.942371000	1.385181000	1.061169000
6	-1.870749000	1.102522000	2.653563000
1	-2.890282000	1.489676000	2.629435000
1	-1.919182000	0.033726000	2.878379000
1	-1.346442000	1.595396000	3.476402000
6	-1.054175000	3.169697000	0.521921000
1	-0.480253000	3.804506000	1.202632000
1	-0.634364000	3.292397000	-0.479648000
1	-2.081673000	3.538788000	0.507828000

5SiTS^{H-H} (T.E.= -1585.698680)

6	0.562347000	-0.517495000	1.481947000
6	1.231011000	-0.148513000	0.138199000
1	0.720094000	-1.576575000	1.722773000
1	0.959056000	0.048919000	2.329959000
14	-0.205662000	-0.391572000	-1.039402000
7	-1.464754000	-0.344503000	0.203605000
14	2.706465000	-1.256049000	-0.287091000
14	1.599567000	1.719744000	0.093487000
6	2.450710000	-2.993338000	0.366784000
1	1.509313000	-3.444676000	0.048007000
1	3.265967000	-3.617468000	-0.010440000
1	2.494480000	-3.027134000	1.457992000
6	4.287031000	-0.646371000	0.511745000
1	5.072994000	-1.387555000	0.342174000
1	4.637504000	0.306112000	0.110473000
1	4.162756000	-0.538243000	1.592656000
6	2.633089000	2.251494000	1.560927000
1	3.634820000	1.821433000	1.563680000
1	2.736352000	3.339696000	1.525069000
1	2.152642000	2.005967000	2.510726000
6	2.461472000	2.197527000	-1.496501000
1	2.543414000	3.286941000	-1.537643000
1	3.471498000	1.789165000	-1.574156000

1	1.894557000	1.876999000	-2.374597000
6	2.953682000	-1.345020000	-2.141444000
1	3.069120000	-0.361972000	-2.601451000
1	3.861777000	-1.917115000	-2.350648000
1	2.128810000	-1.857435000	-2.643259000
6	0.002846000	2.700463000	0.196266000
1	-0.665768000	2.532258000	-0.652393000
1	-0.556320000	2.498977000	1.113409000
1	0.258260000	3.764189000	0.197692000
6	-2.854121000	-0.240178000	-0.050463000
6	-3.781859000	-0.950971000	0.702225000
6	-3.298072000	0.562646000	-1.095040000
6	-5.130312000	-0.847968000	0.411866000
1	-3.442569000	-1.576381000	1.516543000
6	-4.647194000	0.654941000	-1.384573000
1	-2.575481000	1.117392000	-1.685562000
6	-5.570637000	-0.048526000	-0.630179000
1	-5.844668000	-1.404907000	1.007166000
1	-4.976254000	1.285505000	-2.202347000
1	-6.628287000	0.024877000	-0.853634000
6	-0.946512000	-0.335682000	1.483161000
8	-1.587961000	-0.211388000	2.499741000
1	-0.375120000	-1.534641000	-2.012207000
1	-0.078066000	-2.119501000	-1.030585000

8SiTS^{H-H} (T.E.= -1154.306988)

6	0.522609000	-1.629363000	-0.060486000
6	-0.985722000	-1.614945000	0.190593000
6	-1.529154000	-0.242258000	-0.183783000
1	1.009516000	-2.375879000	0.576036000
1	0.717560000	-1.905133000	-1.111331000
1	-1.172326000	-1.841434000	1.250528000
1	-1.437297000	-2.432317000	-0.387084000
7	1.061859000	-0.301945000	0.201881000
14	-0.141403000	0.869011000	-0.315735000
6	2.429459000	-0.100109000	0.131056000
6	3.331501000	-1.132407000	-0.146492000
6	2.955843000	1.180838000	0.349627000
6	4.694819000	-0.887820000	-0.188832000
1	2.970330000	-2.134674000	-0.336355000

6	4.313587000	1.413045000	0.298548000
1	2.273414000	1.994628000	0.577124000
6	5.201336000	0.379593000	0.030524000
1	5.368680000	-1.709903000	-0.405026000
1	4.686009000	2.416180000	0.475595000
1	6.268248000	0.563329000	-0.006525000
1	0.314698000	1.763021000	-1.440053000
1	0.427039000	0.715983000	-2.091897000
15	-3.143550000	0.145539000	0.022381000
6	-3.459913000	1.892760000	-0.250936000
1	-3.179653000	2.162198000	-1.269691000
1	-4.520298000	2.101926000	-0.101457000
1	-2.869663000	2.487529000	0.447223000
6	-4.277311000	-0.731819000	-1.083145000
1	-4.136021000	-1.807127000	-0.957013000
1	-5.317929000	-0.483818000	-0.864204000
1	-4.044931000	-0.472086000	-2.116260000
6	-3.827853000	-0.241753000	1.655563000
1	-3.308560000	0.344755000	2.414304000
1	-4.898997000	-0.036350000	1.698837000
1	-3.665149000	-1.301023000	1.865236000

9SiTS^{H-H} (T.E.= -1153.120910)

6	-0.429144000	-1.535915000	-0.254590000
6	0.910248000	-1.549524000	-0.133485000
6	1.528901000	-0.315742000	0.332567000
14	0.178730000	0.869728000	0.429156000
7	-1.053992000	-0.312905000	0.046970000
15	3.141721000	0.061382000	0.022940000
6	4.309309000	-1.127817000	0.706389000
1	4.049063000	-2.123857000	0.343285000
1	5.329954000	-0.893897000	0.398478000
1	4.238602000	-1.124812000	1.794048000
6	3.555120000	1.676124000	0.689488000
1	4.620171000	1.874102000	0.561424000
1	2.988719000	2.442672000	0.155958000
1	3.301273000	1.713797000	1.748943000
6	3.558223000	0.135035000	-1.733832000
1	2.887102000	0.846544000	-2.219419000
1	4.596195000	0.432192000	-1.893879000

1	3.390670000	-0.850054000	-2.173806000
6	-2.432493000	-0.133897000	0.015109000
6	-2.953343000	1.143708000	-0.200167000
6	-3.324326000	-1.192716000	0.196302000
6	-4.318724000	1.355629000	-0.219237000
1	-2.273746000	1.971002000	-0.379372000
6	-4.688545000	-0.971895000	0.162504000
1	-2.945842000	-2.189524000	0.387882000
6	-5.198883000	0.300370000	-0.041389000
1	-4.698094000	2.356910000	-0.389948000
1	-5.363036000	-1.808310000	0.308961000
1	-6.269137000	0.466446000	-0.063611000
1	-1.039556000	-2.374220000	-0.558533000
1	1.482008000	-2.449226000	-0.339172000
1	0.073023000	2.259663000	-0.131726000
1	0.284471000	1.843817000	-1.348547000

14SiTS^{H-H} (T.E.= -1348.475296)

6	1.670935000	-0.316999000	0.028498000
7	-0.981012000	-0.248114000	-0.141993000
14	0.280476000	-1.461441000	-0.136428000
6	-2.328184000	-0.613124000	0.036949000
6	-3.074682000	-0.093898000	1.092774000
6	-2.930092000	-1.529800000	-0.820121000
6	-4.394340000	-0.465430000	1.268546000
1	-2.602644000	0.607553000	1.772805000
6	-4.249528000	-1.907381000	-0.634359000
1	-2.358066000	-1.924178000	-1.654404000
6	-4.990161000	-1.373921000	0.406276000
1	-4.961312000	-0.048528000	2.093305000
1	-4.702705000	-2.619019000	-1.315215000
1	-6.023798000	-1.666012000	0.548580000
1	0.173267000	-2.599273000	-1.124162000
1	0.379625000	-1.769233000	-1.952625000
15	3.351860000	-0.585540000	0.097107000
6	4.134146000	-0.028262000	1.617802000
1	5.213899000	-0.181843000	1.573742000
1	3.912611000	1.032101000	1.739069000
1	3.718144000	-0.580093000	2.461079000
6	3.698178000	-2.342218000	-0.052035000

1	3.294494000	-2.711030000	-0.997202000
1	4.774613000	-2.518165000	-0.027742000
1	3.225857000	-2.882571000	0.769456000
6	4.252613000	0.219539000	-1.235775000
1	4.062663000	1.291129000	-1.178623000
1	5.323413000	0.026029000	-1.149292000
1	3.885134000	-0.158678000	-2.190573000
6	1.194634000	1.031764000	0.097537000
8	1.953227000	2.004307000	0.274715000
5	-0.412715000	1.089586000	-0.110145000
7	-1.132040000	2.279471000	-0.318845000
6	-2.478531000	2.366088000	-0.834262000
1	-2.813007000	1.419057000	-1.252782000
1	-3.195770000	2.667064000	-0.059292000
1	-2.517015000	3.120020000	-1.628248000
6	-0.578378000	3.590162000	-0.047441000
1	-1.192961000	4.115488000	0.694556000
1	0.441072000	3.499741000	0.320804000
1	-0.572613000	4.202699000	-0.957311000

1GeTS^{H-H} (T.E.= -3299.096076)

6	-0.946325000	0.572631000	1.565920000
6	0.521227000	0.179289000	1.665527000
6	1.212156000	0.049671000	0.277019000
1	-1.432887000	0.400037000	2.532842000
1	-1.043032000	1.647333000	1.334670000
1	0.562503000	-0.776833000	2.200398000
1	1.052691000	0.899207000	2.298738000
32	-0.340137000	-0.379368000	-0.870473000
7	-1.567793000	-0.235773000	0.537804000
14	2.064074000	1.649852000	-0.256225000
14	2.300468000	-1.499246000	0.277850000
6	1.219002000	-3.024650000	0.448178000
1	0.634866000	-3.215020000	-0.456614000
1	1.857584000	-3.896895000	0.613054000
1	0.523336000	-2.960778000	1.288094000
6	3.274869000	-1.670010000	-1.310274000
1	4.044663000	-0.901521000	-1.411103000
1	3.774220000	-2.642383000	-1.321751000
1	2.625957000	-1.621212000	-2.189166000

6	3.482082000	-1.484616000	1.732829000
1	2.967027000	-1.292139000	2.676829000
1	3.956553000	-2.466478000	1.813521000
1	4.273336000	-0.741380000	1.624101000
6	2.346992000	1.707254000	-2.106331000
1	1.411415000	1.699250000	-2.670350000
1	2.865071000	2.638523000	-2.352192000
1	2.967644000	0.882108000	-2.459824000
6	1.092683000	3.166253000	0.259666000
1	0.950878000	3.212942000	1.342279000
1	1.661402000	4.053079000	-0.034966000
1	0.113109000	3.219511000	-0.217927000
6	3.733570000	1.800819000	0.590106000
1	3.650094000	1.694618000	1.675094000
1	4.455873000	1.063685000	0.232180000
1	4.145280000	2.793072000	0.386194000
6	-2.928202000	-0.119566000	0.305647000
6	-3.527678000	-0.867161000	-0.717560000
6	-3.751464000	0.713329000	1.070241000
6	-4.881602000	-0.782714000	-0.962507000
1	-2.910505000	-1.536014000	-1.310640000
6	-5.112409000	0.784287000	0.818363000
1	-3.329352000	1.312686000	1.866533000
6	-5.691073000	0.045043000	-0.196190000
1	-5.313481000	-1.377670000	-1.759680000
1	-5.725443000	1.437952000	1.429416000
1	-6.755156000	0.107753000	-0.388396000
1	-0.821472000	0.295669000	-2.190675000
1	-0.669777000	1.333455000	-1.406702000

2GeTS^{H-H} (T.E.= -3296.726623)

6	0.822604000	0.134214000	-1.648380000
6	-0.500834000	-0.060413000	-1.597745000
6	-1.215517000	-0.003178000	-0.274159000
32	0.226036000	0.704129000	0.876031000
7	1.505809000	0.462706000	-0.486745000
14	-2.734529000	1.118564000	-0.310416000
14	-1.477166000	-1.798489000	0.303334000
6	0.190019000	-2.601825000	0.612331000
1	0.706110000	-2.189567000	1.484388000

1	0.042842000	-3.669386000	0.798090000
1	0.851896000	-2.502309000	-0.252013000
6	-2.460568000	-1.856624000	1.895865000
1	-3.493307000	-1.526381000	1.763535000
1	-2.487361000	-2.882771000	2.271596000
1	-2.002131000	-1.234643000	2.669932000
6	-2.332565000	-2.797148000	-1.027418000
1	-1.751651000	-2.788055000	-1.952491000
1	-2.409036000	-3.836572000	-0.697080000
1	-3.339596000	-2.442950000	-1.251609000
6	-3.147714000	1.718104000	1.415120000
1	-2.370171000	2.372723000	1.817498000
1	-4.074115000	2.297961000	1.385877000
1	-3.295157000	0.894054000	2.116279000
6	-2.435804000	2.579270000	-1.437611000
1	-2.329883000	2.255999000	-2.475899000
1	-3.290545000	3.259143000	-1.383119000
1	-1.537462000	3.135844000	-1.164515000
6	-4.215406000	0.206468000	-1.012119000
1	-3.979630000	-0.234055000	-1.984843000
1	-4.586650000	-0.586797000	-0.359902000
1	-5.031509000	0.918630000	-1.162707000
6	2.869144000	0.278394000	-0.321127000
6	3.527777000	0.918697000	0.732100000
6	3.619682000	-0.539686000	-1.170188000
6	4.884837000	0.752009000	0.924045000
1	2.959800000	1.565784000	1.393713000
6	4.981430000	-0.687589000	-0.976836000
1	3.128694000	-1.080388000	-1.970947000
6	5.626934000	-0.046846000	0.067648000
1	5.370660000	1.262555000	1.748088000
1	5.542513000	-1.328296000	-1.648159000
1	6.692694000	-0.171014000	0.215370000
1	0.326765000	2.052754000	1.646987000
1	-0.063746000	2.433643000	0.449290000
1	1.389288000	0.082920000	-2.571764000
1	-1.063531000	-0.274022000	-2.501378000

3GeTS^{H-H} (T.E.= -3419.198949)

6	-0.745157000	1.389664000	-0.381767000
6	-1.445303000	0.046782000	-0.020476000
32	0.016724000	-1.263649000	-0.265291000
7	1.390361000	0.006008000	-0.379078000
14	-1.986785000	0.096107000	1.785389000
14	-2.771974000	-0.348839000	-1.299563000
6	-1.947184000	-0.633368000	-2.963247000
1	-1.418978000	-1.590266000	-2.991446000
1	-2.702619000	-0.651596000	-3.753357000
1	-1.229180000	0.152624000	-3.212525000
6	-3.726979000	-1.893173000	-0.846585000
1	-4.396072000	-1.719722000	-0.000634000
1	-4.339506000	-2.214100000	-1.692955000
1	-3.059875000	-2.720011000	-0.586341000
6	-3.966628000	1.082459000	-1.496675000
1	-3.444426000	2.029040000	-1.655325000
1	-4.601088000	0.905063000	-2.369112000
1	-4.617821000	1.200247000	-0.629314000
6	-2.469064000	-1.587548000	2.453785000
1	-1.727424000	-2.361546000	2.246026000
1	-2.576478000	-1.521479000	3.539859000
1	-3.427697000	-1.915375000	2.047228000
6	-0.631716000	0.854473000	2.837881000
1	-0.415889000	1.884026000	2.539270000
1	-0.959062000	0.875638000	3.881035000
1	0.296520000	0.281334000	2.788755000
6	-3.491543000	1.208101000	1.966402000
1	-3.354462000	2.172427000	1.470402000
1	-4.391030000	0.741978000	1.556430000
1	-3.674812000	1.402674000	3.026700000
6	2.692430000	-0.447448000	-0.116253000
6	3.306380000	-1.373860000	-0.955807000
6	3.377679000	-0.016350000	1.018811000
6	4.581248000	-1.837797000	-0.680697000
1	2.772700000	-1.711656000	-1.838693000
6	4.655760000	-0.473292000	1.283568000
1	2.892369000	0.692169000	1.682634000
6	5.264583000	-1.386500000	0.436275000
1	5.046401000	-2.552571000	-1.350093000

1	5.178039000	-0.119508000	2.165352000
1	6.264279000	-1.746613000	0.648102000
1	0.444529000	-2.508326000	0.578098000
1	0.389021000	-1.621936000	1.502300000
5	0.854302000	1.332180000	-0.417606000
7	1.615601000	2.516994000	-0.582544000
6	1.055357000	3.842772000	-0.480365000
1	1.634121000	4.454021000	0.223401000
1	1.074010000	4.360745000	-1.448341000
1	0.026048000	3.818238000	-0.128684000
6	3.010847000	2.567771000	-0.951683000
1	3.641334000	2.930056000	-0.128855000
1	3.381633000	1.592070000	-1.256994000
1	3.147058000	3.256225000	-1.794249000
1	-1.065919000	1.742227000	-1.373638000
1	-1.088085000	2.177923000	0.298969000

4GeTS^{H-H} (T.E.= -3629.106442)

6	0.906607000	0.089016000	1.586081000
6	1.441697000	-0.010062000	0.126068000
1	1.226310000	-0.783860000	2.171371000
1	1.337398000	0.955658000	2.105500000
7	-1.479917000	0.047455000	0.065329000
14	2.887925000	-1.233279000	0.076356000
14	1.864714000	1.719414000	-0.546992000
6	2.378031000	-2.969916000	0.568118000
1	1.804917000	-3.473875000	-0.211796000
1	3.289862000	-3.549281000	0.742986000
1	1.785981000	-2.997232000	1.485785000
6	4.208341000	-0.730953000	1.312519000
1	4.922337000	-1.553155000	1.409952000
1	4.761795000	0.157289000	1.009087000
1	3.786463000	-0.543170000	2.302833000
6	3.443705000	2.393781000	0.203459000
1	4.334757000	1.910408000	-0.201808000
1	3.508212000	3.459389000	-0.033777000
1	3.463982000	2.293045000	1.291017000
6	2.046854000	1.735221000	-2.412090000
1	2.354222000	2.740719000	-2.714689000
1	2.796979000	1.033633000	-2.779662000

1	1.104104000	1.516486000	-2.920081000
6	3.656181000	-1.343718000	-1.629623000
1	4.202961000	-0.437184000	-1.899022000
1	4.366036000	-2.174965000	-1.649782000
1	2.906798000	-1.529585000	-2.404480000
6	0.511694000	2.947212000	-0.125991000
1	-0.469291000	2.637764000	-0.495102000
1	0.433501000	3.119982000	0.949850000
1	0.762870000	3.903785000	-0.593099000
14	-0.984577000	0.118369000	1.733612000
6	-1.616507000	1.614250000	2.654482000
1	-1.414524000	2.547961000	2.126844000
1	-2.693479000	1.539820000	2.822039000
1	-1.134503000	1.666298000	3.634717000
6	-1.592218000	-1.411149000	2.614995000
1	-1.259733000	-2.312262000	2.091798000
1	-1.224850000	-1.457220000	3.643151000
1	-2.685150000	-1.421844000	2.645871000
32	-0.086600000	-0.593101000	-0.998267000
6	-2.824779000	-0.062907000	-0.310237000
6	-3.317621000	-1.198720000	-0.954088000
6	-3.716092000	0.977008000	-0.035366000
6	-4.650651000	-1.286724000	-1.316572000
1	-2.646741000	-2.028708000	-1.152694000
6	-5.049607000	0.877899000	-0.386721000
1	-3.338470000	1.875874000	0.441228000
6	-5.526078000	-0.252396000	-1.033046000
1	-5.008612000	-2.178962000	-1.818166000
1	-5.721464000	1.699733000	-0.165418000
1	-6.569570000	-0.323921000	-1.315365000
1	-0.272436000	-2.037896000	-1.571099000
1	-0.130245000	-2.277784000	-0.314365000

5GeTS^{H-H} (T.E.= -3373.163675)

6	-0.606013000	0.138125000	1.641190000
6	-1.284934000	0.005557000	0.264250000
1	-0.995999000	0.982358000	2.218648000
1	-0.781657000	-0.755765000	2.252860000
7	1.471039000	-0.239118000	0.473317000
14	-1.532136000	1.723805000	-0.518326000

14	-2.814188000	-1.113166000	0.274656000
6	0.122358000	2.578307000	-0.747412000
1	0.818649000	2.037080000	-1.394419000
1	-0.055982000	3.555232000	-1.205873000
1	0.620476000	2.754046000	0.210050000
6	-2.542566000	2.834173000	0.597678000
1	-2.576696000	3.830235000	0.147454000
1	-3.569595000	2.493915000	0.730934000
1	-2.085771000	2.941930000	1.584035000
6	-4.360729000	-0.164322000	0.740118000
1	-4.666413000	0.561188000	-0.016347000
1	-5.181581000	-0.875690000	0.866794000
1	-4.232745000	0.363235000	1.689201000
6	-3.065787000	-1.884385000	-1.414298000
1	-3.990137000	-2.468397000	-1.404446000
1	-3.155318000	-1.139058000	-2.207535000
1	-2.257397000	-2.569832000	-1.682862000
6	-2.358774000	1.580023000	-2.190847000
1	-3.402409000	1.264665000	-2.122850000
1	-2.345524000	2.559817000	-2.675693000
1	-1.834112000	0.882360000	-2.849269000
6	-2.640981000	-2.474441000	1.548340000
1	-1.727578000	-3.060912000	1.432395000
1	-2.669862000	-2.080926000	2.567123000
1	-3.491782000	-3.152668000	1.436946000
6	2.854720000	-0.212190000	0.205024000
6	3.639812000	0.901391000	0.489134000
6	3.438372000	-1.315463000	-0.407896000
6	4.983677000	0.897821000	0.162324000
1	3.194379000	1.761811000	0.969449000
6	4.781664000	-1.308481000	-0.738186000
1	2.832223000	-2.192906000	-0.610712000
6	5.561781000	-0.201260000	-0.452530000
1	5.585321000	1.770863000	0.388018000
1	5.220266000	-2.177120000	-1.215614000
1	6.614757000	-0.193921000	-0.707421000
6	0.909741000	0.293005000	1.603242000
8	1.518984000	0.800453000	2.519804000
32	0.174926000	-0.802680000	-0.779937000
1	0.365252000	-2.266103000	-1.272625000

1 -0.023048000 -2.425606000 -0.031304000

8GeTS^{H-H} (T.E.= -2940.803130)

6 0.547546000 1.729960000 0.129110000
6 -0.961274000 1.737207000 -0.097606000
6 -1.558424000 0.414190000 0.366322000
1 1.013289000 2.532408000 -0.453919000
1 0.755582000 1.924852000 1.196559000
1 -1.147396000 1.925453000 -1.167364000
1 -1.380955000 2.591996000 0.447449000
32 -0.154409000 -0.845110000 0.310258000
7 1.089121000 0.441021000 -0.258539000
6 2.452276000 0.231724000 -0.187888000
6 2.979491000 -1.035286000 -0.480715000
6 3.358045000 1.244231000 0.151704000
6 4.336370000 -1.272899000 -0.440019000
1 2.297574000 -1.833428000 -0.760377000
6 4.720482000 0.994646000 0.181970000
1 2.998523000 2.234819000 0.398386000
6 5.225805000 -0.258896000 -0.109879000
1 4.707251000 -2.264810000 -0.674700000
1 5.395345000 1.801500000 0.447376000
1 6.292212000 -0.446793000 -0.081020000
1 0.419548000 -1.877275000 1.311673000
1 0.543799000 -0.768901000 2.074129000
15 -3.126443000 0.003381000 -0.072313000
6 -3.512565000 -0.148700000 -1.843582000
1 -4.575140000 -0.331046000 -2.017799000
1 -3.222836000 0.774054000 -2.350585000
1 -2.928173000 -0.969729000 -2.263292000
6 -4.318496000 1.237556000 0.486775000
1 -5.332105000 0.968385000 0.184859000
1 -4.263968000 1.328468000 1.571543000
1 -4.063922000 2.201800000 0.042288000
6 -3.624287000 -1.572498000 0.632971000
1 -2.959918000 -2.359247000 0.269680000
1 -3.556957000 -1.525866000 1.719556000
1 -4.647699000 -1.808381000 0.336783000

9GeTS^{H-H} (T.E.= -2940.584042)

6	-0.454401000	1.659359000	-0.110415000
6	0.880998000	1.681426000	0.060509000
6	1.549036000	0.444372000	0.434508000
7	-1.099233000	0.429080000	0.032308000
15	3.119781000	0.091653000	-0.073352000
6	3.360763000	0.106901000	-1.864667000
1	3.166624000	1.115788000	-2.234244000
1	4.372340000	-0.193738000	-2.142802000
1	2.632095000	-0.572014000	-2.315298000
6	3.604232000	-1.550923000	0.464362000
1	4.642136000	-1.745827000	0.191169000
1	3.486001000	-1.637409000	1.544452000
1	2.967070000	-2.287872000	-0.030411000
6	4.337029000	1.260391000	0.554270000
1	4.366288000	1.206530000	1.642426000
1	5.326227000	1.051963000	0.143161000
1	4.037185000	2.268491000	0.261995000
32	0.190857000	-0.867472000	0.404406000
6	-2.470568000	0.256303000	-0.034825000
6	-3.368486000	1.307105000	0.178477000
6	-2.993547000	-1.008837000	-0.320714000
6	-4.731744000	1.090370000	0.107214000
1	-2.995259000	2.293671000	0.424778000
6	-4.357754000	-1.216008000	-0.377092000
1	-2.312645000	-1.829907000	-0.523853000
6	-5.241462000	-0.169021000	-0.166365000
1	-5.407158000	1.921004000	0.280823000
1	-4.734256000	-2.207706000	-0.602222000
1	-6.311205000	-0.331677000	-0.216372000
1	-1.047415000	2.529605000	-0.355820000
1	1.429904000	2.613087000	-0.038350000
1	0.068510000	-2.278660000	-0.202782000
1	0.419470000	-1.703219000	-1.445091000

14GeTS^{H-H} (T.E.= -3134.759421)

6	-1.672499000	-0.146826000	-0.108534000
32	-0.271241000	-1.407146000	0.050702000
7	1.051177000	-0.088726000	0.112246000
6	2.395246000	-0.453205000	-0.050785000

6	3.169765000	0.099300000	-1.070860000
6	2.977625000	-1.403206000	0.785516000
6	4.491904000	-0.271008000	-1.229474000
1	2.716177000	0.826748000	-1.736033000
6	4.299480000	-1.778498000	0.616906000
1	2.385015000	-1.824911000	1.592129000
6	5.065975000	-1.211550000	-0.387298000
1	5.078439000	0.172770000	-2.026181000
1	4.734943000	-2.515096000	1.282780000
1	6.101566000	-1.502675000	-0.516738000
1	-0.107946000	-2.654358000	0.955939000
1	-0.379227000	-1.786085000	1.912028000
15	-3.361336000	-0.372880000	-0.100780000
6	-4.210660000	0.250396000	-1.558608000
1	-5.286946000	0.091041000	-1.469430000
1	-3.997398000	1.315712000	-1.645183000
1	-3.834393000	-0.263354000	-2.443511000
6	-4.177713000	0.400043000	1.304221000
1	-5.256518000	0.239530000	1.258873000
1	-3.778487000	-0.029719000	2.223969000
1	-3.959762000	1.467561000	1.284026000
6	-3.738744000	-2.126160000	0.008305000
1	-3.310437000	-2.652193000	-0.846120000
1	-3.311605000	-2.530945000	0.928209000
1	-4.819059000	-2.278045000	0.019448000
5	0.459800000	1.229159000	0.087853000
6	-1.151387000	1.182045000	-0.124656000
8	-1.897679000	2.173352000	-0.248815000
7	1.165695000	2.426808000	0.323743000
6	0.626782000	3.740144000	0.039997000
1	0.592491000	4.350124000	0.951262000
1	1.268614000	4.266157000	-0.678576000
1	-0.380302000	3.657418000	-0.360951000
6	2.497188000	2.508899000	0.876061000
1	2.818336000	1.559270000	1.299427000
1	3.237738000	2.812416000	0.123837000
1	2.515080000	3.259090000	1.674644000

Cartesian coordinates of the intermediates involved in the activation of N – H bond of NH₃ by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and NacNacSi (**IIa**), along with their total energies (in hartrees) including zero point vibrational correction.

1SiInt^{N-H} (T.E.= -1567.044271)

6	-0.917348000	-0.398974000	-1.589565000
6	0.535800000	0.016472000	-1.657411000
6	1.145499000	0.032785000	-0.227167000
1	-1.456606000	-0.091262000	-2.493409000
1	-0.999828000	-1.503105000	-1.547784000
1	0.569318000	1.017044000	-2.106085000
1	1.087701000	-0.631363000	-2.350159000
7	-1.483097000	0.229668000	-0.411717000
14	-0.351474000	0.202796000	0.994721000
14	2.268813000	-1.431934000	0.065388000
14	2.039764000	1.687391000	-0.023042000
6	3.021919000	1.795716000	1.569830000
1	3.883639000	1.123567000	1.561332000
1	3.399894000	2.814522000	1.691525000
1	2.409860000	1.557879000	2.443178000
6	0.794306000	3.096807000	-0.041126000
1	0.125943000	3.075502000	0.823181000
1	1.336566000	4.046757000	-0.021501000
1	0.176191000	3.085729000	-0.942100000
6	3.215207000	2.027077000	-1.450325000
1	3.481555000	3.087786000	-1.439988000
1	4.139325000	1.452398000	-1.375955000
1	2.763041000	1.812173000	-2.421336000
6	2.643002000	-1.712505000	1.886077000
1	3.114847000	-2.691011000	2.013091000
1	3.336918000	-0.961139000	2.267880000
1	1.759934000	-1.679907000	2.528446000
6	1.533055000	-3.028741000	-0.624030000
1	0.716253000	-3.449786000	-0.034171000
1	1.177899000	-2.906466000	-1.650368000
1	2.323621000	-3.784375000	-0.644567000
6	3.920236000	-1.274256000	-0.815713000
1	4.555944000	-0.503375000	-0.374012000
1	4.457015000	-2.224886000	-0.750685000
1	3.790439000	-1.036563000	-1.874948000

6	-2.858979000	0.186775000	-0.240593000
6	-3.702414000	-0.570127000	-1.063569000
6	-3.456670000	0.916402000	0.800099000
6	-5.072477000	-0.593608000	-0.848928000
1	-3.289342000	-1.146735000	-1.882046000
6	-4.818884000	0.877588000	1.008026000
1	-2.824611000	1.530018000	1.433607000
6	-5.644819000	0.120730000	0.186431000
1	-5.697117000	-1.187224000	-1.507969000
1	-5.246178000	1.459282000	1.817642000
1	-6.715685000	0.099095000	0.348079000
7	-0.899709000	-1.834532000	1.325986000
1	-1.806080000	-1.763458000	1.780790000
1	-1.025721000	-2.389044000	0.482538000
1	-0.289118000	-2.346374000	1.954734000

2SiInt^{N-H} (T.E.= -1565.858236)

6	-1.152884000	-0.031200000	-0.196675000
6	-0.509047000	-0.009394000	-1.552711000
6	0.823929000	-0.133153000	-1.573546000
1	-1.073623000	0.141564000	-2.469287000
1	1.421767000	-0.090718000	-2.478110000
14	0.239390000	-0.698108000	0.974191000
7	1.452700000	-0.359145000	-0.352640000
14	-2.789675000	-0.942484000	-0.148809000
14	-1.302964000	1.798836000	0.307944000
6	-4.209107000	0.049831000	-0.872947000
1	-5.103343000	-0.579078000	-0.903305000
1	-4.447954000	0.941768000	-0.290784000
1	-3.988792000	0.363514000	-1.897064000
6	-3.255130000	-1.448030000	1.596099000
1	-4.212792000	-1.975989000	1.580124000
1	-2.515934000	-2.115729000	2.046421000
1	-3.358799000	-0.587208000	2.259088000
6	-2.731766000	-2.506703000	-1.201679000
1	-3.757299000	-2.823420000	-1.409608000
1	-2.242652000	-2.332558000	-2.163646000
1	-2.238881000	-3.351620000	-0.716231000
6	-2.260881000	2.012244000	1.906873000
1	-2.250932000	3.069264000	2.187284000

1	-3.304541000	1.700981000	1.827809000
1	-1.795956000	1.447150000	2.719111000
6	0.378593000	2.593759000	0.575191000
1	0.939302000	2.157593000	1.405519000
1	1.001124000	2.544578000	-0.321505000
1	0.214148000	3.650826000	0.806819000
6	-2.117459000	2.816962000	-1.041424000
1	-3.145633000	2.522102000	-1.253597000
1	-2.126295000	3.864957000	-0.728078000
1	-1.544979000	2.756624000	-1.970020000
6	2.825035000	-0.216367000	-0.196344000
6	3.463758000	-0.781321000	0.914892000
6	3.615813000	0.490165000	-1.109172000
6	4.826892000	-0.655328000	1.094351000
1	2.868563000	-1.312122000	1.651757000
6	4.982906000	0.598519000	-0.926699000
1	3.152546000	0.982040000	-1.956201000
6	5.604094000	0.027446000	0.171105000
1	5.288920000	-1.102981000	1.967575000
1	5.568215000	1.153194000	-1.652054000
1	6.674243000	0.119914000	0.310324000
7	0.196230000	-2.667512000	0.290895000
1	1.124847000	-3.049958000	0.444280000
1	-0.467779000	-3.277610000	0.756290000
1	0.017006000	-2.690473000	-0.711153000

3SiInt^{N-H} (T.E.= -1687.144782)

6	0.743155000	1.195556000	0.789183000
6	1.386897000	0.014438000	0.008733000
1	1.012834000	1.179227000	1.854179000
1	1.135042000	2.165090000	0.446559000
14	0.065254000	-0.591634000	-1.272558000
7	-1.282135000	0.186274000	-0.341419000
5	-0.835333000	1.200582000	0.580576000
7	-1.651416000	2.205737000	1.163795000
6	-1.171054000	3.097282000	2.191721000
1	-1.149549000	4.137908000	1.841733000
1	-1.826705000	3.067537000	3.071351000
1	-0.168219000	2.825450000	2.514672000
6	-3.004717000	2.527530000	0.779594000

1	-3.092448000	3.605373000	0.595780000
1	-3.296935000	2.006219000	-0.129656000
1	-3.729584000	2.270595000	1.563436000
14	1.523423000	-1.466401000	1.181278000
14	3.046171000	0.451517000	-0.740966000
6	-0.170047000	-2.118465000	1.674958000
1	-0.762817000	-2.483545000	0.832328000
1	-0.030422000	-2.948779000	2.373955000
1	-0.758978000	-1.350162000	2.183885000
6	2.336055000	-1.023046000	2.818759000
1	2.363672000	-1.929522000	3.431241000
1	3.357303000	-0.654911000	2.720895000
1	1.757043000	-0.279626000	3.371617000
6	4.453032000	0.493119000	0.504727000
1	4.704800000	-0.490033000	0.906664000
1	5.348714000	0.895364000	0.022790000
1	4.204447000	1.148636000	1.344463000
6	3.530411000	-0.701301000	-2.141870000
1	4.484851000	-0.376298000	-2.566095000
1	3.645806000	-1.734054000	-1.809702000
1	2.791260000	-0.704598000	-2.947599000
6	2.467114000	-2.907545000	0.437261000
1	3.533339000	-2.704090000	0.314595000
1	2.372470000	-3.767515000	1.106437000
1	2.058255000	-3.194797000	-0.534594000
6	3.087064000	2.197920000	-1.466830000
1	2.470595000	2.355856000	-2.354042000
1	2.824990000	2.963039000	-0.732236000
1	4.120525000	2.390734000	-1.769946000
6	-2.580661000	-0.331436000	-0.442641000
6	-3.323828000	-0.634906000	0.700983000
6	-3.161995000	-0.603083000	-1.682226000
6	-4.600073000	-1.154967000	0.606182000
1	-2.880304000	-0.455045000	1.674752000
6	-4.437451000	-1.133513000	-1.775097000
1	-2.601634000	-0.393335000	-2.587572000
6	-5.169785000	-1.406533000	-0.632835000
1	-5.152744000	-1.377387000	1.512365000
1	-4.862452000	-1.329979000	-2.753235000
1	-6.169654000	-1.817423000	-0.705605000

7	0.184090000	1.079974000	-2.533187000
1	-0.715540000	1.159752000	-2.997172000
1	0.891265000	0.983886000	-3.255268000
1	0.351071000	1.954576000	-2.040337000

4SiInt^{N-H} (T.E.= -1897.053880)

6	-0.903131000	-0.348673000	1.534840000
6	-1.354233000	0.036067000	0.083641000
1	-1.104693000	0.459873000	2.249222000
1	-1.458016000	-1.206925000	1.934220000
14	0.130395000	0.195217000	-1.180470000
7	1.411341000	-0.063520000	0.038814000
14	-1.959507000	1.830341000	0.163697000
14	-2.705836000	-1.126070000	-0.489221000
6	-0.515319000	2.990120000	0.500850000
1	0.163707000	3.061657000	-0.352123000
1	-0.908667000	3.992181000	0.695907000
1	0.068727000	2.687979000	1.374462000
6	-3.169863000	2.139459000	1.570815000
1	-3.396615000	3.210033000	1.579824000
1	-4.111605000	1.601516000	1.455430000
1	-2.756260000	1.888482000	2.549861000
6	-4.309907000	-0.917569000	0.467300000
1	-4.827414000	0.007775000	0.206647000
1	-4.980043000	-1.749424000	0.233506000
1	-4.141680000	-0.917060000	1.547505000
6	-3.122122000	-0.945078000	-2.314011000
1	-3.713143000	-1.806859000	-2.637247000
1	-3.716357000	-0.048670000	-2.500316000
1	-2.240990000	-0.878942000	-2.957069000
6	-2.793251000	2.415532000	-1.411822000
1	-3.785234000	1.975976000	-1.541611000
1	-2.920811000	3.500651000	-1.359316000
1	-2.197170000	2.188408000	-2.298379000
6	-2.228893000	-2.936065000	-0.214486000
1	-1.609442000	-3.349538000	-1.013244000
1	-1.719082000	-3.110642000	0.736280000
1	-3.145988000	-3.531432000	-0.199116000
14	0.940513000	-0.695102000	1.583325000
6	1.245056000	-2.536762000	1.814181000

1	0.835712000	-3.143173000	1.000683000
1	2.309137000	-2.767734000	1.902772000
1	0.760308000	-2.871317000	2.736363000
6	1.845125000	0.203232000	2.947276000
1	1.689611000	1.281924000	2.864014000
1	1.501612000	-0.118153000	3.933341000
1	2.920372000	0.014813000	2.890316000
6	2.756182000	0.151629000	-0.309137000
6	3.697562000	-0.878967000	-0.258146000
6	3.189595000	1.411979000	-0.723943000
6	5.022469000	-0.652827000	-0.594913000
1	3.376310000	-1.871433000	0.045057000
6	4.509762000	1.631843000	-1.070313000
1	2.468248000	2.221050000	-0.760071000
6	5.436581000	0.602353000	-1.005537000
1	5.734024000	-1.469524000	-0.542023000
1	4.820177000	2.621403000	-1.387072000
1	6.471750000	0.778409000	-1.272773000
7	0.390937000	-1.827388000	-1.820192000
1	-0.212905000	-2.139893000	-2.574620000
1	1.342019000	-1.817068000	-2.179773000
1	0.356853000	-2.517016000	-1.073209000

5SiInt^{N-H} (T.E.= -1641.116260)

6	0.576199000	-0.163737000	1.568805000
6	1.208568000	-0.048933000	0.171108000
1	0.720550000	-1.154749000	2.020029000
1	0.989498000	0.529186000	2.310090000
14	-0.237339000	-0.286854000	-1.092466000
7	-1.418706000	-0.001705000	0.264203000
14	2.647848000	-1.223471000	-0.090731000
14	1.711680000	1.767007000	-0.092016000
6	2.283815000	-2.952218000	0.583641000
1	1.720114000	-3.573525000	-0.116204000
1	3.241169000	-3.457959000	0.736152000
1	1.767576000	-2.960926000	1.546333000
6	4.208746000	-0.682335000	0.798530000
1	4.965933000	-1.465648000	0.704743000
1	4.631639000	0.238657000	0.391920000
1	4.022053000	-0.525759000	1.864786000

6	2.702761000	2.430133000	1.357665000
1	3.606486000	1.857179000	1.567788000
1	3.003059000	3.454495000	1.118095000
1	2.106267000	2.476239000	2.271493000
6	2.708675000	2.020322000	-1.658677000
1	2.837657000	3.095371000	-1.813488000
1	3.704940000	1.575888000	-1.606324000
1	2.197925000	1.616860000	-2.536434000
6	3.049772000	-1.459694000	-1.908388000
1	3.443223000	-0.554642000	-2.373030000
1	3.809344000	-2.240893000	-2.004850000
1	2.178844000	-1.771580000	-2.492157000
6	0.208085000	2.887587000	-0.210647000
1	-0.386249000	2.701864000	-1.108437000
1	-0.449656000	2.800481000	0.657658000
1	0.560025000	3.922623000	-0.257559000
6	-2.815587000	0.016836000	0.038151000
6	-3.652722000	-0.894127000	0.675751000
6	-3.359584000	0.910688000	-0.876155000
6	-5.008664000	-0.905998000	0.402028000
1	-3.231462000	-1.583695000	1.398542000
6	-4.716238000	0.892646000	-1.149959000
1	-2.706384000	1.620791000	-1.370753000
6	-5.546047000	-0.014314000	-0.512350000
1	-5.650430000	-1.618010000	0.908278000
1	-5.126837000	1.596028000	-1.865190000
1	-6.608321000	-0.025812000	-0.725938000
6	-0.924373000	0.047950000	1.543514000
8	-1.580743000	0.220173000	2.549043000
7	-0.572037000	-2.334129000	-0.863182000
1	-0.105921000	-2.899047000	-1.566609000
1	-0.337172000	-2.711286000	0.052559000
1	-1.573812000	-2.455069000	-0.996091000

8SiInt^{N-H} (T.E.= -1209.726611)

6	0.409002000	1.643624000	0.221310000
6	-1.070782000	1.698391000	-0.116077000
6	-1.556414000	0.263203000	-0.150760000
1	0.935829000	2.534192000	-0.142329000
1	0.534435000	1.619752000	1.317854000

1	-1.205806000	2.189927000	-1.090976000
1	-1.589335000	2.328754000	0.619617000
14	-0.223445000	-0.918018000	-0.424325000
7	0.958891000	0.435480000	-0.372467000
15	-3.196750000	-0.090024000	-0.100307000
6	-4.030618000	0.389513000	1.435220000
1	-3.860638000	1.453220000	1.613262000
1	-5.105622000	0.205369000	1.383606000
1	-3.599293000	-0.172954000	2.263917000
6	-4.190759000	0.746835000	-1.362835000
1	-3.836561000	0.452216000	-2.351351000
1	-5.250664000	0.505100000	-1.262981000
1	-4.063605000	1.826259000	-1.256088000
6	-3.537811000	-1.844704000	-0.292139000
1	-3.178983000	-2.190887000	-1.261481000
1	-3.029611000	-2.406976000	0.491638000
1	-4.613387000	-2.014325000	-0.219621000
6	2.328636000	0.252501000	-0.330199000
6	3.188755000	1.108136000	0.372188000
6	2.915036000	-0.832467000	-1.003943000
6	4.555210000	0.876455000	0.406187000
1	2.788724000	1.960856000	0.906440000
6	4.274189000	-1.056270000	-0.956153000
1	2.276118000	-1.496681000	-1.576059000
6	5.114202000	-0.204794000	-0.249228000
1	5.189347000	1.560251000	0.960834000
1	4.688275000	-1.904281000	-1.491259000
1	6.183039000	-0.378850000	-0.220757000
7	0.994117000	-1.297316000	2.273123000
1	1.833632000	-1.721873000	1.895391000
1	0.640170000	-1.917266000	2.990703000
1	1.280490000	-0.438873000	2.728769000

9SiInt^{N-H} (T.E.= -1208.554177)

6	0.515383000	0.530845000	1.441555000
6	-0.838438000	0.514328000	1.435448000
6	-1.393145000	-0.245717000	0.347718000
14	-0.080745000	-0.973167000	-0.692020000
7	1.099650000	-0.202258000	0.424739000
15	-3.067648000	-0.277971000	0.037772000

6	-4.022617000	-1.255510000	1.216641000
1	-3.841283000	-0.867646000	2.220814000
1	-5.090864000	-1.204602000	0.997534000
1	-3.686457000	-2.292217000	1.179211000
6	-3.418887000	-0.966910000	-1.581472000
1	-4.497559000	-1.049636000	-1.722006000
1	-2.999620000	-0.315073000	-2.348901000
1	-2.963877000	-1.954262000	-1.669340000
6	-3.820775000	1.355994000	0.079173000
1	-3.289006000	2.000592000	-0.625870000
1	-4.881554000	1.300025000	-0.171374000
1	-3.712755000	1.773053000	1.082167000
6	2.488686000	-0.166090000	0.223237000
6	3.158238000	-1.304883000	-0.220413000
6	3.222906000	1.000225000	0.432952000
6	4.520211000	-1.273665000	-0.454357000
1	2.593811000	-2.219331000	-0.368143000
6	4.588360000	1.020100000	0.211958000
1	2.709102000	1.902089000	0.747201000
6	5.246636000	-0.113829000	-0.234831000
1	5.021601000	-2.171241000	-0.798711000
1	5.141016000	1.938000000	0.379441000
1	6.315655000	-0.094224000	-0.410056000
1	1.140168000	1.014210000	2.183326000
1	-1.418529000	1.020911000	2.201860000
7	-0.970505000	2.605259000	-1.422854000
1	-0.600022000	1.996596000	-2.144057000
1	-0.442947000	3.468634000	-1.470456000
1	-0.735105000	2.157696000	-0.539785000

14SiInt^{N-H} (T.E.= -1403.894695)

6	1.208790000	1.097724000	0.168912000
6	1.632082000	-0.257602000	-0.014638000
7	-0.954381000	-0.091344000	-0.314465000
6	-2.296173000	-0.461480000	-0.182260000
6	-3.034886000	-0.082685000	0.943034000
6	-4.352780000	-0.473253000	1.097416000
6	-4.965160000	-1.272179000	0.144306000
6	-4.238715000	-1.671971000	-0.965775000
6	-2.923024000	-1.273994000	-1.130087000

1	-2.554627000	0.538036000	1.694041000
1	-4.904641000	-0.155284000	1.975281000
1	-5.997136000	-1.579312000	0.265571000
1	-4.704208000	-2.294713000	-1.721916000
1	-2.361800000	-1.575686000	-2.007842000
5	-0.384650000	1.209022000	-0.075565000
7	-1.079119000	2.437880000	-0.162537000
6	-0.524075000	3.693210000	0.292459000
1	-0.485877000	4.421644000	-0.527583000
1	-1.153564000	4.127366000	1.081014000
1	0.485072000	3.543444000	0.670631000
6	-2.405877000	2.602809000	-0.702585000
1	-3.146555000	2.823065000	0.078978000
1	-2.415873000	3.443393000	-1.406617000
1	-2.735114000	1.713835000	-1.237432000
15	3.317963000	-0.495595000	-0.086702000
6	4.191675000	-0.093423000	1.439106000
1	5.267726000	-0.232683000	1.317095000
1	3.974313000	0.945868000	1.685223000
1	3.829278000	-0.736145000	2.242387000
6	4.164782000	0.454742000	-1.364029000
1	5.243948000	0.297095000	-1.317075000
1	3.790649000	0.148444000	-2.341613000
1	3.934500000	1.508291000	-1.205603000
6	3.716293000	-2.217981000	-0.424328000
1	3.305396000	-2.852701000	0.362797000
1	3.275993000	-2.518803000	-1.375732000
1	4.798772000	-2.350945000	-0.464864000
8	1.992295000	2.043794000	0.398163000
14	0.268130000	-1.427857000	-0.512547000
7	-0.156960000	-2.059550000	1.441893000
1	-0.100680000	-1.248450000	2.054187000
1	-1.091529000	-2.453448000	1.514013000
1	0.503210000	-2.756255000	1.770336000

1GeInt^{N-H} (T.E.= -3354.527709)

6	-0.888441000	0.424249000	1.672830000
6	0.582508000	0.060239000	1.731999000
6	1.208455000	0.073268000	0.323530000
1	-1.393646000	0.107279000	2.595920000

1	-1.009067000	1.520014000	1.628011000
1	0.669849000	-0.939473000	2.177156000
1	1.101288000	0.732189000	2.429141000
32	-0.237966000	-0.702280000	-0.881552000
7	-1.477285000	-0.220515000	0.518696000
14	1.369340000	1.834534000	-0.355063000
14	2.834222000	-0.855075000	0.275348000
6	2.861063000	-2.307959000	1.477591000
1	2.083157000	-3.059506000	1.328927000
1	3.823632000	-2.814632000	1.358917000
1	2.802804000	-1.969119000	2.514872000
6	3.198963000	-1.559226000	-1.426765000
1	3.247449000	-0.791343000	-2.200081000
1	4.162610000	-2.076100000	-1.408162000
1	2.441422000	-2.284581000	-1.737371000
6	4.305294000	0.175133000	0.834922000
1	4.153952000	0.526999000	1.859812000
1	5.204199000	-0.448351000	0.832181000
1	4.501728000	1.046043000	0.207757000
6	2.448305000	1.893347000	-1.890377000
1	2.025105000	1.267865000	-2.681772000
1	2.462064000	2.922187000	-2.261387000
1	3.482427000	1.585744000	-1.729919000
6	-0.263773000	2.582599000	-0.928638000
1	-1.014698000	2.666624000	-0.140745000
1	-0.053535000	3.592869000	-1.294215000
1	-0.712965000	2.029451000	-1.758803000
6	2.054547000	2.996305000	0.949018000
1	1.355367000	3.119306000	1.779939000
1	3.007770000	2.656544000	1.357845000
1	2.209917000	3.983391000	0.504583000
6	-2.834837000	-0.098935000	0.319535000
6	-3.464173000	-0.791703000	-0.730551000
6	-3.655801000	0.688295000	1.141886000
6	-4.822255000	-0.696436000	-0.944840000
1	-2.860869000	-1.408770000	-1.390050000
6	-5.020754000	0.770472000	0.918946000
1	-3.224632000	1.246392000	1.963286000
6	-5.621599000	0.084796000	-0.120965000
1	-5.266488000	-1.246476000	-1.767657000

1	-5.621806000	1.389435000	1.576912000
1	-6.689553000	0.153712000	-0.287903000
7	-0.217833000	-2.797630000	-0.015263000
1	0.535420000	-3.406827000	-0.316783000
1	-1.093795000	-3.219559000	-0.306102000
1	-0.223221000	-2.760425000	0.998612000

2GeInt^{N-H} (T.E.= -3353.341754)

6	-1.214032000	0.016636000	-0.299534000
6	-0.520598000	0.065362000	-1.624373000
6	0.811503000	-0.089170000	-1.641570000
1	-1.075984000	0.147949000	-2.555821000
1	1.383693000	-0.151867000	-2.562883000
32	0.288434000	0.095139000	1.072101000
7	1.468776000	-0.254592000	-0.436049000
14	-1.854940000	-1.757432000	-0.107084000
14	-2.534970000	1.327040000	-0.090265000
6	-2.931435000	-1.952147000	1.418776000
1	-3.209479000	-3.004397000	1.526381000
1	-2.390412000	-1.659142000	2.323159000
1	-3.854103000	-1.369368000	1.371787000
6	-4.136529000	0.908863000	-0.979545000
1	-4.642519000	0.027391000	-0.580874000
1	-4.824022000	1.754871000	-0.889337000
1	-3.958628000	0.741180000	-2.045829000
6	-2.921206000	1.635396000	1.720319000
1	-2.038801000	1.967716000	2.274765000
1	-3.679955000	2.418169000	1.807548000
1	-3.304532000	0.743888000	2.220512000
6	-2.000978000	2.966290000	-0.848260000
1	-1.292201000	3.524740000	-0.233588000
1	-1.558155000	2.827487000	-1.837844000
1	-2.883111000	3.601024000	-0.968020000
6	-2.816452000	-2.309637000	-1.618270000
1	-3.160734000	-3.336209000	-1.463406000
1	-3.689766000	-1.689104000	-1.821224000
1	-2.179207000	-2.304196000	-2.505456000
6	-0.442542000	-2.985826000	0.074874000
1	-0.860938000	-3.996617000	0.043708000
1	0.283484000	-2.896356000	-0.735891000

1	0.094427000	-2.884465000	1.022147000
6	2.849432000	-0.169871000	-0.330814000
6	3.485793000	-0.724115000	0.787233000
6	3.647612000	0.481427000	-1.278922000
6	4.853424000	-0.626956000	0.948773000
1	2.882727000	-1.252636000	1.518965000
6	5.020073000	0.558219000	-1.115416000
1	3.185747000	0.944560000	-2.143695000
6	5.636318000	0.010481000	-0.003039000
1	5.316681000	-1.069928000	1.823673000
1	5.613650000	1.066399000	-1.867710000
1	6.710431000	0.075911000	0.120332000
7	0.875297000	2.285808000	0.665946000
1	0.421216000	3.010104000	1.210227000
1	1.871807000	2.331687000	0.854348000
1	0.736732000	2.484012000	-0.321008000

3GeInt^{N-H} (T.E.= -3474.625509)

6	0.690545000	1.050297000	-1.116657000
6	1.407144000	0.014019000	-0.202002000
1	1.186818000	2.029041000	-1.078545000
1	0.762003000	0.768489000	-2.179292000
7	-1.347696000	0.120987000	0.092359000
5	-0.847612000	1.178652000	-0.743738000
7	-1.613410000	2.307046000	-1.145205000
6	-1.160443000	3.246165000	-2.141777000
1	-1.876762000	3.313698000	-2.970849000
1	-1.056802000	4.255998000	-1.723143000
1	-0.199471000	2.948494000	-2.557247000
6	-2.913828000	2.659196000	-0.630266000
1	-3.716905000	2.466215000	-1.354388000
1	-3.145179000	2.104232000	0.278303000
1	-2.940842000	3.728622000	-0.388916000
14	2.834565000	0.781035000	0.714424000
14	1.888078000	-1.478319000	-1.239430000
6	2.400238000	2.553847000	1.225039000
1	1.328188000	2.763751000	1.208326000
1	2.780963000	2.777657000	2.226255000
1	2.868056000	3.265249000	0.539870000
6	4.403014000	0.949910000	-0.305943000

1	5.126687000	1.563691000	0.238489000
1	4.874361000	-0.012104000	-0.519495000
1	4.196089000	1.445063000	-1.259237000
6	2.926916000	-1.019789000	-2.736775000
1	2.937282000	-1.863601000	-3.432719000
1	2.530497000	-0.155404000	-3.274376000
1	3.960789000	-0.800512000	-2.465482000
6	2.845913000	-2.766724000	-0.265965000
1	2.985976000	-3.656469000	-0.886210000
1	3.838320000	-2.408651000	0.020529000
1	2.319174000	-3.074125000	0.641205000
6	3.289345000	-0.192735000	2.257584000
1	3.573065000	-1.218708000	2.012539000
1	4.144450000	0.278836000	2.750312000
1	2.476445000	-0.250724000	2.986193000
6	0.338388000	-2.305565000	-1.914693000
1	-0.329602000	-2.674242000	-1.130329000
1	-0.236036000	-1.620107000	-2.543275000
1	0.623774000	-3.161955000	-2.532458000
32	0.028867000	-0.798908000	1.072246000
6	-2.659635000	-0.344276000	0.164893000
6	-3.430846000	-0.500364000	-0.992130000
6	-3.238930000	-0.714570000	1.381883000
6	-4.723062000	-0.983932000	-0.928657000
1	-2.991302000	-0.236726000	-1.949133000
6	-4.529937000	-1.210224000	1.440030000
1	-2.661849000	-0.605541000	2.295004000
6	-5.284916000	-1.344489000	0.287382000
1	-5.296055000	-1.092152000	-1.843149000
1	-4.950510000	-1.489459000	2.399913000
1	-6.296712000	-1.728990000	0.333626000
7	-0.082521000	0.943645000	2.643756000
1	0.762972000	1.429501000	2.923495000
1	-0.718426000	1.626522000	2.241383000
1	-0.516186000	0.571830000	3.481653000

4GeInt^{N-H} (T.E.= -3684.535597)

6	-0.917221000	-0.452773000	1.608341000
6	-1.413392000	0.024432000	0.207699000
1	-1.042690000	0.330713000	2.368351000

1	-1.503167000	-1.297236000	1.993331000
7	1.454213000	0.010416000	0.219469000
14	-2.131173000	1.753786000	0.446166000
14	-2.641144000	-1.179258000	-0.518844000
6	-0.740444000	2.939210000	0.904417000
1	-0.084092000	3.147803000	0.054716000
1	-1.167598000	3.892788000	1.227140000
1	-0.117660000	2.558805000	1.718160000
6	-3.388641000	1.842250000	1.840554000
1	-3.542185000	2.893303000	2.102000000
1	-4.354416000	1.429024000	1.546866000
1	-3.061991000	1.323283000	2.743980000
6	-4.358769000	-1.054004000	0.234771000
1	-4.883233000	-0.143126000	-0.061915000
1	-4.958575000	-1.905959000	-0.099089000
1	-4.318379000	-1.083044000	1.327181000
6	-2.846599000	-0.968703000	-2.375461000
1	-3.600961000	-1.674440000	-2.734961000
1	-3.187088000	0.036867000	-2.631458000
1	-1.927637000	-1.152540000	-2.936081000
6	-2.957414000	2.442379000	-1.092785000
1	-3.871044000	1.901072000	-1.350851000
1	-3.235703000	3.484263000	-0.909457000
1	-2.293335000	2.424625000	-1.960719000
6	-2.154765000	-2.972053000	-0.175220000
1	-1.117150000	-3.241737000	-0.380155000
1	-2.340768000	-3.221398000	0.872894000
1	-2.793576000	-3.625884000	-0.776426000
14	0.911955000	-0.874490000	1.606561000
6	1.175359000	-2.737120000	1.507800000
1	0.952742000	-3.147124000	0.519273000
1	2.204276000	-3.009893000	1.755724000
1	0.523266000	-3.243806000	2.225257000
6	1.771642000	-0.271270000	3.151800000
1	1.621265000	0.803319000	3.280321000
1	1.384368000	-0.779074000	4.038677000
1	2.847380000	-0.457617000	3.104951000
32	0.130995000	0.437472000	-1.095074000
6	2.794997000	0.224620000	-0.107031000
6	3.222835000	1.462468000	-0.600476000

