Supplementary Information

Are Non-Adiabatic Reaction Dynamics the Key to Novel Organosilicon Molecules? The Silicon ($Si(^3P)$) – Dimethylacetylene ($C_4H_6(X^1A_{1g})$) System as a Case Study

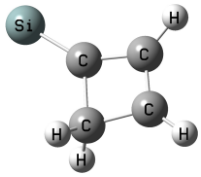
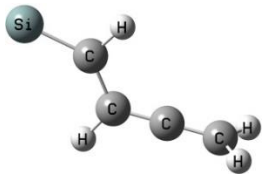
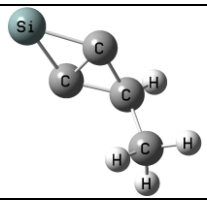
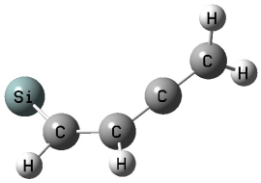
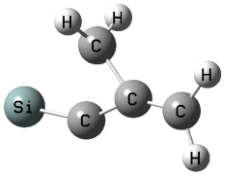
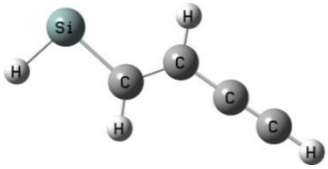
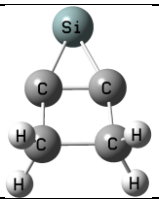
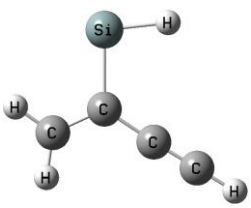
Aaron M. Thomas, Beni B. Dangi, Tao Yang, Ralf I. Kaiser*

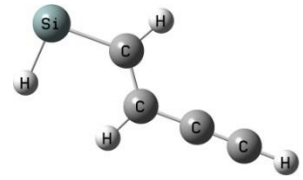
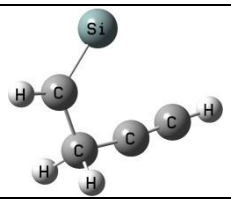
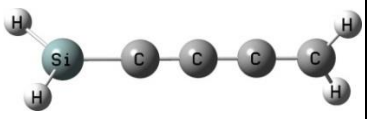
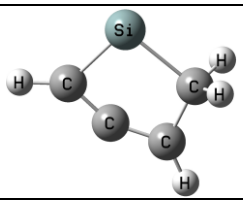
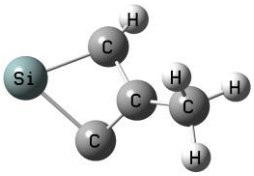
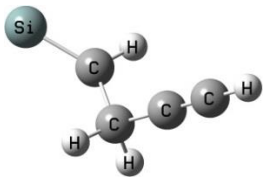
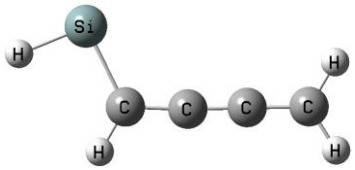
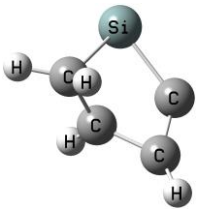
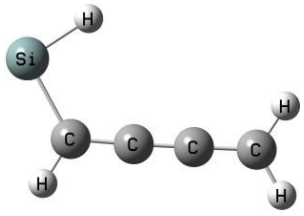
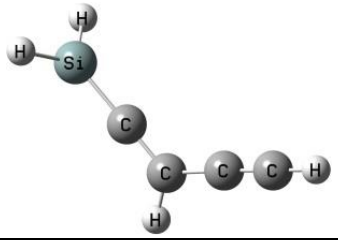
Department of Chemistry, University of Hawai'i at Manoa, Honolulu, Hawaii 96822, USA

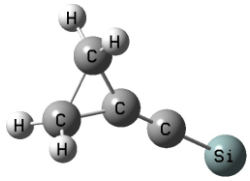
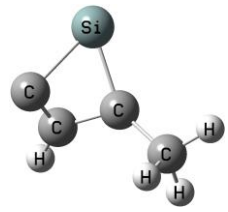
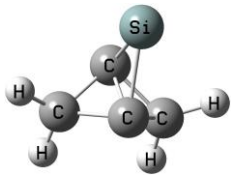
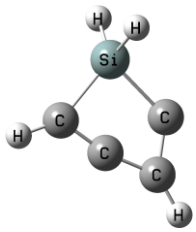
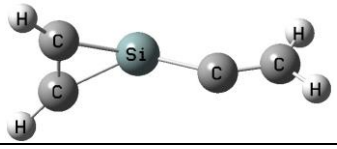
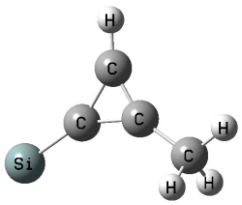
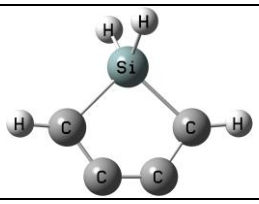
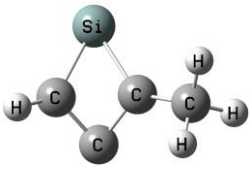
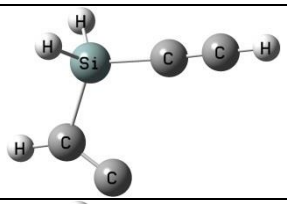
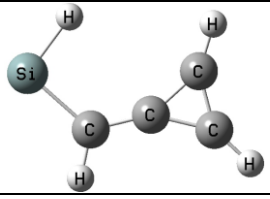
Lin Lin, Tzu-Jung Chou, Agnes H. H. Chang*

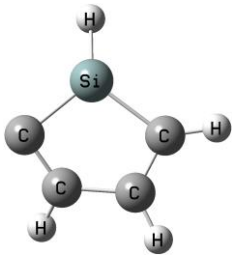
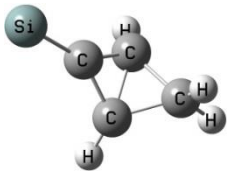
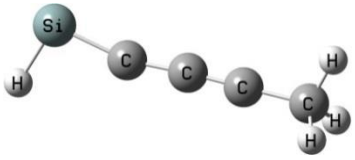
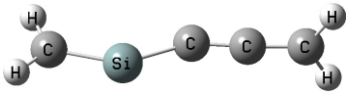
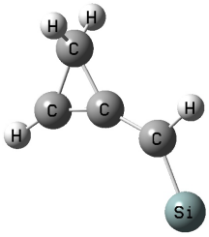
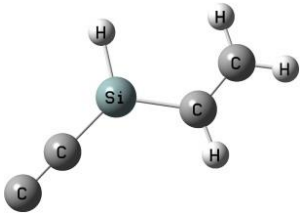
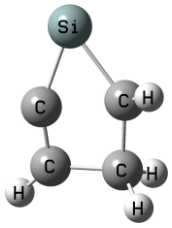
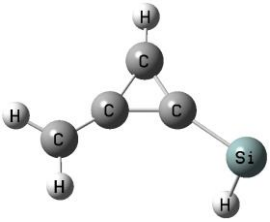
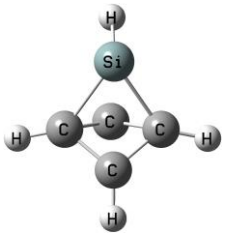
Department of Chemistry, National Dong Hwa University, Hualien 974, Taiwan

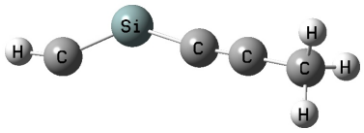
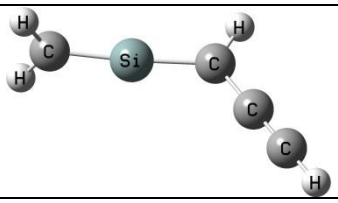
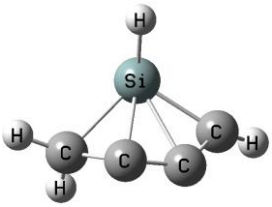
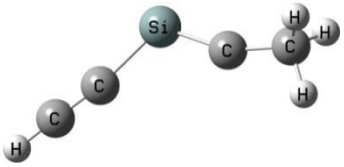
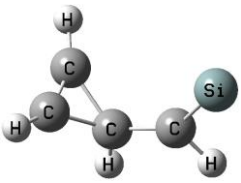
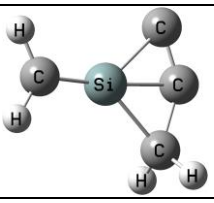
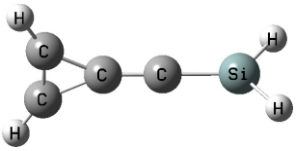
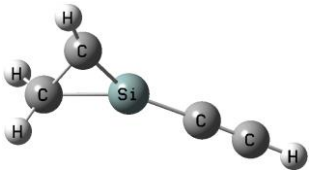
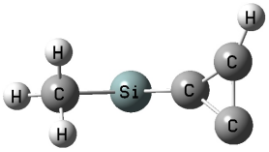
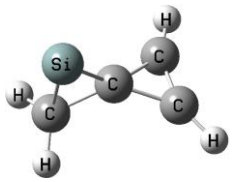
Table S1: Structures, relative energies (E) with respect to the separated reactants, point groups, and electronic wave functions of potential singlet products ^{1}p25-^{1}p153.

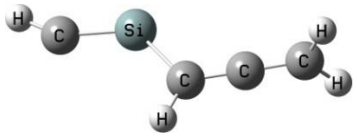
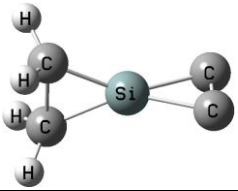
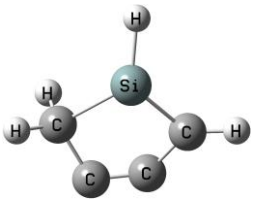
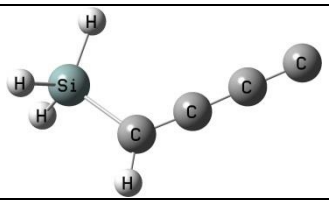
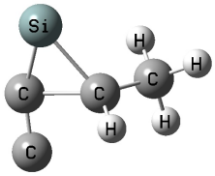
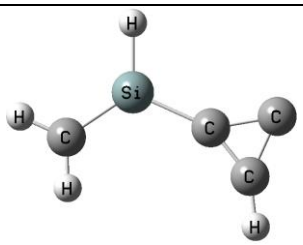
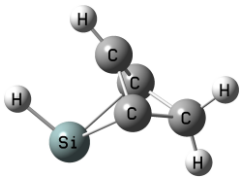
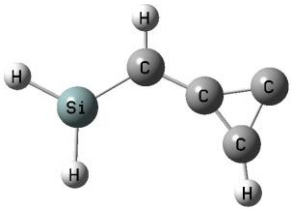
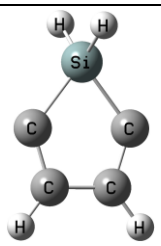
structures	products	E(kJ/mol)	point group	electronic wave function
	p25	-88	C_s	$^{1}A'$
	p26	-87	C_s	$^{1}A'$
	p27	-83	C_s	$^{1}A'$
	p28	-83	C_s	$^{1}A'$
	p29	-82	C_s	$^{1}A'$
	p30	-82	C_s	$^{1}A'$
	p31	-81	C_{2v}	$^{1}A_1$
	p32	-80	C_s	$^{1}A'$

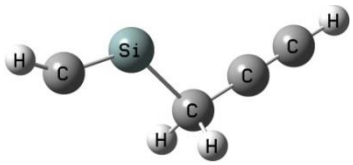
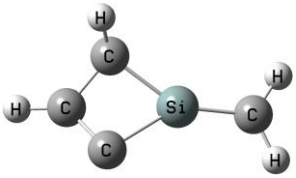
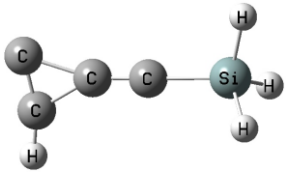
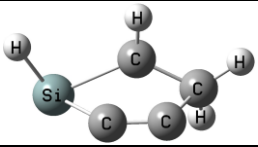
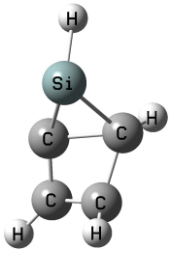
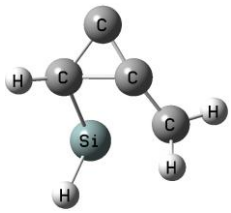
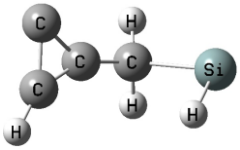
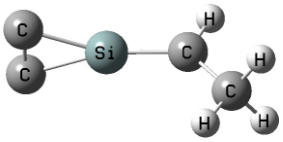
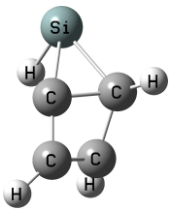
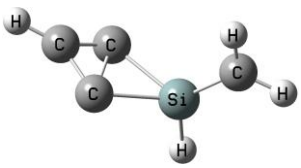
	p33	-80	C_s	$^1A'$
	p34	-72	C_s	$^1A'$
	p35	-67	C_{2v}	$^1A_1$
	p36	-66	C_s	$^1A'$
	p37	-63	C_1	^1A
	p38	-61	C_1	^1A
	p39	-60	C_s	$^1A'$
	p40	-59	C_1	^1A
	p41	-59	C_s	$^1A'$
	p42	-57	C_s	$^1A'$

