

Supporting Information File

Can Main Group Systems Act as Superior Catalysts for Dihydrogen Generation Reactions? A Computational Investigation

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1. The Figures discussed in the manuscript.

Figure S1. Frontier molecular orbitals of GeH-1 and GeH-2.

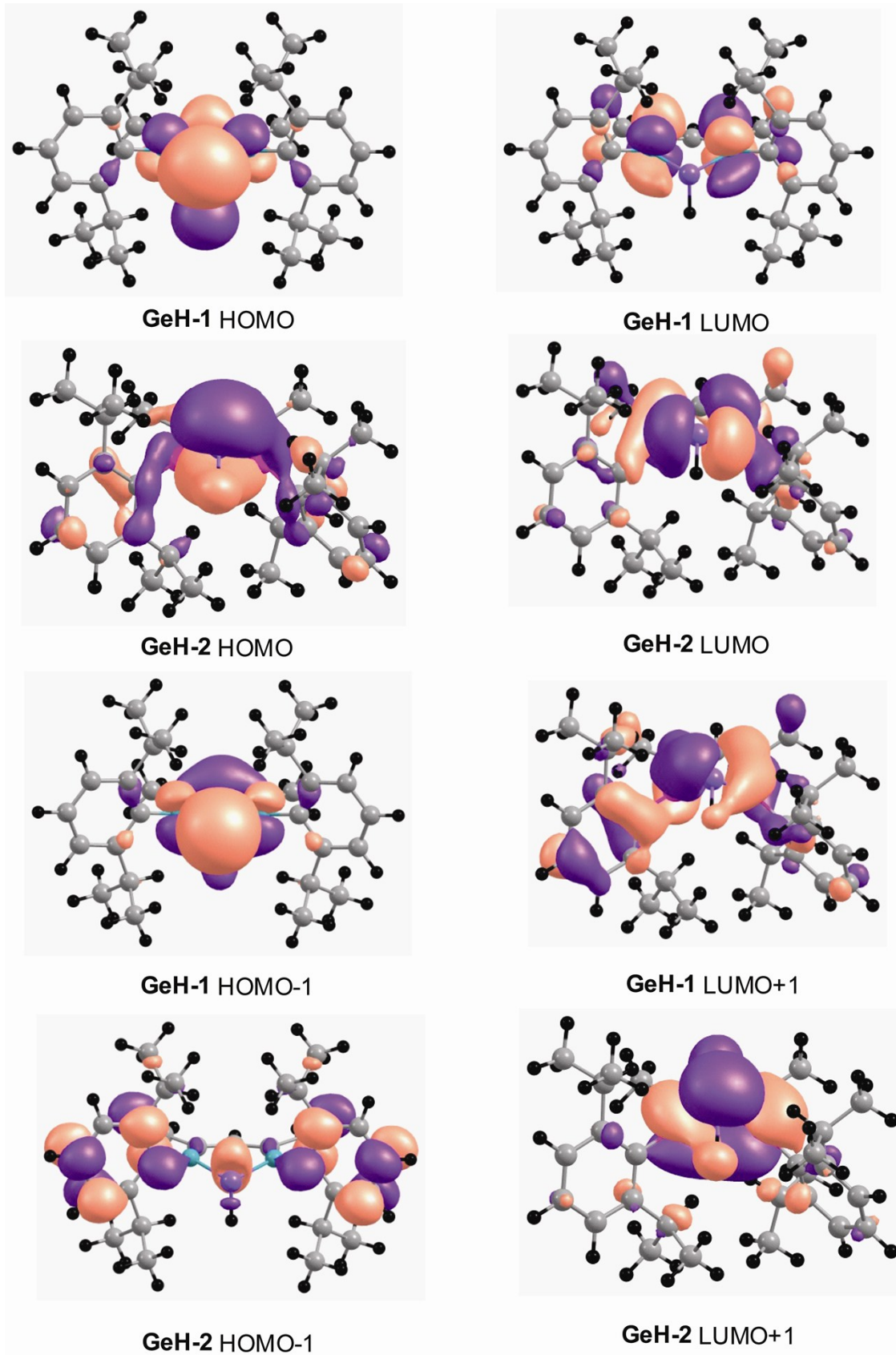


Figure S2. Comparative study for the singlet and triplet states of **GeH-2**; the values outside the parentheses correspond to the gas phase free energies at the B3LYP/QZVP//PBE/TZVP level and the values inside the parentheses correspond to the gas phase free energies at the PBE/TZVP level of theory.

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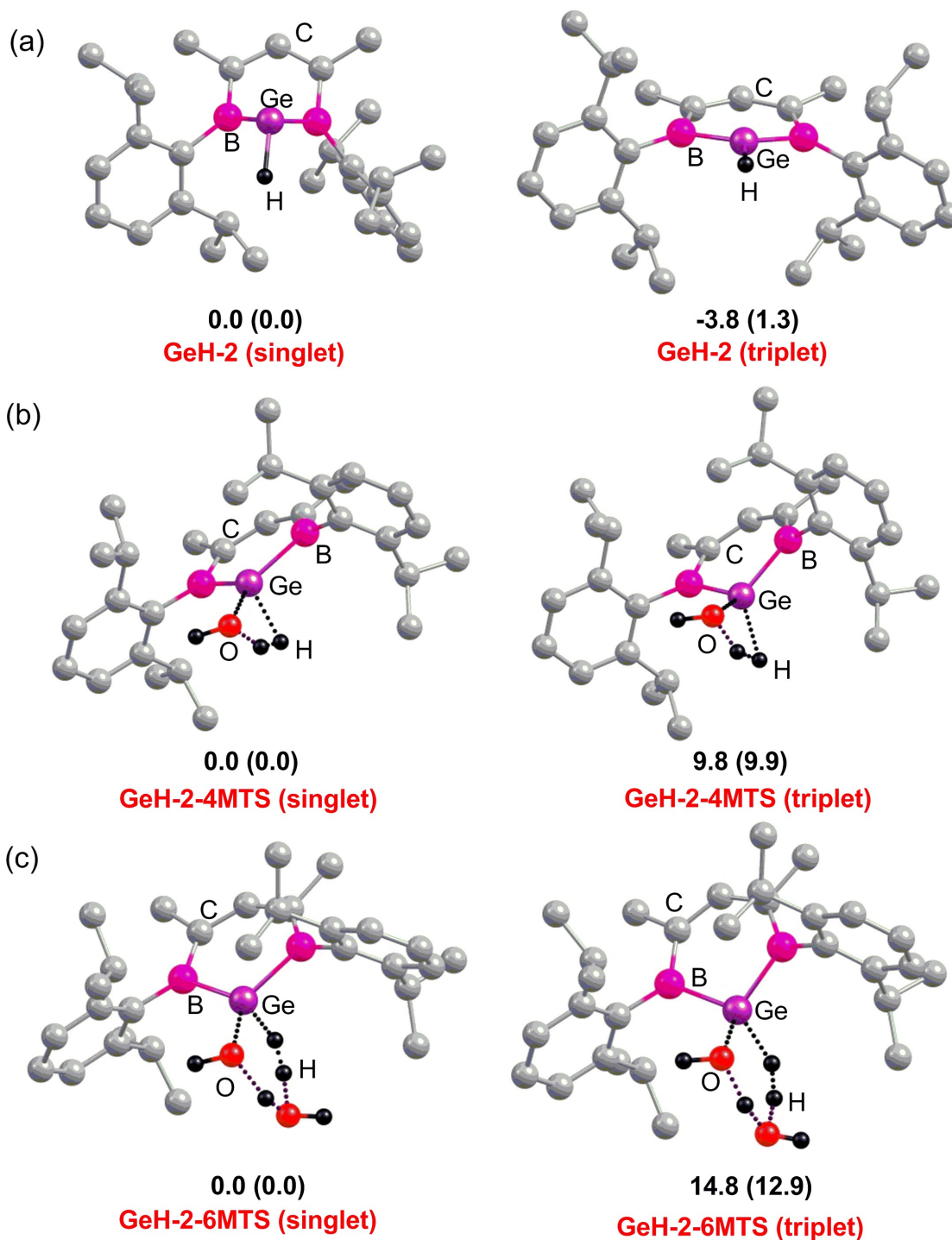
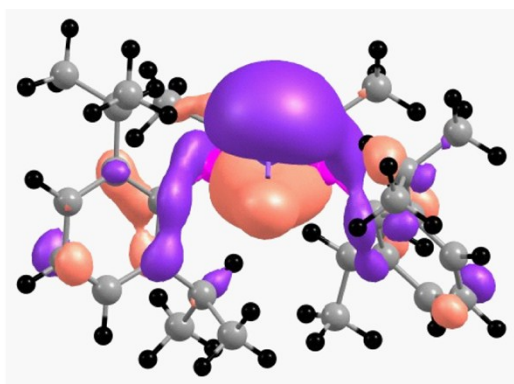
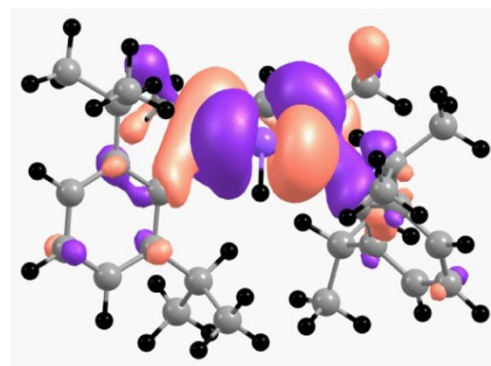


Figure S3. Frontier molecular orbitals of **GeH-2** (singlet) and **GeH-2** (triplet).

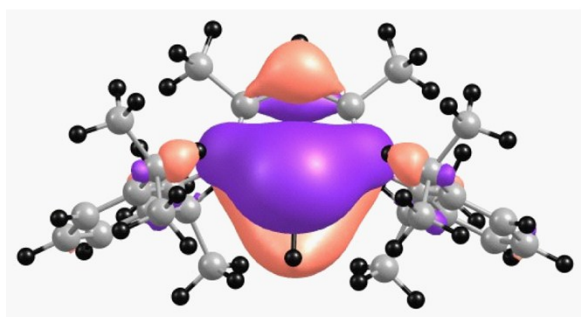
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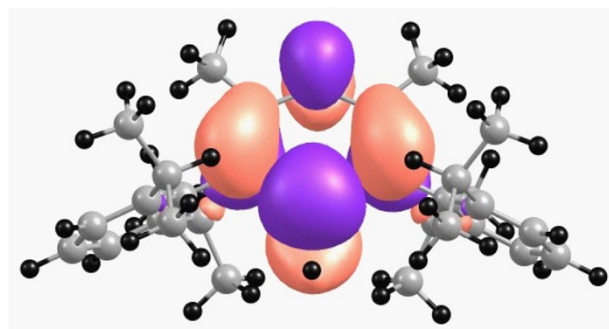
GeH-2 (singlet) HOMO



GeH-2 (singlet) LUMO



GeH-2 (triplet) HOMO



GeH-2 (triplet) LUMO

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2. The Tables discussed in the manuscript.

Table S1: Comparative study of the thermodynamic parameters obtained from full geometry optimization carried out at PBE/TZVP and B3LYP/QZVP.

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System	PBE/TZVP		B3LYP/QZVP	
	Internal Energy	Entropy	Internal Energy	Entropy
H ₂	7.631453	0.032622	7.774857	0.032569
H ₂ O	14.64627	0.046601	15.03824	0.046527
CH ₃ OH	33.01864	0.057048	33.85516	0.05718
C ₂ H ₅ OH	51.10421	0.06441	52.30641	0.064304
SiF ₃ H	13.28633	0.069536	13.84799	0.068709
SiF ₃ OH	17.63384	0.076671	18.19073	0.076205
HC{CMeHB} ₂ GeH	53.18595	0.081283	54.38576	0.080796
HC{CMePhB} ₂ GeH	159.0942	0.134634	163.3437	0.130696

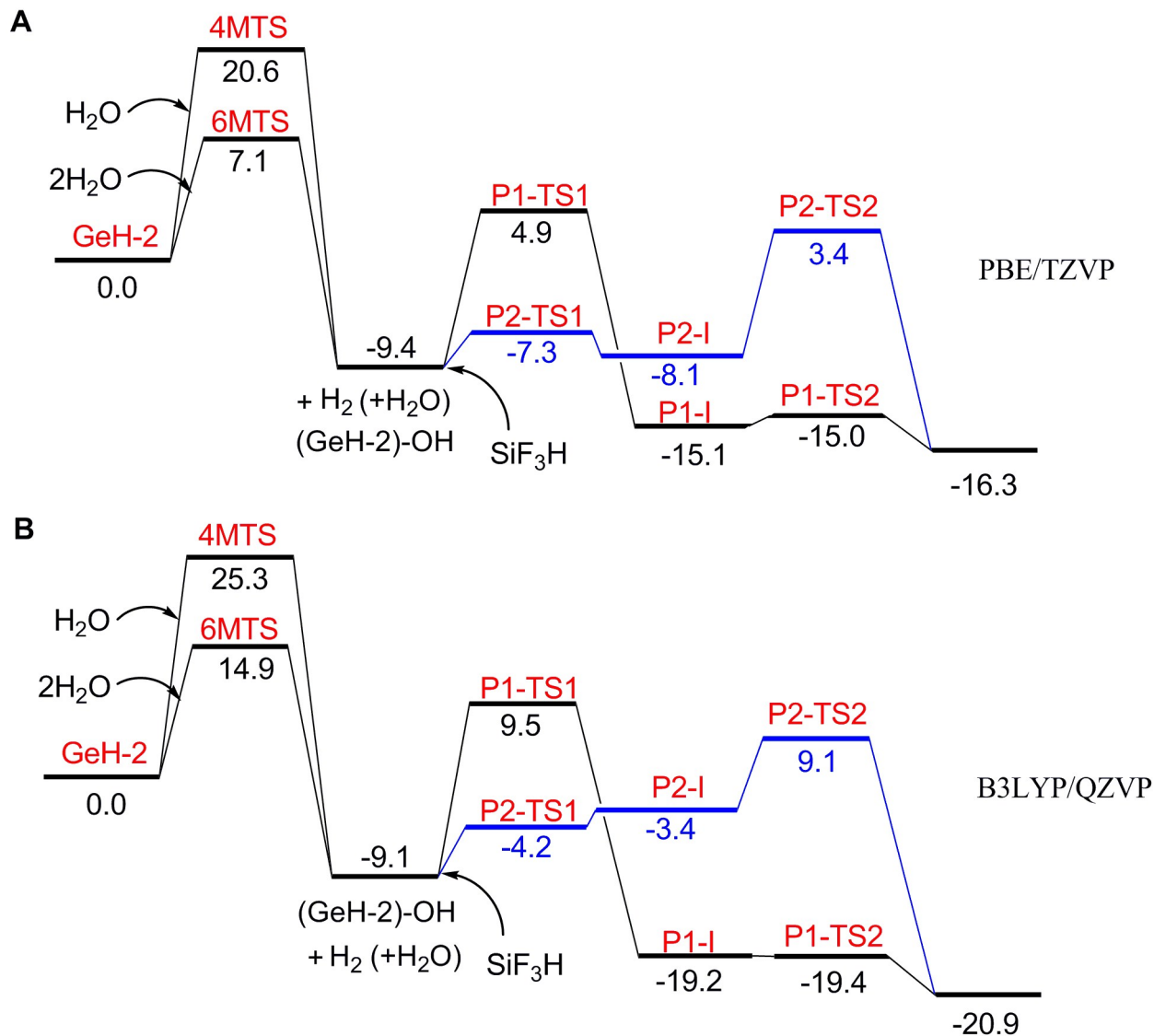
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3. The Schemes discussed in the manuscript.

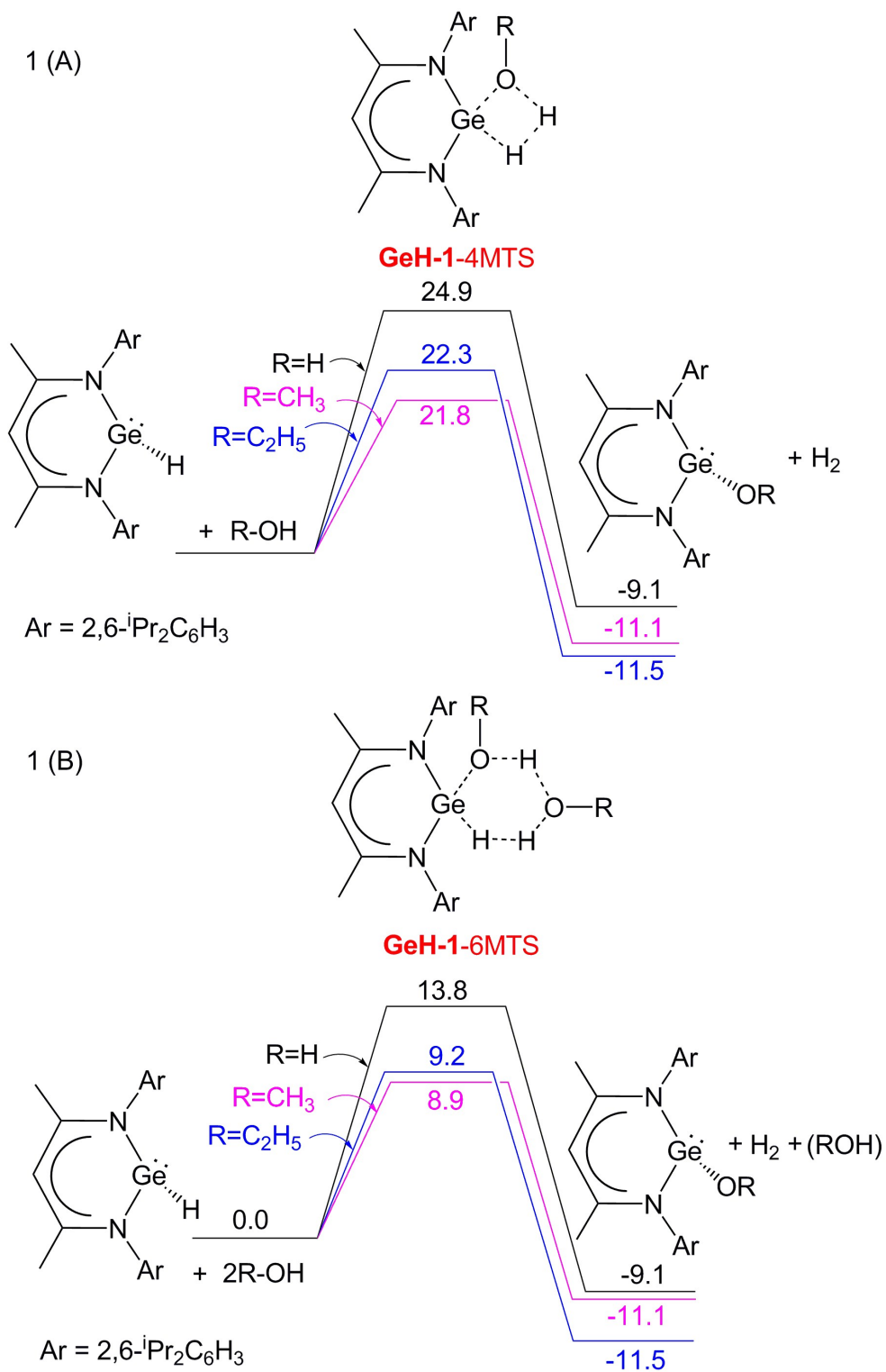
5 **Scheme S1.** Gas phase free energy profiles for the reaction of **GeH-2** with water: comparative study of the calculations at PBE/TZVP and the B3LYP/QZVP//PBE/TZVP level of theory.

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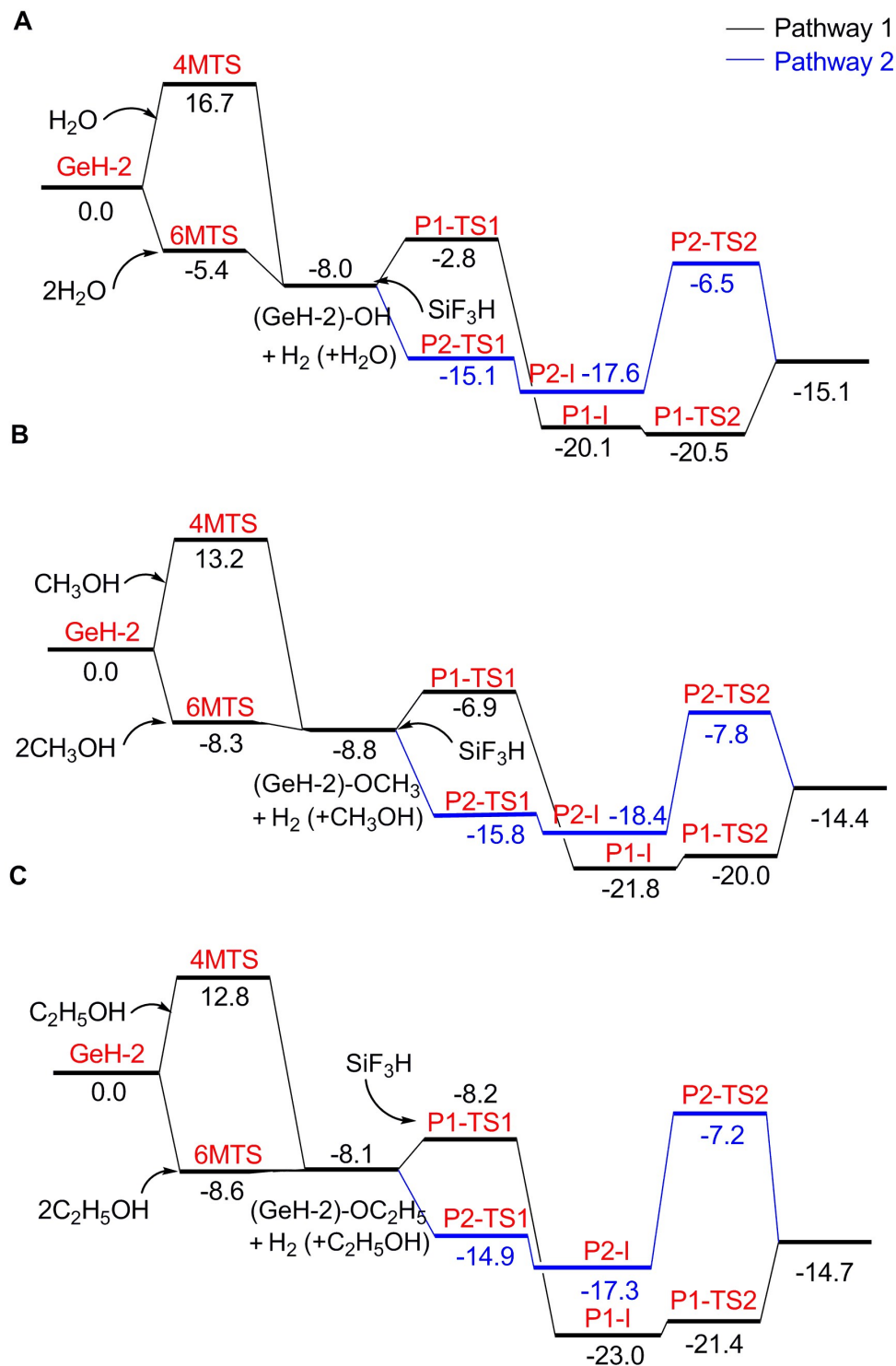


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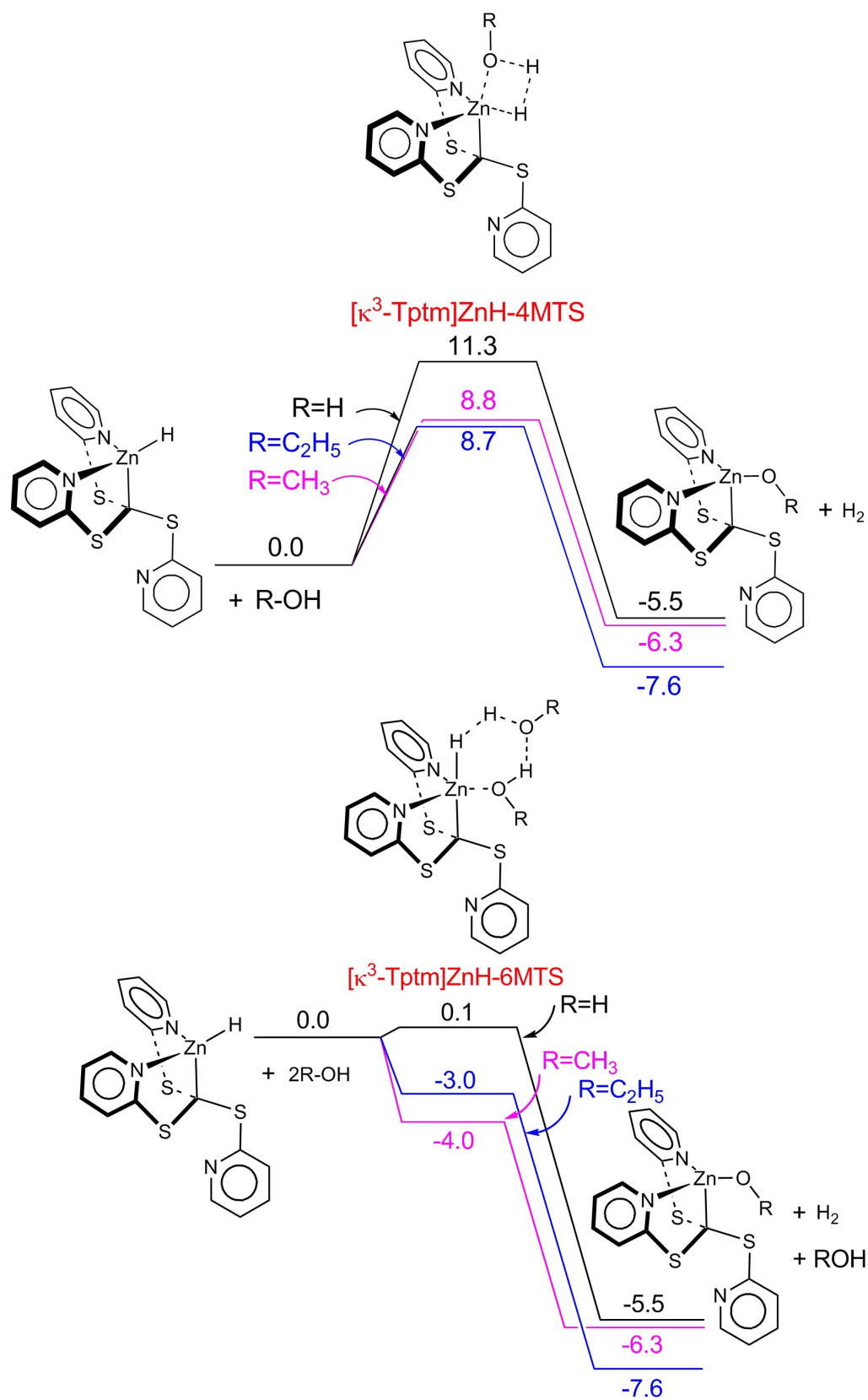
Scheme S2. Enthalpy profiles for the reaction of **GeH-1** with ROH (R=H, CH₃, C₂H₅).