6	3.759950000	-0.779599000	0.032030000
6	4.545076000	1.680864000	-0.937549000
1	2.495226000	2.261481000	-0.699818000
6	5.086484000	-0.552217000	-0.293988000
1	3.456667000	-1.754771000	0.400125000
6	5.490142000	0.677362000	-0.784829000
1	4.843757000	2.653307000	-1.313590000
1	5.809523000	-1.350891000	-0.168251000
1	6.527393000	0.853868000	-1.043024000
7	0.561362000	-1.689537000	-2.045894000
1	-0.023360000	-2.478985000	-1.792991000
1	0.580119000	-1.623497000	-3.057149000
1	1.507392000	-1.884399000	-1.730465000

5GeInt^{N-H} (T.E.= -3428.596519)

6	0.673241000	-0.047319000	1.677848000
6	1.289555000	-0.054959000	0.264615000
1	0.856026000	-0.993867000	2.206775000
1	1.085948000	0.721215000	2.341613000
7	-1.402449000	-0.323638000	0.524946000
14	2.618679000	-1.381441000	0.167948000
14	1.877297000	1.674110000	-0.131695000
6	1.813478000	-3.075898000	0.311334000
1	1.277023000	-3.346293000	-0.602103000
1	2.579893000	-3.837460000	0.479389000
1	1.105961000	-3.134949000	1.143182000
6	3.851437000	-1.234027000	1.572558000
1	4.501694000	-2.113097000	1.580554000
1	4.483043000	-0.350251000	1.473399000
1	3.355001000	-1.183232000	2.544692000
6	3.445130000	2.149556000	0.786955000
1	4.327981000	1.642598000	0.390504000
1	3.608425000	3.226365000	0.684878000
1	3.376835000	1.924881000	1.854521000
6	2.243277000	1.918370000	-1.962509000
1	2.233033000	2.984216000	-2.208013000
1	3.240745000	1.542226000	-2.201571000
1	1.544993000	1.411938000	-2.632032000
6	3.534998000	-1.324993000	-1.466072000
1	4.171601000	-0.441640000	-1.552141000

1	4.176962000	-2.204593000	-1.560662000
1	2.844369000	-1.326610000	-2.314168000
6	0.596418000	2.925984000	0.458763000
1	-0.431671000	2.744847000	0.138250000
1	0.578651000	2.944319000	1.552052000
1	0.883353000	3.927000000	0.123974000
6	-2.796441000	-0.269867000	0.332358000
6	-3.458758000	-1.371695000	-0.200585000
6	-3.520235000	0.893597000	0.589028000
6	-4.814554000	-1.313495000	-0.471697000
1	-2.895143000	-2.278217000	-0.395276000
6	-4.877481000	0.942768000	0.322392000
1	-3.009400000	1.752347000	1.009132000
6	-5.530898000	-0.157226000	-0.209805000
1	-5.314939000	-2.181512000	-0.885643000
1	-5.429256000	1.851896000	0.533464000
1	-6.593354000	-0.113510000	-0.417774000
6	-0.832454000	0.107676000	1.692209000
8	-1.434953000	0.508720000	2.667622000
32	-0.216587000	-0.705737000	-0.964918000
7	-1.042367000	1.217139000	-1.961049000
1	-0.587507000	2.112216000	-1.813480000
1	-1.997240000	1.296949000	-1.615807000
1	-1.092844000	1.053338000	-2.960459000

8GeInt^{N-H} (T.E.= -2997.207170)

6	0.525512000	-1.736474000	0.421462000
6	-0.913493000	-1.515317000	0.852185000
6	-1.492406000	-0.424674000	-0.020205000
1	1.088858000	-2.242466000	1.216730000
1	0.549279000	-2.401824000	-0.458905000
1	-0.921649000	-1.233971000	1.919323000
1	-1.459637000	-2.467025000	0.788849000
32	-0.166539000	0.831550000	-0.576435000
7	1.110331000	-0.446693000	0.116476000
15	-3.145654000	-0.198461000	-0.140843000
6	-4.064133000	-1.603049000	-0.824525000
1	-3.846957000	-2.493548000	-0.231617000
1	-5.140860000	-1.422621000	-0.810275000
1	-3.732675000	-1.780446000	-1.848037000

6	-3.575931000	1.205452000	-1.181016000
1	-3.180823000	2.125117000	-0.747841000
1	-3.150228000	1.073041000	-2.175940000
1	-4.661523000	1.283919000	-1.259208000
6	-4.020750000	0.101802000	1.425112000
1	-5.098735000	0.201444000	1.281092000
1	-3.830419000	-0.735313000	2.100644000
1	-3.628457000	1.011873000	1.883024000
6	2.471373000	-0.333892000	-0.009843000
6	3.061691000	0.932708000	-0.186864000
6	3.342478000	-1.435858000	0.043887000
6	4.426837000	1.080687000	-0.304955000
1	2.418802000	1.806530000	-0.231496000
6	4.712800000	-1.270493000	-0.067799000
1	2.941801000	-2.435045000	0.160793000
6	5.274396000	-0.018248000	-0.243376000
1	4.839423000	2.074891000	-0.442550000
1	5.350986000	-2.147137000	-0.022405000
1	6.347271000	0.102491000	-0.331150000
7	0.123414000	1.914666000	1.846179000
1	-0.621291000	1.464984000	2.365343000
1	0.999776000	1.511823000	2.156903000
1	0.124651000	2.898931000	2.082317000

9GeInt^{N-H} (T.E.= -2996.035431)

6	0.582921000	-1.331509000	-0.907578000
6	-0.770100000	-1.392463000	-0.828685000
6	-1.368630000	-0.422567000	0.040554000
7	1.186159000	-0.350730000	-0.158535000
15	-3.056186000	-0.288630000	0.221624000
6	-3.952139000	-0.353463000	-1.339158000
1	-3.769537000	-1.316827000	-1.818743000
1	-5.024363000	-0.237164000	-1.171548000
1	-3.574556000	0.444161000	-1.984716000
6	-3.504211000	1.265774000	1.000038000
1	-4.580053000	1.295933000	1.178760000
1	-2.977994000	1.369111000	1.950189000
1	-3.220966000	2.088586000	0.342313000
6	-3.801937000	-1.585329000	1.233309000
1	-3.378357000	-1.543138000	2.237409000

1	-4.886880000	-1.474581000	1.284170000
1	-3.557289000	-2.554480000	0.794602000
32	-0.057106000	0.698592000	0.877496000
6	2.578387000	-0.241987000	-0.088498000
6	3.166382000	1.006176000	0.124010000
6	3.415885000	-1.352542000	-0.208363000
6	4.538091000	1.136424000	0.221287000
1	2.525749000	1.878812000	0.197874000
6	4.790018000	-1.211740000	-0.126860000
1	2.981979000	-2.336888000	-0.340883000
6	5.363106000	0.029799000	0.090649000
1	4.968600000	2.117859000	0.386639000
1	5.419057000	-2.089992000	-0.222099000
1	6.439322000	0.134921000	0.156862000
1	1.186331000	-1.963722000	-1.549351000
1	-1.329528000	-2.118147000	-1.413474000
7	-1.523408000	1.741415000	-2.560797000
1	-1.137856000	1.795463000	-3.495918000
1	-1.167583000	2.543824000	-2.053821000
1	-1.111776000	0.926539000	-2.111399000

$^{14}\text{GeInt}^{\text{N-H}}$ (T.E.= -3191.373558)

6	1.173142000	1.246956000	0.129193000
6	1.640675000	-0.094160000	-0.033684000
7	-1.020244000	0.056855000	-0.320130000
6	-2.350998000	-0.312952000	-0.146627000
6	-3.076469000	0.099714000	0.977709000
6	-4.387021000	-0.298124000	1.170547000
6	-5.009869000	-1.138072000	0.260022000
6	-4.299533000	-1.570595000	-0.848203000
6	-2.991720000	-1.165918000	-1.051163000
1	-2.589616000	0.749408000	1.699404000
1	-4.925281000	0.046350000	2.047008000
1	-6.035871000	-1.451007000	0.412678000
1	-4.771823000	-2.225638000	-1.572255000
1	-2.447578000	-1.492837000	-1.931225000
5	-0.426741000	1.345679000	-0.112343000
7	-1.115219000	2.579880000	-0.212128000
6	-0.567143000	3.843559000	0.226786000
1	-0.524404000	4.559589000	-0.604110000

1	-1.205333000	4.288068000	1.002700000
1	0.438532000	3.703482000	0.616584000
6	-2.444619000	2.733453000	-0.748886000
1	-3.185057000	2.953252000	0.033096000
1	-2.462068000	3.569965000	-1.457752000
1	-2.769447000	1.839014000	-1.277417000
15	3.329547000	-0.306415000	-0.005290000
6	4.111884000	0.078907000	1.575523000
1	5.194111000	-0.054359000	1.517656000
1	3.877907000	1.113138000	1.827189000
1	3.704361000	-0.577434000	2.345705000
6	4.246981000	0.662569000	-1.218739000
1	5.321409000	0.499767000	-1.114133000
1	3.927623000	0.374179000	-2.220828000
1	4.009787000	1.713720000	-1.055945000
6	3.762445000	-2.022493000	-0.336789000
1	3.301830000	-2.671264000	0.410344000
1	3.395706000	-2.312121000	-1.322547000
1	4.845817000	-2.149197000	-0.303080000
8	1.935980000	2.207774000	0.368688000
32	0.259745000	-1.398219000	-0.489373000
7	-0.235780000	-1.829348000	1.725589000
1	-0.074676000	-0.940468000	2.189140000
1	-1.213057000	-2.078127000	1.843878000
1	0.330111000	-2.537597000	2.177956000

IIa-Int^{N-H} (T.E.= -1112.372365)

6	-0.025928000	2.359471000	0.338925000
6	-1.215791000	1.723213000	0.378288000
1	-0.045212000	3.436250000	0.454862000
14	0.042803000	-0.759188000	-0.084494000
6	2.381680000	2.585394000	0.348287000
6	1.301824000	1.778920000	0.283434000
1	3.396610000	2.215075000	0.352950000
1	2.237463000	3.654296000	0.431228000
6	-2.602099000	-0.269391000	0.177745000
6	-3.437914000	-0.015676000	-0.907494000
6	-3.004254000	-1.203209000	1.126973000
6	-4.658035000	-0.658303000	-1.023658000
1	-3.122310000	0.697825000	-1.662994000

6	-4.219222000	-1.854191000	1.002985000
1	-2.347354000	-1.405677000	1.965599000
6	-5.053550000	-1.580567000	-0.068264000
1	-5.299075000	-0.443940000	-1.871145000
1	-4.518073000	-2.577063000	1.753264000
1	-6.006988000	-2.086845000	-0.161267000
7	-1.328389000	0.344121000	0.291622000
6	2.658080000	-0.222963000	0.159239000
6	3.110423000	-1.007615000	1.210932000
6	3.454360000	-0.090214000	-0.974707000
6	4.333403000	-1.653968000	1.129057000
1	2.484763000	-1.107388000	2.091082000
6	4.678801000	-0.728473000	-1.052585000
1	3.109016000	0.540174000	-1.788399000
6	5.121554000	-1.515478000	-0.000112000
1	4.671378000	-2.268462000	1.955601000
1	5.289055000	-0.616095000	-1.941454000
1	6.078867000	-2.019542000	-0.062189000
7	1.372740000	0.382863000	0.225021000
6	-2.460163000	2.518354000	0.618668000
1	-3.132702000	2.530040000	-0.241330000
1	-3.028997000	2.096564000	1.451995000
1	-2.203479000	3.548136000	0.861352000
7	-0.061286000	-0.192942000	-2.146388000
1	0.762969000	-0.513638000	-2.644528000
1	-0.872150000	-0.600355000	-2.601763000
1	-0.113487000	0.819166000	-2.238003000

Cartesian coordinates of the transition states involved in the activation of N – H bond of NH₃ by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and NacNacSi (**IIa**), along with their total energies (in hartrees) including zero point vibrational correction.

1SiTS^{N-H} (T.E.= -1566.991204)

6	-0.922725000	-0.385463000	-1.624122000
6	0.524770000	0.067713000	-1.667177000
6	1.156723000	0.054185000	-0.240339000
1	-1.454484000	-0.054250000	-2.523051000
1	-0.987100000	-1.485288000	-1.599077000
1	0.540185000	1.083460000	-2.080410000

1	1.091814000	-0.545228000	-2.377669000
7	-1.517662000	0.203373000	-0.434925000
14	-0.351806000	0.255196000	0.884165000
14	2.134392000	-1.526290000	0.032628000
14	2.175474000	1.639681000	-0.056399000
6	3.171315000	1.679285000	1.527972000
1	4.003300000	0.972130000	1.514177000
1	3.591839000	2.680202000	1.658309000
1	2.551361000	1.463271000	2.401739000
6	1.033711000	3.131021000	-0.049320000
1	0.477271000	3.202623000	0.888030000
1	1.632002000	4.040615000	-0.154236000
1	0.309083000	3.114557000	-0.867334000
6	3.345262000	1.856155000	-1.506919000
1	3.817221000	2.840121000	-1.437352000
1	4.136527000	1.105933000	-1.518878000
1	2.824153000	1.810589000	-2.466027000
6	2.667984000	-1.756103000	1.820714000
1	2.907685000	-2.809669000	1.990847000
1	3.571041000	-1.179851000	2.031246000
1	1.918266000	-1.461729000	2.557236000
6	1.126515000	-3.020674000	-0.503453000
1	0.145693000	-3.087628000	-0.027804000
1	0.968917000	-3.015868000	-1.585019000
1	1.682487000	-3.931084000	-0.261597000
6	3.695133000	-1.577700000	-1.007938000
1	4.469125000	-0.911066000	-0.621341000
1	4.098008000	-2.594474000	-0.992879000
1	3.508332000	-1.310355000	-2.050876000
6	-2.895112000	0.163643000	-0.265779000
6	-3.738551000	-0.533115000	-1.135955000
6	-3.485654000	0.841572000	0.810167000
6	-5.109458000	-0.547232000	-0.932070000
1	-3.324331000	-1.075334000	-1.976746000
6	-4.850229000	0.813844000	1.006655000
1	-2.849986000	1.409730000	1.482776000
6	-5.679534000	0.118831000	0.136873000
1	-5.737526000	-1.096169000	-1.625365000
1	-5.274427000	1.353443000	1.846319000
1	-6.751671000	0.103036000	0.290036000

1	-0.391219000	-0.063071000	2.490515000
7	-0.665817000	-1.284532000	1.949145000
1	-1.649360000	-1.399565000	2.175750000
1	-0.193577000	-2.186966000	1.977777000

2SiTS^{N-H} (T.E.= -1564.723377)

6	-1.159133000	0.003669000	-0.222613000
6	-0.494388000	-0.006170000	-1.575967000
6	0.840208000	-0.073544000	-1.595812000
1	-1.072431000	-0.015195000	-2.494660000
1	1.430703000	-0.149764000	-2.501413000
14	0.317663000	0.174305000	0.943467000
7	1.492381000	-0.114471000	-0.363727000
14	-1.823839000	-1.754192000	0.063274000
14	-2.443349000	1.371652000	-0.099173000
6	-2.823983000	-2.348105000	-1.405287000
1	-3.156156000	-3.371758000	-1.210762000
1	-3.708835000	-1.740627000	-1.597684000
1	-2.216095000	-2.366619000	-2.312589000
6	-2.877711000	-1.845733000	1.608959000
1	-3.150574000	-2.887643000	1.796923000
1	-2.332537000	-1.480123000	2.483033000
1	-3.803192000	-1.272071000	1.517235000
6	-0.405399000	-2.968508000	0.249675000
1	-0.816469000	-3.979647000	0.324282000
1	0.257204000	-2.941690000	-0.618281000
1	0.195556000	-2.788013000	1.144634000
6	-2.881883000	1.768500000	1.680260000
1	-3.653645000	2.543251000	1.694100000
1	-3.280827000	0.895289000	2.200562000
1	-2.032439000	2.138037000	2.258106000
6	-1.767289000	2.904656000	-0.946275000
1	-0.721574000	3.105263000	-0.701901000
1	-1.819895000	2.784953000	-2.031242000
1	-2.359942000	3.783792000	-0.679537000
6	-4.033009000	0.943786000	-0.995038000
1	-4.592535000	0.141368000	-0.509492000
1	-4.674494000	1.829538000	-1.017122000
1	-3.840561000	0.648946000	-2.029962000
6	2.880367000	-0.071388000	-0.239391000

6	3.478308000	-0.554099000	0.927963000
6	3.705298000	0.457594000	-1.233434000
6	4.848213000	-0.500893000	1.095364000
1	2.847765000	-0.990122000	1.697067000
6	5.078078000	0.492567000	-1.062045000
1	3.269119000	0.864479000	-2.137906000
6	5.662130000	0.020049000	0.100872000
1	5.285878000	-0.885902000	2.009705000
1	5.697451000	0.909460000	-1.848502000
1	6.736940000	0.054315000	0.230517000
1	0.285874000	0.945973000	2.385453000
7	0.584584000	1.950782000	1.501010000
1	1.552062000	2.135570000	1.750100000
1	0.129400000	2.815752000	1.209000000

3SiTS^{N-H} (T.E.= -1687.094651)

6	-0.695083000	1.033668000	-1.076354000
6	-1.397492000	-0.078192000	-0.214941000
1	-0.699829000	0.744917000	-2.138135000
1	-1.250655000	1.974662000	-1.032392000
14	0.010873000	-1.334027000	-0.142934000
7	1.320228000	-0.148792000	-0.172126000
5	0.825271000	1.133368000	-0.625329000
7	1.568473000	2.335736000	-0.643879000
6	1.087013000	3.541420000	-1.274897000
1	0.921408000	4.338587000	-0.538220000
1	1.818085000	3.918212000	-2.001024000
1	0.153236000	3.364990000	-1.805422000
6	2.850943000	2.542552000	-0.012598000
1	2.823868000	3.459461000	0.588141000
1	3.107426000	1.718394000	0.650214000
1	3.658931000	2.653079000	-0.747491000
14	-2.867506000	-0.809918000	-1.130918000
14	-1.812399000	0.703999000	1.448257000
6	-2.396578000	-1.209636000	-2.903712000
1	-1.501918000	-1.834776000	-2.958236000
1	-3.218621000	-1.758850000	-3.371723000
1	-2.222958000	-0.310380000	-3.499051000
6	-4.309177000	0.390222000	-1.232016000
1	-5.076235000	-0.021867000	-1.893850000

1	-4.777806000	0.586788000	-0.264978000
1	-3.990159000	1.347406000	-1.654198000
6	-2.591157000	2.399288000	1.222432000
1	-3.415105000	2.410619000	0.507098000
1	-2.979352000	2.734456000	2.188824000
1	-1.848065000	3.133121000	0.898136000
6	-3.016244000	-0.318358000	2.468969000
1	-3.088147000	0.129282000	3.464503000
1	-4.019363000	-0.310826000	2.036161000
1	-2.725067000	-1.363445000	2.596305000
6	-3.460510000	-2.408620000	-0.347354000
1	-3.810035000	-2.282645000	0.678516000
1	-4.292112000	-2.808405000	-0.934391000
1	-2.668860000	-3.163087000	-0.349519000
6	-0.307102000	1.026888000	2.531643000
1	0.167681000	0.114233000	2.895615000
1	0.456325000	1.611853000	2.010839000
1	-0.636851000	1.606333000	3.399645000
6	2.665904000	-0.556685000	-0.109395000
6	3.464838000	-0.541487000	-1.250111000
6	3.221030000	-1.006755000	1.085984000
6	4.785520000	-0.946095000	-1.192190000
1	3.029208000	-0.202593000	-2.184533000
6	4.542100000	-1.420579000	1.139757000
1	2.612645000	-0.990255000	1.984264000
6	5.331357000	-1.389572000	0.003057000
1	5.392753000	-0.923207000	-2.090061000
1	4.958758000	-1.760721000	2.081208000
1	6.365608000	-1.709397000	0.046449000
1	-0.291772000	-2.890223000	0.321955000
7	-0.095371000	-2.266136000	1.487378000
1	0.768569000	-2.719139000	1.767795000
1	-0.686978000	-2.098192000	2.303273000

4SiTS^{N-H} (T.E.= -1897.003615)

6	-0.895056000	-0.104570000	1.580937000
6	-1.372395000	0.065069000	0.092255000
1	-1.094418000	0.801204000	2.166647000
1	-1.448915000	-0.893870000	2.102544000
14	0.130241000	0.042842000	-1.079316000

7	1.424463000	-0.022271000	0.080154000
14	-2.067079000	1.817595000	-0.082203000
14	-2.615952000	-1.285266000	-0.302112000
6	-0.671569000	3.059055000	0.127524000
1	0.036491000	3.023522000	-0.704426000
1	-1.088043000	4.069467000	0.168531000
1	-0.112018000	2.893325000	1.052675000
6	-3.333158000	2.221401000	1.245992000
1	-3.593636000	3.279863000	1.151890000
1	-4.252431000	1.643282000	1.138784000
1	-2.955504000	2.068658000	2.259128000
6	-4.218263000	-1.076530000	0.651180000
1	-4.830058000	-0.272192000	0.235922000
1	-4.798254000	-2.001472000	0.587289000
1	-4.046447000	-0.860726000	1.708624000
6	-3.086109000	-1.372197000	-2.119786000
1	-3.595284000	-2.323070000	-2.303345000
1	-3.784359000	-0.575744000	-2.383149000
1	-2.243673000	-1.309361000	-2.810342000
6	-2.893581000	2.116206000	-1.736085000
1	-3.854469000	1.599382000	-1.799715000
1	-3.088443000	3.186228000	-1.849589000
1	-2.272957000	1.796107000	-2.575808000
6	-1.922524000	-2.957091000	0.215594000
1	-0.925019000	-3.157757000	-0.182658000
1	-1.864526000	-3.049236000	1.302887000
1	-2.591211000	-3.746713000	-0.139048000
14	0.954324000	-0.431561000	1.701550000
6	1.326488000	-2.210858000	2.136060000
1	0.910222000	-2.889760000	1.386884000
1	2.402961000	-2.388031000	2.198403000
1	0.890672000	-2.470711000	3.104695000
6	1.825896000	0.688618000	2.912118000
1	1.613755000	1.737721000	2.689367000
1	1.518980000	0.486698000	3.940816000
1	2.908295000	0.546103000	2.852418000
6	2.777735000	0.103459000	-0.299894000
6	3.586439000	-1.019134000	-0.464802000
6	3.331180000	1.363512000	-0.513278000
6	4.915961000	-0.882284000	-0.829804000

1	3.153388000	-2.002261000	-0.305312000
6	4.657775000	1.496889000	-0.881421000
1	2.697820000	2.234737000	-0.378605000
6	5.456740000	0.374902000	-1.039592000
1	5.531659000	-1.765985000	-0.953925000
1	5.072607000	2.485278000	-1.043959000
1	6.496134000	0.480814000	-1.327028000
1	0.098703000	-0.366948000	-2.668694000
7	0.246806000	-1.581728000	-2.083543000
1	-0.336094000	-2.416960000	-2.093940000
1	1.210355000	-1.822815000	-2.297083000

5SiTS^{N-H} (T.E.= -1639.897650)

6	0.625186000	-0.195040000	1.598627000
6	1.246319000	-0.105144000	0.182991000
1	0.816163000	-1.169647000	2.067053000
1	1.030082000	0.536337000	2.306650000
14	-0.220164000	-0.467198000	-0.956508000
7	-1.410973000	-0.284526000	0.352086000
14	2.527038000	-1.477814000	-0.017341000
14	1.882534000	1.650824000	-0.092577000
6	1.647538000	-3.135083000	0.014037000
1	1.069284000	-3.296485000	-0.898860000
1	2.379888000	-3.942700000	0.096479000
1	0.963251000	-3.225730000	0.862057000
6	3.758225000	-1.476680000	1.396272000
1	4.374351000	-2.377407000	1.327142000
1	4.424462000	-0.613359000	1.371407000
1	3.265277000	-1.492115000	2.371381000
6	3.424808000	1.959595000	0.927199000
1	4.290736000	1.439657000	0.510673000
1	3.647969000	3.030162000	0.918806000
1	3.311794000	1.649549000	1.968636000
6	2.305292000	2.000571000	-1.896407000
1	1.587315000	2.697830000	-2.335197000
1	3.293382000	2.462432000	-1.966426000
1	2.326828000	1.102131000	-2.516854000
6	3.459507000	-1.334147000	-1.633625000
1	4.076968000	-0.433746000	-1.679095000
1	4.123367000	-2.195485000	-1.744960000

1	2.781325000	-1.327993000	-2.491280000
6	0.584375000	2.883135000	0.473056000
1	-0.301114000	2.866962000	-0.166634000
1	0.259950000	2.709281000	1.501977000
1	1.005228000	3.891380000	0.428542000
6	-2.812880000	-0.261684000	0.145908000
6	-3.440733000	-1.353416000	-0.438013000
6	-3.558520000	0.861423000	0.482133000
6	-4.801990000	-1.320692000	-0.686877000
1	-2.851001000	-2.227529000	-0.692370000
6	-4.920277000	0.884663000	0.239475000
1	-3.063629000	1.708270000	0.943728000
6	-5.546293000	-0.203364000	-0.347401000
1	-5.283691000	-2.177523000	-1.143710000
1	-5.496566000	1.761894000	0.510103000
1	-6.612665000	-0.180328000	-0.538291000
6	-0.881568000	-0.054688000	1.601449000
8	-1.521022000	0.177020000	2.602045000
1	-1.019522000	-0.437672000	-2.374114000
7	-0.828829000	0.892203000	-2.089155000
1	-0.233969000	1.173709000	-2.860350000
1	-1.504314000	1.620170000	-1.856332000

8SiTS^{N-H} (T.E.= -1209.672068)

6	0.504465000	-1.694022000	-0.376965000
6	-0.986711000	-1.737979000	-0.077435000
6	-1.531450000	-0.326921000	-0.246061000
1	1.015968000	-2.555875000	0.066435000
1	0.665605000	-1.745615000	-1.466784000
1	-1.125733000	-2.126181000	0.944261000
1	-1.462447000	-2.463175000	-0.750083000
14	-0.179728000	0.836939000	0.068314000
7	1.040101000	-0.450302000	0.158675000
15	-3.131245000	0.001547000	0.129448000
6	-4.299891000	-1.037115000	-0.776849000
1	-4.103314000	-2.084516000	-0.539159000
1	-5.330195000	-0.801374000	-0.504228000
1	-4.157773000	-0.891088000	-1.847921000
6	-3.653402000	-0.229287000	1.856092000
1	-3.080215000	0.453782000	2.485925000

1	-4.721413000	-0.047097000	1.993906000
1	-3.425813000	-1.252296000	2.162660000
6	-3.561396000	1.707156000	-0.242460000
1	-2.898135000	2.370914000	0.316414000
1	-3.431621000	1.894222000	-1.308774000
1	-4.595365000	1.908338000	0.042411000
6	2.407179000	-0.253074000	0.174654000
6	3.314404000	-1.191721000	-0.333283000
6	2.939917000	0.927527000	0.718046000
6	4.679245000	-0.955135000	-0.292908000
1	2.953397000	-2.113654000	-0.771134000
6	4.299239000	1.152867000	0.747182000
1	2.257629000	1.663279000	1.134019000
6	5.188728000	0.213774000	0.241530000
1	5.352884000	-1.704497000	-0.695179000
1	4.672329000	2.075473000	1.179070000
1	6.256861000	0.392034000	0.268447000
1	-0.223410000	2.422966000	-0.349249000
7	0.149295000	1.820375000	-1.519690000
1	1.093868000	2.152298000	-1.689520000
1	-0.355959000	1.664783000	-2.391795000

9SiTS^{N-H} (T.E.= -1208.485093)

6	0.414962000	-1.653299000	0.139086000
6	-0.920360000	-1.602352000	0.286347000
6	-1.519977000	-0.278755000	0.193891000
14	-0.163732000	0.897247000	-0.128373000
7	1.042713000	-0.426330000	-0.125185000
15	-3.157864000	-0.061551000	-0.122423000
6	-3.760071000	-0.668056000	-1.721502000
1	-3.504757000	-1.725843000	-1.811008000
1	-4.840809000	-0.547713000	-1.821586000
1	-3.252422000	-0.123558000	-2.519110000
6	-3.610398000	1.676068000	-0.081194000
1	-4.662052000	1.796753000	-0.346046000
1	-3.436284000	2.079765000	0.916636000
1	-2.992400000	2.224239000	-0.794906000
6	-4.232931000	-0.907626000	1.057469000
1	-4.056830000	-0.509057000	2.056693000
1	-5.283896000	-0.784879000	0.788681000

1	-3.990612000	-1.971997000	1.060555000
6	2.420744000	-0.278713000	-0.146457000
6	2.990369000	0.867394000	-0.717288000
6	3.289892000	-1.230646000	0.398212000
6	4.357377000	1.052438000	-0.735674000
1	2.335147000	1.608486000	-1.166192000
6	4.659999000	-1.038165000	0.366658000
1	2.888965000	-2.117772000	0.872539000
6	5.210669000	0.100680000	-0.195157000
1	4.763068000	1.950363000	-1.189393000
1	5.306365000	-1.793694000	0.800513000
1	6.284015000	0.245166000	-0.214413000
1	1.002007000	-2.561758000	0.137685000
1	-1.499469000	-2.510136000	0.431764000
1	-0.256451000	2.492924000	0.259039000
7	0.144504000	1.906409000	1.438342000
1	1.082036000	2.267869000	1.589305000
1	-0.337583000	1.748294000	2.324357000

¹⁴SiTS^{N-H} (T.E.= -1403.840992)

6	1.218971000	1.140347000	0.122096000
6	1.669953000	-0.212328000	-0.040210000
7	-0.952332000	-0.082631000	-0.274037000
6	-2.301048000	-0.452293000	-0.138427000
6	-3.012508000	-0.112237000	1.011919000
6	-4.336275000	-0.484392000	1.161127000
6	-4.972992000	-1.220565000	0.174223000
6	-4.268343000	-1.580047000	-0.963157000
6	-2.946642000	-1.199948000	-1.121355000
1	-2.507581000	0.462630000	1.782242000
1	-4.873585000	-0.201528000	2.059577000
1	-6.009479000	-1.513644000	0.291938000
1	-4.754743000	-2.155952000	-1.742627000
1	-2.396960000	-1.468478000	-2.017310000
5	-0.386146000	1.230864000	-0.076985000
7	-1.096947000	2.447209000	-0.149560000
6	-0.541160000	3.712117000	0.281092000
1	-0.538982000	4.435037000	-0.544202000
1	-1.150890000	4.141557000	1.086831000
1	0.480686000	3.577753000	0.628388000

6	-2.444820000	2.599607000	-0.642661000
1	-3.155719000	2.822238000	0.164733000
1	-2.483915000	3.435278000	-1.351034000
1	-2.789852000	1.706408000	-1.159528000
15	3.353320000	-0.472784000	-0.050914000
6	4.163914000	-0.072888000	1.507031000
1	5.241751000	-0.229584000	1.431791000
1	3.955628000	0.970791000	1.741956000
1	3.754859000	-0.705110000	2.295735000
6	4.242368000	0.469389000	-1.301512000
1	5.317957000	0.301797000	-1.221788000
1	3.894657000	0.168456000	-2.290281000
1	4.015795000	1.524601000	-1.147259000
6	3.727991000	-2.202882000	-0.366342000
1	3.276969000	-2.822697000	0.410555000
1	3.317550000	-2.499317000	-1.332534000
1	4.808146000	-2.357648000	-0.366965000
8	1.992718000	2.094274000	0.328760000
14	0.287242000	-1.344047000	-0.389867000
1	-0.363842000	-2.843199000	-0.273845000
7	-0.244132000	-2.465095000	1.036366000
1	0.447805000	-3.104185000	1.410648000
1	-0.961012000	-2.244961000	1.727341000

1GeTS^{N-H} (T.E.= -3353.205377)

6	0.849842000	0.485795000	-1.744810000
6	-0.622404000	0.108998000	-1.803739000
6	-1.242147000	0.028810000	-0.383707000
1	1.329077000	0.278644000	-2.710000000
1	0.958109000	1.566267000	-1.565634000
1	-0.699370000	-0.862859000	-2.306425000
1	-1.161094000	0.822702000	-2.436041000
32	0.212844000	-0.967369000	0.522419000
7	1.474183000	-0.287672000	-0.693020000
14	-1.485252000	1.756769000	0.351280000
14	-2.777064000	-1.068913000	-0.384148000
6	-2.408864000	-2.662915000	-1.305256000
1	-1.525410000	-3.175128000	-0.914297000
1	-3.260772000	-3.337954000	-1.185657000
1	-2.263954000	-2.505358000	-2.376023000

6	-3.293966000	-1.545893000	1.353928000
1	-3.787193000	-0.730151000	1.882761000
1	-3.998714000	-2.379881000	1.298777000
1	-2.444650000	-1.876465000	1.959165000
6	-4.222651000	-0.255893000	-1.257020000
1	-3.934735000	0.105781000	-2.247935000
1	-5.026373000	-0.984858000	-1.391067000
1	-4.629770000	0.586741000	-0.694547000
6	-2.467227000	1.702178000	1.950725000
1	-2.107372000	0.954854000	2.661577000
1	-2.395290000	2.681788000	2.431347000
1	-3.527183000	1.504289000	1.775925000
6	0.112726000	2.687563000	0.710156000
1	0.517860000	3.141425000	-0.197039000
1	-0.113669000	3.502824000	1.403953000
1	0.896534000	2.075186000	1.158804000
6	-2.420049000	2.841587000	-0.862232000
1	-1.842251000	3.005969000	-1.775432000
1	-3.394240000	2.438390000	-1.144609000
1	-2.581668000	3.820651000	-0.401709000
6	2.830613000	-0.194976000	-0.469971000
6	3.454018000	-1.028650000	0.471429000
6	3.638291000	0.718511000	-1.159293000
6	4.808312000	-0.943274000	0.715479000
1	2.859438000	-1.773793000	0.993341000
6	4.997528000	0.794078000	-0.904146000
1	3.199652000	1.378214000	-1.896995000
6	5.597393000	-0.026955000	0.033048000
1	5.256767000	-1.608409000	1.445359000
1	5.594608000	1.514304000	-1.453187000
1	6.660927000	0.038417000	0.226923000
1	0.340297000	-1.668657000	2.008316000
7	0.608890000	-0.245180000	2.360646000
1	0.092616000	0.459294000	2.881870000
1	1.599246000	-0.170210000	2.570314000

2GeTS^{N-H} (T.E.= -3353.260612)

6	1.249769000	-0.056741000	0.336154000
6	0.527498000	-0.164417000	1.650183000
6	-0.807493000	-0.260833000	1.657093000

1	1.083364000	-0.196865000	2.582301000
1	-1.378381000	-0.391796000	2.569487000
32	-0.257963000	0.035723000	-0.952256000
7	-1.490884000	-0.259101000	0.451739000
14	2.126566000	-1.701882000	0.006229000
14	2.298972000	1.507733000	0.255138000
6	3.137054000	-1.632495000	-1.569587000
1	3.497729000	-2.635265000	-1.813424000
1	2.542730000	-1.279070000	-2.416945000
1	4.009824000	-0.982932000	-1.473652000
6	3.865763000	1.336509000	1.269440000
1	4.571336000	0.627858000	0.830005000
1	4.364327000	2.307961000	1.329340000
1	3.648104000	1.012271000	2.290528000
6	2.795219000	1.907244000	-1.511140000
1	1.951816000	1.907836000	-2.206344000
1	3.250505000	2.900817000	-1.544831000
1	3.530211000	1.194756000	-1.890625000
6	1.323308000	2.933477000	0.974962000
1	0.357275000	3.056946000	0.479241000
1	1.134702000	2.771891000	2.038713000
1	1.886265000	3.864795000	0.869324000
6	3.235868000	-2.173352000	1.438953000
1	3.643331000	-3.172164000	1.259386000
1	4.075955000	-1.489709000	1.571897000
1	2.674714000	-2.210287000	2.375580000
6	0.851104000	-3.064169000	-0.175218000
1	1.359954000	-4.029549000	-0.245454000
1	0.182669000	-3.101593000	0.688081000
1	0.239820000	-2.950021000	-1.074756000
6	-2.876874000	-0.194161000	0.359650000
6	-3.508611000	-0.585460000	-0.824608000
6	-3.677015000	0.267398000	1.408340000
6	-4.881259000	-0.517730000	-0.953211000
1	-2.903008000	-0.962767000	-1.642843000
6	-5.053427000	0.318319000	1.273627000
1	-3.219395000	0.610432000	2.328245000
6	-5.669370000	-0.069870000	0.096349000
1	-5.341964000	-0.831318000	-1.883376000
1	-5.650299000	0.681561000	2.103033000

1	-6.746730000	-0.022777000	-0.004112000
1	-0.922711000	0.574806000	-2.341713000
7	-0.893143000	1.858788000	-1.529011000
1	-0.256791000	2.531944000	-1.940356000
1	-1.669074000	2.327065000	-1.068685000

3GeTS^{N-H} (T.E.= -3474.555890)

6	0.713937000	0.881374000	-1.223122000
6	1.457803000	0.050772000	-0.135886000
1	1.253231000	1.813757000	-1.421048000
1	0.719712000	0.337220000	-2.179088000
7	-1.344349000	-0.000583000	-0.057837000
5	-0.813154000	1.094436000	-0.822281000
7	-1.528920000	2.272342000	-1.152747000
6	-1.039806000	3.256923000	-2.086695000
1	-1.785445000	3.454024000	-2.867192000
1	-0.830830000	4.213979000	-1.589586000
1	-0.128988000	2.920317000	-2.578442000
6	-2.791137000	2.668013000	-0.574708000
1	-3.615574000	2.609220000	-1.297795000
1	-3.049542000	2.048811000	0.282774000
1	-2.730621000	3.707885000	-0.231335000
14	1.884316000	1.170600000	1.326404000
14	2.904573000	-0.920146000	-0.842893000
6	0.368264000	1.703561000	2.302858000
1	-0.147266000	0.864467000	2.777959000
1	0.703485000	2.373949000	3.100570000
1	-0.360442000	2.248965000	1.697306000
6	2.681228000	2.762732000	0.735936000
1	3.001624000	3.341102000	1.607111000
1	3.551704000	2.604865000	0.097317000
1	1.961566000	3.375481000	0.185698000
6	4.419617000	0.158434000	-1.094983000
1	5.185724000	-0.413524000	-1.626098000
1	4.167993000	1.025077000	-1.713284000
1	4.860916000	0.522339000	-0.165015000
6	3.355462000	-2.379254000	0.247771000
1	4.182745000	-2.932533000	-0.205186000
1	3.668377000	-2.073709000	1.247339000
1	2.520838000	-3.076642000	0.364017000

6	3.009432000	0.309235000	2.554075000
1	3.994397000	0.072341000	2.146572000
1	3.156524000	0.962513000	3.418450000
1	2.559318000	-0.619903000	2.915476000
6	2.475835000	-1.588301000	-2.543590000
1	1.514434000	-2.106101000	-2.557077000
1	2.440125000	-0.791754000	-3.290334000
1	3.249594000	-2.295637000	-2.855036000
32	0.024818000	-1.155430000	0.508789000
6	-2.683768000	-0.371425000	0.114004000
6	-3.531812000	-0.503346000	-0.986351000
6	-3.199627000	-0.641241000	1.381349000
6	-4.856969000	-0.863225000	-0.819878000
1	-3.131907000	-0.307148000	-1.976619000
6	-4.523093000	-1.011173000	1.542961000
1	-2.548475000	-0.540881000	2.243822000
6	-5.361922000	-1.118418000	0.445357000
1	-5.499831000	-0.952196000	-1.688553000
1	-4.904371000	-1.209542000	2.538422000
1	-6.399290000	-1.403579000	0.573933000
1	-0.561121000	-2.656613000	0.791143000
7	-0.398324000	-2.696802000	-0.713640000
1	0.292137000	-3.399792000	-0.947448000
1	-1.123123000	-2.634183000	-1.422807000

4GeTS^{N-H} (T.E.= -3684.463761)

6	-0.920252000	-0.518146000	1.585668000
6	-1.447963000	0.022860000	0.218820000
1	-1.069773000	0.219923000	2.384626000
1	-1.489764000	-1.396753000	1.913510000
7	1.471960000	-0.026006000	0.234873000
14	-2.160632000	1.750464000	0.504017000
14	-2.630754000	-1.206570000	-0.572043000
6	-0.761665000	2.904839000	0.996589000
1	-0.109904000	3.127404000	0.146902000
1	-1.174422000	3.853889000	1.349233000
1	-0.137662000	2.495022000	1.794729000
6	-3.426436000	1.770705000	1.887572000
1	-3.653001000	2.811139000	2.137328000
1	-4.359998000	1.290352000	1.591886000

1	-3.071363000	1.284164000	2.798190000
6	-4.256952000	-1.295805000	0.358378000
1	-4.871369000	-0.406406000	0.201690000
1	-4.827255000	-2.158887000	0.003925000
1	-4.104231000	-1.417769000	1.433891000
6	-3.019389000	-0.775894000	-2.359507000
1	-3.439243000	-1.656942000	-2.853308000
1	-3.762318000	0.020562000	-2.428288000
1	-2.149308000	-0.458787000	-2.939509000
6	-2.968357000	2.461202000	-1.029937000
1	-3.906190000	1.955121000	-1.270748000
1	-3.197975000	3.516254000	-0.857468000
1	-2.315819000	2.401635000	-1.904863000
6	-1.893832000	-2.931128000	-0.533805000
1	-0.962954000	-2.982422000	-1.102797000
1	-1.688478000	-3.275002000	0.482603000
1	-2.604295000	-3.632389000	-0.980578000
14	0.922667000	-0.931738000	1.609320000
6	1.186444000	-2.782896000	1.473586000
1	0.930623000	-3.143820000	0.474258000
1	2.221563000	-3.062798000	1.683047000
1	0.551831000	-3.310681000	2.191401000
6	1.751354000	-0.320562000	3.164365000
1	1.585130000	0.750665000	3.298860000
1	1.363801000	-0.841087000	4.043496000
1	2.829867000	-0.492475000	3.125789000
32	0.110921000	0.336773000	-0.990469000
6	2.808706000	0.210035000	-0.109439000
6	3.215315000	1.461853000	-0.578026000
6	3.778558000	-0.788450000	0.005255000
6	4.533686000	1.701567000	-0.916239000
1	2.476730000	2.252540000	-0.663308000
6	5.100932000	-0.539598000	-0.321098000
1	3.481475000	-1.775918000	0.343137000
6	5.488733000	0.704766000	-0.786771000
1	4.820305000	2.683665000	-1.275830000
1	5.832423000	-1.333687000	-0.219044000
1	6.522578000	0.896889000	-1.047363000
1	0.650229000	0.343443000	-2.533436000
7	0.533762000	-1.153021000	-2.306328000

1	-0.143804000	-1.606162000	-2.908243000
1	1.331813000	-1.756496000	-2.129087000

5GeTS^{N-H} (T.E.= -3428.518791)

6	0.671103000	-0.067570000	1.684714000
6	1.314064000	-0.043465000	0.279979000
1	0.871743000	-1.011873000	2.209547000
1	1.071255000	0.708198000	2.346255000
7	-1.416053000	-0.305869000	0.519661000
14	2.703539000	-1.318555000	0.201503000
14	1.779732000	1.731632000	-0.167709000
6	1.949783000	-3.032969000	0.335385000
1	1.418931000	-3.304607000	-0.581211000
1	2.735736000	-3.775912000	0.494437000
1	1.244796000	-3.119132000	1.166720000
6	3.894960000	-1.096159000	1.628525000
1	4.566413000	-1.957677000	1.675059000
1	4.509205000	-0.201107000	1.520971000
1	3.375195000	-1.032564000	2.587446000
6	3.267035000	2.284026000	0.830973000
1	4.180041000	1.773629000	0.515571000
1	3.418009000	3.356268000	0.677490000
1	3.136190000	2.118257000	1.903033000
6	2.203573000	1.911286000	-1.994942000
1	1.573272000	2.672457000	-2.461303000
1	3.243441000	2.223436000	-2.118153000
1	2.077384000	0.983751000	-2.557375000
6	3.633797000	-1.228555000	-1.419887000
1	4.185374000	-0.293307000	-1.540502000
1	4.356454000	-2.047109000	-1.470330000
1	2.956727000	-1.336112000	-2.272277000
6	0.368477000	2.887188000	0.267207000
1	-0.525107000	2.695142000	-0.330272000
1	0.090308000	2.827037000	1.322460000
1	0.682839000	3.916121000	0.070905000
6	-2.812698000	-0.247739000	0.317908000
6	-3.477451000	-1.349983000	-0.203769000
6	-3.522042000	0.919459000	0.579581000
6	-4.835283000	-1.286615000	-0.463871000
1	-2.917578000	-2.258279000	-0.401771000

6	-4.880854000	0.973223000	0.326543000
1	-2.998630000	1.777070000	0.986027000
6	-5.542491000	-0.126353000	-0.197055000
1	-5.343515000	-2.152463000	-0.872401000
1	-5.427296000	1.885353000	0.537749000
1	-6.606405000	-0.078011000	-0.396557000
6	-0.841055000	0.069216000	1.703038000
8	-1.441517000	0.423583000	2.694746000
32	-0.186141000	-0.644382000	-0.875776000
1	-0.992940000	-0.874637000	-2.281605000
7	-0.938512000	0.636066000	-2.204555000
1	-0.355795000	0.934374000	-2.977709000
1	-1.666729000	1.318861000	-2.010172000

8GeTS^{N-H} (T.E.= -2997.127166)

6	-0.538280000	1.761765000	0.420046000
6	0.916360000	1.582092000	0.829689000
6	1.513451000	0.473673000	-0.010468000
1	-1.078539000	2.325150000	1.190463000
1	-0.590685000	2.351207000	-0.510481000
1	0.946379000	1.348960000	1.905998000
1	1.440312000	2.538593000	0.704122000
32	0.161494000	-0.808724000	-0.281991000
7	-1.139803000	0.452202000	0.243863000
15	3.157083000	0.228683000	-0.169555000
6	4.042924000	1.611983000	-0.928039000
1	3.829056000	2.521819000	-0.363947000
1	5.121315000	1.442691000	-0.929891000
1	3.686476000	1.746924000	-1.949468000
6	3.524592000	-1.213470000	-1.179903000
1	3.162686000	-2.115584000	-0.683678000
1	3.034047000	-1.120932000	-2.149111000
1	4.602882000	-1.297092000	-1.323796000
6	4.087144000	-0.036340000	1.368424000
1	5.158101000	-0.151448000	1.187629000
1	3.927302000	0.820216000	2.027008000
1	3.698540000	-0.927504000	1.864832000
6	-2.497135000	0.340543000	0.051798000
6	-3.090958000	-0.925186000	-0.089408000
6	-3.348457000	1.454717000	0.005114000

6	-4.450790000	-1.062802000	-0.269126000
1	-2.466650000	-1.811813000	-0.049513000
6	-4.713880000	1.300957000	-0.168141000
1	-2.939208000	2.452696000	0.097519000
6	-5.282760000	0.048061000	-0.308588000
1	-4.870162000	-2.057735000	-0.374936000
1	-5.340545000	2.186209000	-0.198251000
1	-6.351505000	-0.064531000	-0.444101000
1	-0.247707000	-2.390831000	-0.293861000
7	-0.044853000	-2.232944000	1.195695000
1	0.797640000	-2.707699000	1.504323000
1	-0.724454000	-2.191142000	1.950886000

9GeTS^{N-H} (T.E.= -2995.943007)

6	-0.449012000	-1.774827000	0.064845000
6	0.891349000	-1.731980000	0.186468000
6	1.529872000	-0.433191000	0.092781000
7	-1.105095000	-0.565988000	-0.166017000
15	3.189437000	-0.203677000	-0.044150000
6	4.136291000	-0.847698000	1.354807000
1	3.929568000	-1.914353000	1.461469000
1	5.208398000	-0.707678000	1.203349000
1	3.819688000	-0.341441000	2.266891000
6	3.590282000	1.543162000	-0.165641000
1	4.667299000	1.670299000	-0.283941000
1	3.079695000	1.975335000	-1.027816000
1	3.262376000	2.061213000	0.736504000
6	3.990625000	-0.993399000	-1.464185000
1	3.588166000	-0.568458000	-2.384426000
1	5.074630000	-0.864096000	-1.440011000
1	3.756206000	-2.059790000	-1.446356000
32	0.165099000	0.843091000	-0.244955000
6	-2.477499000	-0.418049000	-0.132224000
6	-3.334551000	-1.408603000	0.364498000
6	-3.063126000	0.770363000	-0.591376000
6	-4.703670000	-1.211708000	0.391545000
1	-2.924657000	-2.331046000	0.755809000
6	-4.428908000	0.957959000	-0.552525000
1	-2.422909000	1.548401000	-0.998475000
6	-5.268821000	-0.031783000	-0.061416000

1	-5.338238000	-1.997981000	0.786646000
1	-4.844361000	1.890529000	-0.919012000
1	-6.341463000	0.115772000	-0.033313000
1	-1.019901000	-2.694128000	0.056608000
1	1.457201000	-2.651816000	0.306620000
1	0.006993000	2.466866000	-0.005424000
7	-0.268692000	1.978404000	1.401605000
1	0.305956000	1.996487000	2.241766000
1	-1.249855000	2.073739000	1.649355000

14GeTS^{N-H} (T.E.= -3191.295920)

6	1.170319000	1.290853000	0.105922000
6	1.656027000	-0.047585000	-0.031905000
7	-1.044262000	0.100026000	-0.315173000
6	-2.372350000	-0.292307000	-0.116835000
6	-3.075383000	0.102277000	1.023029000
6	-4.377917000	-0.313150000	1.231220000
6	-5.004445000	-1.151635000	0.321926000
6	-4.308814000	-1.568498000	-0.800971000
6	-3.009832000	-1.143640000	-1.020620000
1	-2.578195000	0.740235000	1.746305000
1	-4.904936000	0.011387000	2.121709000
1	-6.023167000	-1.480077000	0.489932000
1	-4.783722000	-2.226000000	-1.520704000
1	-2.471012000	-1.458392000	-1.908967000
5	-0.437811000	1.390375000	-0.109690000
7	-1.130633000	2.618204000	-0.182861000
6	-0.578086000	3.881629000	0.254891000
1	-0.566848000	4.605507000	-0.569527000
1	-1.196301000	4.310580000	1.054440000
1	0.439383000	3.745424000	0.613107000
6	-2.476282000	2.769317000	-0.681253000
1	-3.192934000	2.983476000	0.123301000
1	-2.515365000	3.608800000	-1.385088000
1	-2.813244000	1.876244000	-1.204100000
15	3.339980000	-0.297062000	0.027478000
6	4.080207000	0.104774000	1.619620000
1	5.161479000	-0.043297000	1.591931000
1	3.854122000	1.146262000	1.847652000
1	3.641171000	-0.532256000	2.388131000

6	4.281276000	0.646177000	-1.183502000
1	5.352285000	0.476440000	-1.058629000
1	3.975633000	0.348657000	-2.187034000
1	4.049622000	1.701237000	-1.036532000
6	3.721684000	-2.028299000	-0.271883000
1	3.219261000	-2.649628000	0.471953000
1	3.370871000	-2.316329000	-1.264012000
1	4.798539000	-2.191827000	-0.208630000
8	1.932528000	2.252921000	0.325875000
32	0.251179000	-1.267867000	-0.413563000
1	0.161256000	-2.901467000	-0.219142000
7	-0.105124000	-2.448161000	1.179691000
1	0.420443000	-2.445768000	2.050870000
1	-1.085207000	-2.646712000	1.356910000

IIa-TS^{N-H} (T.E.= -1112.312055)

6	-0.003396000	2.467974000	-0.036005000
6	-1.196998000	1.853626000	0.075028000
1	-0.014135000	3.548701000	-0.101823000
14	0.044588000	-0.604073000	0.382460000
6	2.411601000	2.636565000	-0.198011000
6	1.315940000	1.870307000	-0.044592000
1	3.415532000	2.235980000	-0.191173000
1	2.295799000	3.703661000	-0.329922000
6	-2.607382000	-0.147420000	0.142793000
6	-3.312374000	-0.163477000	-1.057264000
6	-3.132196000	-0.811332000	1.244949000
6	-4.530943000	-0.811489000	-1.145196000
1	-2.887831000	0.336824000	-1.922300000
6	-4.345736000	-1.472150000	1.149632000
1	-2.576508000	-0.799438000	2.176053000
6	-5.051036000	-1.470250000	-0.041680000
1	-5.072758000	-0.811231000	-2.084007000
1	-4.745204000	-1.985375000	2.016694000
1	-6.002794000	-1.983213000	-0.112597000
7	-1.334240000	0.475882000	0.227751000
6	2.661761000	-0.142991000	0.092500000
6	3.331032000	-0.457093000	1.266107000
6	3.236407000	-0.460686000	-1.132426000
6	4.565298000	-1.084664000	1.216042000

1	2.869791000	-0.202025000	2.214086000
6	4.471507000	-1.083097000	-1.180611000
1	2.701115000	-0.202749000	-2.040806000
6	5.138208000	-1.395194000	-0.005835000
1	5.081499000	-1.330757000	2.136739000
1	4.915410000	-1.327221000	-2.138880000
1	6.104650000	-1.884096000	-0.043893000
7	1.382364000	0.481208000	0.137274000
6	-2.448585000	2.667883000	0.115282000
1	-3.083965000	2.498396000	-0.756589000
1	-3.048760000	2.416520000	0.994430000
1	-2.202569000	3.727425000	0.153443000
1	-0.371185000	-2.173333000	0.206202000
7	-0.172376000	-1.730346000	-1.088011000
1	0.655993000	-2.254151000	-1.354173000
1	-0.807201000	-1.623185000	-1.879296000

Cartesian coordinates of the transition states involved in the activation of C – H bond of CH₃Ph by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**) and CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**), along with their total energies (in hartrees) including zero point vibrational correction.

