Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Unveiling the mechanism and origin of stereocontrol in dinuclear-zinc-catalysed reductive desymmetrization of malonic esters

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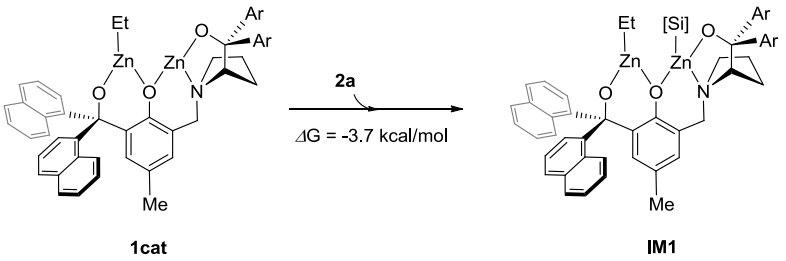

Fig. S1. The formation of dinuclear zinc complex **IM1** via the coordination of silane **2a**.

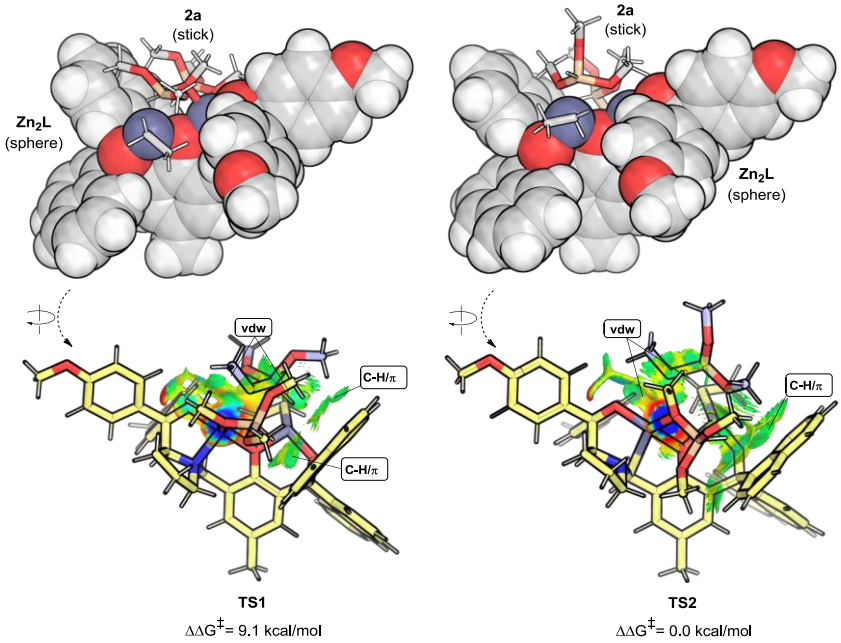

Fig. S2. Optimized geometries (Space-filling model = Zn-PrePhenol sheleton; Stick model = Et group and $HSi(OMe)_3$) and isosurfaces of δg^{inter} = 0.05 a.u. corresponding to IGMH analysis for **TS1** and **TS2**.

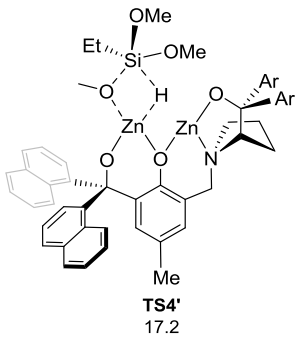

Fig. S3. Possible pathway for the formation of active Zn−H catalyst **IM2** via σ-bond metathesis.

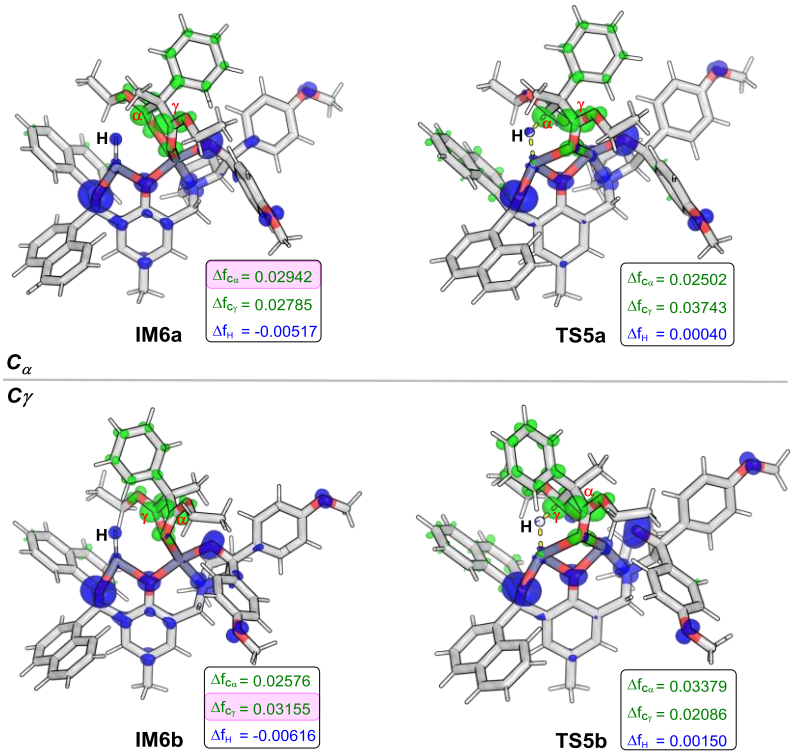

Fig. S4. Topology of dual descriptor isosurfaces and DFT calculations of the condensed dual descriptor.