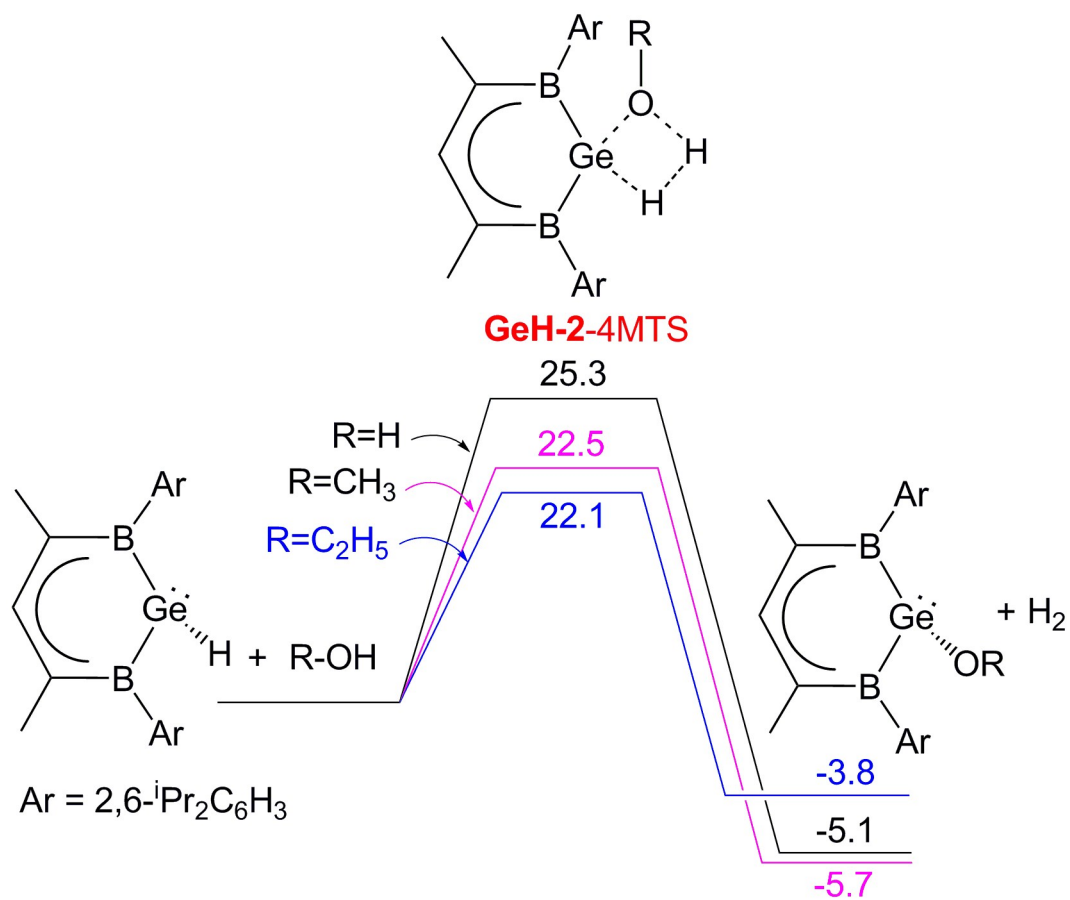
Scheme S3. Enthalpy profiles for the reaction of **GeH-2** with ROH (R=H, CH₃, C₂H₅).



Scheme S4. Enthalpy profiles for the reaction of $[\kappa^3\text{-Tptm}]\text{ZnH}$ with ROH ($\text{R}=\text{H}, \text{CH}_3, \text{C}_2\text{H}_5$).



Scheme S5. Free energy profiles for the reaction of **GeH-2** with ROH (R=H, CH₃, C₂H₅) through a 5 four membered transition state.



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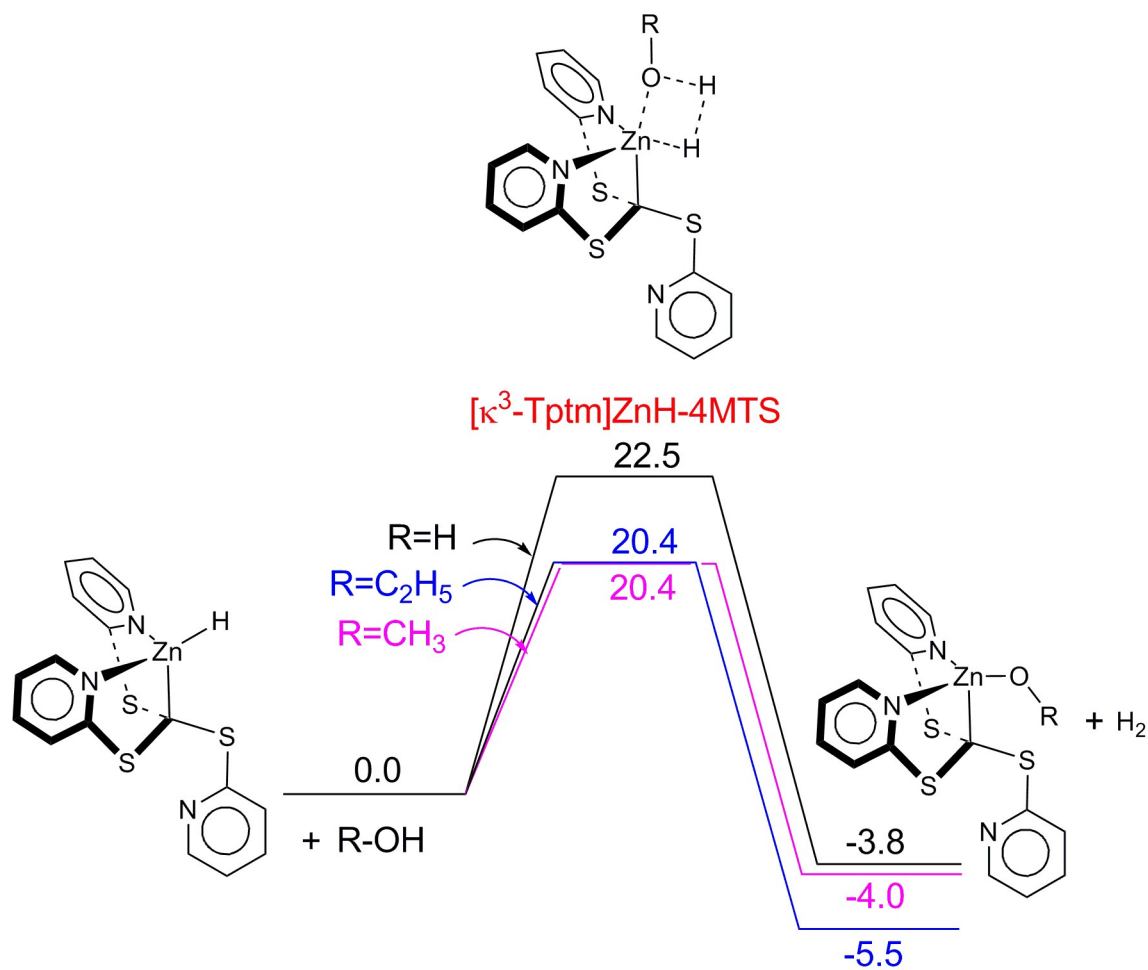
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Scheme S6. Free energy profiles for the reaction of **GeH-2** with ROH (R=H, CH₃, C₂H₅) through a four membered transition state.

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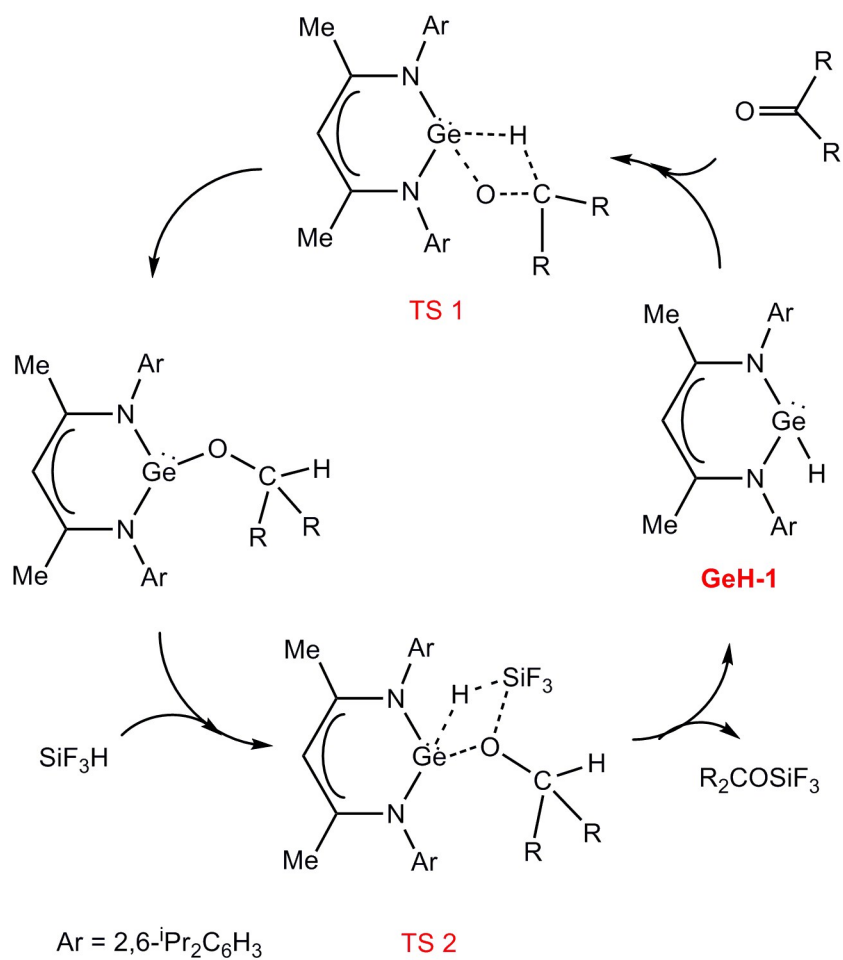


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Scheme S7. Free energy profile for the reaction of **GeH-1** with C=O bond in ketone, with SiF₃H employed to complete the cycle.



3. The xyz coordinates of all the structures discussed in the manuscript.

GeH-I singlet				H -3.283 -2.031 -3.836			C -3.131 -1.582 1.894							
				H -4.221 -1.300 -2.508			H -2.450 -2.310 1.430							
5	H	-2.085	-0.585	-0.000	65	C	-3.291	0.758	-4.105	125	H	-3.972	-1.414	1.206
	Ge	-0.485	-0.897	-0.000		H	-2.792	1.721	-4.292		H	-3.538	-2.035	2.811
	N	-0.182	0.525	1.446		H	-4.292	0.969	-3.701		C	0.096	-0.059	-2.713
	N	-0.182	0.525	-1.446		H	-3.423	0.259	-5.078		C	-1.204	-0.470	-3.096
10	C	-0.282	1.843	1.264	70	C	2.569	-0.010	-2.269	130	C	-1.370	-1.076	-4.348
	C	-0.421	2.446	-0.000		H	2.187	0.434	-1.337		H	-2.368	-1.392	-4.661
	H	-0.511	3.530	0.000		C	3.287	-1.318	-1.897		C	-0.285	-1.291	-5.195
	C	-0.281	1.842	-1.264		H	2.600	-2.011	-1.392		H	-0.433	-1.773	-6.164
15	C	-0.192	2.752	2.466	75	H	4.131	-1.117	-1.221	135	C	0.989	-0.891	-4.802
	H	-0.973	2.509	3.201		H	3.685	-1.822	-2.792		H	1.836	-1.067	-5.469
	H	-0.293	3.803	2.172		C	3.544	0.995	-2.903		C	1.207	-0.262	-3.568
	H	0.770	2.619	2.982		H	3.041	1.938	-3.164		C	-2.409	-0.259	-2.190
20	C	-0.192	2.752	-2.466	80	H	3.993	0.592	-3.824	140	H	-2.035	0.139	-1.236
	H	0.769	2.619	-2.982		H	4.362	1.229	-2.206		C	-3.131	-1.583	-1.895
	H	-0.293	3.803	-2.172		GeH-I triplet			H		-2.450	-2.310	-1.431	
	H	-0.973	2.508	-3.201		H	-0.126	-1.761	0.000		H	-3.538	-2.036	-2.811
25	C	0.047	-0.019	2.754	85	Ge	0.912	-0.561	0.000	145	H	-3.972	-1.415	-1.206
	C	1.373	-0.288	3.168		N	0.261	0.543	1.423		C	-3.379	0.778	-2.780
	C	1.572	-0.845	4.438		N	0.261	0.542	-1.423		H	-2.879	1.741	-2.955
	H	2.589	-1.054	4.777		C	0.177	1.935	1.275		H	-4.219	0.953	-2.091
30	C	0.496	-1.144	5.272	90	C	0.145	2.519	0.000	150	H	-3.795	0.433	-3.739
	H	0.671	-1.580	6.258		H	0.094	3.610	0.000		C	2.616	0.166	-3.181
	C	-0.804	-0.897	4.838		C	0.177	1.935	-1.275		H	2.539	0.771	-2.265
	H	-1.644	-1.148	5.489		H	0.143	2.788	2.511		C	3.496	-1.053	-2.859
35	C	-1.057	-0.337	3.579	95	H	-0.651	2.485	3.211	155	H	3.069	-1.645	-2.035
	C	2.569	-0.010	2.269		H	-0.028	3.838	2.238		H	4.507	-0.735	-2.560
	H	2.187	0.434	1.337		H	1.089	2.740	3.079		C	3.591	-1.713	-3.735
	C	3.544	0.995	2.903		C	0.143	2.788	-2.510		C	3.275	1.039	-4.262
40	H	3.041	1.938	3.164	100	H	1.088	2.739	-3.078	160	H	2.645	1.902	-4.523
	H	4.362	1.229	2.206		H	-0.029	3.837	-2.237		H	3.461	0.471	-5.185
	H	3.993	0.592	3.824		H	-0.651	2.484	-3.210		H	4.244	1.418	-3.906
	C	3.287	-1.318	1.897		C	0.096	-0.059	2.713		GeH-I-4MTS-H ₂ O			
45	H	2.599	-2.011	1.392	105	C	1.207	-0.263	3.568	165	C	-1.477	-0.282	3.581
	H	3.684	-1.822	2.792		C	0.989	-0.892	4.801		C	-0.509	0.124	2.629
	H	4.131	-1.117	1.221		H	1.836	-1.068	5.469		C	0.872	0.123	2.944
	C	-2.494	-0.116	3.124		C	-0.285	-1.291	5.195		C	1.266	-0.287	4.225
50	H	-2.466	0.401	2.154	110	H	-0.433	-1.773	6.164	170	C	0.328	-0.693	5.171
	C	-3.291	0.758	4.106		C	-1.370	-1.076	4.347		C	-1.025	-0.685	4.845
	H	-2.792	1.721	4.292		H	-2.368	-1.392	4.661		N	-0.900	0.511	1.294
	H	-3.423	0.259	5.078		C	-1.204	-0.470	3.095		C	-1.375	1.742	1.045
55	H	-4.292	0.969	3.701	115	C	2.616	0.166	3.181	175	C	-1.717	2.229	-0.226
	C	-3.204	-1.462	2.897		H	2.539	0.771	2.264		C	-1.379	1.705	-1.486
	H	-2.660	-2.081	2.170		C	3.275	1.039	4.262		C	-1.752	2.514	-2.707
	H	-4.221	-1.300	2.508		H	2.645	1.902	4.523		C	1.931	0.621	1.968
60	H	-3.283	-2.031	3.836	120	H	4.245	1.417	3.906	180	C	2.468	1.998	2.397
	C	0.047	-0.019	-2.754		H	3.461	0.470	5.185		C	-2.979	-0.270	3.318
	C	-1.057	-0.337	-3.579		C	3.496	-1.054	2.859		C	-3.700	0.725	4.248
	H	-1.644	-1.149	-5.489		H	3.069	-1.646	2.035		N	-0.722	0.555	-1.619
65	C	0.496	-1.144	-5.272	125	H	3.591	-1.713	3.735	185	Ge	-0.493	-0.925	-0.082
	H	0.671	-1.580	-6.258		H	4.507	-0.736	2.561		O	-1.730	-2.335	1.114
	C	1.571	-0.845	-4.438		C	-2.408	-0.259	2.189		C	-0.214	0.125	-2.885
	H	2.589	-1.054	-4.777		H	-2.035	0.140	1.236		C	1.156	0.352	-3.164
70	C	1.373	-0.288	-3.168	130	C	-3.379	0.778	2.779	190	C	1.671	-0.087	-4.390
	C	-2.494	-0.116	-3.124		H	-2.879	1.742	2.955		C	0.867	-0.756	-5.312
	H	-2.466	0.401	-2.154		H	-3.795	0.434	3.739		C	-0.470	-1.000	-5.011
	C	-3.204	-1.462	-2.897		H	-4.219	0.954	2.091		C	-1.035	-0.574	-3.801
75	H	-2.660	-2.081	-2.170	135				195					

	C	2.049	1.096	-2.179
	C	3.410	0.415	-1.982
	C	-2.491	-0.900	-3.499
	C	-2.666	-2.406	-3.239
5	C	-3.444	-0.427	-4.609
	C	2.224	2.568	-2.593
	C	3.072	-0.388	1.777
	C	-3.604	-1.666	3.481
	C	-1.562	2.718	2.187
10	H	-2.511	-0.993	-0.526
	H	-2.188	3.212	-0.234
	H	-2.619	2.738	2.490
	H	-1.290	3.731	1.865
	H	-0.968	2.446	3.066
15	H	-0.952	2.501	-3.459
	H	-1.983	3.552	-2.440
	H	-2.644	2.077	-3.183
	H	2.326	-0.283	4.485
	H	0.652	-1.013	6.163
20	H	-1.757	-1.001	5.591
	H	1.449	0.758	0.987
	H	1.655	2.734	2.488
	H	3.193	2.377	1.660
	H	2.974	1.937	3.373
25	H	2.685	-1.355	1.427
	H	3.624	-0.561	2.713
	H	3.791	-0.017	1.033
	H	-3.137	0.042	2.274
	H	-3.252	1.728	4.227
30	H	-3.669	0.375	5.291
	H	-4.759	0.814	3.962
	H	-3.110	-2.379	2.810
	H	-4.677	-1.626	3.237
	H	-3.514	-2.020	4.520
35	H	-1.092	-1.538	-5.729
	H	1.287	-1.095	-6.261
	H	2.722	0.091	-4.625
	H	-2.768	-0.380	-2.569
	H	-2.011	-2.747	-2.425
40	H	-2.422	-2.992	-4.138
	H	-3.705	-2.631	-2.953
	H	-3.311	0.641	-4.832
	H	-4.490	-0.587	-4.308
	H	-3.283	-0.983	-5.546
45	H	1.532	1.090	-1.207
	H	3.289	-0.633	-1.676
	H	3.984	0.936	-1.202
	H	4.017	0.435	-2.900
	H	1.256	3.084	-2.663
50	H	2.718	2.641	-3.575
	H	2.843	3.106	-1.859
	H	-2.397	-1.673	0.115
	H	-1.448	-3.233	0.863

55 GeH-1-6MTS-H₂O

	C	5.077	0.210	0.726
	C	4.529	1.508	0.848
	C	5.249	2.558	1.477
60	C	6.544	2.281	1.938
	C	7.106	1.012	1.806
	C	6.372	-0.012	1.215
	N	3.202	1.765	0.352
	C	3.080	2.217	-0.917
65	C	4.330	2.322	-1.768

	C	4.653	3.952	1.660
	C	5.095	4.929	0.553
	C	4.295	-0.939	0.105
	C	5.071	-1.634	-1.025
70	C	1.881	2.529	-1.564
	C	0.560	2.170	-1.203
	C	-0.546	2.548	-2.163
	N	0.310	1.492	-0.097
	Ge	1.709	1.207	1.662
75	O	2.872	1.754	3.354
	C	-0.966	0.931	0.181
	C	-2.006	1.695	0.761
	C	-3.224	1.058	1.042
	C	-3.411	-0.295	0.779
80	C	-2.363	-1.047	0.246
	C	-1.127	-0.461	-0.045
	C	-1.823	3.162	1.121
	C	-1.825	3.350	2.649
	C	0.014	-1.282	-0.630
85	C	0.091	-2.706	-0.068
	C	-0.047	-1.301	-2.168
	C	-2.882	4.065	0.466
	C	4.981	4.554	3.036
	C	3.870	-1.954	1.182
90	O	1.870	3.915	3.823
	H	3.838	1.738	3.224
	H	1.108	3.048	1.825
	H	1.990	2.990	-2.545
	H	4.155	2.975	-2.631
95	H	4.585	1.321	-2.151
	H	5.206	2.679	-1.216
	H	-0.973	3.520	-1.868
	H	-1.363	1.815	-2.147
	H	-0.166	2.649	-3.187
100	H	6.812	-1.008	1.129
	H	8.116	0.820	2.176
	H	7.118	3.074	2.420
	H	3.378	-0.519	-0.334
	H	5.396	-0.916	-1.792
105	H	4.438	-2.392	-1.511
	H	5.967	-2.148	-0.646
	H	3.264	-1.474	1.966
	H	4.750	-2.405	1.665
	H	3.271	-2.763	0.737
110	H	3.561	3.849	1.592
	H	4.728	4.630	-0.436
	H	6.193	4.998	0.506
	H	4.701	5.934	0.763
	H	4.766	3.854	3.853
115	H	4.365	5.449	3.203
	H	6.038	4.854	3.108
	H	-4.039	1.638	1.482
	H	-4.369	-0.770	1.002
	H	-2.509	-2.114	0.065
120	H	-0.834	3.476	0.754
	H	-1.077	2.701	3.127
	H	-2.808	3.098	3.076
	H	-1.595	4.394	2.912
	H	-2.912	3.928	-0.624
125	H	-2.666	5.124	0.674
	H	-3.889	3.851	0.855
	H	0.948	-0.766	-0.350
	H	0.118	-2.701	1.030
	H	1.004	-3.203	-0.430
130	H	-0.760	-3.325	-0.388