1SiTS^{C-H} (T.E.= -1781.754661)

7	0.761380000	0.550529000	-0.419433000
1	0.020029000	-2.972574000	1.186767000
6	1.925899000	-2.096181000	0.652544000
6	2.029647000	-2.489598000	-0.679697000
1	1.133784000	-2.797401000	-1.214241000
6	3.245283000	-2.458662000	-1.331275000
1	3.308653000	-2.758388000	-2.370843000
6	4.383726000	-2.034817000	-0.658498000
1	5.336475000	-1.997138000	-1.173381000
6	4.296523000	-1.655722000	0.668110000
1	5.178618000	-1.315438000	1.197561000
6	3.072270000	-1.680675000	1.316381000
1	2.998532000	-1.358503000	2.350402000
1	0.711997000	-1.907705000	2.410846000
1	-0.285466000	-1.574832000	0.042184000

6	0.612597000	-2.068338000	1.337840000
14	-0.282726000	-0.178793000	0.813347000
6	-1.858218000	0.019868000	-0.288062000
6	0.165811000	0.591984000	-1.741388000
6	-1.232087000	-0.040017000	-1.701446000
1	-1.138775000	-1.087446000	-2.006149000
1	-1.870061000	0.445184000	-2.449951000
1	0.782348000	0.053756000	-2.475755000
1	0.112513000	1.637049000	-2.084538000
6	1.958023000	1.203576000	-0.200417000
6	2.777691000	1.624031000	-1.254968000
6	2.398453000	1.476337000	1.104083000
6	3.979849000	2.267062000	-1.008164000
1	2.484034000	1.429982000	-2.278660000
6	3.592847000	2.121961000	1.337416000
1	1.778313000	1.171689000	1.942778000
6	4.403682000	2.521802000	0.283296000
1	4.593659000	2.571128000	-1.849272000
1	3.895891000	2.318273000	2.360305000
1	5.343913000	3.026693000	0.468945000
14	-3.114994000	-1.358291000	-0.020470000
14	-2.506064000	1.759480000	0.126198000
6	-3.291808000	-1.784350000	1.795757000
1	-4.035737000	-2.577616000	1.911008000
1	-2.351213000	-2.150359000	2.215763000
1	-3.612713000	-0.934078000	2.399152000
6	-4.797473000	-0.913236000	-0.721541000
1	-5.468371000	-1.770644000	-0.618475000
1	-5.266176000	-0.062846000	-0.222225000
1	-4.722991000	-0.680923000	-1.787792000
6	-2.618328000	-2.935294000	-0.915422000
1	-3.347192000	-3.708832000	-0.655969000
1	-2.644195000	-2.815755000	-2.000853000
1	-1.629438000	-3.311156000	-0.642006000

6	-3.526246000	2.416118000	-1.306077000
1	-4.328246000	1.740910000	-1.608712000
1	-3.978421000	3.368705000	-1.016731000
1	-2.894405000	2.607098000	-2.177365000
6	-3.534573000	1.761886000	1.692631000
1	-3.825085000	2.793569000	1.909710000
1	-4.447667000	1.168631000	1.621188000
1	-2.953618000	1.398278000	2.544082000
6	-1.140683000	3.016532000	0.406911000
1	-0.464463000	2.741185000	1.220278000
1	-0.535840000	3.190645000	-0.485502000
1	-1.612669000	3.966004000	0.678344000

2SiTS^{C-H} (T.E.= -1780.562541)

7	-0.690635000	-0.726841000	-0.466389000
1	-0.083679000	2.675147000	1.457095000
6	-1.988911000	1.852681000	0.848619000
6	-2.125696000	2.488814000	-0.382010000
1	-1.248048000	2.910452000	-0.864998000
6	-3.357759000	2.566508000	-1.000768000
1	-3.450777000	3.067115000	-1.957465000
6	-4.471544000	1.992154000	-0.404142000
1	-5.436149000	2.038760000	-0.896053000
6	-4.345699000	1.351555000	0.815217000
1	-5.209499000	0.891896000	1.280778000
6	-3.110333000	1.280964000	1.435875000
1	-3.006488000	0.767154000	2.386678000
1	-0.769407000	1.487633000	2.568470000
1	0.213945000	1.394979000	0.143359000
6	-0.672390000	1.759007000	1.518393000
14	0.320499000	-0.032846000	0.849995000
6	1.909763000	-0.059599000	-0.276053000
6	-0.012142000	-0.612941000	-1.674012000
6	1.279493000	-0.261228000	-1.629935000
6	-1.963403000	-1.282522000	-0.357996000
6	-2.899699000	-1.205305000	-1.390617000
6	-2.338477000	-1.930756000	0.822117000
6	-4.156245000	-1.765284000	-1.244754000

1	-2.653662000	-0.668721000	-2.299896000
6	-3.596564000	-2.481083000	0.961732000
1	-1.622681000	-1.995370000	1.636373000
6	-4.518171000	-2.407387000	-0.072442000
1	-4.868450000	-1.682107000	-2.058513000
1	-3.857204000	-2.981883000	1.887656000
1	-5.504573000	-2.841877000	0.035886000
14	2.925038000	1.522214000	-0.172635000
14	2.812870000	-1.666116000	0.182686000
6	3.188609000	2.055634000	1.605065000
1	3.675225000	3.034769000	1.621392000
1	2.245917000	2.146362000	2.150434000
1	3.822601000	1.359417000	2.156358000
6	4.601044000	1.301197000	-0.984899000
1	5.121401000	2.262556000	-1.007879000
1	5.235523000	0.592323000	-0.448277000
1	4.502024000	0.953168000	-2.016770000
6	2.076154000	2.928672000	-1.080411000
1	2.802093000	3.730371000	-1.244054000
1	1.696189000	2.612858000	-2.054553000
1	1.242774000	3.355650000	-0.517953000
6	3.973344000	-2.185930000	-1.196699000
1	4.765994000	-1.462648000	-1.393659000
1	4.445830000	-3.133943000	-0.924612000
1	3.420658000	-2.348248000	-2.125066000
6	3.777629000	-1.473864000	1.776944000
1	4.180751000	-2.446705000	2.071363000
1	4.618976000	-0.783774000	1.682063000
1	3.134945000	-1.122132000	2.588471000
6	1.608077000	-3.081869000	0.422096000
1	1.001782000	-2.964504000	1.323505000
1	0.937011000	-3.204769000	-0.430463000
1	2.182275000	-4.006567000	0.532434000
1	-0.533022000	-0.861083000	-2.591961000
1	1.872764000	-0.190709000	-2.536870000

3SiTS^{C-H} (T.E.= -1901.857353)

7	-0.622422000	0.774315000	-0.073750000
1	-0.161959000	-3.111436000	-0.867611000
6	-2.040795000	-2.202098000	-0.278154000

6	-2.055500000	-2.345233000	1.106335000
1	-1.114498000	-2.422550000	1.645898000
6	-3.249167000	-2.373952000	1.800470000
1	-3.243178000	-2.491445000	2.877928000
6	-4.452550000	-2.245248000	1.121531000
1	-5.389026000	-2.257849000	1.667004000
6	-4.449536000	-2.084067000	-0.252296000
1	-5.383095000	-1.962058000	-0.789236000
6	-3.250803000	-2.060452000	-0.945279000
1	-3.248639000	-1.910230000	-2.020645000
1	-0.997643000	-2.221395000	-2.127748000
1	0.113661000	-1.552108000	0.100788000
6	-0.773330000	-2.226386000	-1.059987000
14	0.346402000	-0.408206000	-1.006629000
6	1.945926000	-0.205483000	0.067076000
6	1.384570000	0.382444000	1.392907000
6	-1.932008000	1.086116000	-0.464907000
6	-2.960115000	1.160138000	0.475520000
6	-2.252405000	1.292934000	-1.806958000
6	-4.254187000	1.449930000	0.088176000
1	-2.726079000	0.975295000	1.518594000
6	-3.551770000	1.573188000	-2.192213000
1	-1.463139000	1.231753000	-2.550628000
6	-4.562075000	1.657154000	-1.247961000
1	-5.035761000	1.497088000	0.838678000
1	-3.773569000	1.734670000	-3.241417000
1	-5.579022000	1.878058000	-1.549561000
14	2.889626000	-1.810526000	0.326989000
14	2.921950000	1.140291000	-0.852677000
6	3.039625000	-2.805410000	-1.255439000
1	3.541495000	-3.753444000	-1.041918000
1	2.061683000	-3.039089000	-1.684099000
1	3.617672000	-2.286400000	-2.020815000
6	4.607988000	-1.492215000	1.013104000
1	5.078336000	-2.446402000	1.265962000
1	5.263800000	-0.974354000	0.310157000
1	4.555288000	-0.896116000	1.928547000
6	2.058289000	-2.927686000	1.590274000
1	2.706361000	-3.796852000	1.737620000
1	1.934482000	-2.444854000	2.562089000

1	1.082821000	-3.301038000	1.270864000
6	4.141140000	1.983166000	0.301611000
1	4.795321000	1.286988000	0.828275000
1	4.770296000	2.662421000	-0.280637000
1	3.616033000	2.585378000	1.048189000
6	3.838931000	0.458399000	-2.338538000
1	4.289106000	1.294556000	-2.881037000
1	4.642334000	-0.232344000	-2.074394000
1	3.160147000	-0.053913000	-3.025191000
6	1.824724000	2.526010000	-1.493904000
1	1.066083000	2.182380000	-2.201505000
1	1.319667000	3.064183000	-0.687311000
1	2.465995000	3.240900000	-2.018830000
5	0.117560000	1.288183000	1.052153000
1	1.044821000	-0.434031000	2.049047000
1	2.171786000	0.911586000	1.941244000
7	-0.151076000	2.508252000	1.721634000
6	0.488992000	2.876841000	2.960965000
1	1.082373000	2.056050000	3.359671000
1	1.145185000	3.748248000	2.831709000
1	-0.258590000	3.144110000	3.718081000
6	-1.014796000	3.557303000	1.235155000
1	-0.489573000	4.518857000	1.288156000
1	-1.298858000	3.391265000	0.197415000
1	-1.934003000	3.651061000	1.828221000

4SiTS^{C-H} (T.E.= -2111.771804)

7	0.780904000	0.576311000	-0.377358000
1	-0.012424000	-3.076118000	0.820589000
6	1.886621000	-2.095189000	0.913053000
6	2.370392000	-2.631482000	-0.275168000
1	1.677204000	-3.111522000	-0.960751000
6	3.715539000	-2.552748000	-0.587943000
1	4.079108000	-2.972604000	-1.518821000
6	4.594468000	-1.935906000	0.287958000
1	5.647351000	-1.864869000	0.041080000
6	4.123952000	-1.405636000	1.478822000
1	4.806513000	-0.916407000	2.163727000
6	2.778979000	-1.479865000	1.785428000
1	2.403622000	-1.043004000	2.706158000

1	0.242997000	-2.149523000	2.298469000
1	-0.315707000	-1.556274000	-0.062244000
6	0.447317000	-2.173329000	1.230101000
14	-0.313862000	-0.188720000	0.787782000
6	-2.029652000	0.069376000	-0.111869000
6	-1.745159000	0.442233000	-1.600663000
6	1.994525000	1.171259000	-0.015047000
6	3.085580000	1.151288000	-0.885826000
6	2.166413000	1.801498000	1.220309000
6	4.288316000	1.742548000	-0.543234000
1	2.990849000	0.635571000	-1.836401000
6	3.371942000	2.382852000	1.563718000
1	1.339391000	1.819272000	1.923842000
6	4.444630000	2.361257000	0.685326000
1	5.116786000	1.702898000	-1.241999000
1	3.472094000	2.863859000	2.530677000
1	5.388521000	2.818577000	0.956748000
14	-3.080236000	-1.488263000	-0.021946000
14	-2.755919000	1.580304000	0.765785000
6	-3.101969000	-2.272184000	1.682837000
1	-3.776859000	-3.132762000	1.655589000
1	-2.125708000	-2.635261000	2.008539000
1	-3.472948000	-1.585644000	2.445458000
6	-4.862501000	-1.143745000	-0.496361000
1	-5.381941000	-2.092879000	-0.655082000
1	-5.397246000	-0.600221000	0.285637000
1	-4.931687000	-0.564720000	-1.420962000
6	-2.484475000	-2.798022000	-1.235677000
1	-3.100173000	-3.691380000	-1.094578000
1	-2.606545000	-2.481738000	-2.274372000
1	-1.440730000	-3.092041000	-1.099716000
6	-4.291239000	2.239221000	-0.097620000
1	-5.169080000	1.614397000	0.071654000
1	-4.511063000	3.233022000	0.303100000
1	-4.156832000	2.345075000	-1.176277000
6	-3.223204000	1.223730000	2.544115000
1	-3.490958000	2.162488000	3.036777000
1	-4.089930000	0.560887000	2.605515000
1	-2.401992000	0.772158000	3.105385000
6	-1.517754000	2.991136000	0.738651000

1	-0.594952000	2.768998000	1.278444000
1	-1.245585000	3.268875000	-0.283132000
1	-1.974087000	3.867835000	1.207045000
14	0.104308000	0.579705000	-1.980673000
1	-2.186288000	-0.284246000	-2.294358000
1	-2.208099000	1.402322000	-1.863620000
6	0.489905000	2.170675000	-2.879565000
1	1.515379000	2.207089000	-3.250480000
1	-0.179861000	2.282507000	-3.736245000
1	0.341487000	3.029920000	-2.220259000
6	0.624466000	-0.881589000	-3.028176000
1	0.070571000	-0.869074000	-3.971465000
1	1.690610000	-0.869120000	-3.266036000
1	0.399273000	-1.827146000	-2.528405000

5SiTS^{C-H} (T.E.= -1855.825374)

7	0.673585000	-0.680017000	0.445452000
1	0.107111000	2.947512000	-1.054669000
6	2.008202000	1.996938000	-0.717801000
6	2.266609000	2.534281000	0.539994000
1	1.448317000	2.953806000	1.119196000
6	3.547992000	2.526505000	1.055888000
1	3.738303000	2.948901000	2.035488000
6	4.587843000	1.975874000	0.321402000
1	5.591968000	1.964328000	0.728925000
6	4.339945000	1.432559000	-0.927647000
1	5.147247000	0.991201000	-1.499722000
6	3.055304000	1.436463000	-1.440239000
1	2.853358000	0.993973000	-2.411375000
1	0.642465000	1.896328000	-2.366262000
1	-0.229369000	1.526014000	0.026588000
6	0.644125000	2.026264000	-1.285683000
14	-0.321038000	0.159507000	-0.801944000
6	-1.936986000	-0.006529000	0.247001000
6	-1.348713000	-0.217250000	1.653697000
6	1.945493000	-1.252300000	0.204469000
6	2.966920000	-1.162651000	1.142450000
6	2.192802000	-1.890283000	-1.006141000
6	4.208561000	-1.707256000	0.869448000
1	2.783295000	-0.655897000	2.080478000

6	3.438303000	-2.427324000	-1.277026000
1	1.398256000	-1.957753000	-1.742948000
6	4.452675000	-2.341422000	-0.338026000
1	4.997300000	-1.626204000	1.608944000
1	3.612896000	-2.921674000	-2.225857000
1	5.428432000	-2.764309000	-0.546332000
14	-3.016905000	1.533111000	0.110436000
14	-2.757924000	-1.614279000	-0.356135000
6	-3.067693000	2.163370000	-1.654325000
1	-3.742195000	3.022646000	-1.705663000
1	-2.090059000	2.494849000	-2.012018000
1	-3.436323000	1.409059000	-2.351510000
6	-4.776339000	1.229864000	0.681141000
1	-5.308665000	2.185124000	0.698872000
1	-5.334593000	0.552839000	0.031787000
1	-4.795631000	0.822505000	1.695751000
6	-2.387122000	2.920855000	1.208402000
1	-3.004341000	3.803336000	1.016298000
1	-2.493038000	2.676795000	2.268068000
1	-1.346911000	3.202705000	1.031729000
6	-4.055521000	-2.200705000	0.864453000
1	-4.875197000	-1.494099000	0.998421000
1	-4.479663000	-3.136395000	0.488612000
1	-3.624163000	-2.414658000	1.844911000
6	-3.551373000	-1.391091000	-2.036512000
1	-3.879808000	-2.367956000	-2.401752000
1	-4.427601000	-0.739761000	-2.005862000
1	-2.845133000	-0.985221000	-2.765181000
6	-1.506071000	-3.004380000	-0.494646000
1	-0.792125000	-2.845907000	-1.306360000
1	-0.940475000	-3.164236000	0.427095000
1	-2.048654000	-3.928520000	-0.714394000
1	-1.991110000	-0.820494000	2.303669000
6	0.016973000	-0.885468000	1.635475000
8	0.438425000	-1.522893000	2.575955000
1	-1.195830000	0.739784000	2.171626000

8SiTS^{C-H} (T.E.= -1424.429259)

6	-1.824113000	1.701474000	1.113801000
6	-0.338938000	1.990427000	1.364138000

6	0.447804000	1.372003000	0.233191000
1	-2.385512000	1.735314000	2.057578000
1	-2.238716000	2.484764000	0.460475000
1	-0.054997000	1.567701000	2.340582000
1	-0.207976000	3.077493000	1.435601000
14	-0.409404000	-0.190222000	-0.159987000
7	-1.975030000	0.404236000	0.466152000
15	1.870232000	1.938699000	-0.423605000
6	1.859298000	3.727965000	-0.702323000
1	1.686265000	4.242030000	0.244574000
1	2.816809000	4.059606000	-1.108008000
1	1.055465000	3.984694000	-1.392181000
6	3.415302000	1.711624000	0.510176000
1	3.600503000	0.640831000	0.625432000
1	4.266085000	2.176332000	0.005867000
1	3.303542000	2.151963000	1.502982000
6	2.242819000	1.165711000	-2.005904000
1	2.478245000	0.111269000	-1.848702000
1	1.384816000	1.247052000	-2.672753000
1	3.108478000	1.656945000	-2.453960000
6	-3.223569000	-0.028650000	0.099314000
6	-3.381836000	-1.243205000	-0.591601000
6	-4.390030000	0.697442000	0.388351000
6	-4.625407000	-1.688300000	-0.986219000
1	-2.501313000	-1.835730000	-0.821043000
6	-5.632555000	0.234719000	-0.009114000
1	-4.324167000	1.634800000	0.925397000
6	-5.769881000	-0.956068000	-0.700825000
1	-4.703086000	-2.627933000	-1.523034000
1	-6.511015000	0.825409000	0.229171000
1	-6.746079000	-1.311157000	-1.007786000
1	-0.008589000	-0.614988000	1.357351000
6	0.157601000	-2.080486000	0.606740000
1	-0.337581000	-2.712297000	-0.133818000
1	-0.175084000	-2.417077000	1.590489000
6	1.631814000	-2.131343000	0.466623000
6	2.218525000	-2.403422000	-0.765799000
6	2.455564000	-1.898083000	1.562116000
6	3.594584000	-2.455673000	-0.897695000
1	1.577580000	-2.570460000	-1.626871000

6	3.834062000	-1.951223000	1.434074000
1	2.003701000	-1.673705000	2.523976000
6	4.407263000	-2.227385000	0.203535000
1	4.036221000	-2.677244000	-1.862565000
1	4.462979000	-1.775939000	2.299303000
1	5.485379000	-2.268975000	0.102340000

9SiTS^{C-H} (T.E.= -1423.239610)

7	-2.007142000	0.429637000	0.420587000
14	-0.438645000	-0.209570000	-0.188942000
6	0.385900000	1.424988000	0.131726000
6	-1.763206000	1.619406000	1.129417000
6	-0.530804000	2.146137000	0.993878000
6	-3.272496000	-0.029061000	0.128154000
6	-3.443183000	-1.298079000	-0.443913000
6	-4.426822000	0.729423000	0.370889000
6	-4.697215000	-1.776009000	-0.765924000
1	-2.567264000	-1.909964000	-0.636482000
6	-5.678039000	0.233201000	0.056090000
1	-4.338985000	1.726890000	0.782782000
6	-5.832485000	-1.020071000	-0.514810000
1	-4.788524000	-2.760604000	-1.212068000
1	-6.549967000	0.848220000	0.252448000
1	-6.816772000	-1.400175000	-0.759701000
15	1.863199000	2.010189000	-0.401579000
6	1.754784000	3.703954000	-1.026902000
1	1.323822000	4.336940000	-0.249043000
1	2.740123000	4.089822000	-1.294533000
1	1.096051000	3.726916000	-1.894939000
6	3.191491000	2.135499000	0.828235000
1	3.410022000	1.138383000	1.214014000
1	4.097143000	2.569481000	0.398028000
1	2.849837000	2.762957000	1.653881000
6	2.559714000	1.002029000	-1.714484000
1	2.825958000	0.015872000	-1.328254000
1	1.828739000	0.883839000	-2.515061000
1	3.457269000	1.485613000	-2.103620000
1	-2.529737000	2.010833000	1.786291000
1	-0.253017000	3.047746000	1.534713000
1	-0.018821000	-0.503372000	1.335684000

6	0.181595000	-2.071645000	0.651272000
1	-0.095170000	-2.324417000	1.674625000
1	-0.356634000	-2.739228000	-0.022121000
6	1.640324000	-2.110856000	0.426801000
6	2.158178000	-2.561545000	-0.785714000
6	2.524201000	-1.684313000	1.412688000
6	3.523081000	-2.608160000	-0.997808000
1	1.470188000	-2.872495000	-1.566464000
6	3.892875000	-1.724204000	1.200229000
1	2.127706000	-1.319601000	2.355910000
6	4.396280000	-2.185751000	-0.004860000
1	3.910155000	-2.972292000	-1.942506000
1	4.569259000	-1.397223000	1.982029000
1	5.466618000	-2.220113000	-0.170635000

14SiTS^{C-H} (T.E.= -1618.593725)

6	-0.306734000	1.950248000	0.142685000
6	0.644733000	1.027552000	-0.389671000
7	-1.706918000	-0.179110000	0.081276000
6	-2.830396000	-0.891388000	-0.331558000
6	-2.835538000	-2.287975000	-0.338509000
6	-3.934917000	-2.997215000	-0.790534000
6	-5.064541000	-2.335387000	-1.240142000
6	-5.072589000	-0.948238000	-1.238280000
6	-3.974646000	-0.235265000	-0.798243000
1	-1.964785000	-2.819568000	0.031727000
1	-3.907855000	-4.081297000	-0.781432000
1	-5.926548000	-2.890822000	-1.589439000
1	-5.943568000	-0.411067000	-1.597715000
1	-3.983079000	0.849321000	-0.821315000
5	-1.655927000	1.175847000	0.612431000
7	-2.613337000	1.726659000	1.480419000
6	-2.627766000	3.122267000	1.865609000
1	-3.584180000	3.583543000	1.589403000
1	-2.519430000	3.224009000	2.952217000
1	-1.817966000	3.654112000	1.370102000
6	-3.672941000	0.975914000	2.109154000
1	-3.693348000	1.194732000	3.182676000
1	-4.657656000	1.237878000	1.700392000
1	-3.528092000	-0.095156000	1.981020000

15	2.051941000	1.645675000	-1.126667000
6	3.202263000	2.427901000	0.018992000
1	4.063724000	2.835496000	-0.513601000
1	2.678029000	3.228411000	0.541502000
1	3.536920000	1.681777000	0.742229000
6	1.720948000	2.892352000	-2.386271000
1	2.658285000	3.297085000	-2.773127000
1	1.155905000	2.435232000	-3.199256000
1	1.125010000	3.685283000	-1.936143000
6	2.989655000	0.359074000	-1.954838000
1	3.384337000	-0.349415000	-1.225646000
1	2.340205000	-0.176160000	-2.649097000
1	3.818461000	0.810420000	-2.503213000
8	-0.131604000	3.185905000	0.146282000
14	-0.044921000	-0.704555000	-0.322847000
1	0.359710000	-0.530550000	1.218887000
6	0.757800000	-2.142580000	0.989559000
1	0.396925000	-2.181227000	2.019084000
1	0.415710000	-3.050486000	0.488911000
6	2.231794000	-2.012114000	0.910039000
6	2.953332000	-2.744892000	-0.027037000
6	2.920771000	-1.156721000	1.764349000
6	4.331528000	-2.643031000	-0.095887000
1	2.417197000	-3.398753000	-0.708662000
6	4.299207000	-1.047247000	1.692900000
1	2.364142000	-0.570354000	2.489924000
6	5.009030000	-1.790757000	0.763053000
1	4.879522000	-3.228186000	-0.825243000
1	4.822464000	-0.381956000	2.370338000
1	6.088034000	-1.707957000	0.708842000

1GeTS^{C-H} (T.E.= -3569.223137)

7	-0.819611000	0.634325000	0.466037000
1	-0.158515000	-2.892275000	-1.406131000
6	-2.034444000	-2.114019000	-0.627295000
6	-2.007982000	-2.635285000	0.665847000
1	-1.063358000	-2.978926000	1.080615000
6	-3.153924000	-2.681945000	1.430903000
1	-3.115751000	-3.083669000	2.436682000
6	-4.352503000	-2.199784000	0.919235000

1	-5.248793000	-2.218634000	1.527894000
6	-4.395114000	-1.688128000	-0.364114000
1	-5.323648000	-1.302725000	-0.768474000
6	-3.242289000	-1.646370000	-1.130867000
1	-3.274874000	-1.229478000	-2.132154000
1	-1.012958000	-1.756951000	-2.477483000
1	0.245178000	-1.567786000	-0.046100000
6	-0.810412000	-2.021655000	-1.441387000
6	1.865671000	0.036664000	0.368344000
6	-0.174801000	0.720208000	1.754014000
6	1.163593000	-0.020513000	1.737160000
1	0.978778000	-1.066407000	2.004074000
1	1.805601000	0.394946000	2.524321000
1	-0.803637000	0.291496000	2.548256000
1	-0.016847000	1.777798000	2.025928000
6	-1.991810000	1.311038000	0.250588000
6	-2.740003000	1.866686000	1.301416000
6	-2.502012000	1.478148000	-1.049451000
6	-3.939389000	2.513992000	1.057494000
1	-2.391093000	1.771021000	2.321598000
6	-3.693434000	2.130448000	-1.278635000
1	-1.940157000	1.081331000	-1.891250000
6	-4.435860000	2.650800000	-0.226560000
1	-4.494846000	2.918517000	1.897175000
1	-4.049165000	2.235636000	-2.298289000
1	-5.374500000	3.159868000	-0.408359000
14	3.078636000	-1.387611000	0.129205000
14	2.560977000	1.761746000	-0.027509000
6	3.281981000	-1.813405000	-1.684229000
1	4.004634000	-2.627402000	-1.788731000
1	2.336481000	-2.156518000	-2.114703000
1	3.633534000	-0.973921000	-2.285279000
6	4.749123000	-0.982273000	0.883408000
1	5.411726000	-1.846821000	0.788402000
1	5.243270000	-0.129586000	0.413394000
1	4.644280000	-0.764215000	1.950248000
6	2.507287000	-2.955636000	0.991049000
1	3.246373000	-3.735690000	0.785496000
1	2.446525000	-2.840790000	2.075231000
1	1.539752000	-3.315321000	0.631582000

6	3.522216000	2.388817000	1.457106000
1	4.293209000	1.692178000	1.791226000
1	4.008367000	3.333520000	1.199269000
1	2.852280000	2.584210000	2.298499000
6	3.663050000	1.724084000	-1.542510000
1	4.013038000	2.740996000	-1.740637000
1	4.541389000	1.085349000	-1.436900000
1	3.102189000	1.393963000	-2.421162000
6	1.245253000	3.048245000	-0.393661000
1	0.650898000	2.809460000	-1.279385000
1	0.559069000	3.210024000	0.439523000
1	1.757234000	3.995309000	-0.591642000
32	0.268495000	-0.135231000	-0.900184000

2GeTSC^{C-H} (T.E.= -3568.034593)

7	0.731493000	-0.745670000	0.531204000
1	0.224366000	2.690840000	-1.548837000
6	2.097927000	1.868588000	-0.825439000
6	2.175555000	2.546390000	0.390431000
1	1.283518000	3.016872000	0.794937000
6	3.362900000	2.600981000	1.090440000
1	3.409512000	3.132918000	2.033415000
6	4.492336000	1.961547000	0.595539000
1	5.419703000	1.987809000	1.155825000
6	4.427082000	1.277685000	-0.604983000
1	5.297814000	0.755856000	-0.984020000
6	3.237218000	1.232137000	-1.309191000
1	3.179117000	0.678288000	-2.241199000
1	0.977373000	1.468589000	-2.609010000
1	-0.226645000	1.436027000	-0.102978000
6	0.842577000	1.797274000	-1.581616000
6	-1.938186000	-0.060391000	0.375385000
6	0.041968000	-0.622273000	1.717251000
6	-1.250987000	-0.263713000	1.691216000
6	2.001207000	-1.288284000	0.428977000
6	2.918117000	-1.275349000	1.485111000
6	2.405010000	-1.873276000	-0.777624000
6	4.181878000	-1.814154000	1.327816000
1	2.649809000	-0.810672000	2.426748000
6	3.669914000	-2.403259000	-0.926471000

1	1.700390000	-1.906727000	-1.604239000
6	4.574958000	-2.378245000	0.124993000
1	4.876251000	-1.778649000	2.160475000
1	3.950281000	-2.849769000	-1.874340000
1	5.567994000	-2.795330000	0.009400000
14	-2.935685000	1.534645000	0.284418000
14	-2.820688000	-1.677095000	-0.083442000
6	-3.202556000	2.064396000	-1.494016000
1	-3.708174000	3.033659000	-1.515270000
1	-2.255152000	2.176883000	-2.028727000
1	-3.816198000	1.356051000	-2.053145000
6	-4.606997000	1.309470000	1.106655000
1	-5.131102000	2.268368000	1.140157000
1	-5.242311000	0.601061000	0.570089000
1	-4.498455000	0.954385000	2.135254000
6	-2.069890000	2.936108000	1.181706000
1	-2.793677000	3.729860000	1.387616000
1	-1.643728000	2.610067000	2.133050000
1	-1.264271000	3.372381000	0.586210000
6	-3.959570000	-2.198351000	1.312753000
1	-4.755505000	-1.479302000	1.512669000
1	-4.427412000	-3.152453000	1.054397000
1	-3.392738000	-2.346522000	2.234777000
6	-3.810110000	-1.490759000	-1.663449000
1	-4.227479000	-2.461895000	-1.943117000
1	-4.643636000	-0.792777000	-1.556645000
1	-3.182029000	-1.150168000	-2.491101000
6	-1.598730000	-3.076102000	-0.331404000
1	-0.982552000	-2.943704000	-1.224379000
1	-0.934097000	-3.195513000	0.526760000
1	-2.159656000	-4.007123000	-0.454929000
32	-0.327367000	-0.014853000	-0.915858000
1	-1.812543000	-0.161661000	2.615774000
1	0.556013000	-0.850873000	2.645267000

3GeTS^{C-H} (T.E.= -3689.327728)

7	-0.698908000	0.760293000	0.004171000
1	-0.247485000	-3.244491000	-0.590259000
6	-2.113101000	-2.237972000	-0.136534000
6	-2.133153000	-2.239453000	1.256066000

1	-1.193807000	-2.287544000	1.801729000
6	-3.326664000	-2.156603000	1.944588000
1	-3.325181000	-2.161951000	3.028351000
6	-4.524342000	-2.051781000	1.251389000
1	-5.460332000	-1.972927000	1.792177000
6	-4.517520000	-2.033574000	-0.131768000
1	-5.447001000	-1.938595000	-0.680839000
6	-3.319467000	-2.121100000	-0.819210000
1	-3.314270000	-2.103866000	-1.904382000
1	-1.049857000	-2.478938000	-1.970351000
1	0.168716000	-1.583040000	0.302496000
6	-0.859353000	-2.398833000	-0.901286000
6	1.986572000	-0.149714000	0.169727000
6	1.364454000	0.465705000	1.443212000
1	1.047168000	-0.332463000	2.132330000
1	2.121579000	1.050918000	1.977963000
6	-1.999524000	1.060675000	-0.400437000
6	-3.030480000	1.200221000	0.532084000
6	-2.320057000	1.210515000	-1.752324000
6	-4.317404000	1.499912000	0.128739000
1	-2.800790000	1.072495000	1.584727000
6	-3.611980000	1.500973000	-2.152840000
1	-1.533334000	1.101738000	-2.493600000
6	-4.621521000	1.650978000	-1.215813000
1	-5.097511000	1.601475000	0.875747000
1	-3.828812000	1.617810000	-3.209108000
1	-5.633212000	1.880180000	-1.528671000
14	2.965407000	-1.724665000	0.486399000
14	2.895102000	1.198165000	-0.810392000
6	3.109565000	-2.766430000	-1.066095000
1	3.661075000	-3.683960000	-0.842742000
1	2.129893000	-3.058916000	-1.453529000
1	3.637014000	-2.245370000	-1.866518000
6	4.688876000	-1.336385000	1.122879000
1	5.187793000	-2.266983000	1.407072000
1	5.319080000	-0.833388000	0.386519000
1	4.637777000	-0.703750000	2.013558000
6	2.187025000	-2.806982000	1.810104000
1	2.850603000	-3.661966000	1.971023000
1	2.084749000	-2.288169000	2.765773000

1	1.206996000	-3.201044000	1.532168000
6	4.088390000	2.116880000	0.312866000
1	4.809781000	1.467270000	0.810416000
1	4.644802000	2.845690000	-0.283262000
1	3.543369000	2.671121000	1.082329000
6	3.825432000	0.496974000	-2.278660000
1	4.256101000	1.326456000	-2.846459000
1	4.644400000	-0.167732000	-1.996407000
1	3.158454000	-0.050331000	-2.950001000
6	1.747104000	2.524898000	-1.481837000
1	0.986386000	2.140383000	-2.165370000
1	1.240438000	3.073589000	-0.683511000
1	2.359572000	3.241050000	-2.038548000
32	0.329516000	-0.525767000	-0.991569000
5	0.066522000	1.325240000	1.073366000
7	-0.194026000	2.575035000	1.700704000
6	-1.059647000	3.604836000	1.178416000
1	-1.379754000	3.380962000	0.162166000
1	-1.958992000	3.746657000	1.792346000
1	-0.522198000	4.561499000	1.156665000
6	0.491629000	3.013931000	2.891284000
1	1.037444000	2.197963000	3.361287000
1	1.200823000	3.826340000	2.675985000
1	-0.224200000	3.397849000	3.628611000

4GeTS^{C-H} (T.E.= -3899.242269)

7	0.848274000	-0.629077000	0.408556000
1	0.064589000	3.018821000	-1.124388000
6	1.990640000	2.072624000	-0.953676000
6	2.338560000	2.645906000	0.266485000
1	1.571260000	3.138081000	0.857321000
6	3.639485000	2.587554000	0.726709000
1	3.895282000	3.034298000	1.680653000
6	4.614694000	1.956603000	-0.030810000
1	5.634395000	1.903622000	0.332462000
6	4.283337000	1.390385000	-1.251312000
1	5.041375000	0.892352000	-1.843952000
6	2.978493000	1.438206000	-1.703275000
1	2.709889000	0.971842000	-2.646648000
1	0.505786000	1.988323000	-2.505753000

1	-0.294761000	1.546960000	-0.004304000
6	0.606542000	2.127649000	-1.432661000
6	-2.070666000	-0.087298000	0.205812000
6	-1.686565000	-0.440007000	1.662739000
1	-2.119862000	0.267141000	2.382286000
1	-2.093446000	-1.418951000	1.948400000
6	2.052248000	-1.227619000	0.057220000
6	3.142946000	-1.218370000	0.934160000
6	2.230759000	-1.866063000	-1.176253000
6	4.341701000	-1.820868000	0.598766000
1	3.050587000	-0.704459000	1.886155000
6	3.433677000	-2.456438000	-1.511672000
1	1.405373000	-1.890371000	-1.882000000
6	4.502736000	-2.442353000	-0.628250000
1	5.165449000	-1.788372000	1.303799000
1	3.534073000	-2.942040000	-2.476524000
1	5.444344000	-2.908061000	-0.893044000
14	-3.059821000	1.510003000	0.115113000
14	-2.858291000	-1.600187000	-0.610903000
6	-3.112224000	2.216380000	-1.621794000
1	-3.618636000	3.185371000	-1.596260000
1	-2.121236000	2.376559000	-2.052191000
1	-3.667077000	1.570878000	-2.304463000
6	-4.829889000	1.228567000	0.675349000
1	-5.330327000	2.191663000	0.807670000
1	-5.405096000	0.653655000	-0.053664000
1	-4.869659000	0.697085000	1.630121000
6	-2.374931000	2.844056000	1.250194000
1	-3.061756000	3.695260000	1.219044000
1	-2.307364000	2.517446000	2.290582000
1	-1.388461000	3.206082000	0.949821000
6	-4.339616000	-2.220823000	0.364863000
1	-5.188923000	-1.538217000	0.317209000
1	-4.656038000	-3.176862000	-0.062078000
1	-4.105470000	-2.394076000	1.417382000
6	-3.436235000	-1.257448000	-2.359975000
1	-3.730729000	-2.201604000	-2.826492000
1	-4.307474000	-0.598043000	-2.376439000
1	-2.654640000	-0.809845000	-2.978403000
6	-1.633505000	-3.021883000	-0.654387000

1	-0.783512000	-2.833857000	-1.314116000
1	-1.239374000	-3.255994000	0.338000000
1	-2.146192000	-3.914466000	-1.024207000
32	-0.320298000	0.123037000	-0.900717000
14	0.178397000	-0.536737000	1.998683000
6	0.696987000	0.973526000	2.976215000
1	0.201735000	0.965332000	3.951646000
1	1.776283000	1.006999000	3.143393000
1	0.406137000	1.894334000	2.465786000
6	0.549349000	-2.073850000	2.996464000
1	-0.126175000	-2.124957000	3.854785000
1	0.393891000	-2.970229000	2.390268000
1	1.572249000	-2.099064000	3.375242000

5GeTSC^{C-H} (T.E.= -3643.295995)

7	-0.731248000	0.737311000	0.475628000
1	-0.216129000	-2.882854000	-1.282545000
6	-2.099283000	-1.991186000	-0.697498000
6	-2.218754000	-2.562248000	0.567897000
1	-1.336261000	-2.974299000	1.050651000
6	-3.438460000	-2.592131000	1.212429000
1	-3.519457000	-3.040605000	2.195441000
6	-4.557896000	-2.039509000	0.604724000
1	-5.514001000	-2.053702000	1.114643000
6	-4.449328000	-1.460144000	-0.647280000
1	-5.319740000	-1.024741000	-1.123172000
6	-3.225486000	-1.429879000	-1.291064000
1	-3.134100000	-0.964280000	-2.267539000
1	-0.916924000	-1.755996000	-2.469167000
1	0.217676000	-1.524902000	0.004073000
6	-0.815904000	-1.984921000	-1.411165000
6	1.954284000	0.022896000	0.330678000
6	1.279801000	0.202173000	1.694518000
1	1.087758000	-0.766515000	2.176981000
1	1.900167000	0.774626000	2.392544000
6	-1.998146000	1.304937000	0.237148000
6	-3.007477000	1.282577000	1.196555000
6	-2.268594000	1.875445000	-1.004277000
6	-4.250966000	1.815924000	0.910343000
1	-2.809174000	0.845760000	2.165379000

6	-3.515743000	2.402403000	-1.286363000
1	-1.486800000	1.901213000	-1.757437000
6	-4.515920000	2.376818000	-0.328755000
1	-5.026196000	1.785109000	1.667817000
1	-3.702447000	2.841757000	-2.259758000
1	-5.493325000	2.791490000	-0.545468000
14	2.999103000	-1.543104000	0.195982000
14	2.797275000	1.637560000	-0.215534000
6	3.081757000	-2.131561000	-1.581959000
1	3.722754000	-3.015498000	-1.639711000
1	2.100974000	-2.415417000	-1.972577000
1	3.497603000	-1.374659000	-2.249333000
6	4.747298000	-1.277112000	0.818199000
1	5.265710000	-2.239705000	0.842599000
1	5.330908000	-0.603453000	0.187763000
1	4.746700000	-0.875897000	1.835362000
6	2.307973000	-2.941985000	1.239621000
1	2.939437000	-3.820796000	1.079773000
1	2.338591000	-2.709598000	2.306596000
1	1.282862000	-3.221090000	0.984705000
6	4.066415000	2.174010000	1.056330000
1	4.882406000	1.460126000	1.174286000
1	4.498813000	3.124569000	0.731075000
1	3.614537000	2.343166000	2.036203000
6	3.638825000	1.440083000	-1.875842000
1	3.994010000	2.419242000	-2.208441000
1	4.503910000	0.774528000	-1.833063000
1	2.951308000	1.062372000	-2.637005000
6	1.554479000	3.033972000	-0.359937000
1	0.855685000	2.886768000	-1.187370000
1	0.970656000	3.178406000	0.552885000
1	2.100973000	3.961115000	-0.555433000
32	0.324293000	-0.123151000	-0.901808000
6	-0.076628000	0.895568000	1.660733000
8	-0.486287000	1.509281000	2.627656000

8GeTSC-H (T.E.= -3211.890618)

6	-0.785812000	0.686229000	2.121307000
6	-1.950572000	-0.313950000	2.128558000
6	-2.376175000	-0.705517000	0.728070000

7	0.134853000	0.412053000	1.035902000
15	-3.527078000	0.247859000	-0.068324000
6	-5.081486000	0.299703000	0.850298000
1	-4.916736000	0.762839000	1.824326000
1	-5.825530000	0.884453000	0.306637000
1	-5.446454000	-0.716275000	0.999919000
6	-3.926942000	-0.431276000	-1.686386000
1	-4.700293000	0.171295000	-2.165887000
1	-3.033317000	-0.428816000	-2.313043000
1	-4.274632000	-1.457535000	-1.570478000
6	-3.207749000	2.011441000	-0.413613000
1	-2.284168000	2.098127000	-0.991670000
1	-4.026156000	2.481026000	-0.964687000
1	-3.067696000	2.538385000	0.532697000
32	-0.681408000	-0.787511000	-0.241334000
6	1.098891000	1.338885000	0.740389000
6	1.354241000	2.453376000	1.560667000
6	1.894085000	1.209222000	-0.411455000
6	2.339360000	3.370038000	1.234031000
1	0.784030000	2.598225000	2.468787000
6	2.871251000	2.128739000	-0.724068000
1	1.743973000	0.349994000	-1.056507000
6	3.109553000	3.226038000	0.093256000
1	2.504941000	4.215057000	1.894536000
1	3.463208000	1.978360000	-1.621550000
1	3.881370000	3.945477000	-0.151699000
1	-1.197907000	1.704176000	2.006458000
1	-1.630155000	-1.219180000	2.660984000
1	-0.359849000	-1.975791000	0.908167000
6	0.447716000	-2.682531000	-0.530495000
1	0.075971000	-2.879714000	-1.532883000
1	0.202638000	-3.523729000	0.111578000
6	1.872244000	-2.318775000	-0.501464000
6	2.537865000	-1.995025000	-1.681358000
6	2.578037000	-2.291505000	0.697379000
6	3.879414000	-1.662454000	-1.664258000
1	1.985913000	-1.996145000	-2.616991000
6	3.917503000	-1.950329000	0.716448000
1	2.058062000	-2.521876000	1.622244000
6	4.571645000	-1.634399000	-0.463781000

1	4.385926000	-1.415158000	-2.590106000
1	4.453137000	-1.923208000	1.657999000
1	5.619539000	-1.359632000	-0.447209000
1	-2.767841000	0.124681000	2.717539000
1	-0.270745000	0.667964000	3.092826000

9GeTS^{C-H} (T.E.= -3210.702466)

6	-0.517582000	0.688102000	1.690105000
6	-1.721809000	0.090584000	1.793231000
6	-2.323576000	-0.537484000	0.608221000
7	0.103683000	0.721772000	0.451480000
15	-3.807534000	0.086642000	0.072156000
6	-5.043168000	-0.001333000	1.383219000
1	-4.728650000	0.625949000	2.218708000
1	-6.008047000	0.355171000	1.018833000
1	-5.134535000	-1.031293000	1.727501000
6	-4.463791000	-0.839153000	-1.321258000
1	-5.418442000	-0.415293000	-1.637432000
1	-3.756149000	-0.786495000	-2.151314000
1	-4.596349000	-1.882817000	-1.036963000
6	-3.885251000	1.823443000	-0.465123000
1	-3.257143000	1.949571000	-1.349475000
1	-4.903455000	2.143832000	-0.697397000
1	-3.481921000	2.448003000	0.335001000
32	-0.878247000	-0.435845000	-0.750345000
6	1.286187000	1.372648000	0.186200000
6	2.183682000	1.770243000	1.188119000
6	1.635397000	1.663554000	-1.141652000
6	3.358978000	2.423865000	0.866509000
1	1.972839000	1.536054000	2.224650000
6	2.809990000	2.315982000	-1.449896000
1	0.954434000	1.367477000	-1.935771000
6	3.689292000	2.706400000	-0.449011000
1	4.035063000	2.709442000	1.665681000
1	3.041835000	2.525981000	-2.488798000
1	4.611732000	3.220245000	-0.690767000
1	-0.035987000	1.172103000	2.531994000
1	-2.240686000	0.090557000	2.748507000
1	-0.449752000	-1.648276000	0.313738000
6	0.566048000	-2.018286000	-1.193566000

1	0.699442000	-1.819789000	-2.256659000
1	0.076038000	-2.982599000	-1.071479000
6	1.840032000	-1.868237000	-0.455048000
6	2.965273000	-1.383990000	-1.112887000
6	1.954201000	-2.205413000	0.891234000
6	4.176745000	-1.256892000	-0.453031000
1	2.886079000	-1.096524000	-2.156666000
6	3.158585000	-2.081576000	1.552762000
1	1.070323000	-2.537508000	1.429690000
6	4.275899000	-1.603205000	0.882091000
1	5.039218000	-0.868627000	-0.982064000
1	3.226311000	-2.345218000	2.601861000
1	5.218147000	-1.490433000	1.405648000

$^{14}\text{GeTS}^{\text{C-H}}$ (T.E.= -3406.060625)

7	-1.785412000	0.085321000	-0.420288000
1	0.303305000	-2.907610000	-0.706024000
1	0.239748000	-0.628760000	0.841914000
6	0.592258000	-2.255230000	0.117014000
6	0.608660000	1.428422000	-0.307039000
6	-2.631261000	-0.997512000	-0.180481000
6	-3.216700000	-1.191424000	1.073594000
6	-2.858972000	-1.961037000	-1.165838000
6	-4.016774000	-2.292003000	1.320800000
1	-3.024669000	-0.463633000	1.855600000
6	-3.649912000	-3.067060000	-0.910086000
1	-2.409555000	-1.819221000	-2.144485000
6	-4.238089000	-3.239151000	0.332890000
1	-4.462045000	-2.417600000	2.301763000
1	-3.815194000	-3.798225000	-1.693888000
1	-4.860643000	-4.103531000	0.530679000
32	0.029124000	-0.362899000	-0.836166000
15	2.180200000	2.083638000	-0.242980000
6	2.328884000	3.698731000	-1.024243000
1	1.613123000	4.371321000	-0.553753000
1	3.345164000	4.079919000	-0.907176000
1	2.091113000	3.604640000	-2.084265000
6	2.825825000	2.287561000	1.427930000
1	3.817841000	2.743396000	1.411968000
1	2.137475000	2.917456000	1.991576000

1	2.881707000	1.304181000	1.899349000
6	3.354235000	1.016597000	-1.084178000
1	3.410587000	0.051447000	-0.577784000
1	3.030953000	0.855727000	-2.113749000
1	4.342331000	1.479867000	-1.081287000
6	-0.483975000	2.199778000	0.178821000
8	-0.317632000	3.362929000	0.611594000
5	-1.911399000	1.444994000	0.027595000
7	-3.152626000	2.094059000	0.227547000
6	-3.298868000	3.382615000	0.867248000
1	-3.930629000	3.297747000	1.761645000
1	-2.324163000	3.776705000	1.145706000
1	-3.789559000	4.096328000	0.192925000
6	-4.425107000	1.545129000	-0.171081000
1	-5.017651000	2.316365000	-0.677050000
1	-4.302116000	0.710021000	-0.858897000
1	-5.012059000	1.191914000	0.688187000
6	2.053627000	-2.227316000	0.325353000
6	2.916371000	-2.600479000	-0.700929000
6	2.596301000	-1.822300000	1.542363000
6	4.287647000	-2.587922000	-0.512047000
1	2.497938000	-2.900842000	-1.657126000
6	3.966437000	-1.807553000	1.733075000
1	1.928472000	-1.516991000	2.342757000
6	4.816359000	-2.188919000	0.705391000
1	4.946048000	-2.887183000	-1.319118000
1	4.374306000	-1.498351000	2.688626000
1	5.889604000	-2.175430000	0.854324000
1	0.020683000	-2.530735000	1.000181000

Cartesian coordinates of the van der Waals complexes involved in the activation of Si – H bond of SiEt₃H by CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and **IX**, along with their total energies (in hartrees) including zero point vibrational correction.

1Si_v (T.E.= -2038.010412)

6	0.531510000	-1.523809000	1.691105000
6	2.004570000	-1.229691000	1.490294000
6	2.193918000	-0.315588000	0.253960000
1	0.385279000	-2.460693000	2.240239000
1	0.045156000	-0.732750000	2.279226000

1	2.521505000	-2.185696000	1.337801000
1	2.437928000	-0.802860000	2.403424000
7	-0.072115000	-1.615610000	0.365142000
14	0.723036000	-0.696025000	-0.892678000
14	2.201066000	1.513548000	0.714872000
14	3.740737000	-0.864965000	-0.681542000
6	4.202443000	0.288915000	-2.082597000
1	4.537901000	1.269146000	-1.736844000
1	5.023362000	-0.157619000	-2.650534000
1	3.367020000	0.437539000	-2.772018000
6	3.423981000	-2.555997000	-1.440089000
1	2.707155000	-2.498416000	-2.264467000
1	4.355853000	-2.961475000	-1.843929000
1	3.038904000	-3.275251000	-0.712843000
6	5.202942000	-1.045274000	0.478809000
1	6.026355000	-1.527268000	-0.055620000
1	5.561764000	-0.083957000	0.849677000
1	4.961019000	-1.670010000	1.341782000
6	1.791825000	2.602350000	-0.753276000
1	1.885708000	3.652538000	-0.462282000
1	2.439219000	2.431915000	-1.614576000
1	0.759260000	2.441878000	-1.076312000
6	0.903578000	1.881015000	2.021245000
1	-0.096595000	1.598107000	1.684310000
1	1.101334000	1.378669000	2.971235000
1	0.896657000	2.958650000	2.213089000
6	3.842655000	2.052437000	1.445865000
1	4.649698000	2.065967000	0.710559000
1	3.736597000	3.066516000	1.841712000
1	4.146676000	1.403897000	2.271814000
6	-1.368278000	-2.133044000	0.264617000
6	-2.207826000	-2.241145000	1.374645000
6	-1.861588000	-2.554786000	-0.974190000
6	-3.496378000	-2.732585000	1.241293000
1	-1.863160000	-1.925247000	2.351065000
6	-3.147911000	-3.036758000	-1.098680000
1	-1.213070000	-2.511391000	-1.842814000
6	-3.980144000	-3.128624000	0.007816000
1	-4.128340000	-2.798780000	2.120091000
1	-3.502345000	-3.355084000	-2.072751000

1	-4.987629000	-3.514069000	-0.091466000
14	-2.590900000	1.756853000	-0.103558000
6	-4.005369000	0.666277000	-0.671172000
1	-3.969286000	-0.233898000	-0.043492000
1	-4.951317000	1.164614000	-0.428503000
6	-3.969091000	0.268363000	-2.139347000
1	-4.713376000	-0.498057000	-2.370553000
1	-4.166853000	1.121347000	-2.792814000
1	-2.991176000	-0.138901000	-2.418172000
6	-2.256751000	3.253239000	-1.188673000
1	-3.161726000	3.868150000	-1.250267000
1	-1.528785000	3.860285000	-0.633827000
6	-1.720446000	2.944568000	-2.580652000
1	-2.488792000	2.507355000	-3.220396000
1	-1.349192000	3.840242000	-3.084453000
1	-0.895803000	2.225394000	-2.545921000
6	-2.896382000	2.326510000	1.659665000
1	-2.099421000	3.023952000	1.941730000
1	-3.821438000	2.915464000	1.659100000
6	-2.989399000	1.193843000	2.670372000
1	-3.178213000	1.555915000	3.683797000
1	-3.790834000	0.493395000	2.419094000
1	-2.058788000	0.617456000	2.700108000
1	-1.345723000	0.929236000	-0.136353000

2Si_v (T.E.= -2036.820683)

6	2.236531000	-0.078393000	-0.235941000
6	2.090183000	-0.907749000	-1.461567000
6	1.047276000	-1.744913000	-1.466078000
1	2.774323000	-0.840548000	-2.302723000
1	0.799209000	-2.431365000	-2.267667000
7	0.264612000	-1.742558000	-0.311593000
14	2.087554000	1.758729000	-0.665338000
14	3.826033000	-0.588936000	0.656450000
6	3.693943000	2.474318000	-1.313436000
1	3.510389000	3.495029000	-1.661115000
1	4.483251000	2.516814000	-0.559809000
1	4.063914000	1.897470000	-2.165489000
6	1.524885000	2.767951000	0.810142000
1	2.169593000	2.635168000	1.680973000

1	1.528588000	3.829609000	0.546940000
1	0.506112000	2.502401000	1.106912000
6	0.832930000	1.959958000	-2.042324000
1	0.581648000	3.018674000	-2.157044000
1	1.235591000	1.604514000	-2.993552000
1	-0.090779000	1.411089000	-1.844209000
6	4.193485000	0.529494000	2.113238000
1	5.080746000	0.157683000	2.633070000
1	4.393909000	1.562380000	1.818938000
1	3.368367000	0.533736000	2.830581000
6	3.628759000	-2.342425000	1.295978000
1	2.953140000	-2.394382000	2.154053000
1	3.239359000	-3.001546000	0.515332000
1	4.597430000	-2.737969000	1.613447000
6	5.289829000	-0.603942000	-0.510868000
1	5.133458000	-1.313520000	-1.326546000
1	5.506338000	0.373350000	-0.943972000
1	6.175686000	-0.929413000	0.042119000
6	-0.977766000	-2.398941000	-0.279269000
6	-1.744878000	-2.562664000	-1.431592000
6	-1.491791000	-2.852462000	0.934795000
6	-2.987763000	-3.168004000	-1.367005000
1	-1.379967000	-2.186869000	-2.380449000
6	-2.741277000	-3.440693000	0.993897000
1	-0.893303000	-2.746421000	1.833329000
6	-3.497027000	-3.606812000	-0.156678000
1	-3.570579000	-3.278486000	-2.274737000
1	-3.121608000	-3.785788000	1.948542000
1	-4.472913000	-4.074558000	-0.109368000
6	-2.471042000	3.098600000	0.041808000
1	-1.933185000	3.547604000	0.885580000
1	-1.848284000	3.291923000	-0.839573000
6	-3.771929000	0.414830000	-0.804329000
1	-3.819517000	-0.644939000	-0.524446000
1	-4.769953000	0.826554000	-0.618594000
6	-2.801015000	0.796563000	2.117620000
1	-2.821704000	-0.298409000	2.182024000
1	-1.917397000	1.110288000	2.685807000
6	-4.065044000	1.394759000	2.717568000
1	-4.953905000	1.114057000	2.144480000

1	-4.227825000	1.068863000	3.747589000
1	-4.020249000	2.487297000	2.728375000
6	-3.392346000	0.555466000	-2.271665000
1	-4.099702000	0.052348000	-2.936014000
1	-3.344661000	1.604914000	-2.578606000
1	-2.404786000	0.121259000	-2.460349000
6	-3.835948000	3.753712000	-0.125891000
1	-3.758510000	4.836912000	-0.245899000
1	-4.356861000	3.368047000	-1.005916000
1	-4.485488000	3.568323000	0.734013000
1	-1.184450000	0.703056000	-0.076761000
14	-2.518738000	1.236957000	0.318884000
14	0.816746000	-0.593119000	0.923681000

3Si_v (T.E.= -2158.109607)

6	-2.630284000	0.893171000	0.583560000
6	-2.188474000	-0.419373000	-0.119267000
1	-3.510370000	1.326066000	0.084356000
1	-2.979533000	0.713124000	1.608720000
14	-0.629676000	-0.032274000	-1.130205000
7	-0.361849000	1.504540000	-0.316356000
5	-1.470125000	1.971531000	0.503802000
7	-1.590912000	3.253438000	1.086540000
6	-2.678820000	3.581642000	1.979960000
1	-2.294207000	4.016191000	2.910608000
1	-3.353362000	4.321838000	1.530977000
1	-3.262964000	2.701345000	2.239043000
6	-0.769614000	4.417055000	0.834113000
1	-0.184780000	4.698379000	1.719370000
1	-0.078468000	4.259981000	0.010183000
1	-1.408353000	5.270423000	0.578578000
14	-3.522192000	-1.011928000	-1.301894000
14	-1.690056000	-1.659016000	1.211696000
6	-3.612524000	0.217461000	-2.722605000
1	-3.661260000	1.250611000	-2.366709000
1	-2.734646000	0.128737000	-3.369496000
1	-4.496503000	0.037973000	-3.340132000
6	-5.210342000	-1.061876000	-0.486453000
1	-5.453367000	-0.115442000	0.002147000
1	-5.974290000	-1.248002000	-1.246427000

1	-5.281576000	-1.853476000	0.261212000
6	-3.183325000	-2.349783000	2.113863000
1	-3.754999000	-3.042401000	1.491879000
1	-2.843863000	-2.900577000	2.995837000
1	-3.860069000	-1.561863000	2.453983000
6	-0.694339000	-3.102293000	0.547090000
1	-0.282666000	-3.670736000	1.387167000
1	-1.301763000	-3.784160000	-0.050480000
1	0.145448000	-2.774922000	-0.071109000
6	-3.145929000	-2.698430000	-2.026504000
1	-3.252545000	-3.496331000	-1.287690000
1	-3.840601000	-2.910338000	-2.843663000
1	-2.130978000	-2.744414000	-2.430635000
6	-0.636668000	-0.795800000	2.509147000
1	0.283569000	-0.383040000	2.086787000
1	-1.169812000	0.013519000	3.013637000
1	-0.353593000	-1.527090000	3.272290000
6	0.896900000	2.136901000	-0.420644000
6	1.387807000	2.580703000	-1.642961000
6	1.673036000	2.316978000	0.723087000
6	2.608767000	3.231957000	-1.712500000
1	0.787463000	2.432120000	-2.534395000
6	2.887172000	2.973839000	0.651390000
1	1.290300000	1.957821000	1.674192000
6	3.358237000	3.441691000	-0.566755000
1	2.973073000	3.583301000	-2.671222000
1	3.472471000	3.118490000	1.552555000
1	4.308973000	3.958175000	-0.622880000
1	1.600083000	-0.797555000	0.217715000
14	3.009014000	-1.276232000	0.106898000
6	3.929707000	-0.220492000	-1.135689000
1	4.996628000	-0.465673000	-1.072138000
1	3.841286000	0.823856000	-0.816279000
6	3.774947000	-1.135007000	1.814670000
1	4.855412000	-1.302932000	1.743002000
1	3.655307000	-0.093904000	2.138353000
6	2.973222000	-3.065349000	-0.462885000
1	2.420756000	-3.662315000	0.270891000
1	2.390289000	-3.121387000	-1.389824000
6	3.425349000	-0.380959000	-2.562859000

1	2.352308000	-0.173272000	-2.629220000
1	3.931659000	0.296273000	-3.255862000
1	3.579928000	-1.398787000	-2.931777000
6	3.148943000	-2.085990000	2.824826000
1	3.359177000	-3.129005000	2.573440000
1	3.516587000	-1.918183000	3.839945000
1	2.059265000	-1.978570000	2.852269000
6	4.369091000	-3.635786000	-0.674423000
1	4.347266000	-4.684693000	-0.979085000
1	4.910781000	-3.085238000	-1.448732000
1	4.970047000	-3.576685000	0.238418000

4Si_v (T.E.= -2368.023230)

6	-2.291023000	0.444322000	1.520203000
6	-2.215059000	-0.169196000	0.086702000
1	-3.080857000	1.204312000	1.586697000
1	-2.558472000	-0.299632000	2.280016000
14	-0.732710000	0.477570000	-0.933600000
7	-0.025877000	1.456656000	0.316233000
14	-3.702572000	0.470812000	-0.898158000
14	-2.142596000	-2.052100000	0.145838000
6	-3.476230000	2.320386000	-1.163447000
1	-2.680674000	2.533100000	-1.883999000
1	-4.397750000	2.759352000	-1.555230000
1	-3.230395000	2.840761000	-0.233508000
6	-5.314657000	0.239158000	0.032146000
1	-6.098458000	0.797669000	-0.487683000
1	-5.619008000	-0.807645000	0.070598000
1	-5.266584000	0.614541000	1.056257000
6	-3.804168000	-2.835516000	0.529227000
1	-4.507513000	-2.760780000	-0.303075000
1	-3.652513000	-3.897659000	0.741893000
1	-4.269968000	-2.382870000	1.408536000
6	-1.489088000	-2.798665000	-1.446586000
1	-1.532831000	-3.889105000	-1.366176000
1	-2.058241000	-2.503971000	-2.329692000
1	-0.445237000	-2.522283000	-1.622189000
6	-3.879013000	-0.332703000	-2.581572000
1	-4.099257000	-1.400373000	-2.509835000
1	-4.707630000	0.139958000	-3.116357000

1	-2.977807000	-0.212601000	-3.187833000
6	-0.970711000	-2.603957000	1.501792000
1	0.022153000	-2.169936000	1.361603000
1	-1.317925000	-2.348858000	2.505214000
1	-0.864595000	-3.692319000	1.456168000
14	-0.683764000	1.320618000	1.938811000
6	0.424925000	0.358925000	3.100777000
1	0.856262000	-0.522526000	2.619445000
1	1.244156000	0.982623000	3.466819000
1	-0.144932000	0.020345000	3.970470000
6	-0.947479000	3.027793000	2.643353000
1	-1.583441000	3.625640000	1.985799000
1	-1.420512000	2.981235000	3.627019000
1	0.005909000	3.550327000	2.757155000
6	1.097481000	2.261443000	0.030012000
6	2.305569000	2.086247000	0.703583000
6	1.021177000	3.244864000	-0.954453000
6	3.403297000	2.870651000	0.395693000
1	2.388553000	1.307655000	1.454513000
6	2.125143000	4.018396000	-1.267457000
1	0.075872000	3.398033000	-1.465909000
6	3.321947000	3.836544000	-0.594193000
1	4.335296000	2.715269000	0.928286000
1	2.045183000	4.775140000	-2.039469000
1	4.184569000	4.445242000	-0.837183000
1	1.553737000	-0.890437000	0.193479000
14	2.716798000	-1.616427000	-0.394950000
6	2.754187000	-1.298220000	-2.241413000
1	3.477300000	-1.983205000	-2.699625000
1	1.774608000	-1.586502000	-2.641791000
6	4.275063000	-0.990089000	0.443058000
1	4.146043000	-1.088897000	1.527717000
1	4.360658000	0.084921000	0.250942000
6	2.482554000	-3.447381000	-0.043820000
1	3.206905000	-4.016817000	-0.637403000
1	1.496283000	-3.739673000	-0.424630000
6	3.068364000	0.144061000	-2.612740000
1	4.068183000	0.437892000	-2.280430000
1	3.023061000	0.309796000	-3.691516000
1	2.361397000	0.838518000	-2.147794000