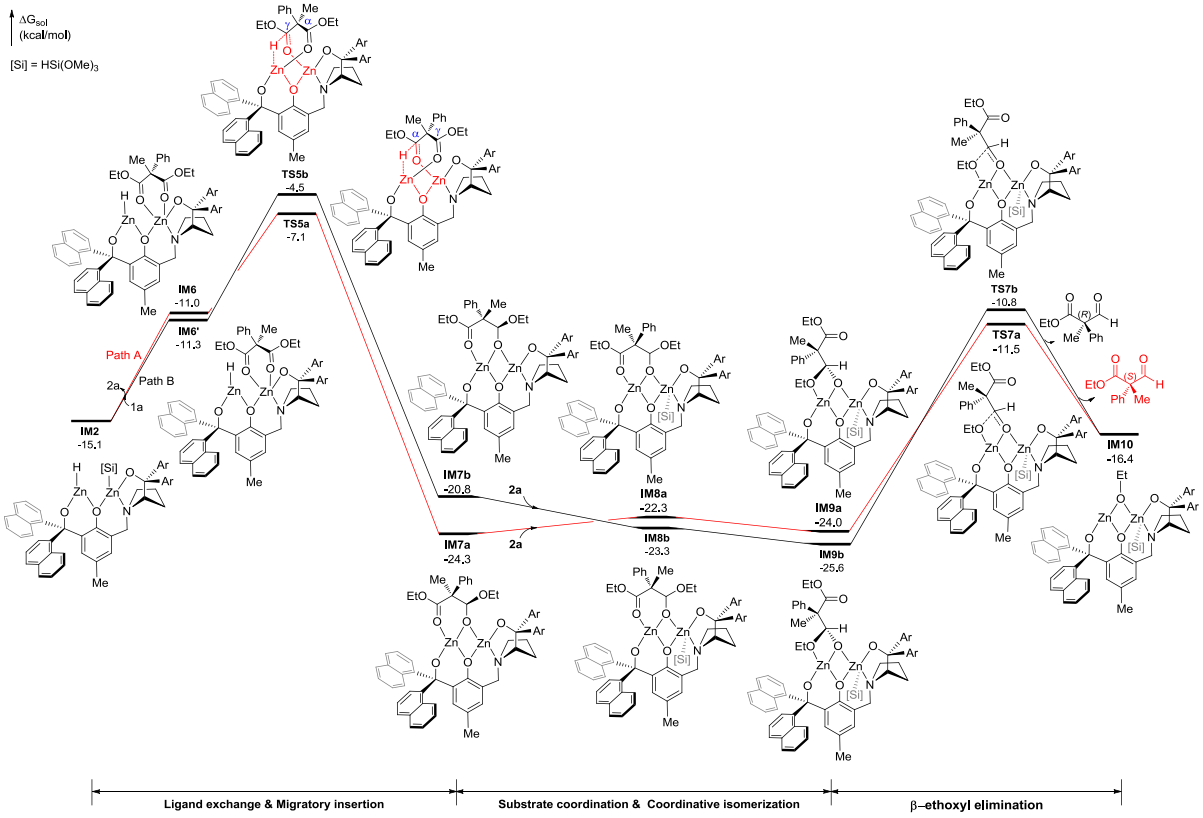

Fig. S5. Free energy profiles for the formation of (*S*)-aldehyde and its enantioisomer (*R*)-aldehyde.

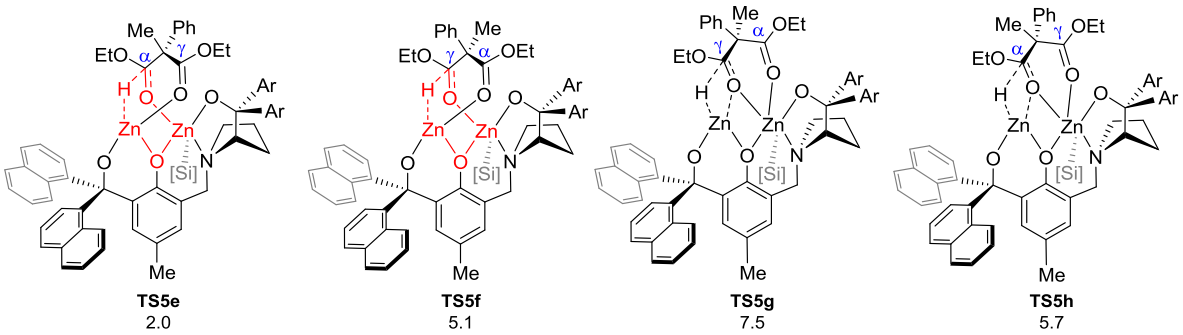

Fig. S6. Possible pathways for migratory insertion of ester C=O into Zn−H with $HSi(OMe)_3$ as a ligand.

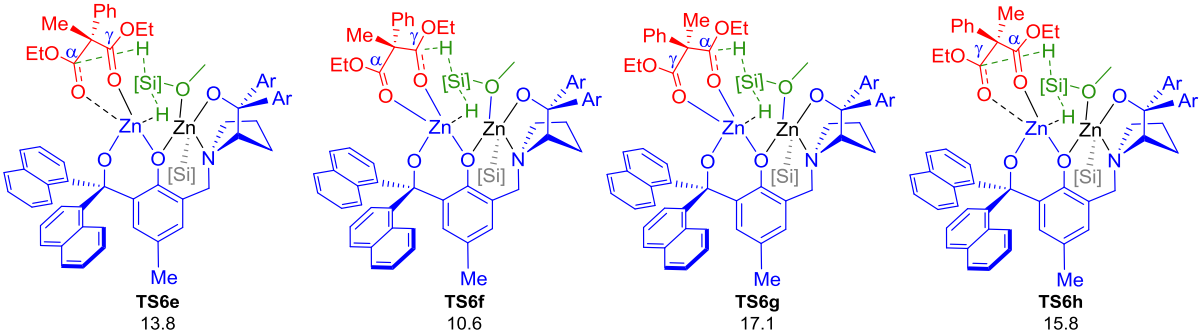

Fig. S7. Possible pathways for H-shuttle mechanism with $HSi(OMe)_3$ as a ligand.

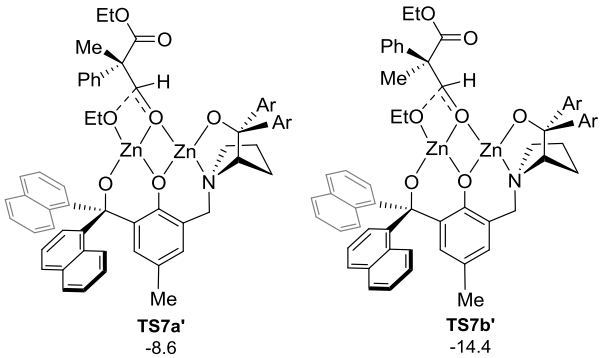

Fig. S8. Possible transition states for decomposition of hemiacetal without $HSi(OMe)_3$ as a ligand.