	H	-0.011	-0.285	-2.586
	H	-0.978	-1.777	-2.514
	H	0.801	-1.867	-2.584
	H	2.432	2.929	3.761
135	H	1.328	3.489	2.603
	H	1.176	3.814	4.497

GeH-1-H₂O-alkoxide intermediate

140	C	-0.068	-0.192	-3.257
	C	-0.028	1.217	-3.382
	C	-0.038	2.056	-2.240
	C	-0.112	1.455	-0.976
	C	-0.168	0.071	-0.836
145	C	-0.149	-0.738	-1.970
	N	0.098	1.811	-4.682
	C	-0.972	2.098	-5.427
	C	-0.890	2.581	-6.746
	C	0.245	2.597	-7.577
150	C	0.010	2.831	-9.051
	C	-0.004	3.576	-2.347
	C	-1.289	4.208	-1.784
	C	-0.049	-1.119	-4.465
	C	-1.382	-1.878	-4.608
155	N	1.485	2.378	-7.131
	Ge	2.023	2.396	-5.139
	O	2.733	0.665	-5.139
	H	3.577	0.705	-4.658
	C	2.598	2.280	-8.031
160	C	3.393	3.428	-8.269
	C	4.508	3.303	-9.108
	C	4.835	2.083	-9.696
	C	4.046	0.962	-9.446
	C	2.925	1.030	-8.608
165	C	3.054	4.790	-7.674
	C	4.181	5.313	-6.768
	C	2.099	-0.224	-8.360
	C	2.945	-1.340	-7.727
	C	1.433	-0.723	-9.656
170	C	2.713	5.813	-8.772
	C	1.241	4.165	-1.664
	C	1.126	-2.105	-4.405
	C	-2.358	1.862	-4.873
	H	-1.837	2.819	-7.227
175	H	-2.707	0.855	-5.147
	H	-3.065	2.585	-5.302
	H	-2.383	1.931	-3.779
	H	0.872	3.305	-9.535
	H	-0.882	3.452	-9.199
180	H	-0.163	1.872	-9.562
	H	-0.128	2.088	-0.085
	H	-0.228	-0.378	0.157
	H	-0.192	-1.824	-1.854
	H	0.052	3.837	-3.414
185	H	-2.185	3.819	-2.289
	H	-1.270	5.301	-1.916
	H	-1.398	4.002	-0.708
	H	2.161	3.755	-2.105
	H	1.249	3.945	-0.585
190	H	1.262	5.259	-1.785
	H	0.093	-0.496	-5.360
	H	-2.243	-1.196	-4.641
	H	-1.537	-2.563	-3.760
	H	-1.385	-2.479	-5.530
195	H	2.076	-1.557	-4.368

	H	1.132	-2.743	-5.302
	H	1.054	-2.765	-3.527
	H	4.307	0.008	-9.909
	H	5.706	2.005	-10.351
5	H	5.129	4.180	-9.308
	H	1.310	0.033	-7.640
	H	3.365	-1.000	-6.773
	H	3.765	-1.649	-8.394
	H	2.321	-2.226	-7.535
10	H	0.834	0.060	-10.141
	H	0.771	-1.576	-9.443
	H	2.187	-1.059	-10.383
	H	2.159	4.669	-7.046
	H	4.388	4.607	-5.951
15	H	3.896	6.278	-6.321
	H	5.113	5.468	-7.333
	H	1.883	5.466	-9.404
	H	3.578	5.997	-9.429
	H	2.422	6.775	-8.324

GeH-1-4MTS-CH₃OH

	C	-1.251	-0.663	-3.705
	C	-0.329	-0.192	-2.737
25	C	1.068	-0.276	-2.952
	C	1.525	-0.818	-4.162
	C	0.633	-1.276	-5.128
	C	-0.736	-1.196	-4.895
	N	-0.796	0.346	-1.482
30	Ge	-0.538	-0.941	0.073
	O	-1.708	-2.436	-1.096
	C	-1.435	-3.751	-0.665
	C	2.075	0.274	-1.948
	C	2.510	1.699	-2.338
35	C	-2.764	-0.591	-3.535
	C	-3.403	0.348	-4.577
	C	-1.281	1.595	-1.407
	C	-1.334	2.469	-2.643
	C	-1.734	2.208	-0.225
40	C	-1.490	1.821	1.100
	C	-1.905	2.763	2.205
	N	-0.859	0.684	1.401
	C	-0.417	0.427	2.739
	C	-1.263	-0.219	3.672
45	C	-0.764	-0.480	4.955
	C	0.533	-0.122	5.316
	C	1.360	0.500	4.384
	C	0.910	0.781	3.087
	C	-2.676	-0.658	3.312
50	C	-2.759	-2.191	3.219
	C	1.848	1.454	2.095
	C	3.094	0.593	1.834
	C	2.241	2.870	2.551
	C	-3.729	-0.115	4.292
55	C	3.290	-0.642	-1.757
	C	-3.419	-1.981	-3.631
	H	-2.620	-0.968	0.346
	H	-2.200	3.184	-0.359
	H	-2.642	2.280	2.863
60	H	-2.344	3.682	1.800
	H	-1.046	3.026	2.840
	H	-0.865	2.001	-3.514
	H	-0.831	3.425	-2.438
	H	-2.381	2.699	-2.890
65	H	2.379	0.772	4.667

	H	0.901	-0.335	6.322
	H	-1.406	-0.978	5.685
	H	1.308	1.553	1.141
	H	1.354	3.501	2.709
70	H	2.875	3.357	1.795
	H	2.804	2.843	3.496
	H	2.815	-0.404	1.467
	H	3.691	0.461	2.749
	H	3.741	1.070	1.081
75	H	-2.908	-0.261	2.312
	H	-3.672	0.978	4.388
	H	-3.606	-0.542	5.299
	H	-4.740	-0.375	3.945
	H	-2.022	-2.587	2.507
80	H	-3.759	-2.505	2.882
	H	-2.565	-2.657	4.198
	H	-1.431	-1.562	-5.653
	H	1.007	-1.697	-6.063
	H	2.598	-0.879	-4.350
85	H	-2.976	-0.197	-2.530
	H	-2.978	-2.652	-2.884
	H	-3.287	-2.415	-4.634
	H	-4.501	-1.899	-3.445
	H	-2.948	1.347	-4.580
90	H	-4.479	0.461	-4.377
	H	-3.297	-0.065	-5.591
	H	1.572	0.349	-0.971
	H	2.979	-1.658	-1.476
	H	3.939	-0.251	-0.960
95	H	3.901	-0.712	-2.669
	H	1.646	2.374	-2.418
	H	3.026	1.697	-3.310
	H	3.199	2.113	-1.586
	H	-2.463	-1.672	-0.250
100	H	-1.786	-3.949	0.369
	H	-1.934	-4.482	-1.327
	H	-0.348	-3.964	-0.690

GeH-1-6MTS-CH₃OH

105	C	-0.984	-0.452	-0.547
	C	-0.930	0.813	0.095
	C	-2.016	1.269	0.880
	C	-3.164	0.468	0.965
110	C	-3.244	-0.756	0.308
	C	-2.155	-1.211	-0.435
	N	0.278	1.560	-0.013
	Ge	1.729	1.190	1.635
	O	2.915	1.774	3.304
115	C	3.515	0.741	4.060
	C	-1.953	2.575	1.660
	C	-3.157	3.490	1.383
	C	0.199	-0.952	-1.363
	C	0.142	-0.443	-2.814
120	C	0.406	2.552	-0.888
	C	-0.790	3.061	-1.661
	C	1.659	3.135	-1.171
	C	2.925	2.731	-0.715
	C	4.087	3.089	-1.618
125	N	3.148	1.997	0.389
	C	4.499	1.603	0.710
	C	4.957	0.329	0.300
	C	6.272	-0.045	0.612
	C	7.119	0.814	1.304
130	C	6.650	2.062	1.713

	C	5.340	2.481	1.442
	C	4.072	-0.642	-0.467
	C	3.804	-1.916	0.350
	C	4.882	3.848	1.935
135	C	5.240	4.073	3.415
	C	5.464	5.001	1.094
	C	4.656	-0.984	-1.849
	C	-1.821	2.292	3.167
	C	0.359	-2.478	-1.337
140	O	2.005	3.928	3.830
	C	1.134	3.952	4.961
	H	1.060	2.966	1.978
	H	1.668	3.859	-1.984
	H	3.883	4.026	-2.153
145	H	4.201	2.296	-2.374
	H	5.042	3.170	-1.090
	H	-1.461	2.241	-1.950
	H	-0.481	3.610	-2.559
	H	-1.376	3.746	-1.029
150	H	6.636	-1.026	0.299
	H	8.143	0.511	1.533
	H	7.314	2.727	2.268
	H	3.105	-0.147	-0.639
	H	4.847	-0.076	-2.439
155	H	3.956	-1.619	-2.413
	H	5.607	-1.531	-1.761
	H	3.322	-1.673	1.309
	H	4.739	-2.454	0.569
	H	3.141	-2.599	-0.199
160	H	3.788	3.883	1.847
	H	5.130	4.969	0.049
	H	6.565	4.973	1.100
	H	5.149	5.968	1.515
	H	4.941	3.214	4.029
165	H	4.713	4.960	3.792
	H	6.320	4.238	3.550
	H	-4.011	0.811	1.564
	H	-4.148	-1.363	0.385
	H	-2.215	-2.182	-0.931
170	H	-1.043	3.109	1.348
	H	-0.938	1.671	3.377
	H	-2.705	1.755	3.544
	H	-1.725	3.232	3.732
	H	-3.287	3.673	0.307
175	H	-3.021	4.461	1.883
	H	-4.093	3.054	1.761
	H	1.099	-0.514	-0.902
	H	0.379	-2.864	-0.308
	H	1.301	-2.763	-1.830
180	H	-0.452	-2.987	-1.879
	H	0.139	0.653	-2.859
	H	-0.766	-0.808	-3.318
	H	1.016	-0.799	-3.382
	H	2.545	2.942	3.780
185	H	1.369	3.461	2.708
	H	0.614	2.988	5.104
	H	1.712	4.178	5.871
	H	0.380	4.740	4.822
	H	3.368	0.902	5.143
190	H	3.072	-0.241	3.804
	H	4.602	0.679	3.860

GeH-1-CH₃OH-alkoxide intermediate

195	C	-0.079	-0.172	-3.264
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C	-0.060	1.239	-3.377	H	-1.342	5.313	-1.914	H	3.475	-0.859	2.561
C	-0.112	2.066	-2.229	H	-1.480	4.030	-0.692	H	3.730	-0.154	0.948
C	-0.206	1.450	-0.974	H	-0.011	-0.460	-5.379	H	-3.065	-0.173	2.048
C	-0.229	0.063	-0.844	H	2.142	-1.318	-4.476	H	-3.383	1.798	3.587
5 C	-0.163	-0.735	-1.983	70 H	1.278	-2.580	-5.387	135 H	-3.678	0.687	4.941
N	0.076	1.837	-4.676	H	1.282	-2.613	-3.607	H	-4.816	0.750	3.577
C	-0.999	2.231	-5.367	H	-2.209	-1.379	-4.578	H	-3.059	-2.488	2.965
C	-2.372	1.947	-4.807	H	-1.351	-2.671	-3.713	H	-4.654	-1.704	3.101
C	-0.069	3.586	-2.311	H	-1.265	-2.585	-5.485	H	-3.638	-1.871	4.546
10 C	-1.363	4.222	-1.770	75 H	4.178	2.512	-2.672	140 H	-1.143	-1.425	-5.825
C	-0.033	-1.091	-4.478	H	4.423	1.550	-4.155	H	1.254	-1.045	-6.319
C	-1.287	-1.979	-4.567	H	4.786	3.297	-4.162	H	2.711	0.037	-4.635
Ge	1.980	1.759	-5.448	GeH-1-4MTS-C₂H₅OH				H	-2.811	-0.327	-2.638
O	2.747	2.844	-4.136	80 C	0.875	0.144	2.930	H	-2.112	-2.720	-2.610
15 C	4.087	2.534	-3.773	C	-0.490	0.123	2.569	145 H	-2.532	-2.870	-4.332
N	1.450	3.306	-6.720	C	-1.489	-0.299	3.481	H	-3.803	-2.533	-3.128
C	2.577	4.033	-7.225	C	-1.081	-0.680	4.766	H	-3.319	0.808	-4.860
C	3.369	3.452	-8.246	85 C	0.261	-0.667	5.140	H	-4.531	-0.412	-4.395
C	4.510	4.142	-8.677	C	1.229	-0.261	4.225	150 H	-3.325	-0.783	-5.642
20 C	4.870	5.365	-8.116	N	-0.866	0.520	1.232	H	1.587	0.801	-1.171
C	4.083	5.920	-7.109	C	-1.289	1.775	1.003	H	3.467	-0.643	-2.021
C	2.933	5.272	-6.638	C	-1.280	2.782	2.132	H	4.017	0.884	-1.291
C	2.999	2.130	-8.907	90 C	-2.974	-0.326	3.133	H	4.019	0.702	-3.050
C	4.095	1.070	-8.706	C	-3.750	0.797	3.848	155 H	1.034	2.957	-2.261
25 C	2.104	5.927	-5.541	C	1.966	0.618	1.977	H	2.445	2.799	-3.334
C	2.932	6.168	-4.269	C	2.692	1.861	2.518	H	2.674	3.009	-1.578
C	0.210	3.533	-7.155	C	-1.673	2.271	-0.252	H	-2.429	-1.653	0.083
C	-0.023	4.509	-8.285	95 C	-1.387	1.735	-1.521	C	-2.246	-4.707	1.285
C	-0.928	2.932	-6.583	C	-1.785	2.545	-2.732	H	-1.462	-3.758	-0.488
30 C	2.683	2.319	-10.401	N	-0.748	0.575	-1.665	160 H	-0.300	-3.857	0.851
C	1.477	7.246	-6.028	Ge	-0.493	-0.909	-0.152	H	-1.977	-5.718	0.940
C	1.156	4.147	-1.572	O	-1.709	-2.350	1.045	H	-2.129	-4.673	2.378
C	1.242	-1.950	-4.485	100 C	-1.366	-3.655	0.618	H	-3.305	-4.530	1.049
H	-1.879	3.158	-7.063	C	-0.248	0.145	-2.936	165 GeH-1-6MTS-C₂H₅OH			
35 H	-0.199	5.518	-7.885	C	-1.079	-0.509	-3.873	C	-1.134	0.324	3.811
H	-0.914	4.219	-8.856	C	-0.513	-0.923	-5.088	C	-0.635	0.049	2.514
H	0.839	4.569	-8.959	C	0.834	-0.715	-5.367	C	-0.526	-1.286	2.045
H	-2.447	0.915	-4.437	105 C	1.651	-0.101	-4.418	170 C	-0.941	-2.326	2.887
H	-3.145	2.119	-5.566	C	1.136	0.327	-3.189	C	-1.445	-2.069	4.160
40 H	-2.582	2.603	-3.950	C	-2.544	-0.810	-3.591	C	-1.537	-0.757	4.608
H	5.125	3.712	-9.470	C	-2.759	-2.322	-3.405	N	-0.176	1.108	1.649
H	5.763	5.886	-8.465	C	2.032	1.003	-2.159	Ge	1.865	1.272	1.536
H	4.370	6.880	-6.673	110 C	3.462	0.449	-2.135	175 O	2.110	1.464	3.695
H	2.086	1.755	-8.422	C	2.044	2.531	-2.344	C	3.148	0.606	4.163
45 H	1.878	3.053	-10.554	C	-3.479	-0.264	-4.683	C	2.613	-0.474	5.096
H	2.365	1.366	-10.851	C	-3.614	-1.684	3.461	C	-0.033	-1.602	0.636
H	3.566	2.674	-10.955	C	2.962	-0.507	1.653	C	-1.180	-1.489	-0.384
H	4.287	0.901	-7.637	115 H	-2.555	-1.027	-0.592	180 C	-1.274	1.728	4.386
H	5.041	1.375	-9.179	H	-2.115	3.267	-0.247	C	-2.746	2.077	4.684
50 H	3.788	0.112	-9.153	H	-1.354	2.324	3.122	C	-1.042	1.862	0.950
H	1.294	5.232	-5.275	H	-2.090	3.511	2.002	C	-2.532	1.696	1.166
H	0.897	7.111	-6.952	H	-0.329	3.338	2.098	C	-0.677	2.825	-0.007
H	2.253	7.999	-6.234	120 H	-1.027	2.486	-3.524	185 C	0.533	2.946	-0.718
H	0.806	7.658	-5.259	H	-1.953	3.596	-2.466	C	0.585	3.926	-1.868
55 H	3.314	5.218	-3.878	H	-2.721	2.147	-3.152	N	1.596	2.202	-0.429
H	2.306	6.632	-3.491	H	2.280	-0.252	4.520	C	2.751	2.212	-1.270
H	3.778	6.845	-4.462	H	0.553	-0.976	6.145	C	3.787	3.158	-1.066
H	-0.253	2.073	-0.078	125 H	-1.834	-1.003	5.487	190 C	4.915	3.102	-1.895
H	-0.297	-0.394	0.143	H	1.483	0.914	1.033	C	5.032	2.143	-2.900
60 H	-0.181	-1.822	-1.878	H	1.984	2.671	2.745	C	4.014	1.210	-3.080
H	0.035	3.861	-3.371	H	3.418	2.234	1.779	C	2.870	1.217	-2.271
H	2.075	3.743	-2.011	H	3.244	1.632	3.443	C	3.720	4.195	0.044
H	1.128	3.896	-0.500	130 H	2.451	-1.368	1.198	195 C	4.650	3.803	1.206
H	1.184	5.244	-1.657								
65 H	-2.259	3.832	-2.273								

C 1.785 0.172 -2.492
 C 2.349 -1.253 -2.385
 C 1.065 0.375 -3.836
 C 4.030 5.619 -0.442
 5 C 0.655 -2.969 0.526
 C -0.444 1.895 5.670
 O 2.414 3.859 3.805
 C 1.482 4.653 4.543
 C 1.701 6.124 4.227
 10 H 1.453 3.177 1.831
 H -1.499 3.437 -0.376
 H -0.389 4.400 -2.035
 H 0.906 3.430 -2.795
 H 1.328 4.710 -1.661
 15 H -2.779 0.740 1.640
 H -3.067 1.774 0.211
 H -2.902 2.502 1.819
 H 4.110 0.455 -3.864
 H 5.918 2.121 -3.537
 20 H 5.720 3.825 -1.747
 H 1.040 0.300 -1.693
 H 0.621 1.379 -3.908
 H 0.256 -0.360 -3.958
 H 1.760 0.255 -4.681
 25 H 2.831 -1.416 -1.410
 H 3.097 -1.451 -3.167
 H 1.545 -1.995 -2.505
 H 2.692 4.199 0.436
 H 3.386 5.909 -1.286
 30 H 5.076 5.721 -0.771
 H 3.871 6.340 0.372
 H 4.432 2.785 1.566
 H 4.525 4.487 2.058
 H 5.703 3.821 0.884
 35 H -1.927 -0.560 5.609
 H -1.762 -2.894 4.801
 H -0.869 -3.358 2.541
 H -0.887 2.439 3.640
 H 0.615 1.708 5.466
 40 H -0.782 1.197 6.451
 H -0.558 2.915 6.068
 H -3.404 1.908 3.822
 H -2.833 3.132 4.984
 H -3.130 1.465 5.515
 45 H 0.718 -0.841 0.369
 H 1.445 -3.083 1.282
 H 1.113 -3.078 -0.465
 H -0.056 -3.800 0.646
 H -1.615 -0.481 -0.396
 50 H -1.982 -2.204 -0.145
 H -0.816 -1.710 -1.400
 H 2.295 2.733 3.940
 H 1.856 3.559 2.561
 H 0.443 4.364 4.292
 55 H 1.620 4.462 5.621
 H 3.648 0.123 3.295
 H 3.922 1.208 4.675
 H 3.424 -1.153 5.406
 H 2.171 -0.032 6.001
 60 H 1.834 -1.065 4.593
 H 1.000 6.754 4.796
 H 2.727 6.425 4.481
 H 1.542 6.317 3.155

65 GeH-1-C₂H₅OH-alkoxide intermediate 130

C 2.995 5.312 -6.670
 C 2.594 4.088 -7.255
 C 3.320 3.515 -8.328
 70 C 4.434 4.208 -8.822
 C 4.827 5.427 -8.275
 C 4.111 5.967 -7.208
 N 1.476 3.370 -6.710
 C 0.235 3.580 -7.153
 75 C -0.901 2.954 -6.606
 C -0.978 2.242 -5.396
 C -2.354 1.954 -4.845
 C 2.921 2.191 -8.971
 C 2.548 2.367 -10.454
 80 C 2.256 5.936 -5.494
 C 1.578 7.260 -5.890
 N 0.097 1.851 -4.707
 Ge 2.014 1.804 -5.479
 O 2.777 2.849 -4.130
 85 C 3.966 2.324 -3.535
 C -0.010 1.308 -3.385
 C 0.125 -0.089 -3.201
 C 0.131 -0.592 -1.893
 C 0.006 0.253 -0.794
 90 C -0.144 1.624 -0.992
 C -0.156 2.180 -2.278
 C 0.221 -1.058 -4.373
 C 1.526 -1.870 -4.343
 C -0.320 3.687 -2.434
 95 C 0.894 4.447 -1.878
 C -1.619 4.187 -1.776
 C -1.003 -1.988 -4.422
 C 4.023 1.132 -8.805
 C 3.192 6.150 -4.294
 100 C -0.000 4.570 -8.270
 H -1.849 3.172 -7.095
 H -0.081 5.588 -7.862
 H -0.938 4.343 -8.792
 H 0.827 4.579 -8.990
 105 H -2.392 0.974 -4.349
 H -3.103 1.990 -5.646
 H -2.630 2.707 -4.092
 H 5.000 3.783 -9.654
 H 5.695 5.954 -8.676
 110 H 4.429 6.919 -6.777
 H 2.028 1.818 -8.449
 H 1.733 3.094 -10.584
 H 2.217 1.408 -10.881
 H 3.407 2.718 -11.045
 115 H 4.258 0.972 -7.743
 H 4.950 1.433 -9.319
 H 3.699 0.170 -9.232
 H 1.476 5.228 -5.177
 H 0.899 7.136 -6.746
 120 H 2.325 8.020 -6.168
 H 0.994 7.659 -5.047
 H 3.623 5.193 -3.976
 H 2.634 6.574 -3.446
 H 4.008 6.847 -4.539
 125 H -0.247 2.283 -0.127
 H 0.019 -0.155 0.217
 H 0.236 -1.668 -1.735
 H -0.375 3.911 -3.510
 H 1.803 4.146 -2.413
 H 1.028 4.249 -0.804