6	5.526476000	-1.721309000	-0.021038000
1	5.668830000	-1.620579000	-1.101047000
1	6.431915000	-1.344408000	0.460374000
1	5.467407000	-2.792252000	0.193334000
6	2.611898000	-3.796220000	1.432613000
1	2.353919000	-4.837843000	1.638403000
1	3.632830000	-3.637679000	1.789243000
1	1.958630000	-3.173892000	2.052951000

5Si_v (T.E.= -2112.069434)

6	2.485043000	-1.259179000	1.100697000
6	2.307009000	-0.086203000	0.125087000
1	3.254439000	-1.963980000	0.757689000
1	2.804103000	-0.972912000	2.108801000
14	0.768067000	-0.476876000	-0.910342000
7	0.348759000	-1.811309000	0.178841000
14	3.760047000	0.006931000	-1.077215000
14	1.982085000	1.502417000	1.105027000
6	3.695397000	-1.518192000	-2.172799000
1	2.859241000	-1.467144000	-2.876808000
1	4.612460000	-1.604395000	-2.761447000
1	3.589659000	-2.440337000	-1.594799000
6	5.400857000	-0.003734000	-0.174720000
1	6.208813000	-0.129848000	-0.900599000
1	5.579635000	0.925647000	0.368833000
1	5.469272000	-0.828334000	0.538930000
6	3.561878000	2.152392000	1.873783000
1	4.237719000	2.586923000	1.133927000
1	3.315089000	2.933874000	2.597536000
1	4.103077000	1.364604000	2.404213000
6	1.223969000	2.855929000	0.052427000
1	1.034227000	3.728903000	0.683942000
1	1.875792000	3.171495000	-0.764796000
1	0.266863000	2.555015000	-0.383173000
6	3.654025000	1.517082000	-2.176031000
1	3.857717000	2.441581000	-1.631116000
1	4.393968000	1.436357000	-2.976517000
1	2.668781000	1.606871000	-2.641634000
6	0.802622000	1.124244000	2.514393000
1	-0.173593000	0.780252000	2.163322000

1	1.201009000	0.370839000	3.198154000
1	0.639542000	2.039030000	3.091850000
6	-0.891100000	-2.496861000	0.091040000
6	-1.290873000	-3.031833000	-1.126556000
6	-1.737298000	-2.588155000	1.190604000
6	-2.522721000	-3.653522000	-1.245080000
1	-0.623194000	-2.964821000	-1.979067000
6	-2.959329000	-3.223330000	1.069294000
1	-1.434767000	-2.156450000	2.136528000
6	-3.358251000	-3.757130000	-0.146204000
1	-2.824041000	-4.066764000	-2.200486000
1	-3.612391000	-3.290362000	1.931758000
1	-4.319380000	-4.249299000	-0.236237000
6	1.227265000	-2.084412000	1.226299000
8	1.041540000	-2.899733000	2.094604000
1	-1.324029000	0.467712000	0.289101000
14	-2.537129000	1.257480000	-0.085515000
6	-2.305280000	1.823462000	-1.863508000
1	-2.509254000	0.962639000	-2.512487000
1	-1.241065000	2.042492000	-2.008092000
6	-4.011597000	0.108772000	0.078647000
1	-4.201408000	-0.057806000	1.145919000
1	-3.688750000	-0.863850000	-0.312204000
6	-5.281736000	0.553652000	-0.632961000
1	-6.089718000	-0.171301000	-0.508277000
1	-5.649002000	1.515015000	-0.262994000
1	-5.113627000	0.664785000	-1.707426000
6	-3.142734000	3.025529000	-2.276476000
1	-2.966833000	3.307267000	-3.317297000
1	-4.213940000	2.835098000	-2.169068000
1	-2.907854000	3.898987000	-1.662068000
6	-2.608148000	2.700391000	1.121713000
1	-1.858556000	3.440660000	0.815691000
1	-2.262289000	2.318731000	2.089458000
6	-3.973044000	3.354359000	1.286951000
1	-3.951039000	4.165469000	2.018588000
1	-4.341209000	3.774860000	0.347692000
1	-4.717782000	2.630627000	1.628975000

8Si_v (T.E.= -1680.699519)

6	-0.439447000	-1.688363000	-1.596725000
6	-1.953744000	-1.668866000	-1.474517000
6	-2.268411000	-0.906823000	-0.201718000
1	-0.093318000	-2.529012000	-2.209789000
1	-0.099557000	-0.761861000	-2.091939000
1	-2.334088000	-2.699468000	-1.426314000
1	-2.386523000	-1.222569000	-2.379496000
14	-0.908287000	-0.954274000	0.971033000
7	0.114372000	-1.762564000	-0.252064000
15	-3.786653000	-0.236859000	0.080738000
6	-4.323217000	0.961288000	-1.165512000
1	-4.307777000	0.491839000	-2.150495000
1	-5.335709000	1.312950000	-0.957933000
1	-3.636080000	1.808672000	-1.172499000
6	-5.155189000	-1.422321000	0.110482000
1	-4.995947000	-2.129375000	0.925398000
1	-6.118130000	-0.923598000	0.236536000
1	-5.161512000	-1.975377000	-0.831329000
6	-3.864334000	0.642767000	1.646571000
1	-3.644541000	-0.035675000	2.470968000
1	-3.133526000	1.452856000	1.649262000
1	-4.864787000	1.058369000	1.777799000
6	1.484545000	-1.926103000	-0.110261000
6	2.374500000	-1.822673000	-1.185928000
6	2.030135000	-2.183141000	1.156220000
6	3.741749000	-1.937811000	-0.991377000
1	2.001116000	-1.628956000	-2.183611000
6	3.392394000	-2.288035000	1.340215000
1	1.358220000	-2.296731000	2.000586000
6	4.267057000	-2.161204000	0.268455000
1	4.403590000	-1.840206000	-1.845465000
1	3.778386000	-2.477443000	2.336149000
1	5.336930000	-2.247499000	0.414540000
1	0.767003000	0.762600000	-0.560076000
14	1.447163000	1.967379000	-0.015925000
6	2.208974000	2.857094000	-1.484656000
1	1.408338000	3.190241000	-2.153990000
1	2.709348000	3.766127000	-1.131765000
6	2.801621000	1.452425000	1.181012000

1	3.570548000	2.234386000	1.182311000
1	3.281519000	0.558196000	0.763003000
6	0.101409000	2.996893000	0.799708000
1	0.504276000	3.963471000	1.121188000
1	-0.211514000	2.477587000	1.713003000
6	2.330460000	1.166134000	2.599283000
1	1.525778000	0.424151000	2.608376000
1	3.137860000	0.778092000	3.225958000
1	1.943622000	2.066804000	3.083637000
6	3.187909000	1.964449000	-2.236176000
1	3.602570000	2.450560000	-3.122770000
1	4.028930000	1.672412000	-1.600846000
1	2.704645000	1.037751000	-2.562310000
6	-1.093790000	3.181565000	-0.125160000
1	-1.471179000	2.206452000	-0.457148000
1	-1.920222000	3.713666000	0.355818000
1	-0.829083000	3.744295000	-1.024385000

9Si_v (T.E.= -1679.521595)

6	0.426605000	-1.657788000	-1.567444000
6	1.712585000	-1.242961000	-1.539022000
6	2.198253000	-0.975699000	-0.210600000
14	0.905557000	-1.279984000	1.038363000
7	-0.174616000	-1.759667000	-0.324043000
15	3.747764000	-0.336668000	0.064736000
6	5.097248000	-1.427129000	-0.431199000
1	4.978913000	-1.678384000	-1.486902000
1	6.066070000	-0.946535000	-0.282076000
1	5.046511000	-2.347562000	0.151213000
6	4.021790000	0.048899000	1.795666000
1	5.034516000	0.434071000	1.924097000
1	3.303080000	0.802748000	2.120087000
1	3.896382000	-0.847043000	2.404027000
6	4.063353000	1.191042000	-0.842944000
1	3.361087000	1.958196000	-0.512576000
1	5.087395000	1.534635000	-0.686764000
1	3.900882000	1.011718000	-1.907355000
6	-1.530014000	-2.104822000	-0.203878000
6	-1.993490000	-2.700005000	0.970481000
6	-2.450690000	-1.854368000	-1.221919000

6	-3.328813000	-3.019941000	1.124062000
1	-1.285543000	-2.917744000	1.762893000
6	-3.782619000	-2.198652000	-1.069623000
1	-2.127871000	-1.360110000	-2.130073000
6	-4.234929000	-2.778446000	0.103164000
1	-3.661129000	-3.479105000	2.048386000
1	-4.477299000	-1.993241000	-1.876597000
1	-5.279566000	-3.040486000	0.220674000
1	-0.117762000	-1.946113000	-2.457549000
1	2.299948000	-1.149050000	-2.448362000
1	-1.575898000	0.952477000	-1.557509000
14	-1.373633000	1.979480000	-0.500083000
6	-2.093966000	1.350314000	1.115641000
1	-1.538641000	0.451850000	1.415514000
1	-1.899277000	2.092032000	1.899176000
6	-2.266900000	3.545744000	-1.038680000
1	-1.859557000	3.842598000	-2.011656000
1	-3.322230000	3.311776000	-1.215956000
6	0.473334000	2.319892000	-0.333446000
1	0.746852000	3.074266000	-1.081337000
1	0.995236000	1.398109000	-0.618684000
6	-2.134888000	4.688355000	-0.041881000
1	-1.085837000	4.952807000	0.122082000
1	-2.647270000	5.594293000	-0.375175000
1	-2.554280000	4.420841000	0.932824000
6	0.920180000	2.754950000	1.055553000
1	1.987156000	3.001139000	1.091745000
1	0.379979000	3.638669000	1.406831000
1	0.746399000	1.960500000	1.787857000
6	-3.582308000	1.050024000	1.024894000
1	-4.159874000	1.953955000	0.809566000
1	-3.792576000	0.330742000	0.227582000
1	-3.975275000	0.626245000	1.952417000

14Si_v (T.E.= -1874.856906)

6	-2.029393000	1.416152000	-0.313233000
6	-2.127757000	0.363244000	0.666468000
7	0.208044000	1.499366000	0.838772000
6	1.610486000	1.529061000	0.865772000
6	2.337355000	1.497624000	-0.326909000

6	3.719278000	1.493745000	-0.316854000
6	4.412669000	1.494059000	0.884574000
6	3.701652000	1.501663000	2.073155000
6	2.316668000	1.522200000	2.067143000
1	1.793426000	1.469720000	-1.267191000
1	4.259893000	1.474778000	-1.257149000
1	5.495937000	1.485755000	0.893071000
1	4.229405000	1.501201000	3.020355000
1	1.763585000	1.545656000	3.000208000
5	-0.634186000	2.207883000	-0.105377000
7	-0.338045000	3.447544000	-0.694536000
6	-1.135823000	4.032354000	-1.752343000
1	-1.533313000	5.006067000	-1.441741000
1	-0.518517000	4.202085000	-2.643268000
1	-1.963993000	3.375220000	-2.008624000
6	0.773707000	4.293555000	-0.328666000
1	1.544427000	4.311184000	-1.109895000
1	0.421938000	5.321697000	-0.189203000
1	1.238929000	3.965479000	0.598841000
15	-3.469275000	-0.685366000	0.524279000
6	-3.554928000	-1.483382000	-1.088304000
1	-4.412973000	-2.155551000	-1.146918000
1	-3.630850000	-0.709558000	-1.852205000
1	-2.632596000	-2.047651000	-1.244256000
6	-5.073019000	0.096208000	0.765641000
1	-5.875370000	-0.631931000	0.631235000
1	-5.122808000	0.513808000	1.771695000
1	-5.177706000	0.901085000	0.038358000
6	-3.385053000	-2.025926000	1.718744000
1	-2.509094000	-2.644815000	1.514192000
1	-3.304492000	-1.625966000	2.730084000
1	-4.282524000	-2.641792000	1.643052000
8	-2.897805000	1.647471000	-1.168494000
14	-0.620352000	0.153310000	1.673821000
1	0.523294000	-0.917681000	-0.247282000
14	1.359660000	-2.054785000	-0.713547000
6	2.902575000	-2.185099000	0.336960000
1	3.460670000	-1.247507000	0.234599000
1	2.605829000	-2.235944000	1.390344000
6	0.297864000	-3.596524000	-0.522780000

1	-0.661284000	-3.405275000	-1.019996000
1	0.751804000	-4.432365000	-1.066747000
6	1.745545000	-1.718843000	-2.518098000
1	2.157794000	-2.623737000	-2.978599000
1	2.539264000	-0.964241000	-2.567605000
6	3.770597000	-3.375557000	-0.045444000
1	4.676854000	-3.439858000	0.561208000
1	3.232295000	-4.320467000	0.075217000
1	4.084867000	-3.318123000	-1.091870000
6	0.074338000	-3.964453000	0.938057000
1	1.001030000	-4.306347000	1.406042000
1	-0.264488000	-3.100503000	1.521757000
1	-0.664946000	-4.760199000	1.062238000
6	0.509509000	-1.245280000	-3.272091000
1	0.107370000	-0.326564000	-2.831759000
1	0.712084000	-1.042284000	-4.326281000
1	-0.291166000	-1.990585000	-3.235499000

1GeV (T.E.= -3825.485721)

6	1.244953000	-2.037944000	1.378990000
6	2.588101000	-1.496466000	0.943241000
6	2.410688000	-0.156693000	0.191703000
1	1.312426000	-3.101759000	1.635215000
1	0.896469000	-1.518505000	2.284603000
1	3.047090000	-2.238363000	0.279369000
1	3.256600000	-1.409750000	1.807541000
32	0.733663000	-0.435206000	-0.887365000
7	0.318810000	-1.845805000	0.273218000
14	2.069399000	1.265132000	1.391783000
14	3.851587000	0.136662000	-0.979572000
6	4.156877000	-1.429597000	-1.974863000
1	3.243624000	-1.784774000	-2.463479000
1	4.888189000	-1.218547000	-2.759807000
1	4.551098000	-2.248992000	-1.370672000
6	3.519508000	1.487741000	-2.238285000
1	3.525978000	2.489343000	-1.808026000
1	4.300698000	1.450698000	-3.002736000
1	2.560540000	1.346158000	-2.744651000
6	5.429248000	0.534680000	-0.046680000
1	5.639223000	-0.225921000	0.710680000

1	6.279235000	0.562828000	-0.733699000
1	5.375973000	1.504063000	0.455568000
6	2.313644000	2.948444000	0.606617000
1	1.693908000	3.068566000	-0.286615000
1	2.001270000	3.709409000	1.327549000
1	3.350332000	3.155019000	0.334276000
6	0.294204000	1.299666000	2.021937000
1	-0.037472000	0.368813000	2.488353000
1	0.211178000	2.094178000	2.770293000
1	-0.408354000	1.541102000	1.218718000
6	3.178818000	1.120890000	2.896700000
1	2.915839000	0.253270000	3.506901000
1	4.235296000	1.041911000	2.631192000
1	3.051546000	2.010697000	3.519318000
6	-0.917312000	-2.488902000	0.315369000
6	-1.662501000	-2.657814000	-0.857168000
6	-1.464526000	-2.959792000	1.511498000
6	-2.912661000	-3.241592000	-0.825848000
1	-1.242587000	-2.328285000	-1.802329000
6	-2.716758000	-3.552030000	1.531273000
1	-0.917737000	-2.845686000	2.439345000
6	-3.453457000	-3.693695000	0.369288000
1	-3.466914000	-3.355777000	-1.751178000
1	-3.119713000	-3.902663000	2.474967000
1	-4.432791000	-4.155955000	0.390005000
1	-1.330642000	1.964090000	-0.810193000
14	-2.783916000	1.929190000	-0.470556000
6	-3.721397000	1.643841000	-2.070291000
1	-4.795448000	1.605797000	-1.856420000
1	-3.572398000	2.513391000	-2.718987000
6	-3.094523000	0.511559000	0.730213000
1	-2.407455000	-0.309058000	0.491659000
1	-2.805954000	0.854377000	1.731512000
6	-3.218268000	3.579013000	0.314790000
1	-2.492012000	3.763224000	1.115569000
1	-3.048343000	4.365474000	-0.428809000
6	-4.635477000	3.659531000	0.863382000
1	-4.790044000	2.930783000	1.663540000
1	-4.864794000	4.645353000	1.274944000
1	-5.379776000	3.449919000	0.089342000

6	-4.524022000	-0.013834000	0.742025000
1	-5.253463000	0.776049000	0.940300000
1	-4.789095000	-0.461368000	-0.219472000
1	-4.663666000	-0.785575000	1.502779000
6	-3.268458000	0.368517000	-2.768663000
1	-3.430244000	-0.509475000	-2.135302000
1	-3.797516000	0.195158000	-3.708894000
1	-2.198034000	0.401086000	-2.993658000

2Ge_v (T.E.= -3824.303231)

6	2.294582000	-0.103399000	0.318688000
6	2.096523000	-1.026363000	1.463404000
6	0.973175000	-1.759576000	1.469299000
1	2.831293000	-1.129029000	2.256942000
1	0.717514000	-2.487367000	2.233512000
32	0.669594000	-0.291097000	-0.844691000
7	0.120169000	-1.612077000	0.392087000
14	3.726758000	-0.736156000	-0.742241000
14	2.434272000	1.653387000	0.987516000
6	3.931376000	0.232556000	-2.334977000
1	4.646297000	-0.292976000	-2.974500000
1	2.992841000	0.315579000	-2.889595000
1	4.315430000	1.240485000	-2.171051000
6	3.790897000	1.788130000	2.273569000
1	4.779034000	1.559107000	1.871450000
1	3.813279000	2.813111000	2.654688000
1	3.608391000	1.126823000	3.123687000
6	2.765658000	2.902161000	-0.368288000
1	2.090774000	2.772229000	-1.219211000
1	2.615081000	3.911169000	0.025139000
1	3.791583000	2.841444000	-0.738162000
6	0.826102000	2.120682000	1.832192000
1	0.060916000	2.396145000	1.102495000
1	0.433172000	1.297737000	2.435646000
1	0.982140000	2.979174000	2.490758000
6	5.345161000	-0.672187000	0.199069000
1	6.106749000	-1.246636000	-0.335083000
1	5.707733000	0.354490000	0.293097000
1	5.250467000	-1.090812000	1.204043000
6	3.379499000	-2.517367000	-1.219017000

1	4.261591000	-2.953629000	-1.695530000
1	3.124987000	-3.130552000	-0.352190000
1	2.553656000	-2.584939000	-1.933626000
6	-1.134020000	-2.237642000	0.368192000
6	-1.603144000	-2.801151000	-0.815663000
6	-1.948193000	-2.266850000	1.498901000
6	-2.859068000	-3.377583000	-0.867724000
1	-0.960724000	-2.792567000	-1.690506000
6	-3.200167000	-2.852203000	1.442380000
1	-1.600925000	-1.797726000	2.413932000
6	-3.663379000	-3.408993000	0.260572000
1	-3.209159000	-3.812562000	-1.796756000
1	-3.826038000	-2.858395000	2.327809000
1	-4.645568000	-3.864243000	0.219443000
1	-1.569860000	0.685998000	0.570957000
14	-2.687152000	1.445476000	-0.059138000
6	-1.957757000	2.945580000	-0.928249000
1	-1.547065000	3.611235000	-0.159651000
1	-1.099881000	2.611190000	-1.524632000
6	-3.576997000	0.301863000	-1.256635000
1	-2.944367000	0.187759000	-2.145793000
1	-3.612872000	-0.692613000	-0.797687000
6	-3.828453000	1.966717000	1.336923000
1	-4.679547000	2.526446000	0.932057000
1	-3.278571000	2.671195000	1.971686000
6	-4.980959000	0.742011000	-1.650225000
1	-5.442755000	0.044300000	-2.353073000
1	-5.639054000	0.801526000	-0.779218000
1	-4.987207000	1.728260000	-2.121252000
6	-2.945111000	3.701447000	-1.804995000
1	-2.509145000	4.607405000	-2.232657000
1	-3.286090000	3.081218000	-2.637600000
1	-3.833721000	4.002126000	-1.241972000
6	-4.309348000	0.776622000	2.155988000
1	-3.464819000	0.222056000	2.576479000
1	-4.956083000	1.073097000	2.985183000
1	-4.870216000	0.067749000	1.539883000

3Ge_v (T.E.= -3945.589486)

6	-2.291402000	-0.604214000	-1.199600000
6	-2.135842000	0.465321000	-0.084251000
1	-3.306716000	-1.024916000	-1.216085000
1	-2.189578000	-0.151680000	-2.196176000
7	-0.271000000	-1.560064000	-0.001696000
5	-1.246742000	-1.788541000	-1.043725000
7	-1.347164000	-2.965489000	-1.827260000
6	-2.234182000	-3.054837000	-2.963029000
1	-1.681106000	-3.353158000	-3.862612000
1	-3.017194000	-3.807174000	-2.800925000
1	-2.715025000	-2.101135000	-3.170511000
6	-0.654707000	-4.214990000	-1.611385000
1	0.098049000	-4.405501000	-2.387931000
1	-0.156158000	-4.241245000	-0.645437000
1	-1.371677000	-5.043887000	-1.640961000
14	-3.596238000	0.342504000	1.092021000
14	-1.829937000	2.163188000	-0.816613000
6	-3.549884000	-1.351758000	1.911254000
1	-2.692028000	-1.461445000	2.583427000
1	-4.452426000	-1.512776000	2.506865000
1	-3.491572000	-2.152714000	1.168784000
6	-5.251963000	0.484281000	0.221973000
1	-6.046894000	0.295650000	0.949462000
1	-5.411180000	1.478954000	-0.197394000
1	-5.364563000	-0.243751000	-0.584060000
6	-3.391411000	2.930049000	-1.519959000
1	-3.140329000	3.813345000	-2.113731000
1	-3.910459000	2.222798000	-2.173293000
1	-4.086962000	3.239831000	-0.736226000
6	-1.107483000	3.365314000	0.432449000
1	-0.806815000	4.283524000	-0.080733000
1	-1.835197000	3.636628000	1.199292000
1	-0.225342000	2.971177000	0.945791000
6	-3.548094000	1.640640000	2.445408000
1	-3.732967000	2.644597000	2.054583000
1	-4.329600000	1.424762000	3.179033000
1	-2.590536000	1.655088000	2.973236000
6	-0.628819000	2.004251000	-2.258041000
1	0.186890000	1.306310000	-2.048368000

1	-1.137864000	1.659028000	-3.161162000
1	-0.191082000	2.980830000	-2.483772000
32	-0.559361000	-0.034244000	1.058197000
6	0.916586000	-2.279955000	0.213353000
6	1.893264000	-2.335293000	-0.779473000
6	1.159719000	-2.919319000	1.426354000
6	3.067399000	-3.036052000	-0.573589000
1	1.707100000	-1.823444000	-1.719642000
6	2.339942000	-3.614092000	1.631969000
1	0.397516000	-2.877708000	2.198580000
6	3.297219000	-3.680073000	0.633265000
1	3.813151000	-3.074664000	-1.360078000
1	2.509957000	-4.110109000	2.580886000
1	4.218313000	-4.227262000	0.794195000
1	1.555706000	0.809304000	-0.309559000
14	2.837213000	1.553739000	-0.098541000
6	2.521568000	3.353590000	-0.534313000
1	1.995142000	3.390209000	-1.494600000
1	1.814439000	3.746872000	0.205180000
6	3.296680000	1.386582000	1.710532000
1	4.142248000	2.049789000	1.927739000
1	2.452454000	1.774387000	2.293538000
6	4.131085000	0.760886000	-1.207937000
1	3.901640000	1.036430000	-2.244018000
1	3.984029000	-0.323177000	-1.148874000
6	3.768884000	4.225068000	-0.582007000
1	3.526875000	5.279363000	-0.735317000
1	4.345519000	4.156424000	0.345262000
1	4.432208000	3.924491000	-1.396934000
6	3.614103000	-0.043827000	2.121805000
1	4.484605000	-0.430120000	1.584296000
1	3.827319000	-0.129910000	3.189850000
1	2.781395000	-0.719645000	1.901315000
6	5.575322000	1.106816000	-0.869262000
1	6.280614000	0.611464000	-1.540868000
1	5.766275000	2.180197000	-0.934364000
1	5.830642000	0.799706000	0.148288000

4Ge_v (T.E.= -4155.501359)

6	2.460727000	-0.873487000	1.211216000
6	2.206207000	0.220088000	0.134187000
1	3.275759000	-1.545016000	0.908837000
1	2.801200000	-0.446313000	2.163871000
7	0.026151000	-1.621447000	0.050261000
14	3.612887000	0.125068000	-1.118391000
14	1.977439000	1.907546000	0.928536000
6	3.469513000	-1.517344000	-2.029808000
1	2.576408000	-1.558499000	-2.662300000
1	4.334171000	-1.660699000	-2.683645000
1	3.429659000	-2.368887000	-1.345059000
6	5.302354000	0.156765000	-0.304856000
1	6.060618000	-0.066925000	-1.060737000
1	5.535538000	1.132960000	0.122322000
1	5.395934000	-0.589342000	0.486977000
6	3.589051000	2.618218000	1.576457000
1	4.263220000	2.918193000	0.771289000
1	3.374277000	3.505011000	2.179471000
1	4.118157000	1.903265000	2.212113000
6	1.215099000	3.161758000	-0.242256000
1	1.150694000	4.126355000	0.270156000
1	1.797303000	3.305688000	-1.153637000
1	0.199359000	2.882512000	-0.535691000
6	3.555870000	1.483035000	-2.410404000
1	3.769225000	2.467337000	-1.987170000
1	4.313158000	1.281375000	-3.173098000
1	2.584748000	1.531860000	-2.910382000
6	0.828782000	1.782349000	2.409494000
1	-0.124835000	1.311294000	2.153526000
1	1.274544000	1.221065000	3.233897000
1	0.614909000	2.791410000	2.774320000
14	0.967316000	-1.982362000	1.482303000
6	0.117311000	-1.616554000	3.114664000
1	-0.497910000	-0.715274000	3.074873000
1	-0.511707000	-2.447591000	3.441953000
1	0.877882000	-1.460252000	3.885425000
6	1.448935000	-3.786973000	1.475918000
1	2.009687000	-4.034216000	0.571151000
1	2.074453000	-4.023724000	2.340402000

1	0.569033000	-4.433717000	1.516040000
32	0.577312000	-0.163351000	-1.002678000
6	-1.159097000	-2.284024000	-0.299309000
6	-1.488320000	-2.509661000	-1.640313000
6	-2.064133000	-2.729330000	0.668559000
6	-2.682590000	-3.109973000	-1.993423000
1	-0.784347000	-2.213422000	-2.411544000
6	-3.250236000	-3.345608000	0.311377000
1	-1.846403000	-2.566585000	1.717708000
6	-3.576121000	-3.531734000	-1.021296000
1	-2.909098000	-3.263328000	-3.042683000
1	-3.932272000	-3.670639000	1.089602000
1	-4.508272000	-4.008295000	-1.299463000
1	-1.296252000	1.034840000	0.233824000
14	-2.644545000	1.581106000	-0.114120000
6	-2.770790000	1.654428000	-1.982111000
1	-1.903608000	2.202178000	-2.368535000
1	-2.656221000	0.626689000	-2.347893000
6	-3.895126000	0.392589000	0.611995000
1	-4.909868000	0.772255000	0.449546000
1	-3.824408000	-0.545458000	0.048251000
6	-2.763683000	3.278827000	0.687836000
1	-2.247791000	3.232821000	1.654058000
1	-2.181842000	3.978687000	0.076161000
6	-4.065129000	2.266233000	-2.498567000
1	-4.142536000	2.207292000	-3.586623000
1	-4.942172000	1.760878000	-2.083317000
1	-4.142277000	3.322388000	-2.227086000
6	-3.642381000	0.137662000	2.090358000
1	-3.749525000	1.052073000	2.681008000
1	-4.325299000	-0.606205000	2.509065000
1	-2.623865000	-0.230495000	2.252677000
6	-4.184525000	3.793522000	0.880216000
1	-4.200823000	4.794520000	1.317571000
1	-4.732186000	3.843695000	-0.064542000
1	-4.757154000	3.141889000	1.545006000

5Ge_v (T.E.= -3899.556518)

6	2.247520000	-1.202787000	-1.333430000
6	2.244251000	-0.116700000	-0.250938000

1	2.565990000	-0.850109000	-2.320766000
1	2.950667000	-2.012841000	-1.094114000
7	0.098702000	-1.739627000	-0.402452000
14	2.003500000	1.588842000	-1.022216000
14	3.755664000	-0.302105000	0.857838000
6	0.776069000	1.476507000	-2.437909000
1	-0.198375000	1.091246000	-2.124075000
1	0.617350000	2.479152000	-2.846168000
1	1.140923000	0.847096000	-3.252796000
6	3.601514000	2.257537000	-1.734863000
1	3.395022000	3.172222000	-2.297237000
1	4.328016000	2.501045000	-0.956407000
1	4.064643000	1.541709000	-2.419225000
6	5.336216000	-0.401522000	-0.142070000
1	5.600201000	0.559625000	-0.586260000
1	6.158839000	-0.705667000	0.510925000
1	5.267478000	-1.135277000	-0.948522000
6	3.903756000	1.089913000	2.101849000
1	4.714601000	0.862519000	2.798991000
1	4.137301000	2.045571000	1.626465000
1	2.990776000	1.216880000	2.690160000
6	1.353851000	2.824669000	0.233883000
1	2.021651000	2.931537000	1.090723000
1	1.260179000	3.807121000	-0.238457000
1	0.364824000	2.555649000	0.617929000
6	3.576505000	-1.907991000	1.820346000
1	2.779505000	-1.840536000	2.568291000
1	3.356437000	-2.761892000	1.173951000
1	4.501922000	-2.133997000	2.356890000
6	-1.189170000	-2.319373000	-0.354147000
6	-2.068577000	-2.229630000	-1.429869000
6	-1.615969000	-2.924347000	0.822445000
6	-3.344576000	-2.751153000	-1.324430000
1	-1.746268000	-1.745036000	-2.343073000
6	-2.901462000	-3.426228000	0.928382000
1	-0.924994000	-3.002318000	1.656180000
6	-3.769942000	-3.346491000	-0.147064000
1	-4.020689000	-2.676065000	-2.168646000
1	-3.220150000	-3.890494000	1.854449000
1	-4.773781000	-3.746845000	-0.069116000

6	0.916613000	-1.901403000	-1.506800000
8	0.647742000	-2.563565000	-2.482336000
32	0.651522000	-0.480905000	0.908556000
1	-1.390657000	0.607072000	-0.273216000
14	-2.555356000	1.474430000	0.091042000
6	-2.602505000	1.605543000	1.963631000
1	-3.354438000	2.352240000	2.242016000
1	-1.643052000	2.010902000	2.307810000
6	-4.113400000	0.660209000	-0.555729000
1	-4.193857000	-0.345879000	-0.128130000
1	-3.990479000	0.509124000	-1.634372000
6	-2.296486000	3.155527000	-0.723765000
1	-1.235664000	3.263564000	-0.971253000
1	-2.821082000	3.138679000	-1.686385000
6	-2.893604000	0.279724000	2.653016000
1	-2.915695000	0.379837000	3.740642000
1	-3.858036000	-0.133055000	2.344260000
1	-2.135797000	-0.471364000	2.410448000
6	-5.361409000	1.482238000	-0.266666000
1	-5.297019000	2.476498000	-0.718713000
1	-6.266802000	1.009297000	-0.653870000
1	-5.507234000	1.627924000	0.807942000
6	-2.748965000	4.346361000	0.110102000
1	-2.624414000	5.290463000	-0.425214000
1	-3.802134000	4.270853000	0.394928000
1	-2.171930000	4.418461000	1.035953000

8Ge_v (T.E.= -3468.175521)

6	-0.253176000	-1.849651000	-1.620073000
6	1.082048000	-1.128267000	-1.714891000
6	1.797147000	-1.292340000	-0.391519000
1	-0.959069000	-1.440309000	-2.354447000
1	-0.119572000	-2.917062000	-1.860626000
1	0.891836000	-0.059920000	-1.922847000
1	1.647090000	-1.516580000	-2.573157000
32	0.594326000	-1.505255000	1.051586000
7	-0.767443000	-1.673394000	-0.274872000
15	3.400541000	-0.798451000	-0.241458000
6	4.583304000	-1.765139000	-1.211344000
1	4.271722000	-1.759098000	-2.257504000

1	5.590910000	-1.351244000	-1.137501000
1	4.580463000	-2.795746000	-0.855132000
6	3.994762000	-0.870624000	1.453958000
1	3.448165000	-0.158606000	2.073983000
1	3.848855000	-1.874653000	1.853730000
1	5.057388000	-0.624250000	1.478281000
6	3.704388000	0.898459000	-0.798580000
1	4.764142000	1.156419000	-0.756261000
1	3.354244000	0.998241000	-1.828351000
1	3.132686000	1.585336000	-0.170660000
6	-2.123098000	-1.685053000	-0.053134000
6	-3.035837000	-2.225160000	-0.972827000
6	-2.655618000	-1.101966000	1.109727000
6	-4.399653000	-2.163756000	-0.744529000
1	-2.669779000	-2.703030000	-1.873607000
6	-4.015777000	-1.055814000	1.330016000
1	-1.976813000	-0.654543000	1.830490000
6	-4.907459000	-1.577754000	0.402177000
1	-5.075546000	-2.586769000	-1.480357000
1	-4.388485000	-0.585240000	2.233885000
1	-5.975992000	-1.527055000	0.572267000
1	-0.295620000	0.886576000	-0.025849000
14	-0.704183000	2.305849000	0.103609000
6	-2.564281000	2.413648000	-0.102548000
1	-3.028133000	1.971179000	0.786311000
1	-2.869518000	3.466200000	-0.113718000
6	0.181861000	3.263846000	-1.250976000
1	1.255022000	3.051247000	-1.176223000
1	-0.129477000	2.850093000	-2.216900000
6	-0.157496000	2.890567000	1.802922000
1	-0.488013000	3.921310000	1.971577000
1	-0.690622000	2.278647000	2.540501000
6	-3.047350000	1.690002000	-1.352019000
1	-2.789821000	0.626121000	-1.306556000
1	-4.131397000	1.751947000	-1.474388000
1	-2.593323000	2.101560000	-2.258951000
6	-0.072134000	4.762792000	-1.201961000
1	-1.136788000	4.989565000	-1.309498000
1	0.250540000	5.191135000	-0.248192000
1	0.453559000	5.302888000	-1.993186000

6	1.345294000	2.766247000	2.005529000
1	1.898314000	3.416057000	1.319874000
1	1.656870000	3.027825000	3.019590000
1	1.678737000	1.738324000	1.818561000

9Ge_v (T.E.= -3467.001277)

6	0.490885000	-1.309821000	-1.746491000
6	1.733940000	-0.770190000	-1.738244000
6	2.348691000	-0.676144000	-0.446855000
7	-0.011572000	-1.691980000	-0.524801000
15	3.748901000	0.245524000	-0.189871000
6	5.138135000	-0.202880000	-1.250431000
1	4.830375000	-0.115133000	-2.293901000
1	5.993778000	0.451413000	-1.074066000
1	5.418736000	-1.238408000	-1.056700000
6	4.337035000	0.109124000	1.501194000
1	5.221359000	0.733511000	1.635502000
1	3.556435000	0.439837000	2.187785000
1	4.587042000	-0.928575000	1.722874000
6	3.510151000	2.010667000	-0.489437000
1	2.765089000	2.386516000	0.214208000
1	4.441830000	2.568985000	-0.379492000
1	3.122329000	2.143610000	-1.501365000
32	1.189278000	-1.307792000	0.939134000
6	-1.343145000	-2.076656000	-0.368806000
6	-1.729991000	-2.795224000	0.766802000
6	-2.336560000	-1.729972000	-1.289072000
6	-3.052414000	-3.124212000	0.985142000
1	-0.970404000	-3.091703000	1.482536000
6	-3.658299000	-2.080653000	-1.071896000
1	-2.079966000	-1.151610000	-2.168504000
6	-4.031977000	-2.771716000	0.067314000
1	-3.320272000	-3.675013000	1.880004000
1	-4.406901000	-1.790956000	-1.801610000
1	-5.068343000	-3.037247000	0.237038000
1	-0.080500000	-1.498673000	-2.648239000
1	2.215892000	-0.470156000	-2.665695000
1	0.040573000	1.253939000	-0.142635000
14	-1.262166000	1.965189000	-0.043332000
6	-2.036396000	2.096873000	-1.761217000

1	-1.717515000	3.051853000	-2.196234000
1	-1.586328000	1.322750000	-2.391566000
6	-0.899266000	3.686706000	0.626281000
1	-0.367407000	3.588391000	1.579472000
1	-0.194621000	4.169535000	-0.060969000
6	-2.394614000	1.048523000	1.142180000
1	-3.356608000	1.573353000	1.175502000
1	-2.611428000	0.061912000	0.719245000
6	-3.553378000	1.978971000	-1.800092000
1	-3.948679000	2.104583000	-2.811332000
1	-3.880659000	0.999198000	-1.441463000
1	-4.038229000	2.727526000	-1.167274000
6	-2.144415000	4.544469000	0.794781000
1	-2.675078000	4.663183000	-0.154955000
1	-2.847747000	4.093153000	1.501058000
1	-1.916168000	5.547529000	1.163806000
6	-1.822369000	0.901218000	2.543878000
1	-2.486674000	0.330385000	3.197850000
1	-0.860632000	0.376519000	2.526604000
1	-1.654440000	1.873017000	3.018350000

14Ge_v (T.E.= -3662.335067)

6	-2.424852000	0.823386000	-0.709260000
6	-2.356510000	-0.220253000	0.279415000
7	-0.321263000	1.499894000	0.538399000
6	1.007190000	1.903261000	0.682157000
6	1.826632000	2.084737000	-0.437364000
6	3.156372000	2.435354000	-0.297918000
6	3.714428000	2.596432000	0.961825000
6	2.917633000	2.407054000	2.079371000
6	1.581731000	2.069967000	1.943510000
1	1.397256000	1.938588000	-1.424073000
1	3.767301000	2.571295000	-1.184130000
1	4.758177000	2.865904000	1.070063000
1	3.337347000	2.530638000	3.071635000
1	0.959429000	1.938165000	2.822950000
5	-1.271176000	1.936969000	-0.453862000
7	-1.285443000	3.211019000	-1.055999000
6	-2.147353000	3.565159000	-2.163306000
1	-2.806027000	4.398489000	-1.888841000

1	-1.547559000	3.895184000	-3.021079000
1	-2.756412000	2.712653000	-2.455061000
6	-0.467780000	4.325411000	-0.639032000
1	0.302726000	4.566373000	-1.383265000
1	-1.094699000	5.216027000	-0.516863000
1	0.028500000	4.127158000	0.308955000
15	-3.484221000	-1.498007000	0.155412000
6	-3.364675000	-2.434514000	-1.379569000
1	-4.108788000	-3.233007000	-1.402291000
1	-3.525475000	-1.753115000	-2.214587000
1	-2.363827000	-2.863040000	-1.454963000
6	-5.206167000	-0.984398000	0.271374000
1	-5.872854000	-1.841292000	0.158530000
1	-5.375688000	-0.512585000	1.239698000
1	-5.396025000	-0.257837000	-0.518794000
6	-3.232075000	-2.701228000	1.468187000
1	-2.233356000	-3.133978000	1.386280000
1	-3.327331000	-2.217793000	2.441266000
1	-3.973888000	-3.497568000	1.387748000
8	-3.276626000	0.840060000	-1.612780000
32	-0.848232000	-0.101604000	1.449192000
1	0.847094000	-0.832820000	-0.477897000
14	2.105770000	-1.605454000	-0.677607000
6	3.307805000	-1.264540000	0.721776000
1	3.528035000	-0.190693000	0.731175000
1	4.254825000	-1.761552000	0.480393000
6	1.615915000	-3.421039000	-0.669649000
1	0.922286000	-3.585607000	-1.502152000
1	1.040841000	-3.617882000	0.243860000
6	2.839386000	-1.111892000	-2.342033000
1	2.341414000	-1.711385000	-3.113154000
1	2.550880000	-0.074370000	-2.541053000
6	4.351038000	-1.255535000	-2.451534000
1	4.713944000	-1.002991000	-3.450848000
1	4.862979000	-0.597279000	-1.744679000
1	4.682255000	-2.275376000	-2.234970000
6	2.802252000	-4.368613000	-0.770648000
1	3.494877000	-4.229307000	0.064683000
1	2.501664000	-5.419146000	-0.770500000
1	3.370338000	-4.195703000	-1.689540000

6	2.814970000	-1.718849000	2.087855000
1	2.646953000	-2.799680000	2.114028000
1	3.530735000	-1.481724000	2.879167000
1	1.868216000	-1.238071000	2.353272000

IX_v (T.E.= -2608.085414)

6	3.076129000	0.174319000	0.483316000
6	2.665337000	1.464780000	-0.216656000
6	1.139696000	1.670412000	-0.045598000
6	2.041264000	-0.930167000	0.158206000
1	4.099400000	-0.114106000	0.207319000
1	3.107999000	0.354905000	1.565150000
1	2.919992000	1.382512000	-1.280422000
1	3.250787000	2.316620000	0.155315000
14	0.354607000	-0.063192000	-0.004483000
14	2.533124000	-1.918916000	-1.378668000
14	1.765990000	-2.094687000	1.630407000
14	0.339571000	2.429902000	-1.588940000
14	0.749378000	2.728543000	1.472871000
6	1.348843000	3.870088000	-2.238627000
1	2.358527000	3.545835000	-2.503370000
1	0.877199000	4.247344000	-3.150459000
1	1.432328000	4.696900000	-1.533261000
6	-1.441186000	2.929943000	-1.282632000
1	-1.898130000	3.210972000	-2.235670000
1	-2.006314000	2.081787000	-0.882839000
1	-1.560338000	3.768474000	-0.594946000
6	0.254651000	1.210449000	-3.022648000
1	-0.099696000	1.756222000	-3.902621000
1	1.220449000	0.773634000	-3.283159000
1	-0.452604000	0.395517000	-2.844762000
6	-0.958624000	2.402080000	2.174357000
1	-1.057215000	2.938747000	3.122251000
1	-1.748388000	2.759150000	1.510371000
1	-1.143577000	1.341863000	2.370675000
6	1.991101000	2.452508000	2.853206000
1	1.754120000	3.162854000	3.650986000
1	1.952760000	1.452325000	3.283620000
1	3.016897000	2.649965000	2.534430000
6	0.887140000	4.573046000	1.136173000

1	1.888327000	4.835805000	0.783443000
1	0.160716000	4.955309000	0.417145000
1	0.725224000	5.098709000	2.082164000
6	3.546228000	-0.887978000	-2.580563000
1	3.020775000	-0.031930000	-3.003968000
1	4.468565000	-0.524392000	-2.121115000
1	3.831509000	-1.541824000	-3.410254000
6	3.678340000	-3.359498000	-0.998163000
1	3.232093000	-4.134345000	-0.372987000
1	3.961597000	-3.821321000	-1.948762000
1	4.596070000	-3.016398000	-0.512484000
6	1.047210000	-2.588030000	-2.303291000
1	0.407903000	-1.785715000	-2.682321000
1	1.392132000	-3.169462000	-3.163148000
1	0.426606000	-3.241406000	-1.686410000
6	0.897823000	-1.223915000	3.057122000
1	1.537945000	-0.495772000	3.557898000
1	-0.035316000	-0.728164000	2.771921000
1	0.638459000	-1.985238000	3.799344000
6	3.395515000	-2.687823000	2.341947000
1	3.211232000	-3.141343000	3.319972000
1	3.891988000	-3.427447000	1.714369000
1	4.084771000	-1.852789000	2.490651000
6	0.661008000	-3.544018000	1.194072000
1	1.042893000	-4.173765000	0.389606000
1	0.543385000	-4.172658000	2.081189000
1	-0.334282000	-3.190002000	0.909322000
1	-2.652042000	-1.221149000	1.425782000
14	-3.774142000	-0.925494000	0.490048000
6	-3.196786000	-1.211808000	-1.273033000
1	-4.013757000	-0.965992000	-1.960869000
1	-2.395545000	-0.490340000	-1.475629000
6	-4.321167000	0.863425000	0.715599000
1	-5.002984000	0.900863000	1.573208000
1	-3.444976000	1.450005000	1.012823000
6	-5.177177000	-2.107597000	0.904707000
1	-4.788597000	-3.131282000	0.863442000
1	-5.458370000	-1.939813000	1.950289000
6	-6.393767000	-1.964437000	0.001648000
1	-7.187429000	-2.670242000	0.258746000

1	-6.822203000	-0.960147000	0.066902000
1	-6.137347000	-2.136002000	-1.048274000
6	-4.973189000	1.496514000	-0.507107000
1	-5.310975000	2.516439000	-0.306670000
1	-4.276093000	1.549095000	-1.347854000
1	-5.841692000	0.927354000	-0.849146000
6	-2.705337000	-2.630289000	-1.511830000
1	-1.894964000	-2.886724000	-0.821612000
1	-3.503296000	-3.362441000	-1.357785000
1	-2.324222000	-2.775188000	-2.526069000

Cartesian coordinates of the transition states involved in the activation of Si – H bond of SiEt₃H by CAASi (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGe (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and **IX**, along with their total energies (in hartrees) including zero point vibrational correction.

1SiTS^{Si-H} (T.E.= -2037.983570)

6	0.195281000	-1.721960000	-1.688074000
6	-1.244485000	-1.891112000	-1.226295000
6	-1.680931000	-0.710479000	-0.297922000
1	0.599616000	-2.668976000	-2.061841000
1	0.254276000	-0.987950000	-2.509849000
1	-1.296397000	-2.841763000	-0.683062000
1	-1.917113000	-2.000691000	-2.085285000
7	0.928585000	-1.282266000	-0.516523000
14	0.005432000	-0.028630000	0.307113000
14	-2.710046000	0.516892000	-1.283115000
14	-2.536823000	-1.446464000	1.216195000
6	-3.356564000	-0.150509000	2.291060000
1	-4.175244000	0.365657000	1.784333000
1	-3.772324000	-0.638056000	3.177194000
1	-2.636808000	0.596662000	2.634527000
6	-1.277729000	-2.334934000	2.291912000
1	-0.570793000	-1.633125000	2.744740000
1	-1.801006000	-2.846284000	3.104911000
1	-0.702140000	-3.083784000	1.742505000
6	-3.838983000	-2.708497000	0.728837000
1	-4.176935000	-3.232170000	1.627547000
1	-4.711978000	-2.241501000	0.270604000
1	-3.457007000	-3.461155000	0.035557000
6	-2.865563000	2.189837000	-0.454082000

1	-3.597714000	2.786168000	-1.005846000
1	-3.200886000	2.127597000	0.583025000
1	-1.921072000	2.738327000	-0.475793000
6	-1.995077000	0.815402000	-2.994650000
1	-1.038120000	1.340285000	-2.960652000
1	-1.854757000	-0.109319000	-3.559119000
1	-2.697985000	1.439124000	-3.554865000
6	-4.449483000	-0.136818000	-1.561741000
1	-5.039400000	-0.157485000	-0.642392000
1	-4.964852000	0.519590000	-2.268472000
1	-4.448960000	-1.144420000	-1.985490000
6	2.283495000	-1.558102000	-0.375553000
6	3.135683000	-1.687284000	-1.474042000
6	2.827349000	-1.712543000	0.902678000
6	4.487699000	-1.927882000	-1.291277000
1	2.738375000	-1.572165000	-2.476557000
6	4.176916000	-1.942065000	1.077097000
1	2.166579000	-1.649289000	1.761800000
6	5.021346000	-2.046585000	-0.019340000
1	5.132123000	-2.014869000	-2.159080000
1	4.573100000	-2.051746000	2.080756000
1	6.079860000	-2.232096000	0.117419000
14	1.160193000	2.101880000	0.211932000
6	2.807229000	1.685793000	1.028435000
1	3.287085000	0.867969000	0.480930000
1	3.425839000	2.574611000	0.840159000
6	2.740905000	1.378544000	2.511037000
1	3.706202000	1.048161000	2.902509000
1	2.435298000	2.256202000	3.086945000
1	2.012195000	0.587616000	2.715576000
6	0.190451000	3.367323000	1.204051000
1	0.974960000	4.085126000	1.486566000
1	-0.462879000	3.915312000	0.517265000
6	-0.577916000	2.917475000	2.430812000
1	0.056633000	2.369444000	3.130586000
1	-1.014460000	3.763343000	2.966953000
1	-1.393631000	2.247747000	2.151121000
6	1.617568000	2.918780000	-1.425224000
1	0.696634000	3.292638000	-1.889186000
1	2.224082000	3.802468000	-1.187017000

6	2.361712000	2.000733000	-2.381183000
1	2.589961000	2.487160000	-3.332176000
1	3.307902000	1.652466000	-1.957313000
1	1.768312000	1.107822000	-2.608513000
1	0.107336000	1.088985000	-0.914328000

2SiTS^{Si-H} (T.E.= -2036.788599)

6	1.860680000	-0.435103000	-0.277808000
6	1.552627000	-1.356014000	-1.431079000
6	0.333669000	-1.905210000	-1.467140000
1	2.314518000	-1.624579000	-2.156443000
1	0.018840000	-2.642927000	-2.196574000
7	-0.542317000	-1.557606000	-0.442748000
14	2.700254000	1.148380000	-0.851523000
14	2.838868000	-1.451195000	0.995369000
6	4.491479000	0.844975000	-1.322167000
1	4.907445000	1.757415000	-1.758502000
1	5.111653000	0.574957000	-0.464453000
1	4.581233000	0.052086000	-2.069528000
6	2.676364000	2.453803000	0.499130000
1	3.479147000	2.280950000	1.218386000
1	2.825430000	3.446223000	0.064838000
1	1.736608000	2.474581000	1.056557000
6	1.874244000	1.792669000	-2.405692000
1	2.350106000	2.730533000	-2.706400000
1	1.999205000	1.075896000	-3.221220000
1	0.803909000	1.973985000	-2.289889000
6	3.522777000	-0.358896000	2.355882000
1	3.914747000	-0.985266000	3.161526000
1	4.338093000	0.276485000	2.003360000
1	2.748418000	0.286110000	2.779657000
6	1.744600000	-2.746760000	1.801738000
1	0.961617000	-2.309833000	2.427627000
1	1.269240000	-3.395379000	1.062581000
1	2.366635000	-3.374569000	2.446792000
6	4.239324000	-2.381638000	0.169487000
1	3.851090000	-3.091271000	-0.564695000
1	4.951650000	-1.726121000	-0.333434000
1	4.784101000	-2.952857000	0.926229000
6	-1.850555000	-2.033149000	-0.370679000

6	-2.584636000	-2.371357000	-1.508133000
6	-2.469593000	-2.147926000	0.876212000
6	-3.900098000	-2.787064000	-1.396405000
1	-2.134155000	-2.274442000	-2.489427000
6	-3.787005000	-2.550535000	0.977330000
1	-1.892904000	-1.920799000	1.767718000
6	-4.515460000	-2.871109000	-0.158631000
1	-4.454346000	-3.034479000	-2.294991000
1	-4.245598000	-2.627306000	1.956861000
1	-5.548167000	-3.187849000	-0.078646000
6	-0.758576000	3.399374000	0.158475000
1	-0.385101000	3.768417000	1.120899000
1	0.111293000	3.341496000	-0.500610000
6	-2.883866000	1.230063000	-0.725609000
1	-3.309330000	0.278468000	-0.383733000
1	-3.665505000	1.980673000	-0.553160000
6	-2.152101000	1.617488000	2.206155000
1	-2.550224000	0.610612000	2.370920000
1	-1.289848000	1.716557000	2.873974000
6	-3.202297000	2.675636000	2.513594000
1	-4.070105000	2.593150000	1.853824000
1	-3.570619000	2.590353000	3.539054000
1	-2.800063000	3.685824000	2.400591000
6	-2.532875000	1.158933000	-2.201096000
1	-3.398713000	0.887526000	-2.810109000
1	-2.154335000	2.114712000	-2.575596000
1	-1.754430000	0.414021000	-2.391050000
6	-1.772149000	4.382707000	-0.418699000
1	-1.342238000	5.381743000	-0.519813000
1	-2.109676000	4.073014000	-1.410549000
1	-2.662536000	4.475573000	0.207319000
1	-0.343734000	0.947414000	-0.669945000
14	-1.480383000	1.676997000	0.441778000
14	0.136514000	-0.188696000	0.489384000

3SiTS^{Si-H} (T.E.= -2158.088133)

6	-1.514975000	2.008227000	-0.373807000
6	-1.744861000	0.466585000	-0.184923000
1	-1.733715000	2.303943000	-1.412284000
1	-2.230524000	2.580803000	0.228765000

14	-0.005524000	-0.203922000	-0.578941000
7	0.866666000	1.278908000	-0.167653000
5	-0.005853000	2.416466000	-0.082880000
7	0.374140000	3.755992000	0.172383000
6	-0.550279000	4.857478000	0.044241000
1	-0.731120000	5.342623000	1.012627000
1	-0.147158000	5.623554000	-0.630203000
1	-1.507151000	4.532358000	-0.359200000
6	1.678013000	4.217909000	0.587179000
1	1.578932000	4.891558000	1.446720000
1	2.323688000	3.395630000	0.884619000
1	2.183702000	4.779016000	-0.209912000
14	-2.971667000	-0.120019000	-1.486506000
14	-2.268141000	0.212249000	1.603089000
6	-2.150313000	-0.105713000	-3.177356000
1	-1.608606000	0.825069000	-3.368774000
1	-1.439084000	-0.929749000	-3.280733000
1	-2.908617000	-0.214268000	-3.957904000
6	-4.462142000	1.016915000	-1.581009000
1	-4.181452000	2.055499000	-1.769092000
1	-5.101995000	0.693065000	-2.406861000
1	-5.058805000	0.989316000	-0.667599000
6	-3.972550000	0.947814000	1.914079000
1	-4.761284000	0.323324000	1.486401000
1	-4.142696000	0.993653000	2.993781000
1	-4.087674000	1.958679000	1.516885000
6	-2.404316000	-1.576160000	2.150760000
1	-2.782109000	-1.582058000	3.177857000
1	-3.105863000	-2.146847000	1.539382000
1	-1.447175000	-2.098277000	2.154339000
6	-3.604007000	-1.857537000	-1.183009000
1	-4.263180000	-1.905564000	-0.313099000
1	-4.179990000	-2.187281000	-2.052065000
1	-2.790572000	-2.572090000	-1.033597000
6	-1.087866000	1.100391000	2.764217000
1	-0.046167000	0.804993000	2.617906000
1	-1.148671000	2.185698000	2.646605000
1	-1.363617000	0.864326000	3.796128000
6	2.276045000	1.242359000	-0.195139000
6	2.976710000	1.602581000	-1.341636000

6	2.985721000	0.807145000	0.919756000
6	4.359138000	1.542396000	-1.366502000
1	2.415065000	1.932651000	-2.209741000
6	4.368678000	0.744053000	0.892300000
1	2.434150000	0.534221000	1.815335000
6	5.060700000	1.112368000	-0.250352000
1	4.893096000	1.829034000	-2.265334000
1	4.908286000	0.406129000	1.770014000
1	6.142692000	1.062768000	-0.272443000
1	0.314806000	-1.032424000	0.949966000
14	1.136339000	-2.256484000	0.095617000
6	2.561565000	-2.290315000	-1.148777000
1	3.142094000	-3.183638000	-0.878865000
1	3.215054000	-1.438699000	-0.925407000
6	2.022636000	-2.715567000	1.706557000
1	2.459637000	-3.707758000	1.534620000
1	2.879568000	-2.036926000	1.797466000
6	-0.188492000	-3.523798000	-0.324106000
1	-1.085236000	-3.347009000	0.277725000
1	-0.483670000	-3.363836000	-1.366346000
6	2.184336000	-2.318922000	-2.614255000
1	1.559339000	-1.459185000	-2.874320000
1	3.063704000	-2.297264000	-3.262361000
1	1.615693000	-3.219546000	-2.864755000
6	1.199595000	-2.706822000	2.979736000
1	0.366897000	-3.415066000	2.926471000
1	1.792047000	-2.973382000	3.858321000
1	0.767035000	-1.718246000	3.166214000
6	0.310059000	-4.950031000	-0.129086000
1	-0.422704000	-5.683780000	-0.471941000
1	1.235075000	-5.131728000	-0.685241000
1	0.517440000	-5.163584000	0.922363000

4SiTS^{Si-H} (T.E. = -2367.998615)

6	1.704522000	-1.459761000	1.318406000
6	1.814232000	-0.484438000	0.097833000
1	2.158999000	-2.434425000	1.098488000
1	2.254731000	-1.086102000	2.189920000
14	0.064638000	0.046647000	-0.468872000
7	-0.899362000	-1.156497000	0.386487000

14	2.449655000	-1.474339000	-1.388518000
14	2.922072000	0.971135000	0.538932000
6	1.212145000	-2.811491000	-1.853875000
1	0.260194000	-2.419250000	-2.218045000
1	1.645527000	-3.414698000	-2.657066000
1	0.997853000	-3.483674000	-1.018712000
6	4.051028000	-2.385918000	-1.024111000
1	4.203170000	-3.134727000	-1.806640000
1	4.919164000	-1.726427000	-1.022691000
1	4.029191000	-2.913186000	-0.067944000
6	4.728635000	0.478117000	0.663932000
1	5.182854000	0.312901000	-0.315242000
1	5.281354000	1.284847000	1.153605000
1	4.864589000	-0.428312000	1.259100000
6	2.826349000	2.367136000	-0.713453000
1	3.314558000	3.252642000	-0.295962000
1	3.343362000	2.109763000	-1.639365000
1	1.806551000	2.651298000	-0.980178000
6	2.724403000	-0.390077000	-2.893664000
1	3.621552000	0.225088000	-2.791479000
1	2.859080000	-1.023329000	-3.774710000
1	1.874820000	0.272117000	-3.083727000
6	2.489687000	1.662875000	2.232215000
1	1.442569000	1.950986000	2.334386000
1	2.721072000	0.953901000	3.031033000
1	3.099905000	2.554932000	2.402612000
14	-0.090143000	-1.758204000	1.811947000
6	-0.504566000	-0.759527000	3.338508000
1	-0.418722000	0.309969000	3.124020000
1	-1.516259000	-0.949459000	3.703596000
1	0.193094000	-0.990834000	4.148001000
6	-0.436684000	-3.571442000	2.085412000
1	-0.328024000	-4.121990000	1.146978000
1	0.278587000	-3.982617000	2.802282000
1	-1.440194000	-3.757453000	2.471073000
6	-2.192086000	-1.508587000	-0.018006000
6	-3.186876000	-1.805253000	0.916300000
6	-2.541152000	-1.556010000	-1.370516000
6	-4.472236000	-2.124741000	0.516597000
1	-2.954808000	-1.747665000	1.974736000