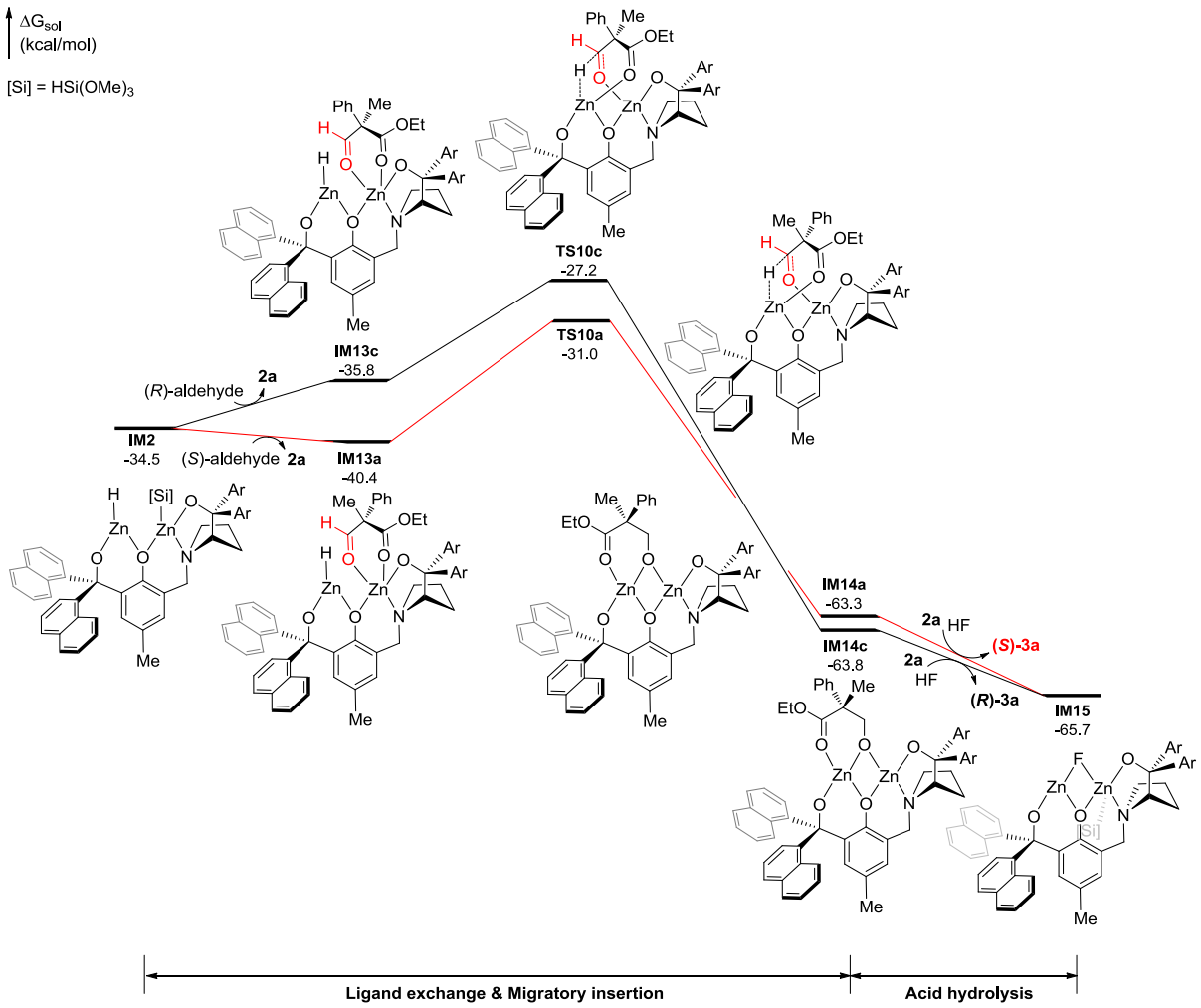

Fig. S9. Free energy profiles for formation of the major product (*S*)-**3a** and minor product (*R*)-**3a**.

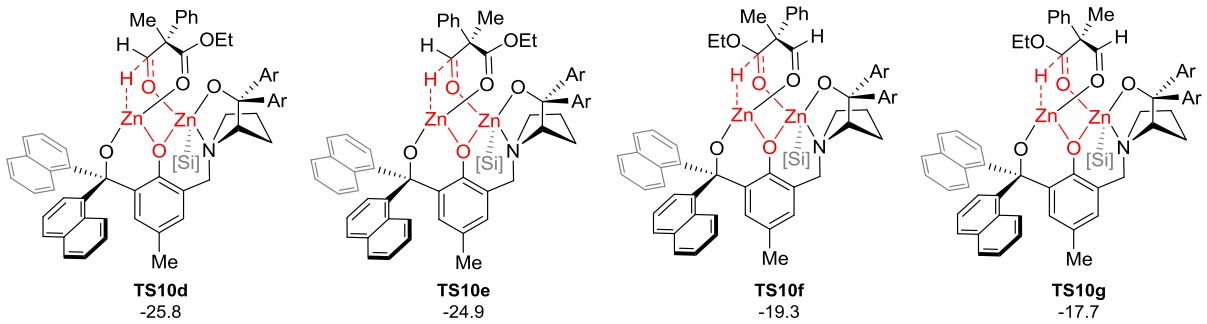

Fig. S10. Possible pathways for the migratory insertion transition states with $HSi(OMe)_3$ as a ligand.

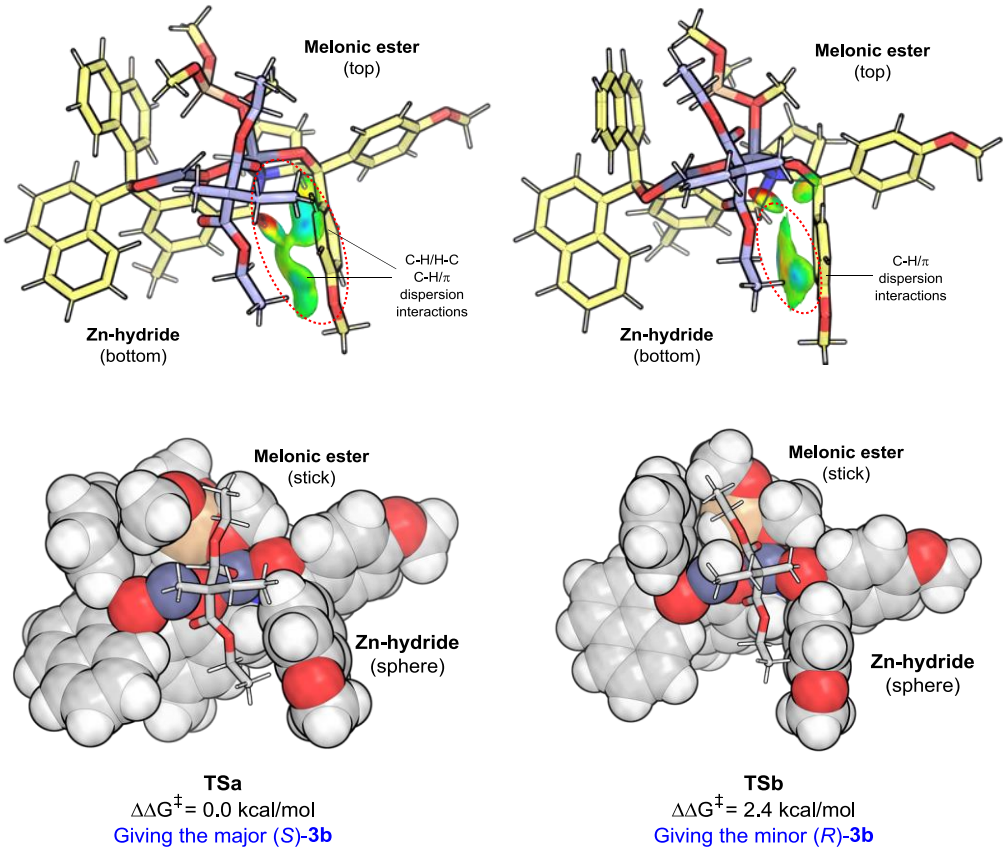

Fig. S11. Origins of stereoselectivity in catalytic reductive desymmetrization of malonic ester **1b** (Et vs Me). Top: Comparison of key NCIs by IGMH analysis. Bottom: TSs shown in sphere (Zn-hydride)-stick (melonic ester) representation.

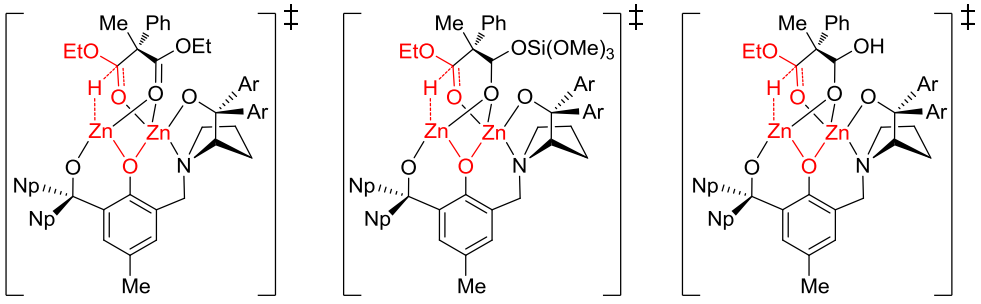

Fig. S12. Key transition states of the migratory insertion step.

Energies and Cartesian Coordinates (Å) for the Optimized Structures

$ZnEt_2$

M06L SCF energy in Solvent: -1937.452342 a.u.

PBE0-D3BJ Free energy in Solvent: -1937.355266 a.u.

Zn	0.000000	0.000000	0.000064
C	0.000000	1.953159	0.000023
H	0.575547	2.294181	0.873303
H	0.575716	2.294141	-0.873160
C	-1.376546	2.612811	-0.000124
H	-1.312351	3.710756	-0.000149
H	-1.969312	2.333003	-0.880540
H	-1.969474	2.333053	0.880198
C	0.000000	-1.953159	0.000023
H	-0.575547	-2.294181	0.873303
H	-0.575716	-2.294141	-0.873160
C	1.376546	-2.612811	-0.000124
H	1.312351	-3.710756	-0.000149
H	1.969312	-2.333003	-0.880540
H	1.969474	-2.333053	0.880198

(*S*)-L

M06L SCF energy in Solvent: -2285.409310 a.u.

