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Supporting Information

Theoretical study of reductive CO_2 functionalization with amines and phenylsilanes: What kind of solvents can be used as catalysts?

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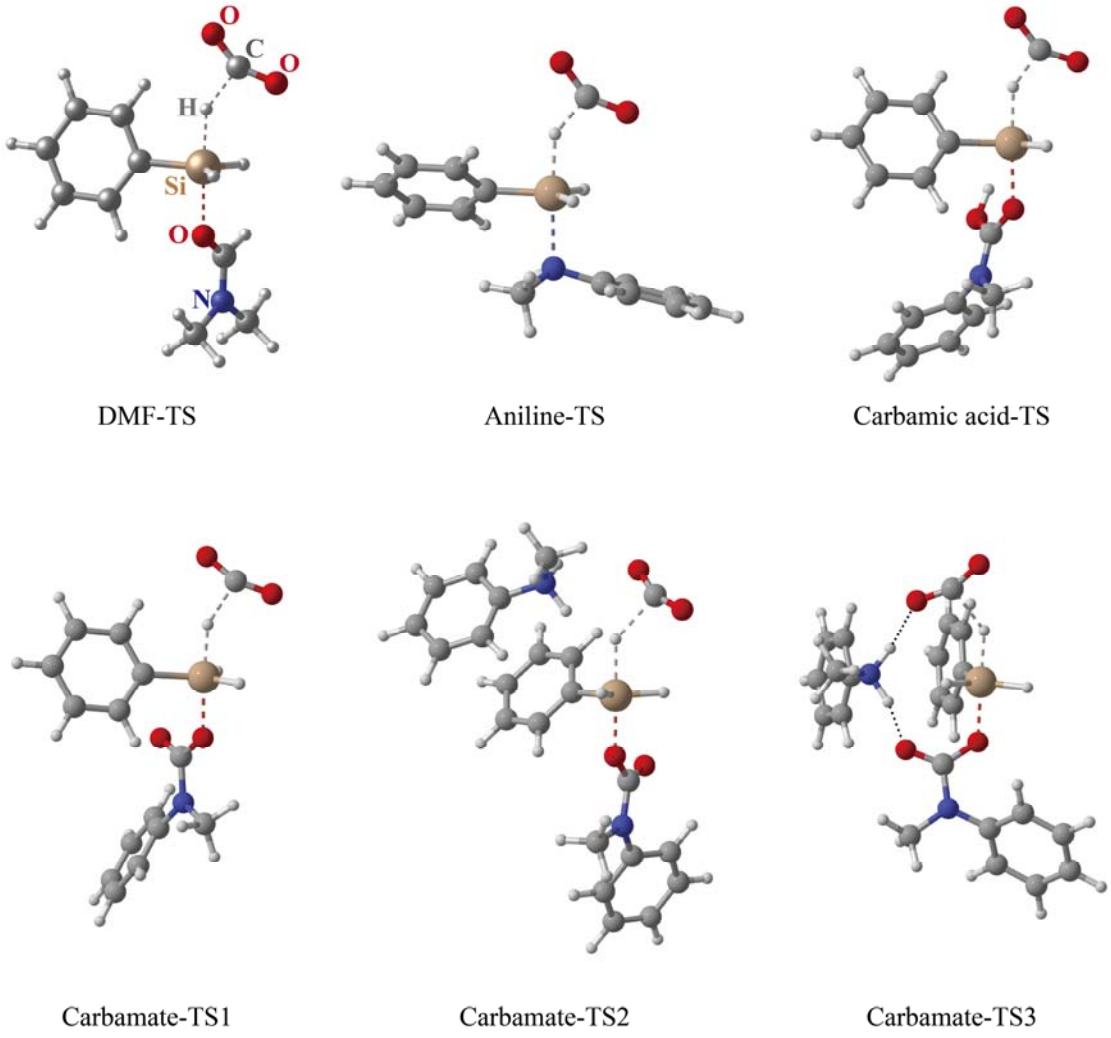

Figure S1. The geometry structures of reduction of CO_2 with $PhSiH_3$ in the presence of different species in the reaction system.

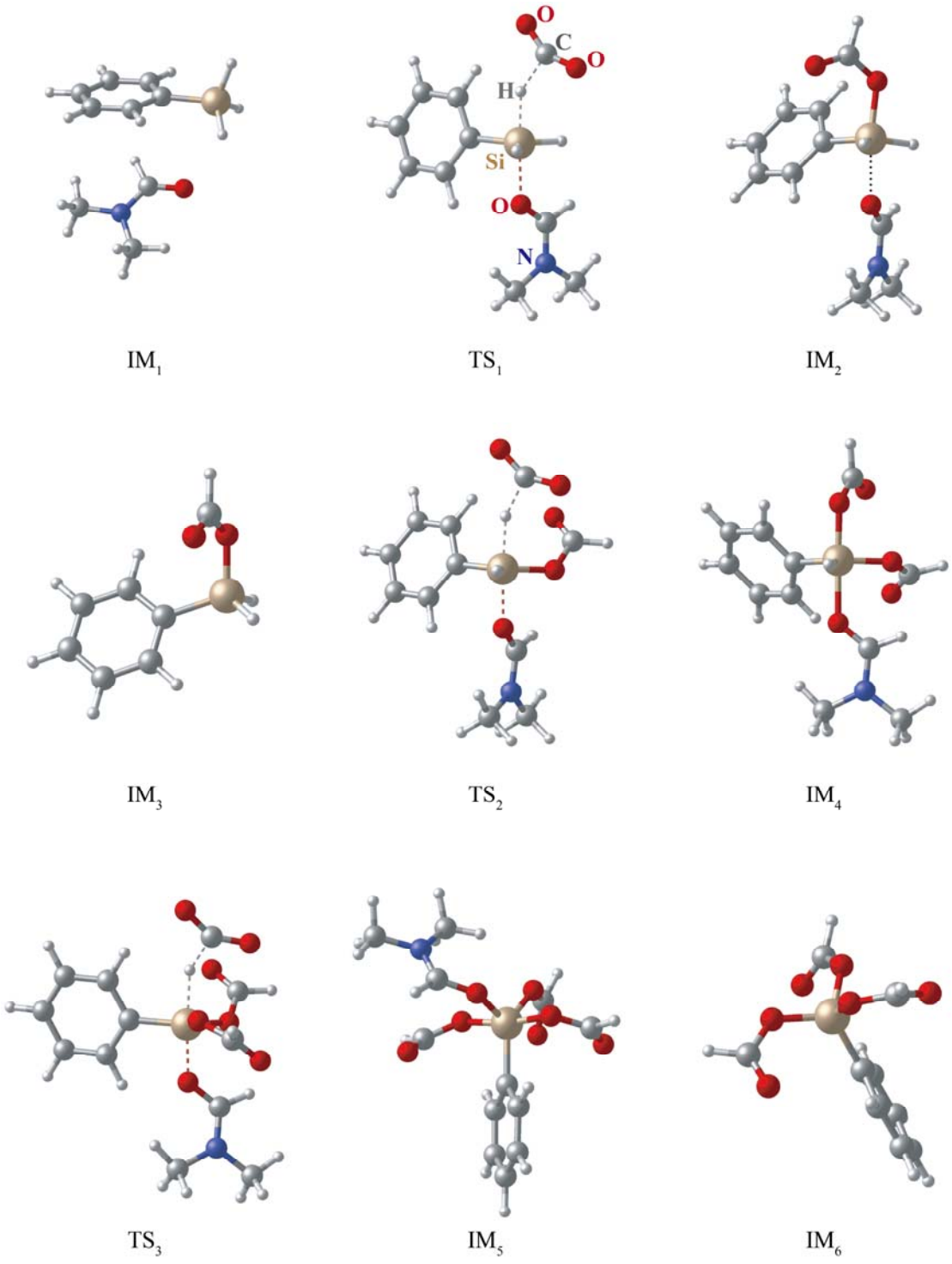

Figure S2. Optimized intermediates and transition states of CO_2 reduction with *N*-methylaniline and $PhSiH_3$ using DMF as catalyst to give triformyloxysilane $[Si](OCHO)_3$.

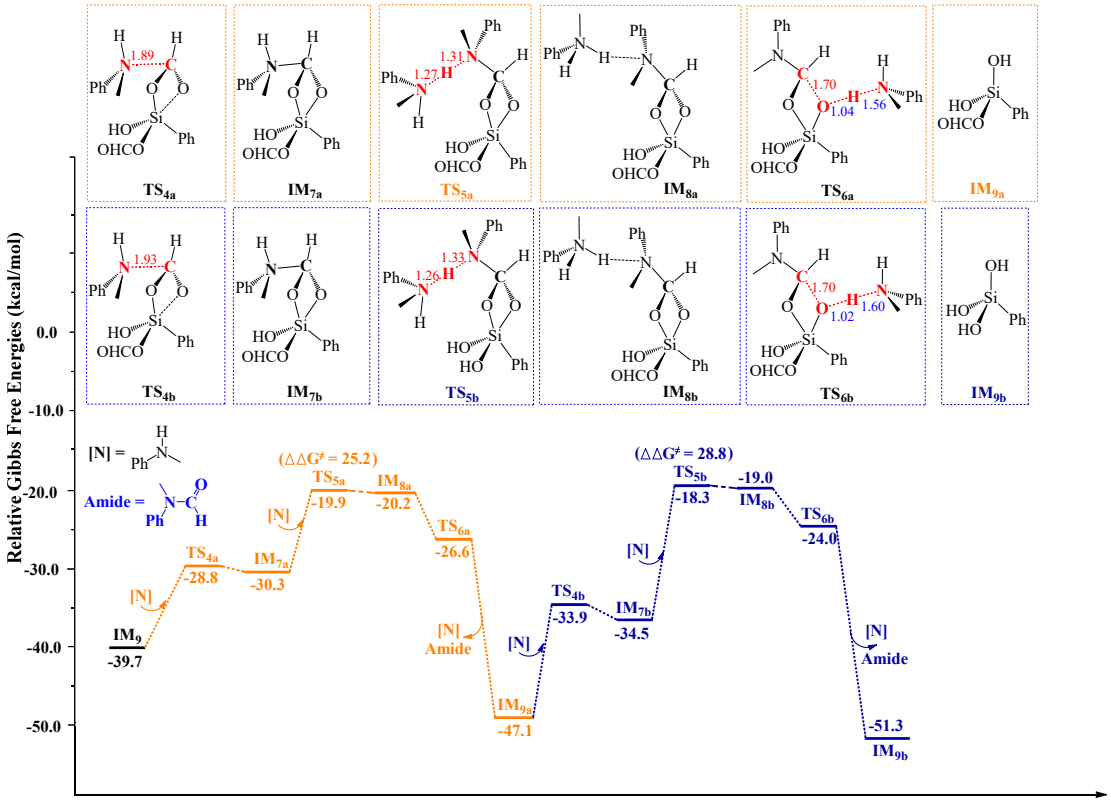

Figure S3. Free energy profile of C−N bond formation to give second and third formamides. The optimized structures of the stationary points are shown (key bond lengths in angstroms).

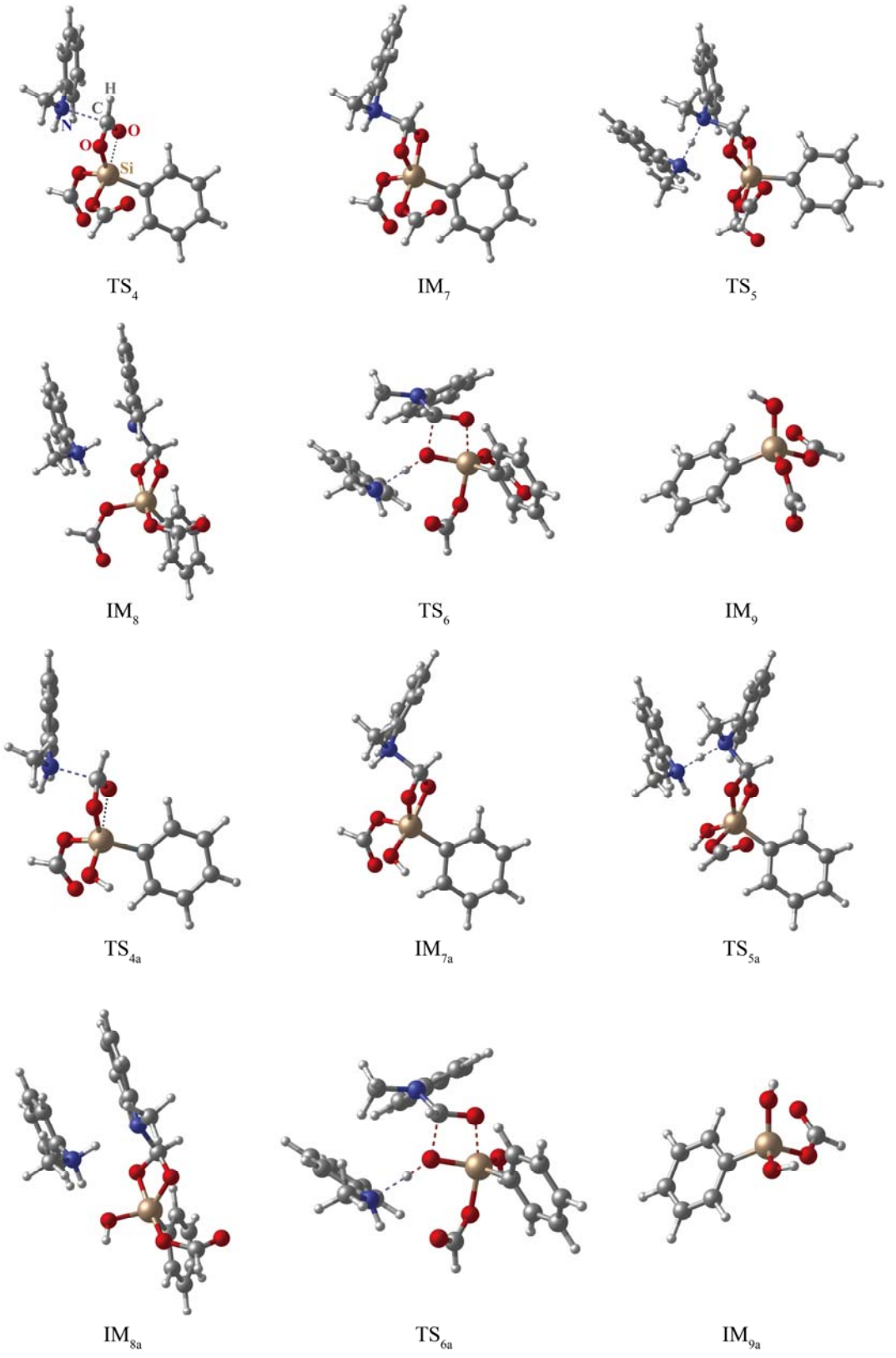

Figure S4. Optimized intermediates and transition states of C−N bond formation to give first and second formamides.

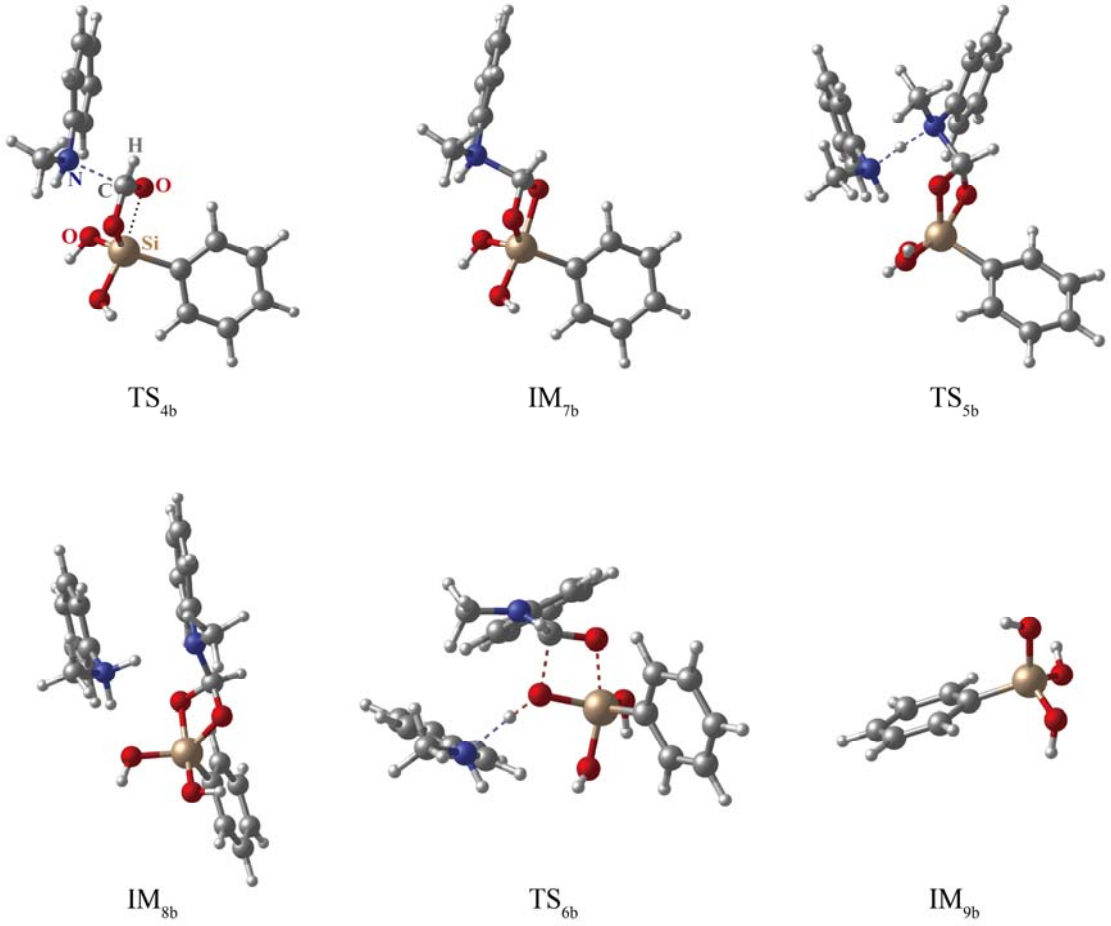

Figure S5. Optimized intermediates and transition states of C−N bond formation to give third formamide.

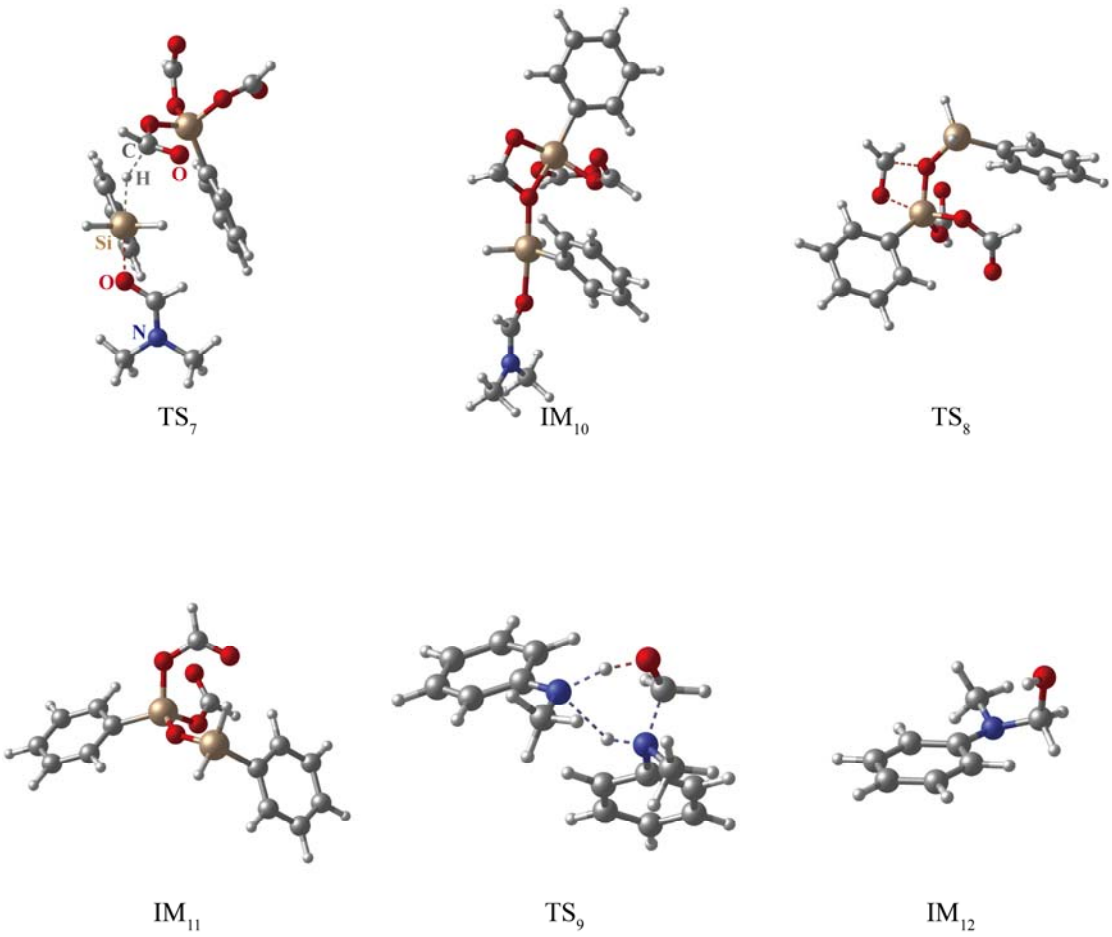

Figure S6. Optimized intermediates and transition states of DMF-catalyzed **IM$_6$** reduction with $PhSiH_3$ to form *N*, *N*-dimethylaniline (part A).

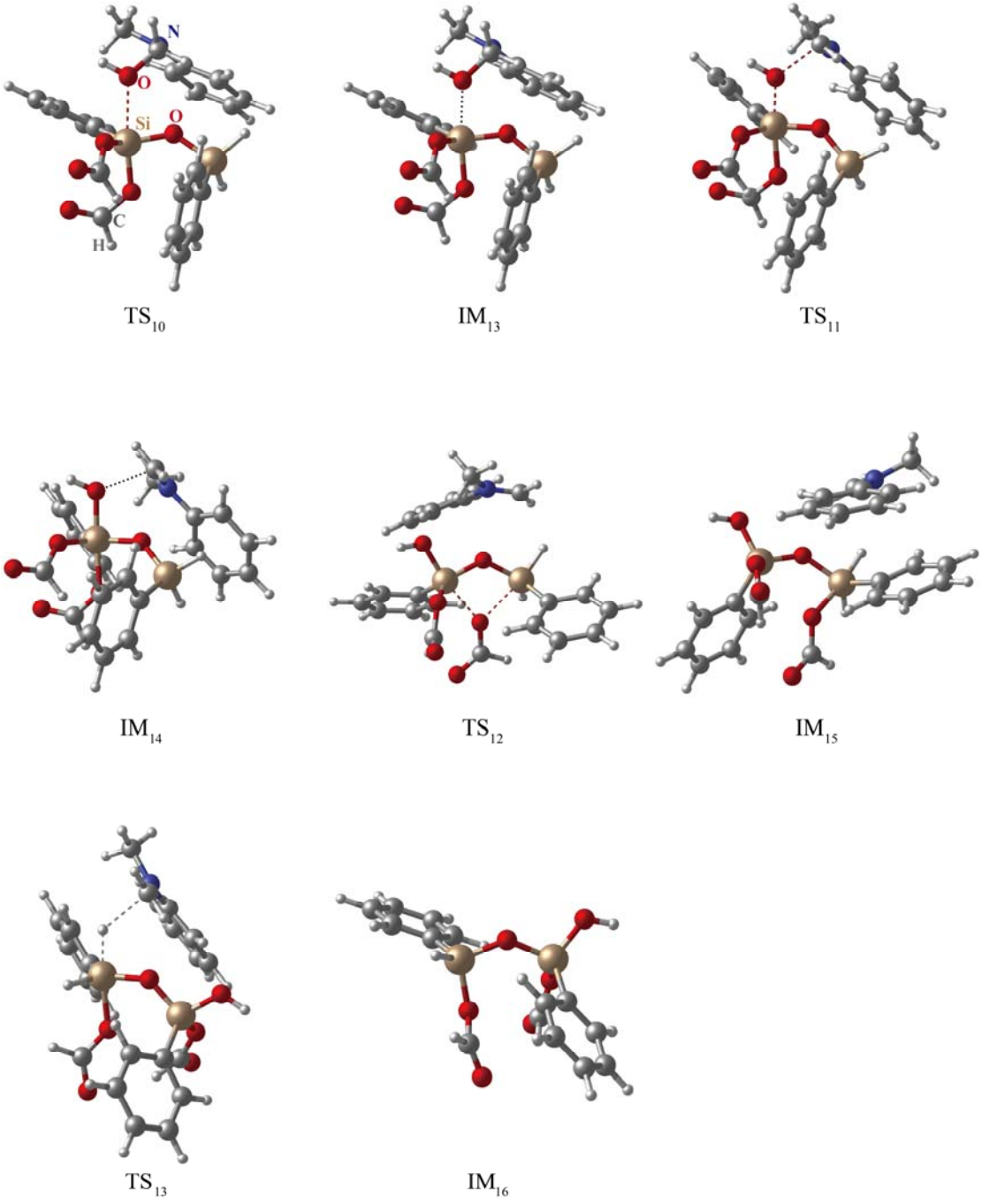

Figure S7. Optimized intermediates and transition states of DMF-catalyzed **IM6** reduction with $PhSiH_3$ to form *N*, *N*-dimethylaniline (part B).