H 0.754 5.532 -2.004
 H -2.502 3.631 -2.125
 H -1.775 5.253 -1.999
 H -1.578 4.082 -0.681
 135 H 0.222 -0.465 -5.301
 H 2.403 -1.206 -4.359
 H 1.587 -2.532 -5.220
 H 1.589 -2.498 -3.441
 H -1.942 -1.416 -4.468
 140 H -1.051 -2.633 -3.531
 H -0.958 -2.641 -5.307
 C 3.680 1.576 -2.237
 H 4.504 1.652 -4.237
 H 4.644 3.175 -3.340
 145 H 4.617 1.233 -1.771
 H 3.151 2.223 -1.523
 H 3.042 0.698 -2.421

GeH-2 singlet

150 C 3.294 4.418 -5.748
 C 2.565 3.812 -6.821
 C 3.169 3.753 -8.107
 C 4.434 4.326 -8.307
 155 C 5.110 4.964 -7.273
 C 4.543 4.996 -6.000
 B 1.129 3.238 -6.503
 Ge -0.517 3.453 -7.838
 H -0.153 4.606 -8.871
 160 C 2.537 3.019 -9.279
 C 3.304 1.723 -9.591
 C 2.779 4.386 -4.310
 C 3.314 3.135 -3.586
 C 0.756 2.146 -5.528
 165 C 1.438 0.807 -5.520
 C -0.304 2.409 -4.643
 C -1.120 3.532 -4.817
 C -2.268 3.744 -3.868
 B -0.907 4.429 -6.047
 170 C -1.571 5.832 -6.376
 C -0.815 7.034 -6.443
 C -1.450 8.243 -6.754
 C -2.819 8.296 -7.004
 C -3.566 7.122 -6.961
 175 C -2.968 5.889 -6.666
 C 0.691 7.034 -6.227
 C 1.438 7.149 -7.567
 C -3.843 4.641 -6.750
 C -4.184 4.321 -8.217
 180 C -5.123 4.745 -5.904
 C 1.149 8.138 -5.260
 C 2.388 3.897 -10.529
 C 3.124 5.628 -3.476
 H -0.521 1.699 -3.832
 185 H -2.033 3.358 -2.864
 H -3.174 3.216 -4.209
 H -2.533 4.809 -3.795
 H 0.864 0.098 -6.141
 H 1.487 0.376 -4.507
 190 H 2.452 0.857 -5.943
 H -4.636 7.162 -7.177
 H -3.300 9.247 -7.241
 H -0.864 9.162 -6.807
 H -3.259 3.789 -6.372
 195 H -4.896 5.007 -4.861

	H	-5.665	3.787	-5.910
	H	-5.807	5.511	-6.298
	H	-3.271	4.179	-8.816
	H	-4.757	5.141	-8.675
5	H	-4.784	3.400	-8.287
	H	0.960	6.059	-5.782
	H	0.691	8.023	-4.266
	H	0.887	9.137	-5.638
	H	2.242	8.120	-5.147
10	H	1.131	6.349	-8.255
	H	2.524	7.072	-7.413
	H	1.219	8.114	-8.050
	H	5.088	5.475	-5.185
	H	6.084	5.424	-7.453
15	H	4.894	4.274	-9.297
	H	1.680	4.313	-4.346
	H	2.840	6.557	-3.984
	H	4.199	5.679	-3.246
	H	2.590	5.591	-2.515
20	H	3.108	2.215	-4.145
	H	2.861	3.041	-2.587
	H	4.405	3.212	-3.462
	H	1.522	2.712	-8.965
	H	1.848	4.826	-10.299
25	H	1.827	3.361	-11.309
	H	3.367	4.168	-10.952
	H	3.354	1.070	-8.706
	H	4.337	1.940	-9.904
	H	2.813	1.167	-10.404

GeH-2 triplet

	C	4.111	3.849	-6.250
	C	3.140	3.273	-7.116
35	C	3.565	2.664	-8.325
	C	4.929	2.627	-8.641
	C	5.876	3.193	-7.787
	C	5.466	3.801	-6.600
	B	1.622	3.341	-6.726
40	Ge	0.280	4.591	-7.598
	H	0.546	5.448	-8.868
	C	2.554	2.010	-9.258
	C	2.759	0.488	-9.341
	C	3.667	4.586	-4.993
45	C	4.531	4.288	-3.761
	C	0.994	2.562	-5.548
	C	1.721	1.316	-5.104
	C	-0.186	2.893	-4.846
	C	-1.131	3.918	-5.044
50	C	-2.284	3.972	-4.072
	B	-1.130	4.967	-6.182
	C	-2.078	6.221	-6.215
	C	-1.675	7.433	-5.607
	C	-2.529	8.543	-5.639
55	C	-3.771	8.468	-6.271
	C	-4.169	7.276	-6.879
	C	-3.337	6.150	-6.859
	C	-0.304	7.534	-4.947
	C	0.610	8.504	-5.712
60	C	-3.761	4.858	-7.549
	C	-3.663	4.992	-9.077
	C	-5.155	4.377	-7.120
	C	-0.390	7.901	-3.459
	C	2.556	2.652	-10.653
65	C	3.582	6.100	-5.258

	H	-0.402	2.232	-3.993
	H	-2.192	3.236	-3.260
	H	-3.245	3.796	-4.584
	H	-2.372	4.980	-3.635
70	H	1.740	0.564	-5.912
	H	1.266	0.851	-4.217
	H	2.781	1.539	-4.893
	H	-5.143	7.225	-7.372
	H	-4.430	9.339	-6.289
75	H	-2.222	9.481	-5.168
	H	-3.036	4.079	-7.244
	H	-5.230	4.290	-6.027
	H	-5.379	3.394	-7.561
	H	-5.939	5.074	-7.453
80	H	-2.648	5.285	-9.385
	H	-4.357	5.763	-9.445
	H	-3.914	4.042	-9.574
	H	0.157	6.529	-5.010
	H	-1.020	7.187	-2.909
85	H	-0.820	8.904	-3.319
	H	0.610	7.900	-3.000
	H	0.716	8.201	-6.764
	H	1.613	8.538	-5.260
	H	0.197	9.525	-5.699
90	H	6.214	4.247	-5.941
	H	6.936	3.159	-8.046
	H	5.259	2.144	-9.564
	H	2.641	4.243	-4.766
	H	2.924	6.315	-6.113
95	H	4.577	6.511	-5.488
	H	3.185	6.630	-4.379
	H	4.603	3.207	-3.573
	H	4.099	4.763	-2.867
	H	5.554	4.679	-3.874
100	H	1.554	2.179	-8.817
	H	2.376	3.735	-10.591
	H	1.774	2.208	-11.288
	H	3.522	2.501	-11.160
	H	2.728	0.027	-8.342
105	H	3.735	0.245	-9.789
	H	1.978	0.023	-9.961

GeH-2-4MTS-H₂O_singlet

110	C	0.450	-2.219	3.335
	C	-0.269	-1.050	2.982
	C	-1.374	-0.648	3.771
	C	-1.740	-1.414	4.886
	C	-1.030	-2.564	5.227
115	C	0.060	-2.963	4.454
	B	0.206	-0.219	1.743
	Ge	1.784	1.084	1.693
	O	2.970	1.594	3.208
	H	3.795	1.959	2.831
120	C	-2.125	0.635	3.445
	C	-3.640	0.422	3.309
	C	1.657	-2.643	2.505
	C	1.594	-4.110	2.059
	C	-0.336	-0.120	0.347
125	C	-1.643	-0.862	0.070
	C	0.230	0.499	-0.813
	C	1.362	1.295	-1.129
	C	1.545	1.614	-2.610
	B	2.394	1.762	-0.148
130	C	3.760	2.505	-0.292

	C	4.960	1.824	0.072
	C	6.185	2.501	0.027
	C	6.244	3.838	-0.373
	C	5.076	4.510	-0.727
135	C	3.833	3.864	-0.692
	C	4.901	0.344	0.428
	C	6.015	-0.142	1.359
	C	2.564	4.643	-1.010
	C	2.236	5.638	0.117
140	C	2.626	5.351	-2.372
	C	4.816	-0.526	-0.838
	C	-1.808	1.731	4.477
	C	2.972	-2.333	3.240
	H	1.099	2.612	2.432
145	H	-0.356	0.252	-1.715
	H	0.880	2.434	-2.934
	H	1.321	0.745	-3.250
	H	2.575	1.932	-2.825
	H	-1.915	-1.522	0.905
150	H	-1.575	-1.478	-0.840
	H	-2.479	-0.157	-0.077
	H	7.107	1.984	0.298
	H	7.206	4.354	-0.407
	H	5.133	5.559	-1.029
155	H	3.935	0.182	0.967
	H	3.968	-0.225	-1.468
	H	4.691	-1.587	-0.574
	H	5.739	-0.423	-1.429
	H	6.106	0.487	2.255
160	H	6.990	-0.150	0.848
	H	5.811	-1.171	1.687
	H	1.739	3.912	-1.050
	H	2.856	4.641	-3.178
	H	3.395	6.139	-2.386
165	H	1.662	5.830	-2.601
	H	2.145	5.123	1.086
	H	1.287	6.159	-0.083
	H	3.027	6.397	0.216
	H	-2.592	-1.109	5.499
170	H	-1.329	-3.154	6.097
	H	0.610	-3.867	4.727
	H	-1.749	0.984	2.466
	H	-0.725	1.906	4.552
	H	-2.167	1.442	5.477
175	H	-2.294	2.681	4.204
	H	-3.866	-0.353	2.564
	H	-4.134	1.354	2.995
	H	-4.091	0.114	4.265
	H	1.635	-2.030	1.583
180	H	3.036	-1.271	3.525
	H	3.841	-2.575	2.608
	H	3.050	-2.927	4.164
	H	0.658	-4.321	1.522
	H	1.650	-4.795	2.919
185	H	2.436	-4.348	1.392
	H	1.909	2.454	2.942

GeH-2-4MTS-H₂O_triplet

190	C	1.026	-2.573	3.564
	C	0.336	-1.402	3.151
	C	-0.734	-0.912	3.941
	C	-1.101	-1.594	5.107
	C	-0.421	-2.744	5.507
195	C	0.637	-3.228	4.738

	B	0.778	-0.672	1.837
	Ge	1.838	1.045	1.733
	O	3.030	1.501	3.284
	H	3.907	1.765	2.941
5	C	-1.505	0.329	3.516
	C	-2.979	0.012	3.212
	C	2.233	-3.062	2.774
	C	2.258	-4.582	2.564
	C	0.526	-1.175	0.393
10	C	-0.563	-2.214	0.256
	C	1.166	-0.778	-0.801
	C	2.167	0.187	-1.047
	C	2.567	0.389	-2.490
	B	2.857	1.092	-0.005
15	C	4.194	1.902	-0.175
	C	5.444	1.270	0.049
	C	6.628	2.009	-0.080
	C	6.592	3.362	-0.419
	C	5.365	3.992	-0.631
20	C	4.165	3.280	-0.513
	C	5.505	-0.207	0.418
	C	6.262	-0.449	1.733
	C	2.835	3.980	-0.760
	C	2.572	5.090	0.269
25	C	2.727	4.517	-2.196
	C	6.097	-1.049	-0.723
	C	-1.377	1.461	4.547
	C	3.535	-2.567	3.427
	H	1.287	2.658	2.575
30	H	0.817	-1.309	-1.698
	H	2.103	1.306	-2.896
	H	2.259	-0.447	-3.134
	H	3.654	0.539	-2.582
	H	-0.406	-3.038	0.971
35	H	-0.630	-2.625	-0.761
	H	-1.546	-1.786	0.517
	H	7.593	1.523	0.085
	H	7.522	3.927	-0.516
	H	5.344	5.051	-0.897
40	H	4.462	-0.545	0.570
	H	5.529	-0.908	-1.654
	H	6.078	-2.120	-0.469
	H	7.142	-0.766	-0.920
	H	5.797	0.093	2.570
45	H	7.309	-0.121	1.660
	H	6.264	-1.518	1.990
	H	2.042	3.218	-0.632
	H	2.904	3.720	-2.933
	H	3.468	5.310	-2.380
50	H	1.729	4.943	-2.380
	H	2.608	4.697	1.295
	H	1.582	5.544	0.112
	H	3.324	5.890	0.189
	H	-1.934	-1.226	5.712
55	H	-0.717	-3.265	6.421
	H	1.168	-4.124	5.064
	H	-1.049	0.685	2.574
	H	-0.322	1.700	4.744
	H	-1.840	1.178	5.505
60	H	-1.877	2.374	4.188
	H	-3.067	-0.782	2.457
	H	-3.500	0.905	2.835
	H	-3.506	-0.327	4.116
	H	2.174	-2.590	1.775
65	H	3.540	-1.471	3.523

	H	4.410	-2.867	2.829
	H	3.648	-2.993	4.436
	H	1.319	-4.941	2.116
	H	2.406	-5.122	3.511
70	H	3.086	-4.861	1.896
	H	2.114	2.436	3.096

GeH-2-6MTS-H₂O singlet

75	C	-1.532	-0.268	3.710
	C	-0.396	-0.802	3.055
	C	0.242	-1.944	3.602
	C	-0.258	-2.530	4.772
	C	-1.383	-2.001	5.408
80	C	-2.014	-0.876	4.877
	B	0.205	-0.157	1.755
	Ge	1.832	1.091	1.684
	O	2.921	1.501	3.189
	C	1.474	-2.522	2.916
85	C	1.301	-4.002	2.544
	C	-2.198	0.990	3.171
	C	-3.691	0.796	2.869
	C	-0.216	-0.303	0.321
	C	-1.492	-1.096	0.040
90	C	0.469	0.135	-0.851
	C	1.672	0.830	-1.160
	C	1.980	0.961	-2.649
	B	2.659	1.366	-0.171
	C	4.081	2.006	-0.322
95	C	4.257	3.334	-0.785
	C	5.545	3.888	-0.828
	C	6.655	3.150	-0.422
	C	6.492	1.842	0.039
	C	5.219	1.260	0.095
100	C	3.050	4.176	-1.175
	C	2.791	5.282	-0.137
	C	5.036	-0.189	0.524
	C	6.021	-0.668	1.596
	C	5.046	-1.125	-0.697
105	C	3.170	4.761	-2.590
	C	2.744	-2.292	3.752
	C	-1.980	2.175	4.128
	O	1.547	3.525	3.760
	H	3.818	1.707	2.865
110	H	0.940	2.619	1.761
	H	-0.050	-0.200	-1.766
	H	1.390	1.770	-3.114
	H	1.753	0.036	-3.204
	H	3.040	1.202	-2.817
115	H	-1.834	-1.634	0.934
	H	-1.346	-1.837	-0.762
	H	-2.315	-0.433	-0.276
	H	7.369	1.271	0.350
	H	7.653	3.593	-0.463
120	H	5.682	4.914	-1.180
	H	4.014	-0.265	0.956
	H	4.283	-0.822	-1.427
	H	4.840	-2.164	-0.395
	H	6.029	-1.097	-1.192
125	H	6.035	0.002	2.469
	H	7.047	-0.733	1.205
	H	5.742	-1.673	1.947
	H	2.175	3.502	-1.165
	H	3.341	3.969	-3.332
130	H	4.004	5.476	-2.662

	H	2.250	5.298	-2.865
	H	2.673	4.861	0.872
	H	1.877	5.845	-0.383
	H	3.629	5.995	-0.103
135	H	-2.895	-0.467	5.380
	H	-1.769	-2.469	6.316
	H	0.229	-3.413	5.191
	H	-1.695	1.232	2.217
	H	-0.910	2.271	4.376
140	H	-2.515	2.024	5.078
	H	-2.328	3.121	3.685
	H	-3.844	-0.034	2.167
	H	-4.122	1.707	2.424
	H	-4.260	0.573	3.785
145	H	1.594	-1.969	1.964
	H	2.891	-1.223	3.967
	H	3.635	-2.662	3.220
	H	2.683	-2.824	4.714
	H	0.406	-4.150	1.924
150	H	1.199	-4.631	3.441
	H	2.175	-4.364	1.981
	H	2.229	2.732	3.792
	H	1.110	3.069	2.608
	H	0.851	3.356	4.423

GeH-2-6MTS-H₂O triplet

	C	-1.132	-0.431	3.808
	C	0.016	-1.071	3.274
160	C	0.584	-2.165	3.982
	C	0.007	-2.591	5.185
	C	-1.125	-1.959	5.699
	C	-1.691	-0.887	5.009
	B	0.673	-0.589	1.930
165	Ge	1.795	1.077	1.699
	O	2.803	1.700	3.243
	C	1.860	-2.821	3.472
	C	1.800	-4.355	3.468
	C	-1.780	0.734	3.072
170	C	-3.205	0.402	2.603
	C	0.598	-1.337	0.577
	C	-0.510	-2.358	0.461
	C	1.416	-1.173	-0.563
	C	2.492	-0.290	-0.809
175	C	3.103	-0.344	-2.190
	B	3.064	0.756	0.164
	C	4.465	1.474	0.100
	C	4.576	2.793	-0.411
	C	5.823	3.431	-0.429
180	C	6.961	2.787	0.056
	C	6.858	1.495	0.571
	C	5.624	0.830	0.606
	C	3.348	3.510	-0.956
	C	3.027	4.785	-0.160
185	C	5.539	-0.582	1.170
	C	6.114	-0.683	2.591
	C	6.205	-1.601	0.231
	C	3.480	3.809	-2.459
	C	3.077	-2.311	4.264
190	C	-1.758	2.017	3.920
	O	1.653	3.822	3.539
	H	3.739	1.745	2.969
	H	0.874	2.638	1.781
	H	1.168	-1.839	-1.402
195	H	2.705	0.470	-2.821

	H	2.889	-1.292	-2.708
	H	4.192	-0.190	-2.150
	H	-0.512	-3.034	1.331
	H	-0.440	-2.954	-0.460
5	H	-1.499	-1.866	0.473
	H	7.754	0.999	0.953
	H	7.929	3.294	0.035
	H	5.909	4.444	-0.831
	H	4.465	-0.842	1.229
10	H	5.760	-1.563	-0.773
	H	6.089	-2.625	0.619
	H	7.283	-1.397	0.130
	H	5.599	-0.001	3.284
	H	7.186	-0.434	2.612
15	H	6.003	-1.704	2.984
	H	2.494	2.818	-0.833
	H	3.691	2.892	-3.028
	H	4.301	4.517	-2.651
	H	2.553	4.255	-2.851
20	H	2.908	4.570	0.911
	H	2.095	5.246	-0.522
	H	3.831	5.529	-0.263
	H	-2.584	-0.402	5.412
	H	-1.567	-2.304	6.636
25	H	0.450	-3.426	5.733
	H	-1.173	0.922	2.168
	H	-0.738	2.225	4.277
	H	-2.402	1.921	4.808
	H	-2.111	2.882	3.338
30	H	-3.212	-0.500	1.976
	H	-3.630	1.232	2.018
	H	-3.872	0.217	3.459
	H	1.993	-2.491	2.426
	H	3.151	-1.215	4.210
35	H	4.009	-2.741	3.866
	H	2.997	-2.593	5.325
	H	0.926	-4.720	2.910
	H	1.742	-4.765	4.489
	H	2.704	-4.772	3.000
40	H	2.290	2.917	3.593
	H	1.089	3.286	2.533
	H	1.016	3.803	4.278

GeH-2-H₂O-alkoxide intermediate

45	C	3.206	4.511	-5.680
	C	2.501	3.921	-6.774
	C	3.091	3.943	-8.064
	C	4.317	4.597	-8.252
50	C	4.966	5.229	-7.196
	C	4.415	5.173	-5.915
	B	1.121	3.240	-6.455
	Ge	-0.739	3.162	-7.654
	O	-0.681	4.457	-8.978
55	H	-0.800	4.055	-9.856
	C	2.483	3.199	-9.242
	C	3.313	1.950	-9.584
	C	2.696	4.358	-4.249
	C	3.304	3.095	-3.609
60	C	0.880	1.985	-5.648
	C	1.665	0.713	-5.806
	C	-0.126	2.118	-4.682
	C	-0.968	3.245	-4.681
	C	-2.014	3.356	-3.603
65	B	-0.845	4.243	-5.837

	C	-1.577	5.641	-6.012
	C	-0.876	6.875	-6.123
	C	-1.582	8.076	-6.254
	C	-2.973	8.097	-6.296
70	C	-3.671	6.896	-6.227
	C	-3.004	5.669	-6.101
	C	0.642	6.919	-6.169
	C	1.133	6.990	-7.626
	C	-3.862	4.407	-6.172
75	C	-4.374	4.194	-7.609
	C	-5.037	4.410	-5.180
	C	1.251	8.067	-5.351
	C	2.274	4.088	-10.474
	C	2.952	5.562	-3.333
80	H	-0.257	1.339	-3.917
	H	-1.609	3.016	-2.636
	H	-2.893	2.724	-3.818
	H	-2.373	4.387	-3.495
	H	1.156	0.034	-6.511
85	H	1.760	0.173	-4.851
	H	2.670	0.903	-6.210
	H	-4.761	6.908	-6.289
	H	-3.510	9.043	-6.394
	H	-1.033	9.017	-6.333
90	H	-3.227	3.544	-5.930
	H	-4.699	4.603	-4.152
	H	-5.555	3.439	-5.195
	H	-5.780	5.179	-5.436
	H	-3.543	4.186	-8.331
95	H	-5.054	5.007	-7.904
	H	-4.921	3.242	-7.694
	H	1.011	5.972	-5.742
	H	0.901	8.060	-4.308
	H	1.000	9.047	-5.783
100	H	2.349	7.990	-5.356
	H	0.695	6.188	-8.232
	H	2.229	6.907	-7.668
	H	0.840	7.953	-8.075
	H	4.942	5.646	-5.084
105	H	5.910	5.752	-7.365
	H	4.770	4.614	-9.246
	H	1.602	4.218	-4.297
	H	2.571	6.494	-3.764
	H	4.024	5.694	-3.122
110	H	2.451	5.405	-2.366
	H	3.155	2.206	-4.233
	H	2.853	2.903	-2.623
	H	4.388	3.228	-3.469
	H	1.489	2.840	-8.920
115	H	1.651	4.958	-10.228
	H	1.779	3.520	-11.278
	H	3.232	4.451	-10.877
	H	3.411	1.286	-8.711
	H	4.328	2.227	-9.908
120	H	2.841	1.380	-10.399

GeH-2-4MTS-CH₃OH

	C	0.597	-2.134	3.504
125	C	-0.203	-0.996	3.203
	C	-1.232	-0.616	4.100
	C	-1.446	-1.367	5.265
	C	-0.656	-2.478	5.555
	C	0.361	-2.859	4.676
130	B	0.026	-0.233	1.857

	C	0.635	1.105	1.564
	C	1.055	1.968	2.752
	C	-2.147	0.557	3.775
	C	-2.211	1.589	4.911
135	C	1.728	-2.509	2.557
	C	2.979	-1.653	2.828
	C	0.943	1.663	0.288
	C	0.802	1.294	-1.080
	C	1.356	2.315	-2.072
140	B	0.256	0.013	-1.642
	Ge	-0.488	-0.962	0.005
	O	-1.679	-2.529	-0.187
	C	-1.782	-3.435	0.925
	C	0.208	-0.540	-3.106
145	C	-0.697	-0.029	-4.068
	C	-0.724	-0.586	-5.354
	C	0.126	-1.636	-5.697
	C	1.019	-2.146	-4.751
	C	1.068	-1.611	-3.460
150	C	-1.678	1.072	-3.692
	C	-3.104	0.508	-3.554
	C	2.018	-2.187	-2.415
	C	1.478	-3.517	-1.856
	C	3.460	-2.338	-2.918
155	C	-1.644	2.262	-4.663
	C	-3.554	0.068	3.389
	C	2.078	-4.000	2.536
	H	-2.225	-0.340	-0.038
	H	1.469	2.627	0.389
160	H	0.344	2.794	2.921
	H	2.048	2.421	2.599
	H	1.092	1.381	3.680
	H	1.507	1.868	-3.064
	H	2.321	2.728	-1.736
165	H	0.665	3.166	-2.200
	H	0.973	-3.730	4.914
	H	-0.831	-3.052	6.468
	H	-2.245	-1.084	5.955
	H	1.381	-2.236	1.535
170	H	2.746	-0.581	2.763
	H	3.772	-1.877	2.098
	H	3.370	-1.860	3.836
	H	1.188	-4.627	2.377
	H	2.550	-4.319	3.478
175	H	2.795	-4.211	1.729
	H	-1.719	1.060	2.891
	H	-1.207	1.943	5.182
	H	-2.675	1.166	5.815
	H	-2.812	2.459	4.607
180	H	-3.512	-0.638	2.546
	H	-4.196	0.912	3.093
	H	-4.038	-0.446	4.233
	H	-1.421	-0.197	-6.100
	H	0.097	-2.058	-6.704
185	H	1.684	-2.967	-5.030
	H	-1.374	1.445	-2.698
	H	-3.133	-0.327	-2.839
	H	-3.470	0.129	-4.521
	H	-3.802	1.285	-3.207
190	H	-0.626	2.666	-4.759
	H	-2.303	3.069	-4.307
	H	-1.989	1.974	-5.668
	H	2.048	-1.458	-1.582
	H	0.440	-3.415	-1.502
195	H	2.101	-3.879	-1.023