PBE0-D3BJ Free energy in Solvent: -2284.668103 a.u.

O	-0.256334	0.242853	-0.131288
O	2.550801	-1.141626	-0.255938
N	1.726165	0.101818	1.981960
C	-1.025530	0.713477	0.883862
C	-2.421343	0.526052	0.927204
C	-3.125680	1.028618	2.024345
H	-4.204049	0.879404	2.069941
C	-2.497469	1.698672	3.072479
C	-1.107510	1.829412	3.016390
H	-0.578428	2.313861	3.840314
C	-0.361505	1.352419	1.945053
C	-3.285703	2.259343	4.217173
H	-4.267358	1.780159	4.305102
H	-3.465737	3.336799	4.097649
H	-2.764260	2.131903	5.173774
C	1.138282	1.432268	1.931157
H	1.481185	1.919457	1.010656
H	1.482698	2.056939	2.783220
C	1.395697	-0.657324	3.179655
H	1.607568	-0.078797	4.106217
H	0.325023	-0.902218	3.192069
C	2.305598	-1.860106	3.067640
H	1.906376	-2.552430	2.315633
H	2.421024	-2.406194	4.010265
C	3.605870	-1.238908	2.566199
H	4.198141	-1.936196	1.966625
H	4.232928	-0.928360	3.411891
C	3.177331	0.000674	1.751745
H	3.693682	0.905351	2.125634
C	3.444620	-0.153802	0.221086
C	4.856740	-0.639596	-0.070875
C	5.958568	-0.213350	0.668951
H	5.817726	0.442666	1.528966
C	7.254953	-0.618517	0.354158
H	8.085289	-0.269076	0.962367
C	7.463980	-1.471986	-0.729978
C	6.368404	-1.910514	-1.480074
H	6.548824	-2.579803	-2.318779
C	5.087190	-1.498045	-1.152176
H	4.237245	-1.845635	-1.734253
C	3.250559	1.171946	-0.528793
C	3.926181	2.331833	-0.147276
H	4.598918	2.312211	0.711045
C	3.770328	3.532995	-0.834651
H	4.311307	4.414685	-0.500428
C	2.928749	3.583103	-1.948408
C	2.258291	2.426171	-2.354139
C	2.422920	1.241405	-1.653263
H	1.896377	0.343407	-1.966153
C	-3.111098	-0.347552	-0.120639
O	-2.549935	0.097959	-1.400294
C	-4.628060	-0.135564	-0.114257
C	-5.202662	1.113544	-0.523969
C	-5.458780	-1.134211	0.355010
C	-4.441125	2.241814	-0.928588
C	-6.631492	1.255043	-0.486193
C	-6.858441	-0.985174	0.397699
H	-5.023317	-2.070986	0.696206
C	-5.050653	3.419944	-1.293355
H	-3.359378	2.174355	-0.947847

C	-7.224193	2.478067	-0.884385
C	-7.434525	0.183197	-0.029701
H	-7.472990	-1.804852	0.765159
C	-6.454108	3.542715	-1.282566
H	-4.437697	4.268726	-1.591362
H	-8.310964	2.557904	-0.855229
H	-8.516705	0.312987	-0.011257
H	-6.921895	4.479623	-1.580338
C	-2.712253	-1.828873	0.052723
C	-3.015618	-2.796045	-0.966220
C	-1.994008	-2.238591	1.158254
C	-3.840470	-2.535139	-2.096074
C	-2.472111	-4.119677	-0.846425
C	-1.497049	-3.550200	1.289147
H	-1.786061	-1.522335	1.949300
C	-4.066895	-3.489293	-3.063243
H	-4.364476	-1.584024	-2.179605
C	-2.719432	-5.073388	-1.862425
C	-1.708616	-4.466833	0.293151
H	-0.927711	-3.817581	2.177491
C	-3.490082	-4.768856	-2.958248
H	-4.710522	-3.252076	-3.908272
H	-2.285799	-6.066930	-1.749807
H	-1.304433	-5.476285	0.363868
H	-3.669671	-5.514203	-3.730287
O	8.684484	-1.931850	-1.130540
H	1.611014	2.480336	-3.227072
O	2.702489	4.700912	-2.697273
C	3.378226	5.874210	-2.310511
H	4.470329	5.747660	-2.351820
H	3.077751	6.645664	-3.022719
H	3.098156	6.190152	-1.294411
C	9.802406	-1.499123	-0.391883
H	9.912025	-0.404832	-0.422461
H	9.744757	-1.818402	0.659521
H	10.673248	-1.961771	-0.861381
H	1.688970	-0.888274	0.141068
H	-0.868757	0.059760	-0.878614
H	-2.766413	-0.568984	-2.071532

1a

M06L SCF energy in Solvent: -844.652166 a.u.

PBE0-D3BJ Free energy in Solvent: -844.400423 a.u.

C	0.321565	1.012636	-0.408247
O	0.716269	0.917912	-1.551220
O	-0.012724	2.172940	0.178808
C	0.110494	3.335820	-0.668629
H	1.139185	3.382034	-1.044623
H	-0.545451	3.200374	-1.536772
C	-0.262762	4.535579	0.156970
H	0.404138	4.644298	1.018678
H	-0.190537	5.445982	-0.447290
H	-1.289441	4.453907	0.528909
C	0.075862	-0.186305	0.514048
C	1.087768	-1.263675	0.087839
O	0.831222	-2.367040	-0.332025
O	2.339696	-0.802149	0.273505
C	3.385358	-1.699736	-0.150084
H	3.316946	-2.620525	0.441921
H	3.200186	-1.971701	-1.195747
C	4.695419	-0.986505	0.039954
H	4.852462	-0.719634	1.090626
H	5.524359	-1.629143	-0.274952
H	4.730131	-0.067664	-0.554365
C	0.326100	0.167776	1.981683
H	0.168009	-0.709716	2.619196
H	1.353413	0.513445	2.121136
H	-0.347048	0.963033	2.311177
C	-1.352626	-0.650083	0.237417
C	-2.338617	-0.640843	1.225318
C	-1.701317	-1.061962	-1.054472
C	-3.641348	-1.039932	0.933256
H	-2.097785	-0.325205	2.237904
C	-3.000370	-1.457520	-1.345870
H	-0.940955	-1.073596	-1.832046
C	-3.977470	-1.447988	-0.352282
H	-4.394864	-1.028241	1.719228
H	-3.250883	-1.776995	-2.356034
H	-4.995915	-1.757525	-0.580882

2a

M06L SCF energy in Solvent: -635.262656 a.u.

PBE0-D3BJ Free energy in Solvent: -635.160431 a.u.

Si	0.000549	-0.247499	0.302268
H	0.000604	0.102397	1.741517
O	1.293499	-1.167558	-0.109281
O	-1.291004	-1.169808	-0.108709

O	-0.000841	1.177966	-0.536706
C	2.592283	-0.616825	-0.076837
H	3.304766	-1.418693	-0.292578
H	2.712103	0.173779	-0.830697
H	2.840681	-0.196264	0.911016
C	-2.590641	-0.621064	-0.077063
H	-2.710976	0.169987	-0.830385
H	-3.301699	-1.423837	-0.294145
H	-2.840608	-0.201715	0.910907
C	-0.003694	2.433131	0.102763
H	-0.005635	3.208635	-0.669801
H	-0.894580	2.575164	0.733551
H	0.886733	2.579284	0.733246

C_2H_6

M06L SCF energy in Solvent: -79.755064 a.u.

