

Supporting Information

Insights into naturally occurring compounds catalyzed formylation and methylation reactions of amines with CO₂: The origins of chemoselectivity

Zhen Yue^a, Jiyang Zhao^{a}, Pan Du^b, Guang-Xiang Liu^{a*}*

^a Nanjing Key Laboratory of Advanced Functional Materials, School of Environmental Science, Nanjing Xiaozhuang University, Nanjing 211171, People's Republic of China.

^b School of Life Science and Chemistry, Jiangsu Second Normal University, Nanjing 210013, People's Republic of China.

*Corresponding Author(s) E-mail: jyzhao1981@163.com;
E-mail: njuliugx@126.com

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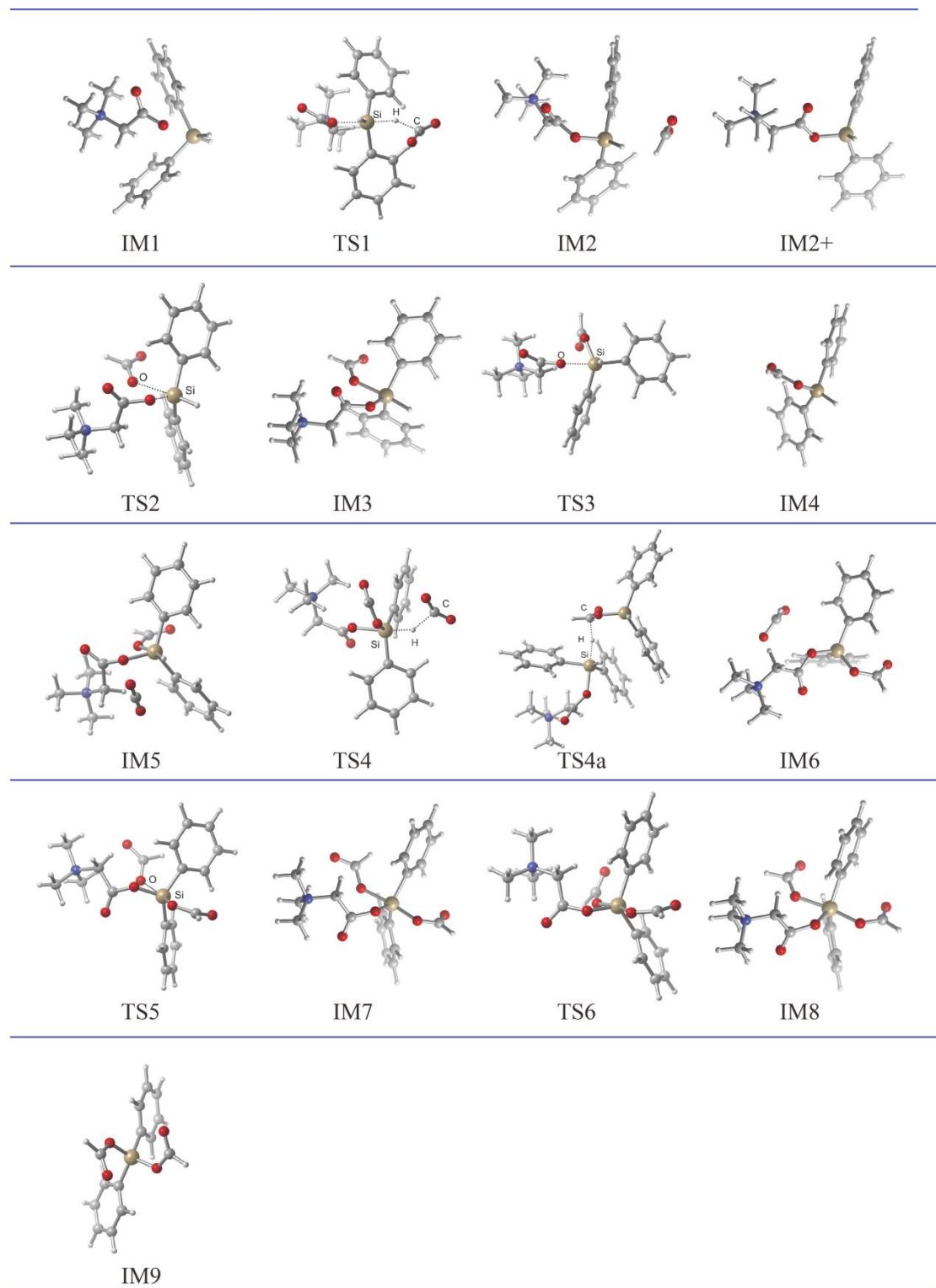


Figure S1. Optimized intermediates and transition states of the reduction of CO_2 with N -methylaniline and PH_2SiH_2 catalyzed by Lewis base GB, giving diformyloxysilane $[\text{Si}](\text{OCHO})_2$, along with the optimized structures of the stationary points.

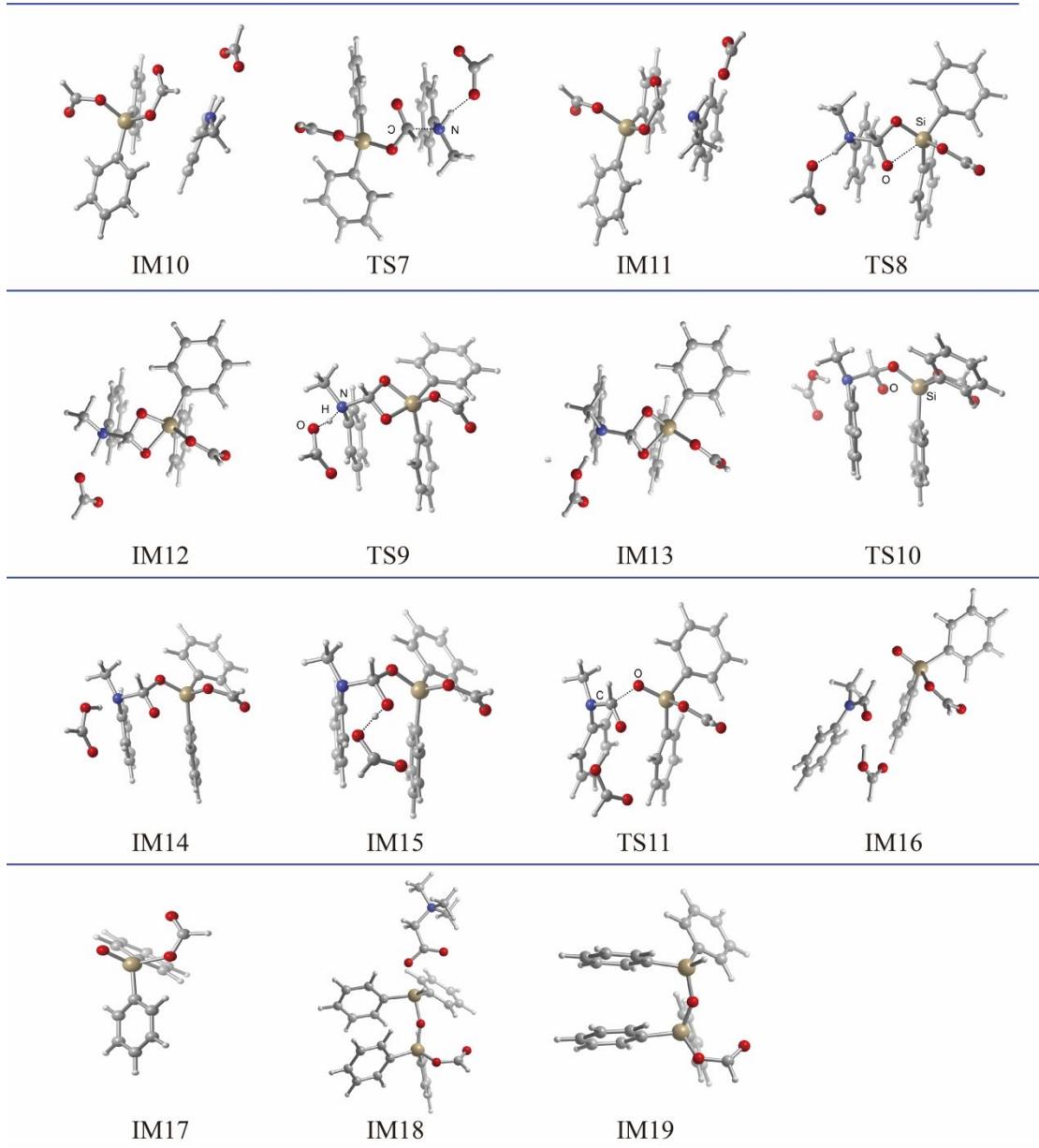


Figure S2. Optimized intermediates and transition states of the C-N bond formation to form formamide, along with the optimized structures of the stationary points.

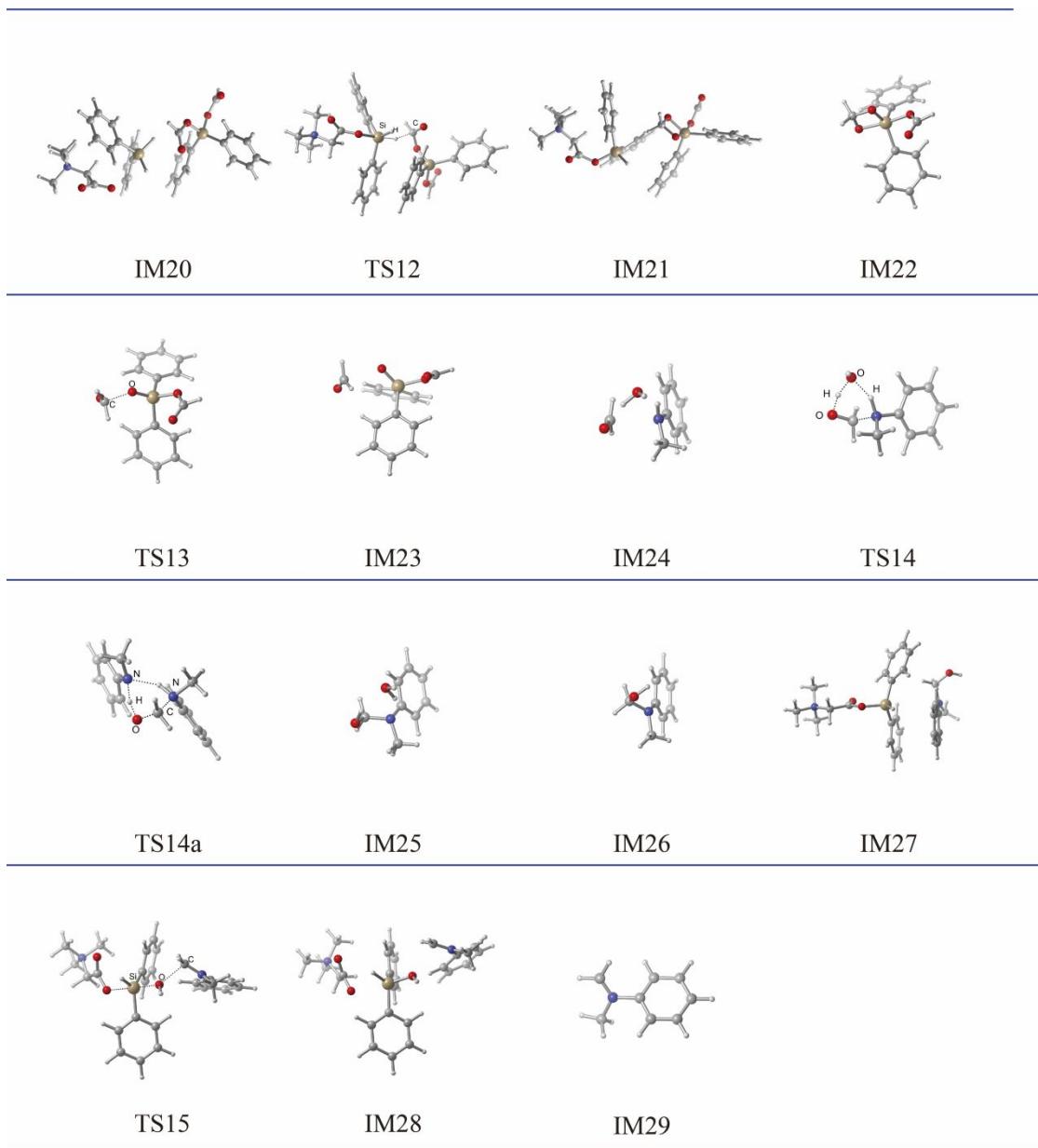


Figure S3. Optimized intermediates and transition states of the reduction of **IM9** with Ph_2SiH_2 catalyzed by GB to form carbocation **IM29**, along with the optimized structures of the stationary points.

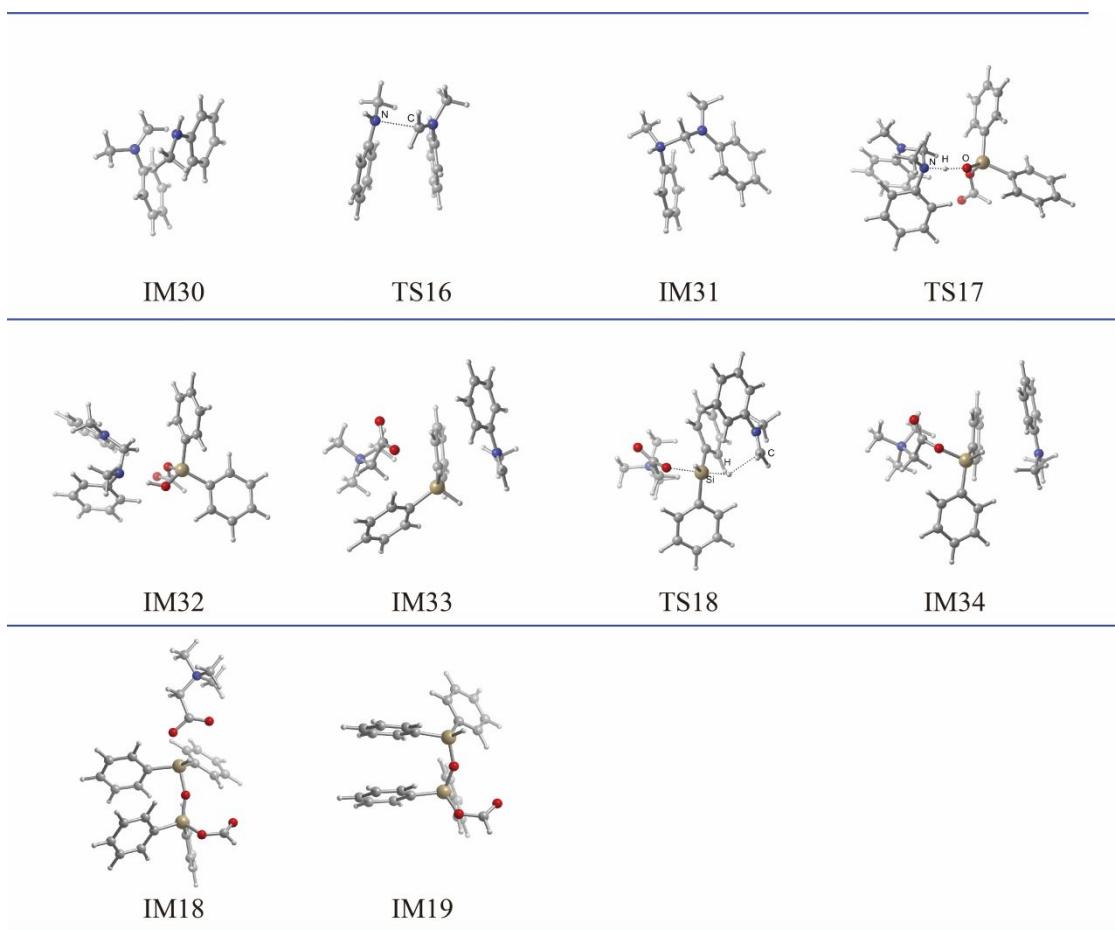


Figure S4. Optimized intermediates and transition states of the generation of aminal and methylamine, along with the optimized structures of the stationary points.

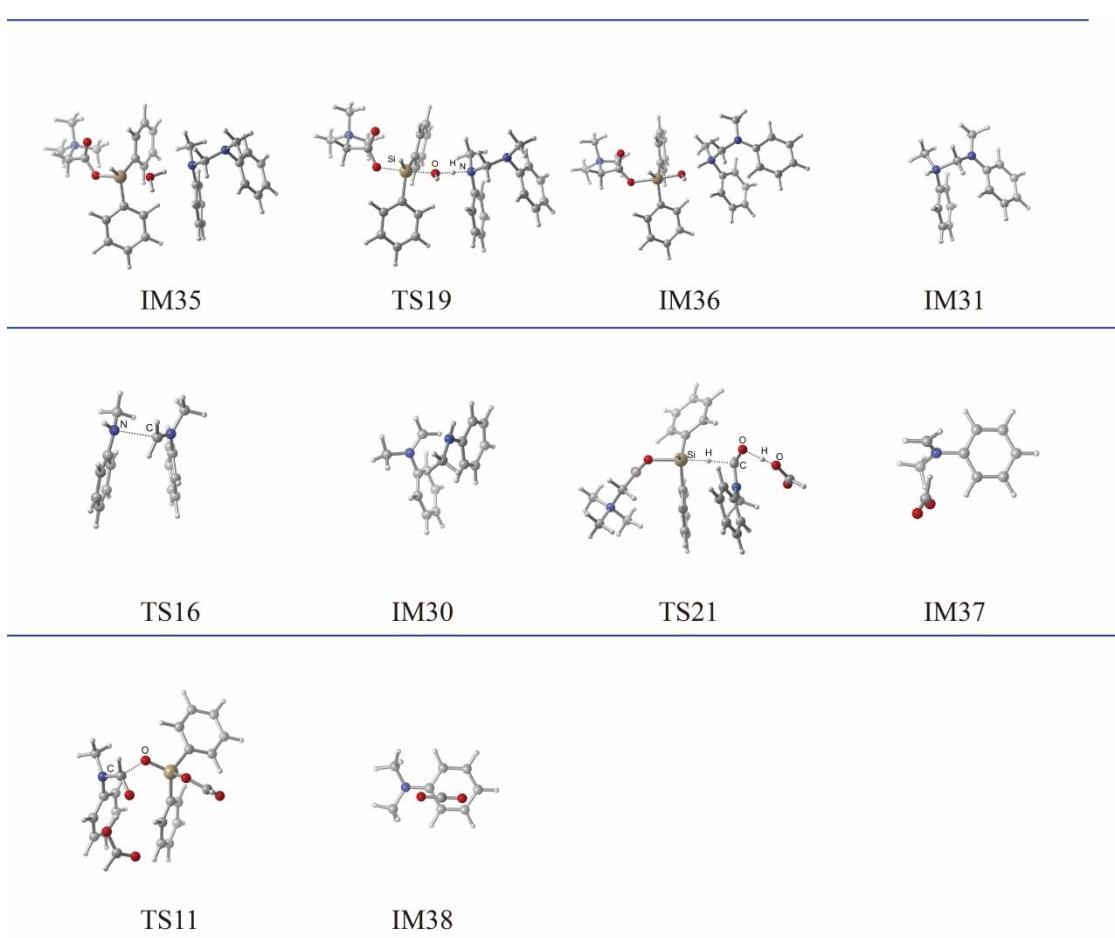


Figure S5. Optimized intermediates and transition states of the generation of methylamine from aminal, along with the optimized structures of the stationary points .

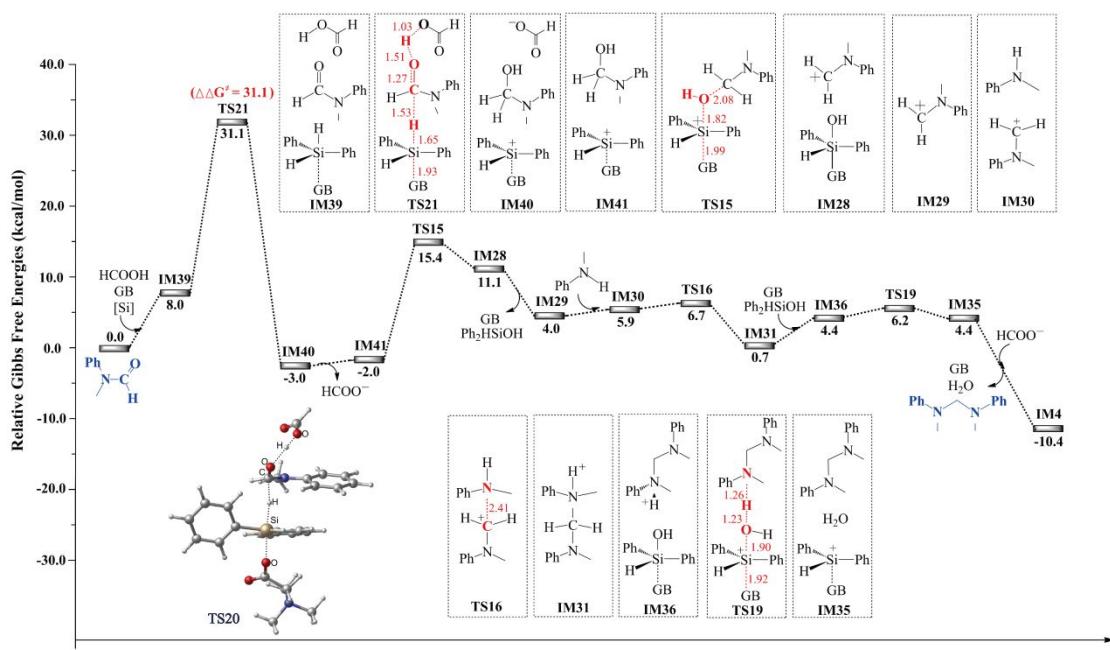


Figure S6. Free energy profile of the formation of aminal from formamide.

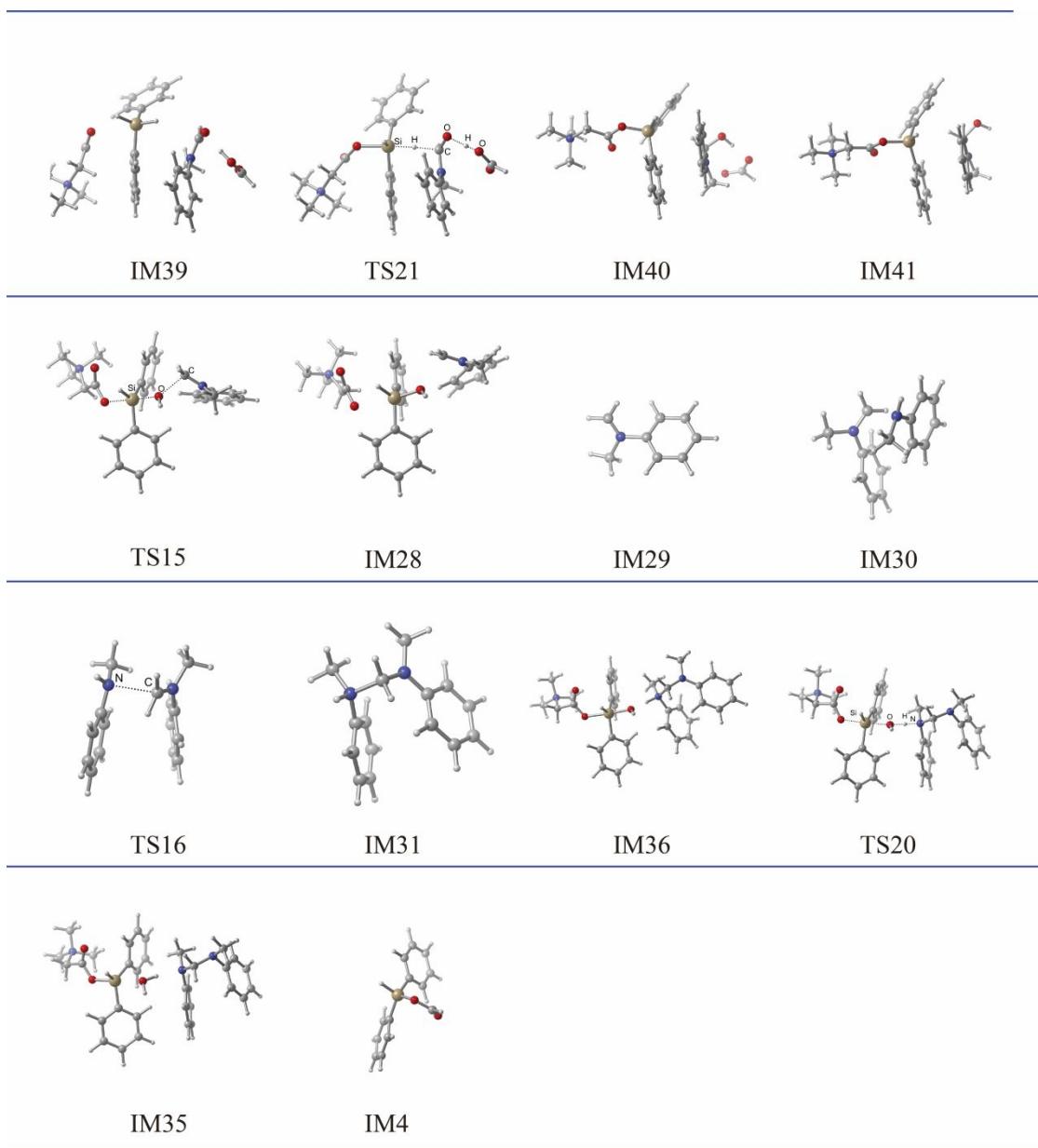


Figure S7. Optimized intermediates and transition states of the formation of aminal from formamide, along with the optimized structures of the stationary points .

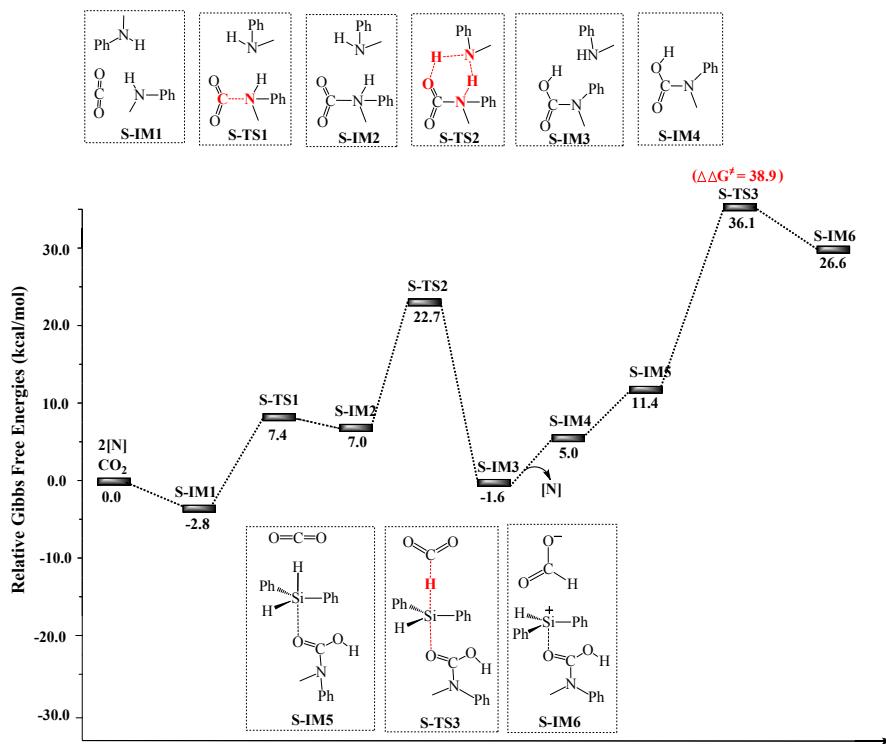


Figure S8. Free energy profile of the reduction of CO_2 with hydrosilane by carbamic acid.

Figures s8 and s9 illustrates the possible pathway for the reaction of CO_2 and PhMeNH to afford an carbamic acid, which then used to promote the reduction of CO_2 . First, the nitrogen center of PhMeNH attacks the carbon atom of CO_2 , producing the **S-IM2** intermediate that exhibits a C-N bond. The transition state of this reaction **S-TS1** lies at 10.2 kcal/mol above **S-IM1**. Then PhMeNH assists in the proton transfer from nitrogen atom to carbonyl oxygen atom via **S-TS2**, resulting in the formation of carbamic acid **S-IM4**. Next, the carbamic acid **S-IM4** like GB participates in the activation of hydrosilane and hydride abstraction by CO_2 through transition state **S-TS3**. The related free energy barrier is as high as 38.9 kcal/mol. So this pathway is unlikely to occur under experimental conditions.