5	H	1.475	-4.292	-2.639	70	H	2.799	4.139	-3.087	135	C	-0.027	-1.472	-2.920		
	H	3.845	-1.384	-3.305		H	3.710	5.548	-2.498		C	3.412	1.969	-9.575		
	H	3.530	-3.083	-3.725		H	1.942	5.504	-2.327		C	3.369	3.215	-3.532		
	H	4.120	-2.672	-2.103		H	3.107	4.800	1.206		C	-0.359	4.545	-8.370		
	H	-2.325	-1.289	-0.083		H	2.148	5.907	0.193		H	-2.321	2.976	-7.395		
	H	-1.973	-2.912	1.876		H	3.924	5.924	0.097		H	-1.303	5.105	-8.273		
	H	-2.608	-4.130	0.716		H	-2.963	-0.506	5.467		H	-0.378	4.060	-9.361		
10	H	-0.849	-4.011	1.028	75	H	-1.665	-2.331	6.527	140	H	0.475	5.257	-8.371		
	GeH-2-6MTS-CH ₃ OH	H	0.422	-3.152		5.467	H	-2.354	0.020		-6.100					
		H	-1.996	1.021		2.157	H	-3.418	1.403		-5.795					
		H	-1.077	2.403		3.995	H	-2.474	0.674		-4.459					
		H	-2.516	2.090		4.989	H	4.814	4.647		-9.216					
		H	-2.665	3.027		3.478	H	5.955	5.736		-7.306					
		H	-4.075	-0.349		2.487	H	4.953	5.607		-5.044					
15	C	5.138	1.058	-0.426	80	H	-4.405	1.401	2.509	145	H	1.556	2.867	-9.028		
	C	4.002	1.911	-0.507		H	-4.383	0.485	4.027		H	1.893	5.027	-10.321		
	C	4.185	3.274	-0.844		H	1.747	-1.699	2.227		H	1.945	3.563	-11.336		
	C	5.477	3.762	-1.087		H	2.943	-1.090	4.348		H	3.446	4.399	-10.905		
	C	6.586	2.921	-1.008		H	3.736	-2.452	3.503		H	3.475	1.311	-8.695		
	C	6.414	1.574	-0.679		H	2.744	-2.753	4.946		H	4.440	2.248	-9.850		
	B	2.583	1.329	-0.172		H	0.553	-3.851	1.994		H	2.979	1.392	-10.407		
20	C	1.475	0.903	-1.087	85	H	1.251	-4.432	3.523	150	H	1.609	4.153	-4.321		
	C	1.653	1.143	-2.585		H	2.314	-4.103	2.134		H	2.372	6.540	-3.933		
	C	2.993	4.220	-0.908		H	2.434	2.936	3.652		H	3.890	5.916	-3.248		
	C	2.854	4.889	-2.285		H	1.272	3.164	2.408		H	2.360	5.548	-2.446		
	C	4.933	-0.416	-0.106		C	1.203	4.281	4.584		H	3.284	2.287	-4.113		
	C	4.591	-1.211	-1.378		H	0.577	5.114	4.241		H	2.918	3.055	-2.541		
	C	0.273	0.217	-0.740		H	0.562	3.485	4.991		H	4.441	3.432	-3.396		
25	C	-0.356	-0.247	0.446	90	H	1.884	4.641	5.369	155	H	-0.487	4.221	-0.921		
	C	-1.642	-1.037	0.212		H	4.746	1.880	4.023		H	0.512	2.384	0.409		
	B	0.138	-0.103	1.856		H	4.681	0.379	3.063		H	1.177	0.274	-0.701		
	Ge	1.857	1.033	1.732		H	4.660	1.966	2.231		H	-0.718	4.237	-4.628		
	O	2.880	1.442	3.258		GeH-2-CH ₃ OH-alkoxide intermediate	100	C	3.208		4.507	-5.677	H	0.278	5.937	-3.041
	C	-0.414	-0.728	3.184				C	2.512		3.918	-6.769	H	-1.220	5.882	-2.085
	C	-1.613	-0.276	3.792				C	3.127		3.956	-8.058	H	-1.266	6.431	-3.766
30	C	-2.043	-0.856	4.994	105	C	4.352	4.618	-8.227	165	H	-2.815	2.997	-3.901		
	C	-1.312	-1.882	5.595		C	5.002	5.223	-7.157		H	-3.102	4.727	-4.212		
	C	-0.137	-2.339	4.998		C	4.431	5.153	-5.888		H	-2.965	4.125	-2.540		
	C	0.320	-1.773	3.802		B	1.111	3.192	-6.604		H	0.968	-0.287	-4.397		
	C	-2.398	0.873	3.174		C	-0.226	3.539	-7.256		H	3.171	-0.100	-3.251		
	C	-2.152	2.176	3.954		C	-1.367	2.810	-6.873		H	2.674	-1.801	-3.467		
	C	1.587	-2.305	3.143		C	-1.304	1.878	-5.828		H	2.548	-1.040	-1.870		
40	C	2.825	-2.138	4.037	110	C	-2.450	0.954	-5.522	170	H	-1.041	-1.161	-3.212		
	C	1.416	-3.757	2.669		C	2.567	3.220	-9.274		H	-0.030	-1.650	-1.834		
	C	-3.899	0.582	3.043		C	2.456	4.106	-10.526		H	0.196	-2.428	-3.419		
	C	3.046	5.270	0.213		C	2.684	4.389	-4.254		H	4.117	-0.890	-5.385		
	C	6.093	-1.071	0.651		C	2.832	5.676	-3.431		H	3.164	-1.073	-6.886		
	O	1.976	3.827	3.456		B	-0.024	1.944	-5.029		H	4.603	-0.010	-6.862		
	C	4.317	1.416	3.122		Ge	1.301	1.077	-6.589		180	GeH-2-4MTS- C ₂ H ₅ OH	C	1.057	-1.621	-3.455
H	0.927	2.615	1.769	O	2.966	0.764	-5.850	C	0.199	-0.547		-3.101				
H	-0.298	-0.068	-1.640	C	3.737	-0.354	-6.270	C	-0.704	-0.035		-4.064				
H	1.017	1.974	-2.936	C	0.128	2.001	-3.467	C	-0.732	-0.593		-5.350				
H	1.380	0.255	-3.180	C	0.653	0.939	-2.688	C	0.116	-1.645		-5.692				
H	2.691	1.407	-2.829	C	0.773	1.093	-1.299	C	1.007	-2.156		-4.746				
H	-1.931	-1.604	1.108	C	0.391	2.273	-0.670	B	0.250	0.007		-1.638				
55	H	-1.537	-1.754	-0.618	120	C	-0.164	3.307	-1.423	190	Ge	-0.491	-0.968	0.011		
	H	-2.486	-0.372	-0.038		C	-0.327	3.184	-2.807		O	-1.671	-2.537	-0.172		
	H	7.289	0.923	-0.621		C	1.013	-0.405	-3.300		C	-1.766	-3.442	0.954		
	H	7.587	3.313	-1.201		C	2.436	-0.859	-2.950		C	-1.685	1.067	-3.688		
	H	5.621	4.816	-1.340		C	-1.057	4.281	-3.579		C	-1.652	2.255	-4.661		
	H	4.035	-0.470	0.545		C	-0.792	5.709	-3.085		C	2.006	-2.199	-2.410		
	H	3.706	-0.794	-1.876		C	-2.574	4.012	-3.563		C	3.447	-2.355	-2.913		
60	H	4.383	-2.266	-1.137	125	130	195									
	H	5.433	-1.179	-2.086												
	H	6.388	-0.486	1.535												
	H	6.982	-1.182	0.012												
	H	5.807	-2.079	0.985												
	H	2.090	3.604	-0.747												

C	0.799	1.288	-1.080	H	-0.803	-3.975	1.047	H	3.674	5.601	-2.410			
C	1.352	2.307	-2.074	H	-2.964	-5.138	1.541	H	1.905	5.555	-2.249			
C	0.942	1.659	0.287	H	-3.863	-3.889	0.642	H	3.045	4.774	1.275			
C	0.638	1.104	1.564	H	-2.743	-4.974	-0.223	H	2.086	5.898	0.283			
5	C	1.059	1.968	2.751	70	135								
B	0.031	-0.234	1.859	GeH-2-6MTS- C ₂ H ₅ OH										
C	-0.197	-0.997	3.206	C	-1.589	-0.237	3.817	H	-2.923	-0.398	5.513			
C	0.606	-2.132	3.509	C	-0.412	-0.733	3.203	H	-1.652	-2.229	6.596			
C	0.367	-2.860	4.679	C	-0.307	-1.781	3.832	H	0.401	-3.122	5.528			
10	C	-0.655	-2.485	5.554	75	C	0.307	-1.781	3.832	140	H	-1.949	1.035	2.157
C	-1.449	-1.378	5.262	C	-0.147	-2.309	5.047	H	-0.971	2.421	3.975			
C	-1.233	-0.624	4.099	C	-1.303	-1.810	5.649	H	-2.428	2.188	4.964			
C	1.743	-2.501	2.566	C	-2.018	-0.780	5.035	H	-2.532	3.091	3.429			
C	2.093	-3.992	2.539	B	0.139	-0.132	1.863	H	-4.060	-0.264	2.527			
15	C	-2.151	0.545	3.769	80	Ge	1.812	1.067	1.743	145	H	-4.344	1.494	2.522
C	-3.556	0.050	3.381	O	2.842	1.483	3.263	H	-4.335	0.601	4.056			
C	-2.222	1.578	4.904	C	4.283	1.535	3.087	H	1.678	-1.810	2.208			
C	2.991	-1.646	2.848	C	4.921	1.925	4.407	H	2.907	-0.964	4.227			
C	-3.110	0.503	-3.546	C	1.568	-2.336	3.178	H	3.732	-2.368	3.489			
20	C	1.462	-3.526	-1.849	85	C	1.445	-3.831	2.849	150	H	2.784	-2.571	4.980
H	-2.229	-0.347	-0.026	C	-2.346	0.921	3.181	H	0.568	-4.026	2.215			
H	1.468	2.625	0.386	C	-3.856	0.671	3.067	H	1.339	-4.431	3.766			
H	0.348	2.795	2.919	C	-0.354	-0.295	0.456	H	2.342	-4.188	2.319			
H	2.052	2.422	2.596	C	-1.627	-1.108	0.231	H	2.372	2.978	3.673			
25	H	1.097	1.383	3.680	90	C	0.261	0.178	-0.734	155	H	1.183	3.179	2.452
H	1.499	1.859	-3.067	C	1.446	0.887	-1.086	H	0.599	3.778	5.062			
H	2.320	2.718	-1.742	C	1.626	1.113	-2.585	H	2.061	4.783	5.275			
H	0.663	3.160	-2.201	B	2.536	1.349	-0.167	H	4.642	0.543	2.770			
H	0.982	-3.729	4.919	C	3.957	1.930	-0.495	H	4.545	2.251	2.290			
30	H	-0.833	-3.062	6.464	95	C	4.144	3.299	-0.798	160	H	6.017	1.921	4.311
H	-2.253	-1.099	5.948	C	5.438	3.792	-1.018	H	4.615	2.937	4.713			
H	1.400	-2.224	1.545	C	5.438	3.792	-1.018	H	4.637	1.218	5.200			
H	2.757	-0.574	2.788	C	6.545	2.947	-0.948	H	0.134	6.294	4.919			
H	3.788	-1.866	2.121	C	6.368	1.592	-0.657	H	1.181	6.360	3.477			
35	H	3.788	-1.866	2.121	100	C	5.089	1.072	-0.428	165	H	-0.337	5.423	3.440
H	3.377	-1.858	3.858	C	2.949	4.242	-0.851	GeH-2-C ₂ H ₅ OH-alkoxide intermediate						
H	1.204	-4.618	2.370	C	2.988	5.267	0.294	C	-0.333	3.179	-2.806			
H	2.558	-4.316	3.483	C	4.879	-0.410	-0.147	C	0.062	1.976	-3.467			
H	2.815	-4.198	1.736	C	6.017	-1.078	0.632	170	C	0.497	0.877	-2.682		
H	-1.723	1.049	2.885	C	4.585	-1.179	-1.447	C	0.600	1.019	-1.290			
40	H	-1.219	1.937	5.175	105	C	2.816	4.938	-2.215	C	0.281	2.218	-0.659	
H	-2.685	1.155	5.808	C	2.822	-2.041	4.017	C	-0.195	3.287	-1.418			
H	-2.826	2.446	4.598	C	-2.054	2.234	3.930	B	-0.072	1.947	-5.040			
H	-3.509	-0.659	2.541	O	1.926	3.864	3.432	175	Ge	1.203	0.956	-6.522		
H	-4.200	0.891	3.082	C	1.271	4.496	4.562	O	2.782	0.397	-5.773			
45	H	-4.040	-0.464	4.226	110	C	0.516	5.713	4.067	C	4.127	0.644	-6.208	
H	-1.429	-0.203	-6.096	H	0.831	2.598	1.830	C	0.781	-0.489	-3.285			
H	0.086	-2.066	-6.700	H	-0.307	-0.124	-1.632	180	C	-0.357	-1.472	-2.966		
H	1.671	-2.978	-5.024	H	0.972	1.924	-2.950	C	-0.983	4.321	-3.586			
50	H	-1.379	1.441	-2.695	115	H	1.378	0.213	-3.173	C	-2.515	4.160	-3.579	
H	-3.137	-0.330	-2.829	H	2.659	1.400	-2.827	C	-1.391	1.892	-5.794			
H	-3.478	0.122	-4.511	H	-1.903	-1.677	1.129	C	-2.559	1.024	-5.424			
H	-3.808	1.281	-3.199	H	-1.515	-1.825	-0.598	C	-1.453	2.802	-6.857			
H	-0.635	2.658	-4.760	H	-2.484	-0.457	-0.017	185	C	-0.286	3.480	-7.256		
H	-2.310	3.063	-4.305	H	7.242	0.938	-0.608	C	-0.384	4.492	-8.366			
55	H	-2.000	1.965	-5.664	120	H	7.549	3.342	-1.120	B	1.020	3.082	-6.556	
H	2.039	-1.469	-1.578	H	5.586	4.852	-1.244	C	2.476	3.696	-6.761			
H	0.424	-3.420	-1.494	H	3.960	-0.482	0.472	C	3.252	4.207	-5.680			
H	2.084	-3.889	-1.016	H	3.715	-0.755	-1.967	190	C	4.557	4.663	-5.900		
H	1.456	-4.302	-2.631	H	4.375	-2.240	-1.237	C	5.134	4.627	-7.167			
60	H	3.835	-1.404	-3.303	125	H	5.451	-1.127	-2.124	C	4.394	4.125	-8.232	
H	3.514	-3.103	-3.719	H	6.280	-0.515	1.539	C	3.085	3.653	-8.058			
H	4.106	-2.690	-2.098	H	6.928	-1.169	0.020	C	2.719	4.223	-4.256			
H	-2.326	-1.296	-0.069	H	5.726	-2.096	0.932	195	C	3.283	3.040	-3.451		
H	-1.918	-2.880	1.892	H	2.047	3.618	-0.711							
65	C	-2.901	-4.418	0.711	130	H	2.765	4.204	-3.031					

	C	2.412	3.048	-9.291
	C	3.082	1.725	-9.703
	C	2.382	4.020	-10.484
	C	2.993	5.544	-3.522
5	C	2.143	-1.062	-2.875
	C	-0.622	5.730	-3.096
	H	-2.406	2.989	-7.374
	H	-1.298	5.096	-8.250
	H	-0.444	4.019	-9.361
10	H	0.482	5.165	-8.375
	H	-2.483	0.047	-5.930
	H	-3.517	1.472	-5.730
	H	-2.585	0.821	-4.343
	H	4.849	4.085	-9.224
15	H	6.155	4.983	-7.321
	H	5.140	5.049	-5.062
	H	1.375	2.804	-9.033
	H	1.938	4.986	-10.206
	H	1.793	3.594	-11.311
20	H	3.393	4.219	-10.870
	H	3.018	0.975	-8.900
	H	4.148	1.871	-9.934
	H	2.592	1.305	-10.595
	H	1.627	4.091	-4.313
25	H	2.597	6.409	-4.075
	H	4.071	5.708	-3.370
	H	2.532	5.523	-2.524
	H	3.052	2.084	-3.938
	H	2.852	3.020	-2.440
30	H	4.378	3.127	-3.363
	H	-0.474	4.216	-0.918
	H	0.388	2.316	0.422
	H	0.940	0.173	-0.689
	H	-0.642	4.246	-4.634
35	H	0.461	5.884	-3.048
	H	-1.040	5.934	-2.098
	H	-1.043	6.481	-3.781
	H	-2.826	3.166	-3.919
	H	-2.987	4.911	-4.232
40	H	-2.904	4.301	-2.559
	H	0.799	-0.366	-4.382
	H	2.949	-0.356	-3.109
	H	2.343	-1.995	-3.422
	H	2.178	-1.291	-1.799
45	H	-1.326	-1.090	-3.320
	H	-0.440	-1.638	-1.880
	H	-0.175	-2.446	-3.445
	C	5.100	0.024	-5.218
	H	4.284	0.198	-7.209
50	H	4.309	1.728	-6.299
	H	6.134	0.169	-5.567
	H	5.003	0.494	-4.229
	H	4.914	-1.053	-5.110

55 PI-TS1-H₂O

	C	3.622	2.605	-9.073
	C	3.993	3.231	-7.844
	C	5.362	3.509	-7.595
60	C	6.318	3.178	-8.564
	C	5.947	2.577	-9.765
	C	4.605	2.284	-10.014
	B	2.879	3.535	-6.802
	C	2.304	4.837	-6.291
65	C	1.053	4.962	-5.658

	C	-0.002	4.090	-5.189
	C	-1.101	4.841	-4.442
	C	5.813	4.085	-6.259
	C	6.620	5.382	-6.424
70	C	2.156	2.356	-9.381
	C	1.446	3.626	-9.878
	Ge	1.534	2.062	-6.235
	O	2.118	0.269	-6.278
	H	1.386	-0.348	-6.089
75	B	-0.202	2.619	-5.378
	C	-1.366	1.642	-5.001
	C	-1.644	1.304	-3.650
	C	-2.678	0.402	-3.361
	C	-3.434	-0.172	-4.380
80	C	-3.160	0.142	-5.712
	C	-2.137	1.038	-6.039
	C	-0.796	1.857	-2.511
	C	0.068	0.751	-1.882
	C	-1.876	1.425	-7.489
85	C	-2.235	0.346	-8.516
	Si	3.395	0.364	-4.537
	F	4.288	0.556	-3.169
	F	2.505	-0.930	-4.090
	F	4.579	0.102	-5.613
90	C	-2.556	2.762	-7.830
	C	-1.638	2.570	-1.441
	C	3.013	6.141	-6.633
	C	6.610	3.047	-5.449
	C	1.871	1.154	-10.282
95	H	0.775	6.019	-5.506
	H	-1.402	5.754	-4.984
	H	-0.764	5.158	-3.441
	H	-1.994	4.216	-4.306
	H	3.570	6.058	-7.578
100	H	3.746	6.414	-5.856
	H	2.308	6.981	-6.726
	H	-2.890	0.137	-2.322
	H	-4.237	-0.871	-4.138
	H	-3.757	-0.317	-6.502
105	H	-0.111	2.603	-2.950
	H	-2.258	3.363	-1.882
	H	-0.988	3.025	-0.680
	H	-2.310	1.867	-0.923
	H	0.672	0.229	-2.637
110	H	-0.560	-0.004	-1.387
	H	0.750	1.170	-1.126
	H	-0.782	1.603	-7.572
	H	-2.226	3.558	-7.148
	H	-3.649	2.666	-7.743
115	H	-2.319	3.071	-8.860
	H	-1.777	-0.622	-8.269
	H	-1.886	0.646	-9.516
	H	-3.323	0.197	-8.588
	H	4.327	1.809	-10.957
120	H	6.706	2.328	-10.510
	H	7.374	3.379	-8.371
	H	1.665	2.116	-8.390
	H	2.384	0.252	-9.923
	H	2.195	1.348	-11.316
125	H	0.791	0.952	-10.314
	H	1.596	4.465	-9.184
	H	0.365	3.454	-9.987
	H	1.852	3.917	-10.859
	H	4.902	4.321	-5.682
130	H	6.052	2.110	-5.327

	H	6.852	3.439	-4.449
	H	7.558	2.802	-5.953
	H	6.065	6.133	-7.004
	H	7.574	5.195	-6.940
135	H	6.859	5.813	-5.440
	H	2.769	1.750	-4.482

PI-I-H₂O

140	C	3.121	-0.651	-1.793
	C	3.003	0.254	-0.704
	C	4.115	0.456	0.151
	C	5.318	-0.216	-0.104
	C	5.435	-1.082	-1.190
145	C	4.339	-1.301	-2.026
	B	1.635	0.982	-0.476
	C	1.254	2.421	-0.710
	C	-0.034	3.061	-0.704
	C	-1.358	2.687	-0.390
150	C	-2.456	3.698	-0.690
	C	3.989	1.339	1.385
	C	5.118	2.373	1.507
	C	1.927	-0.865	-2.715
	C	1.871	0.215	-3.809
155	Ge	0.033	0.308	0.578
	O	-0.899	-1.690	0.189
	H	-1.828	-1.420	-0.096
	B	-1.692	1.304	0.074
	C	-3.003	0.437	0.023
160	C	-3.853	0.325	1.150
	C	-4.914	-0.588	1.131
	C	-5.133	-1.411	0.025
	C	-4.298	-1.317	-1.088
	C	-3.231	-0.400	-1.110
165	C	-3.592	1.196	2.369
	C	-3.335	0.360	3.632
	C	-2.368	-0.219	-2.358
	C	-2.085	-1.516	-3.126
	Si	-0.726	-3.086	1.072
170	F	-1.371	-2.943	2.536
	F	-1.449	-4.304	0.317
	F	0.844	-3.364	1.209
	C	-2.988	0.840	-3.286
	C	-4.722	2.215	2.584
175	C	2.390	3.357	-1.127
	C	3.888	0.477	2.657
	C	1.850	-2.270	-3.325
	H	0.025	4.077	-1.132
	H	-2.253	4.289	-1.598
180	H	-2.577	4.414	0.141
	H	-3.429	3.201	-0.819
	H	3.285	2.796	-1.428
	H	2.686	4.026	-0.301
	H	2.091	4.001	-1.971
185	H	-5.575	-0.669	1.998
	H	-5.957	-2.128	0.031
	H	-4.480	-1.961	-1.951
	H	-2.669	1.769	2.153
	H	-4.868	2.840	1.691
190	H	-4.494	2.875	3.434
	H	-5.675	1.707	2.799
	H	-2.516	-0.357	3.478
	H	-4.231	-0.211	3.921
	H	-3.069	1.010	4.479
195	H	-1.395	0.191	-2.022