PBE0-D3BJ Free energy in Solvent: -79.701025 a.u.

C	0.000000	0.000000	0.758179
H	-0.509536	0.882905	1.161766
H	1.019386	-0.000181	1.161766
H	-0.509850	-0.882724	1.161766
C	0.000000	0.000000	-0.758179
H	0.509850	-0.882724	-1.161766
H	-1.019386	-0.000181	-1.161766
H	0.509536	0.882905	-1.161766

1cat

M06L SCF energy in Solvent: -5921.153863 a.u.

PBE0-D3BJ Free energy in Solvent: -5920.38752 a.u.

Zn	0.875855	0.067543	-0.652333
Zn	-1.645806	1.510195	1.490212
O	-0.579612	-0.176984	0.556696
O	2.640376	0.485536	-1.111646
N	1.486513	-2.016389	-0.668104
C	-1.269124	-1.339663	0.380517
C	-2.637531	-1.313006	0.020792
C	-3.305190	-2.523701	-0.140135
H	-4.351732	-2.511294	-0.441800
C	-2.677225	-3.761342	0.042445
C	-1.313455	-3.759315	0.321669
H	-0.777709	-4.708653	0.398586
C	-0.596907	-2.571237	0.475226
C	-3.448342	-5.039238	-0.088948
H	-4.140940	-5.012212	-0.939075
H	-4.057932	-5.236625	0.803432
H	-2.785028	-5.901612	-0.223400
C	0.900235	-2.586087	0.571614
H	1.256568	-1.980284	1.412873
H	1.270815	-3.617293	0.713780
C	1.071947	-2.753744	-1.880850
H	1.144839	-3.842807	-1.701920
H	0.023783	-2.532529	-2.118644
C	2.070521	-2.305411	-2.921234
H	1.836941	-1.285722	-3.256169
H	2.088644	-2.957135	-3.800921
C	3.374629	-2.297826	-2.138283
H	4.120559	-1.623496	-2.567677
H	3.814373	-3.303393	-2.126592
C	2.983650	-1.883841	-0.707920
H	3.417788	-2.586179	0.018755
C	3.415778	-0.412469	-0.355636
C	4.892020	-0.234065	-0.716453
C	5.876614	-1.013469	-0.110557
H	5.596995	-1.742330	0.651912
C	7.223223	-0.875779	-0.437031
H	7.961166	-1.499953	0.060387
C	7.605051	0.071796	-1.389882
C	6.628755	0.863495	-2.001581
H	6.946137	1.599548	-2.737532
C	5.291337	0.708906	-1.667740
H	4.528552	1.322210	-2.140832
C	3.276345	-0.107411	1.146498
C	3.425928	-1.045343	2.170278
H	3.593400	-2.097263	1.937878
C	3.362680	-0.684546	3.516342
H	3.468682	-1.452359	4.278084
C	3.166236	0.652696	3.864735
C	3.044551	1.612655	2.853918
C	3.099421	1.232249	1.524504
H	3.013835	1.980777	0.739662
C	-3.277311	0.058589	-0.263110
O	-3.268377	0.812700	0.923125
C	-4.741547	-0.046543	-0.724090
C	-5.769509	-0.444274	0.197047
C	-5.100133	0.264712	-2.021154
C	-5.513415	-0.833837	1.539037
C	-7.129179	-0.490861	-0.260388
C	-6.438534	0.224903	-2.462498

H	-4.331266	0.562317	-2.731679
C	-6.531242	-1.238561	2.371407
H	-4.493386	-0.793517	1.905389
C	-8.153018	-0.899811	0.629272
C	-7.435732	-0.141137	-1.597024
H	-6.669550	0.489818	-3.492939
C	-7.865909	-1.269175	1.920119
H	-6.301456	-1.533262	3.394282
H	-9.178733	-0.921784	0.259820
H	-8.475996	-0.175653	-1.921288
H	-8.662600	-1.585773	2.591685
C	-2.391713	0.731227	-1.358744
C	-2.221269	2.152099	-1.423934
C	-1.641775	-0.052118	-2.220456
C	-3.106121	3.070394	-0.790166
C	-1.130498	2.695258	-2.188047
C	-0.562711	0.475642	-2.962158
H	-1.824122	-1.125740	-2.251206
C	-2.914370	4.428461	-0.898056
H	-3.949290	2.676200	-0.232025
C	-0.949626	4.099553	-2.251080
C	-0.269742	1.824030	-2.895622
H	0.031378	-0.184182	-3.594263
C	-1.823113	4.952030	-1.623594
H	-3.620010	5.107755	-0.423194
H	-0.110077	4.486848	-2.827984
H	0.587064	2.235652	-3.428291
H	-1.682062	6.029243	-1.691096
C	-0.281902	2.690105	2.196957
H	0.410259	2.080785	2.794274
H	-0.699535	3.444326	2.875578
C	0.463717	3.368741	1.052220
H	1.347003	3.934875	1.390225
H	0.833893	2.646254	0.303080
H	-0.180287	4.069452	0.505572
O	8.891138	0.298570	-1.781714
H	2.899822	2.653628	3.136569
O	3.082959	1.115842	5.141020
C	3.185630	0.163774	6.176058
H	4.158143	-0.349820	6.160343
H	3.086949	0.720947	7.109598
H	2.385626	-0.588189	6.114642
C	9.891628	-0.478922	-1.165572
H	9.918424	-0.318744	-0.077573
H	9.749888	-1.552391	-1.360672
H	10.838734	-0.154656	-1.601384

IM1

M06L SCF energy in Solvent: -6556.448453 a.u.

PBE0-D3BJ Free energy in Solvent: -6555.550870 a.u.

O	-0.443381	-0.107062	0.214898
C	-0.968916	0.670105	1.195095
C	-2.370837	0.874692	1.263789
C	-2.887563	1.555869	2.365498
H	-3.967997	1.686729	2.430041
C	-2.090512	2.093390	3.377327
C	-0.713013	1.979137	3.224714
H	-0.049663	2.449919	3.954708
C	-0.137250	1.304334	2.146931
C	-2.698732	2.787099	4.558251
H	-3.114945	2.074550	5.284362
H	-3.522255	3.447961	4.261197
H	-1.960100	3.395424	5.093262
C	-3.299595	0.410531	0.115204
O	-2.735203	0.766926	-1.122627
C	-4.661988	1.142699	0.183032
C	-4.738516	2.553458	-0.078794
C	-5.826998	0.462234	0.477174
C	-3.603720	3.366945	-0.338727
C	-6.021733	3.195360	-0.047897
C	-7.085438	1.098280	0.503692
H	-5.788083	-0.602538	0.694833
C	-3.729632	4.718012	-0.566420
H	-2.625026	2.900235	-0.372337
C	-6.114797	4.586726	-0.295843
C	-7.182827	2.438775	0.240081
H	-7.974233	0.512941	0.733991
C	-4.994764	5.338684	-0.552043
H	-2.839135	5.312455	-0.765470
H	-7.102197	5.049315	-0.272768
H	-8.148043	2.945991	0.253892
H	-5.081003	6.408166	-0.739222
C	-3.529130	-1.117894	0.219189
C	-3.934723	-1.898415	-0.918575
C	-3.382321	-1.758685	1.435522
C	-4.268013	-1.338317	-2.185397
C	-4.045359	-3.324948	-0.780804
C	-3.563892	-3.148871	1.581051