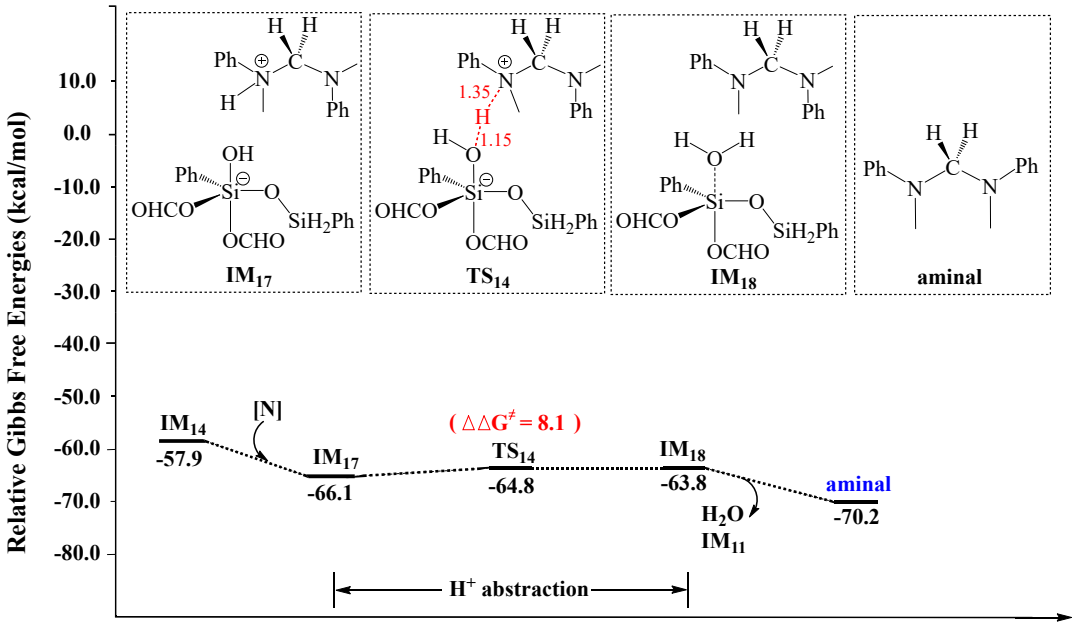

Figure S8. Free energy profile of DMF-catalyzed **IM$_{14}$** reduction with $PhSiH_3$ to form aminal intermediate. The optimized structures of the stationary points are shown (key bond lengths in angstroms).

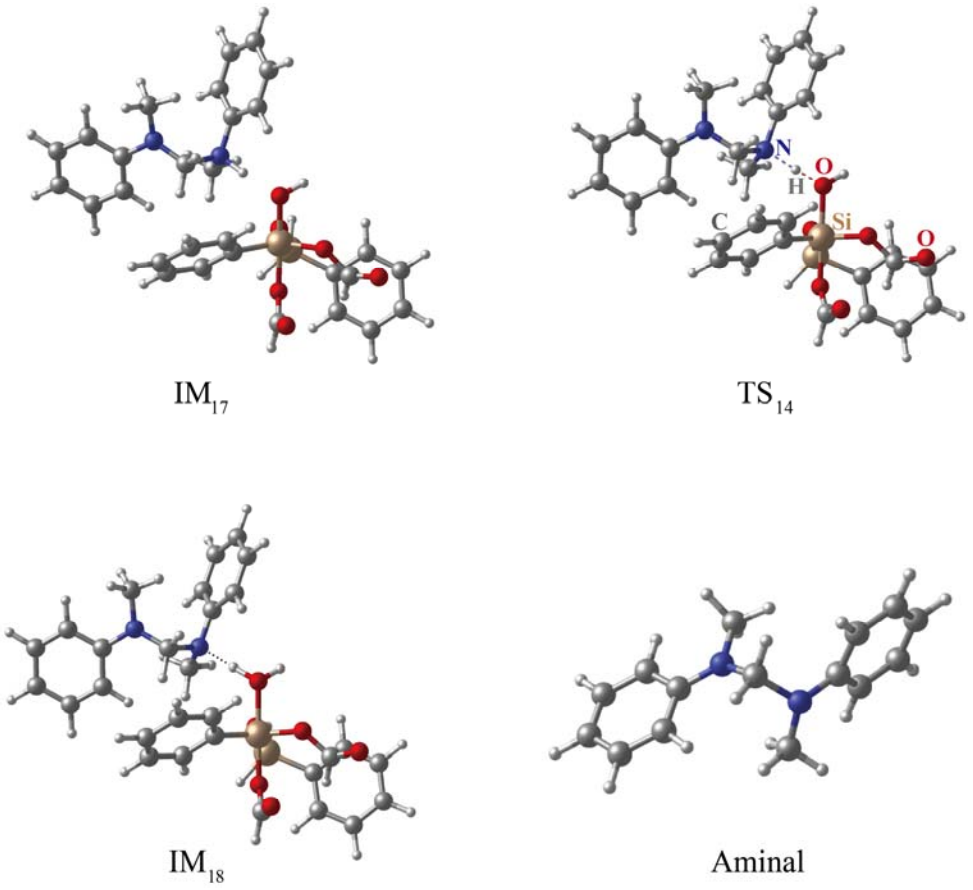

Figure S9. Optimized intermediates and transition states of DMF-catalyzed IM_{14} reduction with $PhSiH_3$ to form aminal intermediate.

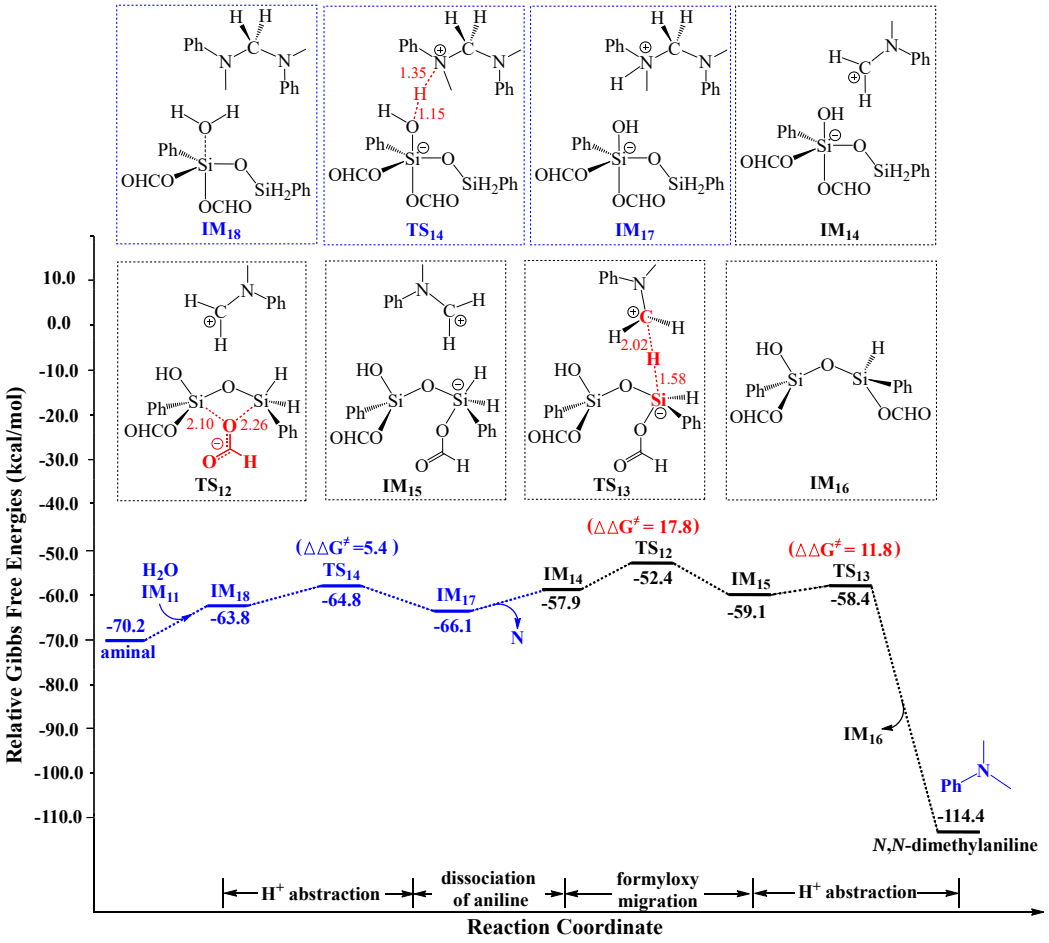

Figure S10. Free energy profile of aminal transforms to *N*, *N*-dimethylaniline. The optimized structures of the stationary points are shown (key bond lengths in angstroms).

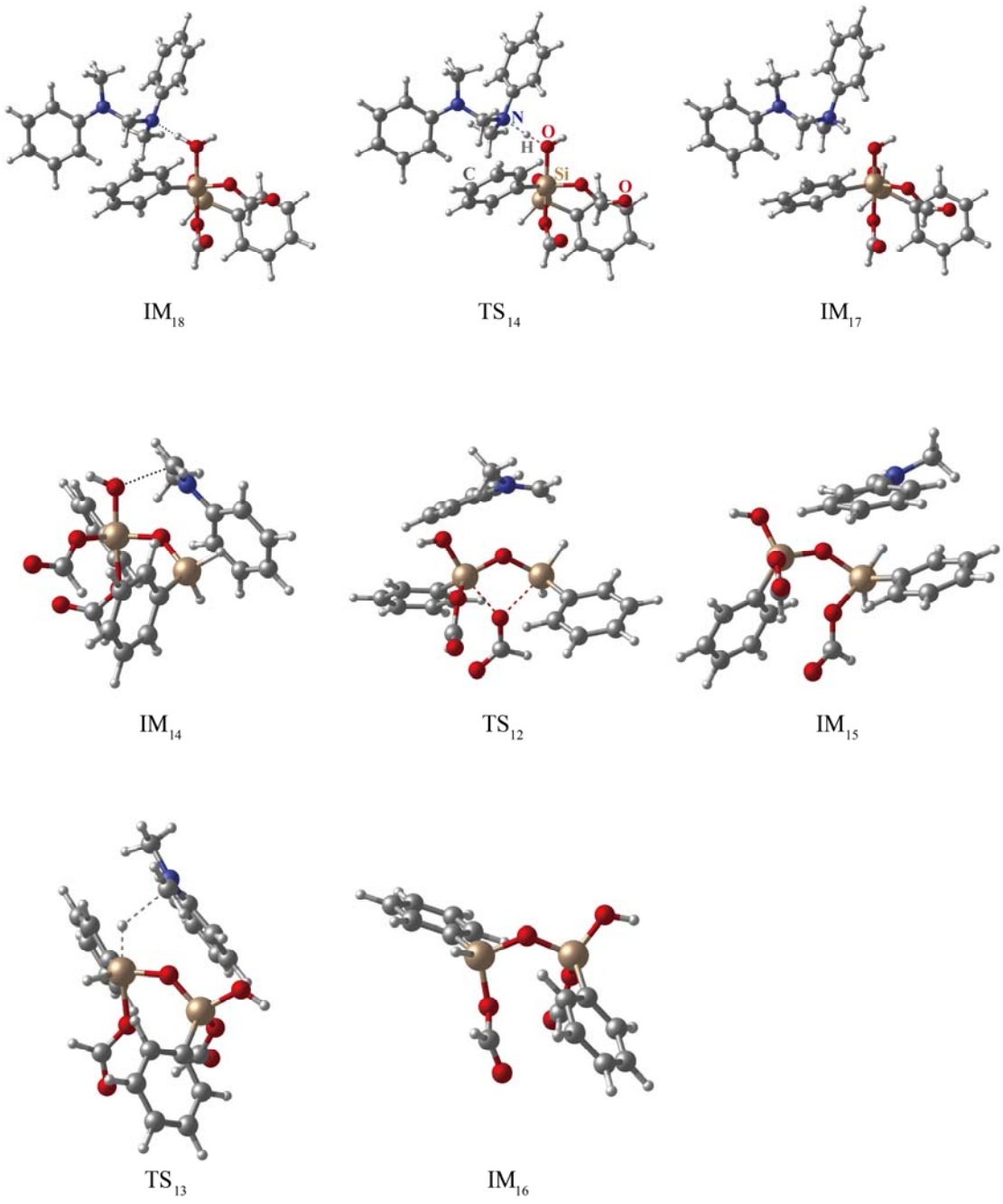

Figure S11. Optimized intermediates and transition states of aminal transforms to *N*, *N*-dimethylaniline.

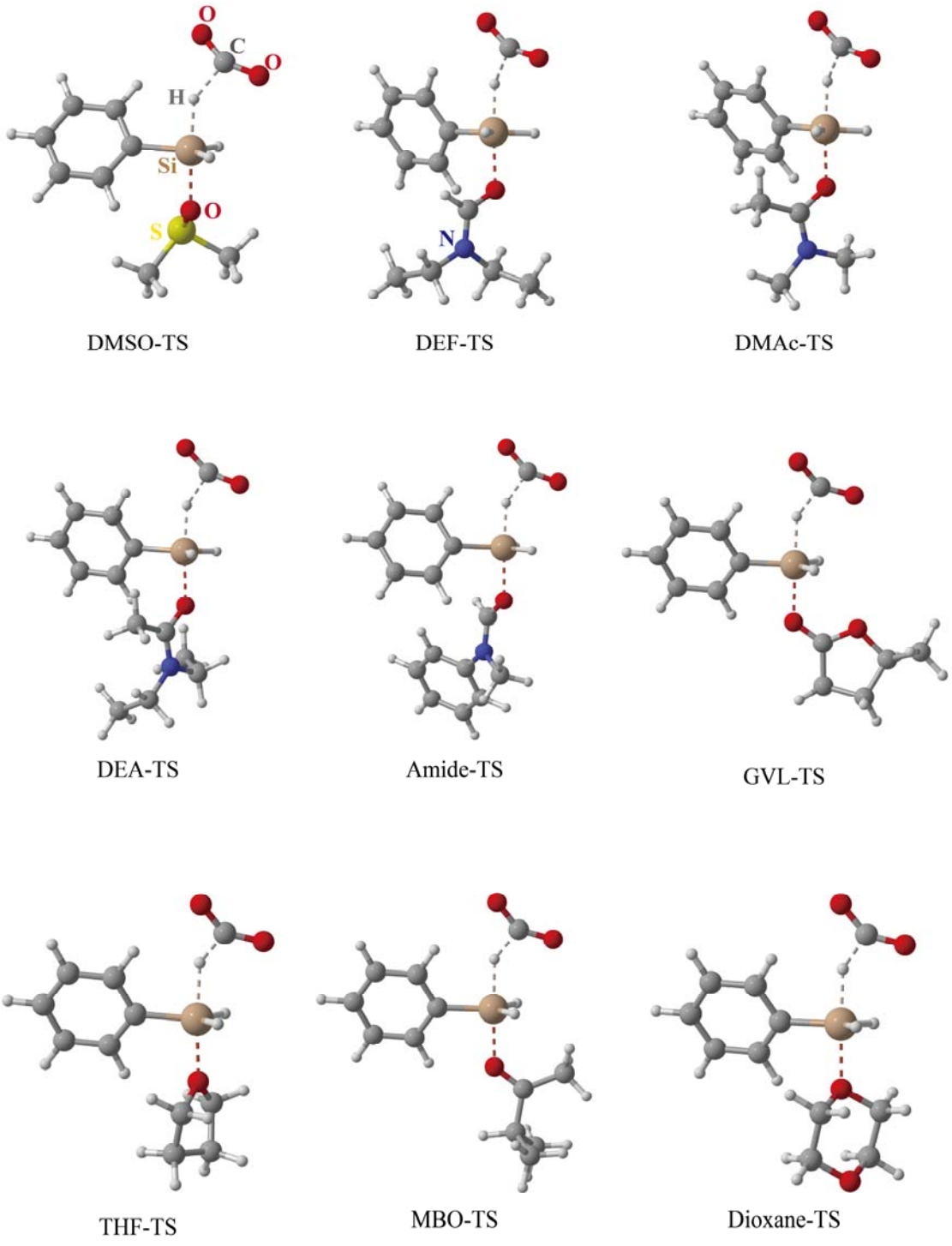

Figure S12. Optimized intermediates and transition states of CO_2 reduction by phenylsilane in different solvents.

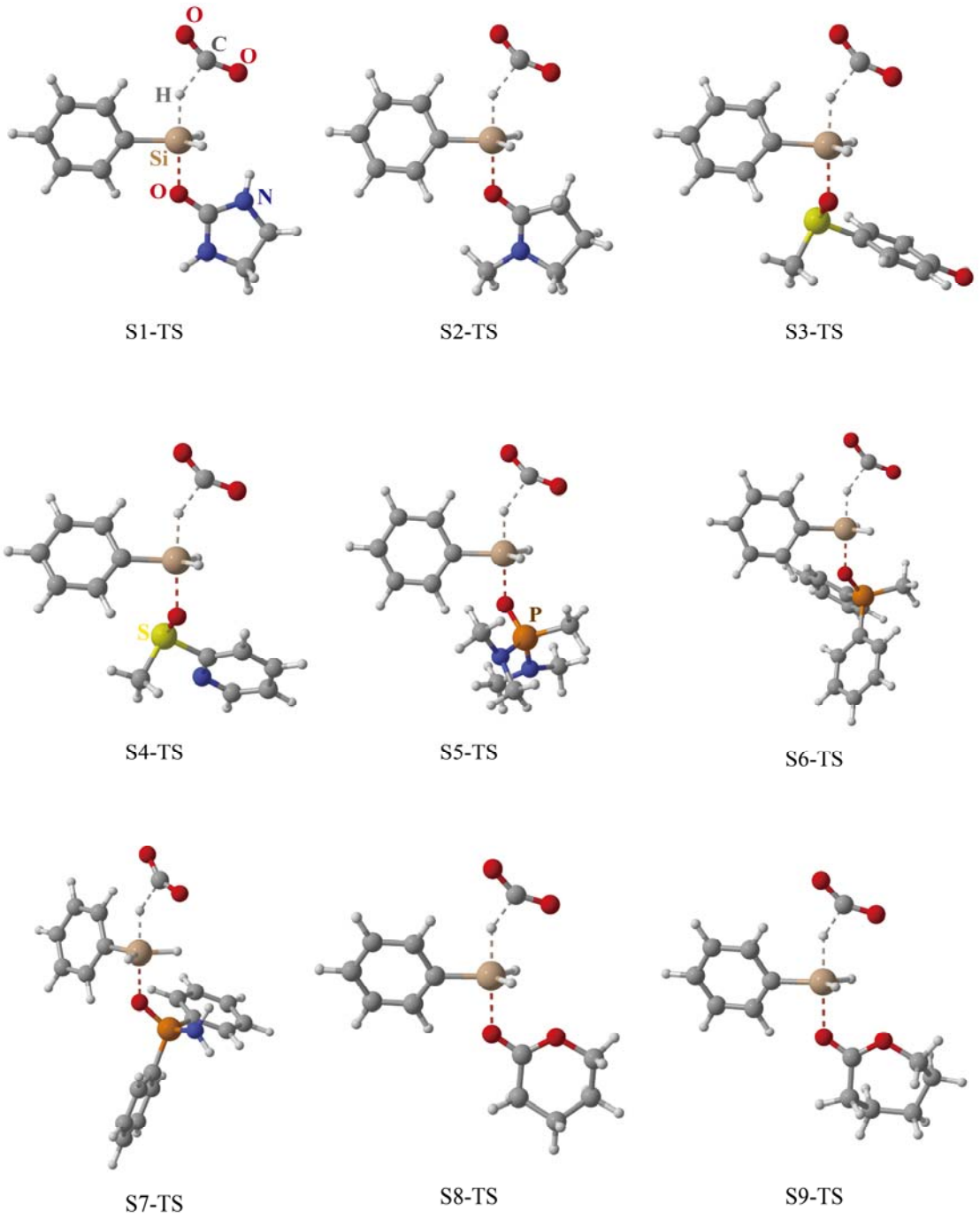

Figure S13. Optimized intermediates and transition states of CO_2 reduction by phenylsilane in other commercial solvents.

Table S1. Detailed information of other commercial solvents.

	S1	**S2**	**S3**
name	2-imidazolidinone	N-methylpyrrolidone	4-(methylsulphinyl)phenol
CAS	120-93-4	872-50-4	14763-64-5
	S4	**S5**	**S6**
name	2-(methylsulfinyl)pyridine	methylphosphonic bis(dimethylamide)	Methyldiphenylphosphine oxide
CAS	21948-75-4	2511-17-3	2129-89-7
	S7	**S8**	**S9**
name	diphenylphosphinamide	δ-valerolactone	ε-caprolactone
CAS	5994-87-6	542-28-9	**502-44-3**

Table S2. Free energies of all species (a.u.).

Species	Free energies	Species	Free energies
CO_2	-188.6009305	**carbamate-TS2**	-1553.516302
Si	-522.8178165	**carbamate-TS3**	-1553.526023
DMF	-248.4279319	**DEA**	-366.2828573
IM_1	-771.2374214	**DEA-CO_2**	-188.6011139
TS_1	-959.80771	**DEA-Si**	-522.8182704
IM_2	-959.8663547	**DEA-TS**	-1077.661763
IM_3	-711.4394603	**DEF**	-326.9948105
TS_2	-1148.432181	**DEF-CO_2**	-188.6009305
IM_4	-1148.488317	**DEF-Si**	-522.81815
TS_3	-1337.058997	**DEF-TS**	-1038.375442
IM_5	-1337.108077	**DMAc**	-287.7163119
IM_6	-1088.692546	**DMAc-CO_2**	-188.6011139
TS_4	-1415.440406	**DMAc-Si**	-522.8182704
IM_7	-1415.447391	**DMAc-TS**	-999.0960535
TS_5	-1742.218178	**DMSO**	-553.1442859
IM_8	-1742.217506	**DMSO-CO_2**	-188.6007722
TS_6	-1742.20849	**DMSO-Si**	-522.816468
IM_9	-975.3669104	**DMSO-TS**	-1264.525647
TS_{4a}	-1302.106017	**THF**	-232.3431659
IM_{7a}	-1302.108325	**THF-CO_2**	-188.6003331
TS_{5a}	-1628.890181	**THF-Si**	-522.8185848
IM_{8a}	-1628.890622	**THF-TS**	-943.7131069
TS_{6a}	-1628.879803	**Amide**	-440.1153146
IM_{9a}	-862.0407393	**Amide-TS**	-1151.492583
TS_{4b}	-1188.776163	**MBO**	-271.649419
IM_{7b}	-1188.777079	**MBO-CO_2**	-188.6008894
TS_{5b}	-1515.549652	**MBO-Si**	-522.8195829
IM_{8b}	-1515.550846	**MBO-TS**	-983.0176205

TS_{6b}	-1515.537835	**Dioxane**	-307.5592068
IM_{9b}	-748.7095188	**Dioxane-TS**	-1018.928264
TS_7	-1859.893755	**GLV**	-345.7120903
IM_{10}	-1859.950596	**GLV-CO_2**	-188.5977195
TS_8	-1611.494574	**GLV-Si**	-522.814939
IM_{11}	-1497.052876	**GLV-TS**	-1057.079594
TS_{9a}	-517.6712136	**S1**	-302.6148064
TS_9	-768.0119626	**S1-TS**	-1013.9937
IM_{12}	-441.2790761	**S2**	-325.8239513
TS_{10}	-1938.316589	**S2-TS**	-1037.202849
IM_{13}	-1938.315914	**S3**	-820.0638572
TS_{11}	-1938.303857	**S3-TS**	-1531.443232
IM_{14}	-1938.308091	**S4**	-760.8837154
TS_{12}	-1938.299301	**S4-TS**	-1472.25992
IM_{15}	-1938.309993	**S5**	-725.5079148
TS_{13}	-1938.308823	**S5-TS**	-1436.891528
IM_{16}	-1572.350153	**S6**	-919.6265811
IM_{17}	-2265.098422	**S6-TS**	-1631.007992
TS_{14}	-2265.096540	**S7**	-935.707871
IM_{18}	-2265.094919	**S7-TS**	-1647.088348
aminal	-691.6286769	**S8**	-345.7023705
Aniline-TS	-1038.150645	**S8-TS**	-1057.072656
carbamic acid-TS	-1226.737219	**S9**	-384.9827813
carbamate-TS1	-1226.305225	**S9-TS**	-1096.353003

Table S3. Imaginary frequencies of all transition states.

Species	Imaginary frequency	Species	Imaginary frequency
TS_1	466.75 cm^{-1}	**carbamic acid-TS**	268.42 cm^{-1}
TS_2	320.10 cm^{-1}	**carbamate-TS1**	440.11 cm^{-1}
TS_3	221.61 cm^{-1}	**carbamate-TS2**	492.91 cm^{-1}
TS_4	172.51 cm^{-1}	**carbamate-TS3**	514.38 cm^{-1}
TS_5	789.56 cm^{-1}	**DEA-TS**	445.89 cm^{-1}
TS_6	298.81 cm^{-1}	**DEF-TS**	430.95 cm^{-1}
TS_{4a}	236.42 cm^{-1}	**DMAc-TS**	447.79 cm^{-1}
TS_{5a}	814.48 cm^{-1}	**DMSO-TS**	450.34 cm^{-1}
TS_{6a}	286.75 cm^{-1}	**THF-TS**	32.64 cm^{-1}
TS_{4b}	214.04 cm^{-1}	**Amide-TS**	393.20 cm^{-1}
TS_{5b}	811.37 cm^{-1}	**MBO-TS**	216.83 cm^{-1}
TS_{6b}	290.93 cm^{-1}	**Dioxane-TS**	172.79 cm^{-1}
TS_7	451.30 cm^{-1}	**GLV-TS**	325.05 cm^{-1}
TS_8	327.84 cm^{-1}	**S1-TS**	429.19 cm^{-1}
TS_{9a}	1022.88 cm^{-1}	**S2-TS**	443.01 cm^{-1}
TS_9	622.26 cm^{-1}	**S3-TS**	438.11 cm^{-1}
TS_{10}	67.93 cm^{-1}	**S4-TS**	422.93 cm^{-1}
TS_{11}	179.24 cm^{-1}	**S5-TS**	448.12 cm^{-1}
TS_{12}	83.32 cm^{-1}	**S6-TS**	447.86 cm^{-1}
TS_{13}	287.71 cm^{-1}	**S7-TS**	447.49 cm^{-1}
TS_{14}	466.18 cm^{-1}	**S8-TS**	374.42 cm^{-1}
Aniline-TS	370.16 cm^{-1}	**S9-TS**	361.95 cm^{-1}

Table S4. Cartesian coordinates of all species (angstroms).