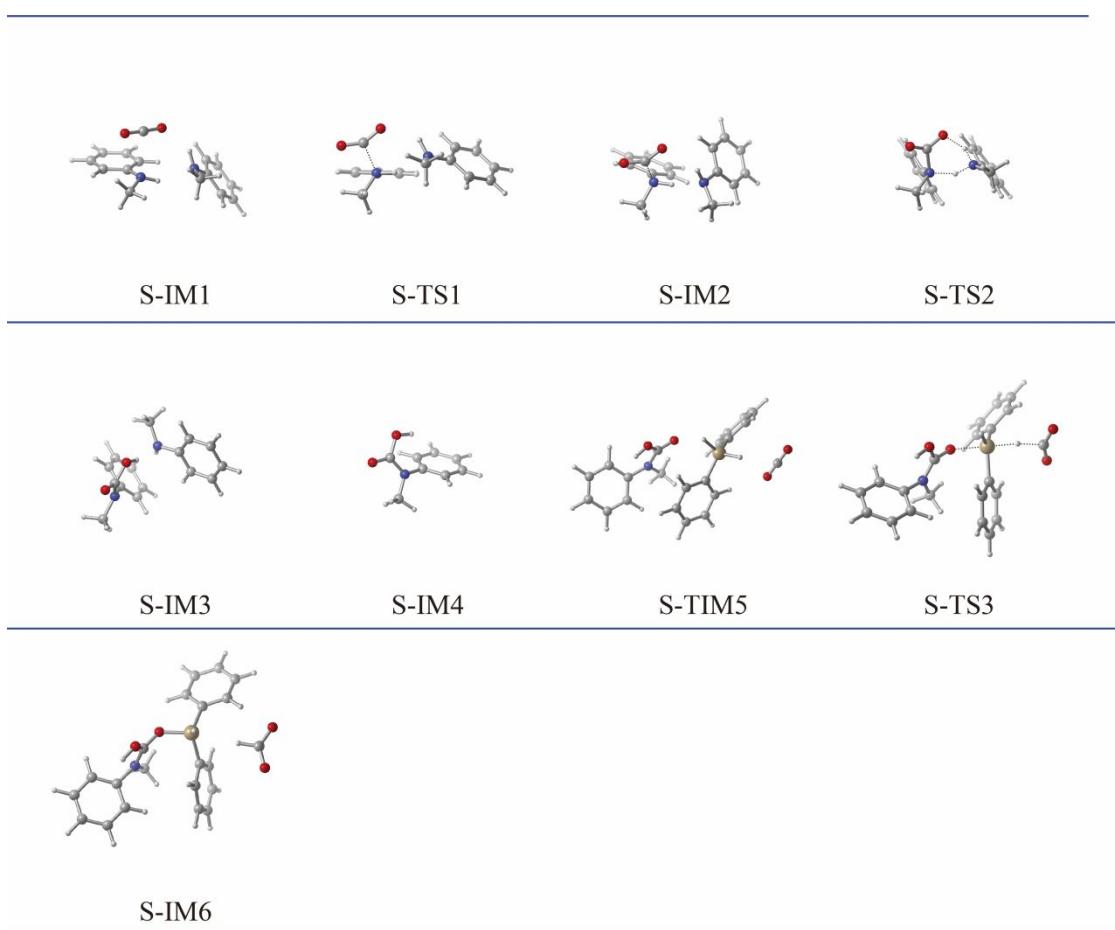


Figure S9. Optimized intermediates and transition states of the reduction of CO₂ with hydrosilane by carbamic acid.

Table S1. Corrected free energies of all species (a.u.).

Species	Corrected free energies	Species	Corrected free energies
[Si]	-326.7395124	[N]	-326.7395124
GB	-402.1696518	CO ₂	-188.586537
H ₂ O	-76.4254896	H[Si]OH	-829.0190761
formamide	-440.065603	aminal	-691.5418697
methylation	-366.005995	HCOO-	-189.2985371
HCOH	-114.4874286	PhSiH ₃	-522.7894771
HCOOH	-189.7464215	IM1	-1155.898358
TS1	-1344.449943	IM2	-1344.474521
TS2	-1344.483715	IM2+	-1155.196411
IM3	-1344.483908	TS3	-1344.486809
IM4	-942.3391752	IM5	-1533.061145
TS4	-1533.049278	TS4a	-2098.191777
IM6	-1533.091249	TS5	-1533.094041
IM7	-1533.097989	TS6	-1533.090355
IM8	-1533.096445	IM9	-1130.941277
IM10	-1646.95673	TS7	-1646.940009
IM11	-1646.942178	TS8	-1646.93575
IM12	-1646.940906	TS9	-1646.941165
IM13	-1646.940799	TS10	-1646.931539
IM14	-1646.952853	IM15	-1646.934484
TS11	-1646.935401	IM16	-1646.957898
IM17	-1017.157631	IM18	-2172.383931
IM19	-1770.213075	IM20	-2286.828701
TS12	-2286.794394	IM21	-2286.823185
IM22	-1131.653878	TS13	-1131.625968
IM23	-1131.634526	IM24	-517.6334968
TS14	-517.6184489	IM25	-517.6447045
IM26	-441.2278399	IM27	-1596.418438
TS15	-1596.39075	IM28	-1596.397684
IM29	-365.2285572	TS14a	-767.9066042
IM30	-691.9613423	TS16	-691.9595211
IM31	-691.9690934	TS17	-1709.155835
IM32	-1709.162001	IM33	-1521.115561
TS18	-1521.107697	IM34	-1521.180778
IM35	-1923.143553	TS19	-1923.140781
IM36	-1923.143557	IM37	-554.5226915
TS20	-554.5151231	IM38	-554.583573

IM39	-1785.696988	TS21	-1785.660076
IM40	-1785.714537	IM41	-1596.418438
BE	-3054.309128	BE-TS	-3996.588438
BE-TD-COFS	-1166.728633	BE-TD-COFS-TS	-2109.008837
Oxamic	-357.9881466	Oxamic-TS	-1300.270761
Salicylic	-479.5436851	Salicylic-TS	-1421.824057
Lecithin	-1351.473397	Lecithin-TS	-2293.753048
S-IM1	-842.0474079	S-IM2	-842.0318768
S-IM3	-842.0454635	S-IM4	-515.3092002
S-IM5	-1457.612772	S-IM6	-1457.588591
S-TS1	-842.0311859	S-TS2	-842.0164652
S-TS3	-1457.573373		

Table S2. Imaginary frequencies of all transition states.

Species	Imaginary frequency
TS1	600.76 cm ⁻¹
TS2	85.02cm ⁻¹
TS3	22.40 cm ⁻¹
TS4	438.22 cm ⁻¹
TS4a	446.76 cm ⁻¹
TS5	32.10 cm ⁻¹
TS6	72.38 cm ⁻¹
TS7	48.73 cm ⁻¹
TS8	161.58 cm ⁻¹
TS9	666.58 cm ⁻¹
TS10	104.79cm ⁻¹
TS11	221.36 cm ⁻¹
TS12	414.67 cm ⁻¹
TS13	151.58 cm ⁻¹
TS14	1048.99 cm ⁻¹
TS14a	669.86 cm ⁻¹
TS15	169.40 cm ⁻¹
TS16	52.14 cm ⁻¹
TS17	480.07 cm ⁻¹
TS18	79.04 cm ⁻¹
TS19	641.94 cm ⁻¹
TS20	294.47 cm ⁻¹
TS21	600.76 cm ⁻¹
BE-TS	487.62cm ⁻¹
BE-TD-COFS-TS	476.30cm ⁻¹
Oxamic-TS	433.63 cm ⁻¹
Salicylic-TS	494.60 cm ⁻¹
Lecithin-TS	394.71cm ⁻¹
S-TS1	177.0 cm ⁻¹
S-TS2	534.4 cm ⁻¹
S-TS3	439.4 cm ⁻¹

Table S3. Cartesian coordinates of all species (angstroms).

[Si]				GB			
Symbol	X	Y	Z	Symbol	X	Y	Z
Si	-1.244864	-0.373940	-0.034150	H	-5.750612	-2.345638	-1.019051
H	-0.739462	-1.764391	-0.127233	H	-5.794374	1.350422	1.156758
H	-0.780762	0.396366	-1.213034	C	-7.013543	-0.520991	0.083844
C	-3.123117	-0.438414	0.021838	C	-0.594122	0.474417	1.506211
C	-3.829383	-1.490829	-0.574425	C	-0.112883	1.788573	1.462679
C	-3.854106	0.579712	0.647137	C	-0.622721	-0.180341	2.745447
C	-5.220806	-1.522180	-0.554099	C	0.323649	2.430718	2.618770
H	-3.290043	-2.300027	-1.057364	H	-0.077275	2.319523	0.516515
C	-5.245250	0.553680	0.668641	C	-0.183725	0.454825	3.901592
H	-3.331613	1.401161	1.129316	H	-0.989652	-1.200682	2.810602
C	-5.930139	-0.498179	0.066451	C	0.289356	1.763597	3.838693
H	-5.750612	-2.345638	-1.019051	H	0.690807	3.449181	2.566784
H	-5.794374	1.350422	1.156758	H	-0.208933	-0.067887	4.850583
H	-7.013543	-0.520991	0.083844	H	0.631162	2.260959	4.738892
C	-0.594122	0.474417	1.506211	[N]			
C	-0.112883	1.788573	1.462679	Symbol	X	Y	Z
C	-0.622721	-0.180341	2.745447	Symbol	X	Y	Z
C	0.323649	2.430718	2.618770	Si	-1.244864	-0.373940	-0.034150
H	-0.077275	2.319523	0.516515	H	-0.739462	-1.764391	-0.127233
C	-0.183725	0.454825	3.901592	H	-0.780762	0.396366	-1.213034
H	-0.989652	-1.200682	2.810602	C	-3.123117	-0.438414	0.021838
C	0.289356	1.763597	3.838693	C	-3.829383	-1.490829	-0.574425
H	0.690807	3.449181	2.566784	C	-3.854106	0.579712	0.647137
H	-0.208933	-0.067887	4.850583	C	-5.220806	-1.522180	-0.554099
H	0.631162	2.260959	4.738892	H	-3.290043	-2.300027	-1.057364
[N]				C	-5.245250	0.553680	0.668641
Symbol	X	Y	Z	H	-3.331613	1.401161	1.129316
Si	-1.244864	-0.373940	-0.034150	C	-5.930139	-0.498179	0.066451
H	-0.739462	-1.764391	-0.127233	CO ₂			
H	-0.780762	0.396366	-1.213034	Symbol	X	Y	Z
C	-3.123117	-0.438414	0.021838	Symbol	X	Y	Z
C	-3.829383	-1.490829	-0.574425	C	-1.432834	1.296296	-0.285009
C	-3.854106	0.579712	0.647137	O	-2.587323	1.296296	-0.285009
C	-5.220806	-1.522180	-0.554099				
H	-3.290043	-2.300027	-1.057364				
C	-5.245250	0.553680	0.668641				
H	-3.331613	1.401161	1.129316				
C	-5.930139	-0.498179	0.066451				

O	-0.278346	1.296296	-0.285008	H	1.236684	-1.786562	3.618480
H2O				H	0.329967	-0.292787	3.899025
Symbol	X	Y	Z	H	-0.153193	-1.376381	2.585864
O	-2.450149	1.599660	0.385712	C	2.429950	-0.977774	1.359348
H	-3.029511	1.692558	1.144214	C	2.057117	-2.278015	1.003713
H	-2.856960	0.904712	-0.138316	C	3.627025	-0.452210	0.857571
				C	2.858787	-3.032704	0.154604
				H	1.139794	-2.708139	1.382769
HSiOH				C	4.416892	-1.217259	0.008707
Symbol	X	Y	Z	H	3.935000	0.544467	1.130723
Si	-0.005366	1.319101	0.385285	C	4.041521	-2.507908	-0.351392
H	0.110115	1.932775	1.731004	H	2.548848	-4.036759	-0.109393
C	1.540948	0.305031	0.109795	H	5.341221	-0.796128	-0.369073
C	2.661105	0.467042	0.933828	H	4.665324	-3.096180	-1.012845
C	1.615548	-0.624426	-0.937881				
C	3.822659	-0.270295	0.718469				
H	2.627333	1.175290	1.756093				
C	2.773305	-1.361937	-1.158517	Aminal			
H	0.756095	-0.779409	-1.583934	Symbol	X	Y	Z
C	3.878637	-1.183926	-0.329121	H	0.426548	-0.598575	-0.716567
H	4.680461	-0.133490	1.366382	H	-0.142769	-1.711652	0.523354
H	2.815170	-2.076907	-1.971809	C	0.698650	-1.086041	0.219517
H	4.780784	-1.760162	-0.498224	N	1.821395	-1.981795	0.004835
C	-1.525813	0.246988	0.220246	C	1.821009	-3.274327	0.667319
C	-1.521697	-1.083252	0.659816	H	2.473184	-3.293905	1.549880
C	-2.708613	0.764001	-0.323494	H	0.806588	-3.509045	0.983890
C	-2.664074	-1.872015	0.564554	H	2.149290	-4.059683	-0.018232
H	-0.614476	-1.513280	1.074142	C	3.019598	-1.486540	-0.490759
C	-3.852418	-0.022538	-0.423755	C	4.202961	-2.247129	-0.418525
H	-2.729981	1.788527	-0.679764	C	3.097256	-0.215990	-1.095760
C	-3.831165	-1.340922	0.022378	C	5.397128	-1.758342	-0.936186
H	-2.643467	-2.899618	0.907984	H	4.198403	-3.225211	0.041716
H	-4.758730	0.391313	-0.850205	C	4.298766	0.255836	-1.605356
H	-4.721119	-1.954498	-0.055236	H	2.221676	0.413065	-1.176205
O	-0.224850	2.503380	-0.762914	C	5.462702	-0.504858	-1.532952
H	0.441207	3.192498	-0.825015	H	6.287472	-2.372751	-0.863861
				H	4.319773	1.237749	-2.064773
				H	6.396653	-0.127822	-1.930113
Formamide				N	0.939869	-0.057270	1.227314
Symbol	X	Y	Z	C	1.622456	-0.530011	2.416605
H	0.821137	1.494382	2.996337	H	1.449093	0.159019	3.243353
C	1.530323	1.125350	2.240417	H	1.207905	-1.500255	2.695928
O	2.137511	1.879518	1.510808	H	2.705607	-0.647306	2.271833
N	1.608268	-0.238985	2.252077	C	1.008740	1.290608	0.886633
C	0.700422	-0.971122	3.133098	C	1.908310	2.163701	1.522336
				C	0.152142	1.828331	-0.092633

C	1.955106	3.509537	1.177217	O	0.594488	-1.689485	0.255108
H	2.592926	1.787231	2.270878				
C	0.224870	3.170192	-0.441078				
H	-0.594944	1.200222	-0.561768				
C	1.124812	4.026474	0.188361				
H	2.663623	4.156048	1.682666				
H	-0.447421	3.552688	-1.200695				
H	1.170840	5.074214	-0.080537				
Methylamine							
Symbol	X	Y	Z				
H	-2.085591	1.414886	-3.112381				
H	-3.530525	2.441808	-3.016699				
H	-3.675140	0.671951	-2.989377				
C	-3.071681	1.512455	-2.653024				
N	-2.972805	1.471145	-1.204740				
C	-4.039880	0.805075	-0.478858				
H	-4.812344	1.504704	-0.131978				
H	-4.504910	0.069738	-1.132033				
H	-3.645643	0.272654	0.389516				
C	-2.255624	2.463790	-0.562634				
C	-1.403366	3.331261	-1.277299				
C	-2.339560	2.641305	0.834372				
C	-0.657635	4.299831	-0.618071				
H	-1.319498	3.252087	-2.352121				
C	-1.585676	3.615684	1.475205				
H	-2.994667	2.017064	1.425772				
C	-0.734095	4.454202	0.762559				
H	-0.010866	4.946576	-1.200529				
H	-1.673948	3.720395	2.550884				
H	-0.151117	5.212970	1.268936				
HCOO⁻							
Symbol	X	Y	Z				
H	-2.346105	1.765507	-0.000914				
C	-2.285888	2.761741	0.525421				
O	-2.001321	3.735368	-0.196889				
O	-2.523160	2.734484	1.749773				
HCOH							
Symbol	X	Y	Z				
H	0.566800	-1.416405	2.249177				
H	1.921120	-2.498990	1.533599				
C	1.030428	-1.873577	1.359751				
PhSiH₃							
Symbol	X	Y	Z				
Si	-3.463075	1.887478	-0.027426				
H	-2.972907	0.490636	-0.035450				
H	-2.968961	2.589689	1.178513				
H	-4.944602	1.884465	-0.017123				
C	-2.823111	2.774488	-1.563742				
C	-2.591437	4.153849	-1.544918				
C	-2.580585	2.066892	-2.745497				
C	-2.134554	4.812322	-2.683394				
H	-2.766467	4.721721	-0.637376				
C	-2.123688	2.723909	-3.885109				
H	-2.747061	0.995582	-2.781277				
C	-1.900297	4.096559	-3.853276				
H	-1.957437	5.881064	-2.658655				
H	-1.938135	2.166559	-4.795680				
H	-1.541224	4.607781	-4.738178				
HCOOH							
Symbol	X	Y	Z				
H	3.168507	2.167293	0.196599				
H	4.905569	2.577171	-1.966095				
C	3.972421	2.244076	-1.498107				
O	3.053150	1.744901	-2.082402				
O	4.003223	2.472135	-0.188182				
IM1							
Symbol	X	Y	Z				
Si	1.652396	1.066361	0.850684				
H	1.682889	1.014475	2.326339				
H	2.809680	1.862541	0.361886				
C	1.802830	-0.661414	0.125615				
C	1.830532	-1.796455	0.943408				
C	1.799932	-0.845750	-1.263996				
C	1.841208	-3.074978	0.392424				
H	1.798791	-1.680400	2.020044				
C	1.797373	-2.121959	-1.820183				
H	1.782699	0.013729	-1.928213				
C	1.813008	-3.239822	-0.989613				
H	1.856336	-3.943482	1.040907				
H	1.782542	-2.244386	-2.897144				
H	1.807576	-4.235008	-1.418862				

C	0.111989	1.952190	0.226397	H	-1.515688	-4.477087	-1.185848
C	0.076443	2.451858	-1.085008	H	-3.151738	-2.571256	2.290019
C	-1.004107	2.170042	1.044336	H	-2.637933	-4.639031	1.019514
C	-1.038559	3.130500	-1.567950	C	-0.059281	1.733871	-0.113721
H	0.935042	2.326937	-1.738569	C	-0.298903	1.944317	1.250705
C	-2.116822	2.859248	0.568199	C	0.988173	2.448986	-0.711607
H	-1.014073	1.774637	2.053413	C	0.496152	2.808052	1.999985
C	-2.138090	3.337589	-0.737926	H	-1.124077	1.431556	1.736386
H	-1.045537	3.506300	-2.584525	C	1.761275	3.345200	0.023080
H	-2.971000	3.013766	1.217541	H	1.207138	2.302238	-1.764550
H	-3.005488	3.871294	-1.108882	C	1.525113	3.516473	1.383899
N	-2.583573	-1.489840	-0.692071	H	0.303786	2.939640	3.058535
C	-1.484467	-1.488526	0.338935	H	2.554977	3.900434	-0.463794
H	-1.234152	-2.531615	0.541774	H	2.135772	4.201444	1.960472
H	-0.624321	-1.021703	-0.137879	N	2.844049	-1.127233	0.611637
C	-1.754940	-0.756442	1.682868	C	1.552389	-1.142877	-0.155412
O	-0.724843	-0.665266	2.373210	H	1.259412	-2.186358	-0.293795
O	-2.904430	-0.349684	1.932528	H	0.809220	-0.671467	0.485607
C	-3.781519	-2.234164	-0.196742	C	1.578107	-0.457667	-1.531640
H	-4.124665	-1.740542	0.706794	O	0.412489	-0.164930	-2.000169
H	-4.541917	-2.217080	-0.975573	O	2.625606	-0.268121	-2.120311
H	-3.481248	-3.259969	0.011510	C	3.901505	-1.951538	-0.059198
C	-2.061406	-2.162401	-1.919275	H	4.104950	-1.520798	-1.032969
H	-2.851972	-2.187706	-2.667177	H	4.787751	-1.936382	0.572277
H	-1.207094	-1.596643	-2.287787	H	3.527414	-2.969326	-0.156691
H	-1.752302	-3.173362	-1.659709	C	2.565226	-1.714081	1.961617
C	-2.958539	-0.082304	-1.036640	H	3.496709	-1.744129	2.522873
H	-3.387042	0.375260	-0.151069	H	1.836807	-1.085405	2.470795
H	-2.051984	0.448505	-1.330938	H	2.171297	-2.719945	1.830352
H	-3.669738	-0.109009	-1.860843	C	3.320508	0.282320	0.792938
				H	3.573266	0.689864	-0.181403
				H	2.515332	0.858117	1.250338
				H	4.192236	0.265030	1.443994

TS1

Symbol	X	Y	Z
Si	-1.149402	0.544704	-1.122664
H	-1.624031	0.930387	-2.468954
H	-2.456675	1.213837	-0.438123
C	-1.645847	-1.151915	-0.424384
C	-1.367068	-2.334400	-1.124910
C	-2.310968	-1.267172	0.803397
C	-1.731148	-3.578734	-0.618531
H	-0.853318	-2.281894	-2.078903
C	-2.652709	-2.510365	1.329674
H	-2.577783	-0.373963	1.359843
C	-2.364711	-3.670342	0.617480

H	-2.637933	-4.639031	1.019514
C	-0.059281	1.733871	-0.113721
C	-0.298903	1.944317	1.250705
C	0.988173	2.448986	-0.711607
C	0.496152	2.808052	1.999985
H	-1.124077	1.431556	1.736386
C	1.761275	3.345200	0.023080
H	1.207138	2.302238	-1.764550
C	1.525113	3.516473	1.383899
H	0.303786	2.939640	3.058535
H	2.554977	3.900434	-0.463794
H	2.135772	4.201444	1.960472
N	2.844049	-1.127233	0.611637
C	1.552389	-1.142877	-0.155412
H	1.259412	-2.186358	-0.293795
H	0.809220	-0.671467	0.485607
C	1.578107	-0.457667	-1.531640
O	0.412489	-0.164930	-2.000169
O	2.625606	-0.268121	-2.120311
C	3.901505	-1.951538	-0.059198
H	4.104950	-1.520798	-1.032969
H	4.787751	-1.936382	0.572277
H	3.527414	-2.969326	-0.156691
C	2.565226	-1.714081	1.961617
H	3.496709	-1.744129	2.522873
H	1.836807	-1.085405	2.470795
H	2.171297	-2.719945	1.830352
C	3.320508	0.282320	0.792938
H	3.573266	0.689864	-0.181403
H	2.515332	0.858117	1.250338
H	4.192236	0.265030	1.443994

IM2

Symbol	X	Y	Z
Si	0.899625	0.123479	1.209197
H	1.635026	0.658612	2.361093
H	3.373777	1.444148	0.786236
C	1.817698	-1.134073	0.179477
C	1.608852	-2.497049	0.436429

				Symbol	X	Y	Z
C	2.718854	-0.772920	-0.835660	Si	-0.540400	-0.330611	-0.635529
C	2.270232	-3.474285	-0.300582	H	-0.288696	-0.247000	-2.086248
H	0.929187	-2.802860	1.225748	C	-1.880946	-1.523216	-0.150195
C	3.375807	-1.753576	-1.572736	C	-1.585085	-2.829041	0.259456
H	2.916479	0.274478	-1.054879	C	-3.224532	-1.129018	-0.215562
C	3.153501	-3.102020	-1.308741	C	-2.603304	-3.715947	0.595252
H	2.097059	-4.522277	-0.086706	H	-0.552459	-3.154019	0.323432
H	4.065414	-1.462338	-2.356565	C	-4.243296	-2.015468	0.116520
H	3.668795	-3.861028	-1.885697	H	-3.482302	-0.119264	-0.521544
C	-0.008489	1.412843	0.208251	C	-3.932207	-3.309934	0.522838
C	0.069402	1.490692	-1.187167	C	-0.871718	2.290014	0.881449
C	-0.871718	2.290014	0.881449	H	-2.359820	-4.722494	0.914110
C	-0.688998	2.423094	-1.890124	H	-5.277090	-1.695809	0.062662
H	0.724889	0.822164	-1.734489	H	-4.725357	-4.000212	0.784860
C	-1.630316	3.222068	0.181808	C	-0.795488	1.362519	0.087604
H	-0.952107	2.250199	1.964185	C	-1.527075	1.543218	1.269110
C	-1.537698	3.289169	-1.206429	C	-0.246925	2.488140	-0.541600
H	-0.615569	2.474784	-2.969776	C	-1.700593	2.813244	1.809624
H	-2.289705	3.894717	0.717241	H	-1.970482	0.687527	1.769206
H	-2.126437	4.015333	-1.754308	C	-0.421984	3.758589	-0.004711
N	-3.110048	-1.287227	-0.451996	H	0.326963	2.368023	-1.454648
C	-1.769201	-1.477095	0.189361	C	-1.148328	3.920310	1.172098
H	-1.566029	-2.550114	0.240501	H	-2.267554	2.940561	2.724089
H	-1.030009	-1.028214	-0.474777	H	0.007027	4.620793	-0.501295
C	-1.635363	-0.903644	1.597792	H	-1.285662	4.910034	1.591651
O	-0.374874	-0.751707	1.981617	N	4.514534	-0.980389	0.486380
O	-2.565142	-0.673570	2.317395	C	3.094116	-1.443777	0.570257
C	-4.170889	-2.095247	0.237706	H	3.036875	-2.444934	0.139975
H	-4.260198	-1.750808	1.262135	H	2.820572	-1.513411	1.624067
H	-5.103851	-1.949689	-0.302222	C	2.073748	-0.564752	-0.130793
H	-3.877634	-3.142809	0.205082	O	0.867283	-1.067666	0.047343
C	-2.992015	-1.757695	-1.872266	O	2.312752	0.434856	-0.756605
H	-3.972426	-1.684756	-2.337033	C	4.987889	-0.921601	-0.937550
H	-2.279273	-1.119066	-2.391223	H	4.427618	-0.154144	-1.461267
H	-2.648343	-2.789920	-1.872606	H	6.048317	-0.679759	-0.923690
C	-3.488681	0.166245	-0.461642	H	4.831395	-1.896411	-1.394995
H	-3.665792	0.490829	0.559274	C	5.352110	-1.979965	1.229345
H	-2.671330	0.731247	-0.910440	H	6.387434	-1.650104	1.189345
H	-4.392416	0.273358	-1.057772	H	5.009089	-2.025360	2.260636
C	3.094714	2.428597	0.307529	H	5.245132	-2.950983	0.750148
O	2.675137	3.301099	1.086440	C	4.684080	0.364226	1.131951
O	3.247749	2.476371	-0.930632	H	4.105099	1.094328	0.575665
				H	4.340422	0.298011	2.162298
				H	5.742246	0.614462	1.105052

IM2⁺

TS2

Symbol	X	Y	Z
Si	0.807069	0.456464	-1.204280
H	1.061906	0.921119	-2.601299
C	-0.099463	1.936672	-0.498236
C	-0.889202	2.691012	-1.376190
C	0.005013	2.357651	0.834174
C	-1.584021	3.814610	-0.934896
H	-0.966230	2.398461	-2.419655
C	-0.664157	3.497245	1.269741
H	0.609366	1.778813	1.525005
C	-1.467782	4.220459	0.390480
H	-2.203541	4.376069	-1.624484
H	-0.566740	3.819608	2.300304
H	-1.997798	5.100242	0.737063
C	2.498379	-0.027869	-0.583323
C	2.824149	-1.359663	-0.306046
C	3.495982	0.943607	-0.461307
C	4.108604	-1.708578	0.095899
H	2.058411	-2.124594	-0.390447
C	4.780188	0.601055	-0.044263
H	3.272847	1.984161	-0.682411
C	5.087788	-0.726842	0.233676
H	4.347099	-2.744536	0.308032
H	5.538802	1.368112	0.060437
H	6.086920	-0.997257	0.555021
N	-3.240177	-1.562928	0.254572
C	-2.248181	-0.835881	-0.602540
H	-2.770879	-0.501513	-1.501612
H	-1.901148	0.032421	-0.043606
C	-1.033545	-1.646505	-1.030451
O	-0.140862	-0.895581	-1.658266
O	-0.941284	-2.840815	-0.946840
C	-3.884914	-2.692262	-0.491416
H	-3.121958	-3.418513	-0.749123
H	-4.638574	-3.134373	0.156747
H	-4.351608	-2.285612	-1.386702
C	-4.302084	-0.577647	0.637372
H	-5.038563	-1.090323	1.251908
H	-3.839795	0.232653	1.197152
H	-4.767135	-0.196337	-0.269385
C	-2.588749	-2.074994	1.505225
H	-1.843812	-2.815045	1.230370
H	-2.112374	-1.235219	2.004456

H	-3.365646	-2.514262	2.127500
H	0.378406	-1.652135	2.587598
C	0.689851	-0.736219	2.031020
O	0.132939	-0.599817	0.899762
O	1.502134	0.013648	2.574410