6	-3.829681000	-1.861642000	-1.765574000
1	-1.789720000	-1.323621000	-2.118396000
6	-4.807975000	-2.149281000	-0.826467000
1	-5.222768000	-2.341807000	1.268549000
1	-4.069212000	-1.880685000	-2.822969000
1	-5.817025000	-2.390861000	-1.137662000
1	-0.100976000	1.258407000	0.761220000
14	-1.001755000	2.273101000	-0.284615000
6	-0.934362000	2.894837000	-2.068302000
1	-1.446849000	3.866511000	-2.043691000
1	0.107313000	3.117086000	-2.326318000
6	-2.752432000	1.792553000	0.190915000
1	-2.748307000	1.466232000	1.237399000
1	-3.081830000	0.926199000	-0.388801000
6	-0.427226000	3.737000000	0.767461000
1	-0.824567000	4.648980000	0.306004000
1	0.662467000	3.817457000	0.682055000
6	-1.561335000	1.982934000	-3.102377000
1	-2.615812000	1.790970000	-2.881468000
1	-1.508336000	2.406854000	-4.107705000
1	-1.054765000	1.013212000	-3.119959000
6	-3.718565000	2.953970000	-0.011925000
1	-3.778613000	3.246581000	-1.063630000
1	-4.729923000	2.690637000	0.305388000
1	-3.423128000	3.842405000	0.553316000
6	-0.839549000	3.658700000	2.228403000
1	-0.377852000	4.445048000	2.829813000
1	-1.921994000	3.753120000	2.343469000
1	-0.557558000	2.701972000	2.679386000

5SiTS^{Si-H} (T.E.= -2112.045659)

6	1.949094000	-2.025055000	0.017430000
6	1.952214000	-0.473775000	-0.070949000
1	2.336695000	-2.486301000	-0.901331000
1	2.585783000	-2.411190000	0.820501000
14	0.169671000	-0.109994000	-0.670208000
7	-0.394502000	-1.756444000	-0.266173000
14	3.162389000	0.064032000	-1.414582000
14	2.277068000	0.169948000	1.676128000
6	2.499178000	-0.477946000	-3.085415000

1	1.621034000	0.103399000	-3.376688000
1	3.267072000	-0.331421000	-3.849981000
1	2.220290000	-1.535300000	-3.101474000
6	4.841389000	-0.739558000	-1.201108000
1	5.446010000	-0.534618000	-2.088801000
1	5.380528000	-0.355573000	-0.334545000
1	4.769293000	-1.824783000	-1.097945000
6	4.064924000	-0.147229000	2.153464000
1	4.740783000	0.543765000	1.643190000
1	4.181574000	0.014866000	3.228624000
1	4.392878000	-1.165773000	1.933537000
6	1.990045000	2.006834000	1.924934000
1	2.385662000	2.268690000	2.910898000
1	2.504301000	2.629688000	1.190407000
1	0.931043000	2.272998000	1.921268000
6	3.372154000	1.922919000	-1.442539000
1	3.866293000	2.292937000	-0.540809000
1	3.984941000	2.213317000	-2.299663000
1	2.408041000	2.431075000	-1.538295000
6	1.191016000	-0.738359000	2.907698000
1	0.128637000	-0.539669000	2.741814000
1	1.341017000	-1.820438000	2.895867000
1	1.438581000	-0.383571000	3.912229000
6	-1.771502000	-2.085335000	-0.210509000
6	-2.501781000	-2.218315000	-1.382279000
6	-2.408751000	-2.206041000	1.017941000
6	-3.864004000	-2.458763000	-1.327015000
1	-1.990319000	-2.121993000	-2.334298000
6	-3.770465000	-2.444949000	1.069486000
1	-1.821307000	-2.111569000	1.925653000
6	-4.501995000	-2.566813000	-0.102234000
1	-4.429342000	-2.559790000	-2.246137000
1	-4.263535000	-2.537034000	2.030259000
1	-5.568556000	-2.753118000	-0.059419000
6	0.564290000	-2.616487000	0.198441000
8	0.361767000	-3.724933000	0.640754000
1	-0.358244000	0.553031000	0.764032000
14	-1.502564000	1.585342000	-0.136260000
6	-0.492001000	3.123103000	-0.512620000
1	-0.483301000	3.230071000	-1.602820000

1	0.548309000	2.948277000	-0.223692000
6	-2.836975000	1.272601000	-1.437899000
1	-3.504302000	0.484004000	-1.069398000
1	-2.352806000	0.871210000	-2.331234000
6	-3.619264000	2.533393000	-1.791559000
1	-4.384511000	2.323447000	-2.542719000
1	-4.125713000	2.967155000	-0.927454000
1	-2.965197000	3.304834000	-2.206051000
6	-1.008316000	4.388009000	0.160503000
1	-0.413679000	5.260707000	-0.117628000
1	-2.045844000	4.601844000	-0.110288000
1	-0.969381000	4.302150000	1.249579000
6	-2.343181000	1.611549000	1.559249000
1	-1.616576000	2.000960000	2.282899000
1	-2.473350000	0.554415000	1.823585000
6	-3.678288000	2.328031000	1.689869000
1	-4.064799000	2.262124000	2.709628000
1	-3.608066000	3.389660000	1.439841000
1	-4.431122000	1.884616000	1.033614000

8SiTS^{Si-H} (T.E.= -1680.662085)

6	0.153040000	-2.397542000	-1.057981000
6	-1.362738000	-2.426060000	-0.853672000
6	-1.801666000	-1.076382000	-0.296235000
1	0.570290000	-3.409836000	-1.015617000
1	0.383220000	-1.987251000	-2.057129000
1	-1.607761000	-3.247055000	-0.163111000
1	-1.837989000	-2.674592000	-1.811603000
14	-0.339383000	-0.184387000	0.252934000
7	0.737425000	-1.557295000	-0.026621000
15	-3.363199000	-0.858022000	0.265502000
6	-4.642520000	-1.008510000	-1.006911000
1	-4.569178000	-1.993420000	-1.472527000
1	-5.641164000	-0.893357000	-0.580691000
1	-4.478546000	-0.249818000	-1.773465000
6	-3.934648000	-2.044241000	1.516567000
1	-3.317037000	-1.944791000	2.410264000
1	-4.983323000	-1.882209000	1.773936000
1	-3.821115000	-3.058443000	1.128978000
6	-3.616746000	0.764357000	0.999284000

1	-2.857486000	0.955845000	1.760012000
1	-3.547956000	1.532571000	0.228161000
1	-4.606688000	0.806087000	1.456429000
6	2.107779000	-1.534967000	0.154210000
6	2.997857000	-2.200604000	-0.695049000
6	2.650451000	-0.824463000	1.235555000
6	4.365120000	-2.138772000	-0.475465000
1	2.622998000	-2.757249000	-1.544849000
6	4.011858000	-0.764876000	1.440446000
1	1.973699000	-0.321136000	1.919935000
6	4.887941000	-1.419946000	0.583890000
1	5.030131000	-2.660499000	-1.155314000
1	4.395697000	-0.203530000	2.285733000
1	5.957778000	-1.373748000	0.746783000
1	0.150476000	0.607431000	-1.256442000
14	0.472049000	2.005299000	-0.253171000
6	1.802368000	2.452043000	-1.521687000
1	1.317200000	2.492416000	-2.503723000
1	2.129300000	3.474533000	-1.291202000
6	1.193626000	2.688830000	1.368398000
1	1.386701000	3.749261000	1.153575000
1	2.179608000	2.232595000	1.517428000
6	-1.106909000	2.960013000	-0.633378000
1	-0.779614000	4.003952000	-0.732612000
1	-1.757444000	2.941894000	0.246858000
6	0.337223000	2.541296000	2.606430000
1	0.094740000	1.489285000	2.791814000
1	0.827447000	2.930307000	3.502559000
1	-0.614476000	3.071603000	2.501798000
6	2.998646000	1.515848000	-1.570833000
1	3.733384000	1.823538000	-2.318954000
1	3.514621000	1.467156000	-0.607338000
1	2.692454000	0.493399000	-1.816222000
6	-1.863794000	2.523408000	-1.876182000
1	-2.181889000	1.478361000	-1.798248000
1	-2.753201000	3.135156000	-2.053300000
1	-1.237512000	2.593564000	-2.769104000

9SiTS^{Si-H} (T.E.= -1679.471170)

6	0.219271000	-2.817190000	-0.495062000
6	1.527369000	-2.508820000	-0.594986000
6	1.921087000	-1.249919000	0.019000000
14	0.383454000	-0.431604000	0.502365000
7	-0.565923000	-1.904318000	0.222880000
15	3.503119000	-0.694028000	0.126388000
6	4.640862000	-1.860353000	0.907299000
1	4.597591000	-2.807777000	0.366605000
1	5.666320000	-1.486623000	0.890744000
1	4.325989000	-2.036206000	1.936061000
6	3.610773000	0.833747000	1.068005000
1	4.659363000	1.095965000	1.217153000
1	3.118584000	1.645337000	0.529273000
1	3.127509000	0.704832000	2.037089000
6	4.308095000	-0.345628000	-1.457782000
1	3.753183000	0.433782000	-1.982081000
1	5.344581000	-0.031603000	-1.319213000
1	4.286481000	-1.251401000	-2.067101000
6	-1.954899000	-1.878486000	0.121280000
6	-2.710382000	-1.339958000	1.165797000
6	-2.624288000	-2.329752000	-1.017486000
6	-4.084656000	-1.244150000	1.068781000
1	-2.198344000	-1.007087000	2.062847000
6	-4.004037000	-2.244405000	-1.099738000
1	-2.051126000	-2.722411000	-1.849528000
6	-4.744319000	-1.698216000	-0.064768000
1	-4.647515000	-0.819669000	1.892932000
1	-4.504012000	-2.597139000	-1.995168000
1	-5.822892000	-1.628628000	-0.137691000
1	-0.231715000	-3.746522000	-0.821189000
1	2.233842000	-3.203312000	-1.040739000
1	-0.153637000	0.213872000	-1.102147000
14	-0.493666000	1.671024000	-0.222937000
6	-0.656602000	2.683052000	1.382099000
1	0.346810000	2.765366000	1.818053000
1	-0.963065000	3.702840000	1.112704000
6	-2.209126000	1.694048000	-1.012187000
1	-2.093868000	1.278313000	-2.018633000
1	-2.861490000	0.993084000	-0.478773000

6	0.841679000	2.501885000	-1.280162000
1	0.453622000	2.481754000	-2.305867000
1	1.706422000	1.826975000	-1.294653000
6	-2.841654000	3.076344000	-1.070541000
1	-2.193629000	3.796443000	-1.580890000
1	-3.792695000	3.064713000	-1.609190000
1	-3.042558000	3.475797000	-0.073712000
6	1.268844000	3.909140000	-0.896769000
1	2.020294000	4.308004000	-1.583363000
1	0.425810000	4.604882000	-0.902329000
1	1.697017000	3.942467000	0.108603000
6	-1.615675000	2.090057000	2.396245000
1	-2.623231000	1.971658000	1.984352000
1	-1.280547000	1.093848000	2.703654000
1	-1.699513000	2.698828000	3.300060000

14SiTS^{Si-H} (T.E.= -1874.826079)

6	-1.806435000	1.793906000	-0.282675000
6	-1.892154000	0.416850000	0.114577000
7	0.601461000	1.269992000	0.270460000
6	2.008422000	1.267161000	0.272074000
6	2.721508000	1.590789000	-0.880126000
6	4.104574000	1.570992000	-0.881152000
6	4.801814000	1.209413000	0.261403000
6	4.099974000	0.871638000	1.407569000
6	2.716060000	0.899685000	1.414041000
1	2.169043000	1.858827000	-1.775179000
1	4.642989000	1.830513000	-1.785834000
1	5.885075000	1.190718000	0.258055000
1	4.633955000	0.588372000	2.307731000
1	2.161845000	0.641844000	2.311227000
5	-0.283862000	2.335595000	-0.138039000
7	0.070016000	3.694106000	-0.272365000
6	-0.791412000	4.671118000	-0.904360000
1	-1.026114000	5.487202000	-0.209570000
1	-0.288076000	5.117913000	-1.771643000
1	-1.722750000	4.207475000	-1.220471000
6	1.305451000	4.290027000	0.177041000
1	1.970881000	4.541964000	-0.659722000
1	1.087716000	5.221525000	0.712283000

1	1.847972000	3.635017000	0.855187000
15	-3.452370000	-0.213247000	0.392001000
6	-4.456695000	-0.427392000	-1.088436000
1	-5.454440000	-0.787437000	-0.829856000
1	-4.530822000	0.536546000	-1.591854000
1	-3.972257000	-1.142584000	-1.754407000
6	-4.453827000	0.797010000	1.496413000
1	-5.450403000	0.365090000	1.604844000
1	-3.968649000	0.848705000	2.471665000
1	-4.524358000	1.799670000	1.076575000
6	-3.369093000	-1.833705000	1.167231000
1	-2.881450000	-2.542473000	0.497144000
1	-2.796589000	-1.770284000	2.093987000
1	-4.377027000	-2.189307000	1.387490000
8	-2.801684000	2.475225000	-0.590029000
14	-0.247038000	-0.271816000	0.488563000
1	0.218082000	-0.835302000	-1.124149000
14	0.739364000	-2.308180000	-0.417991000
6	2.591754000	-2.071763000	-0.607476000
1	2.762879000	-1.407249000	-1.459936000
1	2.999800000	-1.552968000	0.264227000
6	0.419077000	-3.555755000	0.979437000
1	-0.664717000	-3.684110000	1.082914000
1	0.798997000	-4.517592000	0.608109000
6	0.016054000	-3.150398000	-1.948546000
1	0.324608000	-4.202712000	-1.940123000
1	0.485329000	-2.690010000	-2.825523000
6	3.305996000	-3.401342000	-0.816535000
1	4.378646000	-3.259099000	-0.967176000
1	3.187900000	-4.066344000	0.043154000
1	2.924791000	-3.934169000	-1.692039000
6	1.048538000	-3.200948000	2.308866000
1	2.138339000	-3.143790000	2.231017000
1	0.700539000	-2.219661000	2.649301000
1	0.813512000	-3.926803000	3.091081000
6	-1.496603000	-3.047191000	-2.050402000
1	-1.815701000	-1.999411000	-2.018213000
1	-1.886547000	-3.478744000	-2.975397000
1	-1.985605000	-3.571730000	-1.222833000

1GeTS^{Si-H} (T.E.= -3825.448766)

6	0.361603000	-2.717985000	-0.192111000
6	1.710070000	-2.174046000	-0.626452000
6	1.875563000	-0.698460000	-0.176792000
1	0.174001000	-3.698518000	-0.647949000
1	0.355370000	-2.873229000	0.899361000
1	1.761677000	-2.251210000	-1.719000000
1	2.516204000	-2.800614000	-0.232804000
32	0.058910000	-0.009588000	-0.681628000
7	-0.639536000	-1.772215000	-0.631493000
14	2.271702000	-0.617940000	1.676884000
14	3.111949000	0.200820000	-1.280750000
6	2.769372000	-0.207658000	-3.081263000
1	1.719583000	-0.057238000	-3.349163000
1	3.368214000	0.454779000	-3.712446000
1	3.039088000	-1.235085000	-3.334233000
6	2.961642000	2.064338000	-1.123098000
1	3.199377000	2.437602000	-0.126453000
1	3.649213000	2.539010000	-1.828607000
1	1.950933000	2.397325000	-1.381148000
6	4.875493000	-0.328149000	-0.926060000
1	4.972820000	-1.415826000	-0.987475000
1	5.549858000	0.106505000	-1.668739000
1	5.220781000	-0.013710000	0.060953000
6	3.044185000	1.013006000	2.188853000
1	2.403777000	1.867873000	1.961444000
1	3.179631000	0.985973000	3.274362000
1	4.023933000	1.187980000	1.738852000
6	0.836404000	-0.868726000	2.872007000
1	0.094118000	-1.600057000	2.546540000
1	1.254083000	-1.212553000	3.824353000
1	0.305504000	0.067237000	3.063058000
6	3.516338000	-1.970982000	2.073157000
1	3.061361000	-2.964239000	2.044920000
1	4.369442000	-1.968733000	1.390987000
1	3.895353000	-1.814950000	3.087027000
6	-1.981845000	-2.033660000	-0.415526000
6	-2.951635000	-1.330421000	-1.142359000
6	-2.427829000	-2.974256000	0.518650000
6	-4.297422000	-1.516000000	-0.907167000

1	-2.625194000	-0.637799000	-1.910230000
6	-3.783338000	-3.160111000	0.741808000
1	-1.711127000	-3.553577000	1.088421000
6	-4.729727000	-2.428200000	0.047183000
1	-5.019397000	-0.947635000	-1.484842000
1	-4.099563000	-3.889989000	1.479198000
1	-5.786899000	-2.576980000	0.229881000
1	-0.380982000	0.443524000	0.967080000
14	-1.291875000	1.828715000	0.281535000
6	-1.858216000	2.810554000	-1.235965000
1	-2.534518000	3.587977000	-0.855246000
1	-0.961440000	3.336744000	-1.588670000
6	-2.757250000	1.205386000	1.287244000
1	-2.867194000	0.131063000	1.110777000
1	-2.445669000	1.298491000	2.336085000
6	-0.184139000	2.997377000	1.252163000
1	0.063494000	2.510247000	2.201217000
1	0.763230000	3.132898000	0.716709000
6	-0.850170000	4.343596000	1.508040000
1	-1.818359000	4.222037000	2.004242000
1	-0.237851000	4.981992000	2.148625000
1	-1.028372000	4.889593000	0.579253000
6	-4.080317000	1.912333000	1.043872000
1	-4.011000000	2.989364000	1.218618000
1	-4.416517000	1.770536000	0.013524000
1	-4.866696000	1.524181000	1.695300000
6	-2.507467000	2.063795000	-2.381848000
1	-3.419217000	1.548302000	-2.066206000
1	-2.776549000	2.731899000	-3.203034000
1	-1.825628000	1.308406000	-2.785383000

2GeTS^{Si-H} (T.E.= -3824.258714)

6	1.870778000	-0.642933000	0.187537000
6	1.571878000	-1.966404000	0.844491000
6	0.338880000	-2.484346000	0.766823000
1	2.367978000	-2.526574000	1.323791000
1	0.088962000	-3.460726000	1.169495000
32	0.043520000	-0.076281000	-0.398266000
7	-0.635358000	-1.797851000	0.071151000
14	2.803231000	-0.940644000	-1.438064000

14	2.746452000	0.458866000	1.450556000
6	2.950732000	0.629293000	-2.454208000
1	3.307374000	0.369835000	-3.454988000
1	1.983535000	1.126739000	-2.570374000
1	3.652681000	1.346479000	-2.027746000
6	4.135221000	-0.506602000	2.265782000
1	4.824272000	-0.967145000	1.556085000
1	4.711334000	0.178815000	2.894112000
1	3.739650000	-1.290548000	2.915633000
6	3.502241000	1.996399000	0.686796000
1	2.812140000	2.540596000	0.038864000
1	3.809066000	2.672545000	1.489895000
1	4.393717000	1.755876000	0.102704000
6	1.620516000	0.975130000	2.856921000
1	0.908471000	1.755282000	2.581141000
1	1.050322000	0.123766000	3.237195000
1	2.240887000	1.358972000	3.672527000
6	4.521359000	-1.625165000	-1.137142000
1	4.967683000	-1.908224000	-2.094269000
1	5.180866000	-0.891744000	-0.667785000
1	4.497405000	-2.516254000	-0.505190000
6	1.874010000	-2.183807000	-2.490113000
1	2.453458000	-2.373589000	-3.398255000
1	1.733749000	-3.136096000	-1.975691000
1	0.891448000	-1.817406000	-2.800325000
6	-1.982224000	-2.121016000	0.111116000
6	-2.815841000	-1.687425000	-0.924482000
6	-2.557739000	-2.843181000	1.160103000
6	-4.172663000	-1.939276000	-0.899513000
1	-2.369433000	-1.164930000	-1.764958000
6	-3.916742000	-3.105201000	1.167903000
1	-1.942404000	-3.173030000	1.989034000
6	-4.737690000	-2.650021000	0.149172000
1	-4.793644000	-1.587727000	-1.716424000
1	-4.341758000	-3.660717000	1.996645000
1	-5.801710000	-2.851305000	0.168473000
1	-0.482940000	0.641322000	1.089623000
14	-1.365115000	1.902774000	-0.073552000
6	-0.039322000	3.232552000	-0.052769000
1	0.524037000	3.161220000	0.883083000

1	0.670400000	3.038637000	-0.864034000
6	-2.391680000	1.997582000	-1.657212000
1	-1.681228000	2.279369000	-2.444940000
1	-2.732951000	0.991994000	-1.915713000
6	-2.512070000	2.075298000	1.403951000
1	-3.115979000	2.975652000	1.235024000
1	-1.884806000	2.283385000	2.278318000
6	-3.581649000	2.946239000	-1.611134000
1	-4.072492000	3.016748000	-2.584881000
1	-4.333189000	2.603087000	-0.896124000
1	-3.297321000	3.959953000	-1.318057000
6	-0.632448000	4.629048000	-0.203955000
1	0.139159000	5.399221000	-0.142268000
1	-1.132486000	4.748147000	-1.168349000
1	-1.368338000	4.843492000	0.575844000
6	-3.410788000	0.877234000	1.665579000
1	-2.821254000	-0.019147000	1.879460000
1	-4.072612000	1.044049000	2.517905000
1	-4.041691000	0.641620000	0.802924000

3GeTS^{Si-H} (T.E.= -3945.552301)

6	-1.764211000	-1.279025000	-1.099511000
6	-1.916118000	-0.105021000	-0.092762000
1	-2.653909000	-1.923490000	-1.073579000
1	-1.724978000	-0.892344000	-2.130738000
7	0.567052000	-1.405921000	-0.125050000
5	-0.431835000	-2.118612000	-0.860130000
7	-0.315488000	-3.454829000	-1.329673000
6	-1.259559000	-4.036507000	-2.251729000
1	-0.739433000	-4.472803000	-3.114066000
1	-1.838633000	-4.843853000	-1.782509000
1	-1.957013000	-3.291900000	-2.631610000
6	0.685319000	-4.412822000	-0.925519000
1	1.401433000	-4.631483000	-1.729423000
1	1.245434000	-4.067221000	-0.059018000
1	0.202383000	-5.359241000	-0.652757000
14	-2.733320000	-0.731802000	1.496832000
14	-2.820123000	1.315129000	-0.928033000
6	-1.901184000	-2.307806000	2.092916000
1	-0.840147000	-2.171110000	2.316296000

1	-2.398598000	-2.634026000	3.010931000
1	-1.985432000	-3.118941000	1.364962000
6	-4.546417000	-1.155424000	1.258049000
1	-4.878647000	-1.751532000	2.112659000
1	-5.172322000	-0.261682000	1.216834000
1	-4.729474000	-1.739632000	0.353536000
6	-4.515036000	0.780862000	-1.538457000
1	-4.905366000	1.553799000	-2.206811000
1	-4.448011000	-0.146217000	-2.114143000
1	-5.240829000	0.632106000	-0.739031000
6	-3.050532000	2.772324000	0.234943000
1	-3.264433000	3.683164000	-0.330467000
1	-3.893916000	2.595478000	0.907658000
1	-2.169686000	2.960597000	0.853080000
6	-2.626769000	0.510947000	2.898115000
1	-3.175095000	1.430201000	2.684995000
1	-3.064178000	0.063474000	3.795399000
1	-1.594747000	0.782552000	3.134451000
6	-1.961374000	1.875964000	-2.507960000
1	-0.880914000	2.003038000	-2.427496000
1	-2.151619000	1.162932000	-3.314366000
1	-2.397153000	2.832264000	-2.813696000
32	-0.039720000	0.287083000	0.481023000
6	1.918615000	-1.745007000	0.041983000
6	2.773071000	-1.825490000	-1.056610000
6	2.440005000	-2.002834000	1.307940000
6	4.105411000	-2.162154000	-0.892435000
1	2.366364000	-1.626620000	-2.043789000
6	3.772343000	-2.338039000	1.471402000
1	1.774295000	-1.950085000	2.164456000
6	4.612596000	-2.418319000	0.372306000
1	4.753673000	-2.222970000	-1.759402000
1	4.156883000	-2.539678000	2.464929000
1	5.656064000	-2.681000000	0.499602000
1	0.438350000	1.126062000	-1.005212000
14	1.484433000	2.207710000	-0.019091000
6	0.405030000	3.731758000	-0.241614000
1	-0.373923000	3.548272000	-0.985523000
1	-0.110279000	3.921240000	0.706225000
6	2.425615000	2.464271000	1.596182000

1	3.044427000	3.357961000	1.432784000
1	1.684440000	2.732666000	2.356984000
6	2.741739000	1.933667000	-1.394994000
1	2.217997000	2.151644000	-2.334343000
1	2.956295000	0.859054000	-1.425118000
6	1.224382000	4.954744000	-0.640761000
1	0.594489000	5.841237000	-0.741217000
1	1.994796000	5.189361000	0.098161000
1	1.727469000	4.802595000	-1.599386000
6	3.283675000	1.307161000	2.063725000
1	3.979315000	0.976029000	1.286055000
1	3.875545000	1.561246000	2.946266000
1	2.665263000	0.444078000	2.320003000
6	4.037770000	2.724886000	-1.296428000
1	4.679377000	2.547686000	-2.162747000
1	3.859265000	3.801768000	-1.240330000
1	4.612963000	2.446986000	-0.409921000

4GeTS^{Si-H} (T.E.= -4155.466081)

6	1.849365000	-1.692538000	0.980093000
6	1.930370000	-0.434934000	0.062749000
1	2.316538000	-2.563552000	0.501435000
1	2.418464000	-1.550636000	1.907622000
7	-0.828327000	-1.397878000	0.213201000
14	2.719626000	-0.938791000	-1.579212000
14	2.800783000	0.972899000	0.951237000
6	1.588050000	-2.142106000	-2.475871000
1	0.666738000	-1.664100000	-2.819830000
1	2.102959000	-2.531076000	-3.358761000
1	1.307784000	-2.994760000	-1.852409000
6	4.362816000	-1.813280000	-1.344229000
1	4.682111000	-2.211113000	-2.311804000
1	5.144734000	-1.141629000	-0.987587000
1	4.299675000	-2.654486000	-0.650648000
6	4.634475000	0.619460000	1.149377000
1	5.171309000	0.726357000	0.203768000
1	5.069729000	1.328366000	1.859061000
1	4.815501000	-0.388789000	1.531335000
6	2.645532000	2.599506000	0.017011000
1	2.728590000	3.437990000	0.713702000

1	3.446078000	2.701280000	-0.718289000
1	1.700168000	2.712730000	-0.519910000
6	3.006109000	0.528468000	-2.710254000
1	3.785561000	1.190884000	-2.326150000
1	3.330388000	0.167969000	-3.690219000
1	2.098486000	1.120256000	-2.857521000
6	2.137940000	1.192680000	2.695008000
1	1.057929000	1.354944000	2.728479000
1	2.370059000	0.329069000	3.323715000
1	2.625118000	2.063347000	3.144045000
14	0.093505000	-2.224622000	1.428040000
6	-0.287954000	-1.716738000	3.189577000
1	-0.199891000	-0.636773000	3.328111000
1	-1.290439000	-2.018559000	3.501815000
1	0.427599000	-2.195160000	3.865140000
6	-0.098124000	-4.076612000	1.278709000
1	0.032684000	-4.396906000	0.242320000
1	0.658368000	-4.579342000	1.886993000
1	-1.077738000	-4.420407000	1.616079000
32	0.071651000	0.115140000	-0.478687000
6	-2.111361000	-1.727693000	-0.218908000
6	-2.509212000	-1.523733000	-1.545850000
6	-3.058619000	-2.264481000	0.658877000
6	-3.795288000	-1.812065000	-1.960400000
1	-1.791792000	-1.123085000	-2.255613000
6	-4.341636000	-2.563938000	0.235984000
1	-2.788903000	-2.419704000	1.698706000
6	-4.725969000	-2.331798000	-1.073870000
1	-4.070878000	-1.635206000	-2.994334000
1	-5.051844000	-2.972096000	0.946671000
1	-5.733575000	-2.557230000	-1.401358000
1	-0.260597000	1.116134000	0.944403000
14	-1.294951000	2.163340000	-0.145098000
6	-1.613531000	2.657586000	-1.942140000
1	-0.633374000	2.776854000	-2.419497000
1	-2.072870000	1.785672000	-2.422155000
6	-2.891201000	1.548532000	0.621642000
1	-3.596856000	2.383575000	0.521678000
1	-3.293817000	0.745520000	-0.006175000
6	-0.601890000	3.685314000	0.742655000

1	0.063651000	3.378151000	1.553815000
1	0.022464000	4.238644000	0.032000000
6	-2.463962000	3.903218000	-2.141735000
1	-2.645679000	4.101782000	-3.201006000
1	-3.441333000	3.808875000	-1.659849000
1	-1.979904000	4.790835000	-1.726695000
6	-2.793200000	1.098864000	2.068320000
1	-2.368089000	1.877272000	2.709981000
1	-3.769452000	0.829660000	2.478601000
1	-2.146538000	0.223613000	2.158132000
6	-1.697889000	4.594589000	1.290452000
1	-1.277171000	5.499866000	1.734359000
1	-2.399072000	4.910845000	0.514902000
1	-2.282116000	4.095663000	2.067228000

5GeTS^{Si-H} (T.E.= -3899.523532)

6	1.602332000	-1.369032000	-1.486766000
6	1.902948000	-0.427612000	-0.305770000
1	1.514679000	-0.808297000	-2.427529000
1	2.390203000	-2.110064000	-1.655905000
7	-0.605002000	-1.512321000	-0.546838000
14	2.874091000	1.099515000	-0.832415000
14	2.672002000	-1.406744000	1.129523000
6	2.276796000	1.730764000	-2.495894000
1	1.191090000	1.821834000	-2.564225000
1	2.709148000	2.720943000	-2.667103000
1	2.613961000	1.084455000	-3.309947000
6	4.695650000	0.723091000	-1.064392000
1	5.192953000	1.595681000	-1.496912000
1	5.205565000	0.479085000	-0.130093000
1	4.833869000	-0.111649000	-1.757410000
6	4.106095000	-2.450557000	0.528085000
1	4.866580000	-1.877441000	-0.003960000
1	4.583234000	-2.921997000	1.391823000
1	3.762074000	-3.252793000	-0.129113000
6	3.244207000	-0.260294000	2.495345000
1	3.547706000	-0.860168000	3.357396000
1	4.098246000	0.353636000	2.201891000
1	2.442312000	0.407710000	2.822171000
6	2.713907000	2.480227000	0.433783000

1	3.388517000	2.333658000	1.278747000
1	2.978015000	3.432304000	-0.035262000
1	1.704585000	2.587562000	0.841893000
6	1.438913000	-2.596883000	1.892988000
1	0.608887000	-2.083332000	2.386447000
1	1.023381000	-3.298285000	1.165749000
1	1.957685000	-3.182428000	2.657841000
6	-1.922447000	-1.987743000	-0.384063000
6	-2.722610000	-2.284567000	-1.482695000
6	-2.458306000	-2.101345000	0.893402000
6	-4.037198000	-2.672330000	-1.299261000
1	-2.305806000	-2.201075000	-2.478509000
6	-3.777970000	-2.479170000	1.071874000
1	-1.832999000	-1.881438000	1.752538000
6	-4.574051000	-2.764812000	-0.024323000
1	-4.651434000	-2.897825000	-2.163491000
1	-4.182207000	-2.554856000	2.074854000
1	-5.606885000	-3.062362000	0.112998000
6	0.290995000	-2.129714000	-1.373036000
8	0.092113000	-3.160788000	-1.982430000
32	0.075168000	0.049649000	0.316899000
1	-0.326089000	1.059661000	-1.054799000
14	-1.431871000	2.012467000	0.103363000
6	-1.744804000	2.486988000	1.900681000
1	-2.375974000	3.385002000	1.872695000
1	-0.788774000	2.803727000	2.333977000
6	-2.993927000	1.329328000	-0.670545000
1	-3.291621000	0.402566000	-0.169550000
1	-2.770341000	1.054782000	-1.706259000
6	-0.753172000	3.518813000	-0.799965000
1	0.340697000	3.496497000	-0.753447000
1	-0.999803000	3.369448000	-1.858509000
6	-2.393438000	1.408251000	2.743903000
1	-2.547765000	1.732864000	3.775042000
1	-3.368641000	1.117860000	2.341904000
1	-1.772504000	0.507529000	2.773549000
6	-4.123682000	2.351117000	-0.611909000
1	-3.860450000	3.275452000	-1.133937000
1	-5.034210000	1.965177000	-1.074758000
1	-4.373835000	2.617687000	0.418801000

6	-1.267800000	4.863336000	-0.305412000
1	-0.895242000	5.683388000	-0.923076000
1	-2.359707000	4.915740000	-0.320859000
1	-0.948713000	5.059567000	0.720539000

8GeTS^{Si-H} (T.E.= -3468.126472)

6	0.987116000	-2.611754000	0.683148000
6	-0.490315000	-2.584896000	1.051712000
6	-1.218863000	-1.748941000	0.023113000
1	1.581403000	-2.935904000	1.547145000
1	1.150992000	-3.347970000	-0.120555000
1	-0.585296000	-2.166740000	2.068752000
1	-0.857454000	-3.618006000	1.097635000
32	-0.091089000	-0.266412000	-0.308255000
7	1.400592000	-1.288871000	0.252443000
15	-2.886969000	-1.728474000	-0.094788000
6	-3.589157000	-3.363836000	-0.408519000
1	-3.284481000	-4.044785000	0.387976000
1	-4.679407000	-3.320841000	-0.435297000
1	-3.209195000	-3.744589000	-1.356620000
6	-3.456634000	-0.672849000	-1.436338000
1	-3.211112000	0.370058000	-1.228528000
1	-2.971546000	-0.970137000	-2.366313000
1	-4.538736000	-0.763847000	-1.542241000
6	-3.831831000	-1.173224000	1.357385000
1	-4.910267000	-1.231328000	1.194443000
1	-3.566744000	-1.804434000	2.208553000
1	-3.552559000	-0.144824000	1.595799000
6	2.717408000	-1.052624000	-0.049143000
6	3.712225000	-2.032634000	0.101823000
6	3.134092000	0.204559000	-0.518960000
6	5.036687000	-1.755418000	-0.191150000
1	3.449091000	-3.023173000	0.449464000
6	4.455602000	0.466600000	-0.809513000
1	2.392239000	0.982833000	-0.666253000
6	5.429276000	-0.509362000	-0.646215000
1	5.775062000	-2.539736000	-0.060150000
1	4.729311000	1.452787000	-1.169704000
1	6.467824000	-0.301088000	-0.872223000
1	-0.227399000	0.612581000	1.273596000

14	-0.248977000	2.093776000	0.183587000
6	1.149698000	2.862571000	1.181943000
1	2.049301000	2.870374000	0.556809000
1	0.858154000	3.918554000	1.272621000
6	-1.967456000	2.457482000	0.880351000
1	-2.698922000	1.793233000	0.404188000
1	-1.956484000	2.173017000	1.937531000
6	-0.142358000	2.971965000	-1.496850000
1	-0.206071000	4.051343000	-1.302168000
1	0.864078000	2.795229000	-1.893253000
6	1.449119000	2.269479000	2.544075000
1	1.818324000	1.245065000	2.453421000
1	2.204589000	2.847594000	3.082012000
1	0.554446000	2.230984000	3.171677000
6	-2.393885000	3.909001000	0.719589000
1	-1.654850000	4.593574000	1.145871000
1	-2.516255000	4.183139000	-0.330793000
1	-3.344397000	4.110295000	1.219501000
6	-1.187912000	2.545227000	-2.507515000
1	-2.202926000	2.739928000	-2.145356000
1	-1.082094000	3.061612000	-3.464588000
1	-1.115262000	1.470957000	-2.709788000

9GeTS^{Si-H} (T.E.= -3466.940590)

6	0.234271000	-2.911282000	-0.130406000
6	1.552630000	-2.639011000	-0.204698000
6	1.999183000	-1.336602000	0.257171000
7	-0.590921000	-1.916039000	0.394032000
15	3.481505000	-0.640361000	-0.119669000
6	4.858348000	-1.788086000	0.065487000
1	4.718577000	-2.634227000	-0.608955000
1	5.801007000	-1.295798000	-0.179165000
1	4.888068000	-2.156125000	1.090962000
6	3.828052000	0.771507000	0.939505000
1	4.770298000	1.237853000	0.647873000
1	3.026047000	1.506268000	0.842876000
1	3.880763000	0.447149000	1.978609000
6	3.674920000	0.005870000	-1.804041000
1	2.924542000	0.782883000	-1.969819000
1	4.671519000	0.419198000	-1.973760000

1	3.489125000	-0.801915000	-2.514414000
32	0.412683000	-0.322674000	0.536500000
6	-1.967620000	-1.914831000	0.250966000
6	-2.747127000	-1.117657000	1.098936000
6	-2.622230000	-2.651848000	-0.740524000
6	-4.115820000	-1.041926000	0.945398000
1	-2.251555000	-0.560196000	1.888779000
6	-3.998408000	-2.578983000	-0.877207000
1	-2.041167000	-3.256767000	-1.426639000
6	-4.757303000	-1.771544000	-0.046913000
1	-4.691713000	-0.411998000	1.614925000
1	-4.481598000	-3.154112000	-1.659730000
1	-5.832634000	-1.715445000	-0.163924000
1	-0.194398000	-3.887416000	-0.324489000
1	2.254148000	-3.413548000	-0.500183000
1	0.025278000	0.202794000	-1.195441000
14	-0.615836000	1.709912000	-0.227808000
6	-2.157910000	1.499271000	-1.293730000
1	-1.819400000	1.665249000	-2.324352000
1	-2.447829000	0.445582000	-1.254985000
6	0.700691000	2.772411000	-1.065308000
1	1.632758000	2.777055000	-0.489296000
1	0.932606000	2.306917000	-2.028264000
6	-1.116047000	2.625329000	1.359964000
1	-1.600931000	3.564696000	1.066143000
1	-1.889658000	2.029678000	1.858672000
6	-3.348774000	2.383573000	-0.960716000
1	-4.176776000	2.211359000	-1.652877000
1	-3.724968000	2.181639000	0.045025000
1	-3.100177000	3.447595000	-1.006988000
6	0.203714000	4.197709000	-1.272431000
1	-0.743347000	4.209633000	-1.820908000
1	0.031592000	4.710272000	-0.322582000
1	0.914845000	4.799806000	-1.842739000
6	0.034874000	2.895305000	2.309077000
1	-0.290769000	3.379474000	3.232958000
1	0.536230000	1.962989000	2.592622000
1	0.791420000	3.543158000	1.855033000

14GeTS^{Si-H} (T.E.= -3662.295465)

6	-2.508104000	1.033080000	-0.219454000
6	-2.069345000	-0.314032000	-0.029053000
7	-0.070439000	1.485752000	0.325083000
6	1.229759000	1.991561000	0.229705000
6	1.650296000	2.692269000	-0.902976000
6	2.955530000	3.134696000	-1.016596000
6	3.879289000	2.873988000	-0.015268000
6	3.474913000	2.175992000	1.111005000
6	2.165193000	1.744967000	1.235244000
1	0.934576000	2.872027000	-1.698877000
1	3.258814000	3.676838000	-1.905386000
1	4.903589000	3.213365000	-0.112166000
1	4.182870000	1.970238000	1.906536000
1	1.843336000	1.214864000	2.126532000
5	-1.320233000	2.115454000	0.003622000
7	-1.540613000	3.511137000	-0.012659000
6	-2.720905000	4.128776000	-0.576845000
1	-3.233803000	4.743317000	0.173789000
1	-2.444104000	4.794307000	-1.405364000
1	-3.412506000	3.368768000	-0.932656000
6	-0.616507000	4.493549000	0.498265000
1	-0.114881000	5.050123000	-0.305529000
1	-1.158102000	5.223314000	1.111386000
1	0.151096000	4.037797000	1.120943000
15	-3.266043000	-1.527388000	-0.057582000
6	-4.122803000	-1.668176000	-1.634143000
1	-4.889948000	-2.443589000	-1.588716000
1	-4.578075000	-0.703186000	-1.855380000
1	-3.399070000	-1.910518000	-2.412976000
6	-4.560563000	-1.324419000	1.177958000
1	-5.327049000	-2.093478000	1.064472000
1	-4.117241000	-1.392372000	2.172002000
1	-5.001726000	-0.336548000	1.047372000
6	-2.536772000	-3.141797000	0.248771000
1	-1.851932000	-3.390411000	-0.563769000
1	-1.982996000	-3.129257000	1.189770000
1	-3.317645000	-3.902076000	0.301391000
8	-3.701543000	1.306947000	-0.462819000
32	-0.225517000	-0.399506000	0.456687000

1	0.526678000	-0.672280000	-1.170928000
14	1.744566000	-1.660592000	-0.259805000
6	2.609580000	-2.097707000	1.372572000
1	2.945600000	-1.163946000	1.836826000
1	3.522615000	-2.644952000	1.103709000
6	1.091111000	-3.275080000	-0.975751000
1	0.536006000	-3.054252000	-1.892943000
1	0.379287000	-3.724435000	-0.275547000
6	3.013135000	-0.808079000	-1.363363000
1	2.747531000	-1.087439000	-2.390817000
1	2.828208000	0.269281000	-1.301923000
6	4.478343000	-1.098083000	-1.077366000
1	5.128982000	-0.604346000	-1.803587000
1	4.767669000	-0.731984000	-0.089366000
1	4.706956000	-2.167099000	-1.108785000
6	2.225797000	-4.252434000	-1.256663000
1	2.769704000	-4.508507000	-0.342993000
1	1.861819000	-5.187115000	-1.689308000
1	2.950745000	-3.830640000	-1.958306000
6	1.767500000	-2.907794000	2.335715000
1	1.536324000	-3.897387000	1.930542000
1	2.264668000	-3.060047000	3.296586000
1	0.813882000	-2.406441000	2.537507000

IX-TS^{Si-H} (T.E.= -2608.061304)

6	-0.303714000	-2.356176000	0.823910000
6	1.106188000	-2.281451000	0.251090000
6	1.608275000	-0.806034000	0.163529000
6	-1.241844000	-1.307587000	0.160503000
1	-0.691781000	-3.378086000	0.710540000
1	-0.246896000	-2.183396000	1.904232000
1	1.094667000	-2.738870000	-0.746673000
1	1.792849000	-2.903364000	0.841289000
14	-0.009254000	0.007299000	-0.562171000
14	-2.120259000	-2.071322000	-1.337156000
14	-2.479071000	-0.766441000	1.485078000
14	2.945066000	-0.776416000	-1.196782000
14	2.386639000	-0.338488000	1.832138000
6	4.034276000	-2.306690000	-1.104524000
6	4.046490000	0.748064000	-1.178567000

6	2.258310000	-0.856623000	-2.945156000
6	2.427641000	1.496762000	2.219548000
6	1.590408000	-1.153732000	3.326375000
6	4.164613000	-0.946367000	1.993338000
6	-0.935604000	-3.001078000	-2.459744000
1	-0.399622000	-3.804924000	-1.950520000
6	-3.423933000	-3.340348000	-0.861321000
6	-2.964477000	-0.809722000	-2.437823000
6	-1.725180000	0.162589000	2.941887000
6	-3.290198000	-2.245641000	2.318539000
6	-3.861642000	0.336645000	0.867287000
1	-0.328055000	1.232569000	0.693970000
14	-0.427550000	2.538066000	-0.267216000
6	-1.543284000	2.910382000	-1.739998000
6	1.330245000	3.071928000	-0.668988000
6	-1.067247000	3.574136000	1.181793000
6	-1.251169000	5.046016000	0.837858000
6	1.609324000	3.351447000	-2.136831000
6	-3.050875000	2.832271000	-1.604892000

Cartesian coordinates of the H – H splitting product obtained for CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**) and CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**), along with their total energies (in hartrees) including zero point vibrational correction.

1SiP^{H-H} (T.E.= -1511.739046)

6	0.972163000	0.199795000	-1.605659000
6	-0.519615000	-0.115168000	-1.606067000
6	-1.139966000	-0.057227000	-0.174018000
1	1.454008000	-0.286803000	-2.461711000
1	1.148988000	1.279043000	-1.718442000
1	-0.646373000	-1.119142000	-2.027638000
1	-1.037958000	0.560301000	-2.295789000
7	1.542268000	-0.286242000	-0.360482000
14	0.339575000	-0.442930000	0.891617000
14	-1.759363000	1.681084000	0.239839000
14	-2.455038000	-1.412636000	-0.076205000
6	-3.368425000	-1.382910000	1.556762000
1	-4.042660000	-0.527984000	1.638956000
1	-3.969205000	-2.290642000	1.655907000

1	-2.673919000	-1.350921000	2.401724000
6	-1.653670000	-3.103194000	-0.240931000
1	-1.162408000	-3.404622000	0.686035000
1	-2.426351000	-3.843710000	-0.464564000
1	-0.911018000	-3.151448000	-1.040899000
6	-3.682260000	-1.245827000	-1.482692000
1	-4.327073000	-2.128537000	-1.502160000
1	-4.320622000	-0.368213000	-1.376710000
1	-3.182993000	-1.182978000	-2.452591000
6	-2.217116000	1.870628000	2.047561000
1	-2.435108000	2.925678000	2.236895000
1	-3.105442000	1.297854000	2.316791000
1	-1.407989000	1.577395000	2.719621000
6	-0.435345000	2.956571000	-0.137658000
1	0.495288000	2.774751000	0.406421000
1	-0.202229000	3.009788000	-1.203651000
1	-0.805908000	3.940177000	0.165048000
6	-3.272015000	2.135780000	-0.770962000
1	-4.164126000	1.617450000	-0.411169000
1	-3.453631000	3.209620000	-0.672960000
1	-3.156049000	1.913417000	-1.834319000
6	2.910701000	-0.217820000	-0.156647000
6	3.785059000	0.307197000	-1.112764000
6	3.459500000	-0.681271000	1.046055000
6	5.146664000	0.364369000	-0.866515000
1	3.402589000	0.680492000	-2.054069000
6	4.817055000	-0.617033000	1.280344000
1	2.807442000	-1.110633000	1.801312000
6	5.676985000	-0.092099000	0.326466000
1	5.800467000	0.779024000	-1.626000000
1	5.209487000	-0.985858000	2.221496000
1	6.742891000	-0.043071000	0.512218000
1	0.595624000	0.527321000	1.984509000
1	0.347669000	-1.782042000	1.525943000

2SiP^{H-H} (T.E.= -1510.546303)

6	-1.165348000	-0.095927000	-0.174767000
6	-0.513939000	-0.143048000	-1.541089000
6	0.805352000	-0.348222000	-1.588401000
1	-1.097208000	-0.011543000	-2.446448000

1	1.385483000	-0.391954000	-2.502502000
14	0.221738000	-0.797403000	0.859477000
7	1.458927000	-0.570653000	-0.370403000
14	-2.700784000	-1.181526000	-0.089840000
14	-1.377175000	1.742265000	0.241416000
6	-4.150282000	-0.420558000	-0.999976000
1	-4.954018000	-1.156857000	-1.084035000
1	-4.553938000	0.454145000	-0.485164000
1	-3.870762000	-0.117861000	-2.012604000
6	-3.188494000	-1.489722000	1.693087000
1	-3.995683000	-2.226159000	1.728577000
1	-2.360065000	-1.888295000	2.285033000
1	-3.545978000	-0.582964000	2.184207000
6	-2.312892000	-2.818044000	-0.912457000
1	-3.169728000	-3.491706000	-0.830011000
1	-2.094596000	-2.677764000	-1.973783000
1	-1.450648000	-3.312092000	-0.458221000
6	-2.282291000	1.974157000	1.864746000
1	-2.275828000	3.033365000	2.135098000
1	-3.325144000	1.654955000	1.802231000
1	-1.805704000	1.421606000	2.678947000
6	0.300348000	2.569607000	0.380603000
1	0.884622000	2.206670000	1.229429000
1	0.898815000	2.433830000	-0.523652000
1	0.150014000	3.643945000	0.519524000
6	-2.311292000	2.623902000	-1.120020000
1	-3.340156000	2.275659000	-1.220971000
1	-2.340268000	3.693723000	-0.895909000
1	-1.812586000	2.503011000	-2.084426000
6	2.825952000	-0.399238000	-0.194329000
6	3.438538000	-0.906295000	0.954363000
6	3.614826000	0.290267000	-1.117077000
6	4.791409000	-0.732333000	1.169043000
1	2.843104000	-1.456769000	1.677093000
6	4.971694000	0.446668000	-0.898315000
1	3.159917000	0.727466000	-1.998092000
6	5.572315000	-0.059273000	0.242237000
1	5.241930000	-1.136147000	2.068742000
1	5.564464000	0.986720000	-1.628204000
1	6.634445000	0.071615000	0.409079000

1	0.555710000	-0.069400000	2.103145000
1	0.073031000	-2.230978000	1.215099000

3SiP^{H-H} (T.E.= -1631.842506)

6	-0.708845000	0.963146000	-0.945008000
6	-1.409329000	-0.120875000	-0.048696000
1	-0.835467000	0.724329000	-2.011374000
1	-1.196528000	1.939175000	-0.829792000
14	0.018713000	-1.136474000	0.588127000
7	1.332126000	-0.119158000	0.065243000
5	0.852366000	1.041234000	-0.645577000
7	1.639984000	2.150406000	-1.029182000
6	1.142994000	3.181536000	-1.908556000
1	1.074782000	4.148569000	-1.393389000
1	1.815959000	3.317113000	-2.764229000
1	0.158027000	2.931324000	-2.298382000
6	2.982618000	2.438455000	-0.581412000
1	3.039985000	3.474590000	-0.227722000
1	3.280943000	1.790665000	0.240171000
1	3.718644000	2.326070000	-1.388336000
14	-2.562947000	-1.159318000	-1.106566000
14	-2.194830000	0.763740000	1.419378000
6	-1.576863000	-2.033315000	-2.445427000
1	-1.010256000	-2.874196000	-2.041576000
1	-2.259803000	-2.423614000	-3.204749000
1	-0.870757000	-1.367664000	-2.948199000
6	-3.842622000	-0.091015000	-1.967490000
1	-4.351398000	-0.678825000	-2.735931000
1	-4.599181000	0.277401000	-1.272701000
1	-3.388376000	0.773820000	-2.457231000
6	-3.597137000	1.890113000	0.883170000
1	-4.499669000	1.315934000	0.660493000
1	-3.838686000	2.578002000	1.698185000
1	-3.353333000	2.489448000	0.003124000
6	-2.889695000	-0.402409000	2.711643000
1	-3.169923000	0.180686000	3.593489000
1	-3.785644000	-0.917573000	2.359854000
1	-2.167492000	-1.156548000	3.030190000
6	-3.448775000	-2.460487000	-0.089627000
1	-4.251586000	-2.022187000	0.507341000

1	-3.897094000	-3.209273000	-0.747557000
1	-2.770365000	-2.981357000	0.592315000
6	-0.887817000	1.833884000	2.242563000
1	-0.064208000	1.242040000	2.651819000
1	-0.460443000	2.563711000	1.549844000
1	-1.340548000	2.387216000	3.069908000
6	2.663886000	-0.561942000	0.209319000
6	3.446620000	-0.818801000	-0.912746000
6	3.208858000	-0.772729000	1.472034000
6	4.753422000	-1.248362000	-0.772524000
1	3.013480000	-0.667505000	-1.896360000
6	4.515284000	-1.211046000	1.608602000
1	2.601224000	-0.564923000	2.347234000
6	5.294988000	-1.445432000	0.488344000
1	5.352487000	-1.438319000	-1.655877000
1	4.928298000	-1.363006000	2.599347000
1	6.318384000	-1.784659000	0.596074000
1	0.029365000	-1.334481000	2.060642000
1	0.173956000	-2.496464000	0.010572000

4SiP^{H-H} (T.E.= -1841.751758)

6	0.903885000	0.094820000	1.509902000
6	1.383289000	0.004399000	0.013101000
1	1.231406000	-0.781015000	2.083557000
1	1.360027000	0.946614000	2.027890000
14	-0.122349000	0.056448000	-1.108852000
7	-1.427752000	0.005053000	0.015182000
14	2.209487000	-1.675162000	-0.218671000
14	2.459726000	1.502103000	-0.374482000
6	0.950675000	-3.029090000	0.117226000
1	0.071463000	-2.960558000	-0.527479000
1	1.416482000	-4.003150000	-0.056714000
1	0.612512000	-3.012648000	1.156490000
6	3.617154000	-1.955633000	0.990831000
1	3.883580000	-3.016302000	0.973018000
1	4.508501000	-1.387108000	0.721439000
1	3.353552000	-1.700727000	2.019461000
6	4.049367000	1.492506000	0.617579000
1	4.766400000	0.777593000	0.207607000
1	4.511295000	2.482687000	0.580339000

1	3.883077000	1.240041000	1.667272000
6	2.921037000	1.610296000	-2.189082000
1	3.394653000	2.578051000	-2.376579000
1	3.633131000	0.834449000	-2.475789000
1	2.055375000	1.535404000	-2.850922000
6	2.908591000	-1.895903000	-1.943216000
1	3.833164000	-1.326042000	-2.064177000
1	3.150402000	-2.949954000	-2.103805000
1	2.215986000	-1.589272000	-2.730227000
6	1.499757000	3.051322000	0.080030000
1	0.535350000	3.093836000	-0.434511000
1	1.312013000	3.120377000	1.154235000
1	2.070462000	3.937124000	-0.211433000
14	-0.971881000	0.215390000	1.677199000
6	-1.540117000	1.873034000	2.321314000
1	-1.156178000	2.687703000	1.702039000
1	-2.631848000	1.932501000	2.316232000
1	-1.203717000	2.036843000	3.348171000
6	-1.698394000	-1.119946000	2.758601000
1	-1.409394000	-2.115485000	2.413708000
1	-1.363411000	-1.005565000	3.792596000
1	-2.790114000	-1.065348000	2.757704000
6	-2.776762000	-0.026884000	-0.409797000
6	-3.430434000	1.141244000	-0.791286000
6	-3.471011000	-1.232268000	-0.451424000
6	-4.752640000	1.103623000	-1.199346000
1	-2.881585000	2.077919000	-0.760010000
6	-4.793923000	-1.266639000	-0.856874000
1	-2.951342000	-2.140083000	-0.160927000
6	-5.439509000	-0.099240000	-1.231558000
1	-5.250218000	2.020922000	-1.493201000
1	-5.322911000	-2.212605000	-0.882703000
1	-6.474889000	-0.127016000	-1.549788000
1	-0.205297000	-1.079452000	-2.063663000
1	-0.199232000	1.278140000	-1.954835000

5Si^{H-H} (T.E.= -1585.806319)

6	0.555820000	-0.362892000	1.462622000
6	1.216445000	-0.079374000	0.085725000
1	0.756344000	-1.380697000	1.820048000

1	0.931571000	0.285266000	2.261275000
14	-0.243246000	-0.056194000	-1.067282000
7	-1.469890000	-0.133473000	0.186980000
14	2.402377000	-1.489464000	-0.330058000
14	1.952931000	1.666008000	0.116413000
6	1.428294000	-3.087941000	-0.471874000
1	0.860035000	-3.128605000	-1.403303000
1	2.118319000	-3.935698000	-0.466903000
1	0.725811000	-3.233138000	0.352924000
6	3.674129000	-1.718465000	1.024258000
1	4.200039000	-2.663617000	0.865202000
1	4.419148000	-0.921747000	1.032164000
1	3.217428000	-1.760425000	2.015930000
6	3.393190000	1.765536000	1.308208000
1	4.283188000	1.286432000	0.893895000
1	3.638803000	2.814235000	1.494556000
1	3.175799000	1.298371000	2.271432000
6	2.550405000	2.226632000	-1.567029000
1	2.777592000	3.295187000	-1.517248000
1	3.462331000	1.712075000	-1.874203000
1	1.802072000	2.087740000	-2.350378000
6	3.271316000	-1.183754000	-1.958708000
1	4.033768000	-0.406534000	-1.872000000
1	3.767752000	-2.099042000	-2.290627000
1	2.571943000	-0.884120000	-2.744937000
6	0.628489000	2.861019000	0.697025000
1	-0.240195000	2.873779000	0.033357000
1	0.275934000	2.639186000	1.706963000
1	1.045842000	3.871499000	0.711186000
6	-2.869355000	-0.085103000	-0.038997000
6	-3.713251000	-1.039351000	0.514726000
6	-3.397199000	0.912606000	-0.847128000
6	-5.070770000	-0.989622000	0.259237000
1	-3.298240000	-1.812168000	1.149385000
6	-4.756672000	0.951623000	-1.106638000
1	-2.736878000	1.667424000	-1.261786000
6	-5.597781000	0.002249000	-0.553202000
1	-5.723533000	-1.735851000	0.697018000
1	-5.158796000	1.734973000	-1.738464000
1	-6.662353000	0.035144000	-0.752178000

6	-0.955493000	-0.237078000	1.464189000
8	-1.610287000	-0.249131000	2.478608000
1	-0.397153000	-1.191380000	-2.002228000
1	-0.389318000	1.177661000	-1.870298000

8SiP^{H-H} (T.E.= -1154.415569)