H	-3.102125	-1.171542	2.308843
C	-4.602465	-2.138168	-3.254777
H	-4.252600	-0.259289	-2.294184
C	-4.378614	-4.116296	-1.908165
C	-3.852578	-3.926150	0.486155
H	-3.459340	-3.603855	2.565066
C	-4.637897	-3.541338	-3.128038
H	-4.852999	-1.676541	-4.208633
H	-4.442726	-5.197720	-1.777368
H	-3.963778	-5.007491	0.578055
H	-4.895632	-4.160902	-3.985280
H	-1.439413	-2.656794	-0.354695
Si	-0.436983	-3.341393	0.448375
O	1.013369	-2.830772	-0.251806
O	-0.256063	-2.911349	2.018993
O	-0.567870	-4.979008	0.370249
C	2.176586	-3.675236	-0.231037
H	2.054099	-4.470594	-0.973454
H	3.033795	-3.045108	-0.480270
H	2.315549	-4.126414	0.760410
C	-1.001224	-5.602761	-0.827686
H	-0.137053	-5.938086	-1.416210
H	-1.607502	-6.476207	-0.564606
H	-1.612774	-4.931115	-1.449757
C	-0.662301	-3.638784	3.159072
H	-1.204373	-4.554986	2.893112
H	0.226771	-3.912894	3.741829
H	-1.307560	-3.005095	3.780109
Zn	1.364848	-0.773245	0.138722
O	3.131255	-0.766627	-0.526220
N	2.073936	0.133654	1.918223
C	1.349007	1.420659	1.954280
H	1.552259	1.937911	1.010011
H	1.779109	2.047724	2.756738
C	1.949270	-0.605401	3.184690
H	2.220278	0.062143	4.024741
H	0.913246	-0.930522	3.327001
C	2.950831	-1.724802	3.017221
H	2.500540	-2.514597	2.399190
H	3.242161	-2.181134	3.969274
C	4.116670	-1.053953	2.280174
H	4.543935	-1.707413	1.511624
H	4.930220	-0.795408	2.967726
C	3.539856	0.222652	1.632946
H	3.925141	1.130698	2.129578
C	3.819880	0.277503	0.084427
C	5.320157	0.102413	-0.170052
C	6.308821	0.608904	0.672409
H	6.036609	1.138460	1.586321
C	7.666184	0.448376	0.392004
H	8.404401	0.850415	1.080973
C	8.053724	-0.231412	-0.763171
C	7.074023	-0.739335	-1.622634
H	7.393223	-1.267576	-2.518809
C	5.731922	-0.572916	-1.325483
H	4.968341	-0.974976	-1.986947
O	9.347036	-0.454701	-1.133366
C	10.349942	0.044183	-0.279501
H	10.296708	1.138934	-0.184979
H	10.286587	-0.400173	0.725102
H	11.302390	-0.232334	-0.736453
C	3.382733	1.634580	-0.497821
C	2.434187	1.695636	-1.526467
C	3.879699	2.842340	-0.005925
C	1.964905	2.910173	-2.007675
H	2.065769	0.767772	-1.963597
C	3.425338	4.071144	-0.477005
H	4.644183	2.834609	0.772257
C	2.450890	4.109271	-1.479477
H	1.222614	2.954106	-2.802463
H	3.835423	4.988186	-0.061817
O	1.930569	5.251285	-2.006918
C	2.415649	6.471532	-1.494950
H	3.496822	6.581834	-1.664894
H	1.883768	7.258192	-2.033566
H	2.214258	6.568677	-0.417941
Zn	-1.297969	-0.231013	-1.732763
C	-0.116803	-1.190784	-2.957212
H	0.905679	-1.229506	-2.544120
H	-0.459106	-2.239065	-2.958021
C	-0.070097	-0.659604	-4.385333
H	0.311173	0.369330	-4.428894
H	0.578181	-1.264346	-5.036949
H	-1.065577	-0.646084	-4.847885

TS1

M06L SCF energy in Solvent: -7191.686277 a.u.

PBE0-D3BJ Free energy in Solvent: -7190.651661 a.u.

O	0.622524	0.304252	-0.206117
C	1.129827	1.138600	-1.167976
C	2.526943	1.233922	-1.420058
C	2.945283	2.049278	-2.472474
H	4.010662	2.093396	-2.694184
C	2.079618	2.820182	-3.249555
C	0.725994	2.748213	-2.947592
H	0.009142	3.341480	-3.519979
C	0.246193	1.929016	-1.926289
C	2.603312	3.697278	-4.345494
H	3.288976	4.461831	-3.956985
H	1.792420	4.216665	-4.868620
H	3.166755	3.125106	-5.094160
C	3.570152	0.482263	-0.554199
O	3.362769	0.787933	0.799885
C	5.013501	0.971642	-0.847594
C	5.405526	2.311870	-0.498534
C	5.958665	0.135731	-1.408409
C	4.517692	3.281910	0.040463
C	6.758334	2.723731	-0.744791
C	7.290421	0.542015	-1.630678
H	5.683331	-0.876762	-1.692165
C	4.934832	4.563746	0.315857
H	3.492175	2.995473	0.246686
C	7.156363	4.048441	-0.438209
C	7.685223	1.811468	-1.303025
H	7.996954	-0.163295	-2.065136
C	6.266943	4.956890	0.079877
H	4.224889	5.280728	0.725511
H	8.191172	4.332268	-0.632632
H	8.709820	2.143982	-1.471801
H	6.585459	5.973380	0.306252
C	3.479397	-1.033426	-0.860840
C	3.898033	-2.046344	0.068178
C	3.101881	-1.426381	-2.134610
C	4.391903	-1.779031	1.377081
C	3.877932	-3.423497	-0.353310
C	3.115780	-2.769672	-2.551516
H	2.808479	-0.662128	-2.852290
C	4.784765	-2.796760	2.218004
H	4.464677	-0.743995	1.693827
C	4.278715	-4.443864	0.545912
C	3.498472	-3.753676	-1.674673
H	2.821012	-3.021086	-3.569697
C	4.717676	-4.144877	1.811603
H	5.165681	-2.551380	3.209052
H	4.241105	-5.477966	0.199611
H	3.534619	-4.798841	-1.981375
H	5.028055	-4.938618	2.489726
H	1.193550	-2.415003	-0.497078
Si	0.222289	-3.498360	-0.601937
O	-1.227880	-2.665392	-0.772858
O	0.196358	-4.458958	-1.934989
O	0.281701	-4.501835	0.698942
C	-2.455175	-3.397587	-0.899321
H	-2.399219	-4.337048	-0.335250
H	-3.252248	-2.766510	-0.494351
H	-2.642118	-3.626900	-1.954688
C	1.023089	-4.215550	1.872405
H	0.343493	-3.946263	2.690816
H	1.586582	-5.112966	2.153638
H	1.738516	-3.391648	1.722185
C	0.836821	-5.711113	-2.046026
H	1.494628	-5.703532	-2.923953
H	1.432283	-5.960446	-1.156516
H	0.078971	-6.492345	-2.183785
Zn	-1.206352	-0.580083	-0.204846
O	-3.062551	-0.466998	0.221628
N	-1.780129	0.536883	-2.002791
C	-1.224962	1.868465	-1.675367
H	-1.460027	2.080760	-0.621959
H	-1.746130	2.635695	-2.276986
C	-1.394261	0.077380	-3.348487
H	-1.556759	0.895482	-4.075736
H	-0.327514	-0.173976	-3.372342
C	-2.318691	-1.096130	-3.610948
H	-1.857535	-2.019949	-3.240413
H	-2.499776	-1.236450	-4.681657
C	-3.593371	-0.760120	-2.822511
H	-3.890362	-1.583764	-2.165120
H	-4.451072	-0.564268	-3.474392
C	-3.263748	0.485004	-1.985618
H	-3.634191	1.388332	-2.503682
C	-3.816140	0.428783	-0.520123
C	-5.272396	-0.065585	-0.577821
C	-6.215385	0.503284	-1.433654
H	-5.930863	1.332040	-2.083906
C	-7.528060	0.040508	-1.494492