IM3

Symbol	X	Y	Z
Si	-0.859198	0.168160	0.389937
H	-1.279467	0.747484	1.731959
C	-0.398607	1.887659	-0.314995
C	-0.918490	3.007156	0.350760
C	0.429550	2.139232	-1.420284
C	-0.650882	4.307824	-0.070345
H	-1.544625	2.857921	1.224628
C	0.728528	3.434172	-1.832418
H	0.854048	1.315113	-1.981591
C	0.181932	4.525267	-1.162138
H	-1.082307	5.148634	0.460864
H	1.382366	3.591950	-2.682691
H	0.406185	5.534560	-1.487484
C	-2.533178	-0.692126	0.114532
C	-2.675131	-1.993377	-0.382875
C	-3.695405	-0.020999	0.511765
C	-3.925310	-2.597506	-0.485195
H	-1.794324	-2.547910	-0.691206
C	-4.954089	-0.601313	0.378422
H	-3.616385	0.975636	0.938657
C	-5.070711	-1.897160	-0.116325
H	-4.007376	-3.612159	-0.858607
H	-5.840519	-0.050743	0.672848
H	-6.046408	-2.360397	-0.207630
N	3.559617	-1.281716	-0.504191
C	2.505434	-0.602849	0.318526
H	2.992232	-0.178773	1.199334
H	2.098539	0.212419	-0.278640
C	1.355287	-1.488004	0.788795
O	0.359746	-0.771119	1.258785
O	1.401006	-2.691058	0.814766
C	4.314244	-2.301642	0.296755
H	3.624525	-3.079290	0.605095
H	5.101516	-2.705941	-0.336157
H	4.747214	-1.803680	1.162372
C	4.521935	-0.227633	-0.961347

H	5.299849	-0.707994	-1.550285	O	3.067970	-1.198067	2.051320
H	3.984021	0.498485	-1.567111	C	4.773556	-0.050523	-0.084927
H	4.952824	0.254512	-0.086356	H	4.840846	-0.470801	0.912636
C	2.943689	-1.927354	-1.708622	H	5.600817	-0.378914	-0.711357
H	2.272451	-2.713674	-1.377045	H	4.741889	1.036816	-0.044935
H	2.394005	-1.165089	-2.256766	C	3.375303	0.048988	-2.080726
H	3.746114	-2.334931	-2.319540	H	4.241568	-0.253276	-2.665562
H	-0.048108	-1.423534	-2.990240	H	2.458640	-0.328824	-2.531574
C	-0.585679	-0.723092	-2.325541	H	3.332946	1.133485	-1.998536
O	-0.095896	-0.725210	-1.118423	C	3.510583	-2.023431	-0.816652
O	-1.508946	-0.055930	-2.735475	H	3.618467	-2.439339	0.179874

TS3

Symbol	X	Y	Z
Si	-0.993608	-0.335789	1.096098
H	-1.309966	-0.386778	2.532789
C	-0.418580	1.316398	0.388796
C	0.196681	2.266533	1.213311
C	-0.599733	1.633225	-0.962339
C	0.627941	3.488778	0.704435
H	0.361917	2.037094	2.260416
C	-0.140926	2.839473	-1.484220
H	-1.082425	0.916159	-1.617943
C	0.472959	3.770769	-0.650291
H	1.094999	4.214381	1.360380
H	-0.267712	3.056496	-2.538655
H	0.824241	4.713613	-1.053271
C	-2.769868	-0.426247	0.343821
C	-3.391637	-1.618342	-0.051808
C	-3.549236	0.740117	0.290550
C	-4.713446	-1.648037	-0.492962
H	-2.843547	-2.554770	-0.011161
C	-4.872220	0.723133	-0.141929
H	-3.112331	1.690103	0.586260
C	-5.458785	-0.474921	-0.540577
H	-5.160870	-2.587818	-0.796972
H	-5.444022	1.643912	-0.173167
H	-6.486778	-0.493294	-0.883652
N	3.498743	-0.530966	-0.705797
C	2.296213	-0.070557	0.072317
H	2.361882	1.017591	0.149040
H	1.432051	-0.303460	-0.546060
C	2.120011	-0.653440	1.491083
O	0.964171	-0.471149	1.982139

IM4

Symbol	X	Y	Z
Si	0.836211	0.052301	-0.728315
H	0.585946	-0.204663	-2.158023
C	0.684953	1.877723	-0.397387
C	0.181436	2.720048	-1.397082
C	1.085844	2.447969	0.819881
C	0.072555	4.091936	-1.187225
H	-0.128003	2.304417	-2.350827
C	0.979075	3.817635	1.030820
H	1.474037	1.811176	1.607372
C	0.471283	4.639935	0.027246
H	-0.319975	4.730434	-1.969608
H	1.291075	4.245577	1.976129
H	0.389001	5.707815	0.192545
C	2.449062	-0.656731	-0.117956
C	2.543389	-2.010363	0.231751
C	3.598127	0.138140	-0.027961
C	3.749657	-2.553244	0.660318
H	1.666917	-2.648659	0.174697
C	4.807804	-0.403394	0.397988
H	3.550363	1.191611	-0.285879
C	4.883564	-1.749145	0.742651
H	3.805828	-3.600952	0.930926
H	5.688002	0.224945	0.464597
H	5.823866	-2.171105	1.077370

H	-1.472720	-1.501213	1.591259
C	-0.619775	-0.870042	1.317658
O	-0.431476	-0.847698	0.000737
O	0.058276	-0.275972	2.110558

IM5

Symbol	X	Y	Z
Si	-0.847435	0.034882	0.207066
H	-1.567484	0.482655	1.471505
C	-0.390831	1.830813	-0.269770
C	-1.109752	2.857698	0.357950
C	0.616888	2.221433	-1.165210
C	-0.863522	4.201958	0.090534
H	-1.876593	2.598789	1.081364
C	0.893291	3.562094	-1.417862
H	1.207563	1.474232	-1.682420
C	0.146297	4.558794	-0.796619
H	-1.449951	4.968972	0.583564
H	1.687813	3.828502	-2.105773
H	0.352971	5.603235	-0.999610
C	-2.356755	-0.909039	-0.456109
C	-2.293653	-2.173451	-1.054549
C	-3.624077	-0.348486	-0.258400
C	-3.447288	-2.848379	-1.443405
H	-1.327924	-2.642346	-1.215833
C	-4.781998	-0.998779	-0.676990
H	-3.709067	0.615582	0.236698
C	-4.695398	-2.256978	-1.265792
H	-3.373492	-3.833603	-1.890090
H	-5.750146	-0.532959	-0.531394
H	-5.594144	-2.776064	-1.578366
N	3.757804	-0.900383	0.178910
C	2.489193	-0.427114	0.821239
H	2.735315	-0.052661	1.817134
H	2.111927	0.408091	0.230935
C	1.379269	-1.465600	0.954963
O	0.234959	-0.889023	1.259804
O	1.547565	-2.654216	0.882108
C	4.446831	-1.930120	1.023774
H	3.801096	-2.797318	1.108134
H	5.384796	-2.188732	0.537468
H	4.638144	-1.492865	2.001869
C	4.661571	0.286341	0.040032
H	5.590287	-0.044041	-0.419659

H	4.170180	1.027541	-0.587550
H	4.853888	0.694312	1.030010
C	3.479729	-1.455113	-1.185978
H	2.848454	-2.332381	-1.084427
H	2.971545	-0.687355	-1.765907
H	4.432452	-1.712177	-1.644077
H	0.748570	-1.215943	-3.021554
C	0.033571	-0.615065	-2.431510
O	0.276427	-0.684587	-1.153264
O	-0.847377	0.017206	-2.970487
C	0.112184	0.730154	3.490158
O	-0.543090	0.011913	4.112009
O	0.789118	1.467256	2.910742

TS4

Symbol	X	Y	Z
Si	-0.800255	-0.269202	0.428471
H	-1.919534	-1.428755	0.576092
C	-2.147330	0.985850	0.062449
C	-3.305951	0.561769	-0.600492
C	-2.057403	2.330813	0.439579
C	-4.331020	1.454364	-0.900394
H	-3.409115	-0.483752	-0.878377
C	-3.091378	3.221654	0.168855
H	-1.169803	2.687478	0.951411
C	-4.226570	2.786191	-0.509840
H	-5.213751	1.109761	-1.426437
H	-3.009652	4.256720	0.480029
H	-5.027890	3.481847	-0.730487
C	-0.014186	-1.231414	-0.996716
C	0.741579	-2.397609	-0.805021
C	-0.258848	-0.816109	-2.313093
C	1.252736	-3.106717	-1.887947
H	0.937900	-2.751960	0.200530
C	0.243670	-1.531053	-3.398354
H	-0.837940	0.082623	-2.494854
C	1.006018	-2.675067	-3.188638
H	1.841345	-4.000757	-1.715846
H	0.040932	-1.190758	-4.407500
H	1.401228	-3.229736	-4.031749
N	3.464803	1.347587	0.541462
C	2.491914	2.224461	-0.197958
H	2.425997	3.169487	0.344405
H	2.911188	2.414149	-1.183996

C	0.452723	-1.104420	2.715468	C	-3.025284	-3.759799	-0.584118
O	-0.569141	-0.525591	2.132313	H	-2.346853	-2.365647	-2.064405
O	1.454292	-1.489726	2.160672	C	-3.099903	-4.063016	0.772055
C	3.189226	1.352791	2.014980	H	-2.565171	-3.441391	2.761331
H	2.161435	1.045513	2.170143	H	-3.479777	-4.420245	-1.313646
H	3.874958	0.652531	2.487715	H	-3.612880	-4.958502	1.102514
H	3.359256	2.360967	2.388447	N	-5.393573	0.174951	0.236541
C	4.836753	1.901853	0.307371	C	-4.024999	0.655712	-0.153875
H	5.543254	1.334676	0.909619	H	-4.021178	1.745022	-0.072013
H	5.075811	1.801967	-0.749401	H	-3.330915	0.263488	0.588223
H	4.845401	2.949804	0.600659	C	-3.561357	0.274521	-1.567562
C	3.413670	-0.058558	0.017359	O	-2.284904	0.373270	-1.751066
H	2.497323	-0.529411	0.362969	O	-4.356081	-0.036656	-2.431599
H	3.456418	-0.020070	-1.070666	C	-6.467088	0.848079	-0.564909
H	4.278659	-0.590902	0.407951	H	-6.330011	0.590305	-1.608881
H	0.299972	-1.198879	3.797903	H	-7.428823	0.497933	-0.195832
C	1.079240	1.669123	-0.408956	H	-6.377348	1.922637	-0.416580
O	0.620786	0.926619	0.552899	C	-5.591415	0.518335	1.681583
O	0.498463	1.992070	-1.419244	H	-6.589332	0.200838	1.976151
C	-2.117587	-2.985505	0.690914	H	-4.839476	-0.004480	2.269654
O	-1.408687	-3.313494	1.578938	H	-5.486356	1.594490	1.802640
O	-2.903957	-3.206755	-0.163682	C	-5.486051	-1.313735	0.082971
				H	-5.401524	-1.559462	-0.971096
				H	-4.670950	-1.766204	0.648047

TS4a

Symbol	X	Y	Z				
Si	-0.825767	-0.196955	-0.679541	H	-6.447034	-1.635424	0.479319
H	-0.033002	-0.305032	-1.923620	Si	3.333336	-0.699018	-1.086002
H	0.487010	-0.770114	0.163038	H	3.485604	-0.976448	-2.532793
C	-0.812479	1.336859	0.426463	C	2.703220	1.052590	-0.897642
C	-1.367522	2.558717	0.021380	C	2.152324	1.714465	-2.003894
C	-0.234826	1.272932	1.702767	C	2.796308	1.750734	0.312606
C	-1.370621	3.666381	0.863929	C	1.695773	3.024602	-1.903162
H	-1.800831	2.646927	-0.969438	H	2.073550	1.199126	-2.956595
C	-0.260880	2.370131	2.560112	C	2.346390	3.062973	0.416536
H	0.273687	0.367347	2.018393	H	3.203158	1.250198	1.184653
C	-0.829601	3.569055	2.142821	C	1.792694	3.699444	-0.689509
H	-1.796786	4.603572	0.523802	H	1.265468	3.517596	-2.767474
H	0.180371	2.294171	3.547642	H	2.411114	3.584087	1.364673
H	-0.841630	4.426856	2.805674	H	1.430568	4.717654	-0.603877
C	-1.765759	-1.735796	-0.085566	C	5.022953	-0.925867	-0.304316
C	-1.839086	-2.068470	1.274281	C	5.229298	-1.104828	1.071889
C	-2.375365	-2.600882	-1.004614	C	6.146967	-0.877447	-1.140981
C	-2.510307	-3.210780	1.703719	C	6.516059	-1.225513	1.588265
H	-1.363680	-1.426241	2.011335	H	4.368619	-1.153548	1.729631
				C	7.435154	-0.993651	-0.625819

H	6.018902	-0.751280	-2.212144	H	3.842216	1.194207	0.534203
C	7.620535	-1.168096	0.741961	H	5.415818	0.727673	-0.168005
H	6.658757	-1.365711	2.653736	H	3.901506	0.561978	-1.134864
H	8.290575	-0.954361	-1.290193	C	5.066798	-1.793356	-0.429547
H	8.621538	-1.262842	1.146654	H	6.099560	-1.506047	-0.246157
H	0.855302	-2.489540	0.796060	H	4.898250	-2.821360	-0.114455
C	1.538780	-1.641788	0.636852	H	4.817673	-1.670395	-1.481989
O	2.206216	-1.834969	-0.572643	C	4.571417	-0.965713	1.812129
O	2.127883	-1.078144	1.573045	H	3.910899	-0.324523	2.387007

IM6

Symbol	X	Y	Z
Si	-0.975054	-0.141405	0.669007
H	0.768312	-1.311687	-2.713440
C	-2.248259	-1.157762	-0.202356
C	-2.422767	-0.979851	-1.582787
C	-3.031485	-2.107476	0.464949
C	-3.365363	-1.735665	-2.273517
H	-1.804510	-0.269871	-2.126276
C	-3.976121	-2.857679	-0.226836
H	-2.907976	-2.268789	1.530457
C	-4.144460	-2.669523	-1.596019
H	-3.491988	-1.594765	-3.340598
H	-4.579460	-3.587014	0.299900
H	-4.882021	-3.253306	-2.134924
C	-0.950331	1.660709	0.245293
C	0.094403	2.191348	-0.524645
C	-2.000995	2.507561	0.633245
C	0.095402	3.537183	-0.878108
H	0.900684	1.559766	-0.882467
C	-1.993625	3.852801	0.280484
H	-2.825695	2.116330	1.215830
C	-0.943067	4.369061	-0.472884
H	0.905561	3.932110	-1.479353
H	-2.808272	4.496167	0.591788
H	-0.937876	5.417478	-0.748738
N	4.177630	-0.889729	0.369507
C	2.774486	-1.367665	0.151913
H	2.603124	-1.388071	-0.925978
H	2.681934	-2.366976	0.580053
C	1.702503	-0.478268	0.742552
O	0.517459	-0.841925	0.262851
O	1.870316	0.411204	1.532590
C	4.349089	0.514572	-0.143311

H	3.842216	1.194207	0.534203
H	5.415818	0.727673	-0.168005
H	3.901506	0.561978	-1.134864
C	5.066798	-1.793356	-0.429547
H	6.099560	-1.506047	-0.246157
H	4.898250	-2.821360	-0.114455
H	4.817673	-1.670395	-1.481989
C	4.571417	-0.965713	1.812129
H	3.910899	-0.324523	2.387007
H	4.487957	-2.000420	2.140913
H	5.602108	-0.626596	1.896025
H	-1.869047	-0.452020	4.165301
C	-2.065982	-0.164417	3.127719
O	-1.028654	-0.446868	2.339065
O	-3.087904	0.332840	2.745042
C	0.986168	-0.212556	-2.742541
O	2.114637	0.126705	-2.299726
O	0.089137	0.520991	-3.187135

TS5

Symbol	X	Y	Z
Si	0.956094	-0.048187	0.750560
H	-0.225167	1.896300	-2.231353
C	1.346655	1.684170	0.217383
C	2.439268	1.961660	-0.610535
C	0.515380	2.739679	0.610811
C	2.683592	3.259596	-1.050482
H	3.105189	1.160354	-0.912353
C	0.764257	4.038841	0.180932
H	-0.343202	2.543406	1.245597
C	1.846054	4.298860	-0.656063
H	3.528698	3.460196	-1.698533
H	0.111316	4.845927	0.491701
H	2.036561	5.309145	-0.998745
C	1.521287	-1.496031	-0.266564
C	1.670407	-1.424999	-1.656393
C	1.893090	-2.678198	0.386775
C	2.180041	-2.504115	-2.371217
H	1.362657	-0.525891	-2.175326
C	2.382767	-3.765947	-0.328550
H	1.797747	-2.755739	1.465219
C	2.531486	-3.677330	-1.709359
H	2.296405	-2.432688	-3.446279
H	2.653779	-4.677433	0.190905

H	2.920547	-4.520392	-2.268356	C	1.735933	-1.515797	-1.802803
N	-4.047255	-0.418416	0.211508	C	1.896133	-2.643317	0.308541
C	-2.829133	0.163969	0.862436	C	2.329849	-2.605090	-2.433774
H	-2.524979	1.016780	0.256006	H	1.441659	-0.659417	-2.399691
H	-3.110574	0.499514	1.862897	C	2.458473	-3.749529	-0.320654
C	-1.645473	-0.771773	0.974149	H	1.748842	-2.663850	1.383216
O	-0.587385	-0.099014	1.433619	C	2.684392	-3.729125	-1.693928
O	-1.652167	-1.951744	0.765936	H	2.505754	-2.580872	-3.502988
C	-3.731979	-0.970587	-1.151684	H	2.727877	-4.623572	0.260967
H	-3.084181	-1.832822	-1.036986	H	3.134087	-4.584411	-2.184742
H	-4.677531	-1.254962	-1.609627	N	-4.123640	-0.410265	0.252424
H	-3.235530	-0.180471	-1.711280	C	-2.871432	0.161291	0.845573
C	-5.014573	0.712101	0.032177	H	-2.517118	0.935099	0.165633
H	-5.927696	0.314016	-0.405009	H	-3.127015	0.618619	1.803380
H	-5.222795	1.154543	1.004435	C	-1.737105	-0.826075	1.056163
H	-4.550146	1.438542	-0.633315	O	-0.631355	-0.200088	1.432448
C	-4.665653	-1.477741	1.067107	O	-1.834147	-2.018041	0.947022
H	-3.949287	-2.284679	1.188727	C	-3.834331	-1.122715	-1.040890
H	-4.922325	-1.039988	2.030185	H	-3.300408	-2.040369	-0.819804
H	-5.563215	-1.835370	0.566743	H	-4.789129	-1.339266	-1.515736
H	3.404437	-0.361137	3.417246	H	-3.228686	-0.456933	-1.655686
C	3.081583	-0.219051	2.378694	C	-5.030609	0.744286	-0.047683
O	1.762813	-0.272248	2.266003	H	-5.972012	0.350671	-0.424049
O	3.842812	-0.040972	1.464665	H	-5.195605	1.310244	0.866872
C	-1.046186	1.321820	-1.745159	H	-4.549331	1.364830	-0.801808
O	-2.188280	1.813578	-1.788655	C	-4.800339	-1.334629	1.215993
O	-0.713811	0.235847	-1.198399	H	-4.124659	-2.154506	1.439188

IM7

Symbol	X	Y	Z
Si	0.772154	-0.013767	0.439739
H	0.037531	1.739664	-2.096527
C	1.291827	1.770096	0.182217
C	2.403941	2.124954	-0.589143
C	0.499626	2.795249	0.714202
C	2.708124	3.462398	-0.830888
H	3.044055	1.350257	-0.997059
C	0.806666	4.133546	0.483636
H	-0.370667	2.549219	1.316475
C	1.910281	4.469336	-0.295047
H	3.570494	3.718963	-1.435520
H	0.183584	4.912461	0.907907
H	2.148247	5.509966	-0.481850
C	1.517124	-1.508876	-0.419958

C	1.735933	-1.515797	-1.802803
C	1.896133	-2.643317	0.308541
C	2.329849	-2.605090	-2.433774
H	1.441659	-0.659417	-2.399691
C	2.458473	-3.749529	-0.320654
H	1.748842	-2.663850	1.383216
C	2.684392	-3.729125	-1.693928
H	2.505754	-2.580872	-3.502988
H	2.727877	-4.623572	0.260967
H	3.134087	-4.584411	-2.184742
N	-4.123640	-0.410265	0.252424
C	-2.871432	0.161291	0.845573
H	-2.517118	0.935099	0.165633
H	-3.127015	0.618619	1.803380
C	-1.737105	-0.826075	1.056163
O	-0.631355	-0.200088	1.432448
O	-1.834147	-2.018041	0.947022
C	-3.834331	-1.122715	-1.040890
H	-3.300408	-2.040369	-0.819804
H	-4.789129	-1.339266	-1.515736
H	-3.228686	-0.456933	-1.655686
C	-5.030609	0.744286	-0.047683
H	-5.972012	0.350671	-0.424049
H	-5.195605	1.310244	0.866872
H	-4.549331	1.364830	-0.801808
C	-4.800339	-1.334629	1.215993
H	-4.124659	-2.154506	1.439188
H	-5.042114	-0.775022	2.117827
H	-5.709937	-1.704702	0.747665
H	3.359559	-0.272906	3.101399
C	3.005086	-0.160113	2.064817
O	1.703086	-0.219446	1.986627
O	3.773913	-0.007108	1.142505
C	-0.796556	1.071508	-1.826258
O	-1.900981	1.234253	-2.316051
O	-0.514725	0.133818	-0.977703

TS6

Symbol	X	Y	Z
Si	-0.673758	-0.304289	-0.471663
H	0.859426	-1.545292	2.840721
C	-0.447040	1.534852	-0.152707
C	-0.964020	2.198569	0.963868
C	0.238502	2.294343	-1.109339

C	-0.802188	3.571175	1.121269	O	0.298863	-0.908189	1.039594
H	-1.495619	1.641960	1.726390				
C	0.427416	3.664261	-0.945982				
H	0.622277	1.810249	-2.003327				
C	-0.097047	4.306008	0.171561				
H	-1.220969	4.068340	1.988737				
H	0.972047	4.229570	-1.693448				
H	0.037670	5.373789	0.299854				
C	-2.132839	-1.341308	0.125855				
C	-2.553289	-1.302469	1.461601				
C	-2.839314	-2.169344	-0.754510				
C	-3.648807	-2.040951	1.897435				
H	-2.027070	-0.683466	2.181625				
C	-3.913980	-2.939334	-0.317564				
H	-2.547037	-2.215561	-1.797913				
C	-4.327448	-2.870017	1.008700				
H	-3.965880	-1.977808	2.931962				
H	-4.432843	-3.586838	-1.015051				
H	-5.172035	-3.458036	1.348504				
N	4.003313	-0.402037	0.043014				
C	2.678964	-0.137750	-0.606453				
H	2.117518	0.529106	0.050348				
H	2.867219	0.388411	-1.545041				
C	1.827206	-1.365196	-0.915941				
O	0.631914	-1.020366	-1.359690				
O	2.221207	-2.497420	-0.857487				
C	3.810956	-1.082819	1.364369				
H	3.310140	-2.032371	1.199205				
H	4.791271	-1.239661	1.809165				
H	3.213952	-0.429606	1.999364				
C	4.659071	0.926029	0.278511				
H	5.611802	0.752792	0.773585				
H	4.814376	1.412950	-0.681929				
H	4.009583	1.529107	0.909407				
C	4.896560	-1.224940	-0.838695				
H	4.460075	-2.210377	-0.955770				
H	4.979985	-0.722869	-1.800627				
H	5.871780	-1.285626	-0.360695				
H	-2.710870	0.662448	-3.435243				
C	-2.483546	0.603056	-2.358806				
O	-1.374540	-0.047637	-2.132982				
O	-3.210417	1.099519	-1.528228				
C	0.579256	-0.636628	2.278520				
O	0.587429	0.449513	2.816585				

IM8

Symbol	X	Y	Z
Si	-0.699333	0.174743	-0.356355
H	1.281747	0.257851	2.928381
C	-0.749434	2.035931	-0.090034
C	-1.764328	2.693591	0.612885
C	0.283269	2.809748	-0.633235
C	-1.745848	4.075589	0.771617
H	-2.580582	2.119540	1.034894
C	0.307005	4.194320	-0.477147
H	1.080070	2.331730	-1.196183
C	-0.708838	4.830316	0.228261
H	-2.541573	4.566241	1.320764
H	1.115840	4.773377	-0.908197
H	-0.695476	5.907074	0.351943
C	-1.844507	-1.203316	0.216829
C	-2.473961	-1.229788	1.466938
C	-2.072283	-2.274752	-0.657523
C	-3.314804	-2.281666	1.822679
H	-2.306899	-0.420083	2.167072
C	-2.890556	-3.340433	-0.294810
H	-1.605449	-2.275414	-1.637323
C	-3.520335	-3.342907	0.946555
H	-3.806350	-2.274687	2.789049
H	-3.041758	-4.164563	-0.982723
H	-4.167370	-4.165688	1.228115
N	4.131901	-0.934712	-0.125534
C	2.931601	-0.232220	-0.681560
H	2.683526	0.590078	-0.008262
H	3.198737	0.179422	-1.656210
C	1.677253	-1.077297	-0.831352
O	0.681794	-0.328705	-1.267502
O	1.611335	-2.259365	-0.628058
C	3.840428	-1.466755	1.246424
H	3.061481	-2.218315	1.170479
H	4.757233	-1.898851	1.641536
H	3.514951	-0.636598	1.869996
C	5.237325	0.073082	-0.027525
H	6.113842	-0.421265	0.384562
H	5.451377	0.453563	-1.024031
H	4.916559	0.880964	0.626577
C	4.577599	-2.049004	-1.025622

H	3.797739	-2.802144	-1.058959
H	4.760746	-1.635869	-2.015660
H	5.496949	-2.461867	-0.615914
H	-3.040863	0.711235	-3.207271
C	-2.738945	0.676622	-2.148062
O	-1.500150	0.302684	-2.003253
O	-3.512064	0.962240	-1.258999
C	0.353190	0.395637	2.347581
O	-0.626534	0.901389	2.853032
O	0.470763	-0.040061	1.129791

IM9

Symbol	X	Y	Z
Si	0.065744	0.346687	0.314068
H	1.138878	1.520798	3.555471
C	-1.673493	-0.244948	0.125018
C	-2.672641	0.175573	1.012948
C	-2.023753	-1.093626	-0.933731
C	-3.987078	-0.245487	0.848074
H	-2.417235	0.836036	1.833959
C	-3.339428	-1.513224	-1.100145
H	-1.265710	-1.434664	-1.632265
C	-4.319973	-1.089537	-0.208191
H	-4.751653	0.083617	1.541487
H	-3.598326	-2.170787	-1.921140
H	-5.344686	-1.418191	-0.335520
C	1.364209	-0.845875	-0.235995
C	2.576132	-0.387988	-0.769863
C	1.168013	-2.225883	-0.091147
C	3.564253	-1.287698	-1.152495
H	2.743706	0.677138	-0.883500
C	2.157539	-3.126202	-0.471925
H	0.235724	-2.603807	0.317421
C	3.354698	-2.656196	-1.003461
H	4.496863	-0.923389	-1.566292
H	1.994159	-4.190882	-0.356998
H	4.125053	-3.357019	-1.302899
H	0.107292	3.686717	-1.056616
C	-0.219321	2.920991	-0.345432
O	0.367744	1.746400	-0.592573
O	-1.000594	3.107995	0.543600
C	1.244656	1.391358	2.473408
O	2.171061	1.792796	1.828169
O	0.204263	0.728839	1.959497

IM10

Symbol	X	Y	Z
Si	1.090615	0.293121	-1.034872
H	-1.682088	-1.431984	-2.579891
C	2.485116	-0.752202	-0.399794
C	2.406441	-2.149305	-0.479670
C	3.627607	-0.178584	0.177459
C	3.433662	-2.950411	0.008525
H	1.532355	-2.611873	-0.924189
C	4.654356	-0.979226	0.667036
H	3.717893	0.900376	0.236619
C	4.556962	-2.365411	0.585233
H	3.356705	-4.029021	-0.059989
H	5.529930	-0.521716	1.111960
H	5.356549	-2.988477	0.968489
C	0.475667	1.584358	0.142872
C	-0.427980	2.580751	-0.262610
C	0.993862	1.640792	1.440759
C	-0.804378	3.591814	0.611159
H	-0.849135	2.551132	-1.259874
C	0.625309	2.662153	2.312547
H	1.681643	0.877196	1.785316
C	-0.273813	3.636396	1.899951
H	-1.508358	4.349562	0.287924
H	1.032957	2.686179	3.316492
H	-0.564865	4.429852	2.578628
H	2.487344	2.449344	-3.583381
C	2.414853	2.036154	-2.571328
O	1.503744	1.070586	-2.502238
O	3.079436	2.410433	-1.643783
C	-1.184822	-0.533248	-2.208128
O	-1.599849	0.582163	-2.354214
O	-0.020025	-0.830752	-1.617173
N	-2.322757	-1.883889	-0.082965
H	-3.267826	-1.555290	-0.311580
C	-1.969975	-3.177019	-0.617217
H	-1.992813	-3.967511	0.144140
H	-2.688505	-3.429577	-1.397620
H	-0.967952	-3.168114	-1.062562
C	-1.712677	-1.389251	1.040639
C	-0.529204	-1.944971	1.557225
C	-2.277256	-0.277586	1.704666
C	0.031375	-1.440691	2.730233
H	-0.058934	-2.782814	1.057549