	H	-3.135	1.791	-2.758
	H	-3.966	0.498	-3.660
	H	-2.333	1.025	-4.150
	H	-1.644	-2.291	-2.482
5	H	-1.378	-1.319	-3.944
	H	-2.999	-1.930	-3.579
	H	4.439	-1.990	-2.867
	H	6.379	-1.597	-1.381
	H	6.175	-0.067	0.556
10	H	1.025	-0.728	-2.086
	H	1.920	-3.050	-2.552
	H	2.657	-2.444	-4.054
	H	0.899	-2.402	-3.861
	H	1.842	1.221	-3.366
15	H	0.975	0.091	-4.438
	H	2.758	0.151	-4.459
	H	3.039	1.893	1.286
	H	3.058	-0.239	2.585
	H	3.726	1.106	3.546
20	H	4.813	-0.099	2.812
	H	5.193	2.988	0.599
	H	6.094	1.890	1.669
	H	4.936	3.041	2.362
	H	0.248	-0.039	2.089

P1-TS2-H₂O

	C	3.218	-0.266	-1.794
	C	2.941	0.587	-0.692
30	C	3.990	0.930	0.198
	C	5.285	0.449	-0.038
	C	5.555	-0.361	-1.140
	C	4.524	-0.721	-2.009
	B	1.478	1.114	-0.506
35	C	0.921	2.495	-0.737
	C	-0.437	2.974	-0.781
	C	-1.707	2.450	-0.475
	C	-2.919	3.300	-0.820
	C	3.703	1.754	1.446
40	C	4.663	2.940	1.624
	C	2.094	-0.631	-2.755
	C	2.023	0.363	-3.926
	Ge	-0.035	0.261	0.541
	B	-1.865	1.044	0.019
45	C	-3.077	0.042	-0.051
	C	-3.870	-0.210	1.096
	C	-4.865	-1.192	1.050
	C	-5.070	-1.947	-0.107
	C	-4.282	-1.723	-1.235
50	C	-3.280	-0.736	-1.228
	C	-3.620	0.601	2.358
	C	-3.300	-0.288	3.569
	C	-2.462	-0.444	-2.484
	C	-1.924	-1.702	-3.182
55	C	1.943	3.576	-1.096
	C	-3.274	0.419	-3.465
	C	-4.787	1.559	2.650
	C	3.696	0.856	2.697
	C	2.154	-2.080	-3.254
60	O	-0.809	-1.847	0.165
	Si	-0.509	-3.279	0.947
	F	1.072	-3.524	0.902
	F	-0.987	-3.234	2.481
	F	-1.284	-4.479	0.213
65	H	-1.754	-1.635	-0.099

	H	-0.488	3.977	-1.239
	H	-2.764	3.917	-1.720
	H	-3.171	3.988	0.004
	H	-3.808	2.674	-0.988
70	H	2.925	3.143	-1.328
	H	2.086	4.288	-0.265
	H	1.613	4.163	-1.970
	H	-5.486	-1.379	1.929
	H	-5.847	-2.715	-0.129
75	H	-4.449	-2.318	-2.135
	H	-2.729	1.226	2.158
	H	-4.977	2.222	1.794
	H	-4.566	2.183	3.529
	H	-5.713	1.000	2.856
80	H	-2.451	-0.956	3.363
	H	-4.161	-0.916	3.842
	H	-3.047	0.328	4.445
	H	-1.591	0.162	-2.170
	H	-3.611	1.350	-2.990
85	H	-4.164	-0.126	-3.816
	H	-2.665	0.682	-4.343
	H	-1.323	-2.324	-2.503
	H	-1.282	-1.417	-4.028
	H	-2.737	-2.326	-3.583
90	H	4.746	-1.365	-2.863
	H	6.571	-0.721	-1.318
	H	6.095	0.708	0.647
	H	1.151	-0.517	-2.184
	H	2.218	-2.789	-2.416
95	H	3.022	-2.252	-3.908
	H	1.254	-2.320	-3.842
	H	1.902	1.392	-3.557
	H	1.173	0.132	-4.587
	H	2.945	0.321	-4.525
100	H	2.685	2.166	1.330
	H	2.981	0.028	2.587
	H	3.421	1.433	3.593
	H	4.691	0.417	2.867
	H	4.671	3.581	0.731
105	H	5.695	2.603	1.807
	H	4.360	3.554	2.486
	H	0.221	-0.065	2.049

P2-TS1-H₂O

110	C	-1.228	-0.396	3.128
	C	-1.299	-0.753	1.743
	C	-1.050	-2.108	1.385
	C	-0.755	-3.055	2.376
115	C	-0.711	-2.702	3.721
	C	-0.953	-1.381	4.085
	B	-1.530	0.386	0.664
	Ge	0.284	1.460	0.421
	O	1.579	0.183	0.885
120	C	-1.086	-2.575	-0.063
	C	-2.002	-3.796	-0.252
	C	-1.367	1.039	3.633
	C	-2.456	1.187	4.708
	C	-2.726	1.304	0.445
125	C	-3.879	1.399	1.409
	C	-2.702	2.172	-0.666
	C	-1.663	2.107	-1.601
	C	-1.499	3.151	-2.668
	B	-0.776	0.891	-1.446
130	C	-0.296	-0.089	-2.575

	C	-1.285	-0.882	-3.236
	C	-0.892	-1.796	-4.219
	C	0.443	-1.914	-4.600
	C	1.400	-1.096	-4.009
135	C	1.056	-0.184	-3.001
	C	-2.773	-0.698	-2.948
	C	-3.605	-1.987	-2.999
	C	2.141	0.743	-2.480
	C	3.395	0.005	-1.998
140	C	2.487	1.810	-3.535
	C	-3.373	0.327	-3.930
	C	0.323	-2.877	-0.597
	C	-0.021	1.571	4.156
	F	3.491	-1.546	1.472
145	Si	3.822	-0.029	1.961
	F	5.331	-0.197	2.579
	F	2.949	0.358	3.274
	H	1.134	-0.647	1.151
	H	-3.511	2.906	-0.799
150	H	-4.824	1.577	0.871
	H	-3.751	2.241	2.111
	H	-3.977	0.487	2.010
	H	-0.988	2.751	-3.555
	H	-0.888	3.988	-2.291
155	H	-2.469	3.575	-2.974
	H	-0.904	-1.102	5.140
	H	-0.483	-3.452	4.481
	H	-0.560	-4.090	2.089
	H	-1.652	1.676	2.783
160	H	-3.425	0.799	4.364
	H	-2.584	2.246	4.978
	H	-2.188	0.646	5.628
	H	0.769	1.501	3.397
	H	0.324	0.990	5.024
165	H	-0.116	2.623	4.465
	H	-1.501	-1.748	-0.665
	H	-3.035	-3.580	0.057
	H	-1.648	-4.655	0.335
	H	-2.008	-4.111	-1.305
170	H	0.979	-1.999	-0.532
	H	0.279	-3.175	-1.655
	H	0.790	-3.692	-0.024
	H	-1.643	-2.420	-4.706
	H	0.734	-2.634	-5.369
175	H	2.439	-1.165	-4.337
	H	-2.873	-0.289	-1.928
	H	-3.188	-2.771	-2.357
	H	-3.675	-2.385	-4.023
	H	-4.632	-1.782	-2.663
180	H	-2.815	1.270	-3.932
	H	-4.421	0.546	-3.672
	H	-3.350	-0.076	-4.954
	H	1.723	1.283	-1.610
	H	3.148	-0.726	-1.218
185	H	4.120	0.721	-1.582
	H	3.895	-0.523	-2.823
	H	1.591	2.369	-3.845
	H	2.919	1.345	-4.434
	H	3.221	2.527	-3.137
190	H	3.976	1.017	0.940

P2-I-H₂O

	C	-1.063	-0.758	-3.285
195	C	-0.117	0.040	-2.572

	C	1.249	0.007	-2.967
	C	1.641	-0.843	-4.011
	C	0.723	-1.654	-4.669
	C	-0.622	-1.601	-4.310
5	B	-0.668	0.990	-1.451
	Ge	0.312	1.511	0.436
	B	-1.523	0.504	0.752
	C	-2.697	1.427	0.464
	C	-2.649	2.246	-0.679
10	C	-1.594	2.173	-1.602
	C	-1.429	3.221	-2.667
	C	2.297	0.945	-2.390
	C	2.534	2.132	-3.341
	C	-2.560	-0.680	-2.996
15	C	-3.240	0.342	-3.924
	C	-1.246	-0.603	1.842
	C	-0.972	-1.950	1.474
	C	-0.492	-2.856	2.430
	C	-0.300	-2.467	3.753
20	C	-0.608	-1.164	4.134
	C	-1.066	-0.219	3.207
	C	-1.269	-2.456	0.072
	C	-0.046	-3.069	-0.626
	C	-1.327	1.198	3.708
25	C	-0.049	1.873	4.235
	C	-3.859	1.588	1.411
	C	-2.435	1.222	4.775
	C	-2.443	-3.450	0.131
	C	3.615	0.249	-2.031
30	C	-3.284	-2.029	-3.114
	O	1.548	0.094	0.810
	Si	3.400	0.267	1.753
	F	4.911	0.450	2.413
	F	2.548	0.193	3.156
35	F	3.638	-1.220	1.099
	H	1.078	-0.728	1.062
	H	-3.456	2.973	-0.851
	H	-4.782	1.833	0.863
	H	-3.685	2.408	2.127
40	H	-4.024	0.677	2.001
	H	-0.934	2.818	-3.561
	H	-0.797	4.043	-2.291
	H	-2.394	3.664	-2.956
	H	-0.459	-0.864	5.173
45	H	0.087	-3.178	4.486
	H	-0.274	-3.884	2.134
	H	-1.674	1.799	2.856
	H	-3.359	0.752	4.409
	H	-2.665	2.258	5.069
50	H	-2.124	0.683	5.682
	H	0.739	1.900	3.470
	H	0.366	1.331	5.096
	H	-0.265	2.904	4.551
	H	-1.591	-1.584	-0.527
55	H	-3.349	-2.972	0.532
	H	-2.197	-4.299	0.787
	H	-2.678	-3.857	-0.861
	H	0.787	-2.354	-0.683
	H	-0.298	-3.361	-1.656
60	H	0.309	-3.966	-0.097
	H	-1.341	-2.226	-4.842
	H	1.053	-2.322	-5.468
	H	2.689	-0.866	-4.316
	H	-2.686	-0.327	-1.957
65	H	-2.737	-2.831	-2.604

	H	-3.411	-2.326	-4.166
	H	-4.288	-1.963	-2.672
	H	-2.774	1.332	-3.860
	H	-4.306	0.447	-3.669
70	H	-3.170	0.006	-4.970
	H	1.886	1.366	-1.455
	H	3.449	-0.610	-1.370
	H	4.286	0.951	-1.516
	H	4.144	-0.102	-2.930
75	H	1.600	2.674	-3.548
	H	2.940	1.784	-4.303
	H	3.255	2.840	-2.903
	H	3.402	1.527	0.965

80 P2-TS2-H₂O

	C	1.463	-0.920	-2.226
	C	0.076	-0.899	-1.877
	C	-0.711	-2.063	-2.134
85	C	-0.098	-3.222	-2.625
	C	1.264	-3.254	-2.904
	C	2.026	-2.102	-2.729
	B	-0.651	0.364	-1.287
	C	-1.651	1.283	-1.959
90	C	-2.742	1.704	-1.200
	C	-2.798	1.516	0.197
	C	-3.997	2.052	0.933
	C	-2.227	-2.050	-1.963
	C	-2.905	-1.566	-3.261
95	C	2.353	0.316	-2.183
	C	2.388	0.990	-3.567
	B	-1.635	0.873	0.936
	Ge	0.198	1.632	0.262
	O	1.443	-0.366	0.784

100	Si	2.435	0.330	1.985
	F	1.982	0.444	3.550
	C	-1.498	0.441	2.450
	C	-1.436	1.417	3.489
	C	-1.216	1.001	4.809
105	C	-1.041	-0.340	5.130
	C	-1.112	-1.300	4.122
	C	-1.342	-0.927	2.795
	C	-1.570	2.917	3.235
	C	-0.275	3.676	3.576
110	C	-1.550	-1.996	1.739
	C	-0.547	-3.153	1.812
	C	-3.004	-2.498	1.835
	C	-2.761	3.520	4.003
	F	3.456	-0.966	2.130
115	F	3.542	1.447	1.514
	C	-1.471	1.780	-3.368
	C	-2.823	-3.411	-1.575
	C	3.782	0.053	-1.684
	H	1.725	-1.197	0.358
120	H	-3.561	2.244	-1.696
	H	-4.903	2.003	0.309
	H	-3.857	3.111	1.209
	H	-4.171	1.501	1.868
	H	-0.958	1.043	-4.003
125	H	-0.851	2.693	-3.371
	H	-2.435	2.043	-3.830
	H	-1.158	1.749	5.603
	H	-0.846	-0.639	6.162
	H	-0.991	-2.356	4.375
130	H	-1.757	3.065	2.160

	H	-3.696	2.985	3.785
	H	-2.896	4.580	3.736
	H	-2.597	3.471	5.089
	H	0.587	3.274	3.028
135	H	-0.044	3.599	4.649
	H	-0.377	4.743	3.329
	H	-1.417	-1.503	0.756
	H	-3.716	-1.676	1.668
	H	-3.194	-2.905	2.840
140	H	-3.212	-3.289	1.103
	H	0.485	-2.782	1.864
	H	-0.636	-3.797	0.924
	H	-0.719	-3.788	2.694
	H	-0.698	-4.117	-2.796
145	H	1.730	-4.170	-3.274
	H	3.085	-2.119	-2.988
	H	-2.474	-1.329	-1.163
	H	-2.274	-3.882	-0.749
	H	-2.814	-4.108	-2.426
150	H	-3.872	-3.291	-1.269
	H	-2.537	-0.584	-3.578
	H	-3.995	-1.494	-3.122
	H	-2.709	-2.280	-4.075
	H	1.891	1.037	-1.488
155	H	3.804	-0.531	-0.755
	H	4.289	1.007	-1.482
	H	4.382	-0.483	-2.434
	H	1.379	1.259	-3.910
	H	2.828	0.312	-4.314
160	H	2.997	1.906	-3.535
	H	1.259	1.574	1.695

P1-TS1-CH₃OH

165	C	2.396	3.456	-1.471
	C	1.224	3.028	-2.163
	C	0.169	2.431	-1.426
	C	0.301	2.264	-0.040
	C	1.453	2.676	0.626
170	C	2.494	3.273	-0.088
	B	1.123	3.280	-3.706
	Ge	0.735	5.027	-4.607
	O	-0.114	6.438	-3.689
	Si	-2.046	6.396	-4.380
175	F	-1.798	7.935	-4.862
	C	-1.129	2.015	-2.104
	C	-1.451	0.527	-1.887
	C	3.553	4.057	-2.260
	C	4.445	2.948	-2.845
180	B	0.906	5.144	-6.672
	C	1.062	3.719	-7.171
	C	1.297	3.462	-8.653
	C	1.208	6.500	-7.372
	C	2.281	7.307	-6.886
185	C	2.584	8.514	-7.524
	C	1.844	8.940	-8.628
	C	0.773	8.175	-9.086
	C	0.438	6.962	-8.471
	C	3.130	6.828	-5.721
190	C	3.786	7.935	-4.892
	C	-0.809	6.213	-8.916
	C	-2.077	6.989	-8.514
	C	1.200	2.618	-6.315
	C	1.144	2.356	-4.886
195	C	1.184	0.864	-4.570

	C	-0.815	5.900	-10.420
	C	4.151	5.757	-6.139
	C	0.322	6.813	-2.361
	H	1.255	7.390	-2.433
5	C	-2.302	2.901	-1.649
	C	4.383	5.090	-1.491
	F	-3.534	6.158	-5.058
	F	-2.478	6.256	-2.808
	H	1.463	1.698	-6.863
10	H	1.961	0.352	-5.162
	H	0.224	0.376	-4.812
	H	1.386	0.683	-3.506
	H	1.833	4.298	-9.126
	H	0.343	3.352	-9.194
15	H	1.877	2.543	-8.824
	H	-0.512	1.809	0.529
	H	1.541	2.537	1.705
	H	3.391	3.593	0.443
	H	-0.994	2.175	-3.187
20	H	-0.620	-0.115	-2.212
	H	-2.349	0.241	-2.455
	H	-1.648	0.311	-0.826
	H	-2.094	3.968	-1.809
	H	-2.508	2.759	-0.577
25	H	-3.219	2.647	-2.203
	H	3.098	4.579	-3.126
	H	3.857	2.262	-3.472
	H	4.908	2.362	-2.036
	H	5.249	3.376	-3.464
30	H	3.748	5.872	-1.050
	H	5.106	5.574	-2.166
	H	4.964	4.628	-0.679
	H	3.409	9.132	-7.166
	H	2.097	9.880	-9.123
35	H	0.178	8.538	-9.927
	H	2.419	6.305	-5.011
	H	3.062	8.712	-4.609
	H	4.604	8.415	-5.451
	H	4.225	7.513	-3.977
40	H	3.665	4.918	-6.656
	H	4.684	5.360	-5.262
	H	4.891	6.199	-6.823
	H	-0.825	5.255	-8.368
	H	-2.084	7.233	-7.444
45	H	-2.979	6.400	-8.736
	H	-2.142	7.937	-9.069
	H	0.089	5.356	-10.724
	H	-0.873	6.821	-11.019
	H	-1.691	5.285	-10.679
50	H	-1.418	5.236	-5.142
	H	-0.461	7.434	-1.914
	H	0.478	5.917	-1.740

P1-I- CH₃OH

55	C	-1.024	-0.074	4.200
	C	0.075	-0.288	3.335
	C	1.342	0.263	3.670
	C	1.485	1.003	4.851
60	C	0.395	1.208	5.699
	C	-0.850	0.675	5.372
	B	-0.069	-1.059	1.975
	Ge	-0.714	-0.383	0.176
	B	0.115	-1.365	-1.424
65	C	0.359	-2.770	-0.937

	C	0.857	-3.821	-1.923
	C	2.530	0.010	2.749
	C	3.246	-1.300	3.120
	C	-2.397	-0.619	3.830
70	C	-3.023	-1.461	4.952
	C	0.462	-0.690	-2.794
	C	-0.313	-0.911	-3.957
	C	0.001	-0.225	-5.139
	C	1.075	0.660	-5.187
75	C	1.857	0.869	-4.049
	C	1.567	0.205	-2.852
	C	-1.503	-1.860	-3.921
	C	-2.836	-1.104	-4.055
	C	2.455	0.367	-1.623
80	C	3.149	1.731	-1.513
	C	0.276	-3.173	0.415
	C	0.048	-2.530	1.676
	C	0.050	-3.477	2.875
	C	3.486	-0.771	-1.533
85	C	-1.390	-2.970	-4.978
	C	3.531	1.170	2.679
	C	-3.340	0.514	3.390
	O	-0.464	1.838	-0.070
	Si	-1.101	2.739	-1.322
90	F	-2.081	3.864	-0.717
	C	0.288	2.519	0.996
	F	0.057	3.502	-2.129
	F	-1.930	1.760	-2.271
	H	1.316	2.686	0.653
95	H	0.539	-4.237	0.553
	H	0.823	-4.259	2.781
	H	-0.919	-3.994	2.978
	H	0.226	-2.935	3.815
	H	1.370	-3.353	-2.776
100	H	0.022	-4.409	-2.341
	H	1.556	-4.534	-1.457
	H	-1.699	0.845	6.039
	H	0.518	1.788	6.617
	H	2.456	1.426	5.116
105	H	-2.250	-1.285	2.962
	H	-2.352	-2.278	5.253
	H	-3.975	-1.901	4.619
	H	-3.234	-0.852	5.844
	H	-2.907	1.087	2.556
110	H	-3.526	1.214	4.219
	H	-4.310	0.112	3.059
	H	2.112	-0.136	1.732
	H	2.551	-2.149	3.083
	H	3.660	-1.237	4.138
115	H	4.073	-1.504	2.422
	H	3.036	2.129	2.464
	H	4.274	0.983	1.889
	H	4.086	1.287	3.622
	H	2.703	1.558	-4.102
120	H	1.309	1.189	-6.114
	H	-0.601	-0.386	-6.036
	H	1.792	0.254	-0.740
	H	2.443	2.564	-1.646
	H	3.938	1.843	-2.272
125	H	3.634	1.831	-0.530
	H	2.991	-1.752	-1.528
	H	4.082	-0.685	-0.611
	H	4.173	-0.734	-2.393
	H	-1.496	-2.343	-2.927
130	H	-2.944	-0.343	-3.270

	H	-3.687	-1.800	-3.981
	H	-2.901	-0.593	-5.028
	H	-0.441	-3.516	-4.882
	H	-1.441	-2.559	-5.998
135	H	-2.215	-3.691	-4.870
	H	-2.268	-0.203	0.110
	H	-0.204	3.468	1.245
	H	0.275	1.853	1.866

140 P1-TS2- CH₃OH

	C	-0.692	-0.217	4.116
	C	0.430	-0.221	3.251
	C	1.677	0.266	3.722
145	C	1.796	0.716	5.042
	C	0.691	0.702	5.896
	C	-0.541	0.244	5.431
	B	0.409	-0.688	1.762
	Ge	-0.475	-0.031	0.096
150	B	0.453	-0.638	-1.640
	C	1.099	-2.006	-1.415
	C	1.910	-2.697	-2.491
	C	2.881	0.272	2.786
	C	3.898	-0.811	3.171
155	C	-2.061	-0.656	3.615
	C	-2.730	-1.695	4.528
	C	0.689	0.320	-2.853
	C	-0.068	0.115	-4.028
	C	0.099	0.975	-5.121
160	C	1.010	2.028	-5.058
	C	1.763	2.232	-3.899
	C	1.617	1.393	-2.787
	C	-1.107	-0.997	-4.061
	C	-2.534	-0.431	-3.969
165	C	2.466	1.584	-1.533
	C	2.918	3.030	-1.290
	C	1.077	-2.515	-0.135
	C	0.474	-2.054	1.113
	C	0.121	-3.216	2.046
170	C	3.686	0.644	-1.530
	C	-0.952	-1.924	-5.276
	C	3.539	1.655	2.676
	C	-2.975	0.562	3.399
	O	-0.582	2.747	-0.163
175	Si	-1.239	3.654	-1.368
	F	-2.388	4.636	-0.796
	C	-0.090	3.320	1.075
	F	-0.166	4.606	-2.103
	F	-1.894	2.651	-2.434
180	H	0.837	3.881	0.892
	H	1.650	-3.446	0.021
	H	0.969	-3.918	2.127
	H	-0.738	-3.789	1.662
	H	-0.125	-2.869	3.057
185	H	2.545	-1.985	-3.040
	H	1.247	-3.157	-3.243
	H	2.555	-3.492	-2.086
	H	-1.401	0.248	6.105
	H	0.791	1.053	6.925
190	H	2.758	1.078	5.411
	H	-1.910	-1.133	2.631
	H	-2.081	-2.570	4.679
	H	-3.676	-2.042	4.087
	H	-2.963	-1.275	5.518
195	H	-2.514	1.285	2.710

	H	-3.167	1.079	4.352
	H	-3.944	0.255	2.976
	H	2.499	0.013	1.778
	H	3.424	-1.803	3.187
5	H	4.317	-0.620	4.171
	H	4.733	-0.838	2.453
	H	2.810	2.417	2.365
	H	4.354	1.638	1.936
	H	3.970	1.976	3.636
10	H	2.468	3.065	-3.864
	H	1.133	2.698	-5.911
	H	-0.494	0.829	-6.027
	H	1.830	1.290	-0.674
	H	2.085	3.741	-1.365
15	H	3.685	3.339	-2.017
	H	3.368	3.119	-0.290
	H	3.385	-0.407	-1.606
	H	4.263	0.764	-0.599
	H	4.350	0.875	-2.377
20	H	-0.943	-1.615	-3.155
	H	-2.656	0.195	-3.075
	H	-3.275	-1.244	-3.929
	H	-2.761	0.193	-4.846
	H	0.068	-2.326	-5.343
25	H	-1.166	-1.390	-6.214
	H	-1.654	-2.770	-5.210
	H	-2.018	0.148	0.189
	H	-0.846	3.977	1.528
	H	0.117	2.479	1.748