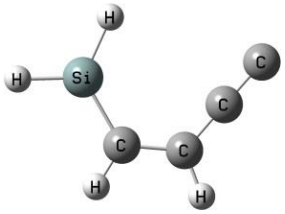
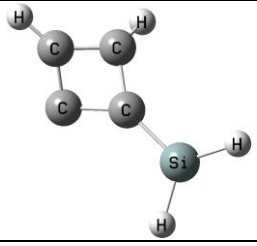
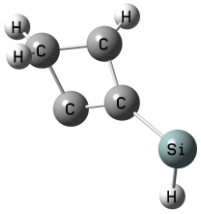
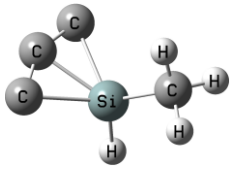
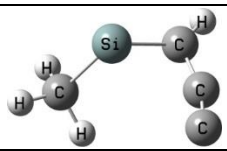
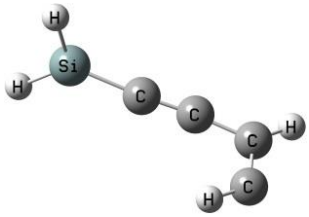
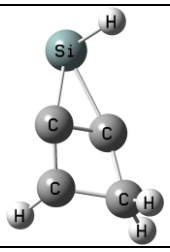
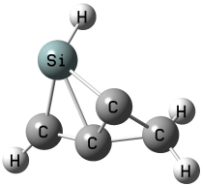
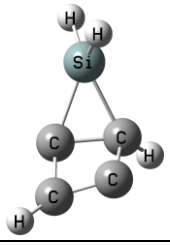
	p43	-55	C_{2v}	$^1A_1$
	p44	-49	C_1	^1A
	p45	-37	C_{2v}	$^1A_1$
	p46	-34	C_s	$^1A'$
	p47	-27	C_s	$^1A'$
	p48	-26	C_s	$^1A'$
	p49	-22	C_{2v}	$^1A_1$
	p50	-21	C_1	^1A
	p51	-20	C_s	$^1A'$
	p52	-19	C_s	$^1A'$

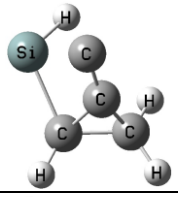
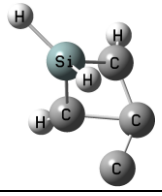
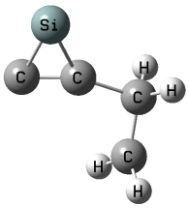
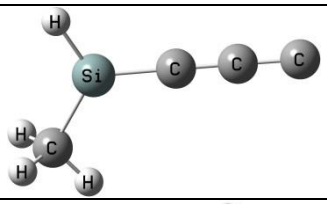
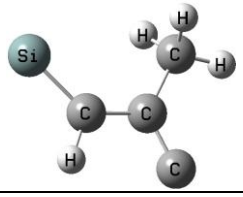
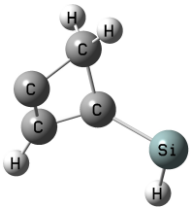
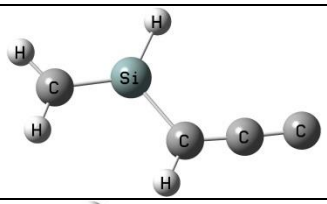
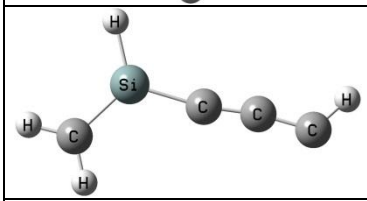
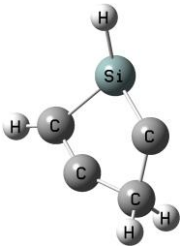
	p53	-16	C_1	^1A
	p54	-13	C_s	$^1A'$
	p55	-12	C_s	$^1A'$
	p56	-12	C_s	$^1A'$
	p57	-10	C_s	$^1A'$
	p58	-8	C_s	$^1A'$
	p59	-8	C_1	^1A
	p60	-7	C_1	^1A
	p61	2	C_s	$^1A'$

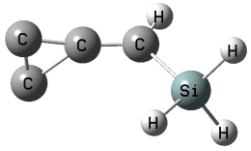
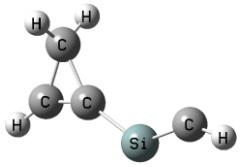
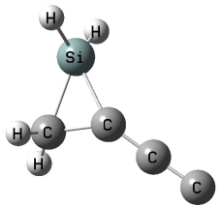
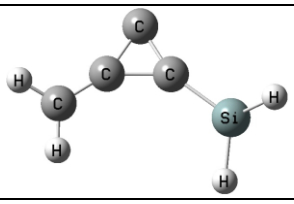
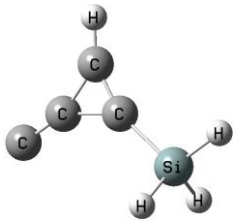
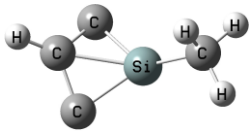
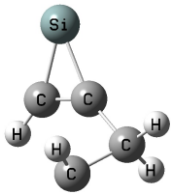
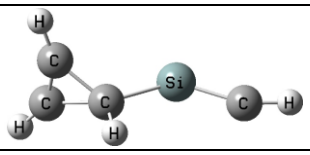
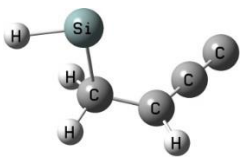
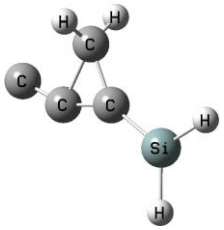
	p62	3	C_1	^1A
	p63	5	C_s	$^1A'$
	p64	10	C_1	^1A
	p65	13	C_s	$^1A'$
	p66	13	C_s	$^1A'$
	p67	15	C_s	$^1A'$
	p68	18	C_{2v}	$^1A_1$
	p69	19	C_1	^1A
	p70	20	C_1	^1A
	p71	26	C_s	$^1A'$

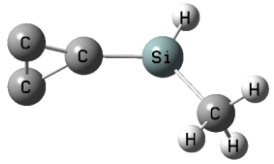
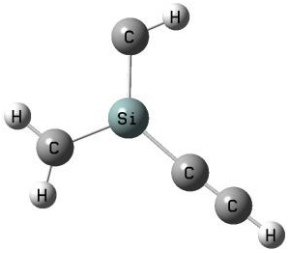
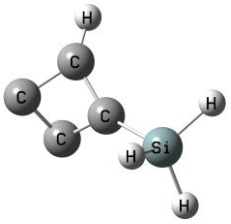
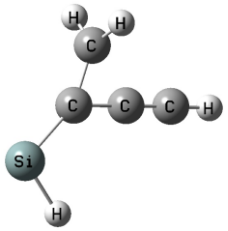
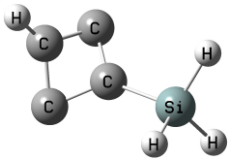
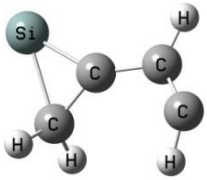
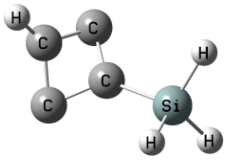
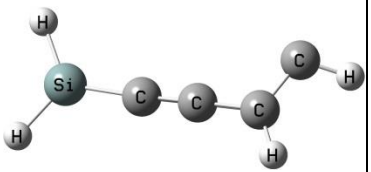
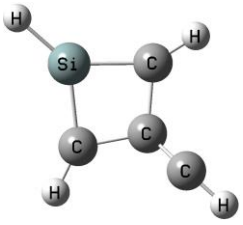
	p72	28	C_s	$^1A'$
	p73	30	C_{2v}	$^1A_1$
	p74	33	C_1	^1A
	p75	34	C_s	$^1A'$
	p76	35	C_1	^1A
	p77	38	C_s	$^1A'$
	p78	41	C_s	$^1A'$
	p79	43	C_s	$^1A'$
	p80	45	C_{2v}	$^1A_1$

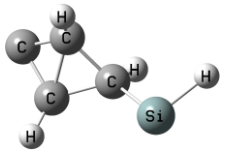
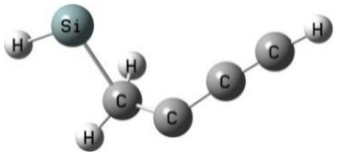
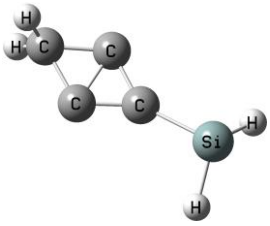
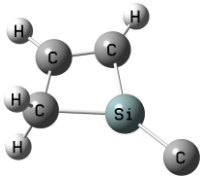
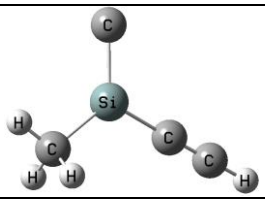
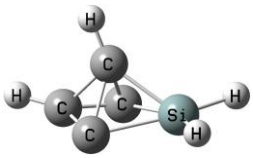
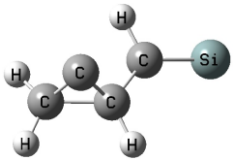
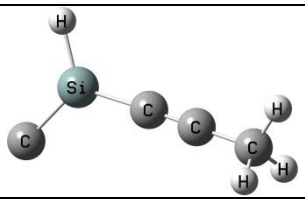
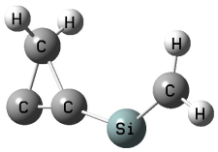
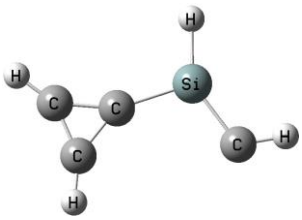
	p81	48	C_s	$^1A'$
	p82	50	C_1	^1A
	p83	55	C_s	$^1A'$
	p84	59	C_1	^1A
	p85	78	C_1	^1A
	p86	78	C_1	^1A
	p87	79	C_1	^1A
	p88	80	C_s	$^1A'$
	p89	83	C_1	^1A
	p90	84	C_s	$^1A'$

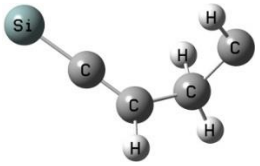
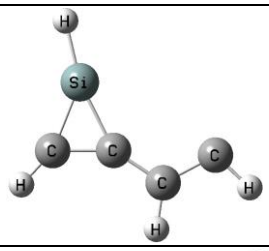
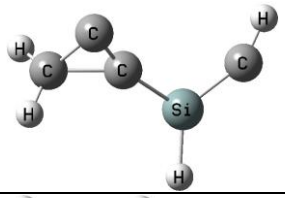
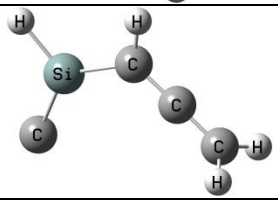
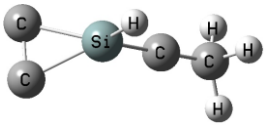
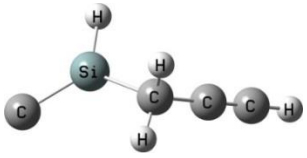
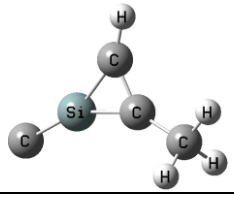
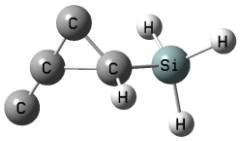
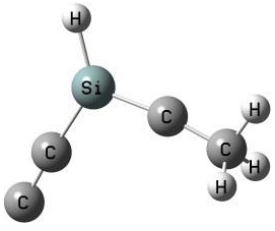
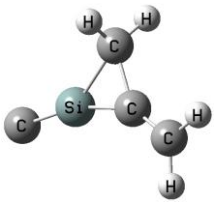
	p91	85	C_s	$^1A'$
	p92	91	C_1	^1A
	p93	93	C_1	^1A
	p94	93	C_s	$^1A'$
	p95	94	C_1	^1A
	p96	94	C_s	$^1A'$
	p97	95	C_1	^1A
	p98	97	C_1	^1A
	p99	97	C_1	^1A

	p100	97	C_1	^1A
	p101	101	C_1	^1A
	p102	102	C_1	^1A
	p103	103	C_s	$^1A'$
	p104	104	C_s	$^1A'$
	p105	105	C_1	^1A
	p106	105	C_s	$^1A'$
	p107	106	C_1	^1A
	p108	107	C_1	^1A

	p109	108	C_1	^1A
	p110	111	C_s	$^1A'$
	p111	111	C_1	^1A
	p112	126	C_1	^1A
	p113	129	C_s	$^1A'$
	p114	133	C_s	$^1A'$
	p115	134	C_1	^1A
	p116	136	C_s	$^1A'$
	p117	141	C_1	^1A
	p118	143	C_s	$^1A'$

	p119	150	C_s	$^1A'$
	p120	151	C_s	$^1A'$
	p121	151	C_1	^1A
	p122	151	C_s	$^1A'$
	p123	153	C_s	$^1A'$
	p124	154	C_1	^1A
	p125	157	C_s	$^1A'$
	p126	157	C_1	^1A
	p127	158	C_s	$^1A'$

	p128	159	C_1	^1A
	p129	161	C_1	^1A
	p130	168	C_s	$^1A'$
	p131	184	C_s	$^1A'$
	p132	186	C_s	$^1A'$
	p133	188	C_s	$^1A'$
	p134	199	C_1	^1A
	p135	199	C_1	^1A
	p136	200	C_1	^1A
	p137	203	C_s	$^1A'$

	p138	206	C_1	^1A
	p139	207	C_s	$^1A'$
	p140	232	C_1	^1A
	p141	233	C_s	$^1A'$
	p142	243	C_s	$^1A'$
	p143	248	C_1	^1A
	p144	255	C_s	$^1A'$
	p145	262	C_1	^1A
	p146	266	C_s	$^1A'$
	p147	284	C_s	$^1A'$