C	-1.707947	0.202911	2.869586
H	-3.168680	0.173081	1.276426
C	-0.555150	-0.379899	3.405857
H	0.941332	-1.892377	3.112549
H	-2.161563	1.053098	3.368255
H	-0.114096	0.008021	4.316184
H	-6.081722	0.208633	-1.742893
C	-5.241246	-0.094400	-1.067197
O	-4.829808	0.771825	-0.277636
O	-4.841507	-1.274624	-1.212006

TS7

Symbol	X	Y	Z
Si	-1.091116	-0.181771	0.934268
H	1.577929	-2.178976	2.000721
C	-2.593984	-0.926656	0.112454
C	-2.544895	-2.241293	-0.370775
C	-3.786864	-0.205563	-0.049910
C	-3.647490	-2.818340	-0.995271
H	-1.633695	-2.816838	-0.250505
C	-4.890543	-0.780558	-0.671449
H	-3.851573	0.812067	0.319495
C	-4.821760	-2.087887	-1.146136
H	-3.590117	-3.836484	-1.362251
H	-5.804372	-0.209336	-0.786357
H	-5.681425	-2.535237	-1.631495
C	-0.644946	1.465877	0.181922
C	0.234982	2.356197	0.816315
C	-1.277293	1.886926	-0.992431
C	0.467943	3.621143	0.292913
H	0.755605	2.034157	1.709802
C	-1.045016	3.155881	-1.520332
H	-1.957728	1.219980	-1.511124
C	-0.173924	4.024962	-0.877362
H	1.152996	4.295198	0.794547
H	-1.542089	3.459199	-2.434712
H	0.008352	5.013212	-1.284174
H	-2.232155	1.041940	4.164747
C	-2.257530	1.004142	3.068893
O	-1.419931	0.092474	2.598643
O	-2.965832	1.707440	2.398811
C	1.308108	-1.262723	1.447708
O	1.618376	-0.135516	1.870934
O	-0.023478	-1.441929	0.980457

N	2.185484	-1.659481	-0.014337
H	3.185631	-1.470672	0.277136
C	2.065549	-3.099581	-0.278789
H	2.488594	-3.348443	-1.252513
H	2.618505	-3.627729	0.496991
H	1.017759	-3.398096	-0.240760
C	1.808175	-0.785787	-1.082178
C	0.813244	-1.136823	-1.994674
C	2.423665	0.462540	-1.150507
C	0.457839	-0.242145	-2.998095
H	0.324635	-2.101101	-1.932815
C	2.050980	1.351712	-2.152558

H	3.201019	0.705637	-0.432308
C	1.075255	1.001969	-3.080441
H	-0.310734	-0.517988	-3.710780
H	2.525446	2.324646	-2.206443
H	0.787241	1.700840	-3.856812
H	6.511054	-0.833775	1.269770
C	5.484897	-0.602916	0.894114
O	5.212164	0.589065	0.703799
O	4.752201	-1.613724	0.717352

IM11

Symbol	X	Y	Z
Si	1.082042	-0.190487	-0.933953
H	-1.593739	-2.163653	-1.995475
C	2.587027	-0.930366	-0.108898
C	2.540206	-2.243670	0.378677
C	3.778674	-0.206922	0.053314
C	3.642989	-2.817063	1.006262
H	1.628775	-2.819528	0.261711
C	4.882535	-0.778171	0.677802
H	3.841617	0.809698	-0.318725
C	4.815908	-2.084128	1.156122
H	3.586663	-3.833887	1.376985
H	5.795151	-0.204702	0.792243
H	5.675625	-2.528666	1.644161
C	0.651288	1.465066	-0.188047
C	-0.213634	2.363330	-0.831351
C	1.279771	1.882624	0.989623
C	-0.434037	3.633499	-0.315069
H	-0.733984	2.043455	-1.725676
C	1.058992	3.156392	1.511060
H	1.947049	1.209336	1.516926

C	0.204258	4.034414	0.857983	C	-4.970224	-1.720720	-1.182392
H	-1.107016	4.313857	-0.824615	H	-3.829219	-3.376054	-1.941686
H	1.552671	3.455958	2.428542	H	-5.837605	0.029577	-0.283013
H	0.032290	5.026510	1.259451	H	-5.892666	-2.032127	-1.658985
H	2.227132	0.999430	-4.176890	C	-0.618654	1.376024	0.270810
C	2.254384	0.970820	-3.080646	C	0.239361	2.247239	0.957987
O	1.409896	0.071228	-2.601505	C	-1.303260	1.875002	-0.841774
O	2.969812	1.674934	-2.418849	C	0.392679	3.567325	0.556460
C	-1.319851	-1.256683	-1.429297	H	0.803061	1.868543	1.801212
O	-1.610302	-0.118378	-1.847915	C	-1.140153	3.195684	-1.259516
O	0.016798	-1.452520	-0.965860	H	-1.970870	1.228483	-1.400929
N	-2.185716	-1.650125	0.016290	C	-0.297129	4.045913	-0.557332
H	-3.197574	-1.467868	-0.262754	H	1.056481	4.225447	1.105948
C	-2.059448	-3.090635	0.283030	H	-1.672897	3.554904	-2.132851
H	-2.494825	-3.339460	1.250974	H	-0.172783	5.075306	-0.874263
H	-2.599190	-3.621629	-0.500212	H	-2.001473	0.227336	4.324202
H	-1.009687	-3.382980	0.258773	C	-2.012442	0.472359	3.254279
C	-1.812318	-0.775592	1.088559	O	-1.293865	-0.392104	2.562534
C	-0.815912	-1.121030	2.001479	O	-2.613059	1.412889	2.803975
C	-2.437482	0.467102	1.157108	C	1.253529	-1.500036	1.075614
C	-0.468689	-0.223874	3.005766	O	1.317573	-0.337396	1.610960
H	-0.318151	-2.080245	1.937813	O	-0.048992	-1.749786	0.585170
C	-2.074469	1.357862	2.161264	N	2.193377	-1.627709	-0.244092
H	-3.215772	0.703655	0.438613	H	3.184612	-1.451617	0.147425
C	-1.096849	1.014899	3.089323	C	2.192494	-3.020012	-0.734329
H	0.301551	-0.494072	3.718743	H	2.750373	-3.081715	-1.667580
H	-2.558129	2.326191	2.216102	H	2.680554	-3.635755	0.019893
H	-0.815937	1.714347	3.867773	H	1.169736	-3.363464	-0.879855
H	-6.485528	-0.855044	-1.309001	C	1.856068	-0.622382	-1.225119
C	-5.470568	-0.610202	-0.913882	C	0.909072	-0.869528	-2.215997
O	-5.215926	0.583156	-0.715856	C	2.463601	0.622964	-1.109968
O	-4.728307	-1.613301	-0.724419	C	0.586217	0.140674	-3.115202
				H	0.426883	-1.835818	-2.290047

TS8

Symbol	X	Y	Z				
Si	-0.957295	-0.367237	0.874012	H	3.198200	0.781638	-0.326431
H	1.601306	-2.380444	1.643018	C	1.190580	1.389859	-3.012291
C	-2.572217	-0.909521	0.057408	H	-0.148058	-0.047999	-3.889411
C	-2.628830	-2.071658	-0.723878	H	2.586878	2.603802	-1.919888
C	-3.752274	-0.162061	0.197799	H	0.925309	2.178929	-3.705947
C	-3.812024	-2.474100	-1.340393	H	6.215425	-0.921017	1.697798
H	-1.733029	-2.670270	-0.846375	C	5.273916	-0.647656	1.167336
C	-4.938296	-0.562541	-0.409279	O	5.029444	0.554349	1.026454
H	-3.739918	0.746602	0.790605	O	4.587976	-1.637310	0.780143

IM12

Symbol	X	Y	Z
Si	-0.768077	-0.509674	0.833342
H	1.593053	-2.556415	1.344293
C	-2.476293	-0.899961	0.033721
C	-2.626437	-1.782878	-1.043228
C	-3.634840	-0.251990	0.490760
C	-3.867434	-2.009865	-1.639454
H	-1.755766	-2.309082	-1.418935
C	-4.879458	-0.476762	-0.089871
H	-3.560593	0.455283	1.312283
C	-4.999323	-1.358114	-1.162585
H	-3.949961	-2.698274	-2.473630
H	-5.756120	0.037133	0.289364
H	-5.966137	-1.533065	-1.620894
C	-0.608407	1.319583	0.335996
C	0.279514	2.163052	1.022428
C	-1.352768	1.883133	-0.704591
C	0.399121	3.509272	0.702163
H	0.894285	1.747403	1.812455
C	-1.221704	3.228652	-1.050739
H	-2.044970	1.265120	-1.266386
C	-0.351938	4.047304	-0.342624
H	1.084092	4.140118	1.258200
H	-1.801682	3.633907	-1.872783
H	-0.253923	5.095611	-0.602079
H	-1.883729	-0.470716	4.355648
C	-1.785115	0.028464	3.380910
O	-1.261362	-0.777502	2.489795
O	-2.132845	1.170127	3.204430
C	1.191068	-1.732905	0.739871
O	1.033465	-0.557572	1.371156
O	-0.063779	-1.996833	0.224116
N	2.206147	-1.610342	-0.417726
H	3.170670	-1.389770	0.099845
C	2.400048	-2.936668	-1.048682
H	3.045197	-2.826377	-1.917739
H	2.881206	-3.584213	-0.316970
H	1.438285	-3.356689	-1.337529
C	1.853427	-0.543121	-1.342120
C	0.924667	-0.757070	-2.356422
C	2.432461	0.703954	-1.147598
C	0.583160	0.297413	-3.195653
H	0.468419	-1.729153	-2.489338

Symbol	X	Y	Z
C	2.079410	1.751726	-1.991458
H	3.141264	0.842480	-0.336427
C	1.157985	1.551605	-3.013156
H	-0.141057	0.138542	-3.985636
H	2.517328	2.730868	-1.839134
H	0.878655	2.374342	-3.660577
H	5.796789	-0.783232	2.088511
C	4.941877	-0.519710	1.428056
O	4.632010	0.667514	1.327977
O	4.402589	-1.519070	0.857577

TS9

Symbol	X	Y	Z
Si	0.769909	-0.514673	-0.830890
H	-1.584708	-2.538971	-1.364540
C	2.474296	-0.913527	-0.022885
C	2.608187	-1.766679	1.080034
C	3.643617	-0.296063	-0.493821
C	3.843775	-1.993738	1.687447
H	1.728350	-2.269421	1.467492
C	4.883122	-0.521158	0.097870
H	3.581998	0.389752	-1.334542
C	4.986807	-1.372527	1.196156
H	3.913594	-2.658303	2.541968
H	5.768397	-0.030973	-0.292745
H	5.949402	-1.547688	1.663236
C	0.626829	1.314993	-0.326620
C	-0.246110	2.168340	-1.020401
C	1.362532	1.868199	0.725175
C	-0.357810	3.514380	-0.697541
H	-0.856332	1.759417	-1.817469
C	1.237512	3.213637	1.075456
H	2.044467	1.242730	1.291555
C	0.384306	4.042344	0.359197
H	-1.030138	4.153329	-1.259904
H	1.810043	3.611142	1.906513
H	0.291940	5.090573	0.621188
H	1.933696	-0.490944	-4.342217
C	1.815274	0.018778	-3.374914
O	1.284914	-0.781194	-2.485069
O	2.153214	1.165543	-3.207362
C	-1.201146	-1.717328	-0.744254
O	-1.014280	-0.543667	-1.384562
O	0.055463	-1.989931	-0.219280

N	-2.225125	-1.591205	0.377321	C	-0.485806	4.055463	-0.140608
H	-3.292378	-1.378121	-0.203163	H	0.855092	4.135499	1.542045
C	-2.426898	-2.914524	1.004956	H	-1.832230	3.651723	-1.764044
H	-3.097010	-2.806702	1.855997	H	-0.411986	5.115903	-0.355198
H	-2.888457	-3.569104	0.265660	H	-1.872914	-0.792201	4.329053
H	-1.476803	-3.341954	1.324273	C	-1.797159	-0.228166	3.387369
C	-1.880373	-0.534374	1.311142	O	-1.251799	-0.953515	2.445726
C	-1.015472	-0.766875	2.378348	O	-2.191243	0.909222	3.290248
C	-2.398492	0.734869	1.082845	C	1.249493	-1.713025	0.601223
C	-0.684306	0.280131	3.231628	O	1.026989	-0.578261	1.319422
H	-0.598075	-1.751768	2.542387	O	-0.029266	-1.988639	0.094851
C	-2.057973	1.776273	1.939268	N	2.241591	-1.512846	-0.493505
H	-3.048119	0.895421	0.229189	H	3.633379	-1.352874	0.310667
C	-1.203959	1.552503	3.013215	C	2.465392	-2.791072	-1.186022
H	-0.010567	0.100801	4.061136	H	3.140767	-2.632495	-2.026338
H	-2.448983	2.769650	1.754122	H	2.935909	-3.484486	-0.485992
H	-0.934163	2.369188	3.672431	H	1.533719	-3.237056	-1.544117
H	-5.845199	-0.786092	-1.980166	C	1.873371	-0.423622	-1.365101
C	-4.936794	-0.506499	-1.411892	C	1.063248	-0.613828	-2.484616
O	-4.569497	0.659832	-1.404938	C	2.315895	0.858044	-1.044194
O	-4.391734	-1.504964	-0.817994	C	0.718630	0.470037	-3.287433
				H	0.697831	-1.602963	-2.729913
				C	1.960521	1.938029	-1.843007

IM13

Symbol	X	Y	Z
Si	-0.750585	-0.572961	0.804823
H	1.635299	-2.559018	1.188287
C	-2.464366	-0.947475	-0.010515
C	-2.598684	-1.749511	-1.151543
C	-3.636355	-0.358775	0.490240
C	-3.834508	-1.953357	-1.766992
H	-1.716223	-2.227039	-1.563856
C	-4.876420	-0.561070	-0.108916
H	-3.575845	0.285367	1.363346
C	-4.979494	-1.359645	-1.246344
H	-3.903169	-2.577167	-2.651974
H	-5.762870	-0.093417	0.306315
H	-5.942121	-1.515681	-1.720224
C	-0.675931	1.294058	0.419287
C	0.141772	2.141497	1.184642
C	-1.384182	1.872587	-0.637029
C	0.226658	3.502646	0.924537
H	0.729509	1.717906	1.991689
C	-1.283868	3.235051	-0.925912
H	-2.024457	1.253186	-1.256517

C	-0.485806	4.055463	-0.140608
H	0.855092	4.135499	1.542045
H	-1.832230	3.651723	-1.764044
H	-0.411986	5.115903	-0.355198
H	-1.872914	-0.792201	4.329053
C	-1.797159	-0.228166	3.387369
O	-1.251799	-0.953515	2.445726
O	-2.191243	0.909222	3.290248
C	1.249493	-1.713025	0.601223
O	1.026989	-0.578261	1.319422
O	-0.029266	-1.988639	0.094851
N	2.241591	-1.512846	-0.493505
H	3.633379	-1.352874	0.310667
C	2.465392	-2.791072	-1.186022
H	3.140767	-2.632495	-2.026338
H	2.935909	-3.484486	-0.485992
H	1.533719	-3.237056	-1.544117
C	1.873371	-0.423622	-1.365101
C	1.063248	-0.613828	-2.484616
C	2.315895	0.858044	-1.044194
C	0.718630	0.470037	-3.287433
H	0.697831	-1.602963	-2.729913
C	1.960521	1.938029	-1.843007

TS10

Symbol	X	Y	Z
Si	-1.017331	-0.394796	0.842742
H	1.586215	-2.373860	1.578973
C	-2.611114	-0.930010	-0.014436
C	-2.670731	-2.149796	-0.702356
C	-3.767825	-0.135081	0.004522
C	-3.837250	-2.564855	-1.341521
H	-1.787558	-2.778273	-0.734784
C	-4.936738	-0.546087	-0.628475
H	-3.750285	0.816812	0.524180

C	-4.973802	-1.763817	-1.303517
H	-3.858524	-3.512159	-1.868402
H	-5.818750	0.083612	-0.598515
H	-5.883335	-2.084121	-1.798795
C	-0.676236	1.371389	0.324191
C	0.077379	2.241329	1.125524
C	-1.238517	1.880601	-0.849104
C	0.247126	3.572703	0.773007
H	0.550332	1.849766	2.017886
C	-1.055263	3.213635	-1.218391
H	-1.825116	1.233714	-1.493274
C	-0.318784	4.063129	-0.404857
H	0.827861	4.231619	1.409026
H	-1.488730	3.582826	-2.141181
H	-0.180283	5.101660	-0.684128
H	-2.163904	0.108274	4.275151
C	-2.167214	0.352319	3.204596
O	-1.360680	-0.446052	2.532701
O	-2.833916	1.240156	2.739315
C	1.311744	-1.457850	1.017214
O	1.368987	-0.327845	1.637048
O	-0.048446	-1.697008	0.537305
N	2.202748	-1.560599	-0.233190
H	3.619451	-1.510284	0.379585
C	2.159254	-2.922346	-0.773669
H	2.786362	-2.986187	-1.664072
H	2.560085	-3.601843	-0.019127
H	1.142225	-3.240092	-1.019301
C	1.918787	-0.529770	-1.185782
C	1.179616	-0.763764	-2.347586
C	2.386298	0.760501	-0.922861
C	0.935638	0.273543	-3.244959
H	0.797315	-1.753373	-2.563406
C	2.127074	1.792182	-1.815179
H	2.951738	0.925625	-0.016545
C	1.406748	1.554162	-2.982791
H	0.367289	0.075545	-4.146784
H	2.486377	2.791094	-1.595248
H	1.206966	2.362814	-3.676337
H	6.229584	-1.132539	1.649254
C	5.293635	-0.780246	1.188844
O	5.042909	0.396751	1.072273
O	4.547288	-1.782317	0.807020

IM14

Symbol	X	Y	Z
Si	1.071922	-0.319523	-0.886482
H	-1.634701	-2.235767	-1.760046
C	2.608611	-0.974249	-0.031242
C	2.583267	-2.241349	0.567493
C	3.794956	-0.229873	0.053963
C	3.700954	-2.751032	1.223892
H	1.673915	-2.830171	0.514721
C	4.914567	-0.736546	0.706298
H	3.840129	0.754168	-0.399676
C	4.869070	-1.998849	1.293127
H	3.660163	-3.733027	1.681177
H	5.822558	-0.146809	0.759625
H	5.740472	-2.392814	1.803492
C	0.708784	1.408398	-0.274947
C	-0.055527	2.307707	-1.032489
C	1.273991	1.865901	0.918221
C	-0.234685	3.619407	-0.616302
H	-0.531596	1.951861	-1.938165
C	1.086324	3.180031	1.347192
H	1.868185	1.193951	1.528998
C	0.337502	4.059698	0.577975
H	-0.825710	4.301986	-1.216792
H	1.525541	3.510904	2.281677
H	0.194588	5.083703	0.904660
H	2.206754	0.537167	-4.247238
C	2.237720	0.632597	-3.154217
O	1.400368	-0.208842	-2.576206
O	2.954995	1.413073	-2.584543
C	-1.383092	-1.325765	-1.175960
O	-1.542302	-0.186524	-1.728499
O	0.015808	-1.564816	-0.754578
N	-2.198689	-1.549089	0.126304
H	-3.622683	-1.514102	-0.404183
C	-2.076241	-2.939979	0.570189
H	-2.656031	-3.089690	1.482441
H	-2.486890	-3.583897	-0.209795
H	-1.036791	-3.229939	0.745510
C	-1.894230	-0.574006	1.126329
C	-1.107207	-0.860618	2.244697
C	-2.391882	0.721180	0.956465
C	-0.845780	0.128278	3.190489
H	-0.702493	-1.854097	2.390778

C	-2.111964	1.705358	1.894636
H	-3.001821	0.922254	0.087358
C	-1.344242	1.413795	3.019437
H	-0.241640	-0.111194	4.058377
H	-2.494905	2.708784	1.746446
H	-1.129338	2.185335	3.749797
H	-6.313868	-1.145948	-1.520788
C	-5.372680	-0.794450	-1.069528
O	-5.171702	0.378166	-0.849869
O	-4.564568	-1.788495	-0.822064

IM15

Symbol	X	Y	Z
Si	-0.936121	-0.490359	-0.788108
H	1.045763	1.251006	-3.018610
C	-2.722820	-0.050800	-0.462575
C	-3.232430	1.182314	-0.891122
C	-3.579232	-0.915664	0.235417
C	-4.554769	1.538364	-0.638804
H	-2.583554	1.867124	-1.426216
C	-4.901071	-0.562934	0.487268
H	-3.206212	-1.874140	0.579251
C	-5.390799	0.665196	0.049599
H	-4.931662	2.496313	-0.978108
H	-5.549211	-1.244076	1.026225
H	-6.420172	0.940675	0.247065
C	-0.084162	-1.026441	0.781424
C	1.094269	-1.789314	0.758255
C	-0.659696	-0.730457	2.020734
C	1.667672	-2.243071	1.937910
H	1.590855	-1.995762	-0.182891
C	-0.084336	-1.185941	3.206514
H	-1.569017	-0.140181	2.069690
C	1.076738	-1.945855	3.165914
H	2.583685	-2.821863	1.899939
H	-0.542194	-0.940942	4.158059
H	1.527522	-2.299982	4.086133
H	-0.970996	-3.708073	-2.485311
C	-1.213051	-3.044393	-1.646387
O	-0.847746	-1.796714	-1.899544
O	-1.745565	-3.422247	-0.636720
C	0.983145	1.028587	-1.947269
O	1.642303	-0.113478	-1.595662
O	-0.395063	0.795035	-1.669359

N	1.434976	2.225858	-1.255730
H	2.667970	-0.052182	-1.637203
C	0.850866	3.420112	-1.859409
H	1.227748	4.305282	-1.346830
H	1.158949	3.469805	-2.905084
H	-0.246040	3.431958	-1.826539
C	1.339813	2.154101	0.166107
C	0.329323	2.804435	0.878606
C	2.298065	1.416678	0.869656
C	0.288214	2.732929	2.269874
H	-0.427475	3.373503	0.352973
C	2.239037	1.331484	2.253020

H	3.087493	0.927147	0.312145
C	1.238532	1.994115	2.961771
H	-0.497746	3.251245	2.807804
H	2.980115	0.744457	2.783290
H	1.201241	1.929664	4.043095
H	5.784383	-1.149420	-1.241856
C	4.670585	-1.150645	-1.280564
O	4.086694	-2.195858	-0.986538
O	4.162636	-0.043528	-1.635805

TS11

Symbol	X	Y	Z
Si	-1.328680	0.199974	-0.656761
H	0.701592	2.842841	-1.839281
C	-3.125070	0.357018	-0.107009
C	-3.619767	1.631572	0.199670
C	-3.997670	-0.733759	0.026951
C	-4.934597	1.816742	0.621185
H	-2.957235	2.485433	0.103841
C	-5.312390	-0.554998	0.447964
H	-3.642371	-1.731090	-0.208498
C	-5.783481	0.721591	0.745999
H	-5.295645	2.812506	0.852735
H	-5.971038	-1.410807	0.544432
H	-6.807112	0.860518	1.074755
C	-0.470748	-1.142082	0.335180
C	0.787517	-1.615799	-0.063777
C	-1.025260	-1.659008	1.511710
C	1.458365	-2.580743	0.678078
H	1.269471	-1.205189	-0.943310
C	-0.355483	-2.626199	2.260111
H	-1.993689	-1.306637	1.853691

C	0.886688	-3.091311	1.841674	C	-6.720791	0.197528	-0.029291
H	2.435013	-2.915906	0.346947	H	-6.914874	-0.623074	-2.006993
H	-0.803422	-3.014219	3.168468	H	-6.215985	0.981675	1.907980
H	1.410539	-3.841507	2.424027	H	-7.786974	0.344086	0.101497
H	-1.580262	-1.698331	-3.785581	C	-1.152569	0.891153	0.267793
C	-1.743752	-1.572850	-2.706162	C	0.019223	0.619569	0.986737
O	-1.358781	-0.383046	-2.297935	C	-1.533899	2.233052	0.130680
O	-2.221241	-2.440522	-2.018876	C	0.785300	1.643575	1.537724
C	1.081679	2.026056	-1.216404	H	0.367170	-0.401826	1.115693
O	1.548023	0.984737	-1.754979	C	-0.777258	3.265173	0.680204
O	-0.661118	1.645773	-0.688318	H	-2.441405	2.479040	-0.415176
N	1.631270	2.528462	-0.033507	C	0.388916	2.970210	1.382430
H	2.949327	0.627032	-2.009117	H	1.695850	1.392598	2.068404
C	0.955042	3.692364	0.524202	H	-1.094172	4.295198	0.560525
H	1.597700	4.155403	1.273572	H	0.984989	3.770020	1.807813
H	0.779962	4.414097	-0.275335	H	-1.461806	-3.148202	1.744421
H	-0.009509	3.434462	0.970155	C	-1.824190	-2.146193	1.472005
C	2.105640	1.568712	0.916123	O	-1.673425	-1.914123	0.186887
C	1.287504	1.110435	1.948849	O	-2.290809	-1.385392	2.283050
C	3.409826	1.093835	0.809351	C	1.402321	-1.126435	-1.346214
C	1.774655	0.186917	2.866061	O	1.886120	-2.115192	-0.795209
H	0.263361	1.458728	2.010262	O	-1.713102	-0.629115	-2.171969
C	3.891675	0.159767	1.721566	N	2.009304	0.066829	-1.512370
H	4.036402	1.463552	0.007623	H	3.044704	-2.311221	0.345136
C	3.075975	-0.293118	2.753733	C	1.235011	1.173744	-2.078206
H	1.127417	-0.178337	3.654805	H	1.788170	1.619382	-2.906054
H	4.906301	-0.210262	1.626771	H	0.278240	0.779444	-2.423273
H	3.449240	-1.022768	3.463073	H	1.031232	1.930275	-1.318032
H	5.327737	-0.973109	-2.379772	C	3.336648	0.318636	-1.058423
C	4.269508	-0.809778	-2.126940	C	3.634858	1.517030	-0.408348
O	3.547815	-1.709217	-1.764832	C	4.349216	-0.611593	-1.292329
O	3.932018	0.445091	-2.279279	C	4.929243	1.763121	0.032652
				H	2.855329	2.245599	-0.227975
				C	5.638943	-0.360944	-0.839706

IM16

Symbol	X	Y	Z				
Si	-2.107992	-0.441961	-0.665136	H	4.122711	-1.530396	-1.816642
H	0.384084	-1.145244	-1.759005	C	5.934502	0.822484	-0.170905
C	-3.952534	-0.182414	-0.365992	H	5.149454	2.692798	0.543655
C	-4.858889	-0.527287	-1.376704	H	6.415637	-1.095194	-1.016835
C	-4.468020	0.364331	0.817005	H	6.941139	1.014850	0.179841
C	-6.230367	-0.346185	-1.213005	H	4.483620	-1.713867	2.711664
H	-4.478261	-0.938291	-2.306406	C	3.672543	-1.590658	1.981778
C	-5.836621	0.555342	0.985984	O	2.836126	-0.726643	2.062587
H	-3.785199	0.632062	1.616057	O	3.736787	-2.505722	1.036778

IM17

Symbol	X	Y	Z
Si	-1.460316	1.042784	-0.686639
C	-1.032389	0.360969	-2.394151
C	-1.911377	0.508736	-3.472099
C	0.171153	-0.320641	-2.619176
C	-1.602184	-0.000665	-4.732003
H	-2.849087	1.034632	-3.320422
C	0.491599	-0.828518	-3.874358
H	0.868875	-0.458120	-1.796976
C	-0.398362	-0.668865	-4.934829
H	-2.297433	0.123883	-5.554740
H	1.430016	-1.349483	-4.028135
H	-0.153920	-1.065167	-5.913774
C	-1.209692	-0.391049	0.520342
C	-0.596116	-0.222423	1.768769
C	-1.706564	-1.664076	0.208655
C	-0.486226	-1.277807	2.670938
H	-0.189287	0.748140	2.034316
C	-1.602872	-2.725158	1.104191
H	-2.176283	-1.832794	-0.757048
C	-0.991475	-2.532345	2.340206
H	-0.004565	-1.124143	3.630218
H	-1.993622	-3.701104	0.838675
H	-0.905774	-3.355968	3.039738
H	1.357456	3.380500	-0.496961
C	0.431226	2.980607	-0.934965
O	-0.027101	1.959322	-0.245243
O	-0.068929	3.450158	-1.926583
O	-2.800662	1.837838	-0.570152

	X	Y	Z
H	-2.010657	2.377044	-3.144638
H	-1.073946	4.664872	-2.927199
C	1.227850	-1.275431	-0.318456
C	1.956339	-1.344578	-1.513099
C	0.756247	-2.477393	0.225592
C	2.199935	-2.561713	-2.145772
H	2.333115	-0.429886	-1.960258
C	1.022840	-3.701180	-0.383929
H	0.147950	-2.452933	1.124588
C	1.739943	-3.746258	-1.576417
H	2.749758	-2.586745	-3.080156
H	0.656707	-4.619079	0.062839
H	1.935360	-4.696196	-2.060883
N	6.266806	0.298736	0.342935
C	4.983712	0.966151	-0.064647
H	5.076519	2.026978	0.171246
H	4.894752	0.862291	-1.146300
C	3.695812	0.424241	0.580062
O	2.678894	0.992474	0.066535
O	3.718419	-0.434932	1.450890
C	6.526190	0.483823	1.807624
H	5.728063	-0.001545	2.358813
H	7.490967	0.036850	2.038679
H	6.548474	1.551819	2.016729
C	7.380891	0.937560	-0.426141
H	8.316382	0.468060	-0.129313
H	7.203655	0.785777	-1.488810
H	7.401015	2.000239	-0.193953
C	6.230242	-1.162440	0.009597
H	5.455198	-1.630692	0.607141
H	6.012765	-1.263365	-1.052428
H	7.207576	-1.584583	0.233810