IM_1

Symbol	X	Y	Z
C	-1.376459	0.527884	0.739396
H	-0.715837	-0.258360	1.136122
O	-1.086717	1.710295	0.824054
N	-2.484646	0.031937	0.158761
C	-3.458953	0.908330	-0.464812
H	-3.541874	0.680711	-1.530808
H	-4.438826	0.772078	-0.000504
H	-3.133460	1.937071	-0.335227
C	-2.734511	-1.394521	0.083657
H	-1.949722	-1.930684	0.615749
H	-3.699771	-1.633334	0.536936
H	-2.744110	-1.727356	-0.958176
Si	2.057578	2.097629	-0.095845
H	3.419994	2.338376	-0.633669
H	1.091401	2.814805	-0.953663
H	2.015622	2.613220	1.291423
C	1.670560	0.260915	-0.091791
C	1.984423	-0.549624	1.006396
C	1.000144	-0.324768	-1.174124
C	1.632178	-1.897761	1.026808
H	2.511051	-0.131479	1.858599
C	0.649394	-1.671017	-1.160315
H	0.728590	0.280964	-2.033398
C	0.961031	-2.459254	-0.055317
H	1.880706	-2.508425	1.886981
H	0.125388	-2.103062	-2.005198
H	0.681446	-3.506221	-0.037770

IM_2

Symbol	X	Y	Z
C	-2.144918	-0.624685	-0.443023
H	-1.837777	-0.401028	-1.470612
O	-1.355329	-1.177405	0.355379
N	-3.373052	-0.272777	-0.134825
C	-3.922883	-0.490251	1.196266
H	-4.237165	0.467918	1.614257
H	-4.789466	-1.150437	1.125265
H	-3.165830	-0.941547	1.831284
C	-4.254227	0.349970	-1.112850
H	-3.729479	0.464431	-2.059440
H	-5.136526	-0.275724	-1.258574
H	-4.566209	1.329875	-0.747595
Si	0.617876	-1.438882	-0.185630
H	4.254635	-2.029166	-0.460379
H	0.622182	-2.270687	1.028750
H	0.044187	-1.941215	-1.451062
C	0.864287	0.434946	-0.056977
C	1.771810	1.071016	-0.915573
C	0.187371	1.231317	0.877105
C	1.983870	2.445847	-0.857145
H	2.324986	0.486108	-1.643475
C	0.412334	2.603297	0.956494
H	-0.522925	0.777059	1.559677
C	1.306758	3.215938	0.083742
H	2.682278	2.913966	-1.541931
H	-0.114257	3.193968	1.697902
H	1.476390	4.285394	0.137692
C	3.323174	-1.723172	0.041994
O	2.277760	-1.858166	-0.737843
O	3.311810	-1.320907	1.181226

IM_3

Symbol	X	Y	Z
Si	-1.244067	1.103761	-0.541661
H	-3.272639	-1.778437	0.220310
H	-1.635975	2.043657	0.523525
H	-1.397205	1.714453	-1.872912
C	0.466882	0.429292	-0.246377
C	0.865176	-0.785233	-0.820551
C	1.385642	1.134278	0.540322
C	2.148692	-1.280210	-0.614676
H	0.170730	-1.355713	-1.430597
C	2.672242	0.642503	0.743061
H	1.098711	2.072394	1.006124
C	3.053557	-0.564879	0.165796
H	2.443334	-2.222553	-1.062264
H	3.373379	1.198016	1.355371
H	4.054046	-0.950397	0.326026
C	-2.581936	-0.958244	0.448756
O	-2.346270	-0.201453	-0.624653
O	-2.100953	-0.762045	1.529784

IM_4

Symbol	X	Y	Z
C	2.474257	-0.239896	-0.385524
H	2.658547	-1.301309	-0.206073
O	1.330767	0.182525	-0.688985
N	3.517169	0.545134	-0.271367
C	3.426505	1.984873	-0.477312
H	3.806083	2.492683	0.411047
H	4.037743	2.263942	-1.338076
H	2.391202	2.265403	-0.651332
C	4.833448	0.015628	0.058111
H	4.776179	-1.064360	0.183560
H	5.529713	0.253386	-0.748156
H	5.185433	0.474434	0.983742
Si	-0.344546	-0.831175	-0.906965
H	0.806698	-2.959590	1.815760
H	-3.422781	-2.862658	-0.666424
H	0.053778	-0.961077	-2.313685
C	-1.257280	0.696465	-0.284252
C	-2.527420	0.979730	-0.807407
C	-0.724445	1.592329	0.652864
C	-3.233461	2.116869	-0.421200
H	-2.978154	0.306671	-1.528905
C	-1.435420	2.717433	1.058726
H	0.248437	1.393751	1.083775
C	-2.690038	2.987166	0.517516
H	-4.209046	2.317568	-0.850160
H	-1.007966	3.387838	1.796474
H	-3.240213	3.868817	0.827488
C	0.593991	-1.971422	1.385089
O	0.326644	-2.063079	0.091084
O	0.626738	-0.953414	2.022155
C	-2.577770	-2.282154	-0.262973
O	-1.802137	-1.822155	-1.215929
O	-2.425035	-2.114668	0.923545

IM_5

Symbol	X	Y	Z
C	2.337610	-0.795275	-1.185260
H	2.352117	-1.713678	-1.765676
O	1.316122	-0.023830	-1.305342
N	3.381912	-0.515573	-0.476839
C	3.534806	0.715095	0.298469
H	3.413785	0.489046	1.358361
H	4.539314	1.095705	0.114969
H	2.797009	1.450639	-0.008565
C	4.482717	-1.473896	-0.370935
H	4.263733	-2.356792	-0.966958
H	5.399119	-0.999165	-0.721094
H	4.592441	-1.754229	0.677675
Si	0.041518	0.528722	-0.248971
H	0.435112	3.386593	1.960981
H	1.319985	-1.796325	2.371987
H	-1.652086	2.726839	-2.668324
C	-1.525996	-0.503759	-0.116326
C	-2.230860	-0.871736	-1.269743
C	-2.011402	-0.951060	1.119660
C	-3.369922	-1.669670	-1.194221
H	-1.888444	-0.536108	-2.242733
C	-3.162421	-1.727743	1.202291
H	-1.492906	-0.667379	2.028659
C	-3.841553	-2.095375	0.043384
H	-3.891427	-1.953249	-2.101693
H	-3.528638	-2.049227	2.171073
H	-4.733927	-2.708211	0.105303
C	-0.018313	2.426519	1.678415
O	0.435842	2.018662	0.502589
O	-0.821399	1.850923	2.358861
C	-1.467439	2.292436	-1.672901
O	-2.115517	2.610281	-0.704972
O	-0.488599	1.421008	-1.701371
C	1.049786	-1.553066	1.332897
O	0.838336	-0.273017	1.164772
O	0.988961	-2.400849	0.470084

IM_6

Symbol	X	Y	Z
Si	-0.877759	-0.077347	0.030184
H	-1.955437	-0.860520	-3.305071
H	-1.296285	-2.851515	2.275022
H	-2.550126	2.920897	1.119756
C	0.946419	0.133187	-0.031734
C	1.553161	1.395130	-0.004411
C	1.756531	-1.010984	-0.073533
C	2.939483	1.509313	-0.027609
H	0.950616	2.295307	0.030066
C	3.140748	-0.893398	-0.096053
H	1.308285	-1.999172	-0.091446
C	3.732228	0.367126	-0.074724

H	3.398858	2.490627	-0.006983
H	3.757342	-1.784043	-0.128109
H	4.812328	0.458346	-0.092625
C	-1.348570	-1.018239	-2.407353
O	-1.662267	-0.131267	-1.447095
O	-0.514526	-1.865510	-2.282123
C	-1.882436	2.371446	0.447905
O	-1.369093	2.825583	-0.531704
O	-1.706926	1.106762	0.868527
C	-0.956816	-1.842049	2.018471
O	-1.314851	-1.515495	0.762067
O	-0.352417	-1.114258	2.748164

IM$_{7a}$

Symbol	X	Y	Z
Si	-1.141739	-0.829221	-0.336424
H	-0.454168	-2.647702	2.750506
H	1.257601	0.495639	-2.056389
C	-2.492131	0.486374	-0.222195
C	-2.284147	1.818737	-0.604720
C	-3.777223	0.130345	0.218308
C	-3.315923	2.754000	-0.563287
H	-1.298805	2.126376	-0.932979
C	-4.806590	1.064261	0.281379
H	-3.963135	-0.887767	0.541369
C	-4.579231	2.379373	-0.116693
H	-3.131336	3.776586	-0.873912
H	-5.786409	0.766761	0.638578
H	-5.381597	3.107777	-0.075293
C	-1.093818	-2.016272	2.117480
O	-0.431032	-1.566634	1.064548
O	-2.235698	-1.761224	2.389490
C	0.838712	-0.130955	-1.259843
O	0.229951	0.475931	-0.244142
O	-0.045986	-1.093044	-1.674588
O	-2.119193	-2.168180	-0.678953
N	2.120885	-0.909641	-0.711333
H	1.736092	-1.518027	0.021146
C	2.711399	-1.767333	-1.772953
H	1.983024	-2.534647	-2.019644
H	2.912455	-1.156272	-2.650963
H	3.631029	-2.212299	-1.399060
C	3.050649	0.018935	-0.076088
C	3.945337	0.749815	-0.846380
C	2.972156	0.185624	1.300126
C	4.787439	1.658975	-0.212989
H	3.994401	0.619013	-1.920190
C	3.822017	1.092597	1.921485
H	2.254263	-0.389322	1.874006
C	4.729611	1.829865	1.166211
H	5.491383	2.232109	-0.804204
H	3.771369	1.222773	2.995722
H	5.391356	2.536900	1.652192
H	-2.908127	-1.965894	-1.186309

IM$_{7b}$

Symbol	X	Y	Z
Si	1.214731	0.977440	0.361133
H	-1.035932	0.387425	-1.921439
C	2.656930	-0.194972	-0.025856
C	2.486165	-1.445931	-0.639029
C	3.965968	0.165385	0.335538
C	3.565280	-2.291169	-0.885942
H	1.489019	-1.757027	-0.923715
C	5.049136	-0.677482	0.100538
H	4.137962	1.123509	0.812338
C	4.851446	-1.910107	-0.514672
H	3.401534	-3.249750	-1.366463
H	6.046834	-0.371302	0.395943
H	5.692550	-2.568187	-0.703082
O	0.502032	0.963309	1.884705
C	-0.649193	0.651159	-0.928577
O	-0.077445	-0.299032	-0.202037
O	0.213822	1.710379	-0.889521
O	2.112214	2.398434	0.664421
N	-1.984031	1.145052	-0.158907
H	-1.621516	1.413912	0.764105
C	-2.558484	2.346955	-0.812812
H	-1.839833	3.154899	-0.706015
H	-2.716202	2.136357	-1.869405
H	-3.501025	2.602174	-0.331763
C	-2.904228	0.031724	0.030883
C	-3.821408	-0.303165	-0.956024
C	-2.788432	-0.715253	1.197748
C	-4.650494	-1.404263	-0.754987
H	-3.900441	0.275756	-1.867862
C	-3.623919	-1.807866	1.388176
H	-2.044355	-0.438048	1.936583

C	-4.556095	-2.153455	0.412401
H	-5.371890	-1.671776	-1.517626
H	-3.544332	-2.390653	2.298063
H	-5.207908	-3.005731	0.563599
H	2.593771	2.746054	-0.090283
H	0.883656	1.651518	2.439274

IM_7

Symbol	X	Y	Z
Si	0.935388	0.590790	0.144627
H	0.429346	1.011215	3.735135
H	3.407129	3.276459	-0.212047
H	-1.473676	0.447278	-1.939769
C	2.239605	-0.709313	-0.231587
C	1.938072	-1.850553	-0.986136
C	3.554693	-0.566820	0.238420
C	2.911208	-2.806703	-1.272595
H	0.929358	-1.991613	-1.353794
C	4.525734	-1.523294	-0.033854
H	3.814673	0.294978	0.842007
C	4.207009	-2.645594	-0.795933
H	2.654318	-3.677032	-1.866218
H	5.533140	-1.394292	0.346593
H	4.965599	-3.389303	-1.014044
C	1.058638	0.729522	2.879650
O	0.347717	0.694703	1.759211
O	2.224763	0.468203	2.979073
C	-1.060032	0.594549	-0.937036
O	-0.484714	-0.467546	-0.346941
O	-0.108726	1.579317	-0.839437
C	2.778372	2.445967	-0.568530
O	2.035692	1.952458	0.394525
O	2.800576	2.065774	-1.713558
N	-2.295026	1.046324	-0.074313
H	-1.912651	1.139870	0.875225
C	-2.794563	2.381719	-0.509276
H	-2.010095	3.107994	-0.316434
H	-3.013906	2.345204	-1.574560
H	-3.691721	2.618744	0.057989
C	-3.317892	-0.000663	-0.046365
C	-4.109717	-0.218491	-1.166801
C	-3.444706	-0.775820	1.097088
C	-5.056045	-1.236839	-1.128444
H	-3.997147	0.389349	-2.056428
C	-4.397951	-1.787711	1.124117
H	-2.807863	-0.588509	1.954299
C	-5.202789	-2.018933	0.013091
H	-5.679612	-1.415608	-1.995972
H	-4.507286	-2.394423	2.014776
H	-5.944216	-2.808527	0.036057

IM_{8a}

Symbol	X	Y	Z
Si	-1.931696	-0.527675	0.454295
H	-4.763635	-2.815561	1.185461
H	-0.283762	-0.954498	-2.050288
C	-3.105191	0.777917	-0.238304
C	-2.742704	1.562947	-1.340596
C	-4.359061	1.021837	0.342667
C	-3.597902	2.536347	-1.854408
H	-1.772702	1.410707	-1.800774
C	-5.209983	2.006281	-0.149665
H	-4.680680	0.433541	1.196561
C	-4.832859	2.763781	-1.256363
H	-3.296673	3.121158	-2.716777
H	-6.169652	2.179448	0.325096
H	-5.497801	3.525702	-1.647873
O	-1.361378	-0.192965	2.015808
C	-0.225041	-1.077198	-0.958212
O	-0.417940	0.120358	-0.281611
O	-1.291263	-1.833856	-0.473088
C	-4.133693	-2.208325	0.514390
O	-3.188620	-1.586510	1.177868
O	-4.338336	-2.153345	-0.672824
N	1.080656	-1.688112	-0.613789
H	1.332299	-0.999723	1.082252
C	1.096385	-3.148057	-0.505233
H	0.151121	-3.469267	-0.079238
H	1.240378	-3.632580	-1.478577
H	1.899104	-3.459993	0.164597
C	2.194662	-1.093482	-1.252011
C	3.404445	-1.790418	-1.391899
C	2.137286	0.236234	-1.710803
C	4.521280	-1.167950	-1.942968
H	3.490332	-2.817988	-1.066454
C	3.256750	0.837816	-2.269941
H	1.228556	0.810561	-1.591545
C	4.461607	0.147958	-2.385153

H	5.444586	-1.730022	-2.029906
H	3.184508	1.865548	-2.609128
H	5.333385	0.626408	-2.815221
N	1.383891	-0.384555	1.933130
H	0.398874	-0.071558	2.046464
C	1.769865	-1.180882	3.126936
H	1.016806	-1.954620	3.267197
H	2.741886	-1.639190	2.962460
H	1.801542	-0.520698	3.991527
C	2.244960	0.753013	1.618152
C	3.607646	0.551874	1.440357
C	1.661719	1.998167	1.441795
C	4.402943	1.632173	1.076557
H	4.040365	-0.434767	1.561491
C	2.467431	3.072354	1.075409
H	0.591806	2.117754	1.569195
C	3.834503	2.890663	0.891858
H	5.466085	1.486106	0.926642
H	2.022324	4.049466	0.930868
H	4.457891	3.728503	0.602741
H	-1.935022	-0.526058	2.713108

IM_{8b}

Symbol	X	Y	Z
Si	-2.134957	-0.862771	0.529954
H	-0.614841	-0.752798	-2.107607
C	-3.435832	0.335970	-0.156427
C	-3.085339	1.447721	-0.937998
C	-4.802499	0.136626	0.094656
C	-4.048560	2.316751	-1.446073
H	-2.037178	1.628953	-1.148643
C	-5.772747	1.001837	-0.405684
H	-5.105964	-0.715456	0.692907
C	-5.397088	2.096252	-1.179829
H	-3.747848	3.166897	-2.049175
H	-6.821302	0.821667	-0.193815
H	-6.149306	2.771136	-1.573413
O	-1.550851	-0.449439	2.087245
C	-0.477022	-1.061211	-1.058533
O	-0.680205	-0.020776	-0.168190
O	-1.455979	-1.960533	-0.655233
O	-3.155445	-2.067179	1.198311
N	0.884969	-1.633318	-0.903082
H	1.154833	-1.199383	0.944582
C	0.993995	-3.080504	-1.086310
H	0.084661	-3.539406	-0.711236
H	1.132615	-3.353783	-2.139891
H	1.836824	-3.467560	-0.511615
C	1.924751	-0.852375	-1.451697
C	3.177592	-1.417582	-1.739911
C	1.755416	0.527876	-1.676713
C	4.224237	-0.626669	-2.205737
H	3.350417	-2.475419	-1.595736
C	2.806496	1.300076	-2.152713
H	0.813277	1.002000	-1.437882
C	4.053028	0.736350	-2.415936
H	5.181743	-1.092880	-2.410790
H	2.646662	2.361455	-2.309933
H	4.870613	1.346868	-2.780255
N	1.179865	-0.694916	1.860443
H	0.179774	-0.437608	2.018525
C	1.615523	-1.607726	2.948782
H	0.908739	-2.435098	2.991537
H	2.612927	-1.984123	2.734472
H	1.610804	-1.056321	3.887053
C	1.980929	0.514968	1.688090
C	3.343645	0.405377	1.443617
C	1.339536	1.743478	1.716417
C	4.080020	1.563622	1.223699
H	3.820041	-0.567758	1.405234
C	2.086630	2.896651	1.493500
H	0.270313	1.788952	1.889688
C	3.452906	2.807808	1.246381
H	5.142392	1.491688	1.023016
H	1.596399	3.862687	1.509244
H	4.030368	3.707318	1.068453
H	-2.054197	-0.894084	2.776952
H	-3.431080	-2.729868	0.560886

IM_{8}

Symbol	X	Y	Z
Si	1.904322	0.112743	0.514963
H	1.583842	-3.203615	2.053809
H	4.662611	0.909240	2.827935
H	0.077087	2.313420	-0.443621
C	3.040782	0.075979	-0.981900
C	2.596412	0.538169	-2.227636
C	4.361810	-0.387983	-0.893085

C	3.437437	0.548743	-3.339637
H	1.576107	0.891015	-2.329361
C	5.201044	-0.395198	-2.001662
H	4.728908	-0.766934	0.054074
C	4.741500	0.079299	-3.228993
H	3.071830	0.918945	-4.291186
H	6.215809	-0.766918	-1.910067
H	5.397077	0.080001	-4.092889
C	2.150323	-2.492433	1.434601
O	1.394729	-1.449291	1.095700
O	3.283332	-2.679795	1.094749
C	0.081858	1.470400	0.262090
O	0.339718	0.258350	-0.371413
O	1.164313	1.539703	1.135662
C	4.022601	1.103810	1.952028
O	3.136317	0.149616	1.790289
O	4.166686	2.080704	1.260044
N	-1.209183	1.449036	0.990521
H	-1.393372	-0.361180	1.259985
C	-1.210280	2.080782	2.311075
H	-0.283291	1.827534	2.815434
H	-1.301606	3.171939	2.249111
H	-2.042242	1.690170	2.898845
C	-2.339063	1.697376	0.172537
C	-3.507162	2.273789	0.690510
C	-2.331167	1.304735	-1.178502
C	-4.637322	2.420155	-0.109844
H	-3.552455	2.604516	1.718867
C	-3.463164	1.465548	-1.965783
H	-1.449668	0.838033	-1.598835
C	-4.629543	2.016490	-1.439120
H	-5.529791	2.861762	0.319528
H	-3.432431	1.145024	-3.001406
H	-5.512782	2.131205	-2.056048
N	-1.443613	-1.404483	1.126387
H	-0.552561	-1.614476	0.657059
C	-1.473413	-2.098215	2.442262
H	-0.599277	-1.779925	3.007425
H	-2.383389	-1.818445	2.968166
H	-1.449382	-3.172297	2.268199
C	-2.566751	-1.700986	0.239370
C	-3.837444	-1.274044	0.603371
C	-2.326729	-2.349216	-0.960815
C	-4.893807	-1.498908	-0.270407
H	-3.991164	-0.755120	1.543767
C	-3.393408	-2.570585	-1.828383
H	-1.320991	-2.663417	-1.218298
C	-4.671959	-2.144307	-1.486065
H	-5.888607	-1.161215	-0.005296
H	-3.219138	-3.072132	-2.772637
H	-5.498134	-2.312103	-2.166720

IM$_{9a}$

Symbol	X	Y	Z
Si	-0.857327	0.047287	0.612596
H	-2.186688	-2.002086	-2.037197
C	0.953512	0.105878	0.262754
C	1.549023	1.272608	-0.235070
C	1.757261	-1.021704	0.477796
C	2.911827	1.310275	-0.511850
H	0.946347	2.159570	-0.400540
C	3.119490	-0.985294	0.199261
H	1.321815	-1.937443	0.864625
C	3.696589	0.180861	-0.295810
H	3.361530	2.219771	-0.893265
H	3.730398	-1.864020	0.370817
H	4.758817	0.210138	-0.510748
C	-1.649519	-1.797901	-1.104502
O	-1.691371	-0.512631	-0.770854
O	-1.087212	-2.642047	-0.454610
O	-1.378353	1.568771	0.861099
O	-1.278074	-0.913416	1.869423
H	-1.228772	-1.860611	1.696853
H	-2.318841	1.723883	0.998241

IM$_{9b}$

Symbol	X	Y	Z
Si	-0.966643	-0.064369	0.603688
C	0.862087	0.036034	0.272783
C	1.466027	1.251870	-0.073454
C	1.667026	-1.109962	0.343687
C	2.828133	1.321065	-0.349768
H	0.870925	2.158604	-0.122188
C	3.029345	-1.044963	0.068027
H	1.230024	-2.065314	0.619446
C	3.610268	0.171533	-0.280125
H	3.279942	2.270135	-0.615029
H	3.637876	-1.940163	0.127502

H	4.671955	0.224056	-0.493561
O	-1.811498	-0.589483	-0.706134
O	-1.583559	1.405427	1.000794
O	-1.250221	-1.107061	1.842072
H	-0.656059	-1.060771	2.597480
H	-1.737466	2.033225	0.288365
H	-1.449110	-1.337542	-1.190965

IM$_9$

Symbol	X	Y	Z
Si	-1.429893	-0.764116	-0.514939
H	-0.287098	-2.121722	2.615800
H	1.248805	1.272201	-1.825788
C	-2.871345	0.339785	-0.184313
C	-2.842269	1.696365	-0.535933
C	-4.051162	-0.188557	0.362299
C	-3.954099	2.506319	-0.330532
H	-1.952134	2.134230	-0.973126
C	-5.161816	0.622160	0.566355
H	-4.098571	-1.235105	0.640694
C	-5.112867	1.970308	0.222656
H	-3.915958	3.554064	-0.604994
H	-6.065299	0.201951	0.992683
H	-5.978897	2.602332	0.383265
C	-1.048430	-1.910199	1.857256
O	-0.527709	-1.242461	0.820340
O	-2.198486	-2.232250	1.940785
C	0.515980	1.011157	-1.054033
O	0.428335	1.550278	0.010338
O	-0.277505	0.010299	-1.462415
O	-1.825139	-2.139749	-1.292646
H	-2.580654	-2.128963	-1.889904

***N*-methylaniline**

Symbol	X	Y	Z
N	1.784437	-0.619777	-0.151182
H	2.000147	-1.545703	0.186787
C	2.811886	0.371725	0.105128
H	3.781653	-0.122426	0.092446
H	2.814261	1.132504	-0.679032
H	2.684011	0.875350	1.072010
C	0.445175	-0.283127	-0.058834
C	0.013574	1.051748	-0.054921
C	-0.527467	-1.298584	-0.005554
C	-1.346110	1.349928	-0.011594
H	0.734281	1.858583	-0.087220
C	-1.875856	-0.986064	0.042838
H	-0.206067	-2.335153	-0.005750
C	-2.301858	0.342982	0.037903
H	-1.655133	2.389406	-0.011617
H	-2.603287	-1.788897	0.086156
H	-3.356985	0.583124	0.074699

***N*-methylformanilide**

Symbol	X	Y	Z
H	3.329301	-0.188904	-0.060125
C	2.305381	-0.582896	-0.143198
O	2.086575	-1.739341	-0.433945
N	1.375122	0.384667	0.113828
C	1.847189	1.751027	0.329739
H	1.299091	2.203393	1.156219
H	2.904101	1.721778	0.586838
H	1.724145	2.366225	-0.563989
C	-0.024907	0.152728	0.050098
C	-0.880319	1.213263	-0.265562
C	-0.575094	-1.102883	0.335967
C	-2.256540	1.019361	-0.306002
H	-0.479683	2.193872	-0.484810
C	-1.951865	-1.282147	0.289857
H	0.069400	-1.928591	0.592207
C	-2.802103	-0.228718	-0.032214
H	-2.899852	1.854736	-0.555365
H	-2.361344	-2.259768	0.515774
H	-3.874059	-0.379086	-0.064097