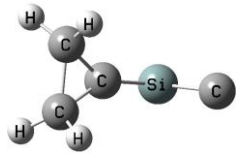
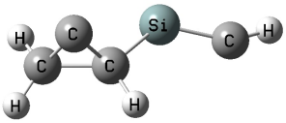
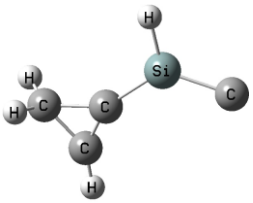
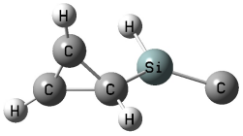
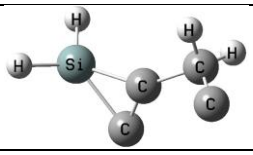
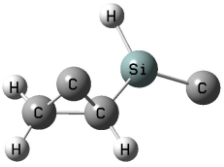
	p148	299	C_s	$^1A'$
	p149	309	C_1	^1A
	p150	312	C_s	$^1A'$
	p151	337	C_s	$^1A'$
	p152	402	C_1	^1A
	p153	506	C_1	^1A

Table S2: Cartesian coordinates of singlet products ^{1}p1-^{1}p153.

Atom	X	Y	Z	Atom	X	Y	Z
p1				**p2**			
C	0.018792	-1.332952	-0.111582	C	0.586426	0.000070	1.029112
C	0.018583	1.332911	-0.111348	C	0.586426	1.029101	0.000000
C	1.215683	0.747384	0.031520	C	0.586426	0.000070	-1.029112
C	1.215813	-0.747216	0.031551	C	0.586820	-1.028956	0.000000
H	-0.097037	-2.408579	-0.099045	H	0.640500	-0.000460	2.103152
H	-0.097289	2.408552	-0.099559	H	0.640948	2.103030	0.000000
H	2.153238	1.281854	0.158228	H	0.640500	-0.000460	-2.103152
H	2.153418	-1.281599	0.158653	H	0.641193	-2.102998	0.000000
Si	-1.351825	-0.000070	0.060063	Si	-1.188552	-0.000059	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p3				**p4**			
C	0.006050	0.290825	0.000530	C	-0.676136	1.060415	0.169589
C	1.443308	0.470421	-0.000132	C	-0.004620	-0.103422	0.106466
C	2.305465	-0.546617	-0.000035	H	-0.398027	2.090358	0.357510
H	1.819724	1.490847	-0.000860	Si	-1.821963	-0.327476	-0.127254
H	1.956811	-1.571441	0.000954	C	2.423428	0.143554	-0.199651
H	3.374944	-0.384449	-0.000516	H	3.423076	-0.268579	-0.169542
C	-1.081120	1.082824	0.000123	H	2.315422	1.147117	-0.591059
H	-1.248526	2.153000	-0.000201	C	1.366429	-0.567542	0.195801
Si	-1.567512	-0.676619	-0.000164	H	1.512409	-1.582267	0.551418
Atom	X	Y	Z	Atom	X	Y	Z
p5				**p6**			
C	0.066634	1.167891	-0.158745	C	-0.421346	0.001759	-0.000608
C	-0.782155	-0.010990	-0.003774	C	0.792869	0.001909	0.000778
C	-2.100820	-0.151876	0.088463	C	2.154069	0.000775	0.000630
C	1.314970	0.799266	0.253963	C	3.359266	-0.001395	-0.000598
Si	0.884921	-0.996101	-0.073803	Si	-2.250759	-0.000691	-0.000057
H	-2.559831	-1.126777	0.195452	H	-2.739758	0.355692	1.351803
H	-2.774674	0.699826	0.086480	H	-2.737106	-1.351003	-0.366234
H	2.184500	1.439712	0.304759	H	-2.742267	0.990305	-0.985176
H	-0.230661	2.106900	-0.632888	H	4.420610	-0.003607	-0.000805

Atom	X	Y	Z	Atom	X	Y	Z
p7				**p8**			
C	1.629747	0.407940	-0.668621	C	1.553281	-0.051069	-0.000014
H	2.232604	0.851515	-1.449191	C	-1.305005	0.070593	-0.000086
C	-1.457871	0.024401	-0.007514	C	-2.314078	0.742910	0.000366
C	-2.600304	0.410789	-0.002667	H	0.628060	1.851757	0.000054
H	-3.607000	0.751431	0.001744	H	2.523033	-0.545655	-0.000010
C	1.624542	0.427327	0.662392	H	2.471113	1.867343	-0.000036
H	2.221024	0.893575	1.434549	H	-3.197643	1.334196	-0.001433
H	0.281665	-2.050198	0.026549	Si	0.046605	-1.200319	-0.000014
Si	0.263930	-0.576362	0.006058	C	1.552965	1.287036	0.000005
Atom	X	Y	Z	Atom	X	Y	Z
p9				**p10**			
Si	2.438615	-0.147436	-0.000073	C	0.862351	1.054744	-0.000005
C	0.790007	0.236488	0.000017	C	-0.720232	-1.438531	-0.000212
C	-0.507863	0.540995	0.000185	C	0.486409	-1.141591	0.000290
C	-1.593273	-0.420621	0.000136	C	1.513283	-0.125226	-0.000192
C	-2.881816	-0.063227	-0.000183	H	1.356165	2.017117	-0.000093
H	-1.312054	-1.466921	0.000335	H	2.576440	-0.319549	0.000236
H	-3.177611	0.978726	-0.000568	Si	-0.958992	0.462320	0.000048
H	-0.818639	1.588556	0.000336	H	-1.678783	0.866752	-1.226578
H	-3.674641	-0.798075	-0.000012	H	-1.678796	0.866825	1.226465
Atom	X	Y	Z	Atom	X	Y	Z
p11				**p12**			
C	1.708201	0.560787	0.000677	C	-1.338762	0.214419	0.000000
C	0.411996	0.341739	-0.001388	H	-2.111318	0.969962	0.000000
C	-0.847859	0.125029	-0.000632	C	0.000000	0.242397	0.000000
H	2.307290	-1.507933	-0.001487	Si	-0.664042	-1.468226	0.000000
H	3.399412	-0.433608	0.880267	H	-0.644187	-2.296512	1.225731
C	2.756687	-0.517037	0.000130	H	-0.644187	-2.296512	-1.225731
Si	-2.523149	-0.163126	0.000378	C	1.034230	1.180942	0.000000
H	3.401270	-0.431597	-0.878447	C	1.959395	1.951940	0.000000
H	2.041966	1.593791	0.001646	H	2.767096	2.640031	0.000000

Atom	X	Y	Z	Atom	X	Y	Z
p13				**p14**			
Si	-2.476094	-0.005394	-0.025479	C	2.066816	-0.989744	-0.000662
H	-2.564254	1.502425	0.198358	C	1.862281	0.329840	0.001649
C	-0.646782	-0.048485	0.019899	C	0.551484	0.979539	-0.001225
C	0.560038	-0.240094	0.018687	C	-0.644919	0.391797	-0.000693
C	1.953133	-0.481428	0.018076	Si	-2.187666	-0.303685	0.000586
H	2.270428	-1.519302	0.041651	H	3.066320	-1.401307	0.001246
C	2.873461	0.488092	-0.022843	H	1.236121	-1.683384	-0.005161
H	3.928571	0.252391	-0.036894	H	2.716658	0.997319	0.005131
H	2.591472	1.531493	-0.049317	H	0.594249	2.070375	-0.003835
Atom	X	Y	Z	Atom	X	Y	Z
p15				**p16**			
C	-1.269553	0.183828	-0.005038	C	-1.498640	1.033224	-0.280352
C	-0.138922	0.641217	-0.000009	C	-0.288424	0.918140	0.144287
C	1.238352	0.969711	0.001076	C	0.784226	0.082707	0.538280
H	1.599189	1.986000	0.002688	H	0.971420	0.040506	1.608188
C	-2.635705	-0.306887	0.001762	Si	-1.013410	-0.827842	-0.037520
H	-3.329559	0.537265	-0.004620	C	2.028867	-0.060392	-0.316592
H	-2.856391	-0.916725	-0.877706	H	1.786586	-0.083834	-1.379119
H	-2.853121	-0.901565	0.892398	H	2.717645	0.771699	-0.152721
Si	1.733918	-0.688013	0.000035	H	2.555915	-0.980671	-0.064808
Atom	X	Y	Z	Atom	X	Y	Z
p17				**p18**			
C	0.000000	-0.678025	-1.659796	C	0.000000	1.754548	-1.067048
H	0.000088	-1.408180	-2.460390	H	0.000000	2.775835	-0.703989
Si	0.000000	0.000000	-0.000027	H	0.000000	1.628296	-2.146818
C	0.677998	-0.000053	1.659881	C	0.000000	0.717347	-0.222020
H	1.408537	0.000125	2.460071	Si	0.000000	0.000000	1.512173
C	0.000000	0.678025	-1.659796	C	0.000000	-0.717347	-0.222020
H	-0.000088	1.408180	-2.460390	C	0.000000	-1.754548	-1.067048
C	-0.677998	0.000053	1.659881	H	0.000000	-2.775835	-0.703989
H	-1.408537	-0.000125	2.460071	H	0.000000	-1.628296	-2.146818

Atom	X	Y	Z	Atom	X	Y	Z
p19				**p20**			
Si	0.114235	1.507509	0.000000	C	-1.435127	0.057946	-0.000459
C	-0.540747	-0.103233	-0.000005	C	2.689711	0.711449	0.000400
C	-1.808496	-0.902665	0.000001	C	1.620188	0.152498	-0.000875
C	0.748421	-0.688476	0.000001	H	-3.109182	0.925007	-0.920301
C	1.915950	-1.036883	0.000004	H	-3.108132	0.924954	0.921213
H	-1.866044	-1.549631	-0.879014	H	0.148879	-2.201911	-0.000093
H	-1.865985	-1.549714	0.878958	H	3.626560	1.212805	0.000429
H	-2.682742	-0.253252	0.000057	C	-2.593766	0.657133	0.000114
H	2.924714	-1.364989	-0.000018	Si	0.053988	-0.738215	0.000263
Atom	X	Y	Z	Atom	X	Y	Z
p21				**p22**			
C	1.036759	0.903620	-0.532963	C	0.116743	1.079811	-0.129699
C	0.084802	0.675466	0.625870	C	-0.869710	0.112736	-0.006878
H	1.957230	1.410566	-0.249583	C	-2.185550	-0.007740	0.029862
H	0.637491	1.260709	-1.475032	C	1.376139	0.998371	0.064886
H	0.189423	1.194873	1.568067	Si	0.831025	-0.949034	0.099549
Si	1.012872	-0.916116	0.030011	H	-2.652869	-0.972348	0.165803
C	-1.212285	0.254619	0.216580	H	-2.835150	0.852886	-0.069230
C	-2.215498	-0.237786	-0.247295	H	0.961572	-1.281037	-1.383239
H	-3.127014	-0.616029	-0.636757	H	2.266366	1.587904	0.143960
Atom	X	Y	Z	Atom	X	Y	Z
p23				**p24**			
C	1.450522	0.491509	0.000000	C	-0.923156	-0.991385	0.000030
H	1.850816	0.949238	0.902192	C	1.111029	1.268077	-0.000052
H	1.850816	0.949238	-0.902192	C	-0.136253	1.113745	0.000095
C	0.000000	0.131583	0.000000	C	-1.452203	0.452060	0.000013
Si	1.049719	-1.391626	0.000000	H	-1.220914	-1.561393	-0.880637
C	-1.174333	0.669945	0.000000	H	-1.221304	-1.561921	0.880229
C	-2.377660	1.173379	0.000000	H	-2.038810	0.717467	0.879638
H	-2.894435	1.392897	-0.926023	H	-2.038400	0.717335	-0.879972
H	-2.894435	1.392897	0.926023	Si	1.065923	-0.669034	0.000016

Atom	X	Y	Z
p25			
C	-0.404506	-1.305215	0.000000
C	0.000000	0.225008	0.000000
C	1.386226	-0.228985	0.000000
C	1.091220	-1.544043	0.000000
H	-0.942258	-1.632036	0.891259
H	-0.942258	-1.632036	-0.891259
H	2.315034	0.324497	0.000000
H	1.681486	-2.449214	0.000000
Si	-1.039260	1.607729	0.000000