IM18

Symbol	X	Y	Z
Si	0.800341	0.382103	0.504639
H	1.171977	0.727443	1.894939
C	0.245010	1.779420	-0.650253
C	0.769202	3.074352	-0.558655
C	-0.767487	1.559610	-1.591474
C	0.293928	4.109504	-1.360050
H	1.566480	3.274844	0.149236
C	-1.232108	2.579986	-2.417631
H	-1.210075	0.571262	-1.688533
C	-0.706986	3.863160	-2.296549
H	0.707240	5.106910	-1.258745

	X	Y	Z
Si	-2.406096	-0.256464	0.986680
C	-3.091981	-1.561756	-0.158181
C	-2.328437	-2.071237	-1.215760
C	-4.393925	-2.052236	0.016432
C	-2.849363	-3.036035	-2.074397
H	-1.307877	-1.730267	-1.358314
C	-4.918840	-3.014963	-0.839745
H	-5.006014	-1.684599	0.835548
C	-4.145314	-3.507047	-1.888229
H	-2.241425	-3.423649	-2.883854
H	-5.926499	-3.383994	-0.688506
H	-4.551135	-4.259049	-2.554830

C	-3.226766	1.399821	0.725232
C	-2.607805	2.549046	1.236293
C	-4.410023	1.553123	-0.004843
C	-3.158147	3.809436	1.033827
H	-1.672569	2.457745	1.781036
C	-4.963306	2.814358	-0.215694
H	-4.902059	0.682664	-0.427844
C	-4.337074	3.942859	0.302936
H	-2.664786	4.688181	1.433115
H	-5.877998	2.916061	-0.788140
H	-4.763472	4.925223	0.135785
H	-3.031961	-1.897897	4.167346
C	-2.577242	-1.817197	3.172010
O	-2.928977	-0.687905	2.570217
O	-1.857198	-2.658029	2.704837
O	-0.814962	-0.140586	0.968118

IM19

Symbol	X	Y	Z
Si	-0.457706	1.553615	1.392745
H	-0.699920	1.941298	2.798749
C	-2.089777	1.485700	0.491730
C	-3.298103	1.536270	1.195182
C	-2.133716	1.270267	-0.893390
C	-4.515726	1.373762	0.538838
H	-3.291800	1.698218	2.268825
C	-3.345147	1.099564	-1.551663
H	-1.211378	1.228679	-1.466944
C	-4.538093	1.150863	-0.833526
H	-5.443300	1.416602	1.097697
H	-3.362016	0.922788	-2.620739
H	-5.483965	1.015822	-1.345402
C	0.758576	2.679921	0.529046
C	0.339244	3.773007	-0.239129
C	2.133766	2.431626	0.641155
C	1.264937	4.596667	-0.874140
H	-0.720847	3.979396	-0.352017
C	3.061633	3.251008	0.007175
H	2.480032	1.576666	1.214839
C	2.626327	4.335347	-0.751035
H	0.924963	5.436652	-1.468355
H	4.121144	3.042475	0.098888
H	3.347608	4.973338	-1.248251
Si	0.458742	-1.409180	0.719906

C	1.917532	-1.436574	-0.428791
C	2.136339	-0.374408	-1.315909
C	2.791707	-2.529774	-0.468455
C	3.202396	-0.399014	-2.209694
H	1.479103	0.490041	-1.307838
C	3.857626	-2.558737	-1.361980
H	2.643748	-3.368672	0.204487
C	4.064184	-1.491934	-2.231972
H	3.361609	0.433773	-2.884540
H	4.527481	-3.410190	-1.377797
H	4.895886	-1.512251	-2.926339
C	-1.112725	-1.942965	-0.110343
C	-2.334489	-1.852191	0.572879
C	-1.123237	-2.350581	-1.448363
C	-3.529593	-2.160574	-0.062710
H	-2.355389	-1.520199	1.606679
C	-2.320537	-2.662914	-2.088583
H	-0.190454	-2.419585	-1.999741
C	-3.522133	-2.565879	-1.396312

H	-4.467117	-2.073781	0.473712
H	-2.314478	-2.976071	-3.125972
H	-4.455343	-2.800586	-1.895260
H	1.714911	-3.236815	3.577224
C	1.737405	-2.422673	2.844010
O	0.729157	-2.527943	1.974588
O	2.565250	-1.556094	2.827612
O	0.244923	0.049742	1.419906

IM20

Symbol	X	Y	Z
Si	3.754965	-0.042987	0.620853
H	1.705641	-3.005711	0.454598
C	5.110670	-0.358990	2.911730
H	5.368137	0.146975	3.848141
C	2.682630	1.369634	0.102496
C	2.138176	1.412729	-1.190740
C	2.411663	2.424522	0.982927
C	1.342534	2.480877	-1.586168
H	2.329604	0.600555	-1.884397
C	1.618594	3.496439	0.582326
H	2.824963	2.409284	1.985155
C	1.085332	3.525051	-0.700477
H	0.917037	2.497245	-2.582869
H	1.409870	4.303161	1.274885

H	0.455603	4.351969	-1.006800	C	-5.960708	-1.451132	0.390092
C	2.229573	-2.141225	0.033235	H	-5.840466	-2.085253	-0.482258
O	2.224045	-1.845341	-1.129910	H	-5.092513	-1.538424	1.042802
O	2.878000	-1.456421	0.975567	H	-6.873015	-1.686456	0.935907
Si	-0.900917	-0.268727	-0.184807	O	4.310757	0.401845	2.156306
H	-0.523214	-0.418502	-1.601574	O	5.493642	-1.450321	2.603206
H	0.302991	-0.441609	0.673707	C	5.128653	-0.438468	-0.555561
C	-1.504834	1.459983	0.249340	C	5.726466	-1.706148	-0.576536
C	-2.100057	2.324377	-0.679594	C	5.580362	0.535004	-1.455282
C	-1.291494	1.935754	1.549180	C	6.750595	-1.989881	-1.471393
C	-2.472859	3.614717	-0.317916	H	5.395229	-2.469768	0.118608
H	-2.289255	1.965374	-1.684839	C	6.609933	0.252797	-2.348564
C	-1.674625	3.222842	1.919981	H	5.124303	1.519973	-1.463997
H	-0.800360	1.303740	2.283833	C	7.193608	-1.009555	-2.356724
C	-2.262976	4.066141	0.983761	H	7.204497	-2.973608	-1.479832
H	-2.927489	4.271468	-1.051324	H	6.951493	1.014804	-3.038695
H	-1.501275	3.569698	2.932319	H	7.992794	-1.231847	-3.054006
H	-2.554577	5.071698	1.264789				
C	-2.050696	-1.659468	0.373181				
C	-2.310532	-1.823489	1.742640	TS12			
C	-2.566938	-2.614378	-0.511350	Symbol	X	Y	Z
C	-3.052461	-2.903208	2.213609	Si	3.072932	-0.003183	0.483944
H	-1.917354	-1.106219	2.458297	H	0.680366	-2.644897	0.278066
C	-3.304903	-3.700366	-0.044793	C	3.902364	0.153923	3.036949
H	-2.405146	-2.496420	-1.576864	H	4.028975	0.850398	3.874161
C	-3.546032	-3.849031	1.317481	C	2.383053	1.378165	-0.549727
H	-3.238834	-3.011033	3.275949	C	2.052843	1.169954	-1.895424
H	-3.694425	-4.428407	-0.747290	C	2.202652	2.658130	-0.006812
H	-4.118284	-4.694904	1.680526	C	1.550014	2.209324	-2.672688
N	-6.044915	-0.032642	-0.079272	H	2.168207	0.181349	-2.325122
C	-4.748478	0.367307	-0.734097	C	1.704885	3.697300	-0.784470
H	-4.849354	1.413487	-1.028917	H	2.441889	2.838570	1.034779
H	-3.982411	0.306856	0.039434	C	1.376826	3.473651	-2.118559
C	-4.273198	-0.461094	-1.959414	H	1.290364	2.030160	-3.709830
O	-3.130704	-0.127169	-2.325131	H	1.561333	4.678211	-0.346397
O	-5.023529	-1.328674	-2.437579	H	0.984031	4.282770	-2.723843
C	-7.194593	0.129691	-1.021797	C	1.293804	-1.842109	-0.155064
H	-7.011789	-0.511346	-1.878089	O	1.814366	-1.922956	-1.271083
H	-8.107040	-0.152514	-0.499343	O	1.985074	-1.199676	0.880021
H	-7.243434	1.174939	-1.322899	Si	-1.177497	-0.250798	-0.896334
C	-6.254371	0.853651	1.104995	H	-0.480746	-0.301227	-2.199757
H	-7.193081	0.581459	1.583991	H	0.154309	-0.908046	-0.196306
H	-5.424099	0.712352	1.794955	C	-1.023313	1.226799	0.281627
H	-6.288884	1.887615	0.767294	C	-1.490405	2.501782	-0.063494
			C	-0.403545	1.077342	1.530873	

C	-1.358920	3.580710	0.807000
H	-1.962405	2.655543	-1.028313
C	-0.290848	2.145829	2.415357
H	0.022498	0.118376	1.807885
C	-0.768111	3.402459	2.053774
H	-1.716554	4.560484	0.510561
H	0.183247	2.001004	3.379705
H	-0.672297	4.239208	2.736231
C	-2.133874	-1.796733	-0.341268
C	-2.071091	-2.264207	0.978745
C	-2.891258	-2.536058	-1.260689
C	-2.757381	-3.410026	1.374035
H	-1.479445	-1.724919	1.713571
C	-3.555011	-3.700576	-0.879640
H	-2.969765	-2.195279	-2.288657
C	-3.496559	-4.134684	0.441310
H	-2.707087	-3.743236	2.404149
H	-4.124497	-4.262390	-1.611085
H	-4.021223	-5.033472	0.743189
N	-5.572690	0.272512	0.505513
C	-4.231517	0.710573	-0.010244
H	-4.156492	1.790405	0.137512
H	-3.484471	0.236585	0.624210
C	-3.948619	0.404275	-1.488677
O	-2.695902	0.436205	-1.808513
O	-4.852416	0.206103	-2.275682
C	-6.688745	1.062298	-0.109607
H	-6.671286	0.902117	-1.181797
H	-7.624107	0.714810	0.324664
H	-6.532904	2.112992	0.128204
C	-5.574657	0.509653	1.985062
H	-6.554480	0.243290	2.374829
H	-4.805509	-0.113989	2.437271
H	-5.366671	1.561360	2.170613
C	-5.776786	-1.192177	0.257638
H	-5.847070	-1.356304	-0.813225
H	-4.924658	-1.730960	0.672150
H	-6.695470	-1.494014	0.756649
O	3.363556	0.762190	1.982359
O	4.212626	-1.003559	3.077091
C	4.665720	-0.689244	-0.183476
C	4.993118	-2.041308	-0.026078
C	5.565123	0.145225	-0.856964
C	6.190779	-2.543843	-0.521097

H	4.302521	-2.702032	0.486483
C	6.767592	-0.353906	-1.351116
H	5.323975	1.193974	-1.004582
C	7.079925	-1.698986	-1.182434
H	6.432532	-3.592662	-0.394672
H	7.455421	0.303314	-1.869898
H	8.013411	-2.091023	-1.569141

IM21

Symbol	X	Y	Z
Si	3.207040	-0.421126	0.150612
H	1.268798	-2.891202	-0.090267
C	4.241954	-0.347232	2.716526
H	4.476332	0.288692	3.586973
C	2.653995	1.249412	-0.564536
C	1.805007	1.275139	-1.681446
C	2.984182	2.483499	0.014652
C	1.285922	2.468020	-2.179566
H	1.542086	0.336246	-2.157253
C	2.481970	3.682005	-0.485335
H	3.626505	2.502847	0.887380
C	1.621716	3.677952	-1.580047
H	0.616817	2.452415	-3.033676
H	2.751381	4.620445	-0.012697
H	1.218681	4.609187	-1.962268
C	1.429462	-1.810662	-0.203469
O	2.459188	-1.501678	-1.086903
O	1.916361	-1.226492	0.989430
Si	-1.945538	0.355890	-1.074119
H	-1.076152	0.259898	-2.257060
H	0.477267	-1.330087	-0.486276
C	-1.461698	1.657510	0.155441
C	-2.180786	2.854276	0.263163
C	-0.336214	1.467559	0.970855
C	-1.790871	3.836393	1.169273
H	-3.046294	3.026399	-0.368912
C	0.055788	2.452003	1.870461
H	0.250879	0.554191	0.909797
C	-0.672505	3.634591	1.972321
H	-2.356008	4.757743	1.244725
H	0.936662	2.297869	2.482638
H	-0.365512	4.400731	2.674692
C	-2.225282	-1.314565	-0.281510
C	-2.160719	-1.507802	1.105608

C	-2.545078	-2.410505	-1.096834	Si	3.240626	-0.441734	0.298672
C	-2.409131	-2.759878	1.661618	H	1.286106	-2.858282	0.288935
H	-1.910743	-0.677392	1.758769	C	4.857863	-0.668774	2.546143
C	-2.798974	-3.661144	-0.542409	H	5.329364	-0.124676	3.382553
H	-2.593989	-2.291655	-2.175438	C	2.742280	1.336458	-0.156342
C	-2.729663	-3.835684	0.837553	C	1.737767	1.553303	-1.112185
H	-2.351335	-2.895679	2.734775	C	3.348231	2.473916	0.400793
H	-3.045447	-4.498069	-1.184460	C	1.351399	2.837058	-1.491227
H	-2.922686	-4.810082	1.270087	H	1.257544	0.691693	-1.562193
N	-6.221698	-0.373113	0.439409	C	2.974118	3.760567	0.021817
C	-5.089505	0.492163	-0.021984	H	4.120088	2.346485	1.150396
H	-5.385771	1.536687	0.101342	C	1.971478	3.946847	-0.925874
H	-4.246152	0.301432	0.642438	H	0.567817	2.971376	-2.228990
C	-4.665125	0.292825	-1.472766	H	3.462752	4.619397	0.468979
O	-3.467462	0.813951	-1.726642	H	1.676648	4.947799	-1.220308
O	-5.347623	-0.214068	-2.314677	C	1.374737	-1.764319	0.253166
C	-7.506681	-0.005893	-0.244932	O	2.144661	-1.328284	-0.825622
H	-7.397595	-0.181112	-1.309693	O	2.142485	-1.278691	1.338607
H	-8.294221	-0.629915	0.171214	H	0.370521	-1.314149	0.258907
H	-7.712329	1.043764	-0.044092	O	4.161232	0.119893	1.784968
C	-6.381089	-0.147665	1.914981	O	5.014306	-1.863844	2.410781
H	-7.224700	-0.740953	2.259531	C	4.840522	-0.947533	-0.606662
H	-5.468043	-0.462374	2.417049	C	4.893757	-2.058394	-1.457195
H	-6.566186	0.910090	2.089226	C	6.006948	-0.177347	-0.482572
C	-5.908019	-1.823857	0.207228	C	6.061970	-2.401069	-2.137123
H	-5.882136	-2.011968	-0.861718	H	3.999417	-2.656725	-1.587763
H	-4.942302	-2.045433	0.661982	C	7.171989	-0.499036	-1.171341
H	-6.691018	-2.414410	0.677552	H	6.002911	0.691680	0.168576
O	3.715414	0.333733	1.742694	C	7.204490	-1.619860	-1.998406
O	4.477854	-1.536522	2.727384	H	6.078435	-3.274424	-2.780059
C	4.997879	-0.856259	-0.326293	H	8.055948	0.119777	-1.062537
C	5.308483	-2.007489	-1.060168	H	8.112291	-1.879027	-2.531417
C	6.056894	0.007502	-0.007066				
C	6.617450	-2.297475	-1.442594				
H	4.506065	-2.681407	-1.336154				
C	7.363740	-0.263259	-0.400161				
H	5.854686	0.910001	0.561742				
C	7.649277	-1.423879	-1.116077				
H	6.830870	-3.202958	-2.000112				
H	8.160908	0.426773	-0.146257				
H	8.667415	-1.642600	-1.417538				

IM22

Symbol X Y Z

TS13

Symbol	X	Y	Z
Si	0.107646	0.773883	0.493085
H	-1.272863	2.219231	-1.934765
C	-1.108956	1.519232	2.794393
H	-0.983720	1.561178	3.884877
C	1.726576	-0.171001	0.415809
C	2.158277	-1.028801	1.435875
C	2.512789	-0.063448	-0.739366
C	3.343299	-1.749019	1.313929
H	1.565070	-1.128139	2.339816

C	3.696399	-0.787091	-0.867358
H	2.180557	0.591166	-1.541578
C	4.114413	-1.628248	0.160132
H	3.666928	-2.402792	2.116023
H	4.295130	-0.693776	-1.766611
H	5.037718	-2.188100	0.063627
C	-0.185388	2.353715	-2.070952
O	0.460661	1.531976	-2.744054
O	0.142732	2.179757	-0.250401
H	0.125774	3.409533	-2.034097
O	-0.066147	0.953841	2.210673
O	-2.085582	1.938071	2.230685
C	-1.271843	-0.406246	-0.006953
C	-1.540705	-0.629925	-1.366583
C	-2.006434	-1.137528	0.935755
C	-2.519381	-1.538579	-1.762831
H	-0.967304	-0.093614	-2.119494
C	-2.984605	-2.047042	0.543265
H	-1.815760	-1.000952	1.995626
C	-3.245385	-2.246755	-0.809418
H	-2.714905	-1.695802	-2.817726
H	-3.542751	-2.598974	1.291082
H	-4.007438	-2.953206	-1.118034

IM23

Symbol	X	Y	Z
Si	0.018060	-0.448979	-0.840352
H	1.321175	2.423570	-1.916809
C	1.288610	-2.792685	-1.430856
H	1.158789	-3.882763	-1.435514
C	-1.645737	-0.406819	0.044781
C	-2.096183	-1.432113	0.887000
C	-2.454833	0.730322	-0.089500
C	-3.310247	-1.336321	1.559374
H	-1.488759	-2.324468	1.006131
C	-3.667508	0.839586	0.588793
H	-2.127294	1.541620	-0.733600
C	-4.099838	-0.197698	1.411500
H	-3.642164	-2.146501	2.201395
H	-4.279544	1.727725	0.470795
H	-5.045022	-0.119414	1.937115
C	0.310933	2.724830	-2.235504
O	-0.464564	3.261859	-1.480635
O	0.044926	0.286218	-2.226894

H	0.073883	2.565679	-3.299433
O	0.241167	-2.180975	-0.923639
O	2.289906	-2.257852	-1.843803
C	1.283632	0.109429	0.452505
C	1.332325	1.470716	0.795273
C	2.147115	-0.761755	1.131852
C	2.215110	1.944135	1.761015
H	0.663925	2.177555	0.302759
C	3.034009	-0.298545	2.101224
H	2.134191	-1.824816	0.904077
C	3.072407	1.059160	2.414495
H	2.235223	2.998955	2.007489
H	3.693213	-0.991514	2.606901
H	3.761285	1.423923	3.167866

IM24

Symbol	X	Y	Z
N	-0.650168	-0.191648	0.597260
H	-1.145348	0.658231	0.845267
C	0.705793	-0.077750	0.357405
C	1.562543	-1.188399	0.383455
C	1.244741	1.178427	0.023841
C	2.912561	-1.038145	0.078257
H	1.177615	-2.166175	0.644114
C	2.591436	1.312000	-0.272744
H	0.590616	2.044256	0.006175
C	3.440405	0.204723	-0.251123
H	3.556858	-1.909694	0.104801
H	2.983603	2.291136	-0.523183
H	4.492156	0.313249	-0.483955
C	-1.230450	-1.393278	1.158424
H	-0.782033	-1.673223	2.118945
H	-2.294022	-1.207601	1.303525
H	-1.124765	-2.234728	0.467560
C	-1.872961	-0.143465	-1.655177
H	-1.154823	-0.900039	-2.008333
O	-3.009619	-0.433696	-1.361801
H	-1.514150	0.897423	-1.638680
O	-3.045769	1.472161	0.743446
H	-3.661346	1.352013	1.471162
H	-3.364378	0.882465	0.044272

TS14

Symbol	X	Y	Z
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N	-0.880022	-0.321963	0.271473
H	-1.375851	0.608017	0.570628
C	0.550230	-0.117117	0.146487
C	1.405862	-1.184816	-0.096753
C	1.028201	1.186598	0.219061
C	2.766141	-0.938324	-0.251922
H	1.025464	-2.196586	-0.164909
C	2.389295	1.422066	0.062675
H	0.330290	1.998383	0.393661
C	3.258738	0.360575	-0.170202
H	3.440161	-1.765022	-0.438633
H	2.768511	2.434502	0.123707
H	4.319125	0.545234	-0.289586
C	-1.294844	-1.372420	1.227913
H	-0.901795	-1.134928	2.214425
H	-2.382565	-1.374491	1.239567
H	-0.930589	-2.345334	0.901408
C	-1.587800	-0.512353	-1.106517
H	-1.360060	-1.539519	-1.418987
O	-2.901124	-0.267160	-0.948477
H	-1.051596	0.199124	-1.752888
O	-2.469349	1.658025	0.387624
H	-3.039019	1.755762	1.154397
H	-2.880310	0.755188	-0.330041

IM25

Symbol	X	Y	Z
N	-0.880076	-0.544060	0.161911
H	-1.628115	1.133580	1.032901
C	0.508437	-0.256659	0.071038
C	1.494540	-1.202456	0.362565
C	0.906870	1.043274	-0.280974
C	2.843871	-0.857237	0.293034
H	1.222780	-2.210271	0.646659
C	2.250505	1.373107	-0.359660
H	0.150501	1.800579	-0.453600
C	3.231763	0.423173	-0.075398
H	3.592155	-1.606125	0.525115
H	2.534236	2.383642	-0.629322
H	4.281038	0.685226	-0.131024
C	-1.246815	-1.812216	0.782379
H	-0.813165	-1.880511	1.780016
H	-2.331825	-1.836967	0.865648
H	-0.922269	-2.677593	0.188433

C	-1.634445	-0.331566	-1.086092
H	-1.556371	-1.219919	-1.725207
O	-2.995422	-0.139655	-0.831949
H	-1.193542	0.520631	-1.606592
O	-2.153229	1.923086	0.815556
H	-2.568936	2.199963	1.636666
H	-3.061193	0.686413	-0.325992

IM26

Symbol	X	Y	Z
N	-0.830868	-0.695531	-0.045640
C	0.508662	-0.297955	-0.059934
C	1.536847	-1.183284	0.297648
C	0.862584	1.025176	-0.385472
C	2.863348	-0.760828	0.317402
H	1.308194	-2.209074	0.553889
C	2.188668	1.428490	-0.375269
H	0.091530	1.749739	-0.617316
C	3.205114	0.540945	-0.024746
H	3.634954	-1.469074	0.597055
H	2.428055	2.454908	-0.628624
H	4.238603	0.863334	-0.011506
C	-1.177631	-2.000162	0.490903
H	-0.751444	-2.128655	1.486448
H	-2.262591	-2.045310	0.577997
H	-0.838696	-2.825143	-0.150156
C	-1.745769	-0.221566	-1.058858
H	-2.045026	-1.046041	-1.714284
O	-2.949891	0.259296	-0.502432
H	-1.248683	0.538306	-1.662270
H	-2.717522	0.956944	0.119168

IM27

Symbol	X	Y	Z
C	-1.190972	1.953433	-1.001749
C	-1.257493	3.231630	-1.505567
C	-0.556461	4.250278	-0.867145
C	0.201713	3.968095	0.265053
C	0.251302	2.676374	0.734668
N	-0.442489	1.704177	0.098045
H	-0.603736	5.262134	-1.248508
H	-1.694194	1.101776	-1.439547
H	-1.853443	3.419007	-2.386969
H	0.751973	4.737643	0.786585

C	-0.389105	0.345056	0.598541	H	0.558072	0.230248	-1.699868
N	0.695824	-0.283588	0.756548	C	0.479792	-3.030561	0.373694
S	3.215268	-0.458208	0.566979	H	0.448013	-1.764181	2.102004
O	1.798215	0.418799	0.323596	C	0.505391	-3.092754	-1.016756
O	4.199903	0.458837	0.068083	H	0.564732	-1.955243	-2.841649
O	3.219919	-0.903121	1.932502	H	0.473062	-3.943724	0.958027
C	2.961318	-1.816338	-0.535907	H	0.508389	-4.052817	-1.519406
H	3.866625	-2.419677	-0.488636	N	4.930308	-0.978660	-0.299967
H	2.100189	-2.380841	-0.184505	C	4.134661	0.294731	-0.345108
H	2.806863	-1.414135	-1.534299	H	4.837653	1.129567	-0.362105
H	0.813931	2.374169	1.606289	H	3.576838	0.290208	-1.281470
C	-1.675900	-0.311204	0.921552	C	3.129504	0.487533	0.799806
C	-2.482155	0.197450	1.935188	O	2.248269	1.360215	0.485284
C	-2.072151	-1.488543	0.287128	O	3.194172	-0.158547	1.833608
C	-3.644794	-0.472819	2.302351	C	5.872231	-0.993844	0.865730
C	-3.211725	-2.178762	0.653878	H	5.288021	-0.932840	1.777389
C	-4.003881	-1.658092	1.671281	H	6.442131	-1.920024	0.824379
H	-4.263568	-0.071208	3.093962	H	6.540445	-0.139234	0.774401
H	-3.474174	-3.091437	0.135999	C	5.732126	-1.062082	-1.561445
H	-4.906420	-2.178801	1.962853	H	6.325647	-1.973386	-1.531429
H	-2.186707	1.101520	2.454652	H	5.050585	-1.083023	-2.409224
O	-1.230051	-3.190144	-1.005696	H	6.381560	-0.190998	-1.619219
O	-0.816646	-1.170808	-1.614921	C	4.009635	-2.162402	-0.234789
N	-1.304896	-1.995145	-0.864405	H	3.484967	-2.143835	0.715616
				H	3.298450	-2.090690	-1.057959
				H	4.611908	-3.063623	-0.330191

TS16

Symbol	X	Y	Z				
Si	0.377149	1.101254	1.122940	H	-1.927022	-1.470798	1.750942
H	0.870747	1.344724	2.493981	H	-2.488377	-0.482101	3.231750
C	-0.094171	2.574063	0.025184	C	-2.614109	-0.767577	2.198298
C	0.755543	3.672498	-0.162013	O	-1.331944	0.778090	1.660569
C	-1.334737	2.595124	-0.627210	N	-3.765818	-0.568202	1.635479
C	0.379797	4.751505	-0.956472	C	-4.801430	0.236993	2.299743
H	1.728877	3.677421	0.314190	H	-5.654943	-0.390129	2.550998
C	-1.706163	3.658964	-1.446411	H	-4.386824	0.657472	3.211988
H	-2.021695	1.766111	-0.489870	H	-5.114240	1.036127	1.629108
C	-0.850687	4.744096	-1.607487	C	-4.018479	-1.022137	0.293409
H	1.050987	5.594677	-1.074619	C	-5.309911	-1.378459	-0.084007
H	-2.664594	3.642893	-1.952882	C	-2.963924	-1.093993	-0.612674
H	-1.140171	5.578952	-2.235446	C	-5.536481	-1.830403	-1.379020
C	0.473209	-0.597226	0.289523	H	-6.131641	-1.320947	0.617327
C	0.532491	-0.681489	-1.108879	C	-3.204198	-1.550844	-1.902640
C	0.461821	-1.793349	1.015722	H	-1.971867	-0.772031	-0.322355
C	0.536790	-1.913929	-1.758379	C	-4.488163	-1.921362	-2.289094
				H	-6.539140	-2.115136	-1.672564

H -2.380627 -1.602484 -2.604873
H -4.673050 -2.273315 -3.296361
H -1.745590 1.565995 2.031608

IM27

Symbol	X	Y	Z
Si	-0.430441	0.104816	1.146346
H	-0.004483	-0.088057	2.538996
H	2.427765	1.693442	-0.737196
C	0.072623	-1.290119	0.023144
C	-0.012790	-2.604382	0.499417
C	0.499001	-1.083716	-1.294771
C	0.306046	-3.683317	-0.319191
H	-0.323822	-2.793349	1.522996
C	0.813744	-2.159987	-2.116618
H	0.591493	-0.076439	-1.687708
C	0.717257	-3.461105	-1.628931
H	0.237598	-4.693902	0.066142
H	1.129302	-1.985300	-3.138809
H	0.964081	-4.299843	-2.269701
C	0.021762	1.808074	0.543743
C	0.808125	2.618505	1.375552
C	-0.322351	2.294446	-0.726707
C	1.258951	3.862822	0.946493
H	1.086134	2.269203	2.365465
C	0.125183	3.539863	-1.155950
H	-0.945520	1.697857	-1.382935
C	0.922869	4.320670	-0.323796
H	1.874806	4.470471	1.598826
H	-0.145907	3.899276	-2.141530
H	1.278635	5.286229	-0.663593
N	-5.504370	-0.140204	-0.152936
C	-4.416788	-0.209673	0.874292
H	-4.628532	0.532323	1.645059
H	-4.450638	-1.197882	1.336343
C	-3.009128	0.026597	0.353032
O	-2.156233	-0.011397	1.352619
O	-2.714670	0.217049	-0.799642
C	-5.556913	1.214666	-0.797036
H	-4.639900	1.374229	-1.354332
H	-6.417667	1.233506	-1.461739
H	-5.670833	1.962241	-0.014207
C	-6.804731	-0.380562	0.556283
H	-7.604355	-0.338332	-0.179706