***N, N*-dimethylaniline**

Symbol	X	Y	Z
H	-3.279182	-1.846695	-2.696745
H	-2.718421	-0.459974	-3.654618
C	-2.590994	-0.990486	-2.712931
N	-2.832188	-0.065479	-1.618634
C	-3.698138	1.069704	-1.887586
H	-3.365309	1.952552	-1.337439
H	-3.648453	1.304300	-2.949213
H	-4.745119	0.871206	-1.620102
C	-2.745843	-0.538272	-0.324027
C	-3.240169	0.210950	0.765793
C	-2.152353	-1.786897	-0.037329

C	-3.116938	-0.258414	2.067271
H	-3.723536	1.163952	0.599374
C	-2.038893	-2.238064	1.271413
H	-1.776457	-2.409716	-0.837576
C	-2.513905	-1.483003	2.340054
H	-3.506820	0.346435	2.879007
H	-1.574271	-3.201414	1.452652
H	-2.423932	-1.843070	3.357632
H	-1.568123	-1.372490	-2.682896

formaldehyde

Symbol	X	Y	Z
C	0.174807	0.258987	-0.000000
H	0.699248	-0.710814	-0.000000
H	-0.927268	0.228128	-0.000000
O	0.774997	1.299326	0.000000

IM_{10}

Symbol	X	Y	Z
C	-4.427452	-0.971521	-0.431943
H	-4.397879	-0.404614	-1.367034
O	-3.362757	-1.336157	0.132954
N	-5.619500	-1.237863	0.037688
C	-5.813099	-1.977610	1.278917
H	-6.375723	-1.356085	1.977718
H	-6.382164	-2.884580	1.067234
H	-4.847853	-2.235590	1.704614
C	-6.826019	-0.810597	-0.659475
H	-6.556215	-0.265537	-1.561936
H	-7.418517	-1.687938	-0.923834
H	-7.410969	-0.165745	-0.001845
Si	-1.597932	-0.751188	-0.526755
H	0.320191	-1.546884	-2.870374
H	-1.069717	-1.646795	0.513578
H	-2.018666	-1.219907	-1.867408
C	-1.981929	1.037352	-0.064958
C	-1.558706	2.086384	-0.889389
C	-2.665258	1.364677	1.114951
C	-1.814507	3.414447	-0.557056
H	-1.003844	1.868502	-1.796369
C	-2.899435	2.690617	1.466981
H	-3.013288	0.575439	1.774280
C	-2.478515	3.719117	0.626914
H	-1.481391	4.209860	-1.214317
H	-3.414041	2.921933	2.393019
H	-2.667428	4.752573	0.895119
Si	1.869253	-0.499571	-0.423584
H	0.363120	0.236662	-3.132933
H	1.493073	-3.696676	1.290667
H	0.720761	2.338303	1.472930
C	3.699303	-0.197784	-0.064718
C	4.667096	-0.347140	-1.068262
C	4.144089	0.158044	1.217253
C	6.021278	-0.151751	-0.805762
H	4.354423	-0.612670	-2.071821
C	5.495451	0.356292	1.486136
H	3.422088	0.269353	2.018182
C	6.438921	0.201203	0.473781
H	6.749342	-0.271390	-1.600732
H	5.813213	0.631996	2.485885
H	7.492052	0.356340	0.680903
C	0.630475	-0.581565	-2.459186
O	0.090424	-0.376602	-1.161753
O	1.988511	-0.557734	-2.123795
C	1.172301	1.784947	0.639062
O	1.594889	2.312264	-0.361696
O	1.214607	0.486916	0.858032
C	1.737885	-2.625863	1.293244
O	1.578187	-2.104876	0.083162
O	2.098160	-2.034609	2.272656

IM_{11}

Symbol	X	Y	Z
Si	-1.343225	1.480423	-1.246753
H	-1.193178	1.786709	-2.682214
H	-1.533002	2.715144	-0.460603
C	-2.776350	0.306215	-1.030444
C	-3.220411	-0.080878	0.243373
C	-3.439013	-0.206351	-2.153172
C	-4.290847	-0.956572	0.386548
H	-2.723715	0.304339	1.128029
C	-4.513690	-1.081371	-2.011498
H	-3.116918	0.077203	-3.150693
C	-4.938204	-1.457488	-0.741551
H	-4.623229	-1.247937	1.376614
H	-5.016493	-1.468574	-2.890387
H	-5.773805	-2.139138	-0.628695
Si	0.847173	0.016834	0.445625

H	-1.202749	-2.287365	2.343559
H	0.615421	2.214088	3.283529
C	2.446608	-0.713443	-0.077858
C	2.881584	-0.620611	-1.404844
C	3.243394	-1.391210	0.856075
C	4.091013	-1.190288	-1.790886
H	2.275557	-0.099619	-2.138630
C	4.451022	-1.959759	0.468833
H	2.920711	-1.475423	1.889674
C	4.873970	-1.858666	-0.854641
H	4.421291	-1.112924	-2.820187
H	5.062042	-2.480910	1.196566
H	5.816173	-2.302325	-1.155842
O	0.088790	0.775044	-0.757717
C	0.207747	1.634236	2.448797
O	-0.963434	1.510971	2.215928
O	1.174098	1.081480	1.710650
C	-0.315385	-1.652201	2.239314
O	-0.224528	-1.154053	1.001403
O	0.471391	-1.436644	3.116172

IM_{12}

Symbol	X	Y	Z
N	-0.759605	-0.997755	-0.552538
C	0.496882	-0.442081	-0.309989
C	1.492664	-1.176313	0.361498
C	0.827768	0.861523	-0.734534
C	2.758195	-0.640013	0.570637
H	1.286081	-2.175222	0.720641
C	2.095934	1.382882	-0.515156
H	0.102944	1.482665	-1.245012
C	3.077458	0.641692	0.136566
H	3.499897	-1.238933	1.087839
H	2.312015	2.389073	-0.857281
H	4.063276	1.056648	0.307177
C	-1.137512	-2.180340	0.210385
H	-1.064136	-2.019013	1.292850
H	-2.167605	-2.434653	-0.035299
H	-0.509958	-3.032854	-0.056721
C	-1.841787	-0.118568	-0.918563
H	-2.686628	-0.734676	-1.220249
O	-2.309699	0.693491	0.144258
H	-1.542386	0.489117	-1.774572
H	-1.620227	1.334164	0.351588

IM_{13}

Symbol	X	Y	Z
C	-2.775588	1.677440	0.792780
H	-3.161391	1.141428	-0.084138
O	-1.486004	1.432865	1.080679
Si	-0.327058	0.627966	0.163250
H	-1.827391	1.421087	-3.107285
C	1.150872	1.651677	-0.302295
C	1.992000	1.212241	-1.328792
C	1.437017	2.870425	0.325526
C	3.107094	1.959178	-1.703813
H	1.787715	0.275140	-1.839244
C	2.540021	3.625914	-0.057918
H	0.787489	3.247816	1.110904
C	3.381297	3.166640	-1.069757
H	3.758558	1.597227	-2.491647
H	2.744132	4.571656	0.431188
H	4.244825	3.752117	-1.364577
O	-0.279450	-1.006322	0.248646
C	-1.535639	1.674700	-2.078933
O	-1.599126	2.792499	-1.634039
O	-1.131198	0.611201	-1.407293
N	2.694072	-0.654037	1.788303
C	2.936470	-1.499099	0.701406
C	2.192810	-2.674379	0.485362
C	3.981908	-1.216607	-0.193533
C	2.461061	-3.497091	-0.598270
H	1.398194	-2.957285	1.161556
C	4.246872	-2.057400	-1.271690
H	4.582985	-0.325819	-0.070561
C	3.487278	-3.198278	-1.494355
H	1.862065	-4.391309	-0.735782
H	5.056902	-1.801746	-1.946188
H	3.692279	-3.846726	-2.337407
C	3.584749	0.472950	2.018934
H	3.525210	1.221837	1.220446
H	3.308626	0.949385	2.961045
H	4.619386	0.132235	2.103148
C	1.461049	-0.627259	2.490880
H	1.638526	-0.460234	3.553446
O	0.559982	0.439509	2.071673
H	0.895757	-1.538597	2.349252
H	0.813344	1.274147	2.490120

Si	-1.201189	-2.194255	-0.465046
H	-0.842994	-2.379115	-1.886088
H	-0.936820	-3.428470	0.302952
C	-2.991835	-1.678960	-0.299941
C	-3.746851	-1.264286	-1.404048
C	-3.561145	-1.567595	0.976523
C	-5.031321	-0.752105	-1.238923
H	-3.324719	-1.324883	-2.402530
C	-4.842679	-1.050778	1.146822
H	-2.997771	-1.875751	1.853540
C	-5.577524	-0.640985	0.037595
H	-5.602575	-0.433460	-2.103545
H	-5.264703	-0.962932	2.141527
H	-6.573953	-0.234088	0.167428
O	-3.443479	2.400823	1.468848

IM$_{14}$

Symbol	X	Y	Z
C	2.865626	-1.899199	0.564466
H	3.095384	-1.167957	-0.220558
O	1.649399	-1.800554	1.086528
Si	0.239157	-0.897893	0.647223
H	1.492339	-1.048841	-2.943270
C	-1.252229	-1.798916	-0.128110
C	-1.755039	-1.481774	-1.398688
C	-1.917847	-2.810035	0.581547
C	-2.861951	-2.136521	-1.934928
H	-1.278514	-0.703519	-1.985465
C	-3.004510	-3.495046	0.041678
H	-1.584289	-3.077830	1.577844
C	-3.484954	-3.155864	-1.219622
H	-3.232732	-1.855403	-2.914981
H	-3.480696	-4.286768	0.609908
H	-4.336932	-3.678305	-1.640384
O	0.194018	0.777245	0.762884
C	1.287597	-1.496465	-1.954734
O	1.389498	-2.690598	-1.773320
O	0.954480	-0.602453	-1.069588
N	-3.049234	0.695823	1.333418
C	-2.783829	1.783886	0.418973
C	-2.296972	2.988113	0.917744
C	-3.059737	1.626974	-0.935610
C	-2.055535	4.037543	0.040254
H	-2.128943	3.116473	1.980408
C	-2.812790	2.686297	-1.802571
H	-3.454701	0.696965	-1.322010
C	-2.309141	3.889384	-1.320223
H	-1.677799	4.976159	0.427334
H	-3.019928	2.564182	-2.858845
H	-2.122902	4.712453	-1.999672
C	-4.202209	-0.174020	1.039317
H	-3.963220	-0.806500	0.184640
H	-4.396603	-0.792136	1.911626
H	-5.061248	0.456020	0.814870
C	-2.322759	0.491595	2.368320
H	-2.611064	-0.285930	3.061163
O	-0.316551	-1.030264	2.279832
H	-1.453381	1.106671	2.548028
H	-0.084012	-1.857542	2.707986
Si	0.995837	1.975596	-0.037726
H	0.460454	2.237640	-1.392931
H	0.838747	3.195863	0.789329
C	2.825104	1.571384	-0.132266
C	3.470033	1.320091	-1.349233
C	3.556159	1.404971	1.051172
C	4.800250	0.911209	-1.384925
H	2.922326	1.425641	-2.281089
C	4.884570	0.986312	1.023196
H	3.083189	1.589916	2.012380
C	5.507180	0.737832	-0.196554
H	5.283974	0.718319	-2.336160
H	5.430907	0.851251	1.950022
H	6.539782	0.408348	-0.222342
O	3.670716	-2.700914	0.956175

IM$_{15}$

Symbol	X	Y	Z
C	1.393857	-0.605425	2.265475
H	2.040102	0.259257	2.072175
O	1.241452	-1.443180	1.227095
Si	1.709369	-1.285332	-0.383074
H	1.820518	3.170800	-0.359563
C	3.409453	-0.542097	-0.440681
C	3.775636	0.320239	-1.482176
C	4.346166	-0.808771	0.565331
C	5.038305	0.901954	-1.515833
H	3.067589	0.547930	-2.273768
C	5.611946	-0.228707	0.534523

H	4.091847	-1.469099	1.390127
C	5.957403	0.628866	-0.504932
H	5.305506	1.570571	-2.326323
H	6.324132	-0.441374	1.323622
H	6.940352	1.085629	-0.527323
O	0.606609	-0.530239	-1.305501
C	1.844488	2.376062	0.409736
O	2.511217	2.509673	1.415780
O	1.122207	1.332617	0.139395
N	-3.084566	-1.320680	-1.732629
C	-2.989748	-1.401618	-0.289672
C	-1.879481	-1.995485	0.309265
C	-4.013367	-0.859387	0.482031
C	-1.782984	-2.006135	1.694109
H	-1.103608	-2.466612	-0.281822
C	-3.906127	-0.886989	1.868083
H	-4.878513	-0.398561	0.026307
C	-2.789896	-1.447479	2.475989
H	-0.905530	-2.434769	2.159113
H	-4.696977	-0.451340	2.466968
H	-2.703534	-1.455653	3.556071
C	-4.416442	-1.096951	-2.324335
H	-4.728757	-0.074236	-2.113780
H	-4.343067	-1.249440	-3.396979
H	-5.117164	-1.803931	-1.884820
C	-2.054889	-1.394002	-2.490514
H	-2.199616	-1.343427	-3.562448
O	1.662208	-2.837457	-0.935648
H	-1.062750	-1.520740	-2.074181
H	2.198782	-3.485402	-0.468141
Si	0.035594	1.081413	-1.406651
H	0.851659	2.132407	-2.087722
H	-0.775314	0.715989	-2.668841
C	-1.512088	1.666182	-0.457990
C	-2.666671	1.964758	-1.197738
C	-1.569948	1.866891	0.930654
C	-3.813108	2.476358	-0.594227
H	-2.668180	1.799569	-2.272154
C	-2.720242	2.358494	1.544979
H	-0.703915	1.639754	1.542538
C	-3.841541	2.675383	0.783324
H	-4.683383	2.714897	-1.196756
H	-2.739082	2.497972	2.620684
H	-4.732564	3.068589	1.260567
O	0.861261	-0.816665	3.317456

IM_{16}

Symbol	X	Y	Z
C	1.950881	-0.477083	2.374582
H	2.846603	0.069505	2.053431
O	1.385460	-1.244048	1.418162
Si	1.614876	-1.245259	-0.245726
H	2.748687	2.926446	-0.647669
C	3.361415	-0.764361	-0.620852
C	3.628751	0.110431	-1.683157
C	4.432959	-1.221186	0.159200
C	4.928745	0.525688	-1.952969
H	2.817751	0.474126	-2.308117
C	5.733325	-0.808350	-0.111193
H	4.258770	-1.899308	0.990078
C	5.980380	0.068228	-1.164325
H	5.119733	1.206457	-2.774421
H	6.552182	-1.165159	0.502575
H	6.993202	0.395646	-1.369516
O	0.588290	-0.146342	-0.896278
C	2.676232	2.444281	0.338142
O	3.542901	2.474430	1.157696
O	1.502823	1.826223	0.566975
O	1.116364	-2.696468	-0.790094
H	1.610278	-3.481549	-0.530338
Si	0.277540	1.431815	-0.536644
H	0.407105	2.283502	-1.726885
C	-1.332654	1.602366	0.344255
C	-2.246195	2.596770	-0.022963
C	-1.653060	0.740533	1.403493
C	-3.454537	2.731227	0.654801
H	-2.018366	3.270901	-0.842932
C	-2.857457	0.878578	2.082714
H	-0.962334	-0.042530	1.704183
C	-3.758017	1.873502	1.707136
H	-4.157489	3.501859	0.360803
H	-3.095850	0.211518	2.902950
H	-4.698658	1.977862	2.235765
O	1.503302	-0.428040	3.478477

IM_{17}

Symbol	X	Y	Z
C	4.183393	0.430196	1.546055

H	4.595820	-0.252938	0.794139
O	2.871834	0.642745	1.463651
Si	1.628653	-0.107076	0.542518
H	3.690739	-3.257979	0.337053
C	0.362691	-1.347858	1.202573
C	-0.037931	-2.443194	0.424873
C	-0.235428	-1.184611	2.458652
C	-1.015849	-3.328658	0.873295
H	0.418125	-2.607062	-0.547424
C	-1.186338	-2.087396	2.929531
H	0.042350	-0.336485	3.075921
C	-1.588634	-3.154991	2.131435
H	-1.328245	-4.155400	0.244387
H	-1.623042	-1.951064	3.912972
H	-2.341410	-3.849535	2.487415
O	1.596060	0.310693	-1.078100
C	3.258157	-2.392899	0.867135
O	3.295947	-2.305690	2.075317
O	2.744306	-1.516193	0.051225
O	0.555271	1.211427	1.013553
H	0.964455	2.079693	0.930393
Si	2.578916	-0.043706	-2.356346
H	2.411575	-1.430879	-2.843240
H	2.187250	0.896980	-3.432713
C	4.371089	0.245910	-1.898697
C	5.281918	-0.812873	-1.800598
C	4.799668	1.527283	-1.527832
C	6.579510	-0.601118	-1.342890
H	4.970491	-1.818686	-2.066258
C	6.093598	1.743595	-1.060765
H	4.114844	2.369131	-1.589573
C	6.983950	0.677815	-0.966445
H	7.272276	-1.432229	-1.270556
H	6.404830	2.739437	-0.765828
H	7.990563	0.842291	-0.598694
O	4.865772	0.978319	2.367643
H	-2.286067	-0.818317	0.645771
H	-2.753399	0.497471	1.737700
C	-2.777401	0.150302	0.704667
N	-4.106219	0.126346	0.200654
C	-5.079324	0.996889	0.858299
H	-5.721298	0.429917	1.541560
H	-4.549713	1.757583	1.428250
H	-5.706735	1.504279	0.122478
C	-4.587818	-0.964108	-0.536212
C	-5.970669	-1.122429	-0.736555
C	-3.732048	-1.924157	-1.108068
C	-6.466943	-2.196203	-1.468645
H	-6.671585	-0.410560	-0.324111
C	-4.245013	-2.995242	-1.827562
H	-2.658269	-1.851054	-1.006846
C	-5.615474	-3.146387	-2.018120
H	-7.539498	-2.283673	-1.602229
H	-3.553365	-3.716571	-2.248939
H	-6.007528	-3.982201	-2.584463
N	-1.868625	1.116808	-0.061567
H	-0.914550	1.112435	0.429919
C	-1.611639	0.650228	-1.449579
H	-1.003732	1.395647	-1.958039
H	-1.060813	-0.286873	-1.383184
H	-2.554640	0.498707	-1.971053
C	-2.359442	2.494967	0.029504
C	-3.203496	3.023048	-0.937964
C	-2.003419	3.224404	1.158123
C	-3.698160	4.312061	-0.764357
H	-3.483845	2.447901	-1.811218
C	-2.503224	4.511682	1.319279
H	-1.349951	2.783920	1.903476
C	-3.352620	5.055113	0.360240
H	-4.359166	4.732080	-1.512903
H	-2.228294	5.086256	2.195557
H	-3.742374	6.058020	0.487708

IM_{18}

Symbol	X	Y	Z
C	4.103387	0.245898	1.589036
H	4.564692	-0.359612	0.799882
O	2.780040	0.422079	1.469098
Si	1.651833	-0.333152	0.448719
H	3.718391	-3.389808	0.049784
C	0.338569	-1.498209	1.103001
C	-0.117613	-2.553082	0.301511
C	-0.214758	-1.348789	2.380812
C	-1.115511	-3.414701	0.750907
H	0.304256	-2.703290	-0.688247
C	-1.189830	-2.226765	2.845809
H	0.115964	-0.536391	3.019402
C	-1.651218	-3.253682	2.026061

H	-1.471914	-4.212471	0.108448
H	-1.597270	-2.103726	3.843115
H	-2.422303	-3.928445	2.380574
O	1.559936	0.275702	-1.089010
C	3.269774	-2.577251	0.640388
O	3.296412	-2.560344	1.847360
O	2.734474	-1.649865	-0.121634
O	0.512098	1.095615	1.025892
H	0.908758	1.973261	0.935431
Si	2.558340	0.129327	-2.407884
H	2.430614	-1.194392	-3.052680
H	2.136545	1.191798	-3.345981
C	4.327012	0.401633	-1.863731
C	5.252036	-0.649349	-1.834242
C	4.716438	1.646271	-1.350150
C	6.526228	-0.465589	-1.304277
H	4.969619	-1.627846	-2.210816
C	5.987099	1.833019	-0.812237
H	4.019114	2.480043	-1.355717
C	6.891821	0.775287	-0.787431
H	7.230216	-1.290057	-1.285716
H	6.268948	2.798863	-0.408477
H	7.880003	0.916867	-0.364473
O	4.725128	0.745017	2.480787
H	-2.304955	-0.770484	0.620652
H	-2.743731	0.532379	1.726187
C	-2.747238	0.222232	0.680027
N	-4.102159	0.214160	0.183611
C	-5.041679	1.133702	0.815455
H	-5.704488	0.614212	1.517983
H	-4.486007	1.892265	1.362272
H	-5.655734	1.641509	0.067392
C	-4.617053	-0.865245	-0.529574
C	-6.008248	-1.004198	-0.706354
C	-3.790802	-1.846548	-1.115985
C	-6.535671	-2.071805	-1.425149
H	-6.690390	-0.279420	-0.284654
C	-4.335585	-2.910525	-1.821509
H	-2.714717	-1.787584	-1.036168
C	-5.712158	-3.039849	-1.987110
H	-7.612091	-2.141113	-1.538786
H	-3.664174	-3.644657	-2.254028
H	-6.129088	-3.870410	-2.543353
N	-1.832004	1.148167	-0.050290
H	-0.456328	1.097516	0.588789
C	-1.630669	0.718834	-1.442622
H	-0.979802	1.432476	-1.947411
H	-1.132275	-0.251408	-1.428620
H	-2.575376	0.633807	-1.987315
C	-2.235690	2.527203	0.099943
C	-2.855890	3.243390	-0.920714
C	-2.007739	3.137786	1.336099
C	-3.253043	4.560600	-0.698114
H	-3.037628	2.784949	-1.884513
C	-2.411566	4.448633	1.552152
H	-1.527096	2.575915	2.130667
C	-3.038487	5.165234	0.534738
H	-3.737702	5.110820	-1.496372
H	-2.231837	4.912344	2.515133
H	-3.351686	6.188920	0.702282

TS_I

Symbol	X	Y	Z
C	-2.277676	-0.835949	-0.343539
H	-1.971993	-1.291633	-1.288866
O	-1.428290	-0.608332	0.554494
N	-3.551406	-0.560446	-0.218268
C	-4.091148	0.054244	0.990834
H	-4.534200	1.017319	0.734264
H	-4.860640	-0.596475	1.407615
H	-3.291676	0.192110	1.712279
C	-4.502218	-0.858705	-1.284199
H	-3.980264	-1.299665	-2.130458
H	-5.251986	-1.558780	-0.914377
H	-4.992345	0.063110	-1.598417
Si	0.488134	-0.933437	0.333968
H	2.061854	-1.292298	0.157827
H	0.466982	-1.559456	1.671464
H	0.168954	-1.764061	-0.853649
C	0.862233	0.911034	0.130327
C	2.131739	1.295672	-0.328034
C	-0.058398	1.927716	0.425046
C	2.464314	2.636458	-0.498871
H	2.875250	0.537143	-0.551340
C	0.274526	3.269897	0.266654
H	-1.046626	1.673282	0.787607
C	1.535633	3.627918	-0.199781
H	3.449938	2.905816	-0.860397

H	-0.452775	4.036721	0.507323
H	1.793292	4.672962	-0.326717
C	3.076318	-2.382159	-0.024223
O	2.502680	-3.406432	0.149090
O	4.073556	-1.788306	-0.274919

TS_2

Symbol	X	Y	Z
C	2.267881	-0.689059	0.123585
H	1.868757	-0.833708	1.127933
O	1.491137	-0.669509	-0.885325
N	3.554570	-0.544921	0.013472
C	4.210517	-0.333492	-1.273771
H	4.738133	0.620919	-1.242659
H	4.929337	-1.137986	-1.435379
H	3.471511	-0.327931	-2.069193
C	4.426543	-0.588323	1.183390
H	3.832297	-0.730645	2.083166
H	5.130400	-1.413632	1.070022
H	4.976588	0.351116	1.247937
Si	-0.357319	-0.623715	-0.786217
H	-2.004115	-0.714828	-0.727024
H	-0.407575	-1.024597	-2.200795
C	-0.449650	1.165758	-0.208942
C	-1.617706	1.640005	0.406626
C	0.603297	2.072294	-0.410649
C	-1.724627	2.964000	0.819875
H	-2.447954	0.961975	0.569183
C	0.493816	3.400424	-0.007994
H	1.518677	1.752422	-0.896466
C	-0.668677	3.847080	0.612341
H	-2.633305	3.307347	1.301330
H	1.316772	4.084998	-0.179539
H	-0.752659	4.880284	0.930099
C	-3.212286	-1.426296	-0.819110
O	-2.956766	-2.594028	-0.860172
O	-4.071126	-0.596685	-0.831702
O	-0.282876	-1.904781	0.351301
C	-1.130959	-2.136204	1.352423
H	-1.057491	-3.174505	1.698953
O	-1.857766	-1.318886	1.843831