Atom	X	Y	Z
p26			
C	-0.475376	-1.668692	0.000000
C	0.367934	-0.659986	0.000000
C	0.000000	0.741007	0.000000
H	-1.672609	-3.102884	0.924119
H	-1.672609	-3.102884	-0.924119
H	-1.082962	0.927119	0.000000
H	1.427043	-0.904099	0.000000
Si	0.820782	2.264531	0.000000
C	-1.307527	-2.665778	0.000000

Atom	X	Y	Z
p27			
C	0.269744	-0.162184	0.718177
C	-0.976203	2.018735	0.000000
C	0.269744	-0.162184	-0.718177
C	0.250638	1.130830	0.000000
Si	0.269744	-1.813114	0.000000
H	-0.977284	2.658198	-0.884009
H	-1.890269	1.427509	0.000000
H	-0.977284	2.658198	0.884009
H	1.184877	1.688515	0.000000

Atom	X	Y	Z
p28			
Si	-1.726951	1.124554	0.000000
C	0.000000	1.124476	0.000000
C	1.141450	0.227646	0.000000
C	1.094611	-1.085906	0.000000
C	1.049038	-2.383837	0.000000
H	1.030009	-2.953568	0.923903
H	1.030009	-2.953568	-0.923903
H	2.130909	0.677681	0.000000
H	0.275794	2.191427	0.000000

Atom	X	Y	Z
p29			
C	-0.274138	-1.068599	0.000000
H	-0.564308	-1.558735	0.920885
H	-0.564308	-1.558735	-0.920885
Si	-1.656218	0.919416	0.000000
C	1.028913	-0.337703	0.000000
C	0.000000	0.578663	0.000000
C	2.336869	-0.574293	0.000000
H	3.046117	0.241192	0.000000
H	2.719681	-1.583950	0.000000

Atom	X	Y	Z	Atom	X	Y	Z
p30				**p31**			
C	0.000000	0.671794	0.000000	C	0.000000	0.698117	0.062944
C	1.101312	1.560134	0.000000	C	0.000000	-0.698117	0.062944
C	2.019988	2.337794	0.000000	C	0.000000	-0.780048	-1.459895
H	1.075897	-1.115714	0.000000	C	0.000000	0.780048	-1.459895
H	-0.851455	-3.041503	0.000000	H	-0.881777	-1.261653	-1.882700
H	-0.980776	1.143739	0.000000	H	0.881777	-1.261653	-1.882700
H	2.837049	3.015507	0.000000	H	-0.881777	1.261653	-1.882700
C	0.081839	-0.678963	0.000000	H	0.881777	1.261653	-1.882700
Si	-1.521396	-1.667613	0.000000	Si	0.000000	0.000000	1.735301
Atom	X	Y	Z	Atom	X	Y	Z
p32				**p33**			
C	2.361933	-0.748311	0.000000	C	0.070204	0.674193	0.000000
C	1.290492	-0.199361	0.000000	C	0.000000	-0.677268	0.000000
C	0.000000	0.393083	0.000000	C	1.115961	-1.549115	0.000000
C	-0.159058	1.734257	0.000000	C	2.048238	-2.310577	0.000000
H	0.678633	2.422900	0.000000	Si	-1.424616	1.823741	0.000000
H	-1.151389	2.168757	0.000000	H	-2.433165	0.671649	0.000000
H	3.306716	-1.230916	0.000000	H	1.068634	1.105370	0.000000
H	-0.980537	-1.983497	0.000000	H	-0.973698	-1.158125	0.000000
Si	-1.629544	-0.603946	0.000000	H	2.876434	-2.974658	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p34				**p35**			
C	0.000000	1.298297	0.000000	C	0.000000	0.000000	0.625492
C	1.295138	0.519156	0.000000	C	0.000000	0.000000	-0.646521
C	0.963849	-0.909430	0.000000	C	0.000000	0.000000	-3.231886
C	0.550973	-2.038797	0.000000	C	0.000000	0.000000	-1.924120
Si	-1.499376	0.425352	0.000000	Si	0.000000	0.000000	2.321101
H	1.913911	0.748060	0.875104	H	0.000000	1.257093	3.085062
H	1.913911	0.748060	-0.875104	H	0.000000	-1.257093	3.085062
H	0.081243	2.381769	0.000000	H	0.924260	0.000000	-3.801665
H	0.222446	-3.048178	0.000000	H	-0.924260	0.000000	-3.801665

Atom	X	Y	Z	Atom	X	Y	Z
p36				**p37**			
C	1.224522	-0.542484	0.000000	C	-0.163997	-0.806015	-0.822402
C	-1.267974	0.728408	0.000000	C	2.118520	-0.103175	0.320879
C	0.000000	1.133545	0.000000	C	-0.273003	1.021565	-0.216393
C	1.304784	0.944063	0.000000	C	0.727237	-0.008340	-0.180466
H	1.630749	-1.018777	0.895947	Si	-1.547276	-0.157023	0.346881
H	1.630749	-1.018777	-0.895947	H	2.745163	0.650254	-0.161744
H	-2.225732	1.209211	0.000000	H	2.142382	0.102349	1.393133
H	2.132385	1.631034	0.000000	H	2.536605	-1.090758	0.133999
Si	-0.766867	-1.027420	0.000000	H	-0.214831	1.912281	-0.831434
Atom	X	Y	Z	Atom	X	Y	Z
p38				**p39**			
C	1.776273	-0.066990	0.076221	C	-1.128030	0.003425	0.000000
C	0.549887	-0.863017	0.075819	H	-2.065362	0.554347	0.000000
C	-0.654097	-0.104639	-0.448020	C	1.112883	1.293126	0.000000
H	0.365145	-1.227419	1.089318	C	0.000000	0.697607	0.000000
H	0.718167	-1.755446	-0.537204	Si	-1.028495	-1.885302	0.000000
Si	-2.209580	0.297014	0.158733	H	-2.547475	-2.083370	0.000000
C	2.777664	0.593254	0.066847	C	2.263687	1.926638	0.000000
H	-0.510990	0.296096	-1.459063	H	3.205056	1.388881	0.000000
H	3.663434	1.176919	0.059483	H	2.315463	3.009591	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p40				**p41**			
C	0.396896	1.263538	0.313127	C	1.106935	1.292415	0.000000
C	-0.603969	-0.984180	0.224398	C	0.000000	0.685455	0.000000
C	-1.656774	-0.238587	0.086400	C	-1.137587	0.009804	0.000000
C	-0.557027	0.518546	-0.579486	H	2.326009	2.998616	0.000000
H	-0.009711	1.517018	1.285452	H	3.200955	1.370603	0.000000
H	0.972807	2.074559	-0.127553	C	2.263394	1.915993	0.000000
H	-2.611357	-0.013212	0.528472	Si	-1.225010	-1.879431	0.000000
H	-0.515689	0.577213	-1.659702	H	0.289871	-2.061276	0.000000
Si	1.192086	-0.536535	-0.020951	H	-2.063154	0.582092	0.000000

Atom	X	Y	Z	Atom	X	Y	Z
p42				**p43**			
C	0.000000	0.620016	0.000000	C	0.000000	0.000000	-0.680904
C	1.087729	-0.123642	0.000000	Si	0.000000	0.000000	2.322022
C	1.102974	-1.546067	0.000000	C	0.000000	0.000000	0.624839
C	1.158542	-2.747019	0.000000	C	0.000000	0.763092	-1.941383
Si	-1.381499	1.584391	0.000000	H	0.911989	1.277921	-2.218829
H	-2.008248	2.026933	1.255636	H	-0.911989	1.277921	-2.218829
H	-2.008248	2.026933	-1.255636	C	0.000000	-0.763092	-1.941383
H	2.069329	0.352494	0.000000	H	-0.911989	-1.277921	-2.218829
H	1.192686	-3.807572	0.000000	H	0.911989	-1.277921	-2.218829
Atom	X	Y	Z	Atom	X	Y	Z
p44				**p45**			
C	0.059783	1.214171	-0.355593	C	0.000000	1.113000	-0.928870
C	-0.522828	-0.085255	-0.235975	C	-0.814411	0.000000	-0.303081
C	-1.935089	-0.384492	0.138343	C	0.000000	-1.113000	-0.928870
C	0.859502	0.954014	0.715071	C	0.814411	0.000000	-0.303081
Si	1.162252	-0.779258	-0.092974	H	0.000000	1.165146	-2.014769
H	-2.127434	-1.456227	0.172986	H	0.000000	2.091296	-0.455428
H	-2.161692	0.033822	1.124310	H	0.000000	-1.165146	-2.014769
H	-2.632821	0.071555	-0.569628	H	0.000000	-2.091296	-0.455428
H	-0.117780	2.069831	-0.997109	Si	0.000000	0.000000	1.408842
Atom	X	Y	Z	Atom	X	Y	Z
p46				**p47**			
C	-1.266098	0.566296	0.000000	C	0.141085	-2.671141	0.000000
C	1.204555	-0.138756	0.000000	H	1.170630	-3.017335	0.000000
C	1.373812	1.178134	0.000000	H	-0.613040	-3.457272	0.000000
C	0.000000	1.012614	0.000000	C	-0.232366	-1.411767	0.000000
H	-2.167261	1.157165	0.000000	Si	0.267850	0.255090	0.000000
H	2.149567	1.927368	0.000000	C	-0.232366	1.852365	0.672694
Si	-0.484036	-1.068927	0.000000	H	-0.485703	2.586203	1.426602
H	-0.539703	-1.914647	1.215020	C	-0.232366	1.852365	-0.672694
H	-0.539703	-1.914647	-1.215020	H	-0.485703	2.586203	-1.426602

Atom	X	Y	Z	Atom	X	Y	Z
p48				**p49**			
Si	1.475460	1.412930	0.000000	C	0.000000	1.429275	-0.241353
C	0.000000	0.510323	0.000000	C	0.000000	-1.429275	-0.241353
C	-0.749010	-0.758491	0.000000	C	0.000000	-0.645461	-1.312973
C	-0.579575	-2.217019	0.000000	C	0.000000	0.645461	-1.312973
H	-0.005862	-2.524394	0.877400	H	0.000000	2.506456	-0.157902
H	-1.538163	-2.733880	0.000000	H	0.000000	-2.506456	-0.157902
H	-0.005862	-2.524394	-0.877400	Si	0.000000	0.000000	1.072707
C	-1.455962	0.325641	0.000000	H	-1.189364	0.000000	1.974909
H	-2.399264	0.838914	0.000000	H	1.189364	0.000000	1.974909
Atom	X	Y	Z	Atom	X	Y	Z
p50				**p51**			
C	-0.127333	1.280615	-0.617066	C	-1.270126	-0.418227	0.000000
C	-0.511387	-0.017376	-0.182817	C	1.791112	0.228857	0.000000
C	-1.910110	-0.423595	0.165105	C	1.734955	-1.047330	0.000000
C	0.743917	0.951783	0.458649	H	-2.922252	-1.970540	0.000000
Si	1.195165	-0.767868	-0.067053	H	-0.143779	1.723476	1.212345
H	-2.394370	-0.766161	-0.753092	H	-0.143779	1.723476	-1.212345
H	-1.939842	-1.240438	0.884926	H	2.593761	0.951588	0.000000
H	0.921311	1.591757	1.315789	Si	0.000000	0.886651	0.000000
H	-2.489938	0.416439	0.547891	C	-2.153267	-1.236820	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p52				**p53**			
C	0.350573	2.209941	0.000000	C	-0.594828	-1.390806	0.166657
H	0.065960	3.248173	0.000000	C	0.578522	1.261775	-0.020754
C	1.328098	1.318433	0.000000	C	1.413476	0.225389	0.069899
H	2.385708	1.119313	0.000000	C	0.707675	-1.122935	-0.082754
C	0.000000	0.828526	0.000000	H	0.863154	2.302103	0.013849
C	-0.892475	-0.191068	0.000000	H	2.495556	0.271225	0.090203
H	-1.937797	0.105867	0.000000	H	1.282271	-1.836428	-0.683058
Si	-0.450006	-1.980654	0.000000	Si	-1.071547	0.328507	0.033827
H	1.069042	-1.739186	0.000000	H	-2.268395	0.823475	-0.692861