H -6.771826 -1.362491 1.023275
H -6.941964 0.394427 1.307444
C -5.326946 -1.200644 -1.200712
H -4.416222 -0.996760 -1.754083
H -5.271053 -2.166869 -0.702922
H -6.192502 -1.167018 -1.858514
H 3.258580 1.661566 -2.306103
C 3.365546 1.447085 -1.239723
O 4.334829 2.300669 -0.652555
N 3.646413 0.045932 -1.101516
C 4.192732 -0.698699 -2.221571
H 3.493233 -1.458790 -2.584964
H 4.399658 -0.007616 -3.037266
H 5.128288 -1.196713 -1.948317
C 3.446600 -0.588311 0.114536
C 3.496897 -1.988736 0.219650
C 3.169903 0.153325 1.279320
C 3.238787 -2.615117 1.431841
H 3.704177 -2.594336 -0.652581
C 2.911030 -0.491210 2.481953
H 3.198052 1.233648 1.244465
C 2.932849 -1.880117 2.572988
H 3.263614 -3.698462 1.475604
H 2.699135 0.106403 3.362513
H 2.730109 -2.376710 3.513715
H 5.179468 2.123807 -1.079120

IM28

Symbol	X	Y	Z
Si	-0.172204	1.419962	-1.060062
H	-0.932737	1.454239	-2.319074
C	-0.283241	2.960998	0.002080
C	-1.395769	3.811102	0.022492
C	0.824724	3.301587	0.791559
C	-1.399305	4.963554	0.801975
H	-2.268864	3.549134	-0.562255
C	0.818433	4.445004	1.586373
H	1.706727	2.667171	0.783424
C	-0.294213	5.280136	1.588527
H	-2.267046	5.613367	0.801531
H	1.681171	4.686651	2.196525
H	-0.300601	6.174732	2.200724
C	-0.283060	-0.188193	-0.104049
C	-0.269959	-0.198765	1.296544

C	-0.309789	-1.416649	-0.774181	C	4.456768	-2.257073	2.146051
C	-0.265043	-1.397909	2.004389	H	6.338672	-2.997711	1.413234
H	-0.270390	0.740718	1.841026	H	2.547512	-1.373139	2.602865
C	-0.294443	-2.620214	-0.070894	H	4.564143	-2.724097	3.117252
H	-0.350755	-1.440681	-1.859919	H	1.839447	2.149512	-1.888588
C	-0.269202	-2.612178	1.321066	IM29			
H	-0.255404	-1.386734	3.088485	Symbol	X	Y	Z
H	-0.309112	-3.561415	-0.609005	H	2.162742	-1.225232	-1.906756
H	-0.256337	-3.546096	1.870713	H	2.836913	-0.073349	-3.240210
N	-4.583093	-1.898526	0.086383	C	2.948032	-0.587345	-2.293820
C	-3.719548	-0.699189	0.384296	N	4.023163	-0.444548	-1.624796
H	-4.281702	-0.068898	1.072746	C	5.141867	0.386153	-2.110927
H	-2.827168	-1.068091	0.897622	H	6.002976	-0.256198	-2.283158
C	-3.254096	0.163987	-0.816169	H	4.844571	0.870711	-3.035915
O	-2.752744	1.242620	-0.432746	H	5.373000	1.118551	-1.340524
O	-3.372924	-0.275739	-1.969067	C	4.180881	-1.067847	-0.324960
C	-5.799602	-1.487010	-0.681724	C	5.316978	-1.825550	-0.069516
H	-5.476606	-1.120697	-1.651047	C	3.188400	-0.877740	0.628223
H	-6.449861	-2.353948	-0.783041	C	5.446437	-2.423033	1.177547
H	-6.306030	-0.701926	-0.122297	H	6.073229	-1.971949	-0.829875
C	-5.010861	-2.497808	1.386947	C	3.336061	-1.479644	1.871973
H	-5.599942	-3.389627	1.180408	H	2.331142	-0.252155	0.410159
H	-4.121741	-2.756703	1.959204	C	4.460765	-2.250584	2.145410
H	-5.608747	-1.768045	1.929351	H	6.319241	-3.026868	1.389728
C	-3.818858	-2.928007	-0.685879	H	2.574031	-1.336143	2.627191
H	-3.472984	-2.467086	-1.605853	H	4.572194	-2.715726	3.116711
H	-2.976560	-3.248841	-0.075463	TS14a			
H	-4.483660	-3.766972	-0.884273	Symbol	X	Y	Z
H	2.132503	-1.154692	-1.854215	H	2.260003	-1.849735	-1.763829
H	2.812361	-0.046496	-3.213611	H	2.256157	-3.082593	-0.469730
C	2.926594	-0.540603	-2.259100	C	1.730819	-2.206576	-0.876478
O	1.473252	1.344746	-1.508388	O	0.408089	-2.381362	-1.076169
N	4.031417	-0.448342	-1.625380	N	1.941606	-1.140054	0.229405
C	5.153252	0.361310	-2.131938	H	1.224633	-1.477350	0.945118
H	6.012567	-0.284001	-2.300346	C	3.313753	-1.176111	0.797229
H	4.854337	0.831453	-3.064213	H	3.491164	-2.162629	1.221342
H	5.393108	1.111834	-1.380820	H	4.032223	-0.977018	0.002577
C	4.189728	-1.068835	-0.326511	H	3.395125	-0.415214	1.570013
C	5.334697	-1.808615	-0.056414	C	1.542201	0.209382	-0.172302
C	3.181905	-0.899444	0.614702	C	2.087209	0.794381	-1.308344
C	5.458091	-2.408595	1.190653	C	0.650309	0.896962	0.638058
H	6.105094	-1.938460	-0.805456	C	1.711642	2.090103	-1.643458

H	2.792544	0.257172	-1.930766
C	0.278046	2.191979	0.291884
H	0.241152	0.418450	1.521052
C	0.806802	2.787821	-0.847842
H	2.127932	2.553046	-2.529279
H	-0.425973	2.729988	0.914401
H	0.516064	3.795637	-1.117092
N	-0.182900	-2.511534	1.334816
H	0.011527	-2.556839	-0.021673
C	0.309875	-3.615885	2.137802
H	1.205142	-4.030144	1.666070
H	0.586719	-3.313158	3.157067
H	-0.421290	-4.432129	2.231761
C	-1.372884	-1.946904	1.728317
C	-2.030105	-2.234622	2.945044
C	-2.002570	-1.009857	0.868693
C	-3.227131	-1.604701	3.281358
H	-1.601857	-2.950542	3.635411
C	-3.190447	-0.393098	1.216722
H	-1.525378	-0.789125	-0.080754
C	-3.821026	-0.679146	2.432168
H	-3.699946	-1.849110	4.227104
H	-3.638105	0.317495	0.529593
H	-4.751787	-0.195242	2.701022

IM30

Symbol	X	Y	Z
H	0.267590	-0.542036	-1.681509
H	0.955625	1.049650	-2.430895
C	0.232917	0.534440	-1.809370
N	-0.684726	1.206378	-1.229101
C	-0.770035	2.673458	-1.343679
H	-0.586740	3.115586	-0.366463
H	-0.019630	3.013665	-2.050822
H	-1.771565	2.927252	-1.685099
C	-1.676281	0.533353	-0.416981
C	-1.940421	1.005609	0.862806
C	-2.300670	-0.597806	-0.926636
C	-2.838383	0.303711	1.657345
H	-1.437942	1.882083	1.251167
C	-3.199957	-1.285590	-0.121767
H	-2.099118	-0.925878	-1.939256
C	-3.463971	-0.839901	1.169309
H	-3.043139	0.651471	2.661800

H	-3.696720	-2.165964	-0.508771
H	-4.163985	-1.380050	1.794328
N	2.948420	1.087521	0.379914
H	3.888387	1.128840	0.015864
C	2.685164	1.947517	1.518068
H	2.831153	1.434892	2.476523
H	3.360085	2.799630	1.470087
H	1.660923	2.328778	1.484094
C	2.334794	-0.141418	0.259219
C	1.211279	-0.488189	1.030106
C	2.792848	-1.063371	-0.703555
C	0.550025	-1.693629	0.809067
H	0.841902	0.187415	1.791486
C	2.132458	-2.265075	-0.902013
H	3.666219	-0.815433	-1.297299
C	0.993267	-2.588757	-0.158815
H	-0.331488	-1.922969	1.399174
H	2.505232	-2.955063	-1.650444
H	0.474680	-3.524283	-0.324583

TS16

Symbol	X	Y	Z
H	-0.397447	-1.123225	-1.598832
H	0.198892	-2.900842	-1.515970
C	0.324828	-1.855373	-1.269083
N	1.430998	-1.462508	-0.744733
C	2.505037	-2.410490	-0.398812
H	2.661937	-2.420050	0.677689
H	2.217072	-3.402678	-0.733784
H	3.415263	-2.087110	-0.900605
C	1.640056	-0.059736	-0.454303
C	2.181677	0.307756	0.771378
C	1.259202	0.892873	-1.392855
C	2.298036	1.658995	1.076097
H	2.485005	-0.436558	1.497120
C	1.379537	2.238988	-1.074684
H	0.884063	0.589838	-2.362812
C	1.888257	2.623879	0.162050
H	2.704047	1.952926	2.035602
H	1.081369	2.985714	-1.799517
H	1.977068	3.674567	0.407934
N	-1.280952	-1.916562	0.525214
H	-1.948745	-2.645438	0.304291
C	-0.465999	-2.215304	1.695332

H	-0.966278	-1.957108	2.633501
H	-0.224340	-3.276572	1.691177
H	0.466794	-1.648470	1.634362
C	-1.817071	-0.623262	0.378959
C	-1.322507	0.467562	1.101161
C	-2.795839	-0.405461	-0.600533
C	-1.791382	1.749981	0.831447
H	-0.568210	0.330686	1.864698
C	-3.257980	0.877695	-0.856009
H	-3.184829	-1.248777	-1.162241
C	-2.754953	1.966539	-0.146484
H	-1.391060	2.584353	1.395444
H	-4.015503	1.026909	-1.616229
H	-3.114166	2.967062	-0.351496

IM31

Symbol	X	Y	Z
H	0.354890	-1.388784	-1.884108
H	1.113541	-2.809459	-1.137986
C	0.663729	-1.837050	-0.943736
N	1.507432	-1.018184	-0.183392
C	2.529939	-1.647371	0.650293
H	2.380242	-1.429276	1.711371
H	2.486380	-2.725834	0.513356
H	3.524915	-1.302333	0.360167
C	1.502220	0.387916	-0.304328
C	2.327274	1.153295	0.531131
C	0.686252	1.063802	-1.225519
C	2.330558	2.542177	0.446760
H	2.964733	0.678156	1.262774
C	0.702358	2.449213	-1.299405
H	0.011445	0.533071	-1.881925
C	1.520853	3.204885	-0.465170
H	2.976840	3.103710	1.110983
H	0.056240	2.939191	-2.018355
H	1.522666	4.285729	-0.524707
N	-0.681699	-2.180683	-0.211894
H	-1.219880	-2.735198	-0.884161
C	-0.450671	-3.050909	0.979968
H	-1.409178	-3.248093	1.453089
H	0.006637	-3.976595	0.638397
H	0.213198	-2.540045	1.670825
C	-1.465838	-0.967730	0.073641
C	-1.198022	-0.214299	1.207511

C	-2.409040	-0.571500	-0.863665
C	-1.890846	0.976393	1.393044
H	-0.454260	-0.522330	1.930177
C	-3.095131	0.620650	-0.665192
H	-2.603644	-1.177675	-1.741653
C	-2.831927	1.396655	0.458918
H	-1.685619	1.577659	2.269499
H	-3.833524	0.938272	-1.390039
H	-3.364549	2.327216	0.609543

TS17

Symbol	X	Y	Z
H	-0.741244	0.851903	0.067693
H	-0.745333	1.943552	1.449485
C	-1.287079	1.128423	0.965524
N	-2.609704	1.528109	0.641574
C	-3.296382	2.461371	1.515867
H	-4.127389	1.993508	2.058611
H	-2.586396	2.849469	2.244643
H	-3.694672	3.305123	0.945805
C	-3.271617	1.024987	-0.486568
C	-4.619217	1.347112	-0.709561
C	-2.633074	0.184768	-1.418088
C	-5.291545	0.860014	-1.826882
H	-5.159087	1.970976	-0.010842
C	-3.315548	-0.283013	-2.529868
H	-1.606978	-0.136699	-1.301153
C	-4.651425	0.044888	-2.749536
H	-6.332807	1.127359	-1.966504
H	-2.779716	-0.925089	-3.220026
H	-5.179533	-0.331185	-3.616650
N	-1.156417	-0.053591	1.908199
H	0.038893	-0.281777	1.810655
C	-1.427614	0.309001	3.314227
H	-1.258642	-0.568785	3.935938
H	-0.731212	1.096272	3.604121
H	-2.451260	0.658833	3.452007
C	-1.916947	-1.208325	1.448019
C	-3.298463	-1.263274	1.607496
C	-1.239989	-2.228720	0.789997
C	-4.006163	-2.333847	1.075864
H	-3.828061	-0.466089	2.114976
C	-1.955521	-3.294671	0.255470
H	-0.161018	-2.184970	0.711920

C	-3.338493	-3.344757	0.390588	C	-4.527249	1.385266	-0.820479
H	-5.083022	-2.369255	1.185787	C	-2.601642	0.074937	-1.433984
H	-1.428772	-4.084218	-0.266106	C	-5.204929	0.893474	-1.932261
H	-3.896082	-4.171071	-0.032893	H	-5.042193	2.071285	-0.162605
Si	1.995454	-0.016645	0.268707	C	-3.293056	-0.403206	-2.536184
C	3.553385	-1.003834	-0.006221	H	-1.598902	-0.298232	-1.275523
C	4.451770	-0.690658	-1.034567	C	-4.601248	-0.003420	-2.803596
C	3.830229	-2.106054	0.810936	H	-6.223683	1.220569	-2.107816
C	5.589992	-1.461133	-1.245832	H	-2.790703	-1.107936	-3.189825
H	4.264032	0.169006	-1.672226	H	-5.134229	-0.386111	-3.664816
C	4.969952	-2.877937	0.604800	N	-1.210083	-0.097454	1.948951
H	3.144668	-2.350049	1.616042	H	0.514905	-0.425687	1.849054
C	5.848246	-2.556300	-0.425220	C	-1.543788	0.333340	3.313159
H	6.277017	-1.208252	-2.044833	H	-1.407869	-0.509751	3.990654
H	5.174244	-3.727168	1.246400	H	-0.856599	1.129883	3.604316
H	6.736393	-3.156003	-0.587227	H	-2.568430	0.703413	3.417337
C	2.291601	1.810716	0.003743	C	-1.972341	-1.239482	1.498680
C	3.235159	2.473676	0.801524	C	-3.357366	-1.304624	1.657020
C	1.601837	2.556695	-0.960067	C	-1.308587	-2.270313	0.837703
C	3.480002	3.833301	0.645514	C	-4.068010	-2.380920	1.138567
H	3.792557	1.919542	1.551885	H	-3.887220	-0.506090	2.163155
C	1.841129	3.919522	-1.117899	C	-2.022740	-3.341600	0.310803
H	0.870952	2.065811	-1.594526	H	-0.230746	-2.228153	0.741101
C	2.780910	4.558204	-0.316138	C	-3.404954	-3.397669	0.456356
H	4.215559	4.327481	1.269345	H	-5.144327	-2.419083	1.257993
H	1.297310	4.480469	-1.869012	H	-1.495692	-4.131679	-0.210673
H	2.970927	5.617885	-0.440851	H	-3.962832	-4.230604	0.045789
H	1.717452	-2.094279	-1.759477	Si	2.073271	-0.062225	0.210152
C	0.852913	-1.416353	-1.838707	C	3.735770	-0.849373	-0.024724
O	0.915319	-0.359811	-1.035160	C	4.685964	-0.271660	-0.876909
O	-0.062168	-1.608144	-2.587897	C	4.055858	-2.049169	0.624973
O	1.278025	-0.416257	1.638086	C	5.921149	-0.878570	-1.079299
				H	4.463067	0.663941	-1.381194
				C	5.290333	-2.657594	0.423808

IM32

Symbol	X	Y	Z				
H	-0.708190	0.680426	0.081757	H	3.335195	-2.503646	1.296823
H	-0.676415	1.835429	1.407205	C	6.222095	-2.072203	-0.429302
C	-1.246212	1.014053	0.965278	H	6.648689	-0.421106	-1.738992
N	-2.540155	1.498746	0.567536	H	5.527446	-3.584254	0.932728
C	-3.201854	2.481489	1.406993	H	7.184778	-2.544849	-0.584880
H	-4.070933	2.066056	1.931950	C	2.093419	1.781992	-0.017582
H	-2.493156	2.841703	2.150854	C	2.896019	2.565699	0.823283
H	-3.538508	3.337602	0.815131	C	1.323408	2.424275	-0.995532
C	-3.205145	0.990125	-0.545181	C	2.922804	3.950382	0.696732
				H	3.509366	2.093212	1.585299

C	1.347871	3.809763	-1.124087
H	0.696509	1.836464	-1.658472
C	2.146240	4.572761	-0.277141
H	3.547091	4.543155	1.354589
H	0.745406	4.293332	-1.883833
H	2.165416	5.651646	-0.376864
H	1.927023	-2.267925	-1.674095
C	0.997082	-1.684755	-1.746830
O	0.986876	-0.577275	-1.001463
O	0.071583	-2.001712	-2.435181
O	1.481325	-0.568376	1.644736

IM33

Symbol	X	Y	Z
Si	-0.030133	1.901741	-0.139803
H	0.630862	1.872909	-1.459981
H	0.543170	3.035827	0.644215
C	-1.874065	2.214503	-0.294004
C	-2.510036	2.213646	-1.540822
C	-2.660713	2.382590	0.853237
C	-3.890437	2.361489	-1.637571
H	-1.924577	2.051745	-2.437452
C	-4.044028	2.511931	0.762387
H	-2.198774	2.403509	1.835871
C	-4.660726	2.498276	-0.485687
H	-4.367804	2.355926	-2.610708
H	-4.637634	2.626985	1.661804
H	-5.737215	2.598920	-0.560245
C	0.390960	0.370944	0.879401
C	0.160077	0.377531	2.265164
C	0.992200	-0.764206	0.318465
C	0.509861	-0.709777	3.060744
H	-0.281163	1.248694	2.740588
C	1.361965	-1.847151	1.114199
H	1.154458	-0.810448	-0.752267
C	1.120128	-1.823208	2.484946
H	0.319973	-0.684036	4.127291
H	1.831110	-2.711676	0.658520
H	1.403837	-2.666994	3.102981
N	-3.137122	-2.154086	0.196714
C	-2.583664	-1.044674	-0.658954
H	-3.399532	-0.685045	-1.289090
H	-2.311616	-0.243499	0.027080
C	-1.350980	-1.365855	-1.548674

O	-0.890559	-0.340945	-2.084582
O	-0.951619	-2.539898	-1.635640
C	-3.661881	-3.271988	-0.646100
H	-2.836731	-3.653849	-1.238356
H	-4.067356	-4.036664	0.014078
H	-4.447866	-2.874669	-1.286376
C	-4.255126	-1.589959	1.011504
H	-4.671288	-2.382872	1.630385
H	-3.860722	-0.789107	1.635149
H	-5.014724	-1.197604	0.337900
C	-2.074160	-2.661600	1.120415
H	-1.291222	-3.107205	0.515446
H	-1.680068	-1.813599	1.681416
H	-2.524133	-3.388369	1.794832
H	3.577357	3.108664	-0.660554
H	3.104324	3.499793	1.116820
C	3.414517	2.790367	0.360879
N	3.605375	1.571057	0.690144
C	3.470604	1.147849	2.101617
H	4.467554	1.069883	2.532386
H	2.891791	1.897821	2.632798
H	2.964942	0.185236	2.125302
C	3.977784	0.559568	-0.277151
C	4.744948	-0.521382	0.142173
C	3.530271	0.666052	-1.590385
C	5.077783	-1.505759	-0.780070
H	5.090386	-0.602499	1.163646
C	3.869829	-0.326116	-2.499363
H	2.895532	1.485062	-1.902728
C	4.640474	-1.412588	-2.096663
H	5.678699	-2.347769	-0.461867
H	3.512533	-0.255620	-3.518491
H	4.893901	-2.188766	-2.807504

TS18

Symbol	X	Y	Z
Si	-0.105013	1.244769	-0.745383
H	0.596796	1.431301	-2.036363
H	0.799616	2.257564	0.045897
C	-1.705428	2.197061	-0.379761
C	-2.809931	2.190376	-1.244133
C	-1.796648	2.979339	0.779986
C	-3.959282	2.920886	-0.956040
H	-2.768865	1.601915	-2.153770

C	-2.953553	3.690399	1.089504
H	-0.944557	3.044333	1.450139
C	-4.038329	3.663766	0.218767
H	-4.794762	2.907878	-1.646651
H	-3.003049	4.273664	2.001764
H	-4.936588	4.224330	0.449971
C	0.352943	-0.186797	0.426101
C	-0.010943	-0.132435	1.780112
C	1.059139	-1.315852	-0.011955
C	0.289512	-1.172921	2.656953
H	-0.553145	0.730250	2.159142
C	1.398004	-2.343733	0.867825
H	1.346153	-1.398105	-1.056419
C	1.004736	-2.279435	2.202977
H	-0.022384	-1.114644	3.693470
H	1.955888	-3.200543	0.507642
H	1.252864	-3.085189	2.883687
N	-3.269194	-2.289251	0.153179
C	-2.738284	-1.014028	-0.438466
H	-3.594310	-0.428842	-0.781663
H	-2.262948	-0.463957	0.372741
C	-1.750287	-1.170065	-1.607119
O	-1.107490	-0.098163	-1.878010
O	-1.661451	-2.224962	-2.217125
C	-4.165900	-3.005607	-0.809900
H	-3.594175	-3.229545	-1.703776
H	-4.516991	-3.916143	-0.328662
H	-5.007782	-2.354292	-1.038266
C	-4.062302	-1.925690	1.369597
H	-4.513069	-2.831336	1.769896
H	-3.389943	-1.482714	2.102692
H	-4.834123	-1.213925	1.084245
C	-2.139641	-3.181419	0.571421
H	-1.611181	-3.509210	-0.317582
H	-1.478621	-2.607636	1.220323
H	-2.559469	-4.028403	1.110727
H	2.924537	3.025798	0.002825
H	2.212252	2.922035	1.735260
C	2.745959	2.469024	0.911390
N	3.278599	1.308445	1.073683
C	3.194705	0.617021	2.372175
H	4.166028	0.669482	2.862043
H	2.446401	1.114061	2.982403
H	2.912302	-0.419055	2.195963

C	3.967209	0.631224	0.001909
C	4.992442	-0.259533	0.303020
C	3.565399	0.847961	-1.312713
C	5.633510	-0.925244	-0.735288
H	5.301291	-0.433011	1.324797
C	4.213968	0.175047	-2.339267
H	2.734690	1.504410	-1.537117
C	5.248483	-0.710771	-2.054113
H	6.436257	-1.614289	-0.506073
H	3.896058	0.334405	-3.361734
H	5.747805	-1.238163	-2.857055

IM34

Symbol	X	Y	Z
Si	-0.582577	0.827150	-1.232604
H	0.301098	1.184153	-2.353746
H	1.808766	2.338571	-0.467374
C	-1.566055	2.254412	-0.547428
C	-2.888027	2.444739	-0.974093
C	-1.022860	3.171212	0.364965
C	-3.645391	3.511080	-0.499516
H	-3.331700	1.759049	-1.688951
C	-1.778631	4.237543	0.839713
H	-0.002331	3.059955	0.715956
C	-3.091258	4.407234	0.408526
H	-4.665328	3.642207	-0.840429
H	-1.343646	4.934139	1.546033
H	-3.680435	5.237610	0.779162
C	0.271052	-0.207624	0.064976
C	0.229475	0.075217	1.436071
C	0.910649	-1.385001	-0.358153
C	0.811674	-0.792323	2.358543
H	-0.271065	0.968139	1.796288
C	1.482054	-2.255518	0.561193
H	0.970338	-1.624133	-1.415989
C	1.435210	-1.956657	1.920934
H	0.773223	-0.559532	3.416170
H	1.977694	-3.154893	0.217259
H	1.886816	-2.631155	2.638937
N	-3.296588	-2.295501	0.681332
C	-3.012260	-1.076524	-0.141833
H	-3.965009	-0.597975	-0.383182
H	-2.443226	-0.390743	0.486161
C	-2.273334	-1.335688	-1.451834

O	-1.715991	-0.238392	-1.959425	H	0.223323	1.948853	0.268624
O	-2.245966	-2.392301	-2.012379	C	-1.248287	5.001021	0.318494
C	-4.293076	-3.194361	0.007917	H	-3.140954	5.480874	-0.583391
H	-3.873251	-3.541649	-0.929636	H	0.591707	4.221168	1.115931
H	-4.491983	-4.028644	0.676385	H	-1.076501	6.006177	0.685446
H	-5.204359	-2.624113	-0.162054	C	-1.578867	-0.773427	-0.176133
C	-3.876841	-1.828103	1.984300	C	-1.305083	-0.570510	1.183343
H	-4.128285	-2.704342	2.577384	C	-1.640245	-2.089350	-0.653862
H	-3.132317	-1.223988	2.499077	C	-1.102772	-1.649680	2.041128
H	-4.769532	-1.241520	1.778660	H	-1.261779	0.437234	1.585508
C	-2.027062	-3.045071	0.967702	C	-1.446003	-3.170299	0.202635
H	-1.643025	-3.456721	0.039180	H	-1.862241	-2.273354	-1.699480
H	-1.311134	-2.351683	1.410300	C	-1.179827	-2.951339	1.552141
H	-2.260846	-3.843476	1.668429	H	-0.890894	-1.474133	3.089420
H	3.334419	3.030074	-1.040461	H	-1.503198	-4.181830	-0.181967
H	2.663911	3.547550	0.506271	H	-1.030579	-3.791845	2.219541
C	2.800624	2.689461	-0.148976	N	-5.994790	-1.315205	0.753188
N	3.542979	1.666778	0.551225	C	-5.921846	-0.209323	-0.269425
C	3.636432	1.721659	1.998556	H	-6.768374	-0.330633	-0.943879
H	4.670230	1.593697	2.332455	H	-5.994677	0.733759	0.267125
H	3.295695	2.697502	2.337941	C	-4.609030	-0.270668	-1.051697
H	3.020631	0.950222	2.477491	O	-3.797710	0.702839	-0.750127
C	3.844547	0.490356	-0.101414	O	-4.380745	-1.169333	-1.831043
C	4.459592	-0.582483	0.576842	C	-6.210161	-2.646069	0.095771
C	3.561722	0.318982	-1.473138	H	-5.395684	-2.828974	-0.598657
C	4.768623	-1.759911	-0.089175				
H	4.688225	-0.502377	1.630871				
C	3.877223	-0.868396	-2.120665				
H	3.085616	1.109164	-2.037866	TS19			
C	4.480761	-1.922444	-1.441628	Symbol	X	Y	Z
H	5.237364	-2.565897	0.464983	Si	-1.801607	0.595592	-1.252249
H	3.639909	-0.967099	-3.174402	H	-2.157071	0.378539	-2.668691
H	4.721479	-2.846340	-1.952634	C	-1.557446	2.360385	-0.635493

IM35

Symbol	X	Y	Z
Si	-2.060649	0.670321	-1.265194
H	-2.283844	0.468923	-2.700825
C	-1.691152	2.394062	-0.631609
C	-2.629594	3.411744	-0.851777
C	-0.526965	2.711224	0.080273
C	-2.407783	4.706000	-0.392493
H	-3.548125	3.190295	-1.385093
C	-0.311091	4.001146	0.558631

Symbol	X	Y	Z
Si	-1.801607	0.595592	-1.252249
H	-2.157071	0.378539	-2.668691
C	-1.557446	2.360385	-0.635493
C	-2.451414	3.384041	-0.974376
C	-0.460130	2.693114	0.167459
C	-2.247235	4.692154	-0.544108
H	-3.321482	3.154467	-1.580291
C	-0.259134	3.994697	0.619740
H	0.252619	1.925083	0.448074
C	-1.151116	4.999687	0.257893
H	-2.945356	5.470836	-0.829459
H	0.596074	4.220904	1.247144
H	-0.994875	6.016342	0.599638
C	-1.630770	-0.778627	0.025499
C	-1.518540	-0.471549	1.387841
C	-1.674014	-2.129205	-0.343326