6	0.498450000	-1.615534000	0.090452000
6	-0.960148000	-1.537070000	0.529245000
6	-1.509959000	-0.196944000	0.069415000
1	1.049077000	-2.330400000	0.712436000
1	0.560284000	-1.972468000	-0.949400000
1	-1.005192000	-1.659394000	1.622325000
1	-1.506180000	-2.388379000	0.103425000
14	-0.143467000	0.965647000	0.109999000
7	1.083876000	-0.287521000	0.210017000
15	-3.140291000	0.104888000	-0.094815000
6	-3.999301000	-1.006065000	-1.237238000
1	-3.860725000	-2.036869000	-0.905854000
1	-5.068751000	-0.789773000	-1.271500000
1	-3.567237000	-0.900691000	-2.232654000
6	-4.159823000	-0.033063000	1.402868000
1	-3.815882000	0.696172000	2.137633000
1	-5.219905000	0.126419000	1.194218000
1	-4.027795000	-1.032693000	1.823417000
6	-3.432766000	1.771507000	-0.705468000
1	-3.031712000	2.499192000	0.002240000
1	-2.937489000	1.900385000	-1.668327000
1	-4.503412000	1.945993000	-0.822001000
6	2.444190000	-0.111276000	0.074677000
6	3.322473000	-1.168568000	-0.194115000
6	2.998926000	1.171126000	0.206380000
6	4.684175000	-0.945131000	-0.313420000
1	2.940942000	-2.173876000	-0.318592000
6	4.356126000	1.380155000	0.082843000
1	2.346906000	2.011776000	0.424563000
6	5.217965000	0.323562000	-0.177278000
1	5.336381000	-1.786524000	-0.522214000
1	4.748010000	2.385397000	0.194098000
1	6.284136000	0.489319000	-0.272519000
1	0.048259000	1.844160000	-1.078443000

1 -0.005791000 1.896326000 1.269086000

9SiP^{H-H} (T.E.= -1153.226561)

6 0.434419000 -1.569016000 0.162545000
6 -0.907148000 -1.529168000 0.125996000
6 -1.513842000 -0.206944000 0.024780000
14 -0.135771000 0.965916000 0.014304000
7 1.079436000 -0.314819000 0.105058000
15 -3.165756000 0.065788000 -0.033888000
6 -4.028826000 -0.728555000 -1.411953000
1 -3.841303000 -1.803426000 -1.368939000
1 -5.105571000 -0.553287000 -1.365443000
1 -3.630916000 -0.347446000 -2.352813000
6 -3.508463000 1.824660000 -0.173153000
1 -4.584941000 1.997082000 -0.208525000
1 -3.092170000 2.349149000 0.688449000
1 -3.053018000 2.215855000 -1.084163000
6 -4.103125000 -0.514312000 1.401858000
1 -3.754645000 0.006928000 2.293855000
1 -5.175207000 -0.353320000 1.272140000
1 -3.916939000 -1.582333000 1.532457000
6 2.449930000 -0.150085000 0.042345000
6 3.345265000 -1.218333000 -0.091155000
6 2.989708000 1.141843000 0.107347000
6 4.708520000 -0.993132000 -0.150183000
1 2.976599000 -2.233192000 -0.163639000
6 4.351872000 1.353768000 0.043558000
1 2.325406000 1.993263000 0.222523000
6 5.229852000 0.288300000 -0.084179000
1 5.375104000 -1.842445000 -0.255441000
1 4.731719000 2.368090000 0.098703000
1 6.299125000 0.453998000 -0.132371000
1 1.023091000 -2.467462000 0.269275000
1 -1.492835000 -2.441899000 0.185122000
1 0.082186000 1.811453000 -1.193836000
1 -0.023561000 1.928925000 1.148461000

14SiP^{H-H} (T.E.= -1348.586265)

6 1.200529000 1.032423000 0.072255000
6 1.658959000 -0.323353000 -0.014525000

7	-0.980504000	-0.219503000	-0.205218000
6	-2.320918000	-0.599446000	-0.009316000
6	-3.047756000	-0.119128000	1.079037000
6	-4.359101000	-0.508720000	1.276811000
6	-4.967642000	-1.400327000	0.406002000
6	-4.246976000	-1.897619000	-0.666054000
6	-2.936914000	-1.500170000	-0.874941000
1	-2.565528000	0.566257000	1.768127000
1	-4.909120000	-0.119925000	2.126482000
1	-5.994407000	-1.707168000	0.565786000
1	-4.709143000	-2.596314000	-1.354340000
1	-2.380434000	-1.872028000	-1.729365000
5	-0.408585000	1.109595000	-0.125749000
7	-1.121841000	2.311177000	-0.292006000
6	-0.561654000	3.610300000	0.015143000
1	-0.567626000	4.253853000	-0.873264000
1	-1.163219000	4.111935000	0.783973000
1	0.463113000	3.505479000	0.364314000
6	-2.475826000	2.415009000	-0.782538000
1	-3.179927000	2.696302000	0.011894000
1	-2.527003000	3.189844000	-1.555686000
1	-2.819405000	1.479488000	-1.219749000
15	3.336856000	-0.595312000	0.080863000
6	4.079016000	-0.068798000	1.633718000
1	5.158326000	-0.231741000	1.621950000
1	3.864004000	0.991509000	1.766152000
1	3.631255000	-0.629905000	2.454403000
6	4.295735000	0.221756000	-1.205217000
1	5.361035000	0.020732000	-1.077566000
1	3.968124000	-0.139663000	-2.180436000
1	4.109588000	1.293507000	-1.139950000
6	3.684198000	-2.352827000	-0.074896000
1	3.172880000	-2.898124000	0.720159000
1	3.324313000	-2.713640000	-1.039890000
1	4.757236000	-2.535705000	-0.001501000
8	1.968253000	1.998835000	0.239238000
14	0.263863000	-1.449577000	-0.247216000
1	0.258202000	-2.222449000	-1.519108000
1	0.004227000	-2.453470000	0.818237000

1Ge^{PH-H} (T.E.= -3299.187182)

6	-0.890193000	0.327066000	1.687258000
6	0.593201000	-0.016555000	1.720052000
6	1.216069000	-0.005067000	0.297222000
1	-1.361955000	0.018062000	2.628361000
1	-1.034408000	1.417249000	1.612720000
1	0.691774000	-1.014415000	2.163474000
1	1.120553000	0.669873000	2.391250000
32	-0.212375000	-0.923820000	-0.664616000
7	-1.496647000	-0.361069000	0.566559000
14	1.372447000	1.759689000	-0.378541000
14	2.806987000	-1.015706000	0.248670000
6	2.613848000	-2.573216000	1.276692000
1	1.726079000	-3.147896000	0.999981000
1	3.485744000	-3.211606000	1.109405000
1	2.562355000	-2.362912000	2.347123000
6	3.201022000	-1.570782000	-1.497999000
1	3.389245000	-0.744621000	-2.183910000
1	4.094584000	-2.200774000	-1.483588000
1	2.387845000	-2.175155000	-1.911345000
6	4.249877000	-0.059992000	0.967440000
1	4.015718000	0.284338000	1.978908000
1	5.127809000	-0.707847000	1.033784000
1	4.522574000	0.811758000	0.368567000
6	2.483974000	1.829669000	-1.885434000
1	2.112001000	1.183473000	-2.685313000
1	2.480786000	2.854839000	-2.266444000
1	3.520625000	1.556934000	-1.679163000
6	-0.260909000	2.501825000	-0.939103000
1	-1.037220000	2.494623000	-0.171905000
1	-0.077279000	3.544941000	-1.213812000
1	-0.661019000	1.999558000	-1.823240000
6	2.064315000	2.879065000	0.956270000
1	1.350185000	3.025240000	1.770428000
1	2.991713000	2.493512000	1.384658000
1	2.275028000	3.862318000	0.527202000
6	-2.845290000	-0.244796000	0.320344000
6	-3.425634000	-0.922465000	-0.762361000
6	-3.688519000	0.531831000	1.125518000
6	-4.775667000	-0.825185000	-1.025045000

1	-2.802137000	-1.547339000	-1.395968000
6	-5.042947000	0.619223000	0.850912000
1	-3.283263000	1.071183000	1.972531000
6	-5.602105000	-0.052363000	-0.221659000
1	-5.190013000	-1.365767000	-1.868960000
1	-5.669325000	1.228913000	1.493244000
1	-6.662586000	0.020965000	-0.428883000
1	-0.130373000	-2.468531000	-0.678610000
1	-0.530829000	-0.426496000	-2.091114000

2Ge^{P^H-H} (T.E.= -3297.995708)

6	1.208493000	0.019484000	0.257863000
6	0.503185000	0.111968000	1.591332000
6	-0.822759000	-0.055892000	1.647817000
1	1.069303000	0.319081000	2.493795000
1	-1.386233000	0.009858000	2.571601000
32	-0.239234000	-0.682466000	-0.865246000
7	-1.508818000	-0.379685000	0.483911000
14	2.629619000	-1.218667000	0.307500000
14	1.608838000	1.795191000	-0.268800000
6	3.173894000	-1.671578000	-1.428142000
1	3.939596000	-2.450222000	-1.377125000
1	2.350973000	-2.066214000	-2.030325000
1	3.601784000	-0.819726000	-1.960144000
6	2.577511000	2.674827000	1.069468000
1	3.552139000	2.221494000	1.253873000
1	2.741903000	3.712775000	0.767595000
1	2.023520000	2.689261000	2.010907000
6	2.588544000	1.821997000	-1.865607000
1	2.112555000	1.224782000	-2.648193000
1	2.667147000	2.848166000	-2.233721000
1	3.603876000	1.443388000	-1.724461000
6	0.020740000	2.761619000	-0.511463000
1	-0.568967000	2.414010000	-1.362469000
1	-0.608919000	2.713432000	0.380625000
1	0.267641000	3.812070000	-0.688306000
6	4.105674000	-0.542659000	1.242010000
1	4.847619000	-1.334135000	1.377107000
1	4.588313000	0.277112000	0.704462000
1	3.825047000	-0.177754000	2.233499000

6	2.039226000	-2.761660000	1.187364000
1	2.819374000	-3.527001000	1.174465000
1	1.794656000	-2.545325000	2.229806000
1	1.147123000	-3.184703000	0.718365000
6	-2.873692000	-0.225096000	0.317669000
6	-3.495578000	-0.784609000	-0.803345000
6	-3.666838000	0.487361000	1.222411000
6	-4.853884000	-0.645487000	-1.005770000
1	-2.899081000	-1.349720000	-1.514193000
6	-5.028754000	0.610109000	1.014823000
1	-3.212053000	0.966668000	2.080980000
6	-5.636515000	0.048346000	-0.095729000
1	-5.307422000	-1.091916000	-1.883737000
1	-5.621419000	1.168686000	1.730968000
1	-6.702852000	0.153821000	-0.253008000
1	-0.179861000	-2.192187000	-1.198470000
1	-0.622433000	0.097304000	-2.139421000

3Ge^{P^H-H} (T.E.= -3419.289627)

6	0.695686000	0.993599000	-1.028573000
6	1.435253000	-0.050791000	-0.124038000
1	1.210121000	1.961272000	-0.981083000
1	0.760687000	0.698610000	-2.087832000
7	-1.388786000	-0.089477000	-0.075985000
5	-0.848632000	1.110215000	-0.656882000
7	-1.573583000	2.311802000	-0.846758000
6	-1.044542000	3.425589000	-1.594876000
1	-1.809299000	3.837263000	-2.264166000
1	-0.718023000	4.241532000	-0.933773000
1	-0.198566000	3.123828000	-2.210567000
6	-2.801018000	2.653386000	-0.169537000
1	-3.642840000	2.766212000	-0.865182000
1	-3.070585000	1.900570000	0.569287000
1	-2.678709000	3.609014000	0.356133000
14	2.047183000	0.833663000	1.426839000
14	2.741441000	-0.933378000	-1.148258000
6	0.653407000	1.870627000	2.142340000
1	-0.221774000	1.267382000	2.401794000
1	1.002318000	2.363016000	3.054151000
1	0.327242000	2.649896000	1.447408000

6	3.476943000	1.983437000	1.039392000
1	3.681827000	2.607967000	1.913206000
1	4.385709000	1.418184000	0.817299000
1	3.275033000	2.646707000	0.195538000
6	3.835347000	0.294900000	-2.048120000
1	4.502177000	-0.247991000	-2.723608000
1	3.245790000	0.987237000	-2.653583000
1	4.454849000	0.884982000	-1.371471000
6	3.811483000	-2.058383000	-0.098450000
1	4.432155000	-2.688838000	-0.740381000
1	4.478400000	-1.492259000	0.556462000
1	3.204774000	-2.719487000	0.528215000
6	2.642359000	-0.333567000	2.767945000
1	3.534273000	-0.886977000	2.469073000
1	2.903292000	0.260600000	3.648593000
1	1.881729000	-1.054671000	3.072382000
6	1.913061000	-1.993516000	-2.459715000
1	1.509303000	-2.915409000	-2.035381000
1	1.092035000	-1.473167000	-2.959985000
1	2.644170000	-2.270900000	-3.223600000
32	-0.014939000	-1.255689000	0.409741000
6	-2.729073000	-0.488845000	0.018261000
6	-3.593227000	-0.354923000	-1.068764000
6	-3.227227000	-1.050860000	1.192968000
6	-4.915050000	-0.746766000	-0.972165000
1	-3.209004000	0.065525000	-1.992307000
6	-4.548995000	-1.452654000	1.281660000
1	-2.567220000	-1.148946000	2.049433000
6	-5.402968000	-1.298127000	0.202893000
1	-5.569854000	-0.629735000	-1.828463000
1	-4.915374000	-1.881435000	2.207745000
1	-6.438476000	-1.608556000	0.274266000
1	-0.186086000	-2.582147000	-0.367033000
1	-0.091639000	-1.577225000	1.921873000

4Ge^{P^H-H} (T.E.= -3629.196543)

6	0.886581000	0.534608000	1.489845000
6	1.436027000	0.022889000	0.112810000
1	1.150215000	-0.158528000	2.298820000
1	1.362339000	1.480015000	1.778271000

7	-1.481417000	0.175722000	0.024299000
14	2.218856000	-1.666713000	0.401468000
14	2.547110000	1.339281000	-0.647482000
6	0.910541000	-2.828698000	1.085287000
1	0.038237000	-2.922988000	0.434034000
1	1.339957000	-3.826044000	1.213468000
1	0.562527000	-2.495458000	2.066626000
6	3.589201000	-1.605711000	1.681118000
1	3.852626000	-2.629956000	1.960288000
1	4.490926000	-1.125663000	1.298310000
1	3.290039000	-1.085071000	2.593502000
6	4.114653000	1.588128000	0.350975000
1	4.821221000	0.770813000	0.187853000
1	4.602918000	2.515572000	0.040159000
1	3.918169000	1.655728000	1.423647000
6	3.056781000	0.930492000	-2.405227000
1	3.604018000	1.783601000	-2.816319000
1	3.719081000	0.064285000	-2.450341000
1	2.206586000	0.741350000	-3.064354000
6	2.941531000	-2.391777000	-1.168243000
1	3.880961000	-1.896713000	-1.426824000
1	3.160773000	-3.451694000	-1.015493000
1	2.271587000	-2.311276000	-2.027431000
6	1.621021000	2.972585000	-0.675677000
1	0.671176000	2.901306000	-1.212634000
1	1.413393000	3.344693000	0.330417000
1	2.230463000	3.725545000	-1.182724000
14	-0.988939000	0.773948000	1.571154000
6	-1.420541000	2.572335000	1.847177000
1	-1.065844000	3.191631000	1.019324000
1	-2.500998000	2.710776000	1.937013000
1	-0.961192000	2.941888000	2.768101000
6	-1.794351000	-0.242151000	2.913810000
1	-1.582709000	-1.305407000	2.774217000
1	-1.450776000	0.052220000	3.908165000
1	-2.879837000	-0.113009000	2.883385000
32	-0.087507000	-0.243375000	-1.114488000
6	-2.826202000	-0.059579000	-0.316771000
6	-3.295517000	-1.357508000	-0.517032000
6	-3.728485000	0.996727000	-0.431814000

6	-4.623611000	-1.589610000	-0.826113000
1	-2.600486000	-2.185182000	-0.412003000
6	-5.059727000	0.760312000	-0.729626000
1	-3.363923000	2.009372000	-0.293850000
6	-5.514033000	-0.532501000	-0.930841000
1	-4.968592000	-2.606544000	-0.976219000
1	-5.745920000	1.595637000	-0.813234000
1	-6.555074000	-0.716074000	-1.168793000
1	-0.130657000	0.713066000	-2.333599000
1	-0.252657000	-1.684413000	-1.658289000

5Ge^{P^H-H} (T.E.= -3373.253489)

6	0.567280000	-0.357999000	1.538804000
6	1.272130000	-0.073588000	0.187880000
1	0.738027000	-1.386112000	1.884313000
1	0.948904000	0.266869000	2.352948000
7	-1.492242000	-0.136982000	0.293338000
14	2.482681000	-1.473216000	-0.185974000
14	1.973715000	1.684500000	0.212429000
6	1.528911000	-3.081314000	-0.356890000
1	0.997552000	-3.131439000	-1.309755000
1	2.224380000	-3.923772000	-0.321534000
1	0.795629000	-3.227418000	0.440471000
6	3.711647000	-1.679899000	1.211316000
1	4.255483000	-2.618753000	1.078074000
1	4.445287000	-0.872908000	1.239454000
1	3.220982000	-1.720312000	2.186812000
6	3.407286000	1.813183000	1.409518000
1	4.303535000	1.333860000	1.008821000
1	3.644285000	2.866314000	1.581528000
1	3.186275000	1.359063000	2.378191000
6	2.569263000	2.244159000	-1.472852000
1	2.815282000	3.308289000	-1.417371000
1	3.469104000	1.716192000	-1.792556000
1	1.812536000	2.126172000	-2.251793000
6	3.398823000	-1.167612000	-1.788945000
1	4.142629000	-0.374314000	-1.687841000
1	3.923298000	-2.076566000	-2.094048000
1	2.718415000	-0.891381000	-2.600215000
6	0.630334000	2.865529000	0.777338000

1	-0.238208000	2.865093000	0.113234000
1	0.278124000	2.645858000	1.787852000
1	1.035266000	3.881202000	0.785514000
6	-2.891119000	-0.089280000	0.091315000
6	-3.734070000	-1.012893000	0.698756000
6	-3.429435000	0.874121000	-0.752212000
6	-5.095210000	-0.965783000	0.462226000
1	-3.315177000	-1.761657000	1.358906000
6	-4.792439000	0.911472000	-0.991263000
1	-2.772425000	1.605875000	-1.211746000
6	-5.630625000	-0.007304000	-0.383997000
1	-5.744510000	-1.689076000	0.941915000
1	-5.199895000	1.668837000	-1.650882000
1	-6.698056000	0.023336000	-0.567446000
6	-0.945146000	-0.205051000	1.548206000
8	-1.571826000	-0.178350000	2.584360000
32	-0.216876000	-0.088858000	-1.078254000
1	-0.415932000	-1.318782000	-1.984490000
1	-0.405781000	1.190235000	-1.918054000

8Ge^{P^H-H} (T.E.= -2941.858049)

6	-0.528667000	1.712614000	0.148492000
6	0.926381000	1.622611000	0.593230000
6	1.517113000	0.336396000	0.052128000
1	-1.064236000	2.447825000	0.760973000
1	-0.576034000	2.061771000	-0.896246000
1	0.954114000	1.674833000	1.693235000
1	1.459820000	2.510505000	0.230857000
32	0.139614000	-0.950108000	0.109402000
7	-1.143834000	0.404957000	0.285499000
15	3.149817000	0.065573000	-0.132251000
6	3.979238000	1.265850000	-1.204111000
1	3.821530000	2.269720000	-0.805436000
1	5.052800000	1.075323000	-1.257064000
1	3.542790000	1.216622000	-2.201870000
6	3.457499000	-1.554004000	-0.852907000
1	3.090477000	-2.331562000	-0.180406000
1	2.938986000	-1.634210000	-1.808795000
1	4.527897000	-1.699181000	-1.005421000
6	4.197933000	0.109968000	1.354674000

1	5.254597000	-0.032911000	1.117082000
1	4.072234000	1.080045000	1.841021000
1	3.869853000	-0.666064000	2.047812000
6	-2.493744000	0.243774000	0.094410000
6	-3.070116000	-1.034537000	0.184010000
6	-3.354789000	1.315660000	-0.184704000
6	-4.424348000	-1.225665000	0.011887000
1	-2.435795000	-1.887424000	0.408382000
6	-4.713660000	1.109144000	-0.352641000
1	-2.959289000	2.319152000	-0.276810000
6	-5.266554000	-0.155561000	-0.258009000
1	-4.830105000	-2.228530000	0.091786000
1	-5.349150000	1.961821000	-0.567840000
1	-6.330524000	-0.307654000	-0.392194000
1	0.008747000	-1.913008000	1.324609000
1	-0.114505000	-1.809402000	-1.158019000

9Ge^{P^H-H} (T.E.= -2940.671599)

6	0.468222000	1.668971000	0.145771000
6	-0.875607000	1.636343000	0.109440000
6	-1.527468000	0.340059000	0.019899000
7	1.138357000	0.436781000	0.103020000
15	-3.182974000	0.100892000	-0.032054000
6	-4.108818000	0.702770000	1.404025000
1	-3.898102000	1.766472000	1.533225000
1	-5.184501000	0.566270000	1.275484000
1	-3.771337000	0.175165000	2.296544000
6	-3.565097000	-1.650375000	-0.167926000
1	-4.645509000	-1.796748000	-0.201847000
1	-3.121054000	-2.053281000	-1.079531000
1	-3.161417000	-2.183839000	0.694243000
6	-4.037310000	0.911237000	-1.407903000
1	-3.656202000	0.515988000	-2.349905000
1	-5.118014000	0.764913000	-1.352845000
1	-3.821173000	1.980972000	-1.371292000
32	-0.134012000	-0.945165000	0.011102000
6	2.503437000	0.284133000	0.040308000
6	3.060101000	-1.003378000	0.087264000
6	3.392532000	1.363609000	-0.073283000
6	4.424344000	-1.200018000	0.026256000

1	2.405494000	-1.864668000	0.184574000
6	4.757449000	1.152124000	-0.130391000
1	3.015329000	2.376459000	-0.129249000
6	5.293192000	-0.124722000	-0.081949000
1	4.813628000	-2.211580000	0.067219000
1	5.415393000	2.010152000	-0.219690000
1	6.364199000	-0.278769000	-0.128630000
1	1.042922000	2.578573000	0.240727000
1	-1.442818000	2.561634000	0.159315000
1	0.112650000	-1.802036000	-1.261218000
1	0.005152000	-1.915750000	1.218223000

$^{14}\text{Ge}^{\text{H-H}}$ (T.E.= -3136.029186)

6	1.152161000	1.170953000	0.111620000
6	1.656061000	-0.161850000	0.004864000
7	-1.055187000	-0.066553000	-0.203169000
6	-2.383893000	-0.436255000	0.032436000
6	-3.128458000	0.162635000	1.051274000
6	-4.433067000	-0.222873000	1.294063000
6	-5.025252000	-1.226864000	0.543023000
6	-4.290611000	-1.840761000	-0.457448000
6	-2.987557000	-1.449638000	-0.712273000
1	-2.662945000	0.934308000	1.655141000
1	-4.990517000	0.259156000	2.089625000
1	-6.046585000	-1.530070000	0.739703000
1	-4.736852000	-2.628929000	-1.053639000
1	-2.424545000	-1.919314000	-1.513445000
5	-0.452468000	1.243934000	-0.133858000
7	-1.143141000	2.452994000	-0.358196000
6	-0.588648000	3.757972000	-0.068496000
1	-0.547548000	4.371685000	-0.977135000
1	-1.222698000	4.289631000	0.652897000
1	0.416946000	3.658422000	0.333612000
6	-2.472346000	2.548411000	-0.911858000
1	-3.210132000	2.862462000	-0.161058000
1	-2.483110000	3.295550000	-1.713659000
1	-2.802866000	1.599165000	-1.329537000
15	3.337511000	-0.386195000	0.148119000
6	4.013308000	0.059051000	1.757066000
1	5.096250000	-0.077793000	1.774414000

1	3.768318000	1.103608000	1.948832000
1	3.551721000	-0.563030000	2.524402000
6	4.312518000	0.542703000	-1.046718000
1	5.379574000	0.389655000	-0.874706000
1	4.051721000	0.218204000	-2.054455000
1	4.062838000	1.597591000	-0.933799000
6	3.749141000	-2.118653000	-0.104584000
1	3.244032000	-2.730152000	0.645093000
1	3.420958000	-2.431156000	-1.097380000
1	4.826540000	-2.268242000	-0.020287000
8	1.898276000	2.145305000	0.337378000
32	0.252671000	-1.401511000	-0.283707000
1	0.234302000	-2.134753000	-1.649644000
1	-0.049261000	-2.450891000	0.813860000

Cartesian coordinates of the N – H splitting product obtained for CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**), CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**) and NacNacSi (**IIa**), along with their total energies (in hartrees) including zero point vibrational correction.

1SiP^{N-H} (T.E.= -1567.109882)

6	-0.882387000	-0.323867000	-1.707073000
6	0.597212000	0.033376000	-1.759228000
6	1.183683000	0.074567000	-0.321434000
1	-1.388308000	0.000931000	-2.624100000
1	-1.014880000	-1.414214000	-1.647830000
1	0.687641000	1.019843000	-2.228632000
1	1.136837000	-0.664111000	-2.408178000
7	-1.452784000	0.340926000	-0.547788000
14	-0.214878000	0.957314000	0.531633000
14	1.378775000	-1.675753000	0.374864000
14	2.763685000	1.101855000	-0.275395000
6	3.135358000	1.745503000	1.444114000
1	3.218819000	0.960594000	2.196106000
1	4.084161000	2.289063000	1.419454000
1	2.364783000	2.446902000	1.774194000
6	2.585335000	2.607033000	-1.383617000
1	1.687763000	3.188294000	-1.158457000
1	3.450323000	3.257017000	-1.223765000
1	2.564607000	2.345369000	-2.443884000
6	4.244298000	0.151015000	-0.924961000

1	5.102747000	0.824802000	-0.993863000
1	4.530558000	-0.688511000	-0.288019000
1	4.046852000	-0.235460000	-1.928885000
6	2.431103000	-1.709060000	1.924403000
1	2.459940000	-2.736801000	2.297330000
1	3.462326000	-1.392636000	1.755085000
1	2.006103000	-1.080730000	2.710454000
6	-0.250645000	-2.509986000	0.827872000
1	-0.905760000	-1.931205000	1.481436000
1	-0.835033000	-2.769088000	-0.058100000
1	-0.014954000	-3.445559000	1.344391000
6	2.154022000	-2.797536000	-0.912840000
1	3.093803000	-2.407843000	-1.307744000
1	2.358083000	-3.770703000	-0.457499000
1	1.476311000	-2.968339000	-1.753081000
6	-2.819494000	0.282266000	-0.336835000
6	-3.647190000	-0.562920000	-1.084175000
6	-3.422862000	1.081453000	0.643599000
6	-5.010827000	-0.609754000	-0.847572000
1	-3.223624000	-1.193275000	-1.855602000
6	-4.781969000	1.022984000	0.872439000
1	-2.811740000	1.764318000	1.223197000
6	-5.592559000	0.175187000	0.130958000
1	-5.624793000	-1.275913000	-1.443960000
1	-5.216712000	1.657946000	1.636642000
1	-6.659988000	0.135186000	0.310427000
1	-0.120185000	2.436984000	0.456821000
7	-0.424020000	0.673733000	2.199444000
1	-0.635931000	-0.218738000	2.612465000
1	-0.666716000	1.433863000	2.812673000

2SiP^{N-H} (T.E.= -1565.916803)

6	-1.170802000	-0.069797000	-0.266610000
6	-0.521655000	0.025404000	-1.628297000
6	0.805523000	-0.125516000	-1.678906000
1	-1.102637000	0.215982000	-2.524239000
1	1.395879000	-0.068624000	-2.586362000
14	0.231152000	-0.800101000	0.736382000
7	1.457358000	-0.435382000	-0.482689000
14	-2.636904000	-1.253091000	-0.260262000

14	-1.545656000	1.718101000	0.233223000
6	-4.150995000	-0.512842000	-1.078624000
1	-4.932651000	-1.273870000	-1.150552000
1	-4.556909000	0.329990000	-0.514451000
1	-3.928699000	-0.168618000	-2.092181000
6	-3.077378000	-1.746189000	1.492978000
1	-3.912740000	-2.451311000	1.472186000
1	-2.242868000	-2.239918000	1.997172000
1	-3.377651000	-0.890814000	2.101311000
6	-2.168677000	-2.784817000	-1.230109000
1	-2.977197000	-3.519512000	-1.189788000
1	-1.988985000	-2.539772000	-2.279693000
1	-1.264274000	-3.257679000	-0.839782000
6	-2.569691000	1.816020000	1.798711000
1	-2.636839000	2.856155000	2.128875000
1	-3.589568000	1.457742000	1.635467000
1	-2.128844000	1.230175000	2.608433000
6	0.048051000	2.686026000	0.469207000
1	0.587033000	2.450939000	1.388371000
1	0.730753000	2.525959000	-0.369397000
1	-0.193226000	3.752131000	0.499955000
6	-2.458821000	2.611441000	-1.137869000
1	-3.418644000	2.157507000	-1.385936000
1	-2.649195000	3.638888000	-0.814429000
1	-1.857053000	2.660348000	-2.048033000
6	2.833060000	-0.300661000	-0.327295000
6	3.503438000	-1.057238000	0.636350000
6	3.575305000	0.591948000	-1.102943000
6	4.866923000	-0.925092000	0.814027000
1	2.945639000	-1.769461000	1.235740000
6	4.942446000	0.707504000	-0.926172000
1	3.071510000	1.214747000	-1.833847000
6	5.599889000	-0.045717000	0.031993000
1	5.364987000	-1.527237000	1.565693000
1	5.497859000	1.407940000	-1.539994000
1	6.669957000	0.051220000	0.169018000
1	0.135779000	-2.265039000	0.953487000
7	0.514772000	-0.200190000	2.301451000
1	0.714646000	0.761333000	2.520028000
1	0.819063000	-0.821769000	3.032180000

3SiP^{N-H} (T.E.= -1687.213007)

6	-0.717535000	0.978083000	-1.064563000
6	-1.404509000	-0.040507000	-0.089328000
1	-0.819143000	0.642697000	-2.106785000
1	-1.218835000	1.952469000	-1.038802000
14	0.007779000	-1.116975000	0.488941000
7	1.311131000	-0.054358000	0.008698000
5	0.833466000	1.088571000	-0.729776000
7	1.614342000	2.208664000	-1.098606000
6	1.138503000	3.213021000	-2.018780000
1	1.024981000	4.187845000	-1.526452000
1	1.848208000	3.348566000	-2.844478000
1	0.178653000	2.933055000	-2.449375000
6	2.924505000	2.533360000	-0.585945000
1	2.941157000	3.576658000	-0.248802000
1	3.189556000	1.906409000	0.263417000
1	3.706578000	2.422917000	-1.348919000
14	-2.758018000	-1.015413000	-0.957381000
14	-1.990408000	0.937960000	1.418668000
6	-2.129712000	-1.635408000	-2.618393000
1	-1.152090000	-2.116713000	-2.555972000
1	-2.835960000	-2.371404000	-3.012640000
1	-2.061856000	-0.826391000	-3.349508000
6	-4.244896000	0.060682000	-1.349056000
1	-4.889432000	-0.453964000	-2.067020000
1	-4.842237000	0.274448000	-0.459556000
1	-3.941102000	1.012783000	-1.792318000
6	-3.108065000	2.376946000	0.964411000
1	-4.054645000	2.065491000	0.521449000
1	-3.333883000	2.925899000	1.883673000
1	-2.626099000	3.078189000	0.279758000
6	-2.927564000	-0.137210000	2.634852000
1	-3.032162000	0.396571000	3.583322000
1	-3.934216000	-0.359666000	2.271849000
1	-2.422444000	-1.084605000	2.835712000
6	-3.356838000	-2.484997000	0.038938000
1	-3.882042000	-2.182204000	0.946401000
1	-4.055596000	-3.067387000	-0.568364000
1	-2.530314000	-3.140169000	0.321059000
6	-0.531595000	1.727928000	2.305015000

1	0.206391000	1.005524000	2.659462000
1	-0.015774000	2.446205000	1.660952000
1	-0.907628000	2.277479000	3.172932000
6	2.647011000	-0.472800000	0.167755000
6	3.451745000	-0.709502000	-0.943790000
6	3.180085000	-0.687190000	1.435527000
6	4.764100000	-1.117506000	-0.789265000
1	3.030477000	-0.557403000	-1.932634000
6	4.492019000	-1.103442000	1.587291000
1	2.558203000	-0.502682000	2.305292000
6	5.292493000	-1.314698000	0.477084000
1	5.378308000	-1.289668000	-1.665931000
1	4.892953000	-1.256423000	2.582943000
1	6.320407000	-1.635847000	0.596726000
1	0.000206000	-1.378547000	1.950306000
7	0.176800000	-2.694131000	-0.159424000
1	0.427531000	-2.860228000	-1.121165000
1	0.519194000	-3.432531000	0.433977000

4SiP^{N-H} (T.E. = -1897.121360)

6	-0.916608000	0.245561000	1.566556000
6	-1.368335000	0.046175000	0.072294000
1	-1.345886000	1.156158000	2.001314000
1	-1.291119000	-0.561605000	2.206875000
14	0.145952000	-0.049522000	-1.043178000
7	1.425400000	-0.006220000	0.119871000
14	-2.313489000	1.584911000	-0.473040000
14	-2.372152000	-1.548426000	0.023500000
6	-1.252898000	3.102247000	-0.140703000
1	-0.276230000	3.054263000	-0.629266000
1	-1.769625000	3.988654000	-0.519259000
1	-1.088860000	3.255009000	0.929120000
6	-3.902652000	1.825870000	0.496006000
1	-4.271239000	2.842183000	0.331151000
1	-4.683174000	1.135296000	0.169060000
1	-3.762523000	1.693297000	1.571542000
6	-3.166131000	-1.909472000	-1.633580000
1	-2.473582000	-1.784970000	-2.466688000
1	-3.534710000	-2.939061000	-1.640061000
1	-4.026347000	-1.255323000	-1.797971000

6	-1.263035000	-2.980633000	0.544690000
1	-1.819491000	-3.918363000	0.459609000
1	-0.343148000	-3.088125000	-0.034555000
1	-0.973806000	-2.873658000	1.594139000
6	-2.768770000	1.548658000	-2.291950000
1	-3.590400000	0.856114000	-2.483962000
1	-3.100995000	2.545388000	-2.595599000
1	-1.934206000	1.266050000	-2.936606000
6	-3.770620000	-1.545406000	1.279006000
1	-3.452106000	-1.262453000	2.284340000
1	-4.587107000	-0.883338000	0.985300000
1	-4.174243000	-2.560874000	1.336948000
14	0.958246000	0.290552000	1.760462000
6	1.598800000	-1.043499000	2.898531000
1	1.269948000	-2.031069000	2.565070000
1	2.691700000	-1.042249000	2.921024000
1	1.246102000	-0.892547000	3.921781000
6	1.586960000	1.942603000	2.359910000
1	1.237552000	2.750573000	1.712026000
1	1.241324000	2.147492000	3.376378000
1	2.679757000	1.965429000	2.370398000
6	2.776920000	-0.037333000	-0.289230000
6	3.496836000	-1.228132000	-0.260859000
6	3.410778000	1.120680000	-0.732508000
6	4.822784000	-1.258143000	-0.657567000
1	2.993319000	-2.128592000	0.078328000
6	4.735904000	1.087926000	-1.131113000
1	2.843116000	2.046465000	-0.755370000
6	5.447370000	-0.100417000	-1.093366000
1	5.371145000	-2.192980000	-0.628765000
1	5.216442000	1.997960000	-1.472386000
1	6.485008000	-0.124430000	-1.404567000
1	0.283605000	1.105334000	-1.967292000
7	0.203749000	-1.353454000	-2.151186000
1	0.647523000	-1.209675000	-3.043881000
1	0.224595000	-2.323947000	-1.884096000

5SiP^{N-H} (T.E.= -1641.178299)

6	0.591713000	-0.076399000	1.583613000
6	1.220482000	-0.005512000	0.167092000

1	0.799598000	-1.030522000	2.084725000
1	0.983944000	0.681333000	2.270614000
14	-0.253008000	-0.079025000	-0.972269000
7	-1.444755000	0.008051000	0.323868000
14	2.397973000	-1.464850000	-0.032304000
14	1.990481000	1.710669000	-0.063195000
6	1.423002000	-3.076669000	0.067056000
1	0.470774000	-2.972422000	0.594929000
1	1.217474000	-3.466299000	-0.932305000
1	2.004090000	-3.834991000	0.596861000
6	3.644006000	-1.508893000	1.369860000
1	4.166405000	-2.469179000	1.341030000
1	4.395288000	-0.722038000	1.289513000
1	3.172590000	-1.424141000	2.352048000
6	3.441909000	1.970702000	1.092091000
1	4.324925000	1.426920000	0.749121000
1	3.696397000	3.033725000	1.113814000
1	3.229908000	1.658562000	2.117310000
6	2.590877000	1.993408000	-1.814575000
1	2.845478000	3.049873000	-1.935399000
1	3.486505000	1.409992000	-2.033944000
1	1.836324000	1.747897000	-2.564867000
6	3.334379000	-1.416158000	-1.649856000
1	4.118015000	-0.655152000	-1.638308000
1	3.816777000	-2.382045000	-1.821443000
1	2.673058000	-1.216045000	-2.496087000
6	0.693797000	3.005459000	0.344003000
1	-0.143440000	2.988445000	-0.358069000
1	0.288477000	2.889288000	1.352350000
1	1.150800000	3.997107000	0.287354000
6	-2.845544000	0.016467000	0.109246000
6	-3.656933000	-0.956816000	0.677342000
6	-3.405250000	0.982997000	-0.714658000
6	-5.015777000	-0.957195000	0.422130000
1	-3.214338000	-1.709038000	1.319457000
6	-4.765217000	0.972520000	-0.974724000
1	-2.766002000	1.748882000	-1.142095000
6	-5.574229000	0.003766000	-0.406402000
1	-5.643985000	-1.717868000	0.870904000
1	-5.193818000	1.730728000	-1.619777000

1	-6.639047000	-0.002895000	-0.607001000
6	-0.918066000	0.050880000	1.594116000
8	-1.557909000	0.156741000	2.614400000
1	-0.415905000	1.077738000	-1.877146000
7	-0.447322000	-1.405423000	-2.018548000
1	-0.899934000	-1.275529000	-2.908603000
1	-0.503704000	-2.361109000	-1.706688000

8SiP^{N-H} (T.E.= -1209.788604)

6	-0.496679000	-1.726241000	0.098518000
6	0.969864000	-1.715548000	-0.314118000
6	1.500671000	-0.314380000	-0.068923000
1	-1.035084000	-2.543159000	-0.395969000
1	-0.575121000	-1.897739000	1.184538000
1	1.041945000	-2.012174000	-1.371706000
1	1.506833000	-2.484675000	0.256804000
14	0.143668000	0.839159000	-0.248352000
7	-1.078141000	-0.442242000	-0.264064000
15	3.139918000	-0.008078000	-0.001166000
6	4.005430000	-0.817428000	1.370044000
1	3.825182000	-1.892995000	1.318243000
1	5.081708000	-0.638044000	1.327884000
1	3.604553000	-0.444783000	2.313211000
6	4.108386000	-0.564196000	-1.432427000
1	3.762442000	-0.042685000	-2.325754000
1	5.176608000	-0.386717000	-1.292207000
1	3.943933000	-1.634960000	-1.573023000
6	3.502038000	1.744803000	0.164177000
1	3.080797000	2.288551000	-0.682610000
1	3.058780000	2.131246000	1.081599000
1	4.582632000	1.894668000	0.186760000
6	-2.440241000	-0.257870000	-0.153811000
6	-3.297984000	-1.234978000	0.368669000
6	-3.022377000	0.950437000	-0.571751000
6	-4.660376000	-1.006386000	0.468406000
1	-2.897492000	-2.181076000	0.709812000
6	-4.379722000	1.166502000	-0.464326000
1	-2.391297000	1.717455000	-1.008727000
6	-5.218152000	0.191462000	0.059234000
1	-5.293818000	-1.785078000	0.880116000

1	-4.792043000	2.111120000	-0.802899000
1	-6.284566000	0.363426000	0.140236000
1	-0.011757000	1.662963000	-1.478027000
7	0.023181000	2.026923000	0.987198000
1	-0.586322000	2.821797000	0.869317000
1	0.051538000	1.735980000	1.952741000

9SiP^{N-H} (T.E.= -1208.600264)

6	0.475033000	-1.596093000	0.570583000
6	-0.860481000	-1.625629000	0.421595000
6	-1.468150000	-0.403001000	-0.083579000
14	-0.145017000	0.819759000	-0.214270000
7	1.091546000	-0.372319000	0.242785000
15	-3.121665000	-0.128805000	-0.154665000
6	-4.046124000	-1.471357000	-0.930864000
1	-3.840943000	-2.399643000	-0.394291000
1	-5.119763000	-1.276992000	-0.906293000
1	-3.712936000	-1.587322000	-1.962247000
6	-3.484540000	1.368452000	-1.079204000
1	-4.556773000	1.569439000	-1.070860000
1	-2.955041000	2.203721000	-0.616194000
1	-3.139352000	1.256136000	-2.107393000
6	-3.970820000	0.091964000	1.432830000
1	-3.555622000	0.970639000	1.929784000
1	-5.048695000	0.215922000	1.307772000
1	-3.777757000	-0.781956000	2.058014000
6	2.460071000	-0.243122000	0.083964000
6	3.314611000	-1.344808000	-0.043633000
6	3.035535000	1.033241000	0.028925000
6	4.675467000	-1.167915000	-0.215251000
1	2.904417000	-2.347007000	-0.036269000
6	4.393613000	1.197749000	-0.156378000
1	2.402058000	1.904898000	0.155345000
6	5.231321000	0.099448000	-0.276734000
1	5.310300000	-2.041867000	-0.314812000
1	4.804794000	2.200726000	-0.195159000
1	6.297965000	0.229491000	-0.413588000
1	1.074627000	-2.397493000	0.978953000
1	-1.435722000	-2.504228000	0.698234000
1	0.256070000	1.413852000	-1.514537000

7	-0.392373000	2.227021000	0.745557000
1	0.129682000	3.071505000	0.564430000
1	-0.609523000	2.139128000	1.726933000

14SiP^{N-H} (T.E.= -1403.959159)

6	1.191949000	1.176415000	0.086232000
6	1.650449000	-0.168035000	-0.099187000
7	-0.979442000	-0.067620000	-0.269821000
6	-2.315511000	-0.462262000	-0.091256000
6	-3.035383000	-0.058902000	1.033172000
6	-4.343645000	-0.464788000	1.218544000
6	-4.957909000	-1.301895000	0.299208000
6	-4.244937000	-1.725984000	-0.809197000
6	-2.938688000	-1.309781000	-1.005652000
1	-2.549288000	0.583918000	1.759821000
1	-4.886584000	-0.132300000	2.096353000
1	-5.982364000	-1.621798000	0.447960000
1	-4.711538000	-2.380549000	-1.536990000
1	-2.389551000	-1.623948000	-1.887346000
5	-0.417486000	1.256739000	-0.112181000
7	-1.135485000	2.464542000	-0.208160000
6	-0.580486000	3.746103000	0.172831000
1	-0.583327000	4.437767000	-0.678758000
1	-1.188265000	4.203071000	0.964444000
1	0.442187000	3.624805000	0.522981000
6	-2.489118000	2.592483000	-0.693028000
1	-3.192985000	2.836902000	0.113887000
1	-2.540346000	3.403812000	-1.428169000
1	-2.832977000	1.679723000	-1.175455000
15	3.325859000	-0.457293000	-0.001370000
6	4.034867000	-0.130263000	1.622059000
1	5.113581000	-0.297699000	1.614746000
1	3.823367000	0.905977000	1.885775000
1	3.565887000	-0.788427000	2.354466000
6	4.306484000	0.521183000	-1.150666000
1	5.371505000	0.329852000	-1.006841000
1	4.022026000	0.265966000	-2.171909000
1	4.085493000	1.573116000	-0.969300000
6	3.689946000	-2.178319000	-0.366885000
1	3.157161000	-2.822541000	0.334099000

1	3.355098000	-2.412214000	-1.378836000
1	4.763121000	-2.359842000	-0.290415000
8	1.951764000	2.131071000	0.336910000
14	0.273492000	-1.299273000	-0.384383000
1	0.203244000	-1.998714000	-1.692443000
7	0.148215000	-2.589249000	0.740807000
1	-0.443346000	-3.377420000	0.524719000
1	0.113322000	-2.381948000	1.727922000

1GeP^{N-H} (T.E.= -3354.538974)

6	-0.877662000	0.532786000	1.683984000
6	0.604647000	0.188049000	1.736172000
6	1.219596000	0.106857000	0.312574000
1	-1.349196000	0.285093000	2.643245000
1	-1.016603000	1.616237000	1.542210000
1	0.706283000	-0.780251000	2.241382000
1	1.134274000	0.915109000	2.361498000
32	-0.202476000	-0.882698000	-0.581084000
7	-1.487712000	-0.218193000	0.607358000
14	1.324522000	1.824142000	-0.493672000
14	2.861181000	-0.829038000	0.336831000
6	2.791371000	-2.257063000	1.549225000
1	1.979265000	-2.949190000	1.319459000
1	3.730406000	-2.813247000	1.477250000
1	2.685795000	-1.923918000	2.584049000
6	3.277895000	-1.545430000	-1.341311000
1	3.370794000	-0.793460000	-2.125360000
1	4.230910000	-2.077907000	-1.277944000
1	2.514477000	-2.268345000	-1.640714000
6	4.258157000	0.275382000	0.930752000
1	4.019533000	0.710837000	1.905383000
1	5.163604000	-0.325513000	1.052243000
1	4.491110000	1.090743000	0.243216000
6	2.405647000	1.800173000	-2.023751000
1	2.027185000	1.085455000	-2.759815000
1	2.370278000	2.791936000	-2.483271000
1	3.452359000	1.564213000	-1.824589000
6	-0.332578000	2.485581000	-1.089996000
1	-1.070087000	2.611830000	-0.295242000
1	-0.152362000	3.471629000	-1.529600000

1	-0.782798000	1.864491000	-1.868067000
6	1.993161000	3.075732000	0.731006000
1	1.304112000	3.238822000	1.563288000
1	2.961666000	2.791418000	1.145514000
1	2.116593000	4.034801000	0.220191000
6	-2.838630000	-0.107739000	0.364438000
6	-3.432175000	-0.828055000	-0.683340000
6	-3.672451000	0.709476000	1.138866000
6	-4.783077000	-0.731664000	-0.942059000
1	-2.818749000	-1.484342000	-1.293239000
6	-5.028287000	0.794470000	0.870183000
1	-3.258560000	1.284422000	1.957501000
6	-5.599379000	0.081288000	-0.168311000
1	-5.206396000	-1.304839000	-1.759653000
1	-5.645729000	1.436298000	1.489465000
1	-6.660673000	0.152926000	-0.371926000
1	-0.506088000	-0.555002000	-2.056728000
7	-0.070003000	-2.716112000	-0.505987000
1	-0.641887000	-3.189211000	-1.193371000
1	-0.283537000	-3.105055000	0.403898000

2GeP^{N-H} (T.E.= -3353.346546)

6	-1.235213000	0.029366000	-0.347424000
6	-0.538196000	0.192528000	-1.677514000
6	0.789833000	0.033268000	-1.737515000
1	-1.103429000	0.445300000	-2.568409000
1	1.358331000	0.155321000	-2.653161000
32	0.196985000	-0.794749000	0.714953000
7	1.474483000	-0.361990000	-0.597561000
14	-2.690725000	-1.163336000	-0.442142000
14	-1.588108000	1.784812000	0.266915000
6	-3.201724000	-1.706274000	1.278341000
1	-4.016139000	-2.431977000	1.205729000
1	-2.383136000	-2.191038000	1.817628000
1	-3.555073000	-0.870684000	1.885585000
6	-2.580882000	2.747751000	-0.995797000
1	-3.590627000	2.358427000	-1.129583000
1	-2.664524000	3.785067000	-0.659484000
1	-2.085164000	2.756964000	-1.969049000
6	-2.538695000	1.783971000	1.883973000

1	-2.092174000	1.133041000	2.639266000
1	-2.570956000	2.798004000	2.291398000
1	-3.571821000	1.460412000	1.733084000
6	0.019304000	2.734674000	0.465929000
1	0.762370000	2.275924000	1.120898000
1	0.489997000	2.865198000	-0.511713000
1	-0.204023000	3.729957000	0.860358000
6	-4.170543000	-0.402478000	-1.300983000
1	-4.927831000	-1.172142000	-1.472218000
1	-4.629988000	0.389945000	-0.705876000
1	-3.898326000	0.018893000	-2.272151000
6	-2.162313000	-2.664771000	-1.427710000
1	-2.958131000	-3.414022000	-1.434550000
1	-1.947571000	-2.392424000	-2.463603000
1	-1.264788000	-3.133577000	-1.016156000
6	2.844464000	-0.205975000	-0.444873000
6	3.531577000	-0.966926000	0.504587000
6	3.573400000	0.706315000	-1.212416000
6	4.894967000	-0.827448000	0.669269000
1	2.984132000	-1.681495000	1.110444000
6	4.941652000	0.829143000	-1.047643000
1	3.059703000	1.337985000	-1.928175000
6	5.615269000	0.066918000	-0.108648000
1	5.403529000	-1.432710000	1.411397000
1	5.484497000	1.544252000	-1.656007000
1	6.685710000	0.170769000	0.020099000
1	0.146638000	-2.327238000	0.920646000
7	0.676395000	-0.149378000	2.350300000
1	0.445966000	0.801143000	2.595073000
1	0.489414000	-0.768774000	3.124577000

3GeP^{N-H} (T.E.= -3474.641981)

6	0.694019000	1.321035000	-0.824931000
6	1.438249000	0.099967000	-0.189553000
1	1.191738000	2.256711000	-0.546882000
1	0.765949000	1.285764000	-1.921910000
7	-1.374297000	0.045302000	-0.096148000
5	-0.857452000	1.336936000	-0.448604000
7	-1.609390000	2.538994000	-0.442928000
6	-1.122418000	3.771453000	-1.011623000

1	-1.843269000	4.176961000	-1.733021000
1	-0.970306000	4.539326000	-0.240985000
1	-0.180246000	3.622547000	-1.536458000
6	-2.903298000	2.709320000	0.172670000
1	-3.700836000	2.855942000	-0.568223000
1	-3.166952000	1.850808000	0.787809000
1	-2.891667000	3.594496000	0.820382000
14	2.017571000	0.619619000	1.529707000
14	2.771280000	-0.582956000	-1.328634000
6	0.552601000	1.094847000	2.612460000
1	-0.201948000	0.313657000	2.727276000
1	0.923314000	1.355953000	3.607895000
1	0.042535000	1.976073000	2.211446000
6	3.083705000	2.163526000	1.473320000
1	3.341849000	2.430175000	2.502621000
1	4.014621000	2.018104000	0.924180000
1	2.560757000	3.018108000	1.038681000
6	4.262432000	0.548425000	-1.422168000
1	4.907590000	0.241711000	-2.249813000
1	3.959599000	1.584078000	-1.599497000
1	4.859213000	0.520901000	-0.507552000
6	3.326576000	-2.291742000	-0.795349000
1	4.059206000	-2.670761000	-1.513404000
1	3.792978000	-2.296050000	0.191057000
1	2.494068000	-3.000213000	-0.771745000
6	3.013650000	-0.713460000	2.388360000
1	4.000867000	-0.820237000	1.931481000
1	3.166385000	-0.432279000	3.434029000
1	2.518507000	-1.686711000	2.360921000
6	2.085150000	-0.738065000	-3.070406000
1	1.118131000	-1.247215000	-3.092236000
1	1.966555000	0.232934000	-3.556104000
1	2.781851000	-1.323788000	-3.676455000
32	0.007429000	-1.217783000	-0.032474000
6	-2.707258000	-0.392178000	-0.089895000
6	-3.525815000	-0.209427000	-1.203838000
6	-3.238105000	-1.042728000	1.023121000
6	-4.838965000	-0.642186000	-1.194122000
1	-3.112903000	0.287545000	-2.075828000
6	-4.549953000	-1.485455000	1.025209000

1	-2.608124000	-1.174748000	1.896670000
6	-5.359194000	-1.283985000	-0.080512000
1	-5.460520000	-0.484062000	-2.068325000
1	-4.945441000	-1.983029000	1.903755000
1	-6.387530000	-1.625035000	-0.075934000
1	-0.206304000	-2.225808000	-1.188101000
7	0.061527000	-2.295346000	1.452856000
1	-0.000620000	-1.837075000	2.351826000
1	-0.596563000	-3.062440000	1.426698000

4GeP^{N-H} (T.E.= -3684.548930)

6	0.919969000	0.837467000	1.421254000
6	1.432125000	0.028471000	0.181763000
1	1.131322000	0.303249000	2.356220000
1	1.454486000	1.789035000	1.527338000
7	-1.490258000	0.108128000	0.184904000
14	2.023535000	-1.649827000	0.830903000
14	2.730613000	1.031850000	-0.750981000
6	0.565610000	-2.552346000	1.600155000
1	-0.232949000	-2.774294000	0.887906000
1	0.913712000	-3.502824000	2.014083000
1	0.126996000	-1.978529000	2.420785000
6	3.309275000	-1.478579000	2.186014000
1	3.443429000	-2.458128000	2.653881000
1	4.278379000	-1.161483000	1.799360000
1	3.014540000	-0.779133000	2.970861000
6	4.280503000	1.246654000	0.285272000
1	4.873434000	0.329966000	0.318655000
1	4.903754000	2.027944000	-0.158015000
1	4.055305000	1.540947000	1.313358000
6	3.209612000	0.254019000	-2.383777000
1	3.886003000	0.930237000	-2.914205000
1	3.724991000	-0.699970000	-2.262511000
1	2.329650000	0.101171000	-3.013003000
6	2.767486000	-2.728388000	-0.509411000
1	3.758347000	-2.370226000	-0.798857000
1	2.885688000	-3.745563000	-0.125908000
1	2.150945000	-2.781051000	-1.409522000
6	2.065646000	2.751566000	-1.105903000
1	1.236418000	2.720094000	-1.815283000

1	1.729954000	3.274171000	-0.207099000
1	2.859745000	3.352672000	-1.557516000
14	-0.931751000	1.204170000	1.415533000
6	-1.186347000	3.009185000	0.982203000
1	-0.871590000	3.202946000	-0.047360000
1	-2.222280000	3.338530000	1.081914000
1	-0.575064000	3.636997000	1.637091000
6	-1.700203000	0.825041000	3.072036000
1	-1.525202000	-0.219062000	3.342407000
1	-1.255106000	1.455130000	3.846393000
1	-2.777767000	0.998952000	3.079911000
32	-0.104145000	-0.380149000	-0.972628000
6	-2.822423000	-0.176119000	-0.119269000
6	-3.180189000	-1.366536000	-0.762122000
6	-3.856035000	0.704330000	0.217672000
6	-4.500111000	-1.657268000	-1.051740000
1	-2.407606000	-2.084697000	-1.015843000
6	-5.176119000	0.403036000	-0.064095000
1	-3.618713000	1.647930000	0.696776000
6	-5.512602000	-0.777869000	-0.703985000
1	-4.739150000	-2.591932000	-1.547272000
1	-5.950413000	1.109725000	0.213633000
1	-6.546640000	-1.009655000	-0.928159000
1	-0.182703000	-1.854380000	-1.425791000
7	-0.259359000	0.560343000	-2.554303000
1	-0.873706000	0.091098000	-3.208543000
1	-0.608982000	1.502925000	-2.428582000

5GeP^{N-H} (T.E.= -3428.608397)

6	0.663752000	0.317660000	1.701251000
6	1.294443000	0.043090000	0.313914000
1	0.869251000	-0.497073000	2.407321000
1	1.060863000	1.218938000	2.177154000
7	-1.429259000	-0.192425000	0.630223000
14	2.813559000	-1.077828000	0.407953000
14	1.560341000	1.703516000	-0.562700000
6	2.472828000	-2.475890000	1.611484000
1	1.522355000	-2.978973000	1.415468000
1	3.266462000	-3.222471000	1.520969000
1	2.466027000	-2.133333000	2.648595000

6	4.332548000	-0.173958000	1.022701000
1	5.117813000	-0.899661000	1.250473000
1	4.730133000	0.525014000	0.283502000
1	4.118475000	0.384489000	1.938086000
6	2.659426000	2.835050000	0.449035000
1	3.681912000	2.468020000	0.541321000
1	2.698284000	3.804771000	-0.055881000
1	2.267882000	3.011207000	1.453329000
6	2.339524000	1.488129000	-2.249340000
1	2.312510000	2.443303000	-2.780687000
1	3.388225000	1.190286000	-2.169441000
1	1.819917000	0.743978000	-2.856876000
6	3.171156000	-1.827579000	-1.270713000
1	3.376344000	-1.072863000	-2.032115000
1	4.049000000	-2.474967000	-1.195264000
1	2.342722000	-2.444290000	-1.629935000
6	-0.066811000	2.628591000	-0.720039000
1	-0.861848000	2.099872000	-1.250427000
1	-0.452954000	2.890255000	0.269426000
1	0.118826000	3.566488000	-1.251261000
6	-2.812010000	-0.165005000	0.362579000
6	-3.434296000	-1.319781000	-0.100409000
6	-3.557650000	1.003730000	0.486639000
6	-4.776219000	-1.308417000	-0.437332000
1	-2.859216000	-2.237243000	-0.182075000
6	-4.900329000	1.005470000	0.154712000
1	-3.079526000	1.905100000	0.846949000
6	-5.516579000	-0.145541000	-0.309897000
1	-5.245669000	-2.217544000	-0.795261000
1	-5.470197000	1.922093000	0.255673000
1	-6.567935000	-0.135575000	-0.571281000
6	-0.853121000	0.461887000	1.685024000
8	-1.446394000	1.062805000	2.554749000
32	-0.151544000	-0.944912000	-0.542018000
1	-0.155902000	-2.481713000	-0.409825000
7	-0.500613000	-0.617142000	-2.299699000
1	-0.768520000	0.325909000	-2.544984000
1	-1.150136000	-1.266561000	-2.721234000

8GeP^{N-H} (T.E.= -2997.214068)

6	-0.588366000	1.838530000	0.233667000
6	0.899397000	1.756345000	0.553248000
6	1.491167000	0.568410000	-0.184756000
1	-1.094756000	2.475315000	0.969055000
1	-0.726341000	2.310826000	-0.753292000
1	1.009985000	1.678107000	1.647826000
1	1.369761000	2.704373000	0.264171000
32	0.154098000	-0.752390000	-0.258296000
7	-1.155104000	0.501742000	0.250025000
15	3.120081000	0.198643000	-0.120408000
6	4.178222000	1.514120000	-0.767573000
1	3.976158000	2.433291000	-0.213778000
1	5.235209000	1.263661000	-0.660824000
1	3.940650000	1.683648000	-1.817922000
6	3.481827000	-1.285189000	-1.068878000
1	2.933771000	-2.124078000	-0.633679000
1	3.165378000	-1.146417000	-2.102946000
1	4.550608000	-1.502086000	-1.037595000
6	3.860024000	-0.121539000	1.510823000
1	4.933619000	-0.310107000	1.441805000
1	3.693783000	0.744963000	2.154369000
1	3.366028000	-0.986392000	1.957516000
6	-2.511197000	0.329552000	0.100662000
6	-3.056545000	-0.965013000	0.074880000
6	-3.406827000	1.402217000	-0.020018000
6	-4.411449000	-1.172519000	-0.068939000
1	-2.394508000	-1.817685000	0.188348000
6	-4.766943000	1.180031000	-0.157369000
1	-3.037941000	2.419816000	-0.013832000
6	-5.287007000	-0.101541000	-0.187178000
1	-4.791715000	-2.188355000	-0.083982000
1	-5.429749000	2.034138000	-0.248847000
1	-6.352006000	-0.265674000	-0.296882000
1	-0.250962000	-1.455356000	-1.575927000
7	0.398722000	-2.172359000	0.904647000
1	0.442237000	-1.894831000	1.877384000
1	-0.270702000	-2.926417000	0.816507000

9GeP^{N-H} (T.E.= -2996.026150)

6	-0.490392000	-1.687648000	0.559716000
6	0.849146000	-1.704233000	0.434229000
6	1.497955000	-0.487667000	-0.028081000
7	-1.144121000	-0.485017000	0.266647000
15	3.155694000	-0.265666000	-0.116265000
6	4.052506000	-0.330715000	1.458478000
1	3.832528000	-1.284488000	1.942665000
1	5.131661000	-0.239781000	1.319250000
1	3.693443000	0.472130000	2.104360000
6	3.548517000	1.338048000	-0.826549000
1	4.629625000	1.471172000	-0.883329000
1	3.122248000	1.408322000	-1.828071000
1	3.124079000	2.125784000	-0.202020000
6	4.025253000	-1.498607000	-1.113616000
1	3.659585000	-1.454161000	-2.139695000
1	5.104753000	-1.336480000	-1.094962000
1	3.809077000	-2.491072000	-0.713220000
32	0.133693000	0.811020000	-0.215851000
6	-2.509785000	-0.372768000	0.104888000
6	-3.098884000	0.898761000	0.057355000
6	-3.351630000	-1.484905000	-0.027851000
6	-4.458567000	1.046861000	-0.126029000
1	-2.472078000	1.773110000	0.201055000
6	-4.714543000	-1.321763000	-0.198135000
1	-2.930737000	-2.482834000	-0.023657000
6	-5.284616000	-0.060467000	-0.253444000
1	-4.881837000	2.045227000	-0.156578000
1	-5.339761000	-2.202306000	-0.301673000
1	-6.352728000	0.058434000	-0.389151000
1	-1.071802000	-2.517350000	0.938591000
1	1.411610000	-2.593869000	0.702855000
1	-0.259687000	1.441582000	-1.574003000
7	0.123335000	2.265464000	0.915881000
1	0.693433000	2.198038000	1.746808000
1	0.238737000	3.168386000	0.478522000

14GeP^{N-H} (T.E.= -3191.385349)

6	1.155991000	1.305623000	0.079237000
6	1.658694000	-0.022326000	-0.085511000

7	-1.052072000	0.081158000	-0.280993000
6	-2.377741000	-0.312890000	-0.065524000
6	-3.086164000	0.123171000	1.055658000
6	-4.386320000	-0.291217000	1.277672000
6	-5.006649000	-1.168711000	0.401172000
6	-4.306905000	-1.624438000	-0.703446000
6	-3.009688000	-1.201033000	-0.936770000
1	-2.596065000	0.794228000	1.753463000
1	-4.917370000	0.066066000	2.153096000
1	-6.023899000	-1.495725000	0.580283000
1	-4.777305000	-2.310665000	-1.398933000
1	-2.473746000	-1.541343000	-1.817456000
5	-0.457042000	1.384859000	-0.127100000
7	-1.161209000	2.603439000	-0.232964000
6	-0.612648000	3.885833000	0.152096000
1	-0.602899000	4.575280000	-0.701477000
1	-1.232908000	4.345411000	0.932752000
1	0.404349000	3.766714000	0.517955000
6	-2.510518000	2.729195000	-0.729241000
1	-3.225172000	2.962093000	0.071803000
1	-2.559048000	3.546692000	-1.457849000
1	-2.843965000	1.818633000	-1.223508000
15	3.335010000	-0.281873000	0.065986000
6	3.989767000	0.085341000	1.703028000
1	5.070310000	-0.066912000	1.732279000
1	3.756051000	1.123362000	1.939192000
1	3.506349000	-0.565610000	2.432385000
6	4.338720000	0.685000000	-1.073204000
1	5.400774000	0.504091000	-0.897105000
1	4.084211000	0.411513000	-2.097570000
1	4.106353000	1.738126000	-0.915469000
6	3.725152000	-2.006295000	-0.254428000
1	3.185157000	-2.642346000	0.449013000
1	3.419221000	-2.265592000	-1.269432000
1	4.797935000	-2.174668000	-0.148409000
8	1.901456000	2.272544000	0.332068000
32	0.264481000	-1.256087000	-0.384759000
1	0.174771000	-2.046496000	-1.709783000
7	0.096441000	-2.540354000	0.921775000
1	-0.037341000	-2.147456000	1.845559000

1 -0.643012000 -3.210365000 0.751494000

IIa-P^{N-H} (T.E.= -1112.430200)

6 -0.012572000 2.466347000 -0.023110000
6 -1.207327000 1.848427000 0.026511000
1 -0.020696000 3.548606000 -0.054461000
14 0.026432000 -0.600327000 0.275244000
6 2.406521000 2.635621000 -0.096794000
6 1.305732000 1.864043000 -0.029813000
1 3.408826000 2.231062000 -0.096226000
1 2.295762000 3.709542000 -0.155569000
6 -2.623352000 -0.154936000 0.068527000
6 -3.312392000 -0.283074000 -1.131663000
6 -3.171145000 -0.685733000 1.228090000
6 -4.542317000 -0.914002000 -1.165397000
1 -2.865541000 0.114741000 -2.037200000
6 -4.398604000 -1.327749000 1.190733000
1 -2.625369000 -0.584294000 2.160216000
6 -5.088081000 -1.439714000 -0.004040000
1 -5.073831000 -1.006192000 -2.105565000
1 -4.818361000 -1.737669000 2.102075000
1 -6.049249000 -1.939227000 -0.033105000
7 -1.340222000 0.462264000 0.105572000
6 2.651713000 -0.149311000 0.029163000
6 3.286861000 -0.441840000 1.227006000
6 3.273115000 -0.460110000 -1.172499000
6 4.535334000 -1.043404000 1.223664000
1 2.792940000 -0.184539000 2.158351000
6 4.521347000 -1.056402000 -1.174798000
1 2.763489000 -0.221756000 -2.100321000
6 5.154707000 -1.348386000 0.023708000
1 5.026160000 -1.271087000 2.162862000
1 5.002348000 -1.296644000 -2.115994000
1 6.132295000 -1.816201000 0.020732000
7 1.364843000 0.464085000 0.032596000
6 -2.465785000 2.649202000 0.037195000
1 -3.083964000 2.448840000 -0.841122000
1 -3.077531000 2.409614000 0.911598000
1 -2.233213000 3.712170000 0.055973000
1 0.047463000 -1.240712000 1.606315000

7	-0.006152000	-1.893727000	-0.811618000
1	-0.006665000	-2.850264000	-0.503412000
1	0.003279000	-1.803650000	-1.813318000

Cartesian coordinates of the C – H splitting product obtained for CAASis (**1Si-5Si**, **8Si-9Si** and **14Si**) and CAAGes (**1Ge-5Ge**, **8Ge-9Ge** and **14Ge**), along with their total energies (in hartrees) including zero point vibrational correction.