TS_3

Symbol	X	Y	Z
C	1.067515	-1.798805	-1.941346
H	0.971678	-2.149398	-2.975635
O	0.034439	-1.034269	-1.596180
Si	-0.210707	-0.302882	-0.075699
H	-0.128589	-2.588740	2.696949
H	-1.641878	-1.186098	-0.039698
H	2.527479	-0.754680	1.012988
C	-1.232606	1.255840	-0.091542
C	-0.684169	2.507886	0.224304
C	-2.593381	1.188484	-0.424411
C	-1.473521	3.653350	0.213292
H	0.364597	2.594539	0.481849
C	-3.378451	2.336593	-0.449644
H	-3.048358	0.232785	-0.665121
C	-2.820266	3.569895	-0.127545
H	-1.035188	4.611566	0.467821
H	-4.426870	2.266794	-0.715860
H	-3.433506	4.463871	-0.140205
C	-0.575538	-1.708108	2.223537
O	0.240426	-1.194254	1.289333
O	-1.629340	-1.234005	2.529626
C	2.484595	0.135234	0.392518
O	1.368236	0.529322	-0.099269
C	-2.174463	-2.377881	-0.350913
O	-3.213066	-2.163054	-0.915386
O	-1.453657	-3.256596	0.042893
N	3.580100	0.793356	0.186029
C	3.626399	2.008280	-0.624652
H	2.683188	2.143746	-1.145551
H	3.820683	2.860227	0.028799
H	4.440622	1.909634	-1.342497
C	4.843188	0.358441	0.777887
H	5.550664	0.142203	-0.023009
H	5.233277	1.163163	1.401859
H	4.679837	-0.532283	1.380578
O	1.988743	-2.076740	-1.223043

TS_{4a}

Symbol	X	Y	Z
Si	1.449066	0.156012	-0.331474
H	-0.442113	1.179761	2.586606
H	-0.007465	-2.321474	-2.100066
C	3.194777	-0.418112	0.015103
C	3.684222	-1.686342	-0.325204

C	4.091664	0.505447	0.575733
C	5.020309	-2.017890	-0.118646
H	3.013007	-2.423472	-0.747003
C	5.422659	0.169959	0.801145
H	3.738347	1.489753	0.862332
C	5.891073	-1.092411	0.448508
H	5.380077	-3.002262	-0.396373
H	6.093924	0.894615	1.248042
H	6.929755	-1.354122	0.616848
C	0.491366	1.027677	2.029617
O	0.270897	0.375091	0.891706
O	1.566173	1.390968	2.417754
C	0.214233	-1.598120	-1.309011
O	0.796809	-1.910634	-0.233085
O	0.583587	-0.358697	-1.722666
O	1.659548	1.766319	-0.710869
N	-1.608780	-1.301944	-0.910056
H	-1.533243	-0.566111	-0.206417
C	-2.273840	-0.799838	-2.119690
H	-1.892240	0.197797	-2.323009
H	-2.031112	-1.447877	-2.963377
H	-3.356276	-0.765737	-1.985867
C	-2.131513	-2.488918	-0.313604
C	-2.783173	-3.455743	-1.075837
C	-1.899481	-2.701795	1.045937
C	-3.212081	-4.632286	-0.465642
H	-2.965549	-3.298175	-2.131427
C	-2.334859	-3.876447	1.643612
H	-1.378409	-1.943449	1.619562
C	-2.992614	-4.846955	0.890062
H	-3.723618	-5.380911	-1.059296
H	-2.159464	-4.034295	2.701387
H	-3.333122	-5.762464	1.358955
H	2.493989	1.994290	-1.129026

TS_{4b}

Symbol	X	Y	Z
Si	1.396313	0.082351	-0.236311
H	0.018602	-2.230113	-2.237666
C	3.185960	-0.436808	0.035435
C	3.638614	-1.764924	0.007219
C	4.135205	0.562164	0.309562
C	4.976263	-2.078906	0.230665
H	2.934650	-2.561976	-0.192287
C	5.472030	0.252834	0.543162
H	3.824335	1.599906	0.345401
C	5.897151	-1.071121	0.501203
H	5.299019	-3.113626	0.196797
H	6.180272	1.045869	0.755957
H	6.938428	-1.316198	0.678589
O	0.331909	0.189873	1.044921
C	0.249646	-1.529439	-1.431356
O	0.811746	-1.881426	-0.349797
O	0.607040	-0.281997	-1.761523
O	1.556011	1.743541	-0.483296
N	-1.615842	-1.261393	-0.996451
H	-1.513658	-0.522091	-0.300557
C	-2.296326	-0.769893	-2.197656
H	-1.892878	0.212808	-2.432327
H	-2.091406	-1.441305	-3.033422
H	-3.375108	-0.701911	-2.044092
C	-2.115579	-2.440163	-0.375125
C	-2.821975	-3.403964	-1.092012
C	-1.806203	-2.649358	0.971192
C	-3.226511	-4.572959	-0.450518
H	-3.064512	-3.250665	-2.136292
C	-2.218629	-3.815912	1.599221
H	-1.237836	-1.892710	1.501535
C	-2.930402	-4.783505	0.891138
H	-3.779992	-5.318991	-1.008920
H	-1.982327	-3.971661	2.645504
H	-3.252464	-5.692885	1.384390
H	2.082837	2.015292	-1.239362
H	0.227441	1.104296	1.329737

TS_4

Symbol	X	Y	Z
Si	1.153947	-0.255392	0.366452
H	-0.216808	-2.053928	-2.460829
H	3.147259	-2.877327	1.899016
H	-1.179994	1.357760	2.162762
C	2.596344	0.829264	-0.087543
C	2.546646	2.229168	-0.070908
C	3.799809	0.214092	-0.468326
C	3.662623	2.988054	-0.414110
H	1.632380	2.734948	0.210086
C	4.910097	0.970422	-0.822276
H	3.867150	-0.867151	-0.507141

C	4.844532	2.361215	-0.792022
H	3.604355	4.070182	-0.388729
H	5.826914	0.474798	-1.120301
H	5.711770	2.952285	-1.064052
C	0.612648	-1.594104	-1.910373
O	0.163495	-0.924285	-0.842559
O	1.761535	-1.668663	-2.235047
C	-0.565282	0.838248	1.428116
O	-0.154261	1.339357	0.355497
O	0.190192	-0.181959	1.813723
C	2.748102	-1.858061	1.814990
O	1.927083	-1.742158	0.779821
O	3.031032	-0.971142	2.574750
N	-2.320355	-0.241420	0.874168
H	-1.915418	-0.877661	0.191648
C	-2.769410	-0.932555	2.080260
H	-2.054951	-1.722246	2.304866
H	-2.788683	-0.234762	2.921131
H	-3.765519	-1.366253	1.956249
C	-3.181620	0.689912	0.258567
C	-4.210102	1.315366	0.966081
C	-2.938535	1.048661	-1.072737
C	-4.990462	2.283471	0.337692
H	-4.409895	1.048720	1.996359
C	-3.725881	2.010591	-1.687967
H	-2.127881	0.566669	-1.608970
C	-4.757269	2.634692	-0.986506
H	-5.789889	2.760042	0.893572
H	-3.533307	2.275552	-2.721337
H	-5.371396	3.384730	-1.470327

TS_{5a}

Symbol	X	Y	Z
Si	1.891667	-0.589065	-0.033127
H	3.936053	-3.123712	1.758727
H	0.684539	1.683893	1.625558
C	3.429390	0.320004	-0.640180
C	3.448607	1.715614	-0.764044
C	4.587375	-0.377073	-1.018447
C	4.577018	2.389637	-1.228080
H	2.562331	2.280733	-0.499136
C	5.710982	0.286139	-1.500677
H	4.615765	-1.459018	-0.936766
C	5.710675	1.675617	-1.601178
H	4.567609	3.471547	-1.303970
H	6.589402	-0.278951	-1.792763
H	6.588155	2.195972	-1.968878
O	1.121025	-1.528253	-1.203113
C	0.433747	0.761491	1.081109
O	0.729478	0.790351	-0.251978
O	1.167248	-0.336881	1.521002
C	3.604748	-2.093674	1.546763
O	2.727421	-2.063655	0.571982
O	4.035160	-1.148307	2.159637
N	-1.034428	0.497423	1.323594
H	-1.276623	-0.581331	0.613136
C	-1.259490	0.169797	2.744781
H	-0.733546	-0.757038	2.962592
H	-0.875081	0.957608	3.397966
H	-2.327230	0.039453	2.918030
C	-1.865571	1.567498	0.805807
C	-2.492820	2.485684	1.644182
C	-2.048690	1.647285	-0.577041
C	-3.310652	3.473094	1.098291
H	-2.359430	2.438736	2.717219
C	-2.868143	2.632814	-1.110906
H	-1.542998	0.942770	-1.224459
C	-3.504073	3.548640	-0.275283
H	-3.797849	4.181925	1.757618
H	-3.012295	2.682343	-2.183979
H	-4.146760	4.313966	-0.694194
N	-1.491215	-1.623050	-0.086471
H	-0.813983	-1.560762	-0.856063
C	-1.150142	-2.814058	0.726313
H	-0.121839	-2.705370	1.072278
H	-1.815012	-2.867732	1.587383
H	-1.248550	-3.720850	0.127638
C	-2.843209	-1.580876	-0.583358
C	-3.894016	-1.457389	0.322133
C	-3.082022	-1.586403	-1.953079
C	-5.194685	-1.339248	-0.153789
H	-3.689033	-1.438473	1.387765
C	-4.386782	-1.461976	-2.420818
H	-2.249079	-1.675227	-2.642833
C	-5.443799	-1.338766	-1.524288
H	-6.013893	-1.237684	0.548253
H	-4.574663	-1.461634	-3.488073
H	-6.458535	-1.240588	-1.891205

H	1.515351	-2.403427	-1.277414

TS_{5b}

Symbol	X	Y	Z
Si	2.062274	-0.897635	0.212643
H	1.021088	1.777378	1.362800
C	3.689169	-0.086075	-0.326590
C	3.726423	1.174666	-0.942506
C	4.917262	-0.733839	-0.119911
C	4.928326	1.761438	-1.332215
H	2.793566	1.699206	-1.114400
C	6.123745	-0.155390	-0.507140
H	4.922596	-1.708862	0.354545
C	6.132145	1.096830	-1.115324
H	4.926185	2.737889	-1.804825
H	7.057142	-0.680296	-0.333864
H	7.069366	1.551512	-1.417121
O	1.308604	-1.868351	-0.960990
C	0.705880	0.778592	1.023041
O	0.977931	0.504094	-0.283440
O	1.357276	-0.249259	1.686790
O	2.670161	-2.280475	1.034527
N	-0.782929	0.671402	1.302462
H	-1.073127	-0.503082	0.751654
C	-1.030151	0.593592	2.753279
H	-0.562346	-0.315284	3.123908
H	-0.600593	1.452115	3.277308
H	-2.104146	0.556985	2.934231
C	-1.537757	1.694461	0.609170
C	-2.131015	2.758944	1.284556
C	-1.686151	1.583487	-0.776753
C	-2.878507	3.698880	0.577676
H	-2.024783	2.863321	2.356306
C	-2.435098	2.523882	-1.471545
H	-1.203952	0.768780	-1.300526
C	-3.036747	3.584574	-0.797575
H	-3.338944	4.521045	1.113082
H	-2.551467	2.423884	-2.544580
H	-3.624422	4.314316	-1.341997
N	-1.305352	-1.613085	0.200283
H	-0.610078	-1.683451	-0.554904
C	-1.033083	-2.694826	1.176584
H	0.004318	-2.608369	1.501698
H	-1.692002	-2.579182	2.036196
H	-1.197329	-3.668851	0.713092
C	-2.644442	-1.591113	-0.333268
C	-3.710343	-1.315675	0.519357
C	-2.852531	-1.774350	-1.695666
C	-4.995494	-1.224978	-0.002952
H	-3.530140	-1.160750	1.578190
C	-4.141489	-1.676408	-2.210646
H	-2.007227	-1.980774	-2.343863
C	-5.213849	-1.402594	-1.367105
H	-5.826755	-1.006161	0.656886
H	-4.305158	-1.815195	-3.272863
H	-6.216551	-1.325859	-1.770411
H	1.620268	-2.776395	-0.886469
H	2.911100	-2.107925	1.947817

TS_5

Symbol	X	Y	Z
Si	1.809468	-0.331117	0.187437
H	0.838992	-3.200457	-1.860565
H	3.718901	-2.592925	2.390868
H	0.452248	2.102797	1.428027
C	3.348846	0.520543	-0.470551
C	3.332832	1.884812	-0.788687
C	4.554880	-0.175234	-0.643682
C	4.476481	2.534475	-1.250863
H	2.410646	2.443732	-0.678851
C	5.695009	0.463538	-1.117376
H	4.593791	-1.235901	-0.423160
C	5.659793	1.824104	-1.417866
H	4.440064	3.593020	-1.483726
H	6.613814	-0.097062	-1.250447
H	6.550236	2.324642	-1.782026
C	1.606730	-2.485859	-1.528140
O	1.052427	-1.454886	-0.896044
O	2.774237	-2.627924	-1.755591
C	0.245993	1.104104	1.016794
O	0.614584	0.943218	-0.290123
O	0.984037	0.102380	1.644345
C	3.409837	-1.600551	2.025425
O	2.579200	-1.703382	1.013720
O	3.818560	-0.580530	2.521428
N	-1.220118	0.832248	1.230107
H	-1.409484	-0.376162	0.711290
C	-1.505974	0.748705	2.676054

H	-0.981516	-0.118090	3.072486
H	-1.160061	1.643389	3.200724
H	-2.578657	0.630392	2.823097
C	-2.052562	1.766435	0.496331
C	-2.735163	2.801194	1.130497
C	-2.177726	1.590580	-0.883834
C	-3.550541	3.649813	0.384494
H	-2.646219	2.951021	2.198660
C	-2.995460	2.439312	-1.617989
H	-1.626938	0.798349	-1.374717
C	-3.686817	3.470937	-0.986479
H	-4.081008	4.451107	0.885441
H	-3.094321	2.290998	-2.687054
H	-4.327591	4.129102	-1.561347
N	-1.600070	-1.513955	0.204308
H	-0.974905	-1.549445	-0.605067
C	-1.171628	-2.556758	1.167622
H	-0.122728	-2.386641	1.410496
H	-1.769039	-2.475617	2.074570
H	-1.297567	-3.547306	0.728353
C	-2.976173	-1.596486	-0.223970
C	-3.988352	-1.367029	0.703383
C	-3.273583	-1.832803	-1.561223
C	-5.312885	-1.376158	0.280773
H	-3.739265	-1.174125	1.741618
C	-4.601667	-1.834842	-1.975817
H	-2.467844	-2.003262	-2.268239
C	-5.622060	-1.607268	-1.057346
H	-6.104204	-1.194654	0.998382
H	-4.836351	-2.015393	-3.018174
H	-6.655437	-1.608306	-1.382856

TS_{6a}

Symbol	X	Y	Z
Si	1.482831	0.427169	-0.543108
H	1.630174	-2.780848	-2.449411
H	0.789449	0.488955	2.442306
C	3.322199	0.232799	-0.178294
C	3.871023	0.623983	1.050377
C	4.200801	-0.291011	-1.139229
C	5.231014	0.482023	1.317889
H	3.228185	1.055409	1.808964
C	5.563304	-0.416704	-0.887612
H	3.819736	-0.605521	-2.105694
C	6.081934	-0.036139	0.347412
H	5.625885	0.783239	2.281962
H	6.219693	-0.816452	-1.652673
H	7.142034	-0.140943	0.549813
O	1.052435	1.508144	-1.729251
C	0.356188	0.974266	1.565600
O	1.161803	1.658881	0.769750
O	0.322722	-0.337483	0.486349
C	1.641361	-2.186530	-1.522027
O	1.378277	-0.925345	-1.746643
O	1.866301	-2.690075	-0.444201
N	-0.909458	1.436104	1.809395
H	-0.143764	-1.268008	0.497925
C	-1.696540	0.607096	2.719645
H	-1.091771	0.375555	3.597124
H	-2.579789	1.161193	3.035477
H	-2.012183	-0.330503	2.249285
C	-1.607562	2.108004	0.756980
C	-2.728381	1.527298	0.164198
C	-1.172696	3.366034	0.340019
C	-3.408550	2.205791	-0.844321
H	-3.071973	0.548411	0.481681
C	-1.852252	4.033125	-0.671176
H	-0.303185	3.805230	0.810926
C	-2.972533	3.456899	-1.266860
H	-4.279431	1.747178	-1.299731
H	-1.509217	5.010415	-0.990983
H	-3.503547	3.982990	-2.051614
N	-0.972378	-2.585298	0.507094
H	-0.480428	-3.141605	-0.188137
C	-0.846964	-3.205714	1.827360
H	0.201428	-3.463650	1.972489
H	-1.138825	-2.493739	2.601178
H	-1.458052	-4.108074	1.921829
C	-2.269590	-2.239247	0.037559
C	-3.392493	-2.240655	0.864340
C	-2.388261	-1.808710	-1.288954
C	-4.619840	-1.805767	0.363820
H	-3.319856	-2.573225	1.892462
C	-3.615110	-1.387565	-1.779413
H	-1.506587	-1.802988	-1.922925
C	-4.739478	-1.378530	-0.952986
H	-5.486396	-1.807742	1.015288
H	-3.693133	-1.055837	-2.808560

H	-5.696277	-1.043229	-1.335339
H	1.033295	1.100327	-2.599572

TS_{6b}

Symbol	X	Y	Z
Si	1.549939	0.063404	-0.595723
H	1.083033	0.397767	2.495075
C	3.420257	-0.084015	-0.330468
C	4.084854	0.482118	0.767610
C	4.203407	-0.791252	-1.257063
C	5.459632	0.339894	0.940741
H	3.516156	1.051095	1.493646
C	5.580434	-0.925650	-1.100074
H	3.727005	-1.242791	-2.120683
C	6.212737	-0.363162	0.004890
H	5.944304	0.783006	1.803986
H	6.158440	-1.471893	-1.837569
H	7.283979	-0.470538	0.134847
O	0.998322	1.138485	-1.747953
C	0.604944	0.789257	1.594560
O	1.346409	1.405317	0.702807
O	0.576835	-0.644639	0.677334
O	1.310826	-1.293977	-1.635631
N	-0.672346	1.233812	1.848708
H	-0.058967	-1.445967	0.615754
C	-1.435719	0.395232	2.765893
H	-0.793068	0.112656	3.600618
H	-2.287508	0.956104	3.149629
H	-1.800412	-0.517571	2.278675
C	-1.390062	1.955782	0.849151
C	-2.605715	1.482105	0.357500
C	-0.895689	3.184201	0.401093
C	-3.318218	2.231802	-0.577387
H	-3.001816	0.530811	0.695391
C	-1.605683	3.918114	-0.538133
H	0.044517	3.547423	0.793119
C	-2.821742	3.446926	-1.031829
H	-4.263606	1.853602	-0.950037
H	-1.212768	4.869034	-0.879668
H	-3.377704	4.027221	-1.758976
N	-1.009517	-2.725218	0.429817
H	-0.490244	-3.237415	-0.279363
C	-1.081631	-3.497734	1.670798
H	-0.080161	-3.858823	1.901424
H	-1.412305	-2.854653	2.487782
H	-1.762617	-4.350645	1.590858
C	-2.219621	-2.230570	-0.127635
C	-3.426931	-2.241645	0.570478
C	-2.161038	-1.658643	-1.404976
C	-4.567627	-1.691029	-0.014971
H	-3.489680	-2.676361	1.560282
C	-3.304293	-1.124310	-1.979661
H	-1.206153	-1.634733	-1.922993
C	-4.516203	-1.136263	-1.287591
H	-5.502132	-1.705580	0.534553
H	-3.248542	-0.685639	-2.969635
H	-5.407118	-0.714577	-1.737782
H	0.885193	0.685701	-2.589206
H	1.670400	-2.123484	-1.309297

TS_{6}

Symbol	X	Y	Z
Si	1.369976	0.248631	-0.140357
H	0.581652	2.551968	-2.833561
H	1.465351	-2.566755	-2.545908
H	0.508384	-0.074352	2.810378
C	3.209168	0.011035	0.154505
C	3.763847	0.181404	1.429795
C	4.069864	-0.371852	-0.885415
C	5.120352	-0.035533	1.663774
H	3.129937	0.494237	2.251340
C	5.427083	-0.573359	-0.661278
H	3.675077	-0.490896	-1.888080
C	5.955450	-0.411534	0.617653
H	5.523489	0.094517	2.661963
H	6.073891	-0.859036	-1.483444
H	7.012629	-0.575096	0.795102
C	1.295063	1.883751	-2.330966
O	0.849956	1.539669	-1.131010
O	2.343392	1.559001	-2.816367
C	0.171071	0.545771	1.978652
O	1.073922	1.275938	1.338312
O	0.162376	-0.610698	0.730937
C	1.483134	-2.139277	-1.531448
O	1.221204	-0.856365	-1.540651
O	1.708267	-2.815487	-0.553655
N	-1.083019	1.051776	2.182360
H	-0.386303	-1.493525	0.531071

C	-1.995484	0.160808	2.895895
H	-1.482470	-0.244927	3.768392
H	-2.863301	0.729176	3.228590
H	-2.332312	-0.668974	2.264527
C	-1.644941	1.915904	1.189043
C	-2.743928	1.508764	0.433759
C	-1.096441	3.183272	0.993871
C	-3.284949	2.368114	-0.519625
H	-3.177634	0.525300	0.580474
C	-1.637039	4.031279	0.036300
H	-0.247525	3.487754	1.591719
C	-2.732209	3.627554	-0.725009
H	-4.139844	2.044278	-1.102970
H	-1.205681	5.014800	-0.111241
H	-3.155649	4.294339	-1.467140
N	-1.243787	-2.694368	0.241826
H	-0.727659	-3.177704	-0.490470
C	-1.290096	-3.526519	1.447794
H	-0.278395	-3.878155	1.646337
H	-1.622631	-2.927295	2.296689
H	-1.956236	-4.385538	1.330471
C	-2.470916	-2.188253	-0.280363
C	-3.669508	-2.249051	0.427649
C	-2.428136	-1.542748	-1.520723
C	-4.815940	-1.660629	-0.106940
H	-3.719992	-2.746839	1.388042
C	-3.575870	-0.969203	-2.047213
H	-1.486002	-1.489810	-2.058235
C	-4.777303	-1.020905	-1.339866
H	-5.744187	-1.710570	0.450731
H	-3.531046	-0.471166	-3.009003
H	-5.672144	-0.567656	-1.749683

TS_7

Symbol	X	Y	Z
Si	-2.390107	-0.392454	-0.276371
H	-1.189855	-0.923911	-3.565396
C	-4.532604	1.247092	-0.164554
H	-4.863777	2.182553	0.301658
C	-1.045465	-0.502526	0.989815
C	-0.118682	-1.554917	0.993728
C	-0.958380	0.473974	1.992610
C	0.877983	-1.616257	1.963249
H	-0.171566	-2.311271	0.219619
C	0.036152	0.408211	2.963998
H	-1.668678	1.293155	2.013358
C	0.958432	-0.633989	2.947416
H	1.589024	-2.435306	1.954804
H	0.094232	1.174589	3.728801
H	1.735313	-0.683540	3.702383
C	-1.072706	-1.058901	-2.480466
O	-0.895591	-2.170295	-1.963511
O	-1.982898	-0.163671	-1.845989
Si	1.668591	-0.114969	-1.897264
H	1.468592	-1.505964	-1.425427
H	0.062854	-0.251590	-2.395376
C	1.234959	1.396055	-0.845427
C	1.988430	1.790438	0.269192
C	0.102724	2.159254	-1.170153
C	1.620358	2.896070	1.033562
H	2.875508	1.238605	0.560465
C	-0.263503	3.268558	-0.414660
H	-0.511593	1.876326	-2.018004
C	0.493967	3.637828	0.693965
H	2.215114	3.175114	1.896468
H	-1.142675	3.841228	-0.688535
H	0.207963	4.498257	1.288574
O	-3.254897	0.991948	0.135124
O	-5.225802	0.554397	-0.851590
H	2.076300	0.142164	-3.296059
C	3.907218	-1.001918	-0.500401
H	3.295520	-1.860302	-0.213449
O	3.469760	-0.154327	-1.335139
N	5.082203	-0.907391	0.054205
C	5.992621	0.197186	-0.229133
H	6.285578	0.656737	0.715766
H	6.879952	-0.192581	-0.730882
H	5.498086	0.928201	-0.862149
C	5.558961	-1.922491	0.987497
H	4.800025	-2.692496	1.110878
H	6.473947	-2.367253	0.593960
H	5.769112	-1.451796	1.948738
H	-4.878019	-2.843719	0.609030
C	-4.273446	-1.948053	0.794747
O	-4.368861	-1.261768	1.773323
O	-3.418868	-1.726933	-0.205681

TS_8

Symbol	X	Y	Z
Si	-1.302210	0.747772	-2.060655
H	1.307317	3.038241	-1.608462
H	-0.800553	-0.230416	-3.043662
H	-1.653734	2.018099	-2.725826
C	-2.707115	0.013836	-1.080112
C	-2.992966	0.478833	0.210114
C	-3.431935	-1.073548	-1.578971
C	-3.970853	-0.135405	0.985385
H	-2.441464	1.319976	0.620086
C	-4.420860	-1.682068	-0.808887
H	-3.218826	-1.463484	-2.569949
C	-4.685655	-1.217589	0.475724
H	-4.175171	0.228114	1.986240
H	-4.974683	-2.524552	-1.207333
H	-5.446461	-1.698244	1.080235
Si	0.823420	0.392496	0.209056
H	0.025763	3.406321	-0.301811
H	-1.512124	-2.452210	0.195146
H	-0.156003	1.576895	3.494811
C	2.519507	-0.323311	-0.062076
C	3.526144	0.334768	-0.778895
C	2.790896	-1.600340	0.449713
C	4.762627	-0.268390	-0.987342
H	3.348738	1.328181	-1.173642
C	4.036276	-2.192582	0.266813
H	2.028081	-2.133697	1.008241
C	5.021739	-1.529657	-0.458952
H	5.526737	0.250274	-1.555057
H	4.234221	-3.173258	0.684241
H	5.989273	-1.994512	-0.611662
C	0.906204	2.836707	-0.609428
O	-0.047366	1.209257	-1.015185
O	1.613826	2.244793	0.249529
C	-0.225137	1.643992	2.402636
O	-0.791832	2.530445	1.825103
O	0.370363	0.606746	1.822202
C	-0.665646	-1.961300	0.698010
O	-0.116729	-1.042674	-0.083962
O	-0.295018	-2.261668	1.799677