Atom	X	Y	Z	Atom	X	Y	Z
p54				**p55**			
C	-0.117740	0.276169	0.000000	C	0.142945	1.718301	0.000000
C	-0.194117	-0.994608	0.746719	C	0.000000	0.499514	0.000000
C	0.841284	-1.780416	0.000000	C	-0.221950	-0.811627	0.000000
H	0.725903	-2.859784	0.000000	H	1.398442	3.369251	0.000000
C	-0.194117	-0.994608	-0.746719	H	-0.100116	3.619596	0.889724
Si	-0.194117	1.992774	0.000000	Si	-0.081562	-2.504695	0.000000
H	-0.943917	-1.325668	1.444957	C	0.326204	3.149907	0.000000
H	1.867703	-1.426932	0.000000	H	-1.539532	-2.879280	0.000000
H	-0.943917	-1.325668	-1.444957	H	-0.100116	3.619596	-0.889724
Atom	X	Y	Z	Atom	X	Y	Z
p56				**p57**			
C	-1.419073	2.710653	0.000000	C	1.017367	1.567960	0.000000
H	-1.712376	3.186779	0.926827	H	2.079378	1.731651	0.000000
H	-1.712376	3.186779	-0.926827	Si	0.016125	-2.182401	0.000000
C	-0.731171	1.588173	0.000000	C	0.000000	0.755199	0.000000
C	1.484641	-2.332029	0.000000	C	-0.328218	2.229221	0.000000
H	1.244919	-3.383422	0.000000	H	-0.702785	2.695515	0.910963
H	2.529394	-2.052110	0.000000	H	-0.702785	2.695515	-0.910963
Si	0.260290	-1.146530	0.000000	C	-0.562155	-0.550751	0.000000
C	0.000000	0.552102	0.000000	H	-1.661520	-0.578834	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p58				**p59**			
C	-1.052211	-0.995569	0.000000	C	-0.001280	-0.905875	-0.012946
C	1.696472	0.520475	0.000000	C	-0.016444	0.817448	-0.214493
C	2.961775	0.519659	0.000000	C	1.308692	0.876014	-0.038305
H	-3.027470	-1.770318	0.000000	C	1.510242	-0.591657	0.093092
H	-0.580702	-1.971778	0.000000	H	-0.270281	-1.687607	-0.733751
H	-0.825546	1.731068	0.000000	H	1.924714	1.718613	0.239083
H	-2.889683	0.062682	0.000000	H	2.094511	-1.090997	-0.681826
Si	0.000000	0.504627	0.000000	H	1.914865	-0.882974	1.067248
C	-2.385468	-0.897305	0.000000	Si	-1.605076	0.054813	0.081797

Atom	X	Y	Z	Atom	X	Y	Z
p60				**p61**			
C	0.236253	0.411208	-0.005280	C	0.411234	-0.030858	1.072831
C	-1.207849	0.036415	-0.001131	C	0.411234	-1.103560	0.000000
Si	1.939351	-0.292739	0.095806	C	0.411234	-0.030858	-1.072831
H	1.781703	-1.009497	-1.240951	H	2.334805	0.520118	0.000000
C	-2.139395	-0.906599	0.028417	C	1.255667	0.427565	0.000000
H	-1.884049	-1.955725	0.007352	Si	-1.183808	0.368098	0.000000
H	-3.185715	-0.640600	0.087691	H	-1.968444	-0.928590	0.000000
C	-0.715281	1.344006	-0.025739	H	0.635368	-0.159313	-2.117844
H	-0.905221	2.393984	-0.172987	H	0.635368	-0.159313	2.117844
Atom	X	Y	Z	Atom	X	Y	Z
p62				**p63**			
C	0.359507	0.035099	-0.000793	C	0.000000	0.981482	0.000000
C	1.569211	-0.024590	-0.000280	C	-1.399609	1.110872	0.000000
C	3.014498	-0.134323	0.000270	C	-2.598567	1.236369	0.000000
H	3.323659	-1.178397	-0.073616	H	2.102685	-2.375225	0.924786
H	3.445037	0.408040	-0.843467	H	2.102685	-2.375225	-0.924786
H	3.434243	0.279818	0.918823	H	0.602831	1.882734	0.000000
C	-2.758257	-0.549003	-0.000007	H	-3.653014	1.348722	0.000000
H	-3.833883	-0.552168	0.000541	C	1.818407	-1.894969	0.000000
Si	-1.391343	0.362829	0.000184	Si	0.851673	-0.505966	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p64				**p65**			
C	0.696923	-0.853204	-0.611582	C	1.225937	-0.373644	0.000000
C	-0.574508	-1.012883	-0.228828	C	-1.708072	0.162882	0.000000
C	-1.541754	-0.269904	0.274216	C	-2.893644	-0.066600	0.000000
H	-2.398016	-0.400057	0.905400	H	3.150056	-0.661157	0.895198
C	1.480503	-0.167084	0.428607	H	3.150056	-0.661157	-0.895198
H	-0.104644	1.719144	-1.275334	H	2.457686	-2.002078	0.000000
H	1.440025	-0.510726	1.463310	H	-3.930357	-0.298995	0.000000
H	2.443645	0.250774	0.153766	C	2.571206	-0.907485	0.000000
Si	-0.124856	0.911380	-0.030115	Si	0.000000	0.766605	0.000000

Atom	X	Y	Z	Atom	X	Y	Z
p66				**p67**			
C	1.161636	-1.304048	0.643091	C	-1.482271	-0.799950	0.000000
H	1.086062	-1.823702	1.581700	C	0.203522	2.095225	0.000000
Si	-1.780827	0.778786	0.000000	C	-0.396592	-1.436940	0.000000
C	1.161636	-1.304048	-0.643091	Si	0.000000	0.413456	0.000000
H	1.086062	-1.823702	-1.581700	C	1.056202	-1.204937	0.000000
C	1.161636	0.067277	0.000000	H	-0.651475	2.752799	0.000000
H	2.095541	0.623807	0.000000	H	1.195811	2.518328	0.000000
C	-0.062241	0.896793	0.000000	H	1.585247	-1.489952	0.903028
H	0.127910	1.984752	0.000000	H	1.585247	-1.489952	-0.903028
Atom	X	Y	Z	Atom	X	Y	Z
p68				**p69**			
C	0.000000	0.655969	-2.188165	C	1.857706	-0.737985	-0.007594
H	0.000000	1.573647	-2.751820	H	2.264866	-1.188358	-0.911829
C	0.000000	0.000000	0.398760	H	2.280902	-1.188469	0.889000
C	0.000000	0.000000	-0.902527	Si	0.176199	0.046872	0.013649
C	0.000000	-0.655969	-2.188165	C	1.644997	0.831690	-0.007441
H	0.000000	-1.573647	-2.751820	H	2.369136	1.627257	-0.024057
Si	0.000000	0.000000	2.073945	C	-1.607436	0.001521	0.005813
H	-1.239694	0.000000	2.874496	C	-2.813071	-0.061078	-0.010899
H	1.239694	0.000000	2.874496	H	-3.874863	-0.111539	-0.023473
Atom	X	Y	Z	Atom	X	Y	Z
p70				**p71**			
C	1.949618	0.202192	-0.548532	C	1.262137	-0.490957	0.000000
C	0.767347	-0.122379	0.018705	C	-0.007818	0.295734	0.000000
H	2.473131	0.308361	-1.484203	H	1.868466	-0.514645	0.903980
C	-1.852341	0.874046	-0.026376	H	1.868466	-0.514645	-0.903980
H	-2.932133	0.734492	-0.012808	Si	-0.392540	-1.524723	0.000000
H	-1.561733	1.475663	0.839323	C	-0.392540	1.610144	-0.641339
H	-1.585199	1.448398	-0.917681	H	-0.528407	2.112511	-1.580968
C	1.932563	0.277420	0.820655	C	-0.392540	1.610144	0.641339
Si	-0.941228	-0.811042	-0.000810	H	-0.528407	2.112511	1.580968

Atom	X	Y	Z	Atom	X	Y	Z
p72				**p73**			
C	1.293146	0.978047	0.000000	Si	0.000000	0.000000	0.166057
C	0.000000	0.810496	0.000000	C	0.000000	0.628584	1.885675
C	-2.407857	-1.240166	0.000000	C	0.000000	-0.628584	1.885675
H	3.140793	1.192726	0.926389	C	0.805545	0.000000	-1.461696
H	3.140793	1.192726	-0.926389	H	1.272390	-0.897585	-1.853132
H	-0.660280	1.671886	0.000000	H	1.272390	0.897585	-1.853132
H	-3.183486	-1.985683	0.000000	C	-0.805545	0.000000	-1.461696
Si	-0.803563	-0.865275	0.000000	H	-1.272390	0.897585	-1.853132
C	2.583387	1.125322	0.000000	H	-1.272390	-0.897585	-1.853132
Atom	X	Y	Z	Atom	X	Y	Z
p74				**p75**			
C	-1.072250	0.947668	-0.075027	C	0.950620	0.041316	0.000000
C	0.857443	-1.133038	-0.047886	C	0.000000	0.916970	0.000000
C	-0.534725	-1.299757	-0.076544	C	-0.981750	1.754437	0.000000
C	-1.429958	-0.463732	0.147884	C	-1.943152	2.592274	0.000000
H	-1.571070	1.716526	0.508368	Si	0.593949	-1.812417	0.000000
H	-1.134406	1.214365	-1.137342	H	-0.869907	-2.013058	0.000000
H	1.642496	-1.869694	-0.084470	H	1.208170	-2.409935	1.208859
Si	0.872288	0.647888	0.104063	H	1.208170	-2.409935	-1.208859
H	1.927891	1.561520	-0.434002	H	1.983970	0.376793	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p76				**p77**			
Si	1.324777	-0.624452	-0.029751	C	0.941478	1.811800	0.000000
C	0.478047	0.933166	-0.303809	C	0.000000	0.866860	0.000000
C	-0.340724	1.868026	0.011323	H	1.992890	2.047700	0.000000
C	-0.475395	-0.151221	0.507763	C	0.512515	-2.187813	0.000000
H	-0.618009	0.042875	1.563516	H	0.177570	-3.216339	0.000000
C	-1.664059	-0.747311	-0.210382	H	1.584580	-2.046106	0.000000
H	-1.972329	-1.669279	0.288052	H	-2.043464	-1.029344	0.000000
H	-2.512240	-0.061236	-0.214863	C	-0.384717	2.255019	0.000000
H	-1.431515	-0.985992	-1.249559	Si	-0.580517	-0.873650	0.000000

Atom	X	Y	Z	Atom	X	Y	Z
p78				**p79**			
C	0.454840	0.086035	0.884956	C	-1.294663	-1.507553	0.000000
C	0.454840	1.195678	0.000000	H	-1.017722	-2.549891	0.000000
C	0.454840	0.086035	-0.884956	C	-2.333863	-0.572320	0.000000
C	1.330423	-0.798767	0.000000	Si	1.706887	0.601637	0.000000
H	0.184763	2.235436	0.000000	H	2.316571	-0.740400	0.000000
H	2.378353	-0.527887	0.000000	H	2.659568	1.727408	0.000000
H	1.141212	-1.866870	0.000000	C	-0.947487	-0.215997	0.000000
Si	-1.282368	-0.309035	0.000000	C	0.000000	0.843680	0.000000
H	-1.920825	1.071927	0.000000	H	-0.398752	1.853101	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p80				**p81**			
C	0.000000	1.140139	-0.118488	C	0.000000	0.931460	0.000000
C	0.000000	-1.140139	-0.118488	C	1.446934	0.973012	0.000000
C	0.000000	-0.730899	-1.400539	C	2.645896	0.994931	0.000000
C	0.000000	0.730899	-1.400539	H	-3.115381	-1.980703	0.000000
H	0.000000	-1.398464	-2.257907	H	-0.409986	1.427953	0.881129
H	0.000000	1.398464	-2.257907	H	-0.409986	1.427953	-0.881129
Si	0.000000	0.000000	1.320160	H	3.706567	1.023661	0.000000
H	1.230463	0.000000	2.130951	C	-2.336132	-1.238581	0.000000
H	-1.230463	0.000000	2.130951	Si	-0.736528	-0.847414	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p82				**p83**			
C	0.979327	-1.048943	-0.314951	C	0.003023	-2.423731	0.000000
C	-2.237470	-0.016901	0.103763	H	0.969393	-2.887462	0.000000
C	1.784611	-0.160950	0.325934	C	-1.265384	-2.230678	0.000000
Si	-0.549686	0.008246	-0.049722	C	-0.357804	-0.952369	0.000000
C	0.993369	0.973644	-0.071493	C	0.000000	0.227276	0.000000
H	-2.789599	0.869782	0.377199	Si	0.494220	1.984734	0.000000
H	-2.781252	-0.949299	0.069936	H	-0.754179	2.782989	0.000000
H	2.773968	-0.235848	0.755684	H	1.293349	2.297604	1.207985
H	1.373460	1.718813	-0.766220	H	1.293349	2.297604	-1.207985