C	-1.439304	-1.477662	2.349411	H	3.351072	3.742763	0.009734
H	-1.500862	0.565662	1.709459	H	3.976060	3.332428	2.378910
C	-1.605582	-3.139086	0.613481	C	2.927155	-0.910080	-1.832189
H	-1.775148	-2.397640	-1.389776	H	2.284068	-1.390357	-2.572617
C	-1.483965	-2.814656	1.962727	H	3.265638	0.046882	-2.246064
H	-1.347546	-1.218321	3.397911	N	3.985967	-1.832551	-1.504505
H	-1.645155	-4.178320	0.307580	C	4.983414	-1.337981	-0.592507
H	-1.427398	-3.599128	2.708248	C	5.368093	-2.167156	0.458804
N	-6.099818	-1.127509	0.599384	C	5.565390	-0.076471	-0.722004
C	-5.853362	-0.045240	-0.422391	C	6.306081	-1.732536	1.389762
H	-6.654381	-0.105590	-1.158750	H	4.913160	-3.148249	0.541181
H	-5.891920	0.906105	0.102822	C	6.489652	0.363476	0.218895
C	-4.484889	-0.214805	-1.099053	H	5.284382	0.574542	-1.542206
O	-3.664920	0.733901	-0.813746	C	6.860130	-0.461073	1.278065
O	-4.261714	-1.190721	-1.794817	H	6.593985	-2.381993	2.207868
C	-6.395516	-2.438685	-0.064213	H	6.922614	1.352259	0.123134
H	-5.557322	-2.700021	-0.702555	H	7.578550	-0.114111	2.010938
H	-6.545569	-3.182993	0.715160	C	4.564047	-2.456621	-2.696270
H	-7.301593	-2.322167	-0.655650	H	5.293038	-3.203468	-2.382660
C	-7.281902	-0.726520	1.425241	H	3.776147	-2.956433	-3.262153
H	-7.507963	-1.535174	2.116801	H	5.067418	-1.730289	-3.349907
H	-7.033631	0.180577	1.971787				
H	-8.125672	-0.551322	0.761036				
C	-4.901218	-1.275975	1.488631	IM36			
H	-4.078757	-1.688118	0.904382	Symbol	X	Y	Z
H	-4.633340	-0.295321	1.878163	Si	-1.800512	0.600924	-1.224274
H	-5.160301	-1.952108	2.300717	H	-2.110968	0.343402	-2.647980
O	0.019082	0.362723	-1.725137	C	-1.731979	2.390932	-0.617834
H	0.268463	0.853928	-2.516034	C	-2.640255	3.365855	-1.048498
H	1.009986	-0.113895	-1.168855	C	-0.726166	2.790577	0.270871
N	2.052851	-0.598043	-0.657202	C	-2.536233	4.688705	-0.626276
C	1.636086	-1.837324	0.036163	H	-3.442795	3.084774	-1.721736
H	1.173421	-2.488920	-0.703786	C	-0.627894	4.105498	0.718619
H	2.492563	-2.346589	0.474000	H	-0.008713	2.058670	0.627027
H	0.903027	-1.583805	0.800348	C	-1.530950	5.061275	0.262271
C	2.584157	0.449071	0.210295	H	-3.242828	5.428541	-0.984876
C	2.909720	0.216684	1.540995	H	0.153771	4.382667	1.417381
C	2.734741	1.722870	-0.335958	H	-1.454115	6.088872	0.598378
C	3.410958	1.259922	2.315627	C	-1.770116	-0.736766	0.110187
H	2.797756	-0.765728	1.979206	C	-1.772517	-0.397434	1.469700
C	3.239270	2.755738	0.441659	C	-1.792400	-2.097501	-0.223947
H	2.445561	1.914311	-1.362967	C	-1.784978	-1.378427	2.460230
C	3.582994	2.526735	1.771287	H	-1.775048	0.647494	1.765657
H	3.671568	1.071726	3.350000	C	-1.813521	-3.083298	0.760576
			H	-1.807649	-2.393320	-1.267859	

C	-1.805550	-2.725236	2.106671	H	3.136134	-0.189191	-1.931987
H	-1.782899	-1.091884	3.505771	N	4.031008	-1.819535	-0.970791
H	-1.834977	-4.129896	0.478314	C	5.279655	-1.212353	-0.757048
H	-1.820442	-3.490159	2.874221	C	6.365474	-1.993739	-0.331057
N	-6.258228	-1.157772	0.332509	C	5.499093	0.162383	-0.950435
C	-5.963206	-0.121934	-0.725054	C	7.612790	-1.419719	-0.107656
H	-6.696758	-0.254643	-1.519933	H	6.246986	-3.054030	-0.160090
H	-6.080587	0.852325	-0.256719	C	6.749567	0.719463	-0.725709
C	-4.532576	-0.272136	-1.272925	H	4.701356	0.822835	-1.257281
O	-3.761260	0.688678	-0.928827	C	7.821219	-0.060808	-0.301143
O	-4.242441	-1.258681	-1.934313	H	8.426411	-2.053862	0.224627
C	-6.457732	-2.511160	-0.279422	H	6.879579	1.784217	-0.881640
H	-5.563359	-2.773076	-0.836342	H	8.792638	0.382449	-0.123561
H	-6.644038	-3.219820	0.525185	C	3.949480	-3.276058	-0.940289
H	-7.317098	-2.460074	-0.945318	H	4.122031	-3.671950	0.063914
C	-7.512343	-0.756657	1.043275	H	2.955297	-3.580936	-1.258054
H	-7.769925	-1.537284	1.755775	H	4.681109	-3.718300	-1.620806
H	-7.334512	0.183641	1.560762				
H	-8.305679	-0.640948	0.307843				
C	-5.127738	-1.219648	1.314831	IM37			
H	-4.253896	-1.635941	0.814820	Symbol	X	Y	Z
H	-4.915632	-0.211350	1.666048	H	0.724229	1.181636	-1.900410
H	-5.428118	-1.859457	2.142126	H	1.961437	2.126549	-0.835369
O	-0.014852	0.425218	-1.498318	C	1.062518	1.531235	-0.932877
H	0.285184	0.891602	-2.285759	N	0.376875	1.254563	0.103086
H	1.131579	-0.186951	-0.702193	C	0.773687	1.672210	1.456430
N	1.992699	-0.640612	-0.216634	H	0.999905	0.768566	2.017489
C	1.491963	-1.807348	0.553799	H	1.661315	2.294938	1.385544
H	0.928532	-2.439983	-0.129279	H	-0.058127	2.222214	1.892842
H	2.325367	-2.365846	0.972382	C	-0.851661	0.491119	-0.005437
H	0.833520	-1.450151	1.344153	C	-0.925434	-0.747945	0.618164
C	2.649920	0.388977	0.592196	C	-1.912408	1.035593	-0.715973
C	3.411197	0.057479	1.704517	C	-2.113315	-1.461728	0.514702
C	2.554133	1.704699	0.151208	H	-0.048298	-1.139458	1.119146
C	4.091831	1.065733	2.379922	C	-3.093050	0.306074	-0.807070
H	3.495466	-0.966173	2.044093	H	-1.819234	2.013256	-1.173508
C	3.235427	2.704159	0.834642	C	-3.193142	-0.937230	-0.191536
H	1.947950	1.943481	-0.715247	H	-2.191522	-2.435501	0.981529
C	4.009634	2.384280	1.946447	H	-3.932720	0.714797	-1.354538
H	4.692138	0.813362	3.244857	H	-4.115041	-1.500828	-0.263615
H	3.159367	3.729766	0.495866	H	2.430303	-0.468216	-1.061956
H	4.544480	3.162876	2.476157	C	2.845436	-0.975273	-0.137060
C	2.889517	-1.093682	-1.379918	O	2.165894	-0.813902	0.901230
H	2.239909	-1.711656	-1.999298	O	3.900497	-1.600421	-0.300694

TS20

Symbol	X	Y	Z
H	-0.749685	1.134795	1.876830
H	-1.937863	2.133650	0.835787
C	-1.137339	1.408347	0.903863
N	-0.394173	1.198574	-0.147351
C	-0.807838	1.655850	-1.478509
H	-1.133015	0.799125	-2.064943
H	-1.636729	2.350654	-1.364720
H	0.035570	2.153919	-1.954406
C	0.816290	0.429503	-0.048142
C	1.042305	-0.619537	-0.933984
C	1.756810	0.769314	0.919569
C	2.225883	-1.340807	-0.835199
H	0.283271	-0.887041	-1.655773
C	2.932837	0.033965	1.013348
H	1.579784	1.612630	1.576568
C	3.169794	-1.019350	0.136327
H	2.405179	-2.164291	-1.515272
H	3.667816	0.296326	1.763934
H	4.089440	-1.586805	0.207197
H	-2.212707	0.172859	0.975585
C	-2.635937	-0.775330	0.353880
O	-2.001019	-0.946393	-0.681296
O	-3.581799	-1.311669	0.910011

IM38

Symbol	X	Y	Z
H	0.439518	2.776081	-1.242663
H	1.851995	2.867559	-0.196322
C	1.113008	2.188044	-0.614974
N	0.387013	1.554735	0.471620
C	1.029905	1.489540	1.771896
H	1.525465	0.524953	1.940626
H	1.774332	2.280053	1.836857
H	0.304465	1.651192	2.572553
C	-0.581221	0.622354	0.164454
C	-1.130792	-0.219830	1.155882
C	-1.057298	0.466659	-1.155759
C	-2.130034	-1.131616	0.841205
H	-0.781634	-0.160591	2.177382
C	-2.057238	-0.451911	-1.448075
H	-0.650871	1.067669	-1.957349
C	-2.611016	-1.256808	-0.458023

H	-2.530670	-1.758281	1.630200
H	-2.400242	-0.539737	-2.472949
H	-3.386768	-1.973579	-0.695438
H	1.628811	1.455921	-1.249422
C	1.206975	-1.770450	-0.483124
O	1.985479	-0.959227	-0.211139
O	0.458930	-2.603824	-0.760809

IM39

Symbol	X	Y	Z
Si	0.562259	1.511216	-1.397328
H	1.203075	1.270870	-2.705286
H	-0.891174	1.711758	-1.674169
C	0.675465	0.020754	-0.254632
C	0.045969	-1.172574	-0.625330
C	1.301535	0.075888	0.996731
C	0.016339	-2.272469	0.229123
H	-0.451467	-1.247500	-1.587798
C	1.284459	-1.021488	1.853006
H	1.809187	0.983118	1.307998
C	0.636042	-2.196575	1.473984
H	-0.505162	-3.175240	-0.070735
H	1.772556	-0.959186	2.819510
H	0.611003	-3.045769	2.147661
C	1.115279	3.090417	-0.538798
C	0.172683	4.108843	-0.337143
C	2.417137	3.288742	-0.052017
C	0.510687	5.286078	0.326133
H	-0.841158	3.986127	-0.705728
C	2.754478	4.463007	0.614828
H	3.163952	2.515560	-0.203806
C	1.804242	5.463456	0.805111
H	-0.234488	6.060366	0.468566
H	3.763492	4.598933	0.987713
H	2.071259	6.376232	1.325173
N	4.745266	-2.459114	-0.015157
C	3.840323	-1.532320	-0.790007
H	3.986641	-1.764283	-1.844476
H	2.812361	-1.783467	-0.513791
C	4.037584	-0.004547	-0.588356
O	3.467234	0.655326	-1.474544
O	4.682989	0.400210	0.395848
C	6.178419	-2.127879	-0.286593
H	6.369150	-1.132227	0.102354

H	6.801404	-2.871165	0.207545	H	0.022235	-1.940340	-0.792725
H	6.338504	-2.159587	-1.363157	C	1.283759	-1.007263	2.739725
C	4.472704	-3.857124	-0.467428	H	1.423514	1.003797	2.011075
H	5.093640	-4.538479	0.111634	C	0.957143	-2.327915	2.443597
H	3.418625	-4.074840	-0.302692	H	0.245843	-3.680959	0.927673
H	4.712175	-3.936310	-1.526083	H	1.632270	-0.743946	3.731996
C	4.477791	-2.370398	1.454583	H	1.049865	-3.095716	3.203122
H	4.615301	-1.336052	1.753874	C	0.653155	2.843000	-0.412617
H	3.452913	-2.691529	1.629447	C	-0.463495	3.674425	-0.590305
H	5.174601	-3.031625	1.967029	C	1.826543	3.421271	0.089955
H	-2.922949	2.472810	0.159732	C	-0.404855	5.033706	-0.295523
C	-3.320679	1.526811	-0.230744	H	-1.394168	3.256414	-0.964277
O	-4.117967	1.510437	-1.162495	C	1.879181	4.775547	0.412257
N	-2.833655	0.451213	0.417515	H	2.707309	2.804848	0.230254
C	-2.093583	0.654472	1.662754	C	0.766413	5.586830	0.213987
H	-1.358360	-0.141404	1.773089	H	-1.275850	5.658992	-0.456135
H	-1.568897	1.609047	1.610778	H	2.794141	5.198947	0.811667
H	-2.767046	0.661103	2.522586	H	0.810542	6.642846	0.455050
C	-3.196252	-0.876061	0.049511	N	4.790358	-1.756754	-0.407043
C	-3.475623	-1.816122	1.037995	C	3.795054	-0.999834	-1.237235
C	-3.211887	-1.251330	-1.294423	H	4.221168	-0.859865	-2.232138
C	-3.767259	-3.128914	0.681984	H	2.906561	-1.627560	-1.327037
H	-3.469392	-1.525266	2.081036	C	3.349161	0.357251	-0.686056
C	-3.506370	-2.563284	-1.640642	O	2.362508	0.822201	-1.373539
H	-2.983094	-0.518949	-2.057705	O	3.885653	0.879721	0.271719
C	-3.784010	-3.508201	-0.655810	C	6.098820	-1.030425	-0.325519
H	-3.980849	-3.855247	1.457034	H	5.928187	-0.067459	0.144014
H	-3.510368	-2.849464	-2.685758	H	6.781452	-1.636781	0.266569
H	-4.010093	-4.531654	-0.929457	H	6.486538	-0.906978	-1.335092
H	-5.444342	0.421037	-0.969810	C	5.015429	-3.082600	-1.065496
H	-7.306480	-0.746023	0.809803	H	5.755964	-3.630864	-0.487094
C	-6.439545	-0.127136	0.546286	H	4.073077	-3.626448	-1.085354
O	-5.773604	0.466641	1.354137	H	5.376906	-2.914214	-2.077828
O	-6.240277	-0.128326	-0.760029	C	4.244506	-1.993936	0.970664
				H	4.174513	-1.041803	1.486334
				H	3.255583	-2.441984	0.874169

TS21

Symbol	X	Y	Z				
Si	0.515988	1.007350	-0.852520	H	4.920928	-2.670962	1.488653
H	0.166138	0.611096	-2.237688	H	-2.047497	1.838400	0.951912
H	-1.088075	1.057965	-0.485977	C	-2.452296	1.155105	0.194806
C	0.713779	-0.330178	0.471620	O	-3.228620	1.601607	-0.699802
C	0.392271	-1.666290	0.191927	N	-2.579894	-0.137623	0.699128
C	1.162794	-0.021142	1.762537	C	-2.327225	-0.365627	2.111553
C	0.509954	-2.656370	1.165733	H	-1.630944	-1.196229	2.249250
				H	-1.879942	0.531604	2.537233

H	-3.263328	-0.569140	2.639326	H	-1.402476	4.913129	-0.862880
C	-2.856466	-1.223054	-0.133782	N	5.988666	0.597811	0.679313
C	-3.242338	-2.452861	0.416433	C	5.072312	0.238357	-0.448050
C	-2.691649	-1.131351	-1.526882	H	5.268909	0.922513	-1.275092
C	-3.441856	-3.560118	-0.401467	H	5.320695	-0.771509	-0.777032
H	-3.384336	-2.549487	1.484685	C	3.586570	0.287501	-0.130892
C	-2.894708	-2.245490	-2.328181	O	2.903435	-0.074118	-1.193551
H	-2.411445	-0.187597	-1.972621	O	3.105731	0.610092	0.925574
C	-3.267226	-3.470125	-1.777592	C	5.759734	2.008836	1.137268
H	-3.738504	-4.500631	0.048737	H	4.760462	2.083567	1.553348
H	-2.756029	-2.153535	-3.399617	H	6.508628	2.237422	1.892250
H	-3.424492	-4.334209	-2.411212	H	5.874453	2.670223	0.280532
H	-4.559013	0.899386	-0.755254	C	7.393619	0.482223	0.165991
H	-6.924694	-0.447886	0.184490	H	8.072249	0.745939	0.973565
C	-5.968809	0.082747	0.308176	H	7.564557	-0.543955	-0.152147
O	-5.477889	0.289567	1.392302	H	7.516820	1.166344	-0.670768
O	-5.475869	0.442681	-0.851850	C	5.821916	-0.347745	1.832936
				H	4.822252	-0.231632	2.238770
				H	5.979729	-1.361422	1.469117

IM40

Symbol	X	Y	Z				
Si	1.167044	-0.216674	-1.227168	H	6.571102	-0.096202	2.580503
H	0.999231	-0.732225	-2.593122	H	-3.266161	1.487584	1.202413
H	-2.204649	1.353219	-0.223535	C	-3.146624	1.023626	0.220592
C	0.693715	-1.447770	0.082093	O	-4.181854	1.427508	-0.636190
C	1.036481	-2.792648	-0.105622	N	-3.073419	-0.407818	0.444595
C	0.028823	-1.084612	1.259775	C	-3.798035	-0.965544	1.573528
C	0.737338	-3.747877	0.860166	H	-3.150030	-1.596463	2.190710
H	1.536615	-3.104423	-1.018289	H	-4.171338	-0.140677	2.179460
C	-0.272650	-2.037233	2.226062	H	-4.652827	-1.570600	1.247212
H	-0.278422	-0.056680	1.417968	C	-2.658455	-1.244070	-0.571475
C	0.083992	-3.368813	2.028103	C	-2.560421	-2.635133	-0.374115
H	1.007062	-4.785013	0.698640	C	-2.287222	-0.736370	-1.834086
H	-0.784864	-1.741795	3.134477	C	-2.063046	-3.461018	-1.372629
H	-0.150269	-4.110594	2.783151	H	-2.839875	-3.068553	0.576892
C	0.412109	1.477979	-1.068450	C	-1.794983	-1.579455	-2.822076
C	-0.273760	1.997869	-2.175227	H	-2.429171	0.313373	-2.048796
C	0.449450	2.240574	0.109053	C	-1.664414	-2.948264	-2.603927
C	-0.922855	3.226077	-2.105817	H	-1.978258	-4.524623	-1.176454
H	-0.317378	1.429237	-3.099474	H	-1.519468	-1.154639	-3.782093
C	-0.198653	3.469530	0.180139	H	-1.278245	-3.600076	-3.377754
H	0.989594	1.874850	0.974617	H	-5.024124	1.356536	-0.113342
C	-0.890944	3.959683	-0.923429	H	-7.250447	1.648825	2.549631
H	-1.455781	3.606500	-2.969070	C	-6.291925	1.618107	1.976642
H	-0.167966	4.043175	1.098931	O	-5.264695	1.957073	2.584401
				O	-6.403664	1.234353	0.783683

IM41

Symbol	X	Y	Z
Si	-0.430441	0.104816	1.146346
H	-0.004483	-0.088057	2.538996
H	2.427765	1.693442	-0.737196
C	0.072623	-1.290119	0.023144
C	-0.012790	-2.604382	0.499417
C	0.499001	-1.083716	-1.294771
C	0.306046	-3.683317	-0.319191
H	-0.323822	-2.793349	1.522996
C	0.813744	-2.159987	-2.116618
H	0.591493	-0.076439	-1.687708
C	0.717257	-3.461105	-1.628931
H	0.237598	-4.693902	0.066142
H	1.129302	-1.985300	-3.138809
H	0.964081	-4.299843	-2.269701
C	0.021762	1.808074	0.543743
C	0.808125	2.618505	1.375552
C	-0.322351	2.294446	-0.726707
C	1.258951	3.862822	0.946493
H	1.086134	2.269203	2.365465
C	0.125183	3.539863	-1.155950
H	-0.945520	1.697857	-1.382935
C	0.922869	4.320670	-0.323796
H	1.874806	4.470471	1.598826
H	-0.145907	3.899276	-2.141530
H	1.278635	5.286229	-0.663593
N	-5.504370	-0.140204	-0.152936
C	-4.416788	-0.209673	0.874292
H	-4.628532	0.532323	1.645059
H	-4.450638	-1.197882	1.336343
C	-3.009128	0.026597	0.353032
O	-2.156233	-0.011397	1.352619
O	-2.714670	0.217049	-0.799642
C	-5.556913	1.214666	-0.797036
H	-4.639900	1.374229	-1.354332
H	-6.417667	1.233506	-1.461739
H	-5.670833	1.962241	-0.014207
C	-6.804731	-0.380562	0.556283
H	-7.604355	-0.338332	-0.179706
H	-6.771826	-1.362491	1.023275
H	-6.941964	0.394427	1.307444
C	-5.326946	-1.200644	-1.200712
H	-4.416222	-0.996760	-1.754083

Symbol	X	Y	Z
H	-5.271053	-2.166869	-0.702922
H	-6.192502	-1.167018	-1.858514
H	3.258580	1.661566	-2.306103
C	3.365546	1.447085	-1.239723
O	4.334829	2.300669	-0.652555
N	3.646413	0.045932	-1.101516
C	4.192732	-0.698699	-2.221571
H	3.493233	-1.458790	-2.584964
H	4.399658	-0.007616	-3.037266
H	5.128288	-1.196713	-1.948317
C	3.446600	-0.588311	0.114536
C	3.496897	-1.988736	0.219650
C	3.169903	0.153325	1.279320
C	3.238787	-2.615117	1.431841
H	3.704177	-2.594336	-0.652581
C	2.911030	-0.491210	2.481953
H	3.198052	1.233648	1.244465
C	2.932849	-1.880117	2.572988
H	3.263614	-3.698462	1.475604
H	2.699135	0.106403	3.362513
H	2.730109	-2.376710	3.513715
H	5.179468	2.123807	-1.079120

BE

Symbol	X	Y	Z
N	-1.761769	2.232334	0.029223
C	-1.339810	0.837171	-0.361553
H	-2.036736	0.143132	0.104368
H	-1.450606	0.765899	-1.444138
C	0.102128	0.377625	0.026525
O	0.325164	-0.772455	-0.373705
O	0.835158	1.154938	0.665662
C	-1.715379	2.396751	1.517080
H	-0.674085	2.338596	1.816340
H	-2.154321	3.360514	1.771157
H	-2.279286	1.589919	1.979162
C	-3.151054	2.517988	-0.490886
H	-3.343466	3.569269	-0.267816
H	-3.098064	2.400703	-1.574623
C	-0.842054	3.233943	-0.603397
H	0.161785	3.029652	-0.246367
H	-0.902057	3.115357	-1.683944
H	-1.171718	4.230591	-0.316169
C	-4.259949	1.646009	0.089345

H	-4.317599	1.756828	1.172906	H	2.081129	-2.927201	1.712738				
H	-4.098905	0.592848	-0.142631	C	1.596393	-1.997187	-0.798132				
C	-5.578654	2.091732	-0.523299	H	2.064934	-2.887786	-1.220166				
H	-5.602041	1.950381	-1.600884	H	0.992103	-1.522626	-1.573810				
H	-5.819845	3.123083	-0.278369	C	-0.482732	-3.215585	-0.489839				
Br	-7.059345	1.021957	0.181193	H	-1.154679	-3.656688	0.239351				
BE-TS											
Symbol	X	Y	Z	H	-1.012563	-2.488733	-1.105792				
Si	-2.264812	1.025180	1.101563	H	-0.027910	-3.983869	-1.112447				
H	-3.262852	1.348588	2.142850	C	2.643510	-1.018136	-0.273121				
H	-2.755616	2.288122	0.206470	H	3.179395	-1.429299	0.584498				
C	-0.517500	1.772163	1.127705	H	2.180154	-0.076301	0.030978				
C	0.361918	1.599331	2.206297	C	3.637375	-0.731414	-1.387332				
C	-0.054048	2.494472	0.019470	H	3.162073	-0.288027	-2.259214				
C	1.658723	2.104372	2.169831	H	4.202498	-1.613387	-1.678042				
H	0.032886	1.047803	3.081226	Br	4.962570	0.576119	-0.784290				
C	1.252508	2.975602	-0.036792	C	-3.818490	2.869435	-0.806242				
H	-0.727718	2.697512	-0.807757	O	-3.141614	3.378443	-1.632469				
C	2.112606	2.779484	1.039093	O	-4.862237	2.570853	-0.341174				
H	2.318368	1.964049	3.018573	BE-TD-COFS							
H	1.593554	3.512451	-0.914719	Symbol	X	Y	Z				
H	3.128421	3.154666	1.000089	N	-4.565215	-0.058889	0.713445				
C	-2.740749	-0.168448	-0.304137	C	-4.959839	-1.087319	-0.317497				
C	-2.348458	0.067584	-1.629018	H	-4.390745	-0.874966	-1.220692				
C	-3.503215	-1.316084	-0.044245	H	-4.646606	-2.058007	0.068648				
C	-2.686725	-0.815527	-2.651709	C	-6.465647	-1.169084	-0.724348				
H	-1.772161	0.954924	-1.872968	O	-6.655992	-2.071166	-1.550680				
C	-3.872909	-2.185722	-1.067725	O	-7.274198	-0.366507	-0.221794				
H	-3.808411	-1.537768	0.973433	C	-4.878990	1.320060	0.221093				
C	-3.457538	-1.941706	-2.373266	H	-5.958996	1.403449	0.159522				
H	-2.358021	-0.619637	-3.665858	H	-4.458497	2.040139	0.921398				
H	-4.475806	-3.058146	-0.842786	H	-4.440819	1.450522	-0.765376				
H	-3.732574	-2.623134	-3.169709	C	-3.093299	-0.184675	1.031430				
N	0.614056	-2.500479	0.243922	H	-2.899515	0.534083	1.830352				
C	0.064506	-1.310427	0.969293	H	-2.957925	-1.189219	1.436035				
H	0.867366	-0.889525	1.575777	C	-5.313589	-0.305468	1.988919				
H	-0.195155	-0.581036	0.204538	H	-6.372945	-0.220494	1.771255				
C	-1.125640	-1.552088	1.907510	H	-5.068714	-1.307101	2.338421				
O	-1.767635	-0.474212	2.213668	H	-4.996444	0.435370	2.720663				
O	-1.368008	-2.657351	2.352187	C	-2.149741	0.050588	-0.137597				
C	1.290828	-3.452664	1.182224	H	-2.303988	1.034714	-0.584146				
H	0.546930	-3.816924	1.883282	H	-2.280693	-0.704749	-0.913790				
H	1.706462	-4.267944	0.593392	C	-0.713316	-0.028331	0.351415				
				H	-0.510066	-0.993370	0.828820				

H	-0.497337	0.768319	1.073399	H	9.231639	-1.806772	-1.467976
O	0.122006	0.125684	-0.795379	H	8.347774	-4.020363	-2.152106
C	1.468106	0.112713	-0.505872	C	4.790209	1.350300	-0.006411
C	2.160315	1.307592	-0.320663	C	4.611120	2.535026	0.716384
C	2.144774	-1.096716	-0.421303	C	4.677461	1.408785	-1.401606
C	3.534156	1.264786	-0.065053	C	4.306011	3.732371	0.072000
C	3.511606	-1.158847	-0.159731	H	4.703517	2.525598	1.798718
H	1.586367	-2.014495	-0.574437	C	4.389140	2.604525	-2.053437
C	4.217703	0.056991	0.019358	H	4.812408	0.503891	-1.988337
H	4.041280	2.210770	0.063401	C	4.193394	3.769034	-1.314694
C	4.103037	-2.510331	-0.098814	H	4.158085	4.636221	0.651966
H	3.374486	-3.307003	-0.310390	H	4.312028	2.628018	-3.134620
N	5.307844	-2.789916	0.169251	H	3.959089	4.700012	-1.817580
C	5.662218	-4.197927	0.176181	C	7.243502	1.348093	2.423908
H	6.061616	-4.458934	1.158928	O	8.189695	1.536527	1.744968
H	6.462478	-4.366257	-0.548177	O	6.568971	1.521178	3.376685
H	4.820121	-4.861154	-0.057719	N	0.764705	-0.389573	-0.819005
O	5.541067	-0.022375	0.259556	C	1.109982	-1.552870	0.072096
C	6.261034	1.189157	0.428224	H	0.499633	-1.478201	0.969664
H	7.292628	0.896450	0.604555	H	0.826600	-2.461819	-0.460329
H	5.888194	1.752739	1.287536	C	2.566284	-1.705987	0.542121
H	6.204290	1.809180	-0.470323	O	2.771719	-2.595474	1.345137
C	1.449746	2.599913	-0.409525	O	3.421605	-0.891846	0.042442
H	0.388593	2.548064	-0.678113	C	1.124799	0.920448	-0.178943
N	2.037649	3.699201	-0.191810	H	2.204030	1.035407	-0.210424
C	1.251363	4.912938	-0.308215	H	0.636921	1.714764	-0.742003
H	1.287838	5.451745	0.641209	H	0.774105	0.917980	0.850773
H	0.205511	4.725925	-0.577976	C	-0.722048	-0.428750	-1.116405
H	1.707045	5.560183	-1.060833	H	-0.881768	0.306654	-1.906623