TS_{9a}

Symbol	X	Y	Z
N	-0.879048	-0.295972	0.291874
H	-1.370104	0.645912	0.543633
C	0.551160	-0.106328	0.155468
C	1.397859	-1.191721	-0.038707
C	1.040607	1.195427	0.164250
C	2.760010	-0.963724	-0.207935
H	1.005943	-2.201611	-0.058895
C	2.403603	1.412078	-0.005555
H	0.351897	2.022508	0.301590
C	3.264204	0.333579	-0.189108
H	3.427313	-1.804292	-0.356807
H	2.790801	2.423920	0.006302
H	4.326378	0.503733	-0.319436
C	-1.294752	-1.293342	1.301626
H	-0.893260	-1.009133	2.273164
H	-2.382879	-1.286346	1.324024
H	-0.941124	-2.284339	1.019722
C	-1.587354	-0.559769	-1.074530
H	-1.351613	-1.601550	-1.330003
O	-2.899152	-0.311960	-0.933476
H	-1.051363	0.118136	-1.757875
O	-2.483856	1.682634	0.305763
H	-3.062675	1.821877	1.059543
H	-2.883984	0.742470	-0.368250

TS_{9}

Symbol	X	Y	Z
N	-1.312686	1.155079	-0.040262
H	-0.352743	1.006665	-0.429629
C	-1.896558	2.330758	-0.734763
H	-2.879525	2.542974	-0.317604
H	-1.230271	3.172370	-0.558515
H	-1.969534	2.111895	-1.798481
C	-2.072796	-0.079467	-0.175001
C	-1.417384	-1.207610	-0.651101
C	-3.403357	-0.124571	0.222243
C	-2.116615	-2.406305	-0.745971
H	-0.373454	-1.144222	-0.943492
C	-4.091362	-1.329391	0.124119
H	-3.898013	0.760662	0.604081
C	-3.452130	-2.467203	-0.360297
H	-1.614798	-3.290198	-1.120685
H	-5.129704	-1.376603	0.429408
H	-3.995111	-3.401794	-0.435259
H	-0.711515	0.503036	1.856946

H	-1.920079	1.830052	1.886561
C	-0.977691	1.487078	1.445171
O	-0.002145	2.413251	1.477416
N	1.511773	1.436649	-0.234106
H	0.809532	2.012764	0.776853
C	1.768583	2.209648	-1.431186
H	2.818161	2.529695	-1.517045
H	1.524769	1.666532	-2.356856
H	1.150834	3.111388	-1.407363
C	2.240268	0.304193	-0.040310
C	3.139433	-0.245753	-0.989133
C	2.098354	-0.407688	1.183983
C	3.821853	-1.432197	-0.728969
H	3.299282	0.256934	-1.935334
C	2.784366	-1.583993	1.423683
H	1.447434	0.008727	1.946845
C	3.655831	-2.120174	0.468342
H	4.498301	-1.822080	-1.483595
H	2.645874	-2.091463	2.373266
H	4.191789	-3.041671	0.660748

TS_{10}

Symbol	X	Y	Z
C	-2.764981	1.669863	0.781831
H	-3.170628	1.166307	-0.105656
O	-1.466790	1.418010	1.028637
Si	-0.339529	0.655797	0.051377
H	-1.859385	1.494159	-3.174852
C	1.152064	1.691214	-0.300763
C	2.025883	1.311332	-1.323841
C	1.409385	2.875635	0.401153
C	3.147370	2.083003	-1.622174
H	1.842557	0.403369	-1.891341
C	2.520400	3.653698	0.096021
H	0.731345	3.204358	1.183835
C	3.394971	3.253573	-0.912938
H	3.823932	1.769133	-2.409338
H	2.704840	4.571483	0.642685
H	4.264266	3.857209	-1.148069
O	-0.244422	-0.966517	0.175586
C	-1.554487	1.729709	-2.146894
O	-1.615768	2.833850	-1.673129
O	-1.130692	0.651864	-1.501995
N	2.718157	-0.750445	1.785429
C	2.912694	-1.565483	0.668821
C	2.182197	-2.754530	0.481928
C	3.895568	-1.249501	-0.283908
C	2.396779	-3.555309	-0.629275
H	1.446227	-3.066798	1.210128
C	4.110005	-2.069930	-1.389096
H	4.484699	-0.347773	-0.183648
C	3.359484	-3.222175	-1.582664
H	1.809977	-4.460946	-0.742355
H	4.872040	-1.788995	-2.108064
H	3.524682	-3.854224	-2.446695
C	3.614644	0.373081	2.004284
H	3.499173	1.160267	1.248872
H	3.402456	0.801386	2.985865
H	4.654089	0.037701	2.002433
C	1.480713	-0.694012	2.496144
H	1.678944	-0.596150	3.565359
O	0.640185	0.415958	2.122454
H	0.882065	-1.577805	2.314180
H	0.986314	1.228396	2.515077
Si	-1.186163	-2.208649	-0.413445
H	-0.860110	-2.492994	-1.825793
H	-0.910632	-3.380176	0.441788
C	-2.970513	-1.674357	-0.247348
C	-3.731544	-1.286997	-1.357550
C	-3.531812	-1.529055	1.029712
C	-5.013938	-0.768231	-1.197957
H	-3.316390	-1.377330	-2.356738
C	-4.811327	-1.005913	1.193772
H	-2.963257	-1.816122	1.910477
C	-5.552194	-0.623864	0.078568
H	-5.590603	-0.471635	-2.066846
H	-5.227109	-0.891617	2.188369
H	-6.547511	-0.212769	0.203995
O	-3.414705	2.369847	1.497238

TS_{11}

Symbol	X	Y	Z
C	2.759844	-1.808938	0.764904
H	3.052238	-1.183065	-0.086907
O	1.512031	-1.632220	1.191553
Si	0.186412	-0.769560	0.527555
H	1.553598	-1.280155	-2.954445
C	-1.239674	-1.783754	-0.197104

C	-1.826117	-1.444593	-1.422525
C	-1.784590	-2.873121	0.497941
C	-2.927805	-2.138690	-1.919543
H	-1.423038	-0.617132	-1.998618
C	-2.862493	-3.594823	-0.006485
H	-1.358717	-3.190509	1.445627
C	-3.448088	-3.218863	-1.212828
H	-3.374979	-1.839655	-2.861596
H	-3.250060	-4.444750	0.544435
H	-4.297812	-3.768500	-1.602128
O	0.188321	0.901281	0.536250
C	1.342727	-1.622618	-1.927186
O	1.464271	-2.784808	-1.610034
O	0.980082	-0.641732	-1.146272
N	-2.882298	0.779796	1.571107
C	-2.763856	1.758749	0.522721
C	-2.185559	2.998852	0.788219
C	-3.265940	1.475938	-0.744218
C	-2.069714	3.934355	-0.231132
H	-1.837354	3.245787	1.783584
C	-3.146561	2.422794	-1.757857
H	-3.737450	0.525597	-0.954781
C	-2.542139	3.649029	-1.509913
H	-1.614693	4.894670	-0.018757
H	-3.530929	2.192108	-2.744409
H	-2.450568	4.383441	-2.301193
C	-3.984215	-0.187636	1.484687
H	-3.788525	-0.901738	0.682858
H	-4.052377	-0.719757	2.430658
H	-4.913358	0.346053	1.287786
C	-2.004698	0.682691	2.527638
H	-2.265623	0.096427	3.396701
O	-0.536477	-0.700321	2.145528
H	-1.213327	1.412366	2.590158
H	-0.680871	-1.544337	2.585008
Si	1.068492	2.034286	-0.281755
H	0.607307	2.228445	-1.674608
H	0.909586	3.300355	0.470399
C	2.881540	1.558015	-0.259034
C	3.566303	1.175766	-1.418913
C	3.552161	1.464996	0.967766
C	4.876693	0.710025	-1.356838
H	3.064819	1.223324	-2.381006
C	4.859897	0.990633	1.037796
H	3.046905	1.751757	1.886546
C	5.522422	0.611114	-0.125975
H	5.392015	0.415686	-2.264454
H	5.359026	0.913091	1.997194
H	6.539072	0.237797	-0.074905
O	3.518237	-2.567396	1.303627

TS_{12}

Symbol	X	Y	Z
C	-1.927152	2.823084	1.259934
H	-1.469715	3.275608	0.370150
O	-1.282894	1.755576	1.735283
Si	-0.080549	0.827808	0.953717
H	-1.977430	1.223056	-2.622638
C	1.251356	1.763863	0.021947
C	1.575566	1.486465	-1.311760
C	2.030133	2.709428	0.701090
C	2.637671	2.124320	-1.943679
H	0.997058	0.755345	-1.868626
C	3.076722	3.375284	0.066166
H	1.821106	2.942484	1.741524
C	3.387310	3.077094	-1.257114
H	2.879021	1.882849	-2.973016
H	3.653760	4.117259	0.606904
H	4.208447	3.584054	-1.751509
O	-0.393580	-0.749625	0.544710
C	-1.531841	1.770347	-1.769855
O	-1.309208	2.960361	-1.848450
O	-1.308191	1.005784	-0.744548
N	1.680047	-2.986529	0.914943
C	2.797708	-2.294237	0.313121
C	3.546400	-2.934937	-0.670787
C	3.110793	-1.011139	0.746564
C	4.607934	-2.256960	-1.255014
H	3.322295	-3.955335	-0.958044
C	4.178332	-0.347250	0.150829
H	2.522714	-0.520132	1.513231
C	4.922264	-0.961918	-0.850002
H	5.197440	-2.749565	-2.018596
H	4.416040	0.661763	0.468507
H	5.752006	-0.437674	-1.309144
C	1.411515	-2.738318	2.342535
H	1.027320	-1.722404	2.448800
H	0.672940	-3.461087	2.678891

H	2.345116	-2.857945	2.890222
C	0.933100	-3.767193	0.235716
H	0.139280	-4.303538	0.738927
O	0.731042	0.443222	2.394120
H	1.110323	-3.900788	-0.824101
H	0.794830	1.162244	3.036301
Si	-1.324022	-1.251488	-0.754325
H	-0.800874	-0.984433	-2.115879
H	-1.111720	-2.736030	-0.639130
C	-3.203477	-1.190373	-0.593564
C	-3.914019	-2.326611	-1.008717
C	-3.941290	-0.118586	-0.071867
C	-5.303094	-2.384298	-0.933644
H	-3.376139	-3.187018	-1.397667
C	-5.328541	-0.179521	0.028787
H	-3.430423	0.776063	0.261699
C	-6.013983	-1.309278	-0.408942
H	-5.827761	-3.270522	-1.272932
H	-5.874669	0.659505	0.445831
H	-7.095038	-1.352804	-0.337984
O	-2.913756	3.257265	1.786600

TS_{13}

Symbol	X	Y	Z
C	1.392479	-0.586995	2.283569
H	2.056731	0.263568	2.085242
O	1.249625	-1.442344	1.258188
Si	1.727122	-1.303579	-0.350390
H	1.787415	3.174486	-0.428270
C	3.416108	-0.539281	-0.421944
C	3.754145	0.339212	-1.459486
C	4.372550	-0.807779	0.564663
C	5.009922	0.934070	-1.509098
H	3.028693	0.569329	-2.234611
C	5.631520	-0.213981	0.517714
H	4.139709	-1.479903	1.386255
C	5.949597	0.658425	-0.518100
H	5.255676	1.614913	-2.316170
H	6.359835	-0.427719	1.291625
H	6.927375	1.125387	-0.552915
O	0.612190	-0.558513	-1.268377
C	1.843399	2.400016	0.358833
O	2.536226	2.556811	1.340557
O	1.121522	1.340740	0.135007
N	-3.033930	-1.118144	-1.866787
C	-2.992304	-1.368659	-0.445001
C	-1.898907	-2.014485	0.134637
C	-4.047044	-0.922640	0.348499
C	-1.848132	-2.166016	1.513775
H	-1.089544	-2.408968	-0.465520
C	-3.988445	-1.094739	1.727449
H	-4.902716	-0.423499	-0.084220
C	-2.886807	-1.702225	2.316033
H	-0.978589	-2.631458	1.959243
H	-4.806827	-0.732654	2.338503
H	-2.836435	-1.818739	3.392077
C	-4.321467	-0.728619	-2.464963
H	-4.613177	0.256474	-2.102493
H	-4.203133	-0.704563	-3.544583
H	-5.073842	-1.465527	-2.187650
C	-1.974199	-1.156604	-2.605622
H	-2.088921	-0.996450	-3.669367
O	1.691283	-2.856837	-0.895105
H	-1.032152	-1.505506	-2.209571
H	2.249038	-3.496671	-0.441339
Si	-0.016260	1.026659	-1.317561
H	0.695982	2.056011	-2.128239
H	-0.946123	0.577508	-2.514750
C	-1.525503	1.619706	-0.323306
C	-2.665845	2.030129	-1.027356
C	-1.560496	1.711683	1.076500
C	-3.783325	2.542525	-0.373271
H	-2.680749	1.949388	-2.111950
C	-2.686001	2.195355	1.740369
H	-0.695752	1.408498	1.656715
C	-3.796908	2.621223	1.016868
H	-4.644956	2.870242	-0.945369
H	-2.693050	2.245924	2.823975
H	-4.668325	3.008784	1.533082
O	0.835813	-0.768218	3.327797

TS_{14}

Symbol	X	Y	Z
C	4.077989	0.331252	1.582184
H	4.545803	-0.301607	0.818886
O	2.757085	0.499017	1.449381
Si	1.622114	-0.290786	0.453088
H	3.730612	-3.353242	0.200949

C	0.331067	-1.484795	1.112659
C	-0.108334	-2.552295	0.318797
C	-0.232645	-1.331593	2.385522
C	-1.100708	-3.420516	0.768682
H	0.321789	-2.706529	-0.666872
C	-1.199655	-2.217008	2.853426
H	0.083022	-0.507983	3.017701
C	-1.645954	-3.255225	2.039317
H	-1.445653	-4.226587	0.130179
H	-1.614313	-2.090230	3.847381
H	-2.412335	-3.934948	2.394633
O	1.566388	0.231443	-1.123032
C	3.267634	-2.520110	0.751812
O	3.277446	-2.460248	1.958893
O	2.740480	-1.627889	-0.051464
O	0.478153	1.093167	0.951537
H	0.877794	1.971141	0.893697
Si	2.583527	0.003443	-2.412407
H	2.476909	-1.358475	-2.977310
H	2.168461	0.998172	-3.426283
C	4.345166	0.327972	-1.871920
C	5.286688	-0.705062	-1.786915
C	4.711880	1.601692	-1.416379
C	6.554603	-0.475581	-1.259535
H	5.022081	-1.705036	-2.117355
C	5.975847	1.834613	-0.880727
H	4.001669	2.423080	-1.465591
C	6.897250	0.794194	-0.800374
H	7.271555	-1.286679	-1.197417
H	6.239618	2.823154	-0.522125
H	7.880286	0.971525	-0.378857
O	4.696408	0.866721	2.456453
H	-2.281743	-0.775558	0.616390
H	-2.709653	0.533243	1.721790
C	-2.727697	0.214842	0.678473
N	-4.078908	0.213058	0.188143
C	-5.017581	1.124542	0.834737
H	-5.674121	0.595236	1.535409
H	-4.460666	1.879136	1.385863
H	-5.636584	1.637585	0.094737
C	-4.596833	-0.867101	-0.526282
C	-5.988175	-1.003411	-0.698160
C	-3.773148	-1.847887	-1.115645
C	-6.519358	-2.070108	-1.415570
H	-6.667951	-0.278081	-0.273722
C	-4.321484	-2.911218	-1.819703
H	-2.696576	-1.791473	-1.039705
C	-5.698593	-3.038637	-1.980471
H	-7.596169	-2.138207	-1.525643
H	-3.652321	-3.646063	-2.254315
H	-6.118339	-3.868660	-2.535392
N	-1.810998	1.144927	-0.064316
H	-0.580317	1.096179	0.496825
C	-1.615302	0.709361	-1.459962
H	-0.975872	1.428928	-1.970133
H	-1.108903	-0.256106	-1.442033
H	-2.565849	0.615985	-1.989168
C	-2.234450	2.525999	0.078168
C	-2.915349	3.203677	-0.927956
C	-1.969460	3.156306	1.294556
C	-3.335115	4.514016	-0.709337
H	-3.126851	2.722087	-1.874190
C	-2.394340	4.461907	1.505262
H	-1.446137	2.616584	2.077343
C	-3.080784	5.144197	0.503410
H	-3.867388	5.039091	-1.493891
H	-2.186517	4.946504	2.451987
H	-3.411602	6.162909	0.667358

Aniline-TS

Symbol	X	Y	Z
C	-0.902690	3.302903	-0.720173
O	-1.999884	3.773825	-0.740986
O	0.273087	3.514687	-0.763129
H	0.613988	-1.908428	-0.430330
H	-1.111251	1.910395	-0.592982
Si	-0.312169	0.502017	-0.231370
H	0.247865	1.127985	0.983947
H	0.420283	0.563883	-1.511331
N	0.814643	-1.195995	0.273824
C	0.404285	-1.725492	1.596401
H	-0.567414	-2.202783	1.486613
H	1.133938	-2.450146	1.959173
H	0.316385	-0.905266	2.309414
C	-1.937561	-0.433239	-0.126247
C	-2.176941	-1.589309	-0.879996
C	-2.951386	0.032841	0.719912
C	-3.390326	-2.265137	-0.783405

H	-1.414837	-1.972344	-1.553711
C	-4.160679	-0.647264	0.828260
H	-2.799086	0.939354	1.299238
C	-4.381017	-1.797807	0.075950
H	-3.561530	-3.156039	-1.376953
H	-4.931696	-0.277549	1.494678
H	-5.323840	-2.326815	0.155948
C	2.212199	-0.850741	0.160841
C	2.882933	-0.241275	1.217820
C	2.858318	-1.066367	-1.054443
C	4.212456	0.138016	1.053630
H	2.382521	-0.064445	2.161849
C	4.185312	-0.684157	-1.207190
H	2.320214	-1.537258	-1.870702
C	4.866888	-0.080894	-0.153599
H	4.734937	0.607594	1.878731
H	4.686176	-0.860903	-2.151668
H	5.902066	0.215499	-0.273476

Carbamate acid-TS

Symbol	X	Y	Z
C	-2.048062	-0.495345	2.365232
H	-3.096031	-0.532818	2.652837
H	-1.602863	0.436867	2.717447
H	-1.520355	-1.341236	2.799813
N	-1.982613	-0.578365	0.899481
C	-3.118923	-0.151513	0.127340
C	-3.800285	-1.064895	-0.668398
C	-3.535972	1.170479	0.229329
C	-4.911731	-0.638860	-1.386494
H	-3.458909	-2.092173	-0.721404
C	-4.655793	1.584214	-0.484685
H	-2.985601	1.861687	0.858044
C	-5.340803	0.682643	-1.294048
H	-5.446535	-1.342904	-2.012752
H	-4.987939	2.612894	-0.411562
H	-6.210416	1.009141	-1.852050
C	-0.854659	-0.953312	0.321478
O	0.143393	-1.310239	1.003479
H	1.759823	-2.080208	-0.702572
H	2.339392	-1.830035	1.767983
H	3.618943	-1.193459	0.068910
C	4.703339	-1.991768	-0.217850
O	5.560873	-1.243978	-0.592238
O	4.423485	-3.135712	0.001899
Si	2.004922	-1.214942	0.476228
C	1.923041	0.645860	0.180037
C	2.777596	1.214724	-0.774629
C	1.042325	1.493067	0.867779
C	2.739789	2.578259	-1.049621
H	3.487044	0.587609	-1.306739
C	1.013656	2.859853	0.605849
H	0.377338	1.094461	1.627433
C	1.857866	3.403292	-0.358118
H	3.402154	2.996391	-1.799006
H	0.331718	3.499292	1.154972
H	1.831138	4.466812	-0.566462
O	-0.838194	-0.924698	-0.997942
H	-0.008389	-1.303122	-1.331025

Carbamate-TS$_1$

Symbol	X	Y	Z
C	-2.157991	-0.855154	2.238715
H	-3.165623	-1.179446	2.498284
H	-1.941408	0.081321	2.763424
H	-1.448272	-1.608303	2.567344
N	-2.065399	-0.714054	0.787858
C	-3.203432	-0.255905	0.086449
C	-3.456274	-0.644010	-1.236917
C	-4.134914	0.564816	0.733835
C	-4.601639	-0.205537	-1.888254
H	-2.750913	-1.283325	-1.746666
C	-5.283865	0.991322	0.074037
H	-3.960071	0.881475	1.754792
C	-5.524561	0.614021	-1.241631
H	-4.778652	-0.519017	-2.911196
H	-5.988554	1.628105	0.597043
H	-6.417987	0.948392	-1.755633
C	-0.807765	-0.754943	0.173472
O	0.147545	-1.067323	1.006116
O	-0.656173	-0.512214	-1.012636
H	1.640236	-2.038213	-0.645380
H	2.219900	-1.737540	1.817995
H	3.526858	-1.234095	0.149699
C	4.570383	-2.360135	-0.640438
O	5.131285	-1.652568	-1.392599
O	4.300109	-3.368595	-0.104056
Si	1.938951	-1.124661	0.489893

C	2.062281	0.769279	0.257580
C	3.107845	1.309761	-0.503579
C	1.156007	1.671326	0.834763
C	3.238118	2.683579	-0.697062
H	3.837317	0.641551	-0.951981
C	1.291855	3.047053	0.666791
H	0.330572	1.296176	1.430577
C	2.331411	3.558075	-0.106013
H	4.050914	3.070589	-1.302211
H	0.582779	3.721120	1.135398
H	2.433915	4.628698	-0.244709

Carbamate-TS$_2$

Symbol	X	Y	Z
C	3.498378	-0.077693	2.436384
H	4.495527	-0.075885	2.875936
H	3.054917	-1.069918	2.568032
H	2.882432	0.651002	2.954638
N	3.602782	0.299020	1.028309
C	4.749295	-0.110538	0.307595
C	5.265029	0.658182	-0.744329
C	5.420912	-1.280363	0.679277
C	6.413077	0.249867	-1.410264
H	4.761076	1.568282	-1.034931
C	6.576014	-1.675673	0.010685
H	5.037592	-1.890574	1.488020
C	7.077952	-0.917552	-1.040418
H	6.797755	0.859204	-2.220558
H	7.078541	-2.586869	0.315125
H	7.975989	-1.226820	-1.561970
C	2.488493	0.810985	0.366532
O	1.483843	1.047132	1.176358
O	2.469163	1.007834	-0.836421
H	0.401617	2.797291	-0.164416
H	-0.594743	1.776429	1.950913
H	-1.681541	2.173511	0.100117
C	-2.396246	3.664731	-0.514022
O	-3.186455	3.225626	-1.271063
O	-1.808488	4.485387	0.076067
Si	-0.138927	1.616073	0.545696
C	-0.537021	0.000770	-0.377067
C	-1.361854	-0.001236	-1.509178
C	-0.058237	-1.235945	0.078639
C	-1.713423	-1.186033	-2.152555
H	-1.746431	0.940936	-1.893313
C	-0.419016	-2.426329	-0.547187
H	0.599309	-1.271755	0.941776
C	-1.254922	-2.405252	-1.661383
H	-2.353398	-1.158690	-3.028053
H	-0.052234	-3.372279	-0.163280
H	-1.540620	-3.331632	-2.147412
H	-4.300829	1.052101	-0.875013
N	-4.017975	0.802169	0.078498
C	-4.841891	1.575493	1.056527
H	-4.720521	2.635667	0.845085
H	-5.880419	1.275802	0.936603
H	-4.484679	1.340029	2.056588
H	-3.028144	1.110766	0.164864
C	-4.117200	-0.650140	0.250147
C	-4.966774	-1.367029	-0.577373
C	-3.366896	-1.253411	1.246866
C	-5.059044	-2.743863	-0.402452
H	-5.534171	-0.858593	-1.349621
C	-3.468443	-2.630597	1.411049
H	-2.708315	-0.656948	1.869947
C	-4.310857	-3.373588	0.588020
H	-5.712511	-3.322036	-1.044295
H	-2.881176	-3.122035	2.177390
H	-4.382153	-4.446865	0.717948

Carbamate-TS$_3$

Symbol	X	Y	Z
C	-1.656900	-0.257960	-0.769248
O	-1.661534	0.714868	0.078616
O	-0.648916	-0.669944	-1.371301
C	2.082547	3.789430	-0.688796
O	2.477471	2.817274	-1.231617
O	2.066811	4.929053	-0.421745
H	0.788875	3.214141	0.261418
Si	-0.304704	2.016519	0.223583
H	-1.323449	2.887341	0.860744
H	-0.139240	1.972322	-1.257615
N	-2.863228	-0.878029	-0.989987
C	-2.866362	-2.093670	-1.801382
H	-2.525011	-2.963781	-1.232960
H	-3.879303	-2.273393	-2.157589
H	-2.206851	-1.952616	-2.654367
H	2.194972	0.829280	-1.051127