P2-TS1- CH₃OH

	C	-1.094	-1.307	-3.222
	C	-0.157	-0.354	-2.711
35	C	1.175	-0.367	-3.213
	C	1.566	-1.379	-4.101
	C	0.675	-2.364	-4.513
	C	-0.652	-2.309	-4.092
	B	-0.659	0.698	-1.661
40	C	-1.552	1.897	-1.836
	C	-1.430	2.819	-3.022
	C	2.168	0.752	-2.935
	C	2.249	1.695	-4.151
	C	-2.588	-1.180	-2.932
45	C	-3.232	-0.198	-3.932
	C	-2.502	2.177	-0.838
	C	-2.491	1.550	0.413
	C	-3.486	2.002	1.451
	B	-1.412	0.527	0.748
50	Ge	0.489	1.218	0.107
	O	1.772	-0.117	0.373
	C	1.468	-1.519	0.310
	C	-1.332	-0.427	2.002
	C	-1.613	-1.815	1.896
55	C	-1.508	-2.644	3.018
	C	-1.123	-2.125	4.254
	C	-0.869	-0.763	4.376
	C	-0.973	0.102	3.277
	C	-2.123	-2.382	0.583
60	C	-1.594	-3.787	0.269
	C	-0.693	1.584	3.513
	C	0.788	1.838	3.829
	C	-1.593	2.172	4.614
	C	-3.664	-2.350	0.589
65	C	3.564	0.261	-2.537

	C	-3.360	-2.506	-2.983
	Si	3.980	0.377	1.540
	F	4.475	-0.745	0.475
	F	5.381	0.823	2.263
70	F	3.167	-0.338	2.748
	H	-3.254	2.954	-1.035
	H	-4.404	2.393	0.984
	H	-3.072	2.813	2.074
	H	-3.747	1.183	2.136
75	H	-1.008	2.308	-3.898
	H	-0.759	3.659	-2.782
	H	-2.405	3.253	-3.295
	H	-0.578	-0.359	5.348
	H	-1.029	-2.782	5.121
80	H	-1.728	-3.709	2.929
	H	-0.918	2.124	2.580
	H	-2.656	1.978	4.414
	H	-1.447	3.261	4.686
	H	-1.355	1.743	5.599
85	H	1.433	1.467	3.022
	H	1.094	1.320	4.749
	H	0.978	2.914	3.961
	H	-1.770	-1.705	-0.217
	H	-4.037	-1.324	0.725
90	H	-4.050	-2.961	1.419
	H	-4.078	-2.747	-0.347
	H	-0.498	-3.830	0.347
	H	-1.871	-4.087	-0.750
	H	-2.012	-4.541	0.952
95	H	-1.358	-3.053	-4.463
	H	1.005	-3.160	-5.184
	H	2.590	-1.392	-4.479
	H	-2.708	-0.752	-1.920
	H	-2.893	-3.283	-2.365
100	H	-3.429	-2.888	-4.012
	H	-4.389	-2.355	-2.628
	H	-2.735	0.776	-3.928
	H	-4.295	-0.044	-3.692
	H	-3.166	-0.606	-4.953
105	H	1.775	1.348	-2.093
	H	3.519	-0.441	-1.698
	H	4.193	1.112	-2.233
	H	4.075	-0.232	-3.378
	H	1.261	2.096	-4.421
110	H	2.644	1.162	-5.030
	H	2.919	2.542	-3.938
	H	3.451	1.642	1.003
	H	1.074	-1.866	1.278
	H	0.733	-1.729	-0.481
115	H	2.397	-2.061	0.081

P2-I- CH₃OH

	C	-1.020	-1.026	-3.320
120	C	-0.099	-0.084	-2.773
	C	1.210	0.005	-3.329
	C	1.574	-0.870	-4.362
	C	0.688	-1.822	-4.854
	C	-0.605	-1.888	-4.341
125	B	-0.616	0.891	-1.657
	Ge	0.530	1.329	0.101
	B	-1.359	0.736	0.844
	C	-2.413	1.779	0.499
	C	-2.462	2.365	-0.771
130	C	-1.546	2.068	-1.795

	C	-1.482	2.968	-3.003
	C	2.214	1.079	-2.934
	C	2.280	2.175	-4.013
	C	-2.477	-1.056	-2.870
135	C	-3.337	-0.141	-3.762
	C	-1.240	-0.192	2.109
	C	-1.574	-1.573	2.054
	C	-1.394	-2.382	3.179
	C	-0.888	-1.851	4.366
140	C	-0.599	-0.493	4.443
	C	-0.775	0.355	3.341
	C	-2.210	-2.137	0.793
	C	-1.946	-3.631	0.574
	C	-0.490	1.842	3.541
145	C	0.993	2.126	3.812
	C	-3.348	2.300	1.560
	C	-1.368	2.432	4.660
	C	-3.723	-1.842	0.807
	C	3.612	0.527	-2.630
150	C	-3.083	-2.466	-2.850
	O	1.731	-0.145	0.301
	C	1.319	-1.519	0.137
	Si	3.538	0.203	1.395
	F	4.918	0.599	2.223
155	F	2.746	-0.550	2.615
	F	4.192	-0.874	0.348
	H	-3.217	3.141	-0.961
	H	-4.265	2.719	1.116
	H	-2.876	3.107	2.145
160	H	-3.617	1.511	2.276
	H	-1.130	2.429	-3.894
	H	-0.776	3.795	-2.824
	H	-2.462	3.423	-3.219
	H	-0.220	-0.080	5.380
165	H	-0.728	-2.496	5.232
	H	-1.643	-3.442	3.134
	H	-0.750	2.367	2.608
	H	-2.433	2.219	4.495
	H	-1.236	3.524	4.715
170	H	-1.094	2.017	5.642
	H	1.620	1.809	2.969
	H	1.352	1.588	4.702
	H	1.157	3.203	3.973
	H	-1.768	-1.587	-0.059
175	H	-3.918	-0.763	0.890
	H	-4.198	-2.339	1.666
	H	-4.206	-2.207	-0.110
	H	-0.871	-3.858	0.592
	H	-2.350	-3.955	-0.393
180	H	-2.437	-4.244	1.344
	H	-1.305	-2.618	-4.751
	H	1.000	-2.507	-5.646
	H	2.577	-0.802	-4.790
	H	-2.519	-0.654	-1.842
185	H	-2.441	-3.177	-2.314
	H	-3.234	-2.852	-3.869
	H	-4.069	-2.451	-2.365
	H	-2.960	0.888	-3.776
	H	-4.377	-0.120	-3.404
190	H	-3.337	-0.514	-4.798
	H	1.845	1.560	-2.012
	H	3.578	-0.283	-1.892
	H	4.254	1.324	-2.226
	H	4.102	0.145	-3.539
195	H	1.292	2.615	-4.206

	H	2.654	1.763	-4.963
	H	2.963	2.981	-3.702
	H	3.185	1.579	0.960
	H	0.905	-1.898	1.082
5	H	0.570	-1.594	-0.662
	H	2.203	-2.106	-0.143

P2-TS2- CH₃OH

10	C	0.764	0.371	-8.616
	C	1.717	1.236	-8.000
	C	3.056	1.229	-8.479
	C	3.429	0.361	-9.509
	C	2.498	-0.500	-10.088
15	C	1.178	-0.478	-9.651
	B	1.296	2.161	-6.791
	C	0.466	3.436	-6.834
	C	-0.273	3.812	-8.091
	C	4.048	2.247	-7.938
20	C	3.872	3.581	-8.689
	C	-0.707	0.326	-8.213
	C	-1.624	0.701	-9.391
	Ge	0.992	1.096	-5.024
	B	1.869	2.891	-4.308
25	C	0.801	3.962	-4.453
	C	0.257	4.641	-3.224
	C	3.093	2.908	-3.329
	C	4.144	3.830	-3.609
	C	5.210	3.965	-2.714
30	C	5.254	3.218	-1.537
	C	4.221	2.334	-1.245
	C	3.139	2.152	-2.120
	C	4.094	4.713	-4.850
	C	5.453	4.848	-5.550
35	C	2.042	1.191	-1.678
	C	2.569	-0.204	-1.314
	C	0.269	4.259	-5.703
	C	1.228	1.790	-0.516
	C	3.537	6.106	-4.505
40	C	5.509	1.786	-7.986
	C	-1.116	-1.044	-7.645
	O	3.047	0.008	-4.898
	Si	2.463	-1.585	-5.218
	F	1.661	-2.365	-4.013
45	C	4.437	0.367	-4.707
	H	4.700	0.312	-3.642
	F	2.147	-2.128	-6.734
	F	3.920	-2.348	-5.036
	H	-0.408	5.119	-5.795
50	H	-0.376	4.904	-8.184
	H	-1.294	3.393	-8.087
	H	0.228	3.415	-8.985
	H	1.043	4.812	-2.474
	H	-0.505	4.004	-2.745
55	H	-0.226	5.598	-3.473
	H	0.452	-1.149	-10.114
	H	2.802	-1.186	-10.881
	H	4.458	0.354	-9.871
	H	-0.865	1.072	-7.417
60	H	-1.341	1.664	-9.839
	H	-2.672	0.767	-9.059
	H	-1.578	-0.058	-10.186
	H	-0.484	-1.341	-6.798
	H	-1.025	-1.830	-8.409
65	H	-2.164	-1.022	-7.308

	H	3.775	2.424	-6.880
	H	2.848	3.968	-8.579
	H	4.065	3.439	-9.763
	H	4.569	4.343	-8.313
70	H	5.636	0.795	-7.527
	H	6.155	2.498	-7.454
	H	5.881	1.730	-9.020
	H	6.016	4.667	-2.934
	H	6.094	3.330	-0.848
75	H	4.254	1.762	-0.315
	H	3.395	4.239	-5.565
	H	5.895	3.866	-5.768
	H	6.170	5.411	-4.934
	H	5.343	5.395	-6.497
80	H	2.552	6.043	-4.024
	H	3.433	6.717	-5.415
	H	4.217	6.630	-3.816
	H	1.347	1.065	-2.524
	H	3.171	-0.635	-2.125
85	H	1.729	-0.890	-1.128
	H	3.187	-0.182	-0.404
	H	0.804	2.769	-0.785
	H	1.860	1.934	0.373
	H	0.401	1.120	-0.239
90	H	1.059	-0.654	-5.390
	H	5.076	-0.309	-5.285
	H	4.563	1.398	-5.052

P1-TS1-C₂H₅OH

95	C	2.433	3.466	-1.493
	C	1.254	3.029	-2.169
	C	0.211	2.424	-1.421
	C	0.346	2.292	-0.033
100	C	1.490	2.743	0.622
	C	2.532	3.317	-0.106
	B	1.157	3.228	-3.709
	C	0.287	4.174	-4.519
	C	0.613	4.604	-5.812
105	C	1.622	4.312	-6.816
	C	1.344	5.020	-8.139
	C	-1.002	1.830	-2.120
	C	-2.330	2.362	-1.558
	C	3.547	4.141	-2.277
110	C	3.209	5.596	-2.642
	Ge	2.641	2.561	-5.002
	O	3.408	0.858	-4.704
	C	4.798	0.582	-5.050
	B	2.882	3.501	-6.758
115	C	4.049	3.284	-7.782
	C	3.875	2.532	-8.973
	C	4.967	2.331	-9.830
	C	6.221	2.857	-9.530
	C	6.403	3.598	-8.361
120	C	5.337	3.820	-7.483
	C	2.534	1.899	-9.324
	C	2.609	0.363	-9.269
	C	5.522	4.683	-6.242
	C	6.935	4.659	-5.650
125	Si	1.843	-0.416	-4.921
	F	0.422	-1.237	-5.135
	F	2.702	-1.118	-6.124
	F	2.223	-0.981	-3.436
	C	5.063	6.128	-6.514
130	C	2.011	2.370	-10.691

	C	-0.875	4.881	-3.840
	C	-0.966	0.292	-2.062
	C	4.938	4.045	-1.645
	H	-0.046	5.417	-6.157
135	H	1.064	6.074	-7.973
	H	0.506	4.548	-8.681
	H	2.220	4.997	-8.799
	H	-0.664	5.072	-2.777
	H	-1.789	4.265	-3.874
140	H	-1.111	5.842	-4.321
	H	4.836	1.747	-10.744
	H	7.062	2.691	-10.208
	H	7.389	4.009	-8.138
	H	1.811	2.223	-8.557
145	H	1.958	3.466	-10.747
	H	1.004	1.967	-10.878
	H	2.662	2.024	-11.509
	H	2.960	0.007	-8.291
	H	3.298	-0.023	-10.036
150	H	1.618	-0.079	-9.455
	H	4.833	4.276	-5.474
	H	4.016	6.151	-6.846
	H	5.683	6.583	-7.302
	H	5.151	6.746	-5.607
155	H	7.293	3.631	-5.491
	H	6.948	5.181	-4.681
	H	7.660	5.172	-6.299
	H	3.427	3.656	0.418
	H	1.577	2.637	1.706
160	H	-0.449	1.816	0.543
	H	3.612	3.586	-3.257
	H	5.185	3.015	-1.354
	H	5.010	4.682	-0.751
	H	5.701	4.397	-2.354
165	H	2.244	5.670	-3.162
	H	3.984	6.026	-3.296
	H	3.153	6.204	-1.727
	H	-0.941	2.121	-3.184
	H	-0.011	-0.109	-2.426
170	H	-1.773	-0.139	-2.673
	H	-1.098	-0.059	-1.027
	H	-2.368	3.460	-1.580
	H	-2.480	2.040	-0.517
	H	-3.177	1.975	-2.146
175	H	1.165	0.937	-5.124
	H	4.885	-0.510	-5.096
	H	4.995	0.987	-6.057
	C	5.737	1.170	-4.016
	H	6.776	0.908	-4.265
180	H	5.672	2.268	-3.992
	H	5.508	0.782	-3.014

P1-I- C₂H₅OH

185	C	0.651	1.596	3.005
	C	-0.317	0.552	2.999
	C	-0.501	-0.231	4.164
	C	0.290	0.014	5.295
	C	1.245	1.029	5.292
190	C	1.418	1.819	4.154
	B	-1.125	0.280	1.685
	C	-2.551	0.617	1.335
	C	-3.105	0.576	0.032
	C	-2.618	0.329	-1.289
195	C	-3.678	0.421	-2.385

C -1.529 -1.355 4.188
 C -2.548 -1.181 5.326
 C 0.786 2.493 1.779
 C -0.320 3.563 1.751
 5 Ge -0.375 -0.593 -0.013
 O 1.867 -0.563 -0.011
 C 2.493 -0.296 -1.342
 B -1.194 0.114 -1.732
 C -0.554 0.239 -3.159
 10 C -0.519 -0.848 -4.064
 C 0.130 -0.703 -5.299
 C 0.738 0.502 -5.647
 C 0.706 1.580 -4.760
 C 0.070 1.465 -3.518
 15 C -1.147 -2.178 -3.675
 C -0.068 -3.234 -3.380
 C 0.004 2.641 -2.548
 C 1.224 3.569 -2.594
 Si 2.781 -1.190 1.239
 20 F 3.862 -2.214 0.623
 F 3.590 -0.053 2.029
 F 1.812 -1.975 2.238
 C -1.291 3.446 -2.747
 C -2.153 -2.686 -4.718
 25 C -3.465 1.168 2.425
 C -0.862 -2.739 4.256
 C 2.163 3.148 1.615
 H -4.159 0.902 0.016
 H -4.398 1.235 -2.194
 30 H -4.259 -0.513 -2.458
 H -3.222 0.593 -3.371
 H -2.882 1.585 3.259
 H -4.107 0.377 2.851
 H -4.131 1.961 2.049
 35 H 0.162 -1.542 -5.998
 H 1.239 0.603 -6.613
 H 1.184 2.520 -5.045
 H -1.705 -2.002 -2.737
 H -2.932 -1.935 -4.913
 40 H -2.643 -3.607 -4.367
 H -1.661 -2.918 -5.676
 H 0.617 -2.889 -2.592
 H 0.530 -3.447 -4.279
 H -0.523 -4.178 -3.042
 45 H -0.048 2.204 -1.531
 H -2.174 2.805 -2.627
 H -1.318 3.887 -3.756
 H -1.360 4.263 -2.011
 H 2.169 3.012 -2.509
 50 H 1.179 4.295 -1.768
 H 1.261 4.147 -3.530
 H 2.164 2.616 4.167
 H 1.856 1.209 6.180
 H 0.159 -0.595 6.192
 55 H 0.617 1.844 0.895
 H 2.979 2.415 1.693
 H 2.335 3.922 2.379
 H 2.230 3.645 0.636
 H -1.317 3.104 1.780
 60 H -0.251 4.170 0.834
 H -0.221 4.236 2.617
 H -2.083 -1.301 3.233
 H -0.175 -2.893 3.413
 H -1.621 -3.537 4.234
 65 H -0.283 -2.851 5.186

H -3.029 -0.194 5.283
 H -2.067 -1.279 6.312
 H -3.333 -1.951 5.262
 H -0.355 -2.158 0.017
 70 H 2.841 -1.261 -1.734
 H 1.663 0.059 -1.963
 C 3.604 0.722 -1.241
 H 3.954 0.952 -2.259
 H 3.247 1.653 -0.782
 75 H 4.469 0.351 -0.671

P1-TS2- C₂H₅OH

C 0.056 1.553 -3.534
 80 C -0.525 0.321 -3.126
 C -0.459 -0.800 -3.988
 C 0.165 -0.672 -5.237
 C 0.726 0.540 -5.637
 C 0.673 1.647 -4.787
 85 B -1.111 0.277 -1.677
 Ge -0.422 -0.578 -0.009
 B -1.167 0.267 1.716
 C -2.565 0.819 1.446
 C -3.349 1.534 2.530
 90 C -1.011 -2.149 -3.549
 C -2.020 -2.732 -4.550
 C -0.037 2.755 -2.601
 C -1.326 3.552 -2.869
 C -0.282 0.539 2.975
 95 C 0.703 1.560 2.970
 C 1.479 1.757 4.119
 C 1.297 0.961 5.253
 C 0.336 -0.048 5.251
 C -0.459 -0.268 4.120
 100 C 0.867 2.440 1.734
 C 2.281 3.002 1.542
 C -1.463 -1.413 4.071
 C -0.749 -2.771 3.946
 C -3.036 0.832 0.145
 105 C -2.513 0.358 -1.128
 C -3.620 0.095 -2.151
 C -2.446 -1.406 5.249
 C -0.162 3.585 1.709
 C 0.127 -3.145 -3.267
 110 C 1.191 3.670 -2.626
 O 2.239 -0.534 0.090
 Si 3.188 -1.132 1.298
 F 4.071 -0.004 2.037
 C 2.722 -0.346 -1.289
 115 C 3.797 0.714 -1.383
 F 2.237 -1.830 2.386
 F 4.228 -2.225 0.721
 H -4.000 1.352 0.006
 H -4.344 0.929 -2.171
 120 H -4.187 -0.815 -1.899
 H -3.216 -0.028 -3.164
 H -2.695 2.159 3.156
 H -3.824 0.809 3.212
 H -4.145 2.174 2.119
 125 H 0.220 -1.534 -5.906
 H 1.210 0.623 -6.613
 H 1.118 2.591 -5.108
 H -1.548 -1.984 -2.599
 H -2.844 -2.029 -4.739
 130 H -2.449 -3.668 -4.163

H -1.545 -2.960 -5.517
 H 0.826 -2.745 -2.518
 H 0.700 -3.356 -4.183
 H -0.270 -4.098 -2.887
 135 H -0.123 2.345 -1.575
 H -2.211 2.907 -2.772
 H -1.317 3.971 -3.887
 H -1.427 4.384 -2.154
 H 2.120 3.105 -2.462
 140 H 1.111 4.435 -1.837
 H 1.287 4.204 -3.584
 H 2.243 2.537 4.134
 H 1.915 1.126 6.138
 H 0.211 -0.676 6.137
 145 H 0.650 1.794 0.859
 H 3.048 2.220 1.613
 H 2.514 3.772 2.293
 H 2.362 3.481 0.554
 H -1.191 3.205 1.752
 150 H -0.060 4.175 0.784
 H -0.005 4.259 2.565
 H -2.059 -1.273 3.146
 H -0.075 -2.788 3.078
 H -1.479 -3.588 3.836
 155 H -0.141 -2.973 4.841
 H -2.963 -0.440 5.332
 H -1.928 -1.595 6.202
 H -3.204 -2.195 5.124
 H -0.205 -2.119 -0.099
 160 H 3.074 -1.318 -1.664
 H 1.827 -0.058 -1.856
 H 4.042 0.878 -2.443
 H 3.448 1.665 -0.959
 H 4.724 0.418 -0.867

P2-TS1- C₂H₅OH

C -1.011 0.298 3.235
 C -1.413 -0.185 1.955
 170 C -1.868 -1.529 1.847
 C -1.867 -2.361 2.971
 C -1.429 -1.894 4.209
 C -1.019 -0.571 4.335
 B -1.374 0.785 0.709
 175 Ge 0.594 1.315 0.106
 O 1.739 -0.138 0.298
 C 1.261 -1.501 0.236
 C -2.441 -2.028 0.531
 C -3.923 -1.621 0.422
 180 C -0.578 1.740 3.484
 C -1.434 2.418 4.568
 C -2.369 1.878 0.354
 C -3.343 2.392 1.385
 C -2.336 2.509 -0.895
 185 C -1.376 2.221 -1.879
 C -1.223 3.157 -3.051
 B -0.478 1.022 -1.728
 C 0.133 0.097 -2.840
 C -0.705 -0.882 -3.445
 190 C -0.189 -1.722 -4.437
 C 1.128 -1.592 -4.871
 C 1.931 -0.589 -4.338
 C 1.462 0.264 -3.329
 C -2.186 -0.956 -3.094
 195 C -2.764 -2.375 -3.165

	C	2.382	1.391	-2.880
	C	3.751	0.894	-2.397
	C	2.541	2.439	-3.998
	C	-3.001	-0.019	-4.006
5	C	-2.268	-3.534	0.307
	C	0.914	1.830	3.836
	Si	4.002	0.295	1.699
	F	3.134	-0.659	2.681
	F	4.648	-0.592	0.506
10	F	5.289	0.717	2.611
	H	-3.057	3.315	-1.094
	H	-4.227	2.848	0.912
	H	-2.879	3.169	2.015
	H	-3.667	1.590	2.064
15	H	-0.855	2.634	-3.944
	H	-0.491	3.948	-2.816
	H	-2.173	3.659	-3.292
	H	-0.694	-0.203	5.310
	H	-1.417	-2.559	5.075
20	H	-2.212	-3.392	2.883
	H	-0.722	2.305	2.550
	H	-2.507	2.339	4.343
	H	-1.175	3.485	4.648
	H	-1.267	1.963	5.556
25	H	1.529	1.382	3.045
	H	1.137	1.288	4.768
	H	1.222	2.878	3.967
	H	-1.894	-1.503	-0.274
	H	-4.046	-0.532	0.515
30	H	-4.509	-2.098	1.222
	H	-4.348	-1.931	-0.544
	H	-1.214	-3.835	0.397
	H	-2.624	-3.818	-0.690
	H	-2.852	-4.122	1.032
35	H	-0.826	-2.484	-4.887
	H	1.522	-2.262	-5.638
	H	2.950	-0.466	-4.709
	H	-2.303	-0.589	-2.058
	H	-2.136	-3.096	-2.624
40	H	-2.852	-2.720	-4.206
	H	-3.774	-2.400	-2.734
	H	-2.642	1.015	-3.948
	H	-4.063	-0.029	-3.719
	H	-2.923	-0.347	-5.054
45	H	1.899	1.900	-2.028
	H	3.645	0.142	-1.607
	H	4.340	1.734	-1.996
	H	4.333	0.451	-3.219
	H	1.568	2.830	-4.327
50	H	3.040	2.002	-4.876
	H	3.154	3.284	-3.648
	H	3.390	1.567	1.282
	H	0.236	-1.507	-0.168
	C	2.157	-2.368	-0.632
55	H	1.216	-1.888	1.268
	H	1.771	-3.399	-0.634
	H	2.168	-2.004	-1.668
	H	3.187	-2.387	-0.253