1Si^{PC-H} (T.E.= -1781.893879)

7	-0.657867000	-0.862560000	-0.702895000
14	0.124354000	0.401477000	0.225557000
6	1.856287000	-0.050033000	-0.292218000
6	0.260658000	-1.436969000	-1.675275000
6	1.513719000	-0.571473000	-1.718033000
1	1.325958000	0.274859000	-2.388656000
1	2.343490000	-1.132411000	-2.161098000
1	-0.200391000	-1.488940000	-2.668837000
1	0.515783000	-2.469557000	-1.393534000
6	-1.845667000	-1.526570000	-0.430488000
6	-2.217860000	-2.686472000	-1.118143000
6	-2.716184000	-1.053778000	0.560190000
6	-3.405295000	-3.336401000	-0.821522000
1	-1.580812000	-3.088402000	-1.895402000
6	-3.895484000	-1.708364000	0.844713000
1	-2.474548000	-0.145771000	1.102627000
6	-4.255541000	-2.858988000	0.157805000
1	-3.664081000	-4.232648000	-1.374998000
1	-4.546486000	-1.303619000	1.612089000
1	-5.184280000	-3.369531000	0.381872000
14	3.092072000	1.372545000	-0.362411000
14	2.444499000	-1.469679000	0.833694000
6	3.058189000	2.401382000	1.206308000
1	3.603263000	3.333392000	1.033073000
1	2.042701000	2.669966000	1.509403000
1	3.530634000	1.894136000	2.048411000
6	4.841558000	0.764141000	-0.657828000
1	5.499344000	1.626406000	-0.797512000
1	5.241687000	0.170523000	0.165922000
1	4.893758000	0.160714000	-1.568471000
6	2.738763000	2.521528000	-1.805299000

1	3.491891000	3.314648000	-1.787939000
1	2.827535000	2.011889000	-2.767533000
1	1.758788000	2.999032000	-1.761539000
6	3.670635000	-2.557023000	-0.078767000
1	4.526539000	-2.004997000	-0.470505000
1	4.048624000	-3.314053000	0.614205000
1	3.200315000	-3.086659000	-0.910699000
6	3.237673000	-0.818008000	2.402737000
1	3.451297000	-1.672151000	3.051324000
1	4.175650000	-0.284546000	2.239077000
1	2.557583000	-0.156193000	2.945725000
6	1.072360000	-2.607748000	1.430114000
1	0.301742000	-2.085367000	2.001562000
1	0.579647000	-3.160960000	0.628675000
1	1.533976000	-3.340685000	2.099296000
1	-0.149866000	0.284460000	1.678930000
6	-0.482802000	2.108483000	-0.304437000
1	0.087493000	2.865531000	0.244162000
1	-0.260963000	2.232319000	-1.368217000
6	-1.945889000	2.254560000	-0.052054000
6	-2.871414000	1.984569000	-1.055368000
6	-2.422400000	2.588227000	1.213314000
6	-4.230209000	2.034111000	-0.801485000
1	-2.514514000	1.716011000	-2.045204000
6	-3.781648000	2.639240000	1.470031000
1	-1.711525000	2.801287000	2.006979000
6	-4.692087000	2.357938000	0.463938000
1	-4.933901000	1.811648000	-1.595397000
1	-4.132054000	2.899497000	2.462488000
1	-5.756334000	2.393183000	0.664804000

2SiP^{C-H} (T.E.= -1780.699514)

7	-0.586670000	-0.983923000	-0.563129000
14	0.219425000	0.315730000	0.321925000
6	1.932876000	-0.148137000	-0.263017000
6	0.296863000	-1.396397000	-1.564928000
6	1.564430000	-0.978293000	-1.473758000
6	-1.907046000	-1.430112000	-0.479118000
6	-2.599555000	-1.921535000	-1.586526000
6	-2.576374000	-1.366913000	0.744396000

6	-3.919268000	-2.320297000	-1.469120000
1	-2.117434000	-1.963458000	-2.555657000
6	-3.897601000	-1.752813000	0.847789000
1	-2.052138000	-0.995640000	1.618883000
6	-4.582119000	-2.236091000	-0.256480000
1	-4.438011000	-2.691202000	-2.346216000
1	-4.396064000	-1.678853000	1.807858000
1	-5.617753000	-2.542002000	-0.172283000
14	3.056984000	1.303659000	-0.684495000
14	2.660707000	-1.374760000	0.995338000
6	3.141113000	2.534698000	0.729247000
1	3.594083000	3.463260000	0.371296000
1	2.155116000	2.785582000	1.128827000
1	3.749825000	2.167204000	1.557322000
6	4.802448000	0.739645000	-1.071126000
1	5.379618000	1.595660000	-1.431392000
1	5.316081000	0.338880000	-0.194253000
1	4.819830000	-0.023719000	-1.853371000
6	2.433668000	2.190716000	-2.214476000
1	3.204655000	2.883653000	-2.562417000
1	2.220561000	1.491820000	-3.026735000
1	1.530221000	2.772621000	-2.024527000
6	4.001503000	-2.428185000	0.219977000
1	4.849198000	-1.851620000	-0.150838000
1	4.374065000	-3.123090000	0.977970000
1	3.604140000	-3.024049000	-0.604702000
6	3.362694000	-0.478997000	2.485026000
1	3.604445000	-1.210774000	3.260516000
1	4.280449000	0.063482000	2.247542000
1	2.646591000	0.229892000	2.909098000
6	1.361219000	-2.577170000	1.616601000
1	0.577606000	-2.094396000	2.204128000
1	0.886525000	-3.128664000	0.802084000
1	1.860135000	-3.303887000	2.264726000
1	-0.066298000	-2.053546000	-2.344754000
1	2.305902000	-1.266509000	-2.211264000
1	0.019773000	0.251010000	1.788341000
6	-0.509744000	1.951020000	-0.264907000
1	-0.369661000	2.005549000	-1.348580000
1	0.043961000	2.779983000	0.187065000

6	-1.960131000	2.010216000	0.087864000
6	-2.369800000	2.367672000	1.369620000
6	-2.932417000	1.633048000	-0.833781000
6	-3.708444000	2.342324000	1.720954000
1	-1.623362000	2.665643000	2.100818000
6	-4.270143000	1.601110000	-0.484104000
1	-2.627243000	1.342602000	-1.835033000
6	-4.664352000	1.953431000	0.796168000
1	-4.006436000	2.625805000	2.724144000
1	-5.008306000	1.291354000	-1.215198000
1	-5.711937000	1.926424000	1.071954000

3SiP^{C-H} (T.E.= -1901.997666)

6	-1.779916000	0.969745000	-1.132289000
6	-1.916728000	-0.251497000	-0.154194000
1	-1.597640000	0.612046000	-2.156262000
1	-2.715648000	1.535360000	-1.182333000
14	-0.124108000	-0.625953000	0.190515000
7	0.514021000	0.978767000	-0.102459000
5	-0.518352000	1.823392000	-0.671577000
7	-0.466365000	3.232883000	-0.747899000
6	-1.419067000	4.008239000	-1.506465000
1	-2.048600000	4.623472000	-0.850133000
1	-0.901917000	4.689462000	-2.192862000
1	-2.066115000	3.366234000	-2.101591000
6	0.461687000	4.075472000	-0.031086000
1	-0.087751000	4.876597000	0.477480000
1	1.006086000	3.514170000	0.726314000
1	1.194376000	4.548521000	-0.697388000
14	-2.868551000	-1.680118000	-0.921713000
14	-2.687143000	0.377641000	1.461038000
6	-2.326659000	-1.967791000	-2.696717000
1	-2.837779000	-2.859086000	-3.071999000
1	-2.615626000	-1.133267000	-3.339778000
1	-1.253430000	-2.128733000	-2.810578000
6	-4.709341000	-1.331335000	-1.025911000
1	-5.197421000	-2.133272000	-1.586596000
1	-5.190649000	-1.266675000	-0.047759000
1	-4.895658000	-0.394316000	-1.558391000
6	-4.192138000	1.444412000	1.113426000

1	-4.940437000	0.958112000	0.486528000
1	-4.664470000	1.701565000	2.065908000
1	-3.902099000	2.382383000	0.632018000
6	-3.172724000	-1.021471000	2.610140000
1	-3.452200000	-0.592602000	3.576405000
1	-4.026217000	-1.597540000	2.247207000
1	-2.342552000	-1.711287000	2.780687000
6	-2.624526000	-3.276330000	0.040745000
1	-1.579786000	-3.466242000	0.301926000
1	-3.197533000	-3.279117000	0.969266000
1	-2.969128000	-4.120877000	-0.562091000
6	-1.532424000	1.494359000	2.439519000
1	-0.609810000	0.999065000	2.749302000
1	-1.262972000	2.397455000	1.885530000
1	-2.062759000	1.808011000	3.344057000
6	1.883991000	1.276385000	0.034396000
6	2.586987000	1.896150000	-0.997579000
6	2.578853000	0.918855000	1.187487000
6	3.936954000	2.167932000	-0.868962000
1	2.059355000	2.158327000	-1.909074000
6	3.934040000	1.171365000	1.303013000
1	2.047386000	0.426174000	1.995004000
6	4.620555000	1.805355000	0.281163000
1	4.462647000	2.655177000	-1.682638000
1	4.456501000	0.869310000	2.203687000
1	5.680750000	2.007691000	0.375676000
1	0.116657000	-1.098857000	1.579313000
6	0.754299000	-1.868534000	-0.932619000
1	0.167964000	-2.792485000	-0.948365000
1	0.753230000	-1.463964000	-1.950017000
6	2.147842000	-2.141846000	-0.469160000
6	3.247338000	-1.600767000	-1.126076000
6	2.374824000	-2.907455000	0.672298000
6	4.531202000	-1.798717000	-0.649348000
1	3.087428000	-0.997024000	-2.014128000
6	3.657087000	-3.109447000	1.150924000
1	1.526271000	-3.342388000	1.194096000
6	4.742263000	-2.550534000	0.494633000
1	5.371108000	-1.356386000	-1.173345000
1	3.810506000	-3.707276000	2.042317000

1 5.746938000 -2.703478000 0.871187000

4SiP^{C-H} (T.E.= -2111.907489)

6 -2.119128000 1.533104000 -0.533668000
6 -1.992031000 0.027432000 -0.087473000
1 -2.595692000 1.617776000 -1.516849000
1 -2.773206000 2.096448000 0.141138000
14 -0.181914000 -0.446193000 -0.285664000
7 0.600711000 1.093474000 -0.159074000
14 -2.990266000 -1.058552000 -1.265598000
14 -2.540300000 -0.067467000 1.717920000
6 -2.638041000 -0.567548000 -3.044429000
1 -1.568290000 -0.492802000 -3.252363000
1 -3.053560000 -1.331714000 -3.707496000
1 -3.103967000 0.383043000 -3.314078000
6 -4.840191000 -0.866606000 -1.027522000
1 -5.360115000 -1.340498000 -1.864694000
1 -5.201720000 -1.328655000 -0.106546000
1 -5.126180000 0.188630000 -1.011835000
6 -4.221175000 0.723128000 1.996883000
1 -5.029191000 0.182128000 1.503077000
1 -4.417580000 0.701325000 3.073326000
1 -4.269742000 1.766916000 1.681269000
6 -2.699272000 -1.816468000 2.378163000
1 -2.990998000 -1.752936000 3.430583000
1 -3.482613000 -2.373316000 1.858144000
1 -1.780111000 -2.400845000 2.327536000
6 -2.534330000 -2.869451000 -1.081846000
1 -2.676061000 -3.243735000 -0.065982000
1 -3.164692000 -3.465698000 -1.747254000
1 -1.494914000 -3.051598000 -1.369035000
6 -1.358290000 0.893239000 2.819917000
1 -0.309590000 0.609974000 2.707225000
1 -1.433100000 1.965879000 2.622631000
1 -1.642437000 0.736760000 3.864565000
14 -0.445586000 2.400455000 -0.640692000
6 -0.292969000 3.898619000 0.458960000
1 -0.477972000 3.660364000 1.508238000
1 0.705460000 4.335573000 0.381052000
1 -1.012541000 4.661417000 0.150571000

6	-0.066398000	2.903603000	-2.398696000
1	-0.150341000	2.039697000	-3.065278000
1	-0.757359000	3.672649000	-2.752875000
1	0.949015000	3.298765000	-2.486252000
6	2.002853000	1.278678000	-0.125535000
6	2.586413000	1.957667000	0.940805000
6	2.822668000	0.803191000	-1.146027000
6	3.956293000	2.153679000	0.986088000
1	1.945064000	2.313438000	1.741209000
6	4.192367000	0.986269000	-1.089455000
1	2.373180000	0.272067000	-1.979473000
6	4.765946000	1.666513000	-0.027071000
1	4.394298000	2.683281000	1.824703000
1	4.816861000	0.592760000	-1.883593000
1	5.839014000	1.811332000	0.013416000
1	0.055999000	-1.051699000	-1.628896000
6	0.521151000	-1.734292000	0.901514000
1	0.445127000	-1.386409000	1.934903000
1	-0.124213000	-2.614944000	0.806366000
6	1.932310000	-2.093955000	0.565306000
6	2.994483000	-1.629248000	1.333633000
6	2.220631000	-2.873145000	-0.552515000
6	4.302882000	-1.925640000	0.994613000
1	2.787576000	-1.018235000	2.207437000
6	3.528093000	-3.168513000	-0.896506000
1	1.403251000	-3.250632000	-1.160489000
6	4.576567000	-2.694148000	-0.125005000
1	5.114010000	-1.550277000	1.608362000
1	3.729322000	-3.777131000	-1.770974000
1	5.600969000	-2.925465000	-0.392581000

5SiP^{C-H} (T.E.= -1855.962785)

6	-1.823382000	-1.557724000	0.995964000
6	-1.977848000	-0.205764000	0.249852000
1	-2.026565000	-1.454957000	2.069235000
1	-2.510293000	-2.333112000	0.644137000
14	-0.238006000	0.451569000	0.388471000
7	0.506896000	-1.125561000	0.631500000
14	-3.136344000	1.009339000	1.118053000
14	-2.443444000	-0.604500000	-1.543861000

6	-2.902031000	0.888014000	2.973647000
1	-1.851415000	0.931130000	3.269770000
1	-3.417708000	1.725968000	3.450541000
1	-3.331807000	-0.031161000	3.378494000
6	-4.945261000	0.676426000	0.773289000
1	-5.556212000	1.325404000	1.406541000
1	-5.217998000	0.870794000	-0.266207000
1	-5.206622000	-0.359220000	1.006273000
6	-4.016098000	-1.621304000	-1.636993000
1	-4.906604000	-1.051345000	-1.370825000
1	-4.133966000	-1.957669000	-2.671343000
1	-3.983753000	-2.515083000	-1.010719000
6	-2.732475000	0.936391000	-2.569348000
1	-2.903247000	0.636818000	-3.607078000
1	-3.626791000	1.468375000	-2.234701000
1	-1.897837000	1.638726000	-2.561443000
6	-2.729802000	2.762072000	0.584409000
1	-2.811316000	2.903197000	-0.495629000
1	-3.427719000	3.454705000	1.062168000
1	-1.721936000	3.057591000	0.890671000
6	-1.121914000	-1.678641000	-2.336537000
1	-0.115467000	-1.255617000	-2.316029000
1	-1.080235000	-2.655760000	-1.846095000
1	-1.392118000	-1.853719000	-3.381640000
6	1.899022000	-1.403639000	0.632037000
6	2.740718000	-0.661637000	1.448692000
6	2.430002000	-2.380258000	-0.199498000
6	4.105198000	-0.886756000	1.428490000
1	2.318821000	0.101755000	2.094055000
6	3.794741000	-2.608354000	-0.207774000
1	1.769231000	-2.957038000	-0.835019000
6	4.636195000	-1.862987000	0.602694000
1	4.755224000	-0.290069000	2.057893000
1	4.204090000	-3.374104000	-0.856534000
1	5.704892000	-2.041835000	0.588074000
6	-0.413680000	-2.116876000	0.910723000
8	-0.149840000	-3.277507000	1.114451000
1	-0.014573000	1.286036000	1.596833000
6	0.480919000	1.433656000	-1.043026000
1	0.338652000	0.899715000	-1.985043000

1	-0.123573000	2.347386000	-1.099747000
6	1.922950000	1.776114000	-0.843599000
6	2.917272000	1.077780000	-1.519837000
6	2.303053000	2.772571000	0.049971000
6	4.254038000	1.365159000	-1.310362000
1	2.633126000	0.290212000	-2.212320000
6	3.640066000	3.060977000	0.263184000
1	1.535767000	3.328479000	0.582455000
6	4.621524000	2.358413000	-0.416909000
1	5.013168000	0.804061000	-1.843464000
1	3.916648000	3.843436000	0.960702000
1	5.668464000	2.584378000	-0.251815000

8SiP^{C-H} (T.E.= -1424.570285)

6	0.775231000	-2.250632000	0.643309000
6	2.227688000	-1.963143000	0.286744000
6	2.368022000	-0.455930000	0.127037000
1	0.513715000	-3.292566000	0.428149000
1	0.621119000	-2.091304000	1.724008000
1	2.475566000	-2.511208000	-0.635625000
1	2.876223000	-2.368534000	1.073877000
14	0.751875000	0.194497000	-0.320867000
7	-0.060628000	-1.353905000	-0.144936000
15	3.857486000	0.262445000	-0.087171000
6	5.032903000	-0.045021000	1.253643000
1	5.158109000	-1.122838000	1.374896000
1	6.006281000	0.400194000	1.040031000
1	4.633271000	0.363564000	2.182238000
6	4.811866000	-0.234377000	-1.552191000
1	4.247267000	0.025685000	-2.448968000
1	5.792201000	0.245941000	-1.583252000
1	4.949222000	-1.317733000	-1.535087000
6	3.710451000	2.050573000	-0.225176000
1	3.046468000	2.300099000	-1.055247000
1	3.297356000	2.457984000	0.697924000
1	4.689173000	2.496181000	-0.409594000
6	-1.417101000	-1.609609000	-0.269664000
6	-2.083728000	-2.540805000	0.532686000
6	-2.170905000	-0.917487000	-1.227117000
6	-3.447588000	-2.746550000	0.393231000

1	-1.539071000	-3.092720000	1.288848000
6	-3.526286000	-1.128058000	-1.355076000
1	-1.671914000	-0.203500000	-1.873757000
6	-4.183251000	-2.043222000	-0.543125000
1	-3.938731000	-3.469045000	1.036371000
1	-4.079421000	-0.567740000	-2.101062000
1	-5.249353000	-2.206426000	-0.644806000
1	0.531760000	0.768813000	-1.681583000
6	0.056453000	1.501618000	0.862364000
1	0.207571000	1.110752000	1.873922000
1	0.694756000	2.387029000	0.757800000
6	-1.372376000	1.843575000	0.621641000
6	-2.385121000	1.227272000	1.351948000
6	-1.739809000	2.733446000	-0.385005000
6	-3.717328000	1.480189000	1.081344000
1	-2.115984000	0.524343000	2.135311000
6	-3.072536000	2.990842000	-0.657765000
1	-0.963279000	3.224790000	-0.964980000
6	-4.068651000	2.362679000	0.072566000
1	-4.486503000	0.976011000	1.655667000
1	-3.335236000	3.687455000	-1.446305000
1	-5.112301000	2.560312000	-0.142885000

9SiP^{C-H} (T.E.= -1423.380748)

6	-0.853768000	-2.279648000	0.406558000
6	-2.126186000	-1.856450000	0.481870000
6	-2.379325000	-0.498223000	0.008814000
14	-0.752632000	0.187103000	-0.393455000
7	0.064213000	-1.359360000	-0.142830000
15	-3.901707000	0.193663000	-0.078560000
6	-5.111083000	-0.744662000	-1.043441000
1	-5.190546000	-1.750018000	-0.625241000
1	-6.095009000	-0.272273000	-1.021177000
1	-4.761358000	-0.826982000	-2.072784000
6	-3.821124000	1.826010000	-0.828672000
1	-4.819942000	2.260255000	-0.892154000
1	-3.190704000	2.479043000	-0.223060000
1	-3.399196000	1.751048000	-1.831711000
6	-4.753988000	0.426568000	1.502737000
1	-4.158693000	1.086992000	2.134511000

1	-5.752639000	0.846003000	1.364308000
1	-4.839341000	-0.541671000	2.000391000
6	1.423203000	-1.631180000	-0.252957000
6	2.190801000	-0.944175000	-1.198915000
6	2.070878000	-2.557006000	0.569227000
6	3.549423000	-1.157269000	-1.302722000
1	1.704290000	-0.230768000	-1.855971000
6	3.434130000	-2.768387000	0.452885000
1	1.509130000	-3.089367000	1.327284000
6	4.187419000	-2.071409000	-0.476931000
1	4.117192000	-0.600040000	-2.039835000
1	3.914212000	-3.485093000	1.110492000
1	5.254680000	-2.238088000	-0.558834000
1	-0.507824000	-3.270217000	0.666388000
1	-2.909503000	-2.510300000	0.853587000
1	-0.528196000	0.764779000	-1.749870000
6	-0.097522000	1.506084000	0.799196000
1	-0.280241000	1.130037000	1.810615000
1	-0.735973000	2.386880000	0.657010000
6	1.337519000	1.845643000	0.595214000
6	2.330446000	1.232524000	1.355022000
6	1.731192000	2.725889000	-0.410229000
6	3.669366000	1.479133000	1.113171000
1	2.041432000	0.536571000	2.137283000
6	3.070829000	2.976058000	-0.654240000
1	0.970398000	3.215227000	-1.012286000
6	4.047297000	2.350928000	0.104649000
1	4.423085000	0.978549000	1.710634000
1	3.354273000	3.664839000	-1.442446000
1	5.096396000	2.543151000	-0.087961000

¹⁴SiP^{C-H} (T.E.= -1618.742079)

6	2.437999000	0.942173000	0.131056000
6	2.163505000	-0.452411000	-0.061520000
7	-0.048228000	0.977815000	-0.325819000
6	-1.408289000	1.331483000	-0.220372000
6	-1.882769000	1.980234000	0.917974000
6	-3.223278000	2.296411000	1.039750000
6	-4.117825000	1.956671000	0.036638000
6	-3.655551000	1.301942000	-1.093003000

6	-2.312247000	0.996786000	-1.224696000
1	-1.178108000	2.232261000	1.704357000
1	-3.574656000	2.804210000	1.931104000
1	-5.169740000	2.196600000	0.137426000
1	-4.346708000	1.020938000	-1.879639000
1	-1.948628000	0.486679000	-2.110957000
5	1.100671000	1.830327000	-0.102329000
7	1.096368000	3.236641000	-0.167711000
6	2.207562000	4.050376000	0.279121000
1	2.584004000	4.672961000	-0.541937000
1	1.884808000	4.728983000	1.079231000
1	3.017228000	3.419417000	0.638547000
6	0.017583000	4.047594000	-0.681330000
1	-0.503624000	4.591999000	0.117422000
1	0.420198000	4.793386000	-1.376377000
1	-0.716748000	3.451777000	-1.218899000
15	3.499345000	-1.507570000	-0.012187000
6	4.334555000	-1.579160000	1.581663000
1	5.183130000	-2.264617000	1.540156000
1	4.679171000	-0.576292000	1.833442000
1	3.627637000	-1.915843000	2.340813000
6	4.787116000	-1.112625000	-1.206892000
1	5.633212000	-1.793730000	-1.099181000
1	4.377180000	-1.192147000	-2.214222000
1	5.108286000	-0.086284000	-1.030280000
6	2.993252000	-3.195367000	-0.376273000
1	2.312214000	-3.556009000	0.395721000
1	2.487122000	-3.228885000	-1.342508000
1	3.866852000	-3.848595000	-0.408582000
8	3.573825000	1.380124000	0.394807000
14	0.405423000	-0.712525000	-0.403746000
1	0.077562000	-1.313640000	-1.726910000
6	-0.532458000	-1.747171000	0.869498000
1	-0.436203000	-1.241007000	1.835732000
1	0.023068000	-2.689405000	0.952326000
6	-1.962490000	-2.022212000	0.539277000
6	-2.998732000	-1.418928000	1.244584000
6	-2.294921000	-2.866409000	-0.518677000
6	-4.320334000	-1.638402000	0.898093000
1	-2.761233000	-0.750322000	2.066318000

6	-3.615313000	-3.089986000	-0.866361000
1	-1.499482000	-3.349406000	-1.079365000
6	-4.636418000	-2.473211000	-0.160676000
1	-5.108835000	-1.149557000	1.459509000
1	-3.849152000	-3.750105000	-1.694247000
1	-5.671276000	-2.645021000	-0.432977000

1GeP^{C-H} (T.E.= -3569.339045)

6	-0.295102000	1.514070000	-1.675875000
6	-1.536577000	0.631584000	-1.721238000
6	-1.902841000	0.091933000	-0.313800000
1	0.124609000	1.614112000	-2.685028000
1	-0.564282000	2.531773000	-1.352648000
1	-1.335698000	-0.204886000	-2.401196000
1	-2.368187000	1.189368000	-2.166365000
32	-0.104960000	-0.428491000	0.258156000
7	0.674185000	0.929814000	-0.769892000
14	-2.488740000	1.481666000	0.844745000
14	-3.103460000	-1.357382000	-0.418422000
6	-2.707801000	-2.461555000	-1.883791000
1	-1.698694000	-2.876545000	-1.859085000
1	-3.408774000	-3.301085000	-1.870913000
1	-2.839308000	-1.942354000	-2.835850000
6	-3.026030000	-2.420592000	1.125166000
1	-3.429052000	-1.917607000	2.005139000
1	-3.610419000	-3.330830000	0.965680000
1	-2.003108000	-2.729639000	1.358616000
6	-4.866374000	-0.782224000	-0.695960000
1	-4.927146000	-0.140685000	-1.579656000
1	-5.504813000	-1.651360000	-0.876301000
1	-5.283320000	-0.233536000	0.150562000
6	-3.254951000	0.786473000	2.408130000
1	-2.557384000	0.127165000	2.931897000
1	-3.480142000	1.621850000	3.076833000
1	-4.183381000	0.238077000	2.239546000
6	-1.112108000	2.613335000	1.442910000
1	-0.622555000	3.169994000	0.642086000
1	-1.563900000	3.341293000	2.123842000
1	-0.336336000	2.084071000	2.001491000

6	-3.738869000	2.568034000	-0.034525000
1	-3.290005000	3.100023000	-0.876840000
1	-4.598845000	2.009152000	-0.407790000
1	-4.107335000	3.321829000	0.666804000
6	1.832001000	1.622825000	-0.478633000
6	2.161744000	2.822635000	-1.123577000
6	2.730965000	1.141887000	0.484435000
6	3.331520000	3.496694000	-0.812953000
1	1.503507000	3.233163000	-1.878602000
6	3.892565000	1.821407000	0.782247000
1	2.521970000	0.207220000	0.995212000
6	4.208773000	3.009421000	0.138221000
1	3.555597000	4.422192000	-1.332841000
1	4.564203000	1.407570000	1.526898000
1	5.123007000	3.540754000	0.373093000
1	0.225666000	-0.286533000	1.763131000
6	0.587841000	-2.173897000	-0.360010000
1	0.374650000	-2.243944000	-1.428463000
1	0.026248000	-2.957024000	0.156655000
6	2.047805000	-2.268778000	-0.090340000
6	2.976353000	-1.967957000	-1.082462000
6	2.519388000	-2.589068000	1.180862000
6	4.333012000	-1.978308000	-0.812742000
1	2.622785000	-1.707861000	-2.075566000
6	3.876111000	-2.599376000	1.453230000
1	1.806064000	-2.824597000	1.966084000
6	4.789451000	-2.290309000	0.457549000
1	5.038814000	-1.733320000	-1.598043000
1	4.222728000	-2.849854000	2.449465000
1	5.851818000	-2.294288000	0.670836000

2GeP^{C-H} (T.E.= -3568.146920)

6	1.993087000	0.207160000	0.254104000
6	1.625940000	1.193063000	1.340268000
6	0.366657000	1.645419000	1.410496000
1	2.385844000	1.575471000	2.014115000
1	0.056318000	2.408807000	2.114683000
32	0.203057000	-0.318002000	-0.360620000
7	-0.571125000	1.164200000	0.509988000
14	3.003473000	-1.238259000	0.919662000

14	2.794815000	1.230521000	-1.133493000
6	3.053777000	-2.655567000	-0.307278000
1	3.542947000	-3.516970000	0.155585000
1	2.055156000	-2.977089000	-0.615020000
1	3.613977000	-2.402974000	-1.208797000
6	4.208803000	2.261915000	-0.466188000
1	5.041523000	1.663556000	-0.095085000
1	4.586306000	2.902162000	-1.268319000
1	3.867441000	2.912826000	0.341936000
6	3.421109000	0.129622000	-2.515090000
1	2.641063000	-0.543481000	-2.881467000
1	3.746014000	0.748888000	-3.355245000
1	4.273163000	-0.478541000	-2.202840000
6	1.560328000	2.440692000	-1.857530000
1	0.739784000	1.955034000	-2.389773000
1	1.132560000	3.079093000	-1.081938000
1	2.082681000	3.084827000	-2.570564000
6	4.762725000	-0.726203000	1.314461000
1	5.267962000	-1.549975000	1.826206000
1	5.342539000	-0.484748000	0.421230000
1	4.789080000	0.141538000	1.978945000
6	2.257318000	-1.857099000	2.521753000
1	2.916889000	-2.611985000	2.958421000
1	2.148821000	-1.046189000	3.245516000
1	1.277648000	-2.317049000	2.382360000
6	-1.901673000	1.567344000	0.486888000
6	-2.544314000	2.091920000	1.610520000
6	-2.639422000	1.429430000	-0.691352000
6	-3.878816000	2.452179000	1.550876000
1	-2.006082000	2.188231000	2.546045000
6	-3.972536000	1.783111000	-0.738011000
1	-2.153960000	1.028722000	-1.576160000
6	-4.606251000	2.299303000	0.382133000
1	-4.358410000	2.848089000	2.439453000
1	-4.522816000	1.651833000	-1.663095000
1	-5.652437000	2.577193000	0.344489000
1	-0.037031000	-0.308515000	-1.888232000
6	-0.684377000	-1.912652000	0.400800000
1	-0.133571000	-2.799185000	0.076367000
1	-0.593131000	-1.828891000	1.485772000

6	-2.111783000	-1.959205000	-0.021102000
6	-3.124644000	-1.544722000	0.838529000
6	-2.462385000	-2.367949000	-1.305480000
6	-4.445265000	-1.531396000	0.427107000
1	-2.868107000	-1.217229000	1.841690000
6	-3.782845000	-2.355935000	-1.719533000
1	-1.684324000	-2.699232000	-1.987962000
6	-4.780317000	-1.933323000	-0.855151000
1	-5.215772000	-1.192501000	1.110472000
1	-4.034486000	-2.679176000	-2.723359000
1	-5.814269000	-1.920182000	-1.179177000

3GeP^{C-H} (T.E.= -3689.440400)

6	1.944898000	1.512373000	-0.318207000
6	2.033428000	-0.035362000	-0.132366000
1	2.730157000	2.014534000	0.257757000
1	2.153247000	1.779972000	-1.365254000
7	-0.545613000	1.080935000	-0.049889000
5	0.487664000	2.077912000	0.010166000
7	0.280983000	3.449491000	0.305120000
6	1.302046000	4.450915000	0.116696000
1	0.938759000	5.256188000	-0.534535000
1	1.592781000	4.912580000	1.069570000
1	2.193591000	4.030647000	-0.345236000
6	-0.941767000	4.029561000	0.808365000
1	-1.472073000	4.609940000	0.041377000
1	-1.620195000	3.265841000	1.181328000
1	-0.715603000	4.710193000	1.637666000
14	2.409550000	-0.383607000	1.684254000
14	3.194745000	-0.849409000	-1.365573000
6	1.005099000	0.159088000	2.811265000
1	0.055879000	-0.341949000	2.610048000
1	1.289202000	-0.057337000	3.845554000
1	0.828017000	1.235537000	2.734946000
6	3.901533000	0.596284000	2.264719000
1	4.141311000	0.285015000	3.285673000
1	4.788601000	0.435964000	1.650315000
1	3.694909000	1.668448000	2.292893000
6	5.002867000	-0.637480000	-0.916348000
1	5.624624000	-1.005798000	-1.737067000

1	5.245435000	0.418356000	-0.766214000
1	5.286988000	-1.183026000	-0.013814000
6	2.810158000	-2.679852000	-1.532325000
1	3.512045000	-3.138939000	-2.233837000
1	2.885007000	-3.220594000	-0.586683000
1	1.804624000	-2.837906000	-1.934432000
6	2.775442000	-2.193445000	2.019436000
1	3.713478000	-2.506452000	1.554085000
1	2.886691000	-2.330330000	3.098904000
1	1.990324000	-2.872086000	1.679721000
6	2.976096000	-0.080801000	-3.063364000
1	1.926254000	-0.017618000	-3.359534000
1	3.404367000	0.922778000	-3.114045000
1	3.495973000	-0.697215000	-3.801913000
32	0.191729000	-0.563863000	-0.541143000
6	-1.923892000	1.302511000	-0.263071000
6	-2.374122000	1.812503000	-1.476904000
6	-2.857415000	0.996513000	0.721567000
6	-3.725882000	2.016071000	-1.697722000
1	-1.642169000	2.048986000	-2.243406000
6	-4.207898000	1.194211000	0.498633000
1	-2.502052000	0.605006000	1.669318000
6	-4.648493000	1.705791000	-0.711887000
1	-4.060662000	2.415459000	-2.648514000
1	-4.921256000	0.942842000	1.275526000
1	-5.706962000	1.858683000	-0.886798000
1	-0.102464000	-0.747096000	-2.060997000
6	-0.549943000	-2.166335000	0.348511000
1	-0.081888000	-2.999995000	-0.186762000
1	-0.196524000	-2.205673000	1.379582000
6	-2.037165000	-2.264872000	0.298752000
6	-2.784652000	-2.237745000	1.471057000
6	-2.717092000	-2.372352000	-0.912687000
6	-4.166817000	-2.308035000	1.439451000
1	-2.268416000	-2.155445000	2.423706000
6	-4.098234000	-2.436226000	-0.947936000
1	-2.152166000	-2.400264000	-1.839926000
6	-4.830456000	-2.403781000	0.228399000
1	-4.727943000	-2.286291000	2.367118000
1	-4.607188000	-2.513730000	-1.902037000

1	-5.912514000	-2.453145000	0.199325000
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4GeP^{C-H} (T.E.= -3899.350210)

6	-1.688893000	0.556763000	1.599756000
6	-2.007896000	0.067223000	0.145689000
1	-2.160804000	1.527244000	1.799541000
1	-2.117007000	-0.113235000	2.354954000
7	0.823793000	0.741948000	0.370113000
14	-2.959350000	1.461994000	-0.707679000
14	-2.912773000	-1.579554000	0.212724000
6	-1.892270000	3.007576000	-0.761967000
1	-0.977399000	2.885590000	-1.345288000
1	-2.470499000	3.816653000	-1.217423000
1	-1.607575000	3.336399000	0.240949000
6	-4.511073000	1.937889000	0.233959000
1	-4.888002000	2.877998000	-0.178977000
1	-5.299830000	1.191501000	0.133288000
1	-4.331031000	2.097043000	1.299317000
6	-4.633581000	-1.425442000	0.941985000
1	-5.340261000	-0.974904000	0.241901000
1	-5.004654000	-2.423940000	1.189948000
1	-4.638894000	-0.832661000	1.860095000
6	-3.091006000	-2.354160000	-1.488627000
1	-3.356235000	-3.409317000	-1.380450000
1	-3.890367000	-1.872652000	-2.055487000
1	-2.183079000	-2.306534000	-2.093922000
6	-3.482111000	1.012091000	-2.451310000
1	-4.324531000	0.316027000	-2.444019000
1	-3.810364000	1.915353000	-2.972716000
1	-2.678017000	0.563593000	-3.038728000
6	-1.988349000	-2.761004000	1.348309000
1	-0.917638000	-2.819273000	1.141799000
1	-2.106857000	-2.474829000	2.396383000
1	-2.402829000	-3.766936000	1.238218000
14	0.149961000	0.780646000	1.971417000
6	0.706734000	-0.602591000	3.103354000
1	0.506766000	-1.578757000	2.653815000
1	1.770738000	-0.556709000	3.344740000
1	0.148268000	-0.550001000	4.042852000
6	0.486491000	2.424988000	2.784858000

1	0.189668000	3.245325000	2.126427000
1	-0.082730000	2.509186000	3.714115000
1	1.542904000	2.553859000	3.027847000
32	-0.302982000	-0.099269000	-0.851492000
6	2.090284000	1.228726000	0.025038000
6	2.312385000	1.865859000	-1.199201000
6	3.173139000	1.113203000	0.899352000
6	3.562447000	2.348080000	-1.537413000
1	1.485858000	1.983209000	-1.891547000
6	4.419602000	1.607381000	0.561724000
1	3.039505000	0.597182000	1.844232000
6	4.628489000	2.223691000	-0.660909000
1	3.701589000	2.835785000	-2.496086000
1	5.241397000	1.492380000	1.260082000
1	5.607704000	2.603762000	-0.926148000
1	-0.329924000	0.680744000	-2.192531000
6	0.456966000	-1.892086000	-1.303824000
1	-0.146419000	-2.674836000	-0.843593000
1	0.354173000	-1.985255000	-2.387894000
6	1.880337000	-2.000041000	-0.882389000
6	2.218376000	-2.562767000	0.344295000
6	2.905204000	-1.492787000	-1.676363000
6	3.534762000	-2.608898000	0.770000000
1	1.434245000	-2.974980000	0.973286000
6	4.222668000	-1.542422000	-1.258206000
1	2.658447000	-1.040736000	-2.633450000
6	4.542993000	-2.096013000	-0.029142000
1	3.772851000	-3.049833000	1.731768000
1	5.001939000	-1.128454000	-1.888341000
1	5.573866000	-2.126780000	0.303728000

5GeP^{C-H} (T.E.= -3643.406827)

6	-1.731910000	1.378038000	-1.107232000
6	-2.004816000	0.173130000	-0.175399000
1	-1.829464000	1.106303000	-2.167189000
1	-2.449772000	2.192285000	-0.963438000
7	0.565580000	1.171329000	-0.389040000
14	-3.028534000	-1.119166000	-1.091264000
14	-2.752176000	0.819657000	1.446011000
6	-2.087908000	-1.757087000	-2.587128000

1	-1.378904000	-2.540615000	-2.314276000
1	-2.798388000	-2.191991000	-3.294744000
1	-1.537471000	-0.975097000	-3.116513000
6	-4.620150000	-0.367515000	-1.731406000
1	-5.085696000	-1.058439000	-2.438980000
1	-5.338731000	-0.171579000	-0.934991000
1	-4.440584000	0.572385000	-2.259538000
6	-4.479782000	1.495147000	1.185066000
1	-5.211662000	0.695836000	1.050470000
1	-4.769839000	2.061036000	2.074768000
1	-4.550259000	2.169441000	0.328833000
6	-2.860493000	-0.495101000	2.776560000
1	-3.127405000	-0.005849000	3.717586000
1	-3.634468000	-1.233559000	2.561633000
1	-1.920340000	-1.025527000	2.940473000
6	-3.418130000	-2.579758000	0.012658000
1	-4.202724000	-2.347003000	0.735679000
1	-3.766637000	-3.419692000	-0.593490000
1	-2.538578000	-2.915985000	0.569857000
6	-1.694557000	2.230265000	2.086043000
1	-0.661940000	1.935736000	2.288277000
1	-1.669230000	3.073150000	1.390960000
1	-2.125137000	2.591583000	3.023930000
6	1.930502000	1.527471000	-0.275176000
6	2.638756000	2.012616000	-1.369341000
6	2.589900000	1.344371000	0.934132000
6	3.984340000	2.305852000	-1.248169000
1	2.129417000	2.154640000	-2.313703000
6	3.939507000	1.627727000	1.045712000
1	2.040635000	0.966709000	1.790426000
6	4.642135000	2.113615000	-0.043262000
1	4.526223000	2.683448000	-2.107767000
1	4.442361000	1.464456000	1.992006000
1	5.698567000	2.338233000	0.044396000
6	-0.347284000	1.995497000	-0.993843000
8	-0.111590000	3.099649000	-1.434408000
32	-0.188188000	-0.428079000	0.257940000
1	0.113390000	-0.551970000	1.770315000
6	0.712425000	-1.937144000	-0.634898000
1	0.648706000	-1.776593000	-1.712247000

1	0.152586000	-2.844034000	-0.390026000
6	2.128190000	-2.022850000	-0.175951000
6	3.160948000	-1.521025000	-0.961439000
6	2.445082000	-2.563021000	1.067791000
6	4.470936000	-1.556851000	-0.519197000
1	2.927705000	-1.085913000	-1.928843000
6	3.754474000	-2.595949000	1.514297000
1	1.650702000	-2.964156000	1.691214000
6	4.773283000	-2.091407000	0.722504000
1	5.260087000	-1.159580000	-1.147152000
1	3.980778000	-3.022057000	2.485132000
1	5.799009000	-2.116594000	1.071016000

8GeP^{C-H} (T.E.= -3212.011251)

6	-0.607406000	-2.215066000	0.943997000
6	-1.921126000	-1.499476000	1.225862000
6	-2.272261000	-0.653133000	0.014452000
1	-0.188633000	-2.614413000	1.876114000
1	-0.793128000	-3.071591000	0.276236000
1	-1.796561000	-0.902166000	2.146469000
1	-2.689524000	-2.249883000	1.448230000
32	-0.620007000	0.122914000	-0.484170000
7	0.323906000	-1.282383000	0.329794000
15	-3.757150000	0.093950000	-0.141823000
6	-5.140597000	-1.069287000	-0.162045000
1	-5.123376000	-1.660711000	0.755305000
1	-6.095729000	-0.544571000	-0.223162000
1	-5.031281000	-1.742888000	-1.011899000
6	-3.852235000	1.034034000	-1.673497000
1	-3.127936000	1.850648000	-1.650037000
1	-3.625316000	0.382122000	-2.517069000
1	-4.850327000	1.457635000	-1.794610000
6	-4.272294000	1.280192000	1.141563000
1	-5.281072000	1.663511000	0.972452000
1	-4.240560000	0.781302000	2.112880000
1	-3.565690000	2.112391000	1.161782000
6	1.586240000	-1.716450000	-0.012277000
6	2.060981000	-2.989013000	0.338751000
6	2.461477000	-0.883772000	-0.728154000
6	3.342571000	-3.389247000	-0.001133000

1	1.425426000	-3.675239000	0.883099000
6	3.733748000	-1.295210000	-1.061573000
1	2.139020000	0.112059000	-1.014404000
6	4.194017000	-2.554422000	-0.701628000
1	3.674964000	-4.380404000	0.289732000
1	4.376530000	-0.614470000	-1.609543000
1	5.194914000	-2.875368000	-0.963648000
1	-0.244706000	0.286427000	-1.980420000
6	-0.189965000	1.824953000	0.454439000
1	-0.563870000	1.681815000	1.472550000
1	-0.796169000	2.599556000	-0.026416000
6	1.251940000	2.169050000	0.441353000
6	2.092071000	1.757432000	1.473240000
6	1.819091000	2.844085000	-0.637727000
6	3.451556000	2.005891000	1.426786000
1	1.666210000	1.217899000	2.313970000
6	3.180081000	3.092704000	-0.687210000
1	1.178612000	3.170241000	-1.452951000
6	4.004043000	2.673092000	0.344916000
1	4.086749000	1.669549000	2.238419000
1	3.600087000	3.618214000	-1.537670000
1	5.069933000	2.864368000	0.306115000

9GeP^{C-H} (T.E.= -3210.824078)

6	-0.751182000	2.125066000	0.975955000
6	-2.023784000	1.699329000	0.890970000
6	-2.291069000	0.477023000	0.151399000
7	0.235504000	1.348177000	0.343967000
15	-3.820208000	-0.139685000	-0.133845000
6	-4.796730000	-0.492193000	1.350245000
1	-4.878152000	0.420052000	1.944649000
1	-5.800339000	-0.840821000	1.098259000
1	-4.280358000	-1.245451000	1.946219000
6	-3.731480000	-1.686853000	-1.044940000
1	-4.736817000	-2.053342000	-1.257162000
1	-3.202718000	-1.528554000	-1.986291000
1	-3.199827000	-2.434126000	-0.454233000
6	-4.927749000	0.931103000	-1.087048000
1	-4.501861000	1.092317000	-2.077882000
1	-5.927881000	0.502104000	-1.177258000

1	-4.997283000	1.897319000	-0.582847000
32	-0.588464000	-0.208480000	-0.328389000
6	1.487876000	1.834669000	0.020013000
6	2.436854000	0.997328000	-0.582930000
6	1.868603000	3.161513000	0.267252000
6	3.697535000	1.455838000	-0.905429000
1	2.187637000	-0.039794000	-0.783936000
6	3.138356000	3.606599000	-0.053265000
1	1.162386000	3.858651000	0.698874000
6	4.069030000	2.765580000	-0.639179000
1	4.401361000	0.770334000	-1.365786000
1	3.398309000	4.639240000	0.154966000
1	5.061050000	3.122766000	-0.887548000
1	-0.448714000	2.991683000	1.546558000
1	-2.813209000	2.251420000	1.393840000
1	-0.186569000	-0.432714000	-1.812099000
6	-0.043767000	-1.837573000	0.673141000
1	-0.301590000	-1.643609000	1.716607000
1	-0.697947000	-2.633400000	0.302485000
6	1.388530000	-2.177958000	0.500339000
6	2.333517000	-1.809601000	1.455001000
6	1.837807000	-2.798984000	-0.663833000
6	3.681243000	-2.044820000	1.250316000
1	2.001149000	-1.315138000	2.362934000
6	3.185867000	-3.031601000	-0.872737000
1	1.114024000	-3.091254000	-1.419751000
6	4.115307000	-2.652865000	0.083194000
1	4.399300000	-1.743791000	2.004642000
1	3.513344000	-3.511978000	-1.787966000
1	5.171557000	-2.832126000	-0.079709000

¹⁴GeP^{C-H} (T.E.= -3406.183411)

6	2.416227000	1.008203000	0.146075000
6	2.187953000	-0.388615000	-0.056674000
7	-0.085663000	1.076123000	-0.324441000
6	-1.441458000	1.422365000	-0.212994000
6	-1.917425000	2.079771000	0.921343000
6	-3.259174000	2.391421000	1.044739000
6	-4.156798000	2.039739000	0.048753000
6	-3.695014000	1.377567000	-1.077405000

6	-2.351688000	1.076257000	-1.210402000
1	-1.212288000	2.341208000	1.704192000
1	-3.609064000	2.905396000	1.933273000
1	-5.209181000	2.276963000	0.151162000
1	-4.387256000	1.089830000	-1.860791000
1	-1.988806000	0.565871000	-2.097146000
5	1.073601000	1.896655000	-0.084603000
7	1.083332000	3.307578000	-0.135653000
6	2.182991000	4.118007000	0.341554000
1	2.579105000	4.746802000	-0.465854000
1	1.841933000	4.791969000	1.138541000
1	2.984474000	3.485477000	0.715217000
6	0.015291000	4.122708000	-0.663205000
1	-0.523247000	4.661401000	0.128371000
1	0.430913000	4.874502000	-1.344400000
1	-0.708121000	3.530343000	-1.219598000
15	3.534083000	-1.424702000	0.044340000
6	4.324901000	-1.474053000	1.662150000
1	5.187670000	-2.142770000	1.648475000
1	4.642900000	-0.463483000	1.918032000
1	3.603493000	-1.820493000	2.403019000
6	4.855021000	-1.034875000	-1.115505000
1	5.703054000	-1.707666000	-0.975390000
1	4.476340000	-1.126375000	-2.133916000
1	5.161858000	-0.004127000	-0.938710000
6	3.040327000	-3.117565000	-0.313611000
1	2.316172000	-3.456446000	0.429156000
1	2.583968000	-3.165861000	-1.303840000
1	3.908279000	-3.778241000	-0.288071000
8	3.544286000	1.459392000	0.429305000
32	0.363570000	-0.737501000	-0.429641000
1	-0.005965000	-1.324642000	-1.819413000
6	-0.627137000	-1.762565000	0.941318000
1	-0.513713000	-1.208144000	1.876600000
1	-0.082718000	-2.706497000	1.049350000
6	-2.057936000	-2.001021000	0.607233000
6	-3.075895000	-1.330820000	1.278129000
6	-2.413435000	-2.878216000	-0.416029000
6	-4.402153000	-1.516710000	0.930624000
1	-2.818922000	-0.639511000	2.074689000

6	-3.738884000	-3.068185000	-0.764138000
1	-1.632927000	-3.414908000	-0.948584000
6	-4.741234000	-2.384609000	-0.093854000
1	-5.175100000	-0.972490000	1.461950000
1	-3.991531000	-3.754917000	-1.564321000
1	-5.779653000	-2.529754000	-0.367956000

Cartesian coordinates of the Si – H splitting product obtained for CAASi (1Si-5Si, 8Si-9Si and 14Si), CAAGes (1Ge-5Ge, 8Ge-9Ge and 14Ge) and IX, along with their total energies (in hartrees) including zero point vibrational correction.