N	1.938344	-0.059928	-1.496274
C	2.157515	0.068293	-2.964826
H	1.542092	0.890052	-3.327290
H	3.211862	0.267600	-3.147204
H	1.859069	-0.866212	-3.436359
H	0.901146	-0.208167	-1.335405
C	0.836423	0.933370	1.316604
C	2.051989	1.439795	1.806654
C	0.513203	-0.386515	1.669963
C	2.905204	0.670774	2.593537
H	2.338520	2.463190	1.590635
C	1.363689	-1.164427	2.453210
H	-0.421613	-0.823189	1.342360
C	2.566559	-0.640658	2.913919
H	3.834998	1.096827	2.954227
H	1.083496	-2.182571	2.701141
H	3.231612	-1.246154	3.519815
C	2.682400	-1.154550	-0.877852
C	3.964834	-0.922540	-0.405587
C	2.080093	-2.402244	-0.793095
C	4.661216	-1.973822	0.182889
H	4.405378	0.065818	-0.485511
C	2.786538	-3.445101	-0.204644
H	1.070384	-2.541564	-1.163661
C	4.072874	-3.230897	0.284852
H	5.661061	-1.806179	0.564855
H	2.327885	-4.423123	-0.122738
H	4.617047	-4.045680	0.747546
C	-4.046957	-0.524080	-0.286269
C	-4.481652	0.802662	-0.226478
C	-4.817166	-1.525558	0.306690
C	-5.659801	1.117739	0.438086
H	-3.894220	1.578087	-0.699944
C	-6.002629	-1.202709	0.961048
H	-4.486409	-2.556751	0.260388
C	-6.426772	0.119126	1.034978
H	-5.986365	2.150629	0.479200
H	-6.589692	-1.990743	1.418576
H	-7.347909	0.370512	1.547379

Amide-TS

Symbol	X	Y	Z
C	2.130738	-0.978477	0.129408
H	1.745083	-1.039905	1.150217
O	1.362710	-1.064714	-0.862445
N	3.429836	-0.816643	-0.000882
C	4.039318	-0.786202	-1.335759
H	4.944377	-0.185166	-1.286663
H	4.281624	-1.798532	-1.662689
H	3.333287	-0.339815	-2.032264
Si	-0.572786	-1.076892	-0.626654
H	-2.204815	-1.153190	-0.489994
H	-0.670937	-1.434784	-2.053618
H	-0.431145	-2.143046	0.390361
C	-0.602494	0.718904	-0.027326
C	-1.678229	1.145330	0.765661
C	0.396216	1.655840	-0.332863
C	-1.743806	2.446558	1.255123
H	-2.481282	0.453169	1.001306
C	0.324867	2.963742	0.140126
H	1.238846	1.376158	-0.956199
C	-0.741521	3.359712	0.941686
H	-2.580428	2.748245	1.875246
H	1.103947	3.672432	-0.117536
H	-0.793379	4.375894	1.316017
C	-3.333977	-2.068174	-0.375190
O	-3.001568	-3.108925	-0.847296
O	-4.181764	-1.419958	0.153503
C	4.265049	-0.723165	1.160284
C	3.895513	0.109515	2.212678
C	5.446312	-1.458000	1.208226
C	4.707700	0.181464	3.339306
H	2.993544	0.706965	2.141053
C	6.256599	-1.366118	2.333600
H	5.721826	-2.099778	0.379499
C	5.887405	-0.553058	3.401911
H	4.422720	0.827817	4.160754
H	7.175523	-1.938423	2.376444
H	6.521902	-0.486745	4.277618

DEA-CO_2

Symbol	X	Y	Z
C	0. 0.000000	0.000000	-0.000078
O	0. 0.000000	0.000000	-1.154565
O	0. 0.000000	0.000000	1.154624

DEA

Symbol	X	Y	Z

N	0. 2.805761	-1.003329	-0.507431
C	0. 3.709717	-0.592490	-1.578336
H	0. 4.432453	-1.399005	-1.731321
H	3.146207	-0.495339	-2.503834
C	3.402139	-1.538016	0.717208
H	2.859993	-2.443890	0.996572
H	4.429353	-1.819695	0.477951
C	1.452923	-0.886506	-0.556560
O	0.745282	-1.260411	0.372095
C	4.442225	0.708399	-1.268943
H	5.079962	0.600082	-0.388684
H	5.075763	0.993259	-2.112307
H	3.728331	1.514746	-1.082084
C	3.378547	-0.549814	1.879198
H	3.843331	-0.997018	2.761584
H	3.922779	0.363615	1.630480
H	2.348928	-0.289120	2.126997
C	0.839290	-0.282750	-1.803196
H	1.277798	0.688630	-2.040150
H	0.981600	-0.937941	-2.665831
H	-0.226551	-0.165070	-1.620018

DEA-Si

Symbol	X	Y	Z
Si	0. 2.341794	0.000378	0.004212
H	0. 2.828769	1.324028	-0.444411
H	0. 2.852115	-1.057221	-0.897266
H	2.861450	-0.261990	1.366639
C	0.464377	0.000815	-0.010886
C	-0.254653	1.203040	-0.008305
C	-0.254178	-1.202930	-0.008765
C	-1.647144	1.204240	0.002692
H	0.273385	2.151835	-0.017236
C	-1.645373	-1.205492	0.002165
H	0.273870	-2.152221	-0.018480
C	-2.343528	-0.000421	0.008491
H	-2.187202	2.144310	0.003803
H	-2.184901	-2.145860	0.002900
H	-3.427710	-0.001179	0.015067

DEA-TS

Symbol	X	Y	Z
N	0. 2.811916	-0.988974	-0.593340
C	0. 3.863637	-0.575698	-1.531982
H	0. 4.578630	-1.398382	-1.590617
H	3.430989	-0.451202	-2.520915
C	3.246151	-1.578594	0.686515
H	2.682605	-2.499398	0.842500
H	4.296430	-1.840650	0.559212
C	1.523489	-0.822283	-0.829911
O	0.700462	-1.204210	0.059751
C	4.550842	0.704352	-1.077877
H	5.057402	0.562545	-0.121005
H	5.297520	1.000677	-1.817140
H	3.823504	1.513427	-0.972620
C	3.072584	-0.642158	1.875611
H	3.518684	-1.102582	2.759843
H	3.569491	0.313984	1.699975
H	2.017756	-0.461373	2.082472
Si	-1.217581	-1.010259	0.216031
H	-1.409077	-1.738322	-1.059505
H	-2.829185	-0.939978	0.432529
H	-1.082887	-1.781708	1.468542
C	-1.140868	0.886782	0.184191
C	-2.284379	1.596338	-0.210456
C	-0.000913	1.629668	0.525590
C	-2.285975	2.986757	-0.284888
H	-3.191937	1.054759	-0.460369
C	-0.003198	3.021091	0.472204
H	0.906302	1.128845	0.846530
C	-1.143980	3.703232	0.059070
H	-3.180592	3.509379	-0.604718
H	0.888195	3.572114	0.751162
H	-1.143525	4.786337	0.009470
C	-4.119915	-1.753951	0.244145
O	-4.939825	-0.916576	0.067823
O	-3.805683	-2.890881	0.350487
C	1.066114	-0.208056	-2.121551
H	1.541818	0.762772	-2.271676
H	1.340166	-0.857766	-2.955751
H	-0.011920	-0.077277	-2.119404

DEF-CO_2

Symbol	X	Y	Z
C	0. 0.000000	0.000000	-0.000078
O	0. 0.000000	0.000000	-1.154565
O	0. 0.000000	0.000000	1.154624

DEF

Symbol	X	Y	Z
N	0. 2.774463	-0.977567	-0.469517
C	0. 3.609373	-0.543433	-1.582514
H	0. 4.241041	-1.381712	-1.892628
H	2.947158	-0.305312	-2.417106
C	3.404998	-1.510221	0.735926
H	2.861083	-2.410272	1.031236
H	4.423091	-1.802170	0.470457
C	1.430589	-0.908714	-0.525813
H	1.061432	-0.496425	-1.479252
O	0.674993	-1.263717	0.364306
C	4.474610	0.662022	-1.237466
H	5.175122	0.429069	-0.432153
H	5.055343	0.965271	-2.111518
H	3.851374	1.502948	-0.923974
C	3.410905	-0.512762	1.889601
H	3.878766	-0.959438	2.770229
H	3.963720	0.391182	1.626444
H	2.387316	-0.235784	2.146932

DEF-Si

Symbol	X	Y	Z
Si	0. 2.341770	0.000376	0.004215
H	0. 2.828724	1.324028	-0.444395
H	0. 2.852095	-1.057202	-0.897266
H	2.861427	-0.261994	1.366627
C	0.464371	0.000811	-0.010885
C	-0.254646	1.203041	-0.008308
C	-0.254175	-1.202936	-0.008764
C	-1.647142	1.204247	0.002691
H	0.273430	2.151802	-0.017246
C	-1.645374	-1.205499	0.002168
H	0.273904	-2.152196	-0.018481
C	-2.343528	-0.000420	0.008493
H	-2.187190	2.144305	0.003798
H	-2.184897	-2.145853	0.002904
H	-3.427695	-0.001176	0.015069

DEF-TS

Symbol	X	Y	Z
N	0. 2.747361	-1.041423	-0.403041
C	0. 3.639936	-0.655050	-1.505009
H	0. 4.507186	-1.315937	-1.461881
H	3.117782	-0.846416	-2.442621
C	3.345526	-1.405861	0.888887
H	4.285287	-0.859281	0.969054
H	2.678035	-1.063477	1.679017
C	1.452959	-1.053036	-0.567294
H	1.083841	-0.773866	-1.559076
O	0.648017	-1.364053	0.357313
C	4.047011	0.806154	-1.395891
H	4.553747	1.005567	-0.449252
H	4.729081	1.060773	-2.209166
H	3.166463	1.449136	-1.463931
C	3.575000	-2.907826	0.977439
H	4.051967	-3.151866	1.928381
H	2.626625	-3.444890	0.917334
H	4.224737	-3.248413	0.168319
Si	-1.253283	-1.073423	0.138971
H	-1.190561	-1.735911	-1.186131
H	-2.869498	-0.909611	-0.011266
H	-1.442507	-1.884450	1.358090
C	-1.062189	0.813405	0.192817
C	-2.070351	1.610400	-0.369926
C	0.040159	1.466096	0.765484
C	-1.974195	2.998977	-0.381673
H	-2.948286	1.139733	-0.802494
C	0.131884	2.855791	0.772452
H	0.837536	0.892043	1.225016
C	-0.871774	3.625348	0.191960
H	-2.762498	3.590895	-0.833162
H	0.989138	3.336468	1.230547
H	-0.797010	4.706961	0.190478
C	-4.113263	-1.617289	-0.465762
O	-4.845538	-0.729582	-0.759565
O	-3.901043	-2.780021	-0.358661

Dioxane

Symbol	X	Y	Z
C	0. -1.163936	0.702755	0.199760
C	0. 1.164899	0.701609	0.199940
C	0. 1.163801	-0.761185	-0.200282
C	-1.164183	-0.760029	-0.200506
H	2.027242	1.216855	-0.225505
H	-1.202126	0.783892	1.295418
H	-2.025671	1.218886	-0.225828
H	1.201488	-0.841044	-1.296071

H	2.025787	-1.278270	0.223690
H	-1.201730	-0.839776	-1.296319
H	-2.026762	-1.276310	0.223233
H	1.203001	0.782701	1.295602
O	-0.000572	-1.410152	0.288711
O	0.000850	1.351611	-0.289498

Dioxane-TS

Symbol	X	Y	Z
Si	0. 0.540092	-0.911571	-0.147516
H	0. 2.178900	-1.202519	-0.235740
H	0. 0.350290	-1.666873	-1.396988
H	0.476028	-1.629155	1.140053
C	0.868218	0.938714	-0.149976
C	2.071461	1.412747	0.391093
C	-0.026601	1.867962	-0.698741
C	2.363285	2.773433	0.402486
H	2.795853	0.713221	0.798101
C	0.270775	3.227375	-0.701087
H	-0.964023	1.532398	-1.128721
C	1.463255	3.682410	-0.145331
H	3.295335	3.121880	0.832558
H	-0.429933	3.931342	-1.135516
H	1.691665	4.742140	-0.142866
C	3.121808	-2.126575	-0.010299
O	2.647225	-3.226427	-0.090340
O	4.139050	-1.521397	0.192615
C	-1.951276	-0.185252	1.189793
C	-2.290501	-1.631667	-0.693666
C	-3.664442	-1.021413	-0.859295
C	-3.333744	0.381454	0.959690
H	-1.855513	-1.886722	-1.657988
H	-1.978107	-1.042320	1.868686
H	-1.267958	0.575004	1.567368
H	-3.609521	-0.176607	-1.558406
H	-4.343131	-1.773533	-1.261704
H	-3.269969	1.263358	0.308712
H	-3.764376	0.675405	1.916864
H	-2.314261	-2.510253	-0.042319
O	-1.415848	-0.642659	-0.083136
O	-4.184999	-0.592615	0.385061

DMAc-CO_2

Symbol	X	Y	Z
C	0. 0.000000	0.000000	-0.000078
O	0. 0.000000	0.000000	-1.154565
O	0. 0.000000	0.000000	1.154624

DMAc

Symbol	X	Y	Z
C	0. -2.252713	-0.895943	-0.218280
C	0. -2.221422	-2.269318	0.418914
H	0. -1.426092	-2.838041	-0.057463
H	-2.024131	-2.201977	1.491005
H	-3.171755	-2.790350	0.284077
N	-3.203444	-0.031245	0.231470
C	-3.367470	1.255052	-0.423268
H	-3.493289	2.037295	0.328759
H	-2.486526	1.464870	-1.023411
H	-4.250914	1.250574	-1.071697
C	-4.278984	-0.414271	1.130967
H	-5.154767	-0.773543	0.578363
H	-3.957860	-1.185773	1.826747
H	-4.575487	0.460711	1.712118
O	-1.446882	-0.587830	-1.086444

DMAc-Si

Symbol	X	Y	Z
Si	0. 2.341794	0.000378	0.004212
H	0. 2.828769	1.324028	-0.444411
H	0. 2.852115	-1.057221	-0.897266
H	2.861450	-0.261990	1.366639
C	0.464377	0.000815	-0.010886
C	-0.254653	1.203040	-0.008305
C	-0.254178	-1.202930	-0.008765
C	-1.647144	1.204240	0.002692
H	0.273385	2.151835	-0.017236
C	-1.645373	-1.205492	0.002165
H	0.273870	-2.152221	-0.018480
C	-2.343528	-0.000421	0.008491
H	-2.187202	2.144310	0.003803
H	-2.184901	-2.145860	0.002900
H	-3.427710	-0.001179	0.015067

DMAc-TS

Symbol	X	Y	Z
N	0. 2.771670	-0.915959	-0.374187
C	0. 3.890639	-0.494025	-1.210510

H	0. 4.448951	-1.373466	-1.537677
H	3.546532	0.057242	-2.079389
C	3.106074	-1.588636	0.881981
H	2.788482	-2.631840	0.849656
H	4.184044	-1.539919	1.016789
C	1.500933	-0.769144	-0.695669
O	0.635498	-1.216263	0.120477
Si	-1.289463	-1.014434	0.182727
H	-1.421335	-1.675647	-1.135377
H	-2.911659	-0.922933	0.312462
H	-1.234054	-1.851150	1.398116
C	-1.177466	0.875883	0.252726
C	-2.231527	1.635188	-0.273958
C	-0.087794	1.563767	0.805366
C	-2.189517	3.026679	-0.276268
H	-3.101850	1.131487	-0.684884
C	-0.051187	2.955731	0.826432
H	0.744110	1.013969	1.234064
C	-1.098285	3.690177	0.277002
H	-3.010990	3.591919	-0.702155
H	0.796454	3.466509	1.269654
H	-1.065924	4.773890	0.284635
C	-4.191084	-1.700447	-0.030108
O	-4.976801	-0.840813	-0.250195
O	-3.909455	-2.847630	0.060195
C	1.115847	-0.097585	-1.980976
H	1.463509	0.937657	-1.981347
H	1.573626	-0.615137	-2.825761
H	0.036888	-0.108906	-2.104916
H	2.609370	-1.093867	1.716571
H	4.547275	0.147169	-0.621050

DMSO-CO_2

Symbol	X	Y	Z
C	0. 0.000000	0.000000	-0.000078
O	0. 0.000000	0.000000	-1.154565
O	0. 0.000000	0.000000	1.154624

DMSO

Symbol	X	Y	Z
S	0. 2.273343	-0.807310	0.483683
C	0. 3.539863	0.361497	-0.048607
H	0. 3.051784	1.324549	-0.197554
H	4.305596	0.449202	0.723217
H	3.964892	0.004355	-0.987921
C	3.345206	-2.255473	0.569297
H	3.790103	-2.415012	-0.414107
H	4.112096	-2.099231	1.329055
H	2.720420	-3.105631	0.842887
O	1.368828	-1.022875	-0.715446

DMSO-Si

Symbol	X	Y	Z
Si	0. 2.341579	0.000375	0.004192
H	0. 2.828367	1.324025	-0.444323
H	0. 2.851881	-1.057082	-0.897298
H	2.861190	-0.262018	1.366529
C	0.464373	0.000783	-0.010874
C	-0.254564	1.203005	-0.008300
C	-0.254121	-1.202942	-0.008732
C	-1.647013	1.204213	0.002675
H	0.273500	2.151755	-0.017222
C	-1.645274	-1.205467	0.002174
H	0.273908	-2.152208	-0.018390
C	-2.343384	-0.000413	0.008468
H	-2.187041	2.144255	0.003772
H	-2.184801	-2.145791	0.002923
H	-3.427527	-0.001156	0.015028

DMSO-TS

Symbol	X	Y	Z
Si	0. -0.490446	-0.970021	-0.610055
H	0. -2.089411	-1.290427	-0.592017
H	0. -0.411440	-1.408876	-2.019525
H	-0.286845	-1.941327	0.495708
C	-0.840129	0.826411	-0.128531
C	-1.926572	1.120296	0.706919
C	-0.057308	1.894571	-0.587511
C	-2.205326	2.427668	1.093817
H	-2.568528	0.315537	1.054160
C	-0.344521	3.207532	-0.220652
H	0.781105	1.702622	-1.249224
C	-1.414307	3.474969	0.628282
H	-3.043204	2.630700	1.751399
H	0.267799	4.019865	-0.596360
H	-1.634331	4.495156	0.921918
C	-3.083693	-2.434722	-0.361908
O	-2.558774	-3.411970	-0.778477

O	-4.007172	-1.891699	0.145394
S	2.233704	-0.411592	0.581807
C	3.379224	0.866836	0.074702
H	2.828156	1.802998	0.002067
H	4.148751	0.944859	0.844374
H	3.807312	0.578660	-0.885343
C	3.349314	-1.811015	0.634759
H	3.862546	-1.880142	-0.324154
H	4.052533	-1.655104	1.453955
H	2.743651	-2.696912	0.822771
O	1.406511	-0.685533	-0.731554

Gvl-CO_2

Symbol	X	Y	Z
C	0. 0.000000	0.000000	-0.000078
O	0. 0.000000	0.000000	-1.154565
O	0. 0.000000	0.000000	1.154624

Gvl

Symbol	X	Y	Z
O	0. -0.059053	-0.946518	0.162525
C	0. 1.046940	-0.035892	0.406545
C	0. 0.565267	1.301122	-0.160964
C	-0.942819	1.216995	0.050616
H	1.035845	2.144758	0.340845
H	0.799998	1.351176	-1.226967
H	-1.236413	1.563470	1.045469
H	-1.548644	1.739276	-0.686539
C	-1.210510	-0.274383	-0.011781
O	-2.257184	-0.835970	-0.173178
C	2.291838	-0.601396	-0.233746
H	3.128675	0.080842	-0.072126
H	2.545400	-1.570565	0.196876
H	2.137435	-0.718396	-1.308238
H	1.163306	0.030662	1.491887

Gvl-Si

Symbol	X	Y	Z
Si	0. 2.341770	0.000376	0.004215
H	0. 2.828724	1.324028	-0.444395
H	0. 2.852095	-1.057202	-0.897266
H	2.861427	-0.261994	1.366627
C	0.464371	0.000811	-0.010885
C	-0.254646	1.203041	-0.008308
C	-0.254175	-1.202936	-0.008764
C	-1.647142	1.204247	0.002691
H	0.273430	2.151802	-0.017246
C	-1.645374	-1.205499	0.002168
H	0.273904	-2.152196	-0.018481
C	-2.343528	-0.000420	0.008493
H	-2.187190	2.144305	0.003798
H	-2.184897	-2.145853	0.002904
H	-3.427695	-0.001176	0.015069

Gvl-TS

Symbol	X	Y	Z
O	0. 2.614255	0.194209	-0.185457
C	0. 4.082539	-0.006994	-0.229260
C	0. 4.263356	-1.402789	0.362763
C	2.956748	-2.100428	-0.011396
H	5.145221	-1.893312	-0.043846
H	4.359302	-1.331728	1.448357
H	2.995164	-2.544332	-1.012081
H	2.601360	-2.852297	0.690208
Si	-0.443673	0.539164	-0.209208
H	-1.431644	1.866464	-0.355830
H	0.144480	0.864544	-1.521353
H	0.168205	1.104695	1.006536
C	-1.951855	-0.577049	-0.056398
C	-3.152526	-0.019260	0.407785
C	-1.945936	-1.935590	-0.402362
C	-4.301333	-0.793738	0.538967
H	-3.196581	1.035161	0.664488
C	-3.098662	-2.707507	-0.288316
H	-1.036038	-2.400430	-0.761862
C	-4.276846	-2.140012	0.187894
H	-5.215858	-0.343910	0.908584
H	-3.074649	-3.754739	-0.568070
H	-5.172407	-2.743771	0.282121
C	-1.449648	3.246666	-0.139766
O	-2.558189	3.496257	0.236191
O	-0.372704	3.690922	-0.408291
C	2.004842	-0.950588	-0.087251
O	0.771762	-1.025629	-0.073894
C	4.737551	1.121308	0.519935
H	5.818849	0.968212	0.504431
H	4.517050	2.082949	0.054779
H	4.400903	1.133632	1.558617

H 4.337687 0.010369 -1.290128

MBO-CO_2

Symbol	X	Y	Z
C	0. 0.000000	0.000000	-0.000078
O	0. 0.000000	0.000000	-1.154565
O	0. 0.000000	0.000000	1.154624

MBO

Symbol	X	Y	Z
C	0. -2.405186	-0.272015	0.022377
C	0. -2.696495	-1.720152	-0.290827
H	0. -1.825874	-2.328519	-0.050396
H	-3.572678	-2.078024	0.254293
H	-2.916737	-1.815573	-1.358544
C	-4.585976	0.471741	-1.045922
H	-5.364722	1.236689	-1.000621
H	-4.108062	0.532337	-2.026932
H	-5.071137	-0.504134	-0.959593
C	-4.256802	0.548790	1.456433
H	-5.062109	1.281196	1.549606
H	-4.691197	-0.447399	1.577829
H	-3.545510	0.717309	2.268298
O	-1.277209	0.111642	0.236132
C	-3.581278	0.690119	0.085234
H	-3.148537	1.690955	0.009895

MBO-Si

Symbol	X	Y	Z
Si	0. 2.341372	0.000905	0.005129
H	0. 2.837683	1.281812	-0.546431
H	0. 2.847769	-1.128592	-0.807098
H	2.858279	-0.149976	1.385661
C	0.464132	0.001541	-0.014221
C	-0.255329	1.203276	0.012762
C	-0.253693	-1.201970	-0.034665
C	-1.647519	1.203709	0.026601
H	0.272211	2.152394	0.019901
C	-1.645213	-1.205336	-0.020729
H	0.275062	-2.150205	-0.065084
C	-2.343635	-0.001273	0.010698
H	-2.187992	2.143298	0.046409
H	-2.184302	-2.145772	-0.037731
H	-3.427754	-0.002476	0.019421

MBO-TS

Symbol	X	Y	Z
Si	0. 0.429903	-0.745879	-0.075571
H	0. 1.870912	-1.604167	-0.212658
H	0. 0.146352	-1.445786	1.189615
H	0.004200	-1.368365	-1.342220
C	1.397975	0.866454	-0.059714
C	2.757849	0.830230	0.284906
C	0.835803	2.105331	-0.399378
C	3.524566	1.991366	0.303851
H	3.230699	-0.115107	0.534564
C	1.605435	3.264962	-0.394313
H	-0.211029	2.172404	-0.669019
C	2.949666	3.211340	-0.038206
H	4.571730	1.940787	0.579668
H	1.152702	4.211839	-0.666151
H	3.546969	4.116089	-0.030260
C	2.382016	-2.835953	-0.023013
O	1.515240	-3.659942	-0.134090
O	3.554594	-2.683411	0.191178
C	-2.435645	-0.269875	-0.014537
C	-2.682975	-1.719717	-0.247180
H	-1.943069	-2.338623	0.260733
H	-3.688217	-2.007873	0.053056
H	-2.584673	-1.894027	-1.326306
C	-4.588833	0.510059	-1.017876
H	-5.366114	1.270005	-0.918711
H	-4.111089	0.633655	-1.992052
H	-5.068610	-0.470424	-0.983759
C	-4.248893	0.451562	1.494220
H	-5.042167	1.190172	1.623269
H	-4.695293	-0.543596	1.553724
H	-3.533983	0.567790	2.311279
O	-1.286009	0.191073	0.058306
C	-3.584789	0.681369	0.126198
H	-3.159176	1.686551	0.101558

THF-CO_2

Symbol	X	Y	Z
C	0. 0.000000	0.000000	-0.000078
O	0. 0.000000	0.000000	-1.154565
O	0. 0.000000	0.000000	1.154624

THF

Symbol	X	Y	Z
C	0. -1.170009	-0.411823	-0.122477
O	0. -0.011837	-1.245517	-0.024282
C	0. 1.152251	-0.437445	0.153393
C	0.742092	0.975692	-0.246427
C	-0.711205	1.001697	0.232351
H	-1.551487	-0.453930	-1.148441
H	-1.939309	-0.793686	0.551560
H	1.461774	-0.467715	1.204985
H	1.955970	-0.848061	-0.459698
H	1.366855	1.742121	0.211662
H	0.783577	1.090590	-1.332623
H	-0.745703	1.155522	1.313810
H	-1.315753	1.770572	-0.248039