60 P2-I- C₂H₅OH

	C	-0.926	0.299	3.406
	C	-1.382	-0.214	2.157
	C	-1.881	-1.546	2.102
65	C	-1.882	-2.340	3.252

	C	-1.397	-1.845	4.463
	C	-0.937	-0.535	4.535
	B	-1.366	0.699	0.873
	C	-2.395	1.760	0.501
70	C	-3.281	2.344	1.570
	C	-2.477	-2.072	0.805
	C	-3.940	-1.605	0.682
	C	-0.434	1.731	3.592
	C	-1.251	2.482	4.658
75	Ge	0.503	1.277	0.100
	O	1.795	-0.080	0.513
	Si	3.774	0.576	0.821
	F	4.181	-0.728	-0.087
	B	-0.592	0.838	-1.679
80	C	-1.582	1.980	-1.815
	C	-1.573	2.853	-3.044
	C	-0.087	-0.062	-2.867
	C	-1.038	-0.924	-3.484
	C	-0.698	-1.619	-4.650
85	C	0.561	-1.480	-5.223
	C	1.497	-0.640	-4.627
	C	1.207	0.070	-3.454
	C	-2.443	-1.091	-2.919
	C	-2.870	-2.565	-2.853
90	C	2.273	1.016	-2.917
	C	3.702	0.466	-3.022
	C	-2.483	2.294	-0.789
	C	2.179	2.392	-3.600
	C	-3.473	-0.276	-3.721
95	C	-2.377	-3.593	0.646
	C	1.064	1.779	3.926
	C	1.498	-1.482	0.789
	F	5.297	1.214	0.983
	F	3.539	0.138	2.385
100	H	-3.244	3.063	-0.985
	H	-4.177	2.817	1.141
	H	-2.744	3.122	2.138
	H	-3.580	1.579	2.301
	H	-1.189	2.318	-3.923
105	H	-0.927	3.733	-2.886
	H	-2.582	3.238	-3.263
	H	-0.572	-0.147	5.488
	H	-1.385	-2.481	5.351
	H	-2.259	-3.362	3.207
110	H	-0.570	2.262	2.636
	H	-2.331	2.433	4.455
	H	-0.952	3.540	4.692
	H	-1.083	2.061	5.660
	H	1.667	1.256	3.175
115	H	1.267	1.299	4.895
	H	1.413	2.821	3.989
	H	-1.903	-1.608	-0.019
	H	-4.019	-0.510	0.732
	H	-4.542	-2.026	1.501
120	H	-4.381	-1.934	-0.270
	H	-1.342	-3.944	0.765
	H	-2.730	-3.899	-0.346
	H	-3.002	-4.119	1.384
	H	-1.430	-2.279	-5.119
125	H	0.818	-2.030	-6.131
	H	2.482	-0.535	-5.083
	H	-2.436	-0.697	-1.888
	H	-2.114	-3.178	-2.343
	H	-3.017	-2.984	-3.859
130	H	-3.825	-2.667	-2.318

	H	-3.212	0.788	-3.754
	H	-4.474	-0.369	-3.272
	H	-3.529	-0.641	-4.758
	H	2.067	1.171	-1.846
135	H	3.785	-0.538	-2.589
	H	4.396	1.121	-2.477
	H	4.049	0.429	-4.066
	H	1.191	2.850	-3.458
	H	2.355	2.296	-4.682
140	H	2.935	3.078	-3.189
	H	3.149	1.805	0.262
	H	0.616	-1.525	1.442
	C	1.295	-2.290	-0.476
	H	2.356	-1.863	1.361
145	H	1.121	-3.345	-0.210
	H	0.427	-1.936	-1.048
	H	2.181	-2.236	-1.121

P2-TS2- C₂H₅OH

150	C	0.863	0.340	-8.600
	C	1.794	1.221	-7.977
	C	3.149	1.225	-8.415
	C	3.541	0.321	-9.416
155	C	2.639	-0.572	-9.983
	C	1.303	-0.551	-9.582
	B	1.243	2.268	-6.947
	Ge	2.068	2.543	-5.021
	B	0.039	2.326	-4.581
160	C	-0.807	3.431	-5.196
	C	-0.561	3.975	-6.478
	C	0.485	3.547	-7.281
	C	0.945	4.388	-8.441
	C	4.196	2.205	-7.900
165	C	4.703	3.117	-9.030
	C	-0.618	0.423	-8.259
	C	-1.347	1.339	-9.260
	C	-0.222	1.562	-3.221
	C	-0.705	0.223	-3.201
170	C	-0.825	-0.460	-1.988
	C	-0.496	0.159	-0.782
	C	-0.084	1.486	-0.783
	C	0.058	2.204	-1.979
	C	-1.197	-0.411	-4.494
175	C	-1.206	-1.944	-4.487
	C	0.489	3.667	-1.876
	C	1.903	3.830	-1.295
	C	-1.906	4.071	-4.387
	C	-0.520	4.487	-1.051
180	C	-2.605	0.125	-4.821
	C	5.366	1.502	-7.193
	C	-1.307	-0.945	-8.194
	O	2.689	0.239	-4.890
	C	2.256	-1.020	-5.492
185	Si	3.574	0.361	-3.423
	F	2.898	0.566	-1.945
	F	3.926	-1.245	-3.248
	F	5.105	0.940	-3.549
	H	-1.162	4.835	-6.806
190	H	-2.741	4.388	-5.032
	H	-1.541	4.976	-3.872
	H	-2.281	3.392	-3.610
	H	1.211	3.767	-9.310
	H	1.857	4.947	-8.167
195	H	0.184	5.126	-8.736

	H	0.150	1.973	0.164
	H	-0.572	-0.392	0.156
	H	-1.181	-1.491	-1.977
	H	0.504	4.088	-2.893
5	H	-1.545	4.368	-1.430
	H	-0.262	5.556	-1.078
	H	-0.518	4.172	0.002
	H	2.650	3.277	-1.879
	H	1.954	3.451	-0.264
10	H	2.191	4.892	-1.279
	H	-0.516	-0.072	-5.296
	H	-2.600	1.219	-4.932
	H	-3.306	-0.130	-4.012
	H	-2.987	-0.310	-5.756
15	H	-0.236	-2.360	-4.181
	H	-1.445	-2.329	-5.488
	H	-1.972	-2.338	-3.802
	H	0.593	-1.234	-10.051
	H	2.972	-1.278	-10.746
20	H	4.580	0.316	-9.752
	H	-0.699	0.891	-7.259
	H	-0.777	-1.634	-7.523
	H	-1.362	-1.416	-9.187
	H	-2.339	-0.836	-7.832
25	H	-0.883	2.333	-9.309
	H	-2.400	1.469	-8.969
	H	-1.319	0.901	-10.270
	H	3.707	2.852	-7.154
	H	5.020	0.902	-6.342
30	H	6.083	2.244	-6.812
	H	5.908	0.835	-7.881
	H	3.873	3.635	-9.532
	H	5.249	2.544	-9.795
	H	5.392	3.876	-8.629
35	H	3.071	1.998	-3.683
	C	3.359	-1.725	-6.254
	H	1.856	-1.656	-4.690
	H	1.434	-0.744	-6.163
	H	2.947	-2.636	-6.716
40	H	3.750	-1.090	-7.058
	H	4.176	-2.017	-5.583

[κ3-Tptm]ZnH

45	Zn	0.693	0.480	0.980
	N	0.063	0.029	2.958
	N	2.761	-0.010	1.045
	C	0.046	1.046	3.841
	C	-0.435	0.863	5.155
50	C	-0.904	-0.385	5.531
	C	-0.893	-1.439	4.603
	C	-0.404	-1.180	3.331
	S	0.625	2.661	3.386
	H	-0.434	1.702	5.853
55	H	-1.283	-0.543	6.543
	H	-1.260	-2.432	4.860
	H	-0.382	-1.947	2.554
	C	3.243	-1.240	0.770
	C	4.600	-1.525	0.724
60	C	5.501	-0.474	0.966
	C	5.016	0.794	1.241
	C	3.620	1.002	1.272
	H	2.487	-2.003	0.574
	H	4.944	-2.534	0.501
65	H	6.578	-0.652	0.937

	H	5.692	1.629	1.432
	S	3.030	2.640	1.618
	C	1.207	2.420	1.660
	H	-0.104	-0.293	-0.126
70	S	0.361	3.508	0.498
	C	0.770	5.167	1.053
	C	0.245	6.269	0.352
	C	0.577	7.544	0.797
	C	1.412	7.686	1.914
75	C	1.876	6.529	2.536
	N	1.566	5.290	2.120
	H	-0.403	6.120	-0.511
	H	0.189	8.423	0.278
	H	1.695	8.669	2.291
80	H	2.528	6.584	3.413

[κ3-Tptm]ZnH-4MTS-H₂O

	N	2.170	4.076	3.088
85	C	1.467	4.543	2.051
	C	1.294	5.916	1.794
	C	1.885	6.824	2.665
	C	2.625	6.348	3.756
	C	2.735	4.968	3.919
90	S	0.717	3.353	0.935
	C	1.170	1.753	1.635
	S	2.980	1.484	1.644
	C	3.199	0.127	0.514
	N	2.148	-0.459	-0.089
95	C	2.348	-1.478	-0.952
	C	3.612	-1.966	-1.246
	C	4.715	-1.366	-0.616
	C	4.515	-0.316	0.266
	Zn	0.269	0.318	0.342
100	N	-0.819	-0.427	1.966
	C	-0.620	0.174	3.155
	C	-1.318	-0.249	4.306
	C	-2.220	-1.296	4.198
	C	-2.422	-1.914	2.953
105	C	-1.700	-1.445	1.866
	S	0.522	1.526	3.330
	H	-1.141	0.250	5.259
	H	-2.768	-1.635	5.079
	H	-3.124	-2.739	2.831
110	H	-1.792	-1.865	0.861
	H	1.434	-1.882	-1.396
	H	3.734	-2.790	-1.948
	H	5.728	-1.719	-0.820
	H	5.353	0.172	0.766
115	H	-0.639	-1.067	-0.870
	H	0.712	6.250	0.933
	H	1.772	7.897	2.496
	H	3.104	7.029	4.459
	H	3.301	4.544	4.754
120	H	-0.871	-0.092	-1.236
	O	-0.733	1.117	-1.281
	H	-1.562	1.588	-1.078

[κ3-Tptm]ZnH-6MTS-H₂O

125	C	-1.843	-1.197	1.931
	N	-0.876	-0.255	1.981
	C	-0.670	0.425	3.124
	C	-1.423	0.148	4.283
130	C	-2.406	-0.827	4.229

	C	-2.634	-1.512	3.026
	Zn	0.365	0.224	0.332
	O	-0.743	1.032	-1.177
	S	0.547	1.718	3.226
135	C	1.173	1.846	1.516
	S	2.994	1.744	1.547
	C	3.344	0.372	0.473
	N	2.357	-0.345	-0.094
	C	2.668	-1.376	-0.908
140	C	3.975	-1.738	-1.196
	C	5.011	-0.997	-0.603
	C	4.699	0.060	0.235
	S	0.602	3.347	0.685
	C	1.228	4.691	1.699
145	N	1.976	4.378	2.761
	C	2.452	5.385	3.514
	C	2.207	6.729	3.243
	C	1.422	7.043	2.125
	C	0.920	6.015	1.336
150	H	-1.230	0.710	5.199
	H	-3.002	-1.051	5.117
	H	-3.407	-2.275	2.939
	H	-1.965	-1.690	0.964
	H	1.806	-1.912	-1.313
155	H	4.179	-2.576	-1.861
	H	6.054	-1.250	-0.798
	H	5.480	0.656	0.711
	H	-0.095	-1.525	-0.394
	H	0.305	6.221	0.458
160	H	1.204	8.083	1.873
	H	2.618	7.508	3.886
	H	3.059	5.086	4.374
	H	-1.442	0.179	-1.476
	H	-1.240	1.831	-0.938
165	O	-1.976	-1.007	-1.576
	H	-0.890	-1.411	-0.942
	H	-1.942	-1.337	-2.490

[κ3-Tptm]ZnOH-intermediate

170	C	2.097	4.021	3.054
	N	1.346	4.533	2.058
	C	1.250	5.864	1.897
	C	1.957	6.748	2.737
175	C	2.746	6.219	3.749
	C	2.819	4.827	3.923
	Zn	0.167	3.347	0.816
	O	-0.002	1.809	1.871
	S	0.211	6.552	0.624
180	C	-0.507	5.065	-0.187
	S	0.054	5.023	-1.938
	C	1.039	3.543	-2.017
	N	1.189	2.763	-0.933
	C	1.908	1.625	-1.011
185	C	2.536	1.223	-2.181
	C	2.401	2.041	-3.316
	C	1.649	3.205	-3.243
	S	-2.306	5.013	-0.048
	C	-2.863	6.493	-0.902
190	N	-1.934	7.290	-1.436
	C	-2.345	8.397	-2.077
	C	-3.686	8.752	-2.212
	C	-4.651	7.908	-1.645
	C	-4.243	6.759	-0.977
195	H	1.870	7.826	2.590

	H	3.299	6.888	4.411
	H	3.419	4.383	4.716
	H	2.074	2.931	3.130
	H	1.945	1.047	-0.083
5	H	3.113	0.300	-2.208
	H	2.880	1.762	-4.256
	H	1.522	3.852	-4.111
	H	-4.966	6.079	-0.523
	H	-5.713	8.147	-1.725
10	H	-3.968	9.661	-2.744
	H	-1.551	9.021	-2.499
	H	-0.579	1.123	1.502

[κ3-Tptm]ZnH-4MTS-CH₃OH

15	C	-0.629	0.135	3.301
	N	-0.912	-0.427	2.111
	C	-1.791	-1.450	2.041
	C	-2.425	-1.964	3.162
20	C	-2.133	-1.387	4.410
	C	-1.234	-0.335	4.485
	Zn	0.050	0.366	0.447
	O	-1.109	1.173	-1.070
	C	-0.439	1.735	-2.194
25	S	0.513	1.492	3.435
	C	1.008	1.800	1.701
	S	2.821	1.604	1.552
	C	2.997	0.262	0.398
	N	1.923	-0.356	-0.129
30	C	2.093	-1.366	-1.010
	C	3.347	-1.810	-1.400
	C	4.474	-1.175	-0.852
	C	4.305	-0.136	0.049
	S	0.439	3.403	1.101
35	C	1.285	4.586	2.154
	C	1.066	5.960	1.943
	C	1.730	6.862	2.766
	C	2.584	6.378	3.767
	C	2.729	4.998	3.892
40	N	2.096	4.112	3.105
	H	-0.991	0.135	5.439
	H	-2.611	-1.761	5.317
	H	-3.129	-2.789	3.065
	H	-1.958	-1.835	1.032
45	H	1.163	-1.800	-1.385
	H	3.443	-2.629	-2.112
	H	5.480	-1.493	-1.133
	H	5.161	0.377	0.489
	H	-0.866	-1.012	-0.766
50	H	0.393	6.300	1.154
	H	1.585	7.936	2.632
	H	3.122	7.054	4.432
	H	3.382	4.568	4.657
	H	-1.123	-0.044	-1.105
55	H	-1.163	1.990	-2.986
	H	0.090	2.655	-1.899
	H	0.306	1.036	-2.625

[κ3-Tptm]ZnH-6MTS-CH₃OH

60	C	-1.164	0.675	3.069
	N	-1.345	0.000	1.921
	C	-2.459	-0.742	1.749
	C	-3.439	-0.852	2.724
65	C	-3.249	-0.164	3.934

	C	-2.108	0.602	4.114
	Zn	0.115	0.259	0.402
	O	-0.902	1.197	-1.107
	C	-1.879	2.197	-0.794
70	S	0.271	1.699	3.327
	C	1.143	1.611	1.729
	S	2.835	0.965	2.019
	C	3.065	-0.134	0.642
	N	2.040	-0.452	-0.168
75	C	2.251	-1.272	-1.217
	C	3.496	-1.808	-1.512
	C	4.567	-1.496	-0.658
	C	4.357	-0.657	0.423
	S	1.185	3.210	0.879
80	C	2.042	4.299	2.023
	C	2.282	5.630	1.634
	C	2.941	6.464	2.530
	C	3.342	5.955	3.773
	C	3.058	4.621	4.057
85	N	2.419	3.801	3.204
	O	-1.876	-0.856	-1.946
	C	-1.454	-1.355	-3.202
	H	-1.935	1.153	5.039
	H	-3.994	-0.229	4.729
90	H	-4.325	-1.459	2.544
	H	-2.532	-1.257	0.787
	H	1.365	-1.503	-1.812
	H	3.624	-2.457	-2.377
	H	5.561	-1.906	-0.846
95	H	5.170	-0.386	1.099
	H	-0.459	-1.465	-0.270
	H	1.957	5.990	0.656
	H	3.143	7.504	2.264
	H	3.861	6.578	4.502
100	H	3.350	4.174	5.012
	H	-1.405	0.335	-1.622
	H	-1.075	-1.287	-0.995
	H	-0.869	-2.290	-3.086
	H	-2.326	-1.590	-3.837
105	H	-0.822	-0.630	-3.751
	H	-2.712	1.784	-0.196
	H	-1.401	3.004	-0.221
	H	-2.293	2.620	-1.723

110 [κ3-Tptm]ZnOCH₃-intermediate

	C	-4.253	6.853	-0.953
	C	-2.877	6.574	-0.864
	N	-1.936	7.343	-1.419
115	C	-2.332	8.436	-2.094
	C	-3.668	8.803	-2.243
	C	-4.645	7.987	-1.656
	S	-2.339	5.114	0.032
	C	-0.542	5.124	-0.135
120	S	-0.010	5.016	-1.892
	C	0.956	3.522	-1.936
	N	1.115	2.775	-0.830
	C	1.827	1.630	-0.884
	C	2.434	1.188	-2.050
125	C	2.289	1.971	-3.207
	C	1.549	3.143	-3.158
	Zn	0.109	3.424	0.898
	O	-0.122	1.902	1.960
	N	1.324	4.602	2.102
130	C	2.080	4.098	3.100

	C	2.847	4.907	3.925
	C	2.821	6.293	3.701
	C	2.032	6.815	2.686
	C	1.272	5.930	1.895
135	S	0.227	6.612	0.625
	H	1.985	7.888	2.499
	H	3.415	6.964	4.326
	H	3.446	4.468	4.723
	H	2.024	3.012	3.211
140	H	1.882	1.082	0.059
	H	3.002	0.259	-2.057
	H	2.753	1.661	-4.145
	H	1.416	3.768	-4.043
	H	-4.986	6.194	-0.484
145	H	-5.704	8.235	-1.749
	H	-3.937	9.699	-2.803
	H	-1.530	9.037	-2.532
	C	-0.940	0.831	1.563
	H	-0.787	-0.031	2.241
150	H	-2.023	1.077	1.597
	H	-0.733	0.466	0.531

[κ3-Tptm]ZnH-4MTS-C₂H₅OH

155	N	2.168	4.117	2.954
	C	1.591	4.562	1.833
	C	1.498	5.928	1.505
	C	2.035	6.852	2.394
	C	2.644	6.398	3.572
160	C	2.683	5.024	3.801
	S	0.906	3.352	0.697
	C	1.242	1.768	1.493
	S	3.036	1.455	1.681
	C	3.328	0.076	0.596
165	N	2.324	-0.499	-0.092
	C	2.581	-1.537	-0.916
	C	3.856	-2.054	-1.086
	C	4.910	-1.465	-0.367
	C	4.651	-0.397	0.477
170	Zn	0.423	0.303	0.179
	O	-0.567	1.085	-1.465
	C	-1.865	1.647	-1.259
	C	-2.528	1.987	-2.587
	N	-0.796	-0.382	1.730
175	C	-0.702	0.272	2.904
	C	-1.507	-0.095	4.003
	C	-2.406	-1.140	3.859
	C	-2.499	-1.813	2.629
	C	-1.676	-1.398	1.594
180	S	0.433	1.622	3.126
	H	-1.414	0.447	4.945
	H	-3.037	-1.435	4.700
	H	-3.195	-2.638	2.480
	H	-1.683	-1.861	0.604
185	H	1.703	-1.932	-1.434
	H	4.024	-2.892	-1.761
	H	5.929	-1.841	-0.472
	H	5.449	0.084	1.043
	H	-0.372	-1.098	-1.092
190	H	1.018	6.244	0.577
	H	1.982	7.920	2.172
	H	3.076	7.093	4.293
	H	3.147	4.617	4.704
	H	-0.593	-0.134	-1.472
195	H	-2.506	0.940	-0.690

H -1.760 2.555 -0.640
H -3.517 2.444 -2.428
H -1.904 2.693 -3.154
H -2.660 1.082 -3.199
5
[κ3-Tptm]ZnH-6MTS-C₂H₅OH

C -0.979 0.516 3.027
N -1.213 -0.024 1.820
10 C -2.363 -0.696 1.597
C -3.327 -0.864 2.581
C -3.079 -0.321 3.852
C -1.902 0.374 4.082
Zn 0.297 0.220 0.337
15 O -0.734 1.127 -1.183
C -1.648 2.215 -0.949
C -1.420 3.334 -1.952
S 0.501 1.456 3.346
C 1.300 1.547 1.707
20 S 3.044 1.018 1.882
C 3.275 -0.037 0.470
N 2.237 -0.394 -0.305
C 2.449 -1.179 -1.381
C 3.707 -1.639 -1.737
25 C 4.794 -1.285 -0.922
C 4.584 -0.482 0.187
S 1.182 3.203 0.978
C 2.015 4.269 2.159
C 2.104 5.645 1.879
30 C 2.749 6.460 2.802
C 3.283 5.889 3.966
C 3.141 4.515 4.146
N 2.519 3.712 3.264
O -1.832 -0.944 -1.850
35 C -1.589 -1.512 -3.126
C -2.291 -2.858 -3.275
H -1.686 0.819 5.055
H -3.810 -0.438 4.655
H -4.245 -1.406 2.360
40 H -2.486 -1.098 0.588
H 1.551 -1.445 -1.945
H 3.834 -2.263 -2.621
H 5.801 -1.635 -1.159
H 5.408 -0.181 0.836
45 H -0.221 -1.501 -0.329
H 1.676 6.054 0.962
H 2.837 7.533 2.619
H 3.795 6.496 4.713
H 3.539 4.020 5.036
50 H -1.279 0.273 -1.626
H -0.920 -1.358 -0.985
H -1.941 -0.815 -3.909
H -0.497 -1.647 -3.299
H -2.681 1.831 -1.017
55 H -1.500 2.591 0.076
H -2.121 -3.287 -4.275
H -1.919 -3.572 -2.525
H -3.374 -2.740 -3.125
H -2.115 4.168 -1.767
60 H -0.392 3.713 -1.870
H -1.575 2.974 -2.980

[κ3-Tptm]Zn-OC₂H₅-intermediate

65 C 1.271 5.917 1.890

N 1.330 4.590 2.101
C 2.069 4.094 3.115
C 2.813 4.912 3.954
C 2.780 6.298 3.726
70 C 2.007 6.811 2.695
Zn 0.132 3.401 0.890
O -0.040 1.875 1.968
C -0.896 0.815 1.623
S 0.250 6.587 0.594
75 C -0.540 5.095 -0.140
S -0.045 4.975 -1.906
C 0.942 3.495 -1.955
N 1.140 2.765 -0.843
C 1.873 1.634 -0.898
80 C 2.463 1.188 -2.072
C 2.274 1.952 -3.236
C 1.512 3.110 -3.186
S -2.334 5.103 0.060
C -2.874 6.563 -0.835
85 C -4.247 6.866 -0.882
C -4.642 7.998 -1.586
C -3.671 8.788 -2.216
C -2.337 8.400 -2.105
N -1.938 7.309 -1.429
90 H 1.951 7.884 2.507
H 3.353 6.974 4.363
H 3.400 4.481 4.764
H 2.017 3.009 3.229
H 1.959 1.098 0.050
95 H 3.051 0.271 -2.080
H 2.722 1.636 -4.180
H 1.347 3.719 -4.076
H -4.975 6.227 -0.380
H -5.699 8.264 -1.646
100 H -3.942 9.682 -2.777
H -1.539 8.981 -2.576
H -0.828 0.039 2.414
C -2.357 1.242 1.479
H -0.582 0.315 0.676
105 H -3.015 0.385 1.261
H -2.704 1.727 2.403
H -2.464 1.969 0.655

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