H	-8.228855	0.507718	-2.181832
C	-7.923150	-1.017008	-0.672026
C	-6.994245	-1.590994	0.199567
H	-7.319119	-2.410955	0.837145
C	-5.690227	-1.119342	0.240121
H	-4.965376	-1.566752	0.916726
O	-9.178139	-1.551913	-0.648859
C	-10.130994	-0.976683	-1.511677
H	-10.296326	0.087005	-1.284354
H	-9.834072	-1.069227	-2.567128
H	-11.059514	-1.528056	-1.349087
C	-3.831523	1.816611	0.150940
C	-3.485349	1.917247	1.505007
C	-4.226856	2.986474	-0.499614
C	-3.524336	3.132566	2.171156
H	-3.165148	1.019273	2.030313
C	-4.263585	4.218844	0.151362
H	-4.513082	2.964415	-1.551040
C	-3.910958	4.295794	1.499934
H	-3.250710	3.207732	3.222550
H	-4.567631	5.105009	-0.400166
O	-3.911835	5.441972	2.238448
C	-4.319875	6.621725	1.586061
H	-5.350892	6.543109	1.210349
H	-4.268199	7.414868	2.334880
H	-3.656112	6.874087	0.745651
Zn	1.685124	0.493318	1.514977
C	1.067812	1.640523	3.082540
H	2.097795	2.022279	3.192065
H	0.802357	1.333314	4.101799
C	0.142492	2.726995	2.557578
H	0.007842	3.553477	3.272121
H	0.533994	3.168616	1.629806
H	-0.854085	2.333311	2.323245
Si	0.113161	-0.720774	2.955355
H	1.404968	-1.166822	2.175780
O	-1.268092	0.093521	3.410400
O	-0.711764	-1.670347	1.792198
O	0.553853	-1.420596	4.390272
C	1.796047	-2.044924	4.631272
H	2.361199	-1.464806	5.371761
H	1.619913	-3.050002	5.034234
H	2.407440	-2.137254	3.719676
C	-1.909325	-2.328929	2.244144
H	-1.995863	-3.259919	1.674562
H	-1.824080	-2.575624	3.309597
H	-2.780965	-1.691686	2.076894
C	-1.504473	0.746125	4.633549
H	-1.310318	1.825631	4.549849
H	-2.563422	0.609703	4.886697
H	-0.892751	0.333393	5.446966

$EtSi(OMe)_3$

M06L SCF energy in Solvent: -713.844842 a.u.

PBE0-D3BJ Free energy in Solvent: -713.689032 a.u.

Si	0.016200	-0.014079	0.023959
O	0.721933	-1.256195	-0.795915
O	-0.661178	0.993994	-1.093100
O	1.129573	0.915203	0.832612
C	1.655986	-1.020543	-1.830173
H	2.008774	-1.990064	-2.196863
H	1.198493	-0.472110	-2.664020
H	2.523240	-0.446815	-1.470844
C	-1.223949	2.233525	-0.725388
H	-0.480413	2.892720	-0.256987
H	-1.603032	2.718462	-1.631059
H	-2.067206	2.108151	-0.027237
C	1.933063	0.364176	1.851005
H	2.653695	1.124393	2.170437
H	1.337104	0.068145	2.728415
H	2.492839	-0.517212	1.502237
C	-1.227559	-0.782622	1.176498
H	-1.611104	-0.004695	1.853185
H	-0.707780	-1.502529	1.825121
C	-2.379793	-1.470508	0.449082
H	-3.097000	-1.918790	1.147167
H	-2.931242	-0.763154	-0.182364
H	-2.012295	-2.267585	-0.207530

IM2

M06L SCF energy in Solvent: -6477.886404 a.u.

PBE0-D3BJ Free energy in Solvent: -6477.043649 a.u.

O	-0.528600	0.217614	-0.129542
C	-1.012928	1.060423	0.817987
C	-2.411285	1.256504	0.958295
C	-2.861032	2.087285	1.984394
H	-3.935698	2.217113	2.108476
C	-2.007799	2.744165	2.872498

C	-0.642650	2.544167	2.705128
H	0.061682	3.042769	3.375340
C	-0.130988	1.731285	1.693095
C	-2.549009	3.637282	3.947081
H	-2.940938	4.576751	3.534369
H	-1.777367	3.901423	4.679347
H	-3.377345	3.166383	4.490992
C	-3.426743	0.497650	0.071888
O	-3.075874	0.575350	-1.292014
C	-4.828680	1.138372	0.177041
C	-5.061104	2.445135	-0.370464
C	-5.877091	0.481149	0.789230
C	-4.043147	3.240962	-0.959691
C	-6.379127	3.007008	-0.289926
C	-7.171162	1.037291	0.863867
H	-5.712283	-0.499036	1.231217
C	-4.312376	4.496911	-1.451913
H	-3.039558	2.835965	-1.030568
C	-6.622939	4.298394	-0.817908
C	-7.420277	2.273178	0.327369
H	-7.966638	0.474712	1.349878
C	-5.613982	5.033430	-1.389998
H	-3.508856	5.081413	-1.897637
H	-7.634627	4.700030	-0.751392
H	-8.415617	2.715809	0.375140
H	-5.814500	6.026502	-1.789406
C	-3.478538	-0.981254	0.543679
C	-4.042252	-2.009475	-0.290289
C	-2.989939	-1.341711	1.787315
C	-4.681825	-1.752844	-1.536554
C	-4.007321	-3.373393	0.163590
C	-2.976240	-2.676987	2.236333
H	-2.588551	-0.571475	2.442493
C	-5.208850	-2.775542	-2.292964
H	-4.748380	-0.727803	-1.884463
C	-4.544332	-4.401185	-0.651280
C	-3.461122	-3.678728	1.433436
H	-2.568375	-2.906100	3.220611
C	-5.131322	-4.114509	-1.859042
H	-5.698373	-2.542912	-3.237353
H	-4.490188	-5.428249	-0.287596
H	-3.462754	-4.716912	1.766233
H	-5.545317	-4.912744	-2.473320
H	-1.345576	-2.356535	0.000766
Si	-0.403123	-3.460813	-0.127916
O	1.025100	-2.639800	-0.497332
O	-0.006763	-4.315411	1.212303
O	-0.840727	-4.541105	-1.281577
C	2.211061	-3.399340	-0.813554
H	2.038495	-3.967485	-1.733963
H	3.020775	-2.678542	-0.952291
H	2.438436	-4.085615	0.009959
C	-1.499566	-4.126075	-2.470471
H	-0.779132	-3.713585	-3.188799
H	-1.989627	-5.002564	-2.905002
H	-2.267341	-3.363423	-2.268510
C	-0.646314	-5.496982	1.652177
H	-1.198932	-5.293497	2.578299
H	-1.341935	-5.897211	0.902620
H	0.120027	-6.252846	1.857209
Zn	1.240193	-0.554433	-0.217628
O	3.011232	-0.447561	-0.849202
N	1.896469	0.274985	1.610650
C	1.358810	1.650267	1.533629
H	1.661042	2.059446	0.561113
H	1.853776	2.273657	2.300218
C	1.550563	-0.424641	2.856876
H	1.824818	0.206143	3.723341
H	0.467423	-0.596680	2.901246
C	2.389573	-1.687855	2.784934
H	1.846415	-2.465749	2.231568
H	2.601979	-2.096283	3.778209
C	3.654968	-1.255352	2.026179
H	3.879915	-1.936042	1.195746
H	4.542560	-1.244319	2.666903
C	3.371968	0.152773	1.470831
H	3.839486	0.925822	2.106607
C	3.830949	0.320039	-0.024149
C	5.273889	-0.188549	-0.155946
C	6.260125	0.065336	0.796761
H	6.019161	0.624226	1.702098
C	7.568324	-0.391616	0.640825
H	8.304054	-0.181488	1.413043
C	7.912307	-1.116633	-0.501417
C	6.938095	-1.370596	-1.471095
H	7.223103	-1.933597	-2.357394
C	5.642375	-0.911998	-1.295739
H	4.883675	-1.107807	-2.049665