THF-Si

Symbol	X	Y	Z
Si	0. 2.340812	0.000903	0.005522
H	0. 2.837542	1.279287	-0.551669
H	0. 2.847117	-1.132176	-0.801811
H	2.858278	-0.143762	1.386425
C	0.463980	0.001519	-0.014297
C	-0.255459	1.202870	0.013851
C	-0.253824	-1.201568	-0.036125
C	-1.647310	1.203403	0.027923
H	0.272327	2.151787	0.021396
C	-1.645042	-1.205063	-0.021946
H	0.275183	-2.149534	-0.068166
C	-2.343285	-0.001313	0.010990
H	-2.187787	2.142884	0.048636
H	-2.184136	-2.145392	-0.040017
H	-3.427326	-0.002512	0.019910

THF-TS

Symbol	X	Y	Z
C	0. -2.598982	-1.021193	-1.011309
O	0. -1.618089	-0.798810	0.054906
C	0. -2.254422	-0.291135	1.271137
C	-3.617067	0.166986	0.788840
C	-3.934852	-0.853274	-0.308341
H	-2.427023	-0.264711	-1.778917
H	-2.424939	-2.015341	-1.418148
H	-2.314145	-1.120298	1.977782
H	-1.620955	0.501735	1.667798
H	-4.347602	0.166293	1.596599
H	-3.551076	1.174258	0.370622
H	-4.248465	-1.800517	0.134807
H	-4.705514	-0.513230	-0.998600
Si	0.270569	-1.009098	-0.113710
H	1.944726	-1.300991	-0.337355
H	0.067999	-1.761082	-1.363378
H	0.334414	-1.719768	1.174143
C	0.649967	0.834030	-0.120113
C	1.925253	1.274782	0.261564
C	-0.297062	1.795107	-0.499788
C	2.236314	2.631038	0.278173
H	2.688733	0.553836	0.539874
C	0.017104	3.150534	-0.497169
H	-1.293223	1.493259	-0.806679
C	1.283704	3.570704	-0.102637
H	3.225764	2.952111	0.582882
H	-0.726963	3.877774	-0.801532
H	1.527878	4.626855	-0.095400
C	2.823998	-2.197216	-0.056573
O	2.385432	-3.307073	-0.238649
O	3.829460	-1.626916	0.296822

S1

Symbol	X	Y	Z
C	1.100327	-0.065434	0.375178
C	0.552464	1.300081	-0.063946
H	0.953491	2.117914	0.532915
H	0.767216	1.482035	-1.121082
C	-1.205385	-0.225483	0.061051
O	-2.325191	-0.693598	-0.000197
H	1.310753	-0.072900	1.449431
H	2.001052	-0.341850	-0.171154
N	-0.877131	1.110572	0.160739
H	-1.541453	1.777562	-0.204649
N	-0.022674	-0.932916	0.044014
H	-0.049437	-1.885158	0.379286

S1-TS

Symbol	X	Y	Z
Si	-0.404576	0.513626	-0.091212
H	-1.356381	1.834323	-0.109737
H	0.177405	0.932550	-1.389703

H	0.260170	1.016630	1.133260
C	-1.926923	-0.605304	0.001288
C	-3.159832	-0.033048	0.349397
C	-1.902020	-1.979848	-0.278304
C	-4.318425	-0.800699	0.428608
H	-3.220237	1.030895	0.556708
C	-3.061362	-2.747880	-0.214575
H	-0.968123	-2.457182	-0.546301
C	-4.271851	-2.161561	0.143253
H	-5.256832	-0.334450	0.707195
H	-3.017877	-3.807373	-0.441574
H	-5.173540	-2.761313	0.197486
C	-1.339349	3.342144	-0.105688
O	-2.488651	3.626818	-0.023178
O	-0.201221	3.667501	-0.185452
C	4.218144	-1.668916	0.028701
C	4.173319	-0.277229	-0.619528
H	4.864022	0.422825	-0.156204
H	4.363436	-0.331007	-1.693669
C	2.027160	-0.981911	-0.162981
O	0.769655	-1.023458	-0.066342
H	4.537007	-1.612993	1.072020
H	4.856066	-2.360802	-0.515704
N	2.779878	0.111435	-0.374259
H	2.384076	0.945041	-0.788300
N	2.810131	-2.064960	-0.050737
H	2.452825	-2.899051	0.395246

S2

Symbol	X	Y	Z
C	1.052767	-0.024267	0.514825
C	0.572998	1.308070	-0.076190
C	-0.951206	1.176711	-0.047336
H	0.946570	2.164453	0.483097
H	0.917698	1.389875	-1.108739
H	-1.371236	1.526563	0.901160
H	-1.468037	1.689982	-0.857350
C	-1.194679	-0.323199	-0.118443
O	-2.256716	-0.877490	-0.344244
H	1.153194	0.023559	1.606285
H	2.003033	-0.360187	0.095307
N	-0.016262	-0.942097	0.147691
C	0.101760	-2.363166	0.368664
H	0.244818	-2.583585	1.432125
H	-0.815316	-2.838838	0.024306
H	0.950851	-2.764404	-0.189584

S2-TS

Symbol	X	Y	Z
Si	-0.412606	0.537704	-0.156824
H	-1.369423	1.853936	-0.089449
H	0.041674	0.929491	-1.510700
H	0.343901	1.051948	1.007900
C	-1.916541	-0.590326	0.057583
C	-3.192186	-0.068199	-0.203899
C	-1.833107	-1.924688	0.482269
C	-4.337092	-0.847871	-0.063821
H	-3.295575	0.966050	-0.518183
C	-2.976767	-2.702949	0.639801
H	-0.865045	-2.362823	0.691697
C	-4.231468	-2.168325	0.361859
H	-5.310357	-0.421812	-0.280442
H	-2.887341	-3.729749	0.976980
H	-5.121271	-2.776822	0.478812
C	-1.389558	3.337231	-0.442115
O	-2.545999	3.567987	-0.568151
O	-0.258246	3.690921	-0.452043
C	4.199071	-1.777166	-0.270840
C	4.278698	-0.266972	-0.521231
C	2.898937	0.247980	-0.095062
H	5.092338	0.197651	0.031290
H	4.425478	-0.081243	-1.585784
H	2.868620	0.539540	0.959858
H	2.532320	1.086346	-0.686991
C	2.022223	-0.967046	-0.249467
O	0.760537	-1.003777	-0.232549
H	4.542417	-2.058622	0.728702
H	4.735829	-2.369929	-1.011323
N	2.761595	-2.048710	-0.373381
C	2.245516	-3.402653	-0.434450
H	2.476270	-3.927971	0.495161
H	1.167755	-3.367306	-0.578706
H	2.713097	-3.926385	-1.269045

S3

Symbol	X	Y	Z
S	0.137129	0.418746	-0.380657
C	-1.074478	0.089621	0.919577

H	-1.947782	0.708203	0.710328
H	-1.348944	-0.965854	0.898558
H	-0.628128	0.362815	1.876656
O	0.629159	1.830345	-0.134302
C	1.423053	-0.680526	0.235902
C	1.387597	-2.040037	-0.061691
C	2.448734	-0.138979	0.995731
C	2.385099	-2.870517	0.424808
H	0.588502	-2.453164	-0.669218
C	3.453738	-0.967846	1.478585
H	2.456134	0.927607	1.191289
C	3.419340	-2.334020	1.196412
H	2.383793	-3.932439	0.210609
H	4.265451	-0.559044	2.072103
O	4.370458	-3.189213	1.639337
H	5.025184	-2.702834	2.156384

S3-TS

Symbol	X	Y	Z
Si	0.622695	-0.944150	0.574521
H	2.246792	-0.824924	0.515705
H	0.694599	-1.483086	1.948312
H	0.655906	-1.853091	-0.599669
C	0.463154	0.909966	0.228971
C	1.387270	1.539426	-0.615668
C	-0.546875	1.697003	0.799204
C	1.292967	2.897858	-0.903328
H	2.196629	0.960109	-1.051123
C	-0.633644	3.061458	0.531943
H	-1.269777	1.243527	1.469644
C	0.281847	3.662381	-0.326946
H	2.011654	3.361312	-1.569911
H	-1.416143	3.653795	0.993160
H	0.211092	4.722525	-0.542653
C	3.523615	-1.654942	0.443220
O	3.210568	-2.771579	0.690474
O	4.348934	-0.850749	0.165181
S	-2.191899	-0.995423	-0.545086
C	-3.693430	-0.343653	0.184335
H	-3.482641	0.675888	0.505149
H	-4.463466	-0.349482	-0.587778
H	-3.970369	-0.977484	1.026393
O	-1.284651	-1.184711	0.729441
C	-2.698497	-2.639808	-0.975861
C	-2.695934	-2.994048	-2.319861
C	-3.067988	-3.547617	0.017338
C	-3.090371	-4.273904	-2.684490
H	-2.390900	-2.284069	-3.080425
C	-3.450294	-4.823692	-0.346572
H	-3.041039	-3.262301	1.062919
C	-3.466540	-5.187192	-1.699281
H	-3.096600	-4.567399	-3.728739
H	-3.738207	-5.554954	0.398614
O	-3.851690	-6.446122	-1.990587
H	-3.818171	-6.585765	-2.946312

S4

Symbol	X	Y	Z
S	0.020633	0.355464	-0.173978
C	-1.272475	-0.907238	-0.122664
H	-2.192824	-0.438076	-0.470550
H	-0.993334	-1.726686	-0.785390
H	-1.377374	-1.245505	0.908891
O	-0.262650	1.307994	0.967983
C	1.356725	-0.734119	0.401632
C	1.845406	-0.570093	1.686280
C	2.771171	-2.430236	-0.093055
C	2.876959	-1.418045	2.075348
H	1.425039	0.190288	2.332377
C	3.348051	-2.362804	1.171438
H	3.118100	-3.153590	-0.823144
H	3.305551	-1.341714	3.067776
H	4.150990	-3.039266	1.435018
N	1.783865	-1.620184	-0.483684

S4-TS

Symbol	X	Y	Z
Si	0.698172	-0.933830	0.503197
H	2.326720	-0.779670	0.454175
H	0.782786	-1.533286	1.849763
H	0.752106	-1.797199	-0.702363
C	0.503334	0.927267	0.237124
C	1.451302	1.617970	-0.530391
C	-0.557507	1.659982	0.787955
C	1.330696	2.984522	-0.764173
H	2.299552	1.081623	-0.945980
C	-0.672239	3.031238	0.572073
H	-1.297339	1.160193	1.404616

C	0.267594	3.693998	-0.211741
H	2.069103	3.496697	-1.370818
H	-1.495328	3.580706	1.015263
H	0.175289	4.759925	-0.386938
C	3.589183	-1.530765	0.238524
O	3.355730	-2.674601	0.462377
O	4.367907	-0.690142	-0.077767
S	-2.116908	-1.043615	-0.629241
C	-3.625740	-0.346567	0.045611
H	-3.430405	0.703435	0.259186
H	-4.395856	-0.443301	-0.720467
H	-3.881934	-0.903694	0.946179
O	-1.210724	-1.223899	0.638276
C	-2.704368	-2.721086	-0.959957
C	-2.233967	-3.792235	-0.224560
C	-4.045146	-3.970780	-2.279133
C	-2.737903	-5.041354	-0.579636
H	-1.521255	-3.656569	0.578157
C	-3.655070	-5.132223	-1.617614
H	-4.758031	-4.005389	-3.095176
H	-2.414839	-5.927644	-0.047064
H	-4.066158	-6.087071	-1.918710
N	-3.568711	-2.766991	-1.957379

S5

Symbol	X	Y	Z
P	1.482355	-0.490032	-0.241918
O	2.186157	0.187221	-1.374718
C	1.847491	-2.256647	-0.152553
H	2.905066	-2.354493	0.106173
H	1.246006	-2.752868	0.611107
H	1.684614	-2.737016	-1.118166
N	-0.194516	-0.397754	-0.193290
N	1.906015	0.207723	1.228883
C	-0.946665	-1.273761	-1.091357
H	-0.601281	-2.304000	-1.009183
H	-1.998401	-1.248951	-0.797530
H	-0.876334	-0.956014	-2.140131
C	-0.758501	0.952366	-0.148250
H	-1.783379	0.894314	0.226113
H	-0.176148	1.577220	0.528927
H	-0.777316	1.422652	-1.139803
C	3.300424	0.619753	1.371511
H	3.640842	1.099241	0.455174
H	3.375402	1.337372	2.192174
H	3.960350	-0.229831	1.597368
C	1.373342	-0.390332	2.450481
H	1.450652	0.334650	3.264555
H	0.323412	-0.648922	2.315349
H	1.928971	-1.292788	2.741533

S5-TS

Symbol	X	Y	Z
Si	-0.501462	0.987402	0.019722
H	-1.926883	1.644933	0.410037
H	0.077789	1.620161	1.234562
H	-0.481760	1.760164	-1.245813
C	-1.282456	-0.748031	0.081860
C	-2.659322	-0.865279	0.328941
C	-0.559176	-1.936095	-0.110633
C	-3.287520	-2.107006	0.384131
H	-3.254327	0.030187	0.478155
C	-1.181351	-3.180525	-0.051682
H	0.504377	-1.887732	-0.311229
C	-2.548032	-3.270147	0.195917
H	-4.353424	-2.164534	0.575196
H	-0.597369	-4.082101	-0.201319
H	-3.032667	-4.239113	0.240375
C	-2.751997	3.007927	0.349980
O	-1.933907	3.855378	0.426079
O	-3.864700	2.621793	0.257781
P	2.685027	0.523549	-0.130659
O	1.199761	0.263722	-0.418529
C	2.971009	2.257193	0.223314
H	2.493744	2.479755	1.180818
H	4.042043	2.451893	0.304260
H	2.533762	2.892985	-0.548025
N	3.689796	0.088486	-1.365349
N	3.132078	-0.444083	1.140493
C	3.894387	1.018102	-2.480111
H	4.083864	2.026829	-2.115799
H	4.773750	0.689556	-3.036516
H	3.035265	1.033437	-3.160610
C	3.653812	-1.315089	-1.791222
H	4.603639	-1.554493	-2.272911
H	3.526806	-1.966805	-0.927081
H	2.839923	-1.495275	-2.502481
C	2.184687	-0.604527	2.246232

H	1.176721	-0.767090	1.865722
H	2.478163	-1.484581	2.821782
H	2.185039	0.265351	2.914670
C	4.525507	-0.379358	1.588937
H	4.759684	-1.298796	2.129023
H	5.194257	-0.299990	0.732233
H	4.693600	0.472920	2.258775

S6

Symbol	X	Y	Z
P	-0.070487	1.251889	-0.296050
O	-0.018369	1.951754	-1.623948
C	1.401889	0.222894	-0.009327
C	1.507986	-0.590699	1.122322
C	2.443642	0.271710	-0.933736
C	2.655467	-1.346935	1.326494
H	0.692891	-0.637347	1.838688
C	3.591866	-0.489483	-0.727066
H	2.347974	0.902897	-1.810505
C	3.697414	-1.295674	0.401330
H	2.737986	-1.978241	2.203579
H	4.401223	-0.452915	-1.447075
H	4.590973	-1.888062	0.561631
C	-1.468012	0.098643	-0.122940
C	-2.606241	0.430967	0.613729
C	-1.420100	-1.118397	-0.810464
C	-3.684468	-0.448734	0.665189
H	-2.658654	1.370644	1.152317
C	-2.498826	-1.992675	-0.759641
H	-0.535526	-1.385211	-1.380847
C	-3.631353	-1.657765	-0.020368
H	-4.564402	-0.188326	1.241767
H	-2.455661	-2.935477	-1.292291
H	-4.471294	-2.341627	0.022330
C	-0.148320	2.362922	1.125257
H	0.760845	2.967982	1.119702
H	-1.013395	3.022754	1.037105
H	-0.203326	1.801621	2.059828

S6-TS

Symbol	X	Y	Z
Si	1.813903	-0.085680	1.012995
H	3.364569	-0.462739	1.285568
H	1.617068	0.120206	2.467777
H	1.595270	-1.453182	0.470675
C	2.350265	1.333093	-0.132530
C	3.714914	1.494640	-0.418991
C	1.455098	2.243286	-0.716668
C	4.167920	2.513122	-1.253692
H	4.439127	0.813895	0.017383
C	1.903736	3.266054	-1.548202
H	0.394523	2.151176	-0.517738
C	3.261765	3.403400	-1.820706
H	5.228199	2.611076	-1.458828
H	1.190521	3.957014	-1.984180
H	3.610788	4.198918	-2.469615
C	4.324237	-1.501601	1.964709
O	3.616009	-2.239007	2.557758
O	5.390096	-1.130519	1.610535
P	-1.274625	-0.599262	0.649972
O	-0.038113	0.319782	0.737075
C	-1.302749	-1.445352	-0.939337
C	-2.219928	-2.473862	-1.174113
C	-0.412876	-1.048168	-1.937718
C	-2.239680	-3.104910	-2.411255
H	-2.916912	-2.777063	-0.399399
C	-0.439422	-1.686231	-3.174101
H	0.294417	-0.246363	-1.752171
C	-1.349935	-2.711335	-3.408901
H	-2.947948	-3.903346	-2.597390
H	0.251388	-1.381825	-3.951176
H	-1.367774	-3.206924	-4.372603
C	-2.770809	0.395265	0.787263
C	-3.186886	0.832316	2.049016
C	-3.480202	0.768771	-0.356443
C	-4.312959	1.637910	2.160875
H	-2.638102	0.550071	2.941157
C	-4.605614	1.576813	-0.234966
H	-3.160479	0.431033	-1.336110
C	-5.021377	2.008526	1.020413
H	-4.637855	1.975137	3.137831
H	-5.157327	1.865904	-1.121414
H	-5.900679	2.635600	1.111752
C	-1.282281	-1.835341	1.952010
H	-1.187370	-1.343001	2.921774
H	-2.216598	-2.398800	1.917375
H	-0.439723	-2.512765	1.800403

S7

Symbol	X	Y	Z
P	1.366053	-0.380324	0.407848
O	2.109708	0.623081	-0.411824
N	1.481156	-0.082869	2.050726
H	2.435127	-0.028684	2.394569
H	0.912933	-0.672025	2.651783
C	1.944658	-2.066843	0.053119
C	1.529014	-3.147082	0.836695
C	2.812692	-2.278275	-1.017389
C	1.980478	-4.429049	0.548426
H	0.850937	-2.989022	1.670456
C	3.264713	-3.564186	-1.303677
H	3.132107	-1.433830	-1.617770
C	2.848671	-4.637120	-0.522372
H	1.658236	-5.265761	1.157287
H	3.940390	-3.726750	-2.135441
H	3.200331	-5.637914	-0.745565
C	-0.430977	-0.421289	0.153231
C	-1.253466	0.467289	0.852592
C	-0.987893	-1.266317	-0.810420
C	-2.620081	0.499248	0.597213
H	-0.825993	1.129250	1.597391
C	-2.354763	-1.228466	-1.065303
H	-0.357716	-1.957742	-1.360257
C	-3.170639	-0.348015	-0.360528
H	-3.254466	1.185941	1.145429
H	-2.782324	-1.888488	-1.810911
H	-4.236281	-0.322182	-0.557427

S7-TS

Symbol	X	Y	Z
Si	-0.383118	0.988016	0.166848
H	-1.775024	1.640438	-0.347499
H	-0.475370	1.776273	1.416571
H	0.313668	1.603771	-0.994304
C	-1.143878	-0.747267	0.041107
C	-2.358250	-0.910744	-0.642147
C	-0.560151	-1.890165	0.609390
C	-2.958639	-2.161255	-0.767611
H	-2.846791	-0.047080	-1.082563
C	-1.163373	-3.140008	0.498561
H	0.378732	-1.801736	1.142852
C	-2.362666	-3.279932	-0.194635
H	-3.893193	-2.259554	-1.308706
H	-0.694926	-4.006561	0.952110
H	-2.829630	-4.254262	-0.285760
C	-2.458512	2.943782	-0.868262
O	-1.691357	3.814042	-0.639490
O	-3.488214	2.542120	-1.291145
P	2.745736	0.560472	0.383464
O	1.291291	0.273560	0.778895
N	3.120071	2.150324	0.631359
H	2.627267	2.828214	0.056949
H	4.103469	2.378216	0.736907
C	2.997216	0.061979	-1.328380
C	4.063222	0.593674	-2.057618
C	2.143876	-0.879406	-1.907852
C	4.273965	0.180597	-3.367585
H	4.722800	1.327845	-1.606466
C	2.359373	-1.285654	-3.220200
H	1.315420	-1.288942	-1.339431
C	3.422552	-0.757143	-3.946828
H	5.098399	0.592636	-3.937091
H	1.696347	-2.012051	-3.674723
H	3.587321	-1.074824	-4.969872
C	3.880418	-0.345007	1.438701
C	4.049829	0.078030	2.761679
C	4.544041	-1.479477	0.968233
C	4.889403	-0.635407	3.606857
H	3.531944	0.958586	3.125911
C	5.381050	-2.188537	1.823460
H	4.413464	-1.808035	-0.056860
C	5.553320	-1.766876	3.137782
H	5.025426	-0.309325	4.630992
H	5.898917	-3.068286	1.460854
H	6.207790	-2.321187	3.800448

S8

Symbol	X	Y	Z
C	1.125536	-0.014666	-0.013826
C	-0.967124	-1.269869	0.168180
C	-1.721570	-0.055859	-0.326437
C	-1.112840	1.187486	0.308158
C	0.346473	1.278672	-0.125221
H	-1.266986	-2.179225	-0.350750
H	-1.656535	0.008166	-1.417347
H	-2.773033	-0.175500	-0.056811

H	-1.645310	2.093021	0.014119
H	-1.175575	1.105378	1.397941
H	0.395871	1.544028	-1.187906
H	0.906831	2.037145	0.421018
H	-1.132709	-1.408818	1.240398
O	2.328288	-0.040243	0.019003
O	0.462287	-1.182105	-0.034726

S8-TS

Symbol	X	Y	Z
Si	-0.427737	0.602353	-0.122368
H	-1.435242	1.900399	-0.234608
H	0.172899	0.959723	-1.421368
H	0.153956	1.146156	1.119052
C	-1.911459	-0.558675	-0.029292
C	-3.140432	-0.039017	0.404272
C	-1.863475	-1.911638	-0.394505
C	-4.274100	-0.842103	0.488172
H	-3.218694	1.010158	0.673396
C	-2.999936	-2.712835	-0.328606
H	-0.931877	-2.348739	-0.732122
C	-4.206299	-2.181736	0.118356
H	-5.210422	-0.419334	0.834639
H	-2.941561	-3.754698	-0.623261
H	-5.089461	-2.808102	0.175365
C	-1.492758	3.330650	-0.136111
O	-2.648484	3.572791	0.034061
O	-0.385319	3.754602	-0.260300
C	2.056844	-0.856887	0.005128
C	4.029958	0.563518	-0.028029
C	4.831154	-0.655017	-0.415180
C	4.350753	-1.848135	0.400664
C	2.883956	-2.102684	0.071464
H	4.188998	1.408747	-0.693147
H	4.717377	-0.855785	-1.484632
H	5.882306	-0.432713	-0.223005
H	4.931125	-2.742838	0.176865
H	4.462918	-1.633870	1.467066
H	2.786651	-2.552525	-0.924048
H	2.392442	-2.776691	0.773724
H	4.227766	0.866344	1.000990
O	0.817898	-0.939569	0.004256
O	2.583409	0.327077	-0.095521

S9

Symbol	X	Y	Z
C	-1.359445	0.025910	0.013965
O	-2.473654	-0.095820	-0.424742
O	-0.773274	1.233713	-0.072091
C	0.552732	1.473762	0.431376
C	-0.586042	-1.118051	0.624416
C	1.637257	0.793408	-0.390719
C	0.614956	-1.552631	-0.236281
C	1.852577	-0.678943	-0.048248
H	0.610071	1.190057	1.486309
H	1.388087	0.912650	-1.450666
H	-1.298457	-1.936201	0.714235
H	0.317686	-1.564521	-1.290765
H	0.657044	2.555760	0.368024
H	-0.245735	-0.852106	1.629624
H	2.568726	1.339471	-0.216672
H	0.861882	-2.581783	0.032845
H	2.666484	-1.075168	-0.661490
H	2.177423	-0.752031	0.996173

S9-TS

Symbol	X	Y	Z
Si	-0.418156	0.535129	-0.175709
H	-1.394526	1.859522	-0.273215
H	0.156391	0.870352	-1.492275
H	0.210948	1.068212	1.046761
C	-1.927159	-0.587206	-0.036648
C	-3.131133	-0.035187	0.425947
C	-1.921676	-1.942476	-0.396315
C	-4.282054	-0.809264	0.541269
H	-3.176166	1.016399	0.693062
C	-3.075651	-2.714742	-0.297960
H	-1.010043	-2.403956	-0.755604
C	-4.256838	-2.151639	0.176075
H	-5.198606	-0.362095	0.909243
H	-3.050692	-3.759034	-0.588654
H	-5.153718	-2.755418	0.257563
C	-1.424712	3.280096	-0.116956
O	-2.569192	3.535658	0.105185
O	-0.316118	3.693642	-0.266516
C	2.029681	-0.991458	-0.129941
O	0.790454	-1.040576	-0.080296
O	2.578713	0.181762	-0.248417

C	4.027072	0.359033	-0.312650
C	2.837802	-2.246956	-0.083592
C	4.623656	-0.189862	-1.593957
C	3.566279	-2.517493	-1.415296
C	4.843832	-1.700901	-1.589546
H	4.469045	-0.087631	0.580452
H	3.986727	0.110754	-2.432383
H	2.140859	-3.050633	0.144872
H	2.879837	-2.336402	-2.248655
H	4.135726	1.439121	-0.258852
H	3.562757	-2.173678	0.733373
H	5.584792	0.313451	-1.728470
H	3.813275	-3.580228	-1.432159
H	5.324819	-1.992408	-2.526217
H	5.536949	-1.953907	-0.779712