Atom	X	Y	Z	Atom	X	Y	Z
p84				**p85**			
C	-0.086677	-1.068699	0.074305	C	-1.182097	0.677355	-0.390699
C	0.361756	0.519043	0.534869	C	-0.001334	0.827538	0.492709
C	1.622829	0.528087	-0.285025	C	-0.340170	-0.688397	0.281712
C	1.165441	-0.865294	-0.028502	C	-1.684116	-0.559079	0.068397
H	0.499672	0.630265	1.603776	H	-1.183642	0.961280	-1.445461
H	2.535676	0.872560	0.187363	H	-0.219657	1.108315	1.515287
H	1.527855	0.819547	-1.327713	H	-2.522010	-1.204486	-0.143325
Si	-1.487243	0.203698	-0.241186	Si	1.499935	-0.141768	-0.264780
H	-2.121894	0.147034	1.139298	H	2.172522	-0.424857	1.067704
Atom	X	Y	Z	Atom	X	Y	Z
p86				**p87**			
C	0.675722	0.945487	0.181270	C	-1.944466	0.504171	0.405674
H	0.864871	1.815261	0.805570	H	-2.447187	1.136134	1.119923
C	0.824936	-0.607662	0.149211	C	-0.906290	-0.260070	0.075715
C	1.828239	0.154500	-0.275301	C	-1.959328	-0.080124	-0.866650
Si	-1.139586	0.479400	-0.228420	Si	1.899515	0.297756	-0.156184
H	-1.739885	0.750335	1.136902	H	1.215554	1.583900	0.299383
C	-0.327705	-1.399820	0.088583	C	0.397660	-0.846101	0.313519
H	-0.340488	-2.209534	-0.630496	H	0.510879	-1.806651	-0.189935
H	-0.837438	-1.622680	1.023321	H	0.602085	-0.989231	1.387654
Atom	X	Y	Z	Atom	X	Y	Z
p88				**p89**			
C	0.297298	2.093305	0.642274	C	0.324171	-0.615108	0.382483
C	0.297298	2.093305	-0.642274	C	0.019385	0.866072	0.388954
C	-0.579755	-1.193275	0.000000	C	1.241536	0.628672	-0.429263
H	-1.655064	-1.347888	0.000000	C	1.678898	-0.582047	0.117229
Si	-0.127097	0.439981	0.000000	H	0.152900	1.344374	1.349139
C	0.297298	-2.419921	0.000000	H	1.312838	0.860115	-1.493574
H	0.101200	-3.037126	0.880175	H	2.438278	-1.306198	-0.135554
H	0.101200	-3.037126	-0.880175	Si	-1.593510	-0.165723	-0.067762
H	1.359186	-2.178073	0.000000	H	-1.178816	-0.363705	-1.527763

Atom	X	Y	Z	Atom	X	Y	Z
p90				**p91**			
C	-0.506518	-0.886699	0.802692	C	0.000000	1.135961	0.000000
C	1.466599	1.462900	0.000000	C	-1.222652	0.419264	0.000000
C	-0.506518	-1.972614	0.000000	C	-1.366648	-0.926193	0.000000
Si	-0.121872	0.838276	0.000000	C	-1.515380	-2.182356	0.000000
C	-0.506518	-0.886699	-0.802692	Si	1.585415	0.415121	0.000000
H	2.352174	0.845551	0.000000	H	1.852580	-1.029272	0.000000
H	1.616084	2.533266	0.000000	H	-0.059129	2.218326	0.000000
H	-0.584828	-3.046153	0.000000	H	-2.129119	1.024762	0.000000
H	-1.359494	1.630149	0.000000	H	2.767946	1.294426	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p92				**p93**			
C	-1.084266	-0.952208	-0.280082	C	-0.874393	-0.898433	-0.338342
C	0.042199	0.005038	-0.019838	C	0.122669	0.029612	-0.109548
C	-1.119870	0.863834	-0.073755	C	-1.070518	0.838686	-0.133496
C	-2.051307	-0.129808	0.289188	C	-2.068082	-0.130359	0.313054
H	-1.271927	1.677196	-0.782487	H	-1.279658	1.504053	-0.969174
H	-3.106192	-0.183804	0.492464	H	-3.044666	-0.170158	-0.160794
Si	1.762206	-0.008826	0.020368	H	-2.098354	-0.356860	1.371521
H	2.486286	-1.288574	0.080273	Si	1.966903	0.075715	0.155419
H	2.500415	1.197612	0.431513	H	2.227986	-1.074086	-0.807427
Atom	X	Y	Z	Atom	X	Y	Z
p94				**p95**			
C	-0.325424	-1.100523	1.287750	C	-0.659175	1.059954	0.438360
C	1.229482	1.489752	0.000000	C	-1.444508	-0.020873	0.326154
C	-0.325424	-1.419176	0.000000	C	-1.853566	-1.145910	-0.135846
Si	-0.324141	0.465759	0.000000	H	1.231150	-1.093433	1.288903
C	-0.325424	-1.100523	-1.287750	H	2.347703	0.262020	1.041853
H	2.108354	0.846048	0.000000	H	2.468081	-1.176318	0.015320
H	1.264201	2.125177	-0.885482	H	-0.880191	1.964143	0.993460
H	1.264201	2.125177	0.885482	C	1.773120	-0.519283	0.536959
H	-1.618040	1.165796	0.000000	Si	0.567002	0.271447	-0.738092

Atom	X	Y	Z	Atom	X	Y	Z
p96				**p97**			
C	0.600660	-0.656100	0.000000	C	0.003402	-0.680056	0.504099
C	1.116795	-1.942076	0.000000	C	0.256387	0.556831	-0.088449
C	0.002296	-2.672270	0.000000	C	1.766880	0.603423	-0.018936
H	-1.022134	-2.313709	0.000000	C	1.269376	-0.813143	-0.061192
C	0.000000	0.442824	0.000000	H	2.144360	0.931722	0.942259
Si	-0.676408	2.007371	0.000000	H	2.336346	1.006141	-0.854569
H	-0.987513	2.720690	1.248929	H	1.574547	-1.557406	-0.795285
H	2.148363	-2.265144	0.000000	Si	-1.709059	0.050098	-0.170075
H	-0.987513	2.720690	-1.248929	H	-1.904700	0.915841	1.075519
Atom	X	Y	Z	Atom	X	Y	Z
p98				**p99**			
C	0.728045	-0.652507	-0.664586	C	-1.243568	0.452680	-0.669170
C	1.707893	-0.117274	0.353808	C	-0.065094	1.004368	0.179179
C	-0.709435	1.223571	0.056304	C	-0.363095	-0.356525	0.652414
C	0.522664	0.642948	-0.242011	C	-1.692819	-0.557057	0.086392
Si	-1.102604	-0.539231	0.006406	H	-0.207591	1.958744	0.659431
H	2.704591	0.126523	0.004545	H	-2.400367	-1.362886	0.021910
H	-1.365439	-1.070709	1.385910	Si	1.332786	-0.217999	-0.107394
H	-1.040122	2.246328	0.076989	H	2.482825	-0.158397	0.817980
H	1.642423	-0.333334	1.421774	H	1.653596	-0.646280	-1.488696
Atom	X	Y	Z	Atom	X	Y	Z
p100				**p101**			
H	1.064446	0.657406	-1.553644	C	1.263021	0.316641	0.448384
C	-0.509246	-0.717733	0.135026	C	0.086405	1.077920	0.240898
C	0.523432	-1.522308	0.102113	C	0.374118	-0.123537	-0.835654
H	-2.626887	-0.014289	-0.050223	C	1.631266	-0.880437	0.136360
H	-1.506209	0.376957	-1.455093	H	0.090965	2.115841	-0.061655
C	-0.602976	0.724143	0.547634	H	0.659618	0.170139	-1.833783
H	-0.881901	0.939798	1.570632	Si	-1.219488	-0.248497	0.097725
C	-1.614147	0.169176	-0.395332	H	-2.489451	0.107815	-0.576351
Si	1.226298	0.437176	-0.060594	H	-1.317156	-1.258363	1.163710

Atom	X	Y	Z	Atom	X	Y	Z
p102				**p103**			
C	-0.733823	1.182159	0.199232	C	0.000000	0.748136	0.000000
C	-0.007115	0.102575	0.119811	C	-0.583067	1.891176	0.000000
C	1.354279	-0.686387	0.245001	C	-1.178066	3.039781	0.000000
H	1.282636	-1.618039	-0.306496	H	-1.269625	-2.154673	0.000000
H	1.425120	-0.903373	1.310970	H	0.031532	-2.969207	0.883546
Si	-1.819761	-0.281490	-0.136583	H	0.031532	-2.969207	-0.883546
C	2.326027	0.246528	-0.248496	H	2.238169	-0.789331	0.000000
H	2.525099	1.151075	0.306073	C	-0.203574	-2.375254	0.000000
H	2.607586	0.241946	-1.291671	Si	0.768331	-0.781473	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p104				**p105**			
Si	-1.728161	0.889754	0.000000	C	-1.030419	1.096318	0.139803
C	0.000000	0.771050	0.000000	C	-0.077773	0.068762	0.293861
C	0.961788	-0.324631	0.000000	C	-1.089998	-1.058257	0.193039
C	0.552574	-1.779015	0.000000	C	-1.677302	0.129985	-0.588945
C	2.222143	0.032548	0.000000	H	-1.038054	2.170438	0.215464
H	0.443467	1.776398	0.000000	H	-1.619003	-1.252475	1.117200
H	-0.043716	-1.997488	0.887647	H	-0.836408	-1.966634	-0.347535
H	-0.043716	-1.997488	-0.887647	Si	1.758954	-0.111846	-0.127955
H	1.419190	-2.437689	0.000000	H	2.121066	1.193672	0.579695
Atom	X	Y	Z	Atom	X	Y	Z
p106				**p107**			
C	0.000000	0.903036	0.000000	C	0.576383	-0.055532	-0.039753
C	1.235231	1.400957	0.000000	C	1.832097	0.054581	0.007569
C	2.442412	1.826196	0.000000	C	3.104727	0.356953	-0.020638
H	-2.264400	-2.488620	0.000000	H	-2.070204	1.800177	-0.037974
H	0.813439	-1.794208	0.000000	H	-1.525130	-1.901767	0.026564
H	-0.850678	1.584796	0.000000	H	-3.393622	0.544409	0.144957
H	-2.817571	-0.746783	0.000000	H	3.862811	-0.374691	0.245650
C	-1.989170	-1.442785	0.000000	C	-2.339474	0.754208	0.017620
Si	-0.357973	-0.905687	0.000000	Si	-1.136875	-0.480671	-0.011999

Atom	X	Y	Z	Atom	X	Y	Z
p108				**p109**			
C	0.484187	-1.122298	-0.143589	C	2.208116	-0.134205	-0.624828
C	-0.503514	1.327883	-0.020672	C	1.014846	0.312697	-0.126269
C	0.727110	0.875405	-0.128459	C	-0.179472	0.793657	0.135952
C	1.652792	-0.230807	0.066049	H	-0.241969	1.816890	0.494146
H	-0.794068	2.369131	0.003016	C	2.143258	-0.489317	0.644797
H	2.456970	-0.341706	-0.660109	Si	-1.745169	-0.232990	-0.032275
H	2.070986	-0.201004	1.073360	H	-2.389939	-0.350752	1.296956
Si	-1.115653	-0.424153	0.111304	H	-2.669826	0.465087	-0.957518
H	-2.278194	-0.989377	-0.614499	H	-1.386392	-1.566357	-0.559639
Atom	X	Y	Z	Atom	X	Y	Z
p110				**p111**			
C	-1.225050	1.624388	0.000000	C	-0.616473	1.221431	0.095279
C	0.000000	0.706912	0.000000	H	-0.924931	1.762412	-0.800855
H	-1.806098	1.717292	0.912991	H	-0.405589	1.885920	0.926549
H	-1.806098	1.717292	-0.912991	C	2.873550	-0.341752	0.038580
C	-0.078315	-2.461539	0.000000	C	1.618954	-0.107434	-0.043077
H	0.032236	-3.531657	0.000000	C	0.325570	0.101713	-0.171280
H	0.930717	2.791900	0.000000	Si	-1.418923	-0.491950	0.021577
C	0.218164	1.986702	0.000000	H	-1.748880	-1.285637	1.218082
Si	0.654318	-0.988115	0.000000	H	-2.265282	-0.719142	-1.162873
Atom	X	Y	Z	Atom	X	Y	Z
p112				**p113**			
H	2.728405	0.144338	1.033113	C	-1.481162	0.018250	0.000000
H	1.929860	-1.625440	-0.530187	C	-2.379818	-0.898242	0.000000
C	0.179108	0.468134	-0.041694	C	0.000000	0.405766	0.000000
C	-1.265260	0.137215	-0.000339	H	2.700957	0.651064	0.000000
C	-2.186342	-0.820756	0.059422	H	1.767278	-1.246008	1.216489
H	-3.168366	-0.591870	0.453001	H	1.767278	-1.246008	-1.216489
H	-1.982718	-1.839970	-0.235668	H	-1.162536	2.381318	0.000000
Si	1.770557	-0.251411	-0.018122	Si	1.671034	-0.411396	0.000000
C	-0.776670	1.454189	-0.095148	C	-0.883596	1.344088	0.000000