BE-TD-COFS-TS

Symbol	X	Y	Z				
Si	5.087808	-0.305737	0.858658	H	2.546063	-0.536929	-1.941433
H	4.475269	-0.541216	2.190524	H	1.143768	-1.418670	-2.626138
H	6.427587	0.245481	1.577378	H	1.220692	0.362152	-2.736154
C	6.111165	-1.571542	-0.103302	C	-1.629330	-0.132990	0.067433
C	5.628957	-2.823203	-0.506015	H	-1.461073	0.875363	0.449644
C	7.425364	-1.230473	-0.454610	H	-1.480192	-0.839459	0.885473
C	6.431184	-3.703866	-1.227867	C	-3.079806	-0.231682	-0.375957
H	4.622706	-3.123186	-0.236575	H	-3.318223	-1.239730	-0.732252
C	8.222676	-2.096358	-1.197293	H	-3.294273	0.481032	-1.181533
H	7.829621	-0.273623	-0.136077	O	-3.878979	0.078144	0.764080
C	7.726623	-3.338786	-1.582419	C	-5.232592	0.067731	0.508848
H	6.043609	-4.674075	-1.517503	C	-5.890507	1.238305	0.136418
				C	-5.949016	-1.113181	0.645517

C	-7.270113	1.200706	-0.086262	C	-0.648084	-3.960856	0.480209
C	-7.323394	-1.169865	0.425137	H	0.728758	-2.781227	-0.652903
H	-5.416010	-2.010505	0.942582	C	-2.617939	-2.830601	1.269824
C	-7.993784	0.020933	0.049377	H	-2.819114	-0.778315	0.686851
H	-7.750308	2.127994	-0.365842	C	-1.848747	-3.986327	1.185196
C	-7.959334	-2.488794	0.613559	H	-0.047181	-4.859837	0.400482
H	-7.250091	-3.263414	0.940970	H	-3.556822	-2.841326	1.812000
N	-9.180691	-2.764821	0.430733	H	-2.183529	-4.901658	1.659682
C	-9.581120	-4.138411	0.677526	C	-0.053481	1.603497	0.111367
H	-10.020946	-4.549441	-0.234086	C	-0.974355	2.093872	1.045915
H	-10.362324	-4.148738	1.441104	C	1.128107	2.333613	-0.075373
H	-8.754229	-4.783112	1.000455	C	-0.722047	3.250622	1.779392
O	-9.323700	-0.051745	-0.153583	H	-1.910695	1.566142	1.202606
C	-10.006707	1.136561	-0.522745	C	1.376539	3.506161	0.632945
H	-11.050417	0.854332	-0.632050	H	1.869183	1.982122	-0.786582
H	-9.631409	1.527705	-1.472103	C	0.453859	3.964478	1.569137
H	-9.913104	1.901675	0.252438	H	-1.445726	3.598899	2.507744
C	-5.137999	2.502488	-0.001810	H	2.292609	4.059267	0.458416
H	-4.076510	2.463296	0.268277	H	0.649337	4.871807	2.128970
N	-5.692516	3.567219	-0.401837	C	2.172904	-0.642851	0.039930
C	-4.867556	4.756884	-0.496381	C	3.666661	-0.809679	-0.361850
H	-4.896282	5.127915	-1.523276	O	4.513860	-1.051427	0.474731
H	-3.825535	4.584551	-0.202962	O	1.871354	-0.686781	1.210386
H	-5.295738	5.536665	0.137328	O	1.387168	-0.462505	-0.975659

Oxamic

Symbol	X	Y	Z
C	-0.118904	-0.762376	-0.112823
C	0.	-0.122926	0.799408
O	-1.123784	1.438874	0.380777
O	-1.213835	-1.321842	0.025915
O	0.996141	-1.248769	-0.396662
N	1.097153	1.347457	-0.067626
H	1.855820	0.727104	-0.301221
H	1.237105	2.339652	0.033282

Oxamic-TS

Symbol	X	Y	Z
Si	-0.449484	0.027088	-0.884814
H	0.	-0.385747	0.105021
H	-2.000552	0.463488	-0.928378
C	-0.972033	-1.603979	-0.048806
C	-0.213835	-2.781464	-0.117269
C	-2.188461	-1.661305	0.645470

C	-0.648084	-3.960856	0.480209
H	0.728758	-2.781227	-0.652903
C	-2.617939	-2.830601	1.269824
H	-2.819114	-0.778315	0.686851
C	-1.848747	-3.986327	1.185196
H	-0.047181	-4.859837	0.400482
H	-3.556822	-2.841326	1.812000
H	-2.183529	-4.901658	1.659682
C	-0.053481	1.603497	0.111367
C	-0.974355	2.093872	1.045915
C	1.128107	2.333613	-0.075373
C	-0.722047	3.250622	1.779392
H	-1.910695	1.566142	1.202606
C	1.376539	3.506161	0.632945
H	1.869183	1.982122	-0.786582
C	0.453859	3.964478	1.569137
H	-1.445726	3.598899	2.507744
H	2.292609	4.059267	0.458416
H	0.649337	4.871807	2.128970
C	2.172904	-0.642851	0.039930
C	3.666661	-0.809679	-0.361850
O	4.513860	-1.051427	0.474731
O	1.871354	-0.686781	1.210386
O	1.387168	-0.462505	-0.975659
N	3.898843	-0.647145	-1.675453
H	3.126632	-0.475105	-2.298874
H	4.835189	-0.742896	-2.035933
C	-3.234662	1.511425	-1.352284
O	-2.801151	2.051322	-2.302240
O	-4.032900	1.275089	-0.519263

Salicylic

Symbol	X	Y	Z
C	-1.480900	0.194744	1.182155
C	0.	-2.873780	0.869727
C	-3.861412	0.605012	2.102743
H	-2.728391	1.922651	0.726342
C	-4.163930	-1.028816	0.301747
C	-4.689555	-0.634313	1.680801
H	-4.508471	1.466264	2.269971
H	-3.305675	0.415867	3.018219
H	-4.920182	-1.382588	-0.397192
H	-3.352702	-1.746021	0.386655
H	-5.753487	-0.400653	1.644689

H	-4.553128	-1.463506	2.371778	C	-0.140007	3.759535	0.275954
N	-3.551385	0.235325	-0.250131	H	-0.706569	2.848044	-1.577013
C	-4.626084	1.146805	-0.747320	C	-0.276821	2.361386	2.231096
H	-4.161874	2.062578	-1.107042	H	-0.930021	0.343984	1.904425
H	-5.157353	0.649297	-1.556479	C	0.022873	3.590083	1.648686
H	-5.311828	1.371772	0.065942	H	0.085131	4.715360	-0.183599
C	-2.606211	-0.053101	-1.365463	H	-0.158293	2.225579	3.300227
H	-2.112154	0.873569	-1.649947	H	0.376591	4.411588	2.260798
H	-1.873061	-0.778016	-1.020848	C	-1.870952	-1.659496	-0.301855
H	-3.175677	-0.456580	-2.200840	C	-1.211265	-2.851446	-0.628566
O	-0.505441	0.866534	0.811580	C	-2.933939	-1.729067	0.608051
O	-1.513290	-0.949327	1.678190	C	-1.601839	-4.066898	-0.075167

Salicylic-TS

Symbol	X	Y	Z
C	1.286859	-0.788514	-0.427171
C	0.2749997	-0.787233	-0.910018
C	3.520360	-2.006516	-0.395430
H	2.779438	-0.654044	-1.989428
C	3.826482	-0.085824	1.108409
C	4.161236	-1.569898	0.945604
H	4.280098	-2.308134	-1.115276
H	2.837032	-2.843141	-0.263303
H	4.640252	0.528735	1.488770
H	2.935591	0.056100	1.714421
H	5.238250	-1.732557	0.931159
H	3.749051	-2.126891	1.784123
N	3.481629	0.393138	-0.282638
C	4.737005	0.650007	-1.055033
H	4.466983	0.941960	-2.067537
H	5.282326	1.452087	-0.562358
H	5.341007	-0.253971	-1.072760
C	2.664288	1.643264	-0.247169
H	2.357656	1.890973	-1.262178
H	1.790978	1.480917	0.382562
H	3.280741	2.438585	0.167871
O	0.446795	-0.464174	-1.345519
O	1.045960	-1.071782	0.733713
Si	-1.411407	0.016295	-1.051087
H	-2.971810	0.461312	-0.953883
H	-1.440019	0.273509	-2.512240
C	-0.876892	1.449696	0.057548
C	-0.588900	2.699350	-0.507657
C	-0.723174	1.303139	1.441691

C	-3.310856	-2.937804	1.188943
H	-3.478273	-0.823416	0.860574
C	-2.648605	-4.111401	0.842521
H	-1.086318	-4.978998	-0.353926
H	-4.126962	-2.965107	1.902042
H	-2.947176	-5.055957	1.282514
C	-3.910883	1.787041	-0.749361
O	-3.729820	2.401686	-1.738688
O	-4.397595	1.587715	0.306322

Lecithin

Symbol	X	Y	Z
C	1.358338	-1.008324	-0.020893
H	1.839310	-1.432257	-0.903386
C	0.978953	0.432345	-0.287089
H	0.232148	0.474103	-1.080789
H	0.570850	0.871141	0.626677
O	2.181146	1.102679	-0.674861
C	2.203857	2.436547	-0.882494
O	3.235809	2.934578	-1.240303
C	0.138249	-1.844210	0.330717
H	-0.370827	-1.413815	1.197999
H	0.453959	-2.859020	0.579978
O	-0.708906	-1.869232	-0.807291
P	-2.303149	-1.587713	-0.610980
O	-2.825173	-2.309392	0.586697
O	-2.931118	-1.714679	-1.953190
O	-2.169913	0.016689	-0.204336
C	-3.248022	0.583842	0.507555
H	-4.168656	0.551697	-0.086829
H	-3.415868	0.043463	1.443869

C	-2.847864	2.022529	0.774247	O	-5.595611	-1.258667	2.574060
H	-2.695211	2.564318	-0.156614	C	-2.173912	0.314911	-1.973595
H	-1.946479	2.069053	1.381342	H	-2.417510	1.380738	-1.997393
H	-3.680375	3.708530	1.702151	H	-2.105022	-0.057310	-2.995950
H	-4.813820	2.732562	1.011939	O	-0.943450	0.082630	-1.286741
H	-4.106820	2.297398	2.438178	P	0.084016	1.295284	-1.069463
N	-3.930433	2.732310	1.528958	O	0.399350	2.055166	-2.300297
O	2.218220	-1.060378	1.118823	O	1.216061	0.704079	-0.238678
C	3.568020	-1.112918	1.025998	O	-0.800047	2.198007	-0.042486
O	4.196467	-1.008256	2.043592	C	-0.316432	3.498136	0.264360
C	0.933864	3.204819	-0.636490	H	0.646124	3.430647	0.781022
H	0.100957	2.780834	-1.198756	H	-0.191974	4.077534	-0.654935
H	0.676022	3.171264	0.424108	C	-1.371956	4.120004	1.159044
H	1.096057	4.235983	-0.936177	H	-1.463544	3.578282	2.097610
C	4.197990	-1.334672	-0.323043	H	-2.334963	4.148282	0.654208
H	3.854673	-2.274989	-0.758134	H	-1.710714	5.963322	2.089788
H	3.940722	-0.522844	-1.002808	H	-0.111424	5.581852	2.002835
H	5.274010	-1.374270	-0.180571	H	-0.909371	6.114050	0.659706
				N	-0.999444	5.530574	1.495837
				O	-4.464030	-0.239059	-1.920359

Lecithin-TS

Symbol	X	Y	Z				
Si	2.417911	-0.745570	-0.461830	C	-5.313411	-1.242958	-2.248076
H	3.420190	-1.969911	-0.698500	O	-6.340102	-0.941956	-2.790661
C	1.642197	-1.677854	1.015457	C	-4.064101	0.560812	2.859884
C	0.537121	-1.210365	1.745613	H	-2.990659	0.368944	2.908421
C	2.196457	-2.904508	1.413109	H	-4.208930	1.523572	2.366857
C	0.006996	-1.935503	2.809400	H	-4.473907	0.596946	3.864916
H	0.088110	-0.261056	1.481057	C	-4.922763	-2.659082	-1.923910
C	1.675598	-3.632347	2.480879	H	-3.985131	-2.929199	-2.412382
H	3.050835	-3.300737	0.873896	H	-4.798609	-2.778907	-0.846935
C	0.574914	-3.150805	3.181154	H	-5.716742	-3.309272	-2.279219
H	-0.850514	-1.551519	3.351217	H	1.900382	-0.927521	-1.849106
H	2.128152	-4.576361	2.762927	C	3.896365	0.409298	-0.151575
H	0.163217	-3.715922	4.009493	C	3.907279	1.758010	-0.531408
C	4.634653	-2.676363	-1.628535	C	5.042886	-0.097104	0.475402
O	5.067405	-3.456119	-0.861620	C	5.021241	2.563477	-0.306203
O	4.544174	-2.098995	-2.646485	H	3.034715	2.183140	-1.015485
C	-3.244983	-0.445172	-1.209988	C	6.150065	0.708038	0.728984
H	-2.976255	-1.500848	-1.161047	H	5.072218	-1.143147	0.768581
C	-3.405355	0.083832	0.199102	C	6.143146	2.042153	0.331972
H	-2.447531	0.017468	0.718040	H	5.012306	3.599974	-0.624527
H	-3.743210	1.122817	0.172627	H	7.019167	0.294030	1.227610
O	-4.383254	-0.749515	0.823281	H	7.006922	2.670485	0.516440
C	-4.753539	-0.543317	2.106399				

S-IM1

Symbol	X	Y	Z			
N	1.452834	-0.700571	0.919556	H	1.861310	-2.452315
H	0.443359	-0.793166	0.921803	H	3.282529	-1.421513
C	2.175685	-1.497254	1.891682	H	1.926080	-0.853911
H	1.593012	-2.391134	2.109797	C	1.836235	0.574114
H	3.138308	-1.815445	1.483463	C	3.146420	1.035678
H	2.359001	-0.956851	2.828581	C	0.764596	1.456586
C	1.892621	0.569304	0.582101	C	3.375678	2.391304
C	3.205936	0.994429	0.829582	H	3.974123	0.339156
C	1.015076	1.449310	-0.077852	C	1.004899	2.810403
C	3.620740	2.259274	0.420200	H	-0.249409	1.085802
H	3.903607	0.339655	1.336071	C	2.309005	3.281236
C	1.442112	2.705376	-0.475968	H	4.393381	2.751899
H	-0.006397	1.130911	-0.258605	H	0.168355	3.494981
C	2.751386	3.124095	-0.233745	H	0.2495125	4.335862
H	4.640610	2.567461	0.621317	C	2.160600	-1.714764
H	0.744463	3.366976	-0.977158	O	3.286507	-2.044918
H	3.081770	4.106906	-0.545552	O	1.239086	-1.693656
C	2.167402	-1.668883	-1.560778	N	-1.303796	-1.405202
O	3.252300	-1.811449	-1.194572	H	-0.830273	-1.375451
O	1.097179	-1.547234	-1.983630	C	-1.426216	-2.761754
N	-1.400956	-1.248640	-0.189976	H	-0.547167	-3.324425
H	-0.943314	-1.194404	-1.090498	H	-1.453422	-2.754848
C	-1.382146	-2.586344	0.381200	H	-2.323321	-3.272862
H	-0.453350	-3.070905	0.080469	C	-2.397272	-0.539958
H	-1.398501	-2.537811	1.472705	C	-3.427964	-0.726607
H	-2.227197	-3.201190	0.049968	C	-2.446803	0.580546
C	-2.550437	-0.468174	-0.104827	C	-4.469469	0.193955
C	-3.545496	-0.711947	0.850612	H	-3.419856	-1.585490
C	-2.705781	0.626134	-0.972862	C	-3.490553	1.488369
C	-4.651361	0.129572	0.939273	H	-1.655811	0.727674
H	-3.458924	-1.553851	1.525671	C	-4.511559	1.305103
C	-3.812908	1.453973	-0.874823	H	-5.257356	0.032006
H	-1.950818	0.812495	-1.730393	H	-3.508854	2.344090
C	-4.796431	1.216186	0.085141	H	-5.326058	2.015016
H	-5.408911	-0.076059	1.686930			
H	-3.911119	2.290241	-1.557404			
H	-5.660664	1.864057	0.159461			

S-TS1

Symbol	X	Y	Z
N	1.583783	-0.832982	0.558458
H	0.567767	-0.983254	0.552069
C	2.201656	-1.422119	1.759495

S-IM2

Symbol	X	Y	Z
N	1.685477	-0.203696	0.353803
H	0.890749	-0.869403	0.393070
C	2.632309	-0.496659	1.455185
H	2.906302	-1.549148	1.404198
H	3.519172	0.116977	1.317975
H	2.155551	-0.274253	2.409012
C	1.166791	1.157524	0.409094

C	2.005351	2.219513	0.085414	C	-0.665509	2.374854	1.219822
C	-0.145536	1.373961	0.810316	H	-0.144524	0.512974	2.156342
C	1.509106	3.516129	0.150582	C	-0.406647	3.248096	0.166895
H	3.025737	2.027521	-0.223470	H	0.829711	3.639329	-1.545683
C	-0.632116	2.676491	0.868751	H	-1.463504	2.586236	1.921315
H	-0.783171	0.536818	1.071783	H	-0.997397	4.148227	0.048630
C	0.191935	3.746856	0.538626	C	2.513616	-0.743598	-0.706156
H	2.154390	4.347336	-0.105240	O	3.720877	-0.649659	-0.696939
H	-1.656775	2.848933	1.174428	O	1.712249	-1.135405	-1.592217
H	-0.189723	4.759306	0.584934	N	-0.141209	-1.886659	-0.086717
C	2.368000	-0.509906	-1.146924	H	0.469137	-1.722290	-0.956204
O	3.547050	-0.252781	-1.146629	C	-0.178421	-3.302317	0.307346
O	1.511684	-0.922945	-1.899305	H	0.821629	-3.712923	0.171478
N	-0.418288	-2.258645	0.002086	H	-0.464573	-3.407555	1.353150
H	0.067974	-2.420533	-0.873193	H	-0.883649	-3.846383	-0.320844
C	-0.385050	-3.401094	0.907337	C	-1.395515	-1.179546	-0.200279
H	0.586372	-3.883960	0.815922	C	-2.426476	-1.387227	0.706828
H	-0.500109	-3.068639	1.940417	C	-1.513187	-0.224663	-1.207379
H	-1.170311	-4.132755	0.686650	C	-3.582545	-0.617649	0.611426
C	-1.627893	-1.575476	-0.194571	H	-2.334378	-2.132689	1.487159
C	-2.667565	-1.629246	0.738692	C	-2.666556	0.541629	-1.288363
C	-1.761976	-0.743912	-1.317524	H	-0.688613	-0.077633	-1.896378
C	-3.807855	-0.848234	0.556594	C	-3.703153	0.349771	-0.378479
H	-2.590958	-2.267539	1.609616	H	-4.388696	-0.777459	1.317057
C	-2.903828	0.022096	-1.488369	H	-2.753795	1.292165	-2.064345
H	-0.943615	-0.691203	-2.027296	H	-4.602993	0.948641	-0.445040
C	-3.935833	-0.018378	-0.549828				
H	-4.602416	-0.897782	1.292186				
H	-2.987790	0.661880	-2.359290				
H	-4.825110	0.584494	-0.684741				

S-TS2

Symbol	X	Y	Z
N	1.793647	-0.343528	0.581158
H	0.642568	-1.273152	0.515172
C	2.692188	-0.364376	1.748313
H	3.119889	-1.361235	1.847714
H	3.505721	0.350291	1.613900
H	2.124549	-0.119952	2.645957
C	1.094925	0.915573	0.447591
C	1.373655	1.801506	-0.589406
C	0.081526	1.214265	1.359413
C	0.614966	2.959489	-0.729848
H	2.170741	1.579747	-1.289695

S-IM3

Symbol	X	Y	Z
N	1.097090	1.567583	1.786780
H	-0.024939	-0.553482	1.418465
C	1.589115	2.889739	2.171532
H	0.876045	3.354685	2.847820
H	2.559995	2.818488	2.669885
H	1.691059	3.500316	1.276477
C	1.535120	1.022418	0.544275
C	2.390214	-0.079183	0.517177
C	1.107502	1.602178	-0.648850
C	2.786413	-0.618907	-0.702196
H	2.729232	-0.515373	1.449812
C	1.519983	1.070254	-1.866102
H	0.440054	2.455821	-0.614865
C	2.351317	-0.047760	-1.895973
H	3.442228	-1.481062	-0.719336

H	1.181032	1.520622	-2.791226
H	2.663395	-0.467286	-2.844328
C	0.501642	0.805956	2.762396
O	0.386013	1.189267	3.906620
O	0.026170	-0.387373	2.395593
N	-0.476908	-1.411783	-0.096490
H	0.076726	-1.049264	-0.866615
C	-0.090095	-2.777701	0.255455
H	0.992272	-2.857057	0.163592
H	-0.356055	-2.986296	1.293190
H	-0.565126	-3.524358	-0.388905
C	-1.846168	-1.122087	-0.262729
C	-2.838060	-1.871131	0.375981
C	-2.220377	-0.017080	-1.038104
C	-4.176681	-1.510573	0.242556
H	-2.573477	-2.731564	0.976957
C	-3.557084	0.329955	-1.166279
H	-1.453643	0.561216	-1.542852
C	-4.546970	-0.412711	-0.524411
H	-4.933599	-2.101821	0.744625
H	-3.827496	1.185206	-1.774445
H	-5.589909	-0.140003	-0.625690

O	-0.495383	-1.597061	1.167227
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S-IM5

Symbol	X	Y	Z
Si	1.883580	0.359819	-1.414948
H	1.192586	-0.330379	-2.525813
H	2.877706	1.286361	-2.027153
C	0.633014	1.365898	-0.440076
C	-0.654380	1.578571	-0.949273
C	0.966468	1.960451	0.784403
C	-1.580657	2.356045	-0.259573
H	-0.942815	1.125764	-1.893353
C	0.043965	2.738152	1.478474
H	1.956550	1.812619	1.203640
C	-1.232426	2.935522	0.958065
H	-2.573673	2.505196	-0.668884
H	0.319299	3.188275	2.425265
H	-1.952509	3.539998	1.498026
C	2.879914	-0.790321	-0.314233
C	4.138422	-1.241345	-0.732733
C	2.415777	-1.193335	0.943865
C	4.914568	-2.062130	0.081142
H	4.525635	-0.945485	-1.703842

S-IM4

Symbol	X	Y	Z
N	-2.078868	-1.240825	-0.477060
H	-0.335938	-0.664736	0.978428
C	-3.109257	-1.783081	-1.363316
H	-2.795880	-2.761224	-1.719350
H	-4.063483	-1.880036	-0.839026
H	-3.232329	-1.111032	-2.209949
C	-1.962488	0.178931	-0.357372
C	-2.302108	0.819487	0.834621
C	-1.525767	0.924597	-1.452135
C	-2.189086	2.202913	0.931730
H	-2.658280	0.234608	1.675117
C	-1.434104	2.307096	-1.353889
H	-1.256346	0.413646	-2.369138
C	-1.761254	2.948132	-0.161567
H	-2.448892	2.696365	1.860116
H	-1.095816	2.883149	-2.206368
H	-1.682675	4.025634	-0.086047
C	-1.452655	-2.114257	0.368070
O	-1.697259	-3.297177	0.409993

C	3.190072	-2.009352	1.763017
H	1.435679	-0.870771	1.278389
C	4.441613	-2.443093	1.333242
H	5.886521	-2.399509	-0.259731
H	2.817994	-2.308243	2.736528
H	5.045683	-3.076932	1.971687
C	5.089068	1.746336	-0.297796
O	5.846157	1.447754	-1.119186
O	4.331834	2.044974	0.523751
N	-2.250319	-1.057859	0.390740
H	-2.889085	-0.980288	-1.888322
C	-1.562474	-0.831931	1.663992
H	-1.030258	0.123178	1.655958
H	-2.300724	-0.836991	2.462758
H	-0.849737	-1.637636	1.826623
C	-3.634591	-0.749457	0.286182
C	-4.136946	0.405613	0.889746
C	-4.507212	-1.619483	-0.372761
C	-5.493417	0.694954	0.811588
H	-3.462987	1.072037	1.414296
C	-5.860056	-1.309727	-0.464430

H	-4.130942	-2.545923	-0.791370	H	0.846651	0.885214	1.875964
C	-6.358153	-0.153747	0.125856	C	3.612979	0.665786	-0.055302
H	-5.873278	1.592818	1.283584	C	4.135810	-0.612842	-0.227159
H	-6.526104	-1.989430	-0.981072	C	4.409134	1.797872	-0.204501
H	-7.413601	0.079450	0.061797	C	5.478791	-0.755642	-0.556744
C	-1.453864	-1.400304	-0.669705	H	3.493539	-1.477608	-0.105900
O	-0.291476	-1.711282	-0.544933	C	5.749527	1.643563	-0.541971
O	-2.003765	-1.366679	-1.898207	H	3.977543	2.780641	-0.054661

S-TS3

Symbol	X	Y	Z
Si	-1.387294	0.019530	-0.853270
H	-0.931527	0.130552	-2.253437
H	-2.590643	-1.013414	-1.342403
C	-0.603900	-1.298656	0.223151
C	0.492257	-2.035609	-0.243077
C	-1.055175	-1.528028	1.528136
C	1.120339	-2.975354	0.571860
H	0.862572	-1.882240	-1.253965
C	-0.423648	-2.458635	2.347575
H	-1.910104	-0.977816	1.907828
C	0.666401	-3.182594	1.871538
H	1.959494	-3.547850	0.192673
H	-0.783335	-2.621907	3.356788
H	1.156694	-3.909496	2.508177
C	-2.638017	1.202479	-0.106236
C	-3.896857	1.363829	-0.699006
C	-2.358911	1.926495	1.059824
C	-4.840509	2.229685	-0.155821
H	-4.148826	0.807657	-1.596909
C	-3.308401	2.776624	1.618876
H	-1.389091	1.831232	1.533900
C	-4.548975	2.933733	1.008642
H	-5.804139	2.348644	-0.636870
H	-3.077424	3.319794	2.527727
H	-5.286146	3.601145	1.439311
C	-3.746562	-1.806211	-1.230532
O	-4.221836	-1.839076	-2.328250
O	-3.845452	-2.157868	-0.093734
N	2.228665	0.817746	0.307562
H	2.594074	1.052124	-2.011585
C	1.864887	0.550668	1.703803
H	1.934265	-0.521842	1.901013
H	2.552802	1.094806	2.349342

S-IM6

Symbol	X	Y	Z
Si	1.135463	-0.483007	-0.712672
H	1.107226	-0.388134	-2.180408
H	2.706004	1.479989	-1.525314
C	0.608574	1.091102	0.119480
C	-0.366423	1.902916	-0.474565
C	1.082795	1.423676	1.394662
C	-0.873728	3.007606	0.203535
H	-0.732499	1.679595	-1.474117
C	0.582633	2.531334	2.069493
H	1.843829	0.809095	1.865366
C	-0.401737	3.317813	1.477772
H	-1.627803	3.630576	-0.262981
H	0.956207	2.779139	3.055808
H	-0.794838	4.179304	2.004536
C	2.582050	-1.341273	0.060961
C	3.888907	-0.889650	-0.183217
C	2.385915	-2.419208	0.933779
C	4.968543	-1.512497	0.434802
H	4.086942	-0.054546	-0.852011
C	3.469809	-3.035535	1.550044
H	1.384444	-2.785078	1.130997
C	4.761752	-2.582432	1.301029
H	5.973957	-1.157920	0.240285
H	3.305244	-3.868903	2.221932
H	5.606167	-3.063503	1.780957
C	3.456437	2.266898	-1.839846

O 4.642396 1.883016 -1.854572
O 2.972589 3.377246 -2.107460
N -2.249107 -0.903422 0.389784
H -2.787065 -1.417315 -1.873752
C -1.796660 -0.567835 1.751540
H -1.744782 0.518118 1.851648
H -2.523381 -0.975767 2.450925
H -0.819501 -1.006595 1.931286
C -3.641380 -0.672444 0.074170
C -4.061838 0.627203 -0.183798
C -4.523662 -1.746844 0.062814
C -5.403317 0.851112 -0.467292
H -3.345418 1.440308 -0.162401
C -5.862309 -1.508240 -0.229410
H -4.164294 -2.745515 0.280767
C -6.299084 -0.214139 -0.491410
H -5.746457 1.857006 -0.671638
H -6.561354 -2.334217 -0.247391
H -7.342997 -0.033905 -0.715786
C -1.434786 -1.336951 -0.539251
O -0.188431 -1.555132 -0.312160
O -1.838375 -1.587697 -1.753898