1Si^{PSi-H} (T.E.= -2038.040401)

6	0.038124000	-1.891006000	-1.298177000
6	1.188588000	-0.928825000	-1.583326000
6	1.733103000	-0.321469000	-0.263191000
1	-0.619918000	-1.945995000	-2.175020000
1	0.407986000	-2.913253000	-1.123149000
1	0.810771000	-0.131437000	-2.233952000
1	1.972979000	-1.437169000	-2.154148000
7	-0.680893000	-1.412598000	-0.130326000
14	0.092192000	0.004819000	0.588341000
14	2.659373000	-1.624698000	0.764782000
14	2.756011000	1.223592000	-0.584360000
6	2.852749000	2.294441000	0.955995000
1	3.620455000	1.938385000	1.644503000
1	3.106919000	3.321415000	0.679300000
1	1.907693000	2.327910000	1.505141000
6	2.012836000	2.224495000	-1.992421000
1	0.941202000	2.409447000	-1.899112000
1	2.511401000	3.197774000	-2.028194000
1	2.187521000	1.732904000	-2.952918000
6	4.501086000	0.840315000	-1.157387000
1	4.997363000	1.775316000	-1.432518000
1	5.112552000	0.351165000	-0.396794000
1	4.488184000	0.203350000	-2.046233000
6	3.640868000	-0.824174000	2.146980000
1	4.072153000	-1.615410000	2.766281000
1	4.461263000	-0.197210000	1.791908000
1	3.000558000	-0.214102000	2.789345000
6	1.559701000	-2.899819000	1.599923000

1	0.871847000	-2.461861000	2.326652000
1	0.968978000	-3.490378000	0.896167000
1	2.215093000	-3.588937000	2.141843000
6	3.825583000	-2.597123000	-0.339088000
1	4.525850000	-1.965135000	-0.887813000
1	4.407834000	-3.282196000	0.283542000
1	3.278039000	-3.204248000	-1.064335000
6	-1.799138000	-2.090951000	0.308512000
6	-2.370777000	-3.142804000	-0.418841000
6	-2.398681000	-1.749757000	1.529836000
6	-3.496921000	-3.798097000	0.050053000
1	-1.936225000	-3.452459000	-1.360177000
6	-3.521959000	-2.408473000	1.983998000
1	-1.961923000	-0.962124000	2.134776000
6	-4.087986000	-3.439582000	1.248052000
1	-3.915730000	-4.606462000	-0.539442000
1	-3.957219000	-2.115121000	2.933012000
1	-4.969022000	-3.956644000	1.607702000
1	0.215896000	-0.117222000	2.070216000
14	-1.317469000	1.837167000	0.047788000
6	-2.758854000	1.728985000	1.271199000
1	-3.348743000	0.841737000	1.011311000
1	-2.328294000	1.513173000	2.256843000
6	-0.520488000	3.547405000	0.207627000
1	-0.583000000	3.826282000	1.266837000
1	0.546958000	3.480266000	-0.014251000
6	-1.931424000	1.472376000	-1.706781000
1	-1.146724000	1.742887000	-2.423622000
1	-2.020905000	0.380318000	-1.768150000
6	-1.145402000	4.627690000	-0.664903000
1	-2.210279000	4.756051000	-0.457444000
1	-0.664788000	5.597744000	-0.515556000
1	-1.051296000	4.379586000	-1.725868000
6	-3.652577000	2.958214000	1.369078000
1	-3.082179000	3.848226000	1.647732000
1	-4.153758000	3.178000000	0.423154000
1	-4.432286000	2.828702000	2.124060000
6	-3.256662000	2.105248000	-2.107376000
1	-3.219435000	3.196457000	-2.075716000
1	-3.549447000	1.819571000	-3.120868000

1 -4.060911000 1.787114000 -1.439775000

2SiP^{Si-H} (T.E.= -2036.843541)

6 -1.660753000 0.807139000 0.023585000
6 -1.404994000 2.302355000 -0.027176000
6 -0.130651000 2.705746000 -0.025455000
1 -2.221555000 3.010484000 -0.120417000
1 0.187641000 3.737621000 -0.127273000
14 0.047930000 0.233299000 0.591285000
7 0.852384000 1.718061000 0.042528000
14 -2.009708000 0.296373000 -1.765036000
14 -3.016085000 0.440626000 1.282234000
6 -3.441208000 1.249008000 -2.511841000
1 -3.455714000 1.053185000 -3.588058000
1 -4.411349000 0.960106000 -2.107961000
1 -3.320062000 2.326572000 -2.378418000
6 -2.416627000 -1.532693000 -1.890480000
1 -2.458829000 -1.828382000 -2.942581000
1 -1.682885000 -2.175274000 -1.396717000
1 -3.394697000 -1.743843000 -1.449595000
6 -0.546989000 0.712105000 -2.867580000
1 -0.725184000 0.298330000 -3.864579000
1 -0.462022000 1.797107000 -2.965737000
1 0.415183000 0.339184000 -2.515024000
6 -3.119791000 -1.380168000 1.706061000
1 -3.968662000 -1.540093000 2.376591000
1 -3.271645000 -2.004340000 0.822801000
1 -2.224904000 -1.732405000 2.223406000
6 -2.691688000 1.400608000 2.855885000
1 -1.714861000 1.168719000 3.285101000
1 -2.730688000 2.477027000 2.674559000
1 -3.456842000 1.155070000 3.597383000
6 -4.701971000 0.968028000 0.652454000
1 -5.079920000 0.292767000 -0.118729000
1 -5.410990000 0.949144000 1.484836000
1 -4.695469000 1.980810000 0.242399000
6 2.213233000 2.042125000 0.049087000
6 3.111961000 1.264650000 -0.678499000
6 2.702740000 3.138755000 0.757615000
6 4.462713000 1.559896000 -0.680096000

1	2.731287000	0.436418000	-1.267892000
6	4.052541000	3.440510000	0.737553000
1	2.017158000	3.743733000	1.340662000
6	4.941983000	2.651427000	0.026115000
1	5.143422000	0.941324000	-1.254194000
1	4.414642000	4.295401000	1.297506000
1	5.999021000	2.888231000	0.018459000
1	0.100405000	0.269051000	2.091590000
14	1.057287000	-1.858393000	0.126601000
6	2.737041000	-1.826378000	0.986722000
1	3.335895000	-1.009154000	0.574174000
1	2.572596000	-1.565253000	2.038483000
6	-0.005358000	-3.162765000	0.990598000
1	-1.038988000	-3.063471000	0.641766000
1	0.325625000	-4.147561000	0.642821000
6	1.263228000	-2.300977000	-1.703628000
1	0.488701000	-1.802630000	-2.292524000
1	2.213422000	-1.864923000	-2.037087000
6	3.495822000	-3.141296000	0.868115000
1	4.446361000	-3.114418000	1.406361000
1	2.921969000	-3.983187000	1.266428000
1	3.722409000	-3.372690000	-0.176404000
6	0.049465000	-3.108327000	2.511700000
1	1.033435000	-3.400542000	2.885163000
1	-0.147226000	-2.103552000	2.897881000
1	-0.681415000	-3.780503000	2.968070000
6	1.234628000	-3.793489000	-2.006494000
1	0.255665000	-4.221920000	-1.776986000
1	1.435744000	-3.992485000	-3.061714000
1	1.972640000	-4.349462000	-1.423237000

3SiP^{Si-H} (T.E.= -2158.148448)

6	1.556992000	-0.694339000	-1.330621000
6	1.853547000	0.135887000	-0.034226000
1	1.161361000	-0.037934000	-2.119466000
1	2.479339000	-1.116610000	-1.741821000
14	0.131928000	0.246426000	0.710978000
7	-0.462699000	-1.279880000	0.041594000
5	0.437050000	-1.769413000	-0.978809000
7	0.385719000	-3.059430000	-1.554051000

6	1.193059000	-3.439118000	-2.688466000
1	1.980663000	-4.149351000	-2.403008000
1	0.577317000	-3.927302000	-3.452795000
1	1.661711000	-2.570945000	-3.147743000
6	-0.354555000	-4.179121000	-1.022788000
1	0.311408000	-5.044149000	-0.917791000
1	-0.763591000	-3.954980000	-0.039244000
1	-1.182682000	-4.479144000	-1.677711000
14	2.614990000	1.808971000	-0.417487000
14	2.916607000	-0.929658000	1.119063000
6	1.781786000	2.577780000	-1.917291000
1	0.690924000	2.546085000	-1.890130000
1	2.081517000	3.627396000	-1.991427000
1	2.106943000	2.079058000	-2.833716000
6	4.427567000	1.696156000	-0.890418000
1	4.764961000	2.670309000	-1.256236000
1	5.070818000	1.414124000	-0.054520000
1	4.575365000	0.969861000	-1.695044000
6	4.401840000	-1.644793000	0.215064000
1	5.107894000	-0.888721000	-0.134437000
1	4.932848000	-2.303690000	0.908905000
1	4.101260000	-2.253967000	-0.643688000
6	3.528663000	0.048486000	2.597399000
1	4.003338000	-0.636833000	3.304786000
1	4.269403000	0.801989000	2.322947000
1	2.709678000	0.551320000	3.117212000
6	2.466483000	2.973111000	1.050850000
1	3.227769000	2.762659000	1.803607000
1	2.602470000	4.007355000	0.722407000
1	1.491807000	2.910412000	1.541871000
6	2.023376000	-2.444494000	1.789432000
1	1.116890000	-2.212650000	2.352414000
1	1.759910000	-3.146935000	0.993058000
1	2.717004000	-2.957106000	2.463272000
6	-1.760273000	-1.736915000	0.330956000
6	-2.695356000	-1.935029000	-0.684813000
6	-2.159481000	-1.954743000	1.648237000
6	-3.984214000	-2.340408000	-0.390755000
1	-2.397020000	-1.762740000	-1.714065000
6	-3.451831000	-2.355969000	1.939986000

1	-1.438365000	-1.806502000	2.445473000
6	-4.372529000	-2.549921000	0.923782000
1	-4.695561000	-2.484333000	-1.196274000
1	-3.740003000	-2.518499000	2.972314000
1	-5.384732000	-2.860734000	1.152935000
1	0.177878000	0.195086000	2.205154000
14	-1.510471000	1.839084000	0.076175000
6	-2.949366000	1.491868000	1.260903000
1	-3.390388000	0.527806000	0.981870000
1	-2.502543000	1.324118000	2.248726000
6	-1.019595000	3.662846000	0.215087000
1	-1.051722000	3.944855000	1.274210000
1	0.024161000	3.778393000	-0.087780000
6	-1.971309000	1.432854000	-1.721077000
1	-1.400183000	2.098667000	-2.378108000
1	-1.602353000	0.423798000	-1.937332000
6	-3.453289000	1.515230000	-2.057260000
1	-3.854027000	2.516119000	-1.877848000
1	-3.645642000	1.271165000	-3.105329000
1	-4.035240000	0.815664000	-1.450643000
6	-4.030326000	2.558447000	1.366016000
1	-4.808651000	2.270602000	2.077445000
1	-3.622256000	3.513690000	1.706075000
1	-4.520495000	2.738899000	0.405994000
6	-1.885038000	4.602020000	-0.615773000
1	-1.838726000	4.344522000	-1.677724000
1	-2.936281000	4.563623000	-0.320858000
1	-1.560222000	5.641242000	-0.522259000

4SiP^{Si-H} (T.E.= -2368.052688)

6	-1.926966000	-1.285932000	1.207165000
6	-1.927934000	-0.213261000	0.058696000
1	-2.186579000	-0.832879000	2.172242000
1	-2.703339000	-2.044593000	1.047976000
14	-0.148207000	0.021785000	-0.567901000
7	0.668434000	-1.315349000	0.217473000
14	-2.685450000	1.353245000	0.772421000
14	-2.893699000	-0.931213000	-1.402241000
6	-1.587227000	2.008092000	2.150829000
1	-0.683084000	2.489945000	1.776917000

1	-2.138449000	2.753501000	2.730681000
1	-1.278814000	1.218462000	2.842784000
6	-4.355934000	1.033170000	1.566918000
1	-4.650438000	1.923718000	2.129416000
1	-5.134671000	0.833115000	0.830086000
1	-4.332043000	0.195008000	2.267006000
6	-4.690110000	-1.270962000	-0.969065000
1	-5.286647000	-0.356130000	-0.966019000
1	-5.107105000	-1.931238000	-1.735288000
1	-4.819380000	-1.763841000	-0.003119000
6	-2.931248000	0.175805000	-2.915776000
1	-3.417565000	-0.375751000	-3.725962000
1	-3.512955000	1.083040000	-2.742735000
1	-1.939396000	0.468354000	-3.263377000
6	-2.927790000	2.683495000	-0.528180000
1	-3.851816000	2.508551000	-1.085338000
1	-3.009371000	3.665850000	-0.054924000
1	-2.108886000	2.727001000	-1.250616000
6	-2.156388000	-2.589082000	-1.889128000
1	-1.080314000	-2.543409000	-2.070635000
1	-2.338355000	-3.347144000	-1.123034000
1	-2.639047000	-2.932548000	-2.808211000
14	-0.256046000	-2.127003000	1.442495000
6	-0.229952000	-3.965684000	1.131106000
1	-0.526257000	-4.196141000	0.105458000
1	0.780414000	-4.355755000	1.282065000
1	-0.896712000	-4.497888000	1.813428000
6	0.333060000	-1.813306000	3.190340000
1	0.409569000	-0.740631000	3.391832000
1	-0.384863000	-2.233655000	3.900545000
1	1.303271000	-2.271905000	3.393974000
6	1.975169000	-1.706028000	-0.139688000
6	2.262719000	-2.107666000	-1.444352000
6	3.012502000	-1.702413000	0.792273000
6	3.545464000	-2.476357000	-1.806491000
1	1.461907000	-2.122248000	-2.175943000
6	4.293909000	-2.080299000	0.428722000
1	2.810341000	-1.376583000	1.807032000
6	4.570016000	-2.463537000	-0.873186000
1	3.744836000	-2.781125000	-2.827684000

1	5.084803000	-2.063485000	1.170164000
1	5.574630000	-2.752421000	-1.157892000
1	-0.121023000	-0.204531000	-2.046084000
14	1.311149000	1.868980000	-0.235013000
6	2.642613000	1.527863000	-1.543536000
1	3.200659000	0.637125000	-1.230267000
1	2.112351000	1.225656000	-2.455100000
6	2.018119000	1.713174000	1.520799000
1	1.485175000	2.414463000	2.171827000
1	1.752994000	0.714975000	1.889045000
6	0.616183000	3.608169000	-0.506976000
1	0.523648000	3.765032000	-1.588399000
1	-0.402719000	3.661913000	-0.114573000
6	1.456131000	4.710064000	0.126383000
1	2.479154000	4.720406000	-0.256724000
1	1.031762000	5.700736000	-0.055021000
1	1.520605000	4.580531000	1.210213000
6	3.520202000	1.922482000	1.650366000
1	3.815739000	2.928040000	1.339093000
1	3.860076000	1.788281000	2.680803000
1	4.075153000	1.211451000	1.031635000
6	3.601845000	2.662977000	-1.874964000
1	3.071319000	3.543009000	-2.248307000
1	4.180750000	2.978800000	-1.003806000
1	4.316887000	2.368686000	-2.647647000

5SiP^{Si-H} (T.E.= -2112.110007)

6	-1.584193000	-1.084049000	1.502637000
6	-1.880027000	-0.272377000	0.214486000
1	-1.500266000	-0.439754000	2.388718000
1	-2.375890000	-1.799385000	1.750989000
14	-0.167323000	-0.120524000	-0.557112000
7	0.511799000	-1.454509000	0.403813000
14	-2.711766000	1.353695000	0.678760000
14	-2.898133000	-1.371959000	-0.957539000
6	-1.588133000	2.410853000	1.749944000
1	-0.808282000	2.912547000	1.174600000
1	-2.198154000	3.190520000	2.214847000
1	-1.106888000	1.851476000	2.556071000
6	-4.243790000	1.056398000	1.717069000

1	-4.583258000	2.010834000	2.128121000
1	-5.069832000	0.623168000	1.153242000
1	-4.030002000	0.395297000	2.561168000
6	-4.608810000	-1.717354000	-0.269258000
1	-5.268019000	-0.853818000	-0.380186000
1	-5.047894000	-2.540886000	-0.839377000
1	-4.606015000	-2.009936000	0.782863000
6	-3.141815000	-0.624037000	-2.657739000
1	-3.602729000	-1.382142000	-3.297603000
1	-3.810054000	0.238227000	-2.637302000
1	-2.206302000	-0.319218000	-3.129907000
6	-3.156798000	2.344648000	-0.846606000
1	-4.061390000	1.965528000	-1.327213000
1	-3.338045000	3.387653000	-0.573865000
1	-2.354080000	2.329979000	-1.590179000
6	-2.051905000	-3.033082000	-1.165924000
1	-1.079906000	-2.956141000	-1.657059000
1	-1.909492000	-3.554786000	-0.216702000
1	-2.689652000	-3.662851000	-1.792769000
6	1.828386000	-1.950975000	0.241920000
6	2.748683000	-1.894916000	1.282622000
6	2.222310000	-2.443988000	-0.994285000
6	4.050457000	-2.312775000	1.076174000
1	2.434162000	-1.522614000	2.250454000
6	3.527518000	-2.857969000	-1.197085000
1	1.496395000	-2.494891000	-1.799071000
6	4.446752000	-2.789852000	-0.164095000
1	4.763245000	-2.261514000	1.891062000
1	3.825568000	-3.236208000	-2.167935000
1	5.469489000	-3.110915000	-0.322054000
6	-0.279907000	-1.857742000	1.451715000
8	0.012861000	-2.704345000	2.265157000
1	-0.186916000	-0.522441000	-1.992626000
14	1.403784000	1.631910000	-0.349673000
6	2.865967000	1.017576000	-1.384984000
1	3.360521000	0.215895000	-0.822974000
1	2.453769000	0.530525000	-2.277021000
6	0.779799000	3.268123000	-1.061665000
1	0.889426000	3.204617000	-2.150645000
1	-0.295953000	3.358276000	-0.881299000

6	1.892045000	1.762971000	1.476946000
1	1.258570000	2.511811000	1.960759000
1	1.627867000	0.809285000	1.952042000
6	3.359828000	2.073257000	1.732487000
1	3.640130000	3.048290000	1.325601000
1	3.588222000	2.089857000	2.800915000
1	4.011643000	1.325953000	1.272416000
6	3.877659000	2.075955000	-1.803689000
1	4.690394000	1.641214000	-2.390866000
1	3.418071000	2.852694000	-2.420281000
1	4.331535000	2.571605000	-0.942190000
6	1.495750000	4.501496000	-0.526897000
1	2.569540000	4.465874000	-0.727343000
1	1.112352000	5.421009000	-0.975610000
1	1.372115000	4.595016000	0.555544000

8SiP^{Si-H} (T.E. = -1680.717651)

6	-0.153375000	-2.486491000	-0.983908000
6	-1.649028000	-2.425205000	-0.711857000
6	-1.950750000	-1.085044000	-0.057994000
1	0.178775000	-3.525066000	-1.095215000
1	0.078959000	-1.965826000	-1.929203000
1	-1.918878000	-3.272847000	-0.062524000
1	-2.188063000	-2.576617000	-1.656555000
14	-0.451361000	-0.522710000	0.780650000
7	0.534352000	-1.847946000	0.128237000
15	-3.521685000	-0.565188000	0.153687000
6	-4.381474000	0.015818000	-1.334708000
1	-4.345026000	-0.768498000	-2.093525000
1	-5.425048000	0.263753000	-1.128845000
1	-3.864176000	0.894232000	-1.723444000
6	-4.670794000	-1.823715000	0.777358000
1	-4.316843000	-2.191007000	1.741472000
1	-5.680786000	-1.422787000	0.883392000
1	-4.697833000	-2.660310000	0.076073000
6	-3.630690000	0.804225000	1.316603000
1	-3.257373000	0.486721000	2.291261000
1	-3.034147000	1.645643000	0.960547000
1	-4.668321000	1.126922000	1.415545000
6	1.910873000	-1.879616000	0.185716000

6	2.702291000	-2.511717000	-0.782354000
6	2.573654000	-1.218744000	1.231757000
6	4.084255000	-2.448175000	-0.717251000
1	2.235938000	-3.033269000	-1.608550000
6	3.950320000	-1.153712000	1.278680000
1	1.986664000	-0.749043000	2.015932000
6	4.724358000	-1.763120000	0.300812000
1	4.668147000	-2.938103000	-1.489144000
1	4.426235000	-0.621141000	2.095356000
1	5.805406000	-1.710069000	0.338281000
1	-0.435209000	-0.580533000	2.281446000
14	0.485143000	1.532422000	0.073740000
6	1.510978000	1.159307000	-1.475035000
1	1.976094000	0.175447000	-1.344484000
1	0.809137000	1.045835000	-2.311461000
6	2.587665000	2.183356000	-1.806200000
1	3.306881000	2.272851000	-0.986941000
1	3.153585000	1.906397000	-2.699693000
1	2.169753000	3.178528000	-1.980219000
6	-0.917795000	2.721353000	-0.400074000
1	-1.692558000	2.104845000	-0.874959000
1	-1.364367000	3.112188000	0.523356000
6	-0.549314000	3.868624000	-1.330127000
1	0.212380000	4.520184000	-0.895513000
1	-0.152130000	3.497634000	-2.278234000
1	-1.413445000	4.495211000	-1.567837000
6	1.555221000	2.288096000	1.443965000
1	2.513148000	1.753957000	1.436026000
1	1.084443000	2.020764000	2.398353000
6	1.789066000	3.791086000	1.392522000
1	2.403942000	4.136608000	2.228077000
1	2.296652000	4.092089000	0.472410000
1	0.847165000	4.344827000	1.436968000

9SiP^{Si-H} (T.E.= -1679.530731)

6	0.035066000	-2.614973000	0.582715000
6	-1.280871000	-2.367505000	0.681087000
6	-1.789466000	-1.235525000	-0.084248000
14	-0.328340000	-0.463550000	-0.867794000
7	0.754962000	-1.741626000	-0.257089000

15	-3.404880000	-0.793391000	-0.074405000
6	-4.544376000	-2.166974000	-0.367603000
1	-4.373238000	-2.938069000	0.385885000
1	-5.582854000	-1.836511000	-0.303977000
1	-4.349983000	-2.595237000	-1.350983000
6	-3.752848000	0.439822000	-1.334994000
1	-4.821213000	0.658294000	-1.362999000
1	-3.212845000	1.360912000	-1.109455000
1	-3.431751000	0.069212000	-2.309437000
6	-4.047405000	-0.089005000	1.470537000
1	-3.516032000	0.836541000	1.698481000
1	-5.120214000	0.108381000	1.413529000
1	-3.855556000	-0.799888000	2.277223000
6	2.134187000	-1.689346000	-0.289620000
6	2.944907000	-2.282753000	0.686439000
6	2.767270000	-0.986045000	-1.322817000
6	4.321462000	-2.168682000	0.621845000
1	2.490980000	-2.812267000	1.515093000
6	4.142288000	-0.870667000	-1.370726000
1	2.160517000	-0.543111000	-2.107420000
6	4.936269000	-1.461726000	-0.399860000
1	4.923755000	-2.633119000	1.395291000
1	4.598740000	-0.317014000	-2.184153000
1	6.015108000	-1.375044000	-0.440212000
1	0.545791000	-3.457752000	1.027213000
1	-1.924504000	-3.016500000	1.267889000
1	-0.357069000	-0.389699000	-2.365265000
14	0.370018000	1.558089000	0.128717000
6	-1.040893000	2.809688000	-0.024082000
1	-1.943984000	2.349290000	0.397425000
1	-0.832678000	3.680193000	0.608624000
6	-1.279087000	3.247981000	-1.462866000
1	-2.154453000	3.894755000	-1.567838000
1	-0.421331000	3.800225000	-1.855108000
1	-1.424491000	2.390770000	-2.129305000
6	1.944206000	2.342539000	-0.568493000
1	2.781574000	1.708698000	-0.253025000
1	1.914604000	2.259054000	-1.661464000
6	2.183023000	3.790465000	-0.162766000
1	3.130503000	4.171648000	-0.552865000

1	1.395419000	4.450178000	-0.535987000
1	2.209159000	3.909881000	0.922879000
6	0.587553000	1.065455000	1.938942000
1	1.283639000	0.218448000	1.971758000
1	-0.377558000	0.660327000	2.269735000
6	1.056042000	2.166528000	2.877877000
1	1.063595000	1.842074000	3.921756000
1	2.072050000	2.486949000	2.634131000
1	0.415328000	3.051416000	2.817165000

14SiP^{Si-H} (T.E.= -1874.885518)

6	0.688264000	-2.178206000	0.454880000
6	1.340697000	-1.276597000	-0.447417000
7	-1.239272000	-0.713123000	-0.274876000
6	-2.529028000	-0.427739000	-0.728089000
6	-3.496316000	-1.432583000	-0.819217000
6	-4.763987000	-1.156833000	-1.292660000
6	-5.103981000	0.122809000	-1.706151000
6	-4.149016000	1.122172000	-1.640831000
6	-2.880316000	0.852617000	-1.157333000
1	-3.232249000	-2.439981000	-0.515658000
1	-5.493935000	-1.956723000	-1.351062000
1	-6.098226000	0.334412000	-2.080661000
1	-4.390752000	2.128568000	-1.964245000
1	-2.147516000	1.651827000	-1.103487000
5	-0.839873000	-1.711852000	0.701821000
7	-1.618861000	-2.122966000	1.798658000
6	-1.267264000	-3.247334000	2.639843000
1	-1.128783000	-2.923343000	3.678532000
1	-2.072100000	-3.993044000	2.635354000
1	-0.346313000	-3.705799000	2.285092000
6	-2.821205000	-1.463642000	2.248422000
1	-3.718506000	-2.067791000	2.060120000
1	-2.761321000	-1.291746000	3.329179000
1	-2.956572000	-0.499062000	1.761253000
15	2.951000000	-1.636132000	-0.869702000
6	3.151496000	-3.270137000	-1.598317000
1	4.202192000	-3.467260000	-1.819558000
1	2.774064000	-4.004208000	-0.886666000
1	2.565356000	-3.325582000	-2.516174000

6	4.129513000	-1.584194000	0.493089000
1	5.126349000	-1.868059000	0.150304000
1	4.160892000	-0.577394000	0.911386000
1	3.790384000	-2.278943000	1.261470000
6	3.556756000	-0.471908000	-2.099924000
1	2.931409000	-0.528465000	-2.992204000
1	3.518844000	0.544007000	-1.703071000
1	4.587133000	-0.710152000	-2.368647000
8	1.252656000	-3.164418000	0.968748000
14	0.195964000	0.042052000	-0.981313000
1	-0.001321000	0.187065000	-2.454725000
14	0.608193000	2.105388000	0.091221000
6	-0.187516000	3.573892000	-0.804159000
1	-1.247531000	3.592055000	-0.523074000
1	-0.174228000	3.356162000	-1.878747000
6	2.483275000	2.348566000	0.242511000
1	2.907703000	1.349043000	0.400254000
1	2.865125000	2.687132000	-0.729039000
6	-0.155484000	1.882669000	1.808282000
1	-1.099256000	1.340783000	1.669906000
1	0.490849000	1.195550000	2.370175000
6	0.436762000	4.937881000	-0.545142000
1	1.486737000	4.961104000	-0.847720000
1	-0.074748000	5.730662000	-1.097042000
1	0.400855000	5.206220000	0.513921000
6	2.968720000	3.270479000	1.352988000
1	4.059944000	3.325602000	1.387492000
1	2.597140000	4.290734000	1.233076000
1	2.632538000	2.917209000	2.331019000
6	-0.409592000	3.157095000	2.601011000
1	-0.862886000	2.948487000	3.573512000
1	0.510406000	3.717485000	2.784264000
1	-1.090511000	3.824436000	2.066007000

1GeP^{Si-H} (T.E.= -3825.501081)

6	0.152661000	-1.725463000	1.616970000
6	-1.123611000	-0.897706000	1.700551000
6	-1.664542000	-0.558109000	0.289700000
1	0.694274000	-1.654425000	2.570637000
1	-0.086659000	-2.792769000	1.477476000

1	-0.889266000	0.024362000	2.248391000
1	-1.869190000	-1.426929000	2.304600000
32	0.031242000	0.031123000	-0.531142000
7	0.958187000	-1.235208000	0.520634000
14	-2.259069000	-2.124405000	-0.609079000
14	-2.969879000	0.793044000	0.362517000
6	-2.481182000	2.124427000	1.595590000
1	-1.478104000	2.525562000	1.440734000
1	-3.184193000	2.957523000	1.502393000
1	-2.542389000	1.758398000	2.623430000
6	-3.213900000	1.599793000	-1.317568000
1	-3.903543000	1.031056000	-1.942668000
1	-3.633469000	2.601386000	-1.188773000
1	-2.278759000	1.704753000	-1.875132000
6	-4.625649000	0.162264000	0.980610000
1	-4.514880000	-0.333892000	1.949037000
1	-5.298222000	1.012703000	1.123793000
1	-5.113853000	-0.534456000	0.296463000
6	-3.311770000	-1.699367000	-2.100791000
1	-2.765219000	-1.066330000	-2.804882000
1	-3.562401000	-2.628955000	-2.619159000
1	-4.247295000	-1.196880000	-1.848038000
6	-0.891733000	-3.229361000	-1.272331000
1	-0.224951000	-3.615759000	-0.499040000
1	-1.372603000	-4.086992000	-1.753665000
1	-0.276495000	-2.734252000	-2.026606000
6	-3.254542000	-3.178731000	0.581342000
1	-2.616991000	-3.598465000	1.363516000
1	-4.063256000	-2.627361000	1.063607000
1	-3.696235000	-4.016903000	0.035673000
6	2.185377000	-1.790010000	0.265312000
6	2.917366000	-1.411694000	-0.871894000
6	2.765438000	-2.747724000	1.111817000
6	4.163673000	-1.941234000	-1.132283000
1	2.486415000	-0.699812000	-1.568785000
6	4.015920000	-3.273727000	0.835298000
1	2.235877000	-3.082231000	1.994722000
6	4.732272000	-2.877392000	-0.280004000
1	4.696425000	-1.621653000	-2.021415000
1	4.434389000	-4.010354000	1.512930000

1	5.710444000	-3.293331000	-0.487470000
1	0.119994000	-0.378607000	-2.031627000
14	1.036833000	2.204738000	-0.171737000
6	-0.091801000	3.597083000	-0.781948000
1	0.097546000	3.704071000	-1.857176000
1	-1.138206000	3.291849000	-0.699012000
6	0.097477000	4.932581000	-0.073104000
1	1.130263000	5.285924000	-0.124426000
1	-0.534182000	5.711026000	-0.507337000
1	-0.162372000	4.857991000	0.985976000
6	2.621243000	2.210071000	-1.193869000
1	3.263274000	1.389011000	-0.858714000
1	2.352260000	1.973492000	-2.230733000
6	3.377403000	3.529611000	-1.129794000
1	2.776826000	4.356257000	-1.518219000
1	3.653703000	3.782744000	-0.101936000
1	4.300986000	3.499289000	-1.712660000
6	1.479255000	2.437714000	1.646235000
1	1.904003000	3.445234000	1.734945000
1	0.565122000	2.455122000	2.249189000
6	2.459385000	1.410672000	2.196035000
1	3.379037000	1.373769000	1.604953000
1	2.746192000	1.636767000	3.225392000
1	2.035839000	0.403110000	2.182669000

2GeP^{Si-H} (T.E.= -3824.302867)

6	-1.700691000	-0.789030000	0.074774000
6	-1.404742000	-2.258426000	0.290989000
6	-0.134225000	-2.657927000	0.434948000
1	-2.215829000	-2.966195000	0.423112000
1	0.134179000	-3.682151000	0.674380000
32	0.115097000	-0.165815000	-0.424311000
7	0.882923000	-1.722077000	0.363540000
14	-2.195853000	-0.108336000	1.772086000
14	-2.983933000	-0.595849000	-1.296474000
6	-2.495062000	1.745168000	1.797171000
1	-2.616250000	2.056965000	2.838981000
1	-1.666316000	2.320220000	1.381252000
1	-3.399945000	2.027717000	1.257633000
6	-4.366979000	-1.843875000	-1.082118000

1	-4.848502000	-1.794484000	-0.103976000
1	-5.130809000	-1.649907000	-1.840566000
1	-4.006579000	-2.863917000	-1.233821000
6	-3.752181000	1.115689000	-1.317489000
1	-3.008963000	1.915074000	-1.256477000
1	-4.308899000	1.247756000	-2.249117000
1	-4.454569000	1.247292000	-0.490739000
6	-2.242044000	-0.933477000	-2.983808000
1	-1.574295000	-0.139775000	-3.326068000
1	-1.675476000	-1.868347000	-2.984235000
1	-3.052284000	-1.028085000	-3.712404000
6	-3.780345000	-0.912909000	2.369741000
1	-3.961003000	-0.619774000	3.407649000
1	-4.641894000	-0.587546000	1.781157000
1	-3.733830000	-2.003611000	2.334206000
6	-0.853657000	-0.469332000	3.029510000
1	-1.172658000	-0.092589000	4.005558000
1	-0.666879000	-1.540653000	3.122740000
1	0.094220000	0.013673000	2.780013000
6	2.213819000	-2.088182000	0.188007000
6	3.217664000	-1.207548000	0.595088000
6	2.596274000	-3.300792000	-0.390282000
6	4.551638000	-1.516023000	0.418306000
1	2.929916000	-0.283587000	1.087306000
6	3.935711000	-3.612614000	-0.544877000
1	1.837501000	-3.990459000	-0.741933000
6	4.923126000	-2.725302000	-0.149776000
1	5.308946000	-0.810948000	0.743609000
1	4.209281000	-4.558969000	-0.998397000
1	5.969441000	-2.973077000	-0.281029000
1	0.377772000	-0.435995000	-1.944427000
14	1.112223000	1.994453000	-0.023959000
6	-0.019294000	3.238260000	-0.876646000
1	0.483442000	4.212180000	-0.845327000
1	-0.935927000	3.362653000	-0.290554000
6	2.777738000	1.957985000	-0.920325000
1	3.518977000	1.574289000	-0.209784000
1	2.736550000	1.212107000	-1.721953000
6	1.356461000	2.419813000	1.790934000
1	0.383372000	2.427581000	2.292818000

1	1.925693000	1.609376000	2.260725000
6	-0.357101000	2.866212000	-2.314058000
1	-0.933162000	3.646820000	-2.815856000
1	0.542505000	2.688072000	-2.910220000
1	-0.953737000	1.949978000	-2.363577000
6	3.233745000	3.299397000	-1.480214000
1	2.562079000	3.658154000	-2.263715000
1	3.270195000	4.074469000	-0.710463000
1	4.231513000	3.230516000	-1.919605000
6	2.072661000	3.747702000	2.000656000
1	1.534145000	4.575167000	1.530337000
1	2.177017000	3.989456000	3.060642000
1	3.077996000	3.728114000	1.572530000

3GeP^{Si-H} (T.E.= -3945.602725)

6	-1.857170000	-1.762223000	-0.323541000
6	-1.894603000	-0.218613000	-0.077001000
1	-2.621006000	-2.260342000	0.287549000
1	-2.148256000	-1.985574000	-1.363157000
7	0.640856000	-1.431446000	-0.113357000
5	-0.407662000	-2.401997000	-0.104760000
7	-0.245446000	-3.804823000	0.053527000
6	-1.323183000	-4.743489000	-0.140638000
1	-1.063046000	-5.478928000	-0.913125000
1	-1.536444000	-5.304577000	0.779013000
1	-2.238172000	-4.245163000	-0.454434000
6	0.984105000	-4.486514000	0.380107000
1	1.371625000	-5.060115000	-0.473008000
1	1.757694000	-3.792020000	0.698800000
1	0.814283000	-5.197088000	1.198409000
14	-2.187977000	0.101185000	1.758076000
14	-3.175800000	0.562224000	-1.213178000
6	-0.976676000	-0.867722000	2.815426000
1	0.061176000	-0.582717000	2.630132000
1	-1.199010000	-0.673707000	3.868792000
1	-1.057172000	-1.945012000	2.649357000
6	-3.908116000	-0.438067000	2.283985000
1	-3.967562000	-0.409841000	3.375584000
1	-4.676073000	0.234740000	1.895320000
1	-4.152433000	-1.453502000	1.964759000

6	-4.800566000	-0.374954000	-1.137521000
1	-5.510882000	0.094259000	-1.824182000
1	-4.674839000	-1.413137000	-1.454135000
1	-5.249134000	-0.379044000	-0.143365000
6	-3.513351000	2.361635000	-0.796181000
1	-4.026978000	2.837160000	-1.636169000
1	-4.156404000	2.460476000	0.081324000
1	-2.597243000	2.926751000	-0.602697000
6	-2.039768000	1.913326000	2.232409000
1	-2.950586000	2.465071000	1.993374000
1	-1.881288000	1.986051000	3.312337000
1	-1.208729000	2.425263000	1.745125000
6	-2.642448000	0.499587000	-3.012714000
1	-1.837936000	1.203380000	-3.235645000
1	-2.305441000	-0.494683000	-3.316086000
1	-3.501130000	0.764729000	-3.636651000
32	-0.043884000	0.267609000	-0.566587000
6	2.028871000	-1.613144000	-0.249581000
6	2.582529000	-1.962411000	-1.479548000
6	2.885000000	-1.408317000	0.830828000
6	3.952059000	-2.104081000	-1.623096000
1	1.914798000	-2.121822000	-2.320686000
6	4.254768000	-1.547561000	0.685861000
1	2.453458000	-1.160427000	1.795599000
6	4.794970000	-1.892355000	-0.543334000
1	4.364931000	-2.378995000	-2.587188000
1	4.903801000	-1.387819000	1.539630000
1	5.866990000	-1.999649000	-0.657940000
1	0.096290000	0.317937000	-2.126610000
14	1.393273000	2.044895000	0.212416000
6	2.950685000	1.816419000	-0.833858000
1	3.535634000	1.004873000	-0.384286000
1	2.637756000	1.432477000	-1.812085000
6	0.593187000	3.695695000	-0.221790000
1	1.314541000	4.489591000	0.006962000
1	-0.257281000	3.871279000	0.446026000
6	0.150594000	3.783758000	-1.675563000
1	-0.263466000	4.763671000	-1.923676000
1	0.978864000	3.594445000	-2.364185000
1	-0.622278000	3.042263000	-1.902722000

6	3.811796000	3.059616000	-1.014868000
1	3.270960000	3.856081000	-1.532439000
1	4.148288000	3.469311000	-0.059386000
1	4.705391000	2.843984000	-1.605834000
6	1.761468000	1.946286000	2.058888000
1	0.894585000	2.339946000	2.600852000
1	1.832482000	0.891211000	2.341265000
6	3.029487000	2.675771000	2.479228000
1	3.011825000	3.728229000	2.181944000
1	3.174460000	2.647428000	3.561765000
1	3.912898000	2.221828000	2.021772000

4GeP^{Si-H} (T.E.= -4155.511833)

6	2.019413000	-1.922707000	0.128892000
6	1.925850000	-0.358407000	0.061817000
1	2.693028000	-2.315188000	-0.642353000
1	2.467565000	-2.249728000	1.075326000
7	-0.736594000	-1.494965000	-0.041759000
14	3.155208000	0.280702000	-1.213829000
14	2.183339000	0.289749000	1.809370000
6	2.985421000	-0.662524000	-2.829665000
1	2.008008000	-0.507501000	-3.291038000
1	3.745265000	-0.298962000	-3.527450000
1	3.136730000	-1.738233000	-2.713291000
6	4.929139000	0.065340000	-0.642115000
1	5.602686000	0.230665000	-1.487486000
1	5.194968000	0.782216000	0.137995000
1	5.116866000	-0.939612000	-0.256061000
6	3.791692000	-0.299637000	2.584050000
1	4.665349000	0.197576000	2.160898000
1	3.757341000	-0.058834000	3.650888000
1	3.943294000	-1.377738000	2.499046000
6	2.242359000	2.163872000	1.889934000
1	2.168097000	2.484274000	2.933149000
1	3.196103000	2.531342000	1.501372000
1	1.442396000	2.656885000	1.335297000
6	2.895821000	2.096124000	-1.608508000
1	3.027904000	2.741363000	-0.737799000
1	3.627681000	2.401749000	-2.361432000
1	1.904738000	2.288891000	-2.026735000

6	0.834504000	-0.362098000	2.941981000
1	-0.174834000	-0.162507000	2.579693000
1	0.934080000	-1.444056000	3.067376000
1	0.938421000	0.095456000	3.930252000
14	0.365852000	-2.819118000	-0.057414000
6	0.006239000	-4.016028000	1.329169000
1	0.051159000	-3.524074000	2.303726000
1	-0.993296000	-4.443847000	1.213488000
1	0.722079000	-4.841606000	1.328314000
6	0.327265000	-3.748007000	-1.680924000
1	0.492961000	-3.056791000	-2.512951000
1	1.104747000	-4.515579000	-1.719313000
1	-0.636762000	-4.239134000	-1.836615000
32	0.079390000	0.106430000	-0.564396000
6	-2.133209000	-1.663168000	-0.067115000
6	-2.828029000	-1.823448000	-1.265522000
6	-2.856972000	-1.673344000	1.124750000
6	-4.203367000	-1.979609000	-1.271542000
1	-2.267413000	-1.811072000	-2.195980000
6	-4.232361000	-1.830435000	1.117772000
1	-2.313995000	-1.553770000	2.057787000
6	-4.912474000	-1.981806000	-0.080646000
1	-4.725631000	-2.098978000	-2.214253000
1	-4.776905000	-1.833842000	2.055429000
1	-5.989134000	-2.103388000	-0.086236000
1	0.093907000	0.107084000	-2.135630000
14	-1.315661000	2.000519000	0.035936000
6	-2.957379000	1.674895000	-0.835030000
1	-2.728626000	1.292960000	-1.837284000
1	-3.448078000	0.844038000	-0.315540000
6	-3.898601000	2.868439000	-0.939728000
1	-4.801099000	2.616009000	-1.501914000
1	-4.220202000	3.223607000	0.040882000
1	-3.430561000	3.715743000	-1.447300000
6	-0.536344000	3.557773000	-0.692569000
1	-1.065791000	4.430422000	-0.292572000
1	0.491947000	3.646764000	-0.326315000
6	-0.552424000	3.592195000	-2.216007000
1	-1.568983000	3.685736000	-2.603925000
1	0.024546000	4.431774000	-2.610472000

1	-0.135496000	2.679531000	-2.652489000
6	-1.550129000	2.148577000	1.899541000
1	-1.901355000	1.175381000	2.262553000
1	-0.569076000	2.300381000	2.362768000
6	-2.515211000	3.239148000	2.344895000
1	-3.538465000	3.012075000	2.038845000
1	-2.521891000	3.350765000	3.431700000
1	-2.258157000	4.213960000	1.921182000

5GeP^{Si-H} (T.E.= -3899.569674)

6	-1.572519000	-1.027279000	1.530990000
6	-1.932639000	-0.241352000	0.248106000
1	-1.433175000	-0.362279000	2.394877000
1	-2.365784000	-1.717990000	1.837507000
7	0.511886000	-1.486164000	0.415110000
14	-2.710421000	1.410951000	0.705616000
14	-2.997156000	-1.351283000	-0.863287000
6	-1.536319000	2.452570000	1.737999000
1	-0.719688000	2.876606000	1.151322000
1	-2.103408000	3.290952000	2.152388000
1	-1.100266000	1.908245000	2.578985000
6	-4.232850000	1.180149000	1.774221000
1	-4.523438000	2.146907000	2.193851000
1	-5.086893000	0.784159000	1.224543000
1	-4.031397000	0.506944000	2.611802000
6	-4.691428000	-1.648667000	-0.115314000
1	-5.334917000	-0.771955000	-0.213873000
1	-5.168680000	-2.469127000	-0.658694000
1	-4.657041000	-1.928942000	0.939739000
6	-3.278689000	-0.632775000	-2.570906000
1	-3.773773000	-1.391900000	-3.183225000
1	-3.929369000	0.242825000	-2.545235000
1	-2.353099000	-0.353953000	-3.077973000
6	-3.146192000	2.396515000	-0.827008000
1	-4.060522000	2.031576000	-1.300002000
1	-3.306211000	3.445022000	-0.562238000
1	-2.348129000	2.361735000	-1.575387000
6	-2.187346000	-3.031282000	-1.055505000
1	-1.217848000	-2.981042000	-1.554314000
1	-2.045283000	-3.537435000	-0.097643000

1	-2.842112000	-3.660359000	-1.665176000
6	1.823319000	-1.987059000	0.268222000
6	2.733185000	-1.952592000	1.321092000
6	2.239264000	-2.455092000	-0.972374000
6	4.037445000	-2.367466000	1.123586000
1	2.410438000	-1.597293000	2.292436000
6	3.546252000	-2.867370000	-1.165381000
1	1.527887000	-2.488128000	-1.791072000
6	4.452048000	-2.821617000	-0.119173000
1	4.738772000	-2.331047000	1.949407000
1	3.856659000	-3.226356000	-2.139792000
1	5.476574000	-3.140869000	-0.268931000
6	-0.286249000	-1.836889000	1.464753000
8	-0.020439000	-2.677584000	2.299037000
32	-0.169431000	-0.055348000	-0.635343000
1	-0.222466000	-0.566897000	-2.103986000
14	1.509668000	1.653898000	-0.345997000
6	2.937240000	1.048166000	-1.423044000
1	3.354438000	0.140077000	-0.972232000
1	2.498051000	0.723936000	-2.374803000
6	0.952028000	3.350804000	-0.957732000
1	1.120437000	3.364037000	-2.040989000
1	-0.128479000	3.466731000	-0.826707000
6	1.680805000	4.512232000	-0.293408000
1	2.764700000	4.429602000	-0.407927000
1	1.381975000	5.473972000	-0.716464000
1	1.472542000	4.552824000	0.778888000
6	4.036237000	2.069328000	-1.686759000
1	3.645219000	2.968688000	-2.170183000
1	4.528606000	2.383718000	-0.763396000
1	4.810020000	1.663270000	-2.342572000
6	1.939034000	1.620487000	1.496860000
1	1.372045000	2.407597000	2.002615000
1	1.548441000	0.676831000	1.898538000
6	3.419259000	1.737197000	1.831387000
1	3.837994000	2.689363000	1.495781000
1	3.590174000	1.669854000	2.908474000
1	3.998522000	0.937106000	1.362259000

8Ge^{PSi-H} (T.E.= -3468.168590)

6	-0.100611000	-2.369804000	1.069153000
6	1.364932000	-2.523568000	0.692202000
6	1.822137000	-1.279429000	-0.047440000
1	-0.539370000	-3.346617000	1.307785000
1	-0.185142000	-1.747768000	1.978057000
1	1.468453000	-3.429512000	0.074932000
1	1.940319000	-2.710159000	1.609534000
32	0.313975000	-0.501586000	-0.906080000
7	-0.803891000	-1.773996000	-0.049681000
15	3.404719000	-0.773066000	-0.025499000
6	4.019830000	-0.013456000	1.511489000
1	3.848273000	-0.709102000	2.336048000
1	5.085195000	0.223696000	1.462323000
1	3.448869000	0.895794000	1.710340000
6	3.747981000	0.453057000	-1.297707000
1	3.505150000	0.038181000	-2.276604000
1	3.144467000	1.346119000	-1.128976000
1	4.801592000	0.735717000	-1.272679000
6	4.610758000	-2.103310000	-0.277155000
1	5.635527000	-1.735569000	-0.195572000
1	4.450890000	-2.871551000	0.482283000
1	4.454810000	-2.551423000	-1.259029000
6	-2.176266000	-1.709215000	-0.040404000
6	-2.861349000	-1.231739000	-1.170855000
6	-2.954264000	-2.113962000	1.054989000
6	-4.237178000	-1.151138000	-1.196857000
1	-2.287509000	-0.937598000	-2.045149000
6	-4.336170000	-2.031696000	1.013958000
1	-2.474135000	-2.485061000	1.951766000
6	-4.994751000	-1.548353000	-0.102768000
1	-4.727330000	-0.777364000	-2.089750000
1	-4.905676000	-2.348909000	1.881326000
1	-6.075775000	-1.486060000	-0.125959000
1	0.196562000	-0.722437000	-2.449709000
14	-0.354514000	1.680232000	-0.126447000
6	-1.984784000	2.251875000	-0.886238000
1	-1.778921000	2.595527000	-1.907330000
1	-2.619246000	1.365455000	-0.993222000
6	1.023918000	2.925330000	-0.500200000

1	1.865646000	2.696832000	0.167052000
1	1.383790000	2.725588000	-1.516692000
6	-0.521388000	1.418189000	1.736543000
1	0.256982000	0.699920000	2.024259000
1	-1.474736000	0.901647000	1.908049000
6	-2.746614000	3.315705000	-0.104681000
1	-2.176372000	4.241599000	0.008039000
1	-3.689817000	3.573799000	-0.592871000
1	-2.992979000	2.961923000	0.900004000
6	0.646422000	4.395757000	-0.381752000
1	-0.160544000	4.651234000	-1.072826000
1	0.301419000	4.648408000	0.623940000
1	1.489151000	5.052688000	-0.611944000
6	-0.416665000	2.661099000	2.609138000
1	-1.179831000	3.402489000	2.359708000
1	-0.528536000	2.424320000	3.670383000
1	0.555653000	3.147604000	2.489047000

${}^9\text{GeP}^{\text{Si-H}}$ (T.E.= -3466.984119)

6	-0.066084000	-2.557249000	0.790375000
6	-1.379666000	-2.276172000	0.846307000
6	-1.901596000	-1.249260000	-0.039965000
7	0.707469000	-1.832380000	-0.128035000
15	-3.464019000	-0.656411000	0.031230000
6	-4.718716000	-1.950967000	0.162148000
1	-4.537824000	-2.538042000	1.064112000
1	-5.718763000	-1.517551000	0.221521000
1	-4.649992000	-2.610678000	-0.702670000
6	-3.864199000	0.293230000	-1.444370000
1	-4.870456000	0.707844000	-1.366175000
1	-3.156903000	1.115994000	-1.566417000
1	-3.801988000	-0.355145000	-2.318821000
6	-3.905699000	0.435902000	1.419230000
1	-3.287317000	1.335053000	1.388067000
1	-4.960836000	0.718863000	1.400139000
1	-3.690776000	-0.091918000	2.350926000
32	-0.385450000	-0.518665000	-0.965742000
6	2.079658000	-1.764351000	-0.071962000
6	2.787763000	-1.206049000	-1.146286000
6	2.824323000	-2.206183000	1.033152000

6	4.162475000	-1.084368000	-1.112924000
1	2.238424000	-0.886094000	-2.027724000
6	4.201266000	-2.086061000	1.050225000
1	2.313143000	-2.617702000	1.895011000
6	4.887618000	-1.522251000	-0.014412000
1	4.674732000	-0.645840000	-1.962852000
1	4.747013000	-2.428437000	1.923160000
1	5.966364000	-1.429109000	0.009811000
1	0.404175000	-3.359221000	1.344546000
1	-2.026809000	-2.852014000	1.502026000
1	-0.387765000	-0.717185000	-2.516336000
14	0.420334000	1.595862000	-0.142282000
6	-0.968146000	2.879659000	-0.260733000
1	-1.926951000	2.357219000	-0.163761000
1	-0.961161000	3.299613000	-1.273658000
6	1.950610000	2.216785000	-1.055733000
1	2.785958000	1.565130000	-0.774969000
1	1.784037000	2.029119000	-2.123539000
6	0.765039000	1.183266000	1.669356000
1	-0.188619000	1.260387000	2.207351000
1	1.038535000	0.123492000	1.719472000
6	-0.901069000	3.988634000	0.780810000
1	0.032938000	4.551109000	0.715905000
1	-1.719654000	4.704749000	0.671512000
1	-0.959541000	3.581155000	1.793832000
6	2.315811000	3.679293000	-0.839563000
1	1.505059000	4.347306000	-1.143105000
1	2.534097000	3.890863000	0.210511000
1	3.199501000	3.963726000	-1.416494000
6	1.843461000	2.014734000	2.348547000
1	1.995415000	1.712267000	3.387621000
1	2.803933000	1.900241000	1.837099000
1	1.602667000	3.081280000	2.352189000

14GeP^{Si-H} (T.E.= -3662.342738)

6	0.525903000	-2.150641000	0.475130000
6	1.213450000	-1.359750000	-0.493683000
7	-1.369427000	-0.581635000	-0.199718000
6	-2.639114000	-0.277280000	-0.673634000
6	-3.673812000	-1.220695000	-0.639533000

6	-4.924318000	-0.926065000	-1.145692000
6	-5.189169000	0.310610000	-1.715669000
6	-4.171342000	1.246614000	-1.775464000
6	-2.918295000	0.959421000	-1.264515000
1	-3.473025000	-2.201786000	-0.223444000
1	-5.701364000	-1.681671000	-1.105371000
1	-6.170836000	0.535892000	-2.114425000
1	-4.350621000	2.218096000	-2.222978000
1	-2.136032000	1.711400000	-1.320014000
5	-0.965664000	-1.585381000	0.763513000
7	-1.714331000	-1.929066000	1.907433000
6	-1.410095000	-3.059471000	2.757826000
1	-1.192726000	-2.726449000	3.780361000
1	-2.270944000	-3.738067000	2.813191000
1	-0.546988000	-3.596722000	2.370974000
6	-2.830532000	-1.162105000	2.402828000
1	-3.784518000	-1.693859000	2.288140000
1	-2.692930000	-0.963550000	3.472296000
1	-2.913328000	-0.204949000	1.889886000
15	2.835940000	-1.749826000	-0.821545000
6	3.078083000	-3.431511000	-1.414090000
1	4.138748000	-3.630997000	-1.578162000
1	2.678243000	-4.112400000	-0.663313000
1	2.529082000	-3.563219000	-2.346880000
6	3.959283000	-1.569705000	0.579292000
1	4.964675000	-1.911449000	0.325831000
1	3.995094000	-0.518959000	0.874049000
1	3.567131000	-2.158685000	1.408851000
6	3.485083000	-0.670282000	-2.105453000
1	2.873467000	-0.765540000	-3.003778000
1	3.454438000	0.366448000	-1.764642000
1	4.517327000	-0.933683000	-2.341332000
8	1.051693000	-3.135159000	1.037741000
32	0.170159000	0.164886000	-1.001114000
1	-0.098650000	0.332873000	-2.523263000
14	0.862170000	2.111745000	0.224298000
6	-0.411685000	3.498892000	0.305922000
1	0.100859000	4.401333000	0.659769000
1	-0.740640000	3.731800000	-0.713719000
6	2.477521000	2.743602000	-0.539520000

1	3.276811000	2.083466000	-0.174934000
1	2.437668000	2.593150000	-1.624620000
6	1.188711000	1.446346000	1.955277000
1	0.246317000	1.050143000	2.353623000
1	1.849628000	0.576610000	1.858419000
6	1.790036000	2.469164000	2.907993000
1	1.927858000	2.065617000	3.914040000
1	2.769425000	2.806543000	2.556749000
1	1.157969000	3.357750000	2.997693000
6	-1.607211000	3.199042000	1.200213000
1	-1.305863000	3.089699000	2.244893000
1	-2.353639000	3.995716000	1.161277000
1	-2.111160000	2.272190000	0.912509000
6	2.821220000	4.196359000	-0.239381000
1	3.794971000	4.478274000	-0.647082000
1	2.080778000	4.873381000	-0.671592000
1	2.846984000	4.396013000	0.835059000

IX-PSi-H (T.E.= -2608.125475)

6	0.674365000	-2.447208000	0.415072000
6	-0.727947000	-2.223224000	0.978709000
6	-1.485866000	-1.094261000	0.214137000
6	1.428536000	-1.096747000	0.181342000
1	1.239791000	-3.110077000	1.083540000
1	0.580846000	-2.997544000	-0.525958000
1	-0.638081000	-1.958240000	2.039263000
1	-1.287330000	-3.168257000	0.957868000
14	-0.033375000	-0.004633000	-0.376788000
14	2.367250000	-0.651690000	1.764478000
14	2.699870000	-1.337392000	-1.222463000
14	-2.711264000	-0.317659000	1.422781000
14	-2.377461000	-1.814527000	-1.300009000
6	-3.769339000	-1.608128000	2.288407000
1	-3.168334000	-2.443283000	2.656738000
1	-4.227431000	-1.130021000	3.159673000
1	-4.570208000	-2.014266000	1.672550000
6	-3.869924000	0.932047000	0.640110000
1	-4.534330000	1.309308000	1.422936000
1	-3.340665000	1.789856000	0.218319000

1	-4.497251000	0.502988000	-0.143755000
6	-1.851659000	0.546623000	2.852380000
1	-2.562143000	1.244502000	3.305719000
1	-1.572380000	-0.176110000	3.622354000
1	-0.962867000	1.113393000	2.576065000
6	-2.905121000	-0.527008000	-2.557728000
1	-3.468385000	-1.041821000	-3.341973000
1	-3.559837000	0.236688000	-2.133286000
1	-2.058634000	-0.025820000	-3.030018000
6	-1.345563000	-3.093407000	-2.211479000
1	-1.932957000	-3.442656000	-3.065923000
1	-0.401945000	-2.704745000	-2.595406000
1	-1.131569000	-3.962615000	-1.584805000
6	-3.939200000	-2.754790000	-0.837590000
1	-3.764178000	-3.505821000	-0.063715000
1	-4.748864000	-2.101754000	-0.505704000
1	-4.285783000	-3.277204000	-1.734310000
6	1.389724000	-0.876830000	3.350275000
1	0.571339000	-0.167780000	3.462696000
1	0.992773000	-1.887898000	3.465498000
1	2.088136000	-0.704926000	4.175219000
6	3.830463000	-1.806950000	2.040819000
1	4.597905000	-1.789744000	1.266818000
1	4.302588000	-1.513000000	2.983043000
1	3.495274000	-2.841058000	2.159432000
6	2.995875000	1.113882000	1.811046000
1	3.521018000	1.259160000	2.759713000
1	3.690000000	1.353421000	1.005236000
1	2.176270000	1.835904000	1.780922000
6	2.074908000	-1.071325000	-2.975063000
1	1.184863000	-1.643234000	-3.238435000
1	1.869816000	-0.018976000	-3.183441000
1	2.884027000	-1.391097000	-3.640233000
6	3.341124000	-3.103938000	-1.204930000
1	4.172614000	-3.175311000	-1.911998000
1	3.699453000	-3.437100000	-0.230251000
1	2.570215000	-3.803289000	-1.538642000
6	4.175677000	-0.173287000	-1.144492000
1	4.788876000	-0.259611000	-0.247413000
1	4.810591000	-0.414091000	-2.002854000

1	3.872611000	0.871246000	-1.251776000
1	-0.071782000	-0.051335000	-1.870183000
14	-0.001899000	2.357005000	-0.336943000
6	1.643771000	2.803462000	-1.169588000
6	1.669565000	4.131449000	-1.914714000
1	1.859188000	1.991063000	-1.876743000
1	2.446347000	2.769636000	-0.425770000
1	2.631540000	4.299564000	-2.405521000
1	0.901780000	4.167516000	-2.691397000
1	1.493995000	4.977395000	-1.246204000
6	-1.374948000	2.791036000	-1.573733000
6	-2.000763000	4.171400000	-1.442801000
1	-2.155875000	2.026819000	-1.516083000
1	-0.933598000	2.663184000	-2.570174000
1	-2.761215000	4.345362000	-2.208331000
1	-2.488557000	4.300234000	-0.472391000
1	-1.258786000	4.968491000	-1.536613000
6	-0.221590000	3.288006000	1.296610000
6	0.325771000	4.708244000	1.313626000
1	0.257798000	2.709231000	2.093444000
1	-1.289553000	3.285695000	1.546323000
1	0.164505000	5.190340000	2.281011000
1	1.402430000	4.719571000	1.122789000
1	-0.144886000	5.338379000	0.554861000