Atom	X	Y	Z	Atom	X	Y	Z
p114				**p115**			
C	-0.065366	-1.118532	1.157944	C	-0.530702	1.023376	0.334225
C	-0.065366	2.115038	0.000000	H	-0.237546	2.030839	0.591162
C	0.719460	-1.427131	0.000000	C	0.117472	-0.153278	0.240856
Si	-0.344267	0.271187	0.000000	Si	-1.671839	-0.318210	-0.183752
C	-0.065366	-1.118532	-1.157944	C	1.922886	0.479658	-0.573193
H	1.007463	2.313694	0.000000	H	1.692339	0.111012	-1.590945
H	-0.500484	2.567357	-0.890009	C	1.553581	-0.611449	0.356269
H	-0.500484	2.567357	0.890009	H	1.652382	-1.654312	0.048975
H	1.673069	-1.950090	0.000000	H	1.919149	-0.462443	1.374404
Atom	X	Y	Z	Atom	X	Y	Z
p116				**p117**			
C	-0.252163	1.911849	0.641469	C	-0.500674	0.818258	0.365687
H	-0.526004	2.352249	1.581695	C	0.764027	0.763920	-0.352379
C	0.480828	-2.490400	0.000000	C	1.778738	-0.059131	-0.063089
H	0.447246	-3.564954	0.000000	C	2.741851	-0.840330	0.211491
C	0.455461	0.740150	0.000000	Si	-1.810137	-0.559547	-0.165062
H	1.543266	0.724806	0.000000	H	-2.820325	-0.010885	0.842751
H	-0.526004	2.352249	-1.581695	H	-1.009531	1.782169	0.295124
C	-0.252163	1.911849	-0.641469	H	-0.389071	0.549869	1.423477
Si	-0.252163	-1.021788	0.000000	H	0.857202	1.416205	-1.220743
Atom	X	Y	Z	Atom	X	Y	Z
p118				**p119**			
H	-0.907140	2.704649	0.000000	C	2.046714	-0.373430	0.726345
H	-2.661520	0.882362	0.000000	C	0.944687	0.094696	-0.130356
C	0.000000	0.100922	0.000000	H	-1.030973	1.967164	0.332779
C	0.300362	-1.261368	0.000000	C	-2.114656	-0.683201	-0.026698
C	1.070755	-2.280108	0.000000	H	-1.722429	-1.668549	-0.272482
H	2.010623	-0.010476	0.923040	H	-2.608090	-0.733514	0.945201
H	2.010623	-0.010476	-0.923040	H	-2.863716	-0.405949	-0.769590
Si	-1.245822	1.275020	0.000000	C	2.199269	-0.210950	-0.628721
C	1.460370	-0.128835	0.000000	Si	-0.730777	0.562726	0.008620

Atom	X	Y	Z	Atom	X	Y	Z
p120				**p121**			
C	1.636889	1.046212	0.000000	C	-1.244399	-0.978891	-0.409785
Si	0.000000	0.444899	0.000000	C	-0.199328	-0.002824	-0.241394
C	-1.228781	1.767401	0.000000	C	-1.295892	0.857867	-0.122187
C	-0.210508	-1.364281	0.000000	C	-1.890671	-0.183512	0.645662
C	-0.435249	-2.550369	0.000000	H	-1.638967	1.751357	-0.621004
H	1.788677	2.117821	0.000000	Si	1.649973	0.004185	0.067189
H	2.533828	0.440485	0.000000	H	2.207670	1.253950	-0.498671
H	-2.270206	1.415350	0.000000	H	1.873960	-0.036411	1.531453
H	-0.626406	-3.596017	0.000000	H	2.239463	-1.183332	-0.586206
Atom	X	Y	Z	Atom	X	Y	Z
p122				**p123**			
H	2.260159	-0.597075	0.000000	C	-1.228655	0.352787	1.051226
H	-1.940008	0.886293	0.918699	C	-0.331059	-0.067976	0.000000
H	-1.940008	0.886293	-0.918699	C	-1.228655	0.352787	-1.051226
C	0.000000	0.386324	0.000000	C	-1.228655	1.323643	0.000000
C	-0.729202	-0.844178	0.000000	H	-1.099665	2.397383	0.000000
C	-1.349261	-1.907877	0.000000	Si	1.408603	-0.800101	0.000000
H	-1.864799	-2.836600	0.000000	H	2.117929	-0.346452	-1.216353
C	-1.385244	0.701750	0.000000	H	2.117929	-0.346452	1.216353
Si	1.733350	0.831784	0.000000	H	1.245525	-2.270512	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p124				**p125**			
C	0.132830	-0.092348	-0.073845	C	0.445919	-0.340177	1.151456
C	1.376524	-0.689662	0.213777	C	0.445919	2.009560	0.000000
H	1.453609	-1.758078	0.377119	C	0.445919	-0.340177	-1.151456
C	2.396443	0.078915	-0.227463	C	0.381320	0.513328	0.000000
H	2.408549	1.157997	-0.078418	Si	-0.689853	-1.186111	0.000000
C	-0.506228	1.189578	0.126950	H	1.496836	2.304237	0.000000
Si	-1.660887	-0.422917	-0.057299	H	-0.021940	2.421008	-0.893208
H	-0.727663	1.812999	-0.741684	H	-0.021940	2.421008	0.893208
H	-0.279491	1.789032	1.008653	H	-2.109465	-1.595893	0.000000

Atom	X	Y	Z	Atom	X	Y	Z
p126				**p127**			
C	-0.716492	-0.306587	-0.059873	C	0.204488	-0.080321	1.183767
C	-2.076695	-0.450045	-0.052014	C	0.204488	2.079506	0.000000
C	-2.799752	0.731119	0.004787	C	0.204488	-0.080321	-1.183767
H	-3.811805	0.551958	0.400296	C	0.434322	0.796150	0.000000
C	0.518587	-0.156695	0.002840	Si	-0.435060	-1.236653	0.000000
Si	2.200270	0.110877	0.015254	H	0.207538	0.228626	2.213168
H	3.152374	-0.986647	0.240639	H	0.207538	0.228626	-2.213168
H	-2.472267	-1.469599	-0.018782	H	0.547572	3.093572	0.000000
H	2.774026	1.445264	-0.210145	H	-1.158526	-2.527763	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p128				**p129**			
C	1.093234	-0.795437	-0.026349	C	-0.612090	0.940338	0.229472
C	-0.039953	0.006058	0.555323	C	0.634007	0.942618	-0.404102
C	1.029690	0.782742	-0.210081	C	1.643619	0.093865	-0.082807
C	2.231545	0.057905	0.004632	C	2.599790	-0.634353	0.138341
H	0.973809	-1.653103	-0.680316	Si	-1.727356	-0.660675	-0.098359
H	0.054847	0.167056	1.624615	H	-2.960630	0.094710	0.394833
H	0.848989	1.466012	-1.032048	H	-1.239771	1.825094	0.162168
Si	-1.815046	-0.094493	-0.181756	H	-0.681500	0.500292	1.275636
H	-2.354098	1.035330	0.691182	H	3.472936	-1.225455	0.258966
Atom	X	Y	Z	Atom	X	Y	Z
p130				**p131**			
C	0.155062	-1.056649	0.737672	C	-1.131774	-0.855638	0.000000
C	0.113893	0.129068	0.000000	C	-0.133053	2.476835	0.000000
C	0.155062	-1.056649	-0.737672	C	0.202510	-1.591098	0.000000
C	0.155062	-2.323747	0.000000	Si	0.000000	0.690860	0.000000
H	1.067935	-2.913766	0.000000	C	1.215156	-0.704896	0.000000
H	-0.755272	-2.921770	0.000000	H	-1.741165	-1.022516	0.887311
Si	-0.338617	1.927111	0.000000	H	2.275192	-0.903213	0.000000
H	0.476747	2.351921	-1.186423	H	0.290103	-2.675001	0.000000
H	0.476747	2.351921	1.186423	H	-1.741165	-1.022516	-0.887311

Atom	X	Y	Z	Atom	X	Y	Z
p132				**p133**			
C	-1.845052	0.824868	0.000000	C	0.466221	0.880518	0.000000
Si	0.000000	0.495279	0.000000	C	0.466221	-0.417189	0.971396
C	1.276950	1.741799	0.000000	C	0.466221	-0.417189	-0.971396
C	0.540724	-1.229367	0.000000	H	2.564627	-0.228925	0.000000
C	0.924580	-2.374263	0.000000	C	1.495108	-0.333535	0.000000
H	-2.305822	0.386205	0.885159	Si	-1.192052	-0.015479	0.000000
H	-2.034906	1.897307	0.000000	H	-2.075908	0.154770	1.181972
H	-2.305822	0.386205	-0.885159	H	0.913287	1.860451	0.000000
H	1.263343	-3.381844	0.000000	H	-2.075908	0.154770	-1.181972
Atom	X	Y	Z	Atom	X	Y	Z
p134				**p135**			
C	-2.056534	0.540950	0.096568	C	-1.500219	-0.012431	-0.000023
C	-0.776491	-0.013654	-0.461716	C	-0.301024	-0.179852	-0.000002
H	-2.772609	0.874737	-0.648667	C	2.603047	1.026006	0.000012
H	-2.132850	1.076308	1.038390	H	-3.245945	0.781446	0.859767
H	-0.693669	-0.004236	-1.542162	H	-3.458349	-0.772877	0.046112
C	0.479582	-0.016690	0.304230	H	-3.257135	0.702542	-0.905650
H	0.345878	-0.074775	1.393225	H	2.032425	-1.735652	0.000050
C	-1.834874	-0.920271	0.134872	C	-2.936557	0.184464	-0.000008
Si	2.170225	0.041854	-0.048893	Si	1.481251	-0.363184	-0.000011
Atom	X	Y	Z	Atom	X	Y	Z
p136				**p137**			
C	-1.867608	0.829166	-0.023701	C	0.029561	2.111633	0.000000
H	-1.954177	1.354089	-0.971382	H	-0.512046	3.040758	0.000000
H	-1.952708	1.460300	0.857657	C	0.000000	0.699207	0.000000
C	-0.794104	-0.371518	0.006991	H	-2.219588	-0.786860	0.000000
C	2.243253	0.605018	0.073796	H	2.255126	1.453166	0.000000
H	2.083259	1.659536	-0.111313	C	0.546767	-2.131800	0.000000
H	3.268191	0.268229	0.114710	H	0.245249	-3.185494	0.000000
C	-2.064725	-0.618395	0.075402	C	1.180159	1.460940	0.000000
Si	0.961038	-0.529127	-0.048900	Si	-0.736262	-0.954389	0.000000

Atom	X	Y	Z	Atom	X	Y	Z
p138				**p139**			
C	-1.813961	-0.254460	0.333651	C	-1.409275	0.625931	0.000000
C	-0.550318	-0.847424	-0.225539	H	-2.008294	1.525613	0.000000
C	0.668552	-0.346467	-0.107030	C	0.000000	0.399922	0.000000
H	-1.664775	1.452605	-0.793840	C	1.262463	0.969587	0.000000
C	-2.443932	0.925454	-0.212554	H	1.275833	2.065830	0.000000
Si	2.234262	0.282451	0.065914	Si	-1.024470	-1.053112	0.000000
H	-0.717167	-1.758963	-0.804129	H	-1.575824	-2.420677	0.000000
H	-2.491510	-0.989707	0.771333	C	2.374467	0.139213	0.000000
H	-1.568267	0.479123	1.172671	H	3.284935	0.764887	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p140				**p141**			
C	-2.122887	-0.279605	-0.286269	C	1.280035	0.754547	0.000000
C	-0.632565	0.158468	0.148513	C	0.000000	1.012123	0.000000
H	-2.498352	-1.140672	0.260794	C	-1.258720	-2.067588	0.000000
H	-2.441854	-0.228496	-1.324616	H	3.093702	0.346746	0.926706
C	2.179923	0.675225	-0.159185	H	3.093702	0.346746	-0.926706
H	2.502374	1.631244	-0.527527	H	-0.329469	2.048203	0.000000
H	1.261821	-1.931479	0.405290	H	-2.712763	0.239044	0.000000
Si	1.031620	-0.523589	0.055678	C	2.546028	0.469243	0.000000
C	-1.635582	0.945855	0.364702	Si	-1.324945	-0.285049	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p142				**p143**			
C	-0.751450	-1.816609	0.633043	C	-1.615126	0.164200	-0.068372
C	-0.751450	-1.816609	-0.633043	C	-0.390475	0.903336	0.165712
C	0.685315	0.899022	0.000000	C	2.550472	-0.057388	-0.729050
C	1.840610	1.716687	0.000000	H	-3.493571	-1.042110	-0.426967
H	1.333673	2.709370	0.000000	H	-0.195634	1.614819	-0.639058
H	2.450816	1.702529	0.908947	H	-0.450598	1.475418	1.094747
H	2.450816	1.702529	-0.908947	H	1.005893	-1.373006	1.274653
Si	-0.751450	-0.066581	0.000000	Si	1.107983	-0.274108	0.287613
H	-1.853164	0.922766	0.000000	C	-2.607847	-0.483083	-0.256615

Atom	X	Y	Z	Atom	X	Y	Z
p144				**p145**			
C	0.561244	-2.626134	0.000000	C	-1.480704	-0.020505	-0.139049
C	0.000000	0.881383	0.000000	C	-1.950539	-1.201341	0.043515
C	0.739017	2.165126	0.000000	C	-0.106455	0.542490	0.500681
H	0.058674	3.018679	0.000000	H	-0.171320	0.780917	1.563370
H	1.384938	2.228203	0.877080	H	2.592835	0.792035	0.155358
H	1.384938	2.228203	-0.877080	H	1.805171	-1.436022	0.719214
Si	-0.063785	-0.955612	0.000000	H	1.417522	-0.544217	-1.521180
C	-1.248253	0.423900	0.000000	C	-0.998609	1.270562	-0.359336
H	-2.247619	0.837841	0.000000	Si	1.540974	-0.224283	-0.085116
Atom	X	Y	Z	Atom	X	Y	Z
p146				**p147**			
C	1.134124	-0.289597	0.000000	C	0.255542	2.621056	0.000000
C	-1.569014	0.269820	0.000000	Si	0.000000	0.871383	0.000000
C	-2.678655	-0.333930	0.000000	C	0.200102	-0.956688	0.000000
H	1.850319	-2.083294	0.904364	C	0.965657	-2.032712	0.000000
H	2.957952	-1.062997	0.000000	H	0.533769	-3.028949	0.000000
H	1.850319	-2.083294	-0.904364	H	2.044930	-1.962036	0.000000
H	0.460167	2.381953	0.000000	C	-1.246636	-0.582096	0.000000
C	1.927086	-1.471844	0.000000	H	-1.813341	-0.752865	0.911089
Si	0.000000	0.985781	0.000000	H	-1.813341	-0.752865	-0.911089
Atom	X	Y	Z	Atom	X	Y	Z
p148				**p149**			
C	0.248502	1.614246	0.756946	C	1.945670	0.516511	0.220327
H	1.153900	1.901046	1.280153	C	0.701299	-0.311498	0.354605
H	-0.664961	1.868521	1.284062	H	2.702730	0.533900	0.997608
C	-1.496644	-1.545605	0.000000	H	1.892707	1.440902	-0.346800
C	0.248502	0.356167	0.000000	H	0.562095	-0.985755	1.196834
H	-0.664961	1.868521	-1.284062	C	-2.462847	-0.192614	0.267156
H	1.153900	1.901046	-1.280153	H	-3.532474	-0.093364	0.201903
C	0.248502	1.614246	-0.756946	C	1.806670	-0.747583	-0.540336
Si	0.252068	-1.412390	0.000000	Si	-0.969272	0.251102	-0.275718

Atom	X	Y	Z	Atom	X	Y	Z
p150				**p151**			
C	-0.640467	2.020050	0.000000	C	-0.117317	1.857429	0.641096
C	0.000000	0.625500	0.000000	H	0.078040	2.339742	1.580498
H	-1.104487	2.384291	0.912996	C	-0.117317	-2.695771	0.000000
H	-1.104487	2.384291	-0.912996	C	-0.633444	0.578953	0.000000
C	0.933717	-2.442810	0.000000	H	-1.708313	0.408739	0.000000
H	1.807812	2.017710	0.000000	H	1.871553	-0.789800	0.000000
H	-1.731361	-1.592820	0.000000	H	0.078040	2.339742	-1.580498
C	0.797153	1.651661	0.000000	C	-0.117317	1.857429	-0.641096
Si	-0.314992	-1.165706	0.000000	Si	0.399504	-0.991905	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
p152				**p153**			
C	0.492991	1.241118	-0.242824	C	-1.876796	0.186441	-0.539519
C	-0.160009	0.132117	-0.102121	C	-0.649323	-0.532619	-0.059133
C	-2.567158	0.181202	0.522919	H	-2.671527	-0.358174	-1.040394
C	-1.676654	-0.430242	-0.308288	H	-1.808765	1.223793	-0.849609
H	-1.778974	-1.418321	0.204993	H	-0.537974	-1.606996	-0.184170
H	-1.819959	-0.563514	-1.380981	C	2.577541	-0.465377	-0.180023
Si	1.606599	-0.238738	0.105554	C	-1.707602	-0.128479	0.902734
H	2.305653	-1.020611	-0.939042	Si	1.000237	0.328864	0.068283
H	2.265880	-0.400389	1.419163	H	0.952029	1.777477	0.373867

Table S3: Cartesian coordinates of potential triplet products ^{3}p1-^{3}p24.

Atom	X	Y	Z	Atom	X	Y	Z
^{3}p1				**^{3}p2**			
C	0.000000	1.369572	0.031897	C	0.477205	-0.018776	1.036596
C	0.000000	-1.369572	0.031897	C	0.477205	1.015092	0.000000
C	0.000000	-0.730307	-1.171501	C	0.477205	-0.018776	-1.036596
C	0.000000	0.730307	-1.171501	C	1.134522	-0.880676	0.000000
H	0.000000	2.438672	0.161314	H	0.664788	0.093506	2.093691
H	0.000000	-2.438672	0.161314	H	0.485900	2.094384	0.000000
H	0.000000	-1.264741	-2.115008	H	0.664788	0.093506	-2.093691
H	0.000000	1.264741	-2.115008	H	1.399930	-1.929085	0.000000
Si	0.000000	0.000000	1.255903	Si	-1.329445	-0.066679	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
^{3}p3				**^{3}p4**			
C	0.885763	1.024475	-0.121763	C	-0.881552	1.022080	-0.123086
C	-0.295224	0.587510	0.168780	C	0.296996	0.584275	0.175927
H	1.212123	2.057438	-0.191740	H	-1.203623	2.056472	-0.191339
Si	1.876629	-0.590613	-0.055710	Si	-1.881387	-0.587165	-0.056711
C	-2.483769	-0.316484	-0.384753	C	2.483984	-0.315037	-0.388176
H	-3.385631	-0.804287	-0.046027	H	3.388677	-0.801118	-0.054577
H	-2.418565	-0.034369	-1.425478	H	2.413847	-0.028605	-1.427368
C	-1.457674	-0.060402	0.490094	C	1.460336	-0.064350	0.491702
H	-1.575317	-0.360789	1.529034	H	1.581936	-0.368248	1.529040
Atom	X	Y	Z	Atom	X	Y	Z
^{3}p5				**^{3}p6**			
C	1.171613	-0.111573	0.000000	C	0.437705	-0.133951	-0.000004
C	0.000000	0.793281	0.000000	C	-0.832421	-0.055986	-0.000037
C	-0.093769	2.114166	0.000000	C	-2.112790	0.073295	-0.000070
C	0.758571	-1.401542	0.000000	C	-3.407403	0.126181	0.000011
Si	-1.022102	-0.834551	0.000000	Si	2.248071	0.024043	0.000006
H	-1.050719	2.618541	0.000000	H	2.792843	-0.628581	-1.214234
H	0.789639	2.744702	0.000000	H	2.793257	-0.631639	1.212436
H	1.354930	-2.298603	0.000000	H	2.648245	1.456195	0.001928
H	2.197092	0.253087	0.000000	H	-4.217884	-0.589820	0.000383

Atom	X	Y	Z	Atom	X	Y	Z
^{3}p7				**^{3}p8**			
C	1.829445	-1.259916	-0.029263	C	-1.655118	-0.206920	-0.000228
H	2.637582	-1.975051	-0.039861	C	1.482929	0.067722	0.000271
C	-1.437277	-0.098296	0.032891	C	2.535087	0.674222	0.000229
C	-2.451179	-0.756659	0.041131	H	-1.104313	1.849654	0.000194
H	-3.339506	-1.339426	0.061031	H	-2.490947	-0.898164	-0.000464
C	1.651494	0.033601	0.096857	H	-2.912820	1.495219	-0.000136
H	2.521850	0.679902	0.262949	H	3.447169	1.219391	0.000434
H	-0.028988	2.166788	0.675725	Si	0.019524	-0.968683	-0.000098
Si	0.046726	0.925386	-0.129253	C	-1.898302	1.114218	-0.000048
Atom	X	Y	Z	Atom	X	Y	Z
^{3}p9				**^{3}p10**			
Si	-1.653581	-1.877997	0.000000	C	-0.555421	-1.207060	-0.120063
C	-0.697326	-0.391732	0.000000	C	0.341053	1.474461	-0.201246
C	0.000000	0.747795	0.000000	C	-0.819874	0.972888	-0.055888
C	1.435484	0.870627	0.000000	C	-1.580801	-0.140276	0.152444
C	2.092889	2.041285	0.000000	H	-0.753934	-1.927026	-0.911909
H	1.999732	-0.054714	0.000000	H	-2.592294	-0.234262	0.509377
H	1.567664	2.987816	0.000000	Si	1.089454	-0.249457	0.088697
H	-0.576131	1.674742	0.000000	H	2.102246	-0.589937	-0.936825
H	3.172593	2.076270	0.000000	H	1.681892	-0.356450	1.446117
Atom	X	Y	Z	Atom	X	Y	Z
^{3}p11				**^{3}p12**			
C	1.752167	0.553516	-0.000002	C	-0.618120	0.830907	-0.027345
C	0.420142	0.331500	0.000027	H	-0.895484	1.886309	0.014006
C	-0.815830	0.129240	0.000010	C	0.662992	0.510130	-0.017890
H	2.350881	-1.510565	0.000005	Si	-1.997052	-0.377998	0.081043
H	3.442157	-0.417809	0.875463	H	-1.650230	-1.735364	-0.399943
C	2.792692	-0.517256	-0.000006	H	-3.272158	0.146882	-0.465609
Si	-2.588344	-0.158407	-0.000007	C	1.876851	0.021560	-0.012417
H	3.442149	-0.417818	-0.875481	C	3.038096	-0.396293	0.008185
H	2.106602	1.581890	-0.000061	H	4.017685	-0.803676	0.013749

Atom	X	Y	Z	Atom	X	Y	Z
^{3}p13				**^{3}p14**			
Si	-0.989851	-2.211842	0.000000	C	0.331265	-2.297058	0.000000
H	-0.051456	-3.366743	0.000000	C	1.310163	-1.376544	0.000000
C	-0.334661	-0.574839	0.000000	C	1.141221	0.058598	0.000000
C	0.000000	0.606931	0.000000	C	0.000000	0.757545	0.000000
C	0.372548	1.959551	0.000000	Si	-1.495618	1.684299	0.000000
H	-0.448876	2.670071	0.000000	H	0.563969	-3.351941	0.000000
C	1.635374	2.415508	0.000000	H	-0.715595	-2.023493	0.000000
H	1.837297	3.476593	0.000000	H	2.339761	-1.714510	0.000000
H	2.481388	1.742963	0.000000	H	2.054619	0.654514	0.000000
Atom	X	Y	Z	Atom	X	Y	Z
^{3}p15							
C	0.000000	0.794785	0.000000	C	0.000000	0.676218	1.651256
C	-1.051138	0.019159	0.000000	H	0.012154	1.422772	2.434875
C	-1.242932	-1.281441	0.000000	Si	0.000000	0.000000	-0.007231
H	-2.034393	-2.001842	0.000000	C	0.714009	0.120207	-1.708286
C	0.510202	2.170788	0.000000	H	1.155640	1.059883	-2.042077
H	-0.303923	2.895449	0.000000	C	0.000000	-0.676218	1.651256
H	1.135592	2.350737	0.877491	H	-0.012154	-1.422772	2.434875
H	1.135592	2.350737	-0.877491	C	-0.714009	-0.120207	-1.708286
Si	0.769310	-1.129631	0.000000	H	-1.155640	-1.059883	-2.042077
Atom	X	Y	Z	Atom	X	Y	Z
^{3}p18				**^{3}p19**			
C	0.095761	1.681469	-1.136381	Si	-1.715567	-0.468613	0.000000
H	-0.360037	2.652604	-0.997229	C	0.000000	0.329021	0.000000
H	0.649878	1.514127	-2.052291	C	0.250262	1.813345	0.000000
C	0.000000	0.702897	-0.158358	C	1.087398	-0.520141	0.000000
Si	0.000000	0.000000	1.545422	C	2.028346	-1.295595	0.000000
C	0.000000	-0.702897	-0.158358	H	0.836108	2.107596	0.876307
C	-0.095761	-1.681469	-1.136381	H	0.836108	2.107596	-0.876307
H	0.360037	-2.652604	-0.997229	H	-0.683266	2.373252	0.000000
H	-0.649878	-1.514127	-2.052291	H	2.832957	-1.987637	0.000000

Atom	X	Y	Z
^{3}p20			
C	1.481552	0.039988	-0.060015
C	-2.551886	-0.848214	-0.031541
C	-1.557418	-0.159817	-0.036631
H	2.300760	-1.883030	0.172381
H	3.502554	-0.530176	-0.173402
H	-0.198127	2.096976	-0.736680
H	-3.424541	-1.454627	-0.040255
C	2.464680	-0.820862	-0.015157
Si	-0.085873	0.893163	0.117001

Atom	X	Y	Z
^{3}p21			
C	0.783099	1.104478	-0.390428
C	-0.224918	0.659810	0.511864
H	1.479802	1.847867	-0.023827
H	0.529233	1.177129	-1.440725
H	-0.098190	0.854780	1.570249
Si	1.535504	-0.792440	0.003253
C	-1.420064	0.045202	0.125509
C	-2.474505	-0.455164	-0.192744
H	-3.389568	-0.911570	-0.476444

Atom	X	Y	Z
^{3}p22			
C	-0.040151	1.235280	-0.046130
C	0.830379	0.060779	-0.015968
C	2.148454	-0.080546	0.039598
C	-1.338453	0.913507	0.089586
Si	-0.829449	-0.868130	-0.113889
H	2.613473	-1.056930	0.060712
H	2.807806	0.779318	0.075769
H	-1.205641	-1.894980	0.911330
H	-2.204732	1.552287	0.144126

Atom	X	Y	Z
^{3}p23			
C	1.409793	0.837473	0.000000
H	1.865265	1.223763	0.907844
H	1.865265	1.223763	-0.907844
C	0.000000	0.780706	0.000000
Si	1.164571	-1.170482	0.000000
C	-1.198681	0.467101	0.000000
C	-2.526873	0.208079	0.000000
H	-3.069981	0.089537	-0.927542
H	-3.069981	0.089537	0.927542

Atom	X	Y	Z
^{3}p24			
C	1.028398	-0.912174	0.000000
C	-1.231286	1.072353	0.000000
C	0.000000	1.195391	0.000000
C	1.354839	0.630831	0.000000
H	1.407061	-1.415519	0.885211
H	1.407061	-1.415519	-0.885211
H	1.927082	0.917330	-0.882817
H	1.927082	0.917330	0.882817
Si	-0.970000	-0.780145	0.000000