O	9.156071	-1.614386	-0.756659
C	10.153281	-1.357329	0.204372
H	10.323487	-0.278324	0.334914
H	9.899013	-1.794723	1.181408
H	11.066031	-1.823369	-0.172739
C	3.812131	1.796466	-0.461000
C	3.181982	2.157358	-1.657767
C	4.418908	2.810096	0.281306
C	3.136552	3.477047	-2.080834
H	2.720147	1.374533	-2.255636
C	4.381040	4.142590	-0.124665
H	4.943138	2.571706	1.207658
C	3.732204	4.482661	-1.314287
H	2.642118	3.755537	-3.009251
H	4.861635	4.901106	0.488043
O	3.632773	5.749171	-1.807060
C	4.243917	6.776395	-1.061179
H	5.327546	6.616181	-0.960753
H	4.065745	7.699813	-1.615973
H	3.804948	6.867523	-0.056524
Zn	-1.574868	-0.330611	-1.849117
H	-0.608230	-1.087002	-2.777474

TS2

M06L SCF energy in Solvent: -7191.695969 a.u.

PBE0-D3BJ Free energy in Solvent: -7190.666131 a.u.

O	0.424213	0.174895	-0.368532
C	0.937673	1.143459	-1.193948
C	2.334946	1.372778	-1.331392
C	2.756989	2.278505	-2.309450
H	3.830128	2.426210	-2.430814
C	1.894906	3.013099	-3.119256
C	0.535062	2.848397	-2.889728
H	-0.185628	3.442566	-3.456471
C	0.047434	1.951632	-1.939885
C	2.415660	3.950069	-4.166011
H	2.766518	3.413770	-5.058842
H	3.266300	4.536404	-3.798203
H	1.643361	4.654018	-4.496893
C	3.424963	0.708751	-0.442448
O	3.011573	0.615946	0.888016
C	4.692105	1.598816	-0.396039
C	4.636008	2.881468	0.248584
C	5.893383	1.175862	-0.927433
C	3.447835	3.439362	0.791221
C	5.833759	3.666841	0.333374
C	7.068690	1.951226	-0.837841
H	5.947714	0.213623	-1.432447
C	3.444749	4.679310	1.386501
H	2.528685	2.865302	0.742835
C	5.796402	4.936734	0.960214
C	7.041228	3.170934	-0.214925
H	7.994484	1.568866	-1.264938
C	4.628348	5.438321	1.479755
H	2.515141	5.076204	1.791544
H	6.721495	5.511564	1.015268
H	7.941220	3.781323	-0.136130
H	4.613802	6.416863	1.957642
C	3.775499	-0.688621	-1.009346
C	4.403083	-1.687073	-0.184822
C	3.497534	-1.003148	-2.325909
C	4.875165	-1.442541	1.136177
C	4.606017	-3.003828	-0.725077
C	3.747651	-2.281560	-2.865142
H	3.046652	-0.245248	-2.964034
C	5.456696	-2.443311	1.882190
H	4.754953	-0.447382	1.551861
C	5.184640	-4.014979	0.082799
C	4.257150	-3.276620	-2.069966
H	3.525419	-2.476601	-3.913350
C	5.599478	-3.746741	1.364507
H	5.811839	-2.221613	2.887283
H	5.315219	-5.008311	-0.349268
H	4.436311	-4.277353	-2.465853
H	6.051690	-4.529342	1.971802
H	1.834852	-2.418727	-0.580309
Si	0.667042	-2.791071	-1.372800
O	-0.704513	-2.510314	-0.434347
O	0.356145	-1.878342	-2.693798
O	0.724769	-4.374954	-1.810878
C	-1.518195	-3.541651	0.154069
H	-1.136684	-3.786860	1.153745
H	-2.532634	-3.140095	0.235665
H	-1.516749	-4.426163	-0.491685
C	1.524032	-5.340485	-1.153389
H	0.920641	-5.904546	-0.429001
H	1.913556	-6.036734	-1.903952
H	2.375551	-4.884226	-0.626122

C	0.678032	-2.189411	-4.032030
H	1.143458	-3.178828	-4.124304
H	-0.242673	-2.177233	-4.629739
H	1.364979	-1.429600	-4.427559
Zn	-1.435857	-0.559492	-0.364038
O	-3.274629	-0.733940	0.051518
N	-2.072497	0.653011	-2.038215
C	-1.433396	1.940262	-1.699268
H	-1.646062	2.156976	-0.645608
H	-1.911051	2.745927	-2.286762
C	-1.808662	0.252608	-3.430123
H	-2.088754	1.083632	-4.106558
H	-0.743846	0.047611	-3.564480
C	-2.723456	-0.937037	-3.608171
H	-2.262604	-1.816461	-3.135139
H	-2.905425	-1.181069	-4.660560
C	-3.989441	-0.518559	-2.853189
H	-4.417915	-1.348279	-2.281686
H	-4.769434	-0.165434	-3.537697
C	-3.558428	0.619852	-1.905849
H	-3.945109	1.593351	-2.258528
C	-3.989509	0.359555	-0.424693
C	-5.488679	0.044561	-0.378137
C	-6.422867	0.655468	-1.214489
H	-6.096094	1.359488	-1.980813
C	-7.787256	0.381054	-1.121105
H	-8.478318	0.874628	-1.799742
C	-8.241879	-0.528091	-0.165407
C	-7.318629	-1.154954	0.677419
H	-7.688216	-1.867655	1.411752
C	-5.967745	-0.870430	0.566123
H	-5.250698	-1.373806	1.210778
O	-9.548742	-0.873178	0.015760
C	-10.492052	-0.257035	-0.829558
H	-10.496700	0.836120	-0.705659
H	-10.302734	-0.490947	-1.887833
H	-11.465933	-0.656866	-0.539641
C	-3.735546	1.616239	0.433002
C	-2.878325	1.570932	1.539949
C	-4.308426	2.847947	0.111845
C	-2.583476	2.714180	2.271472
H	-2.419598	0.625150	1.828386
C	-4.024620	4.004905	0.832721
H	-5.000365	2.920849	-0.727748
C	-3.149516	3.942209	1.920763
H	-1.912625	2.676767	3.127774
H	-4.489277	4.943862	0.542000
O	-2.796891	5.007374	2.692868
C	-3.361444	6.254927	2.359434
H	-4.459013	6.235459	2.427824
H	-2.967113	6.968658	3.085506
H	-3.075476	6.572927	1.345844
Zn	1.458659	-0.315783	1.297550
Si	0.029682	-1.726201	3.223758
O	1.387963	-2.117184	2.206425
O	-1.360642	-1.320346	2.321581
O	-0.322190	-3.401851	3.453488
C	1.882741	-3.426695	1.937287
H	1.136177	-4.022034	1.395503
H	2.112369	-3.936469	2.876722
H	2.791668	-3.318914	1.336555
C	-0.848836	-3.907090	4.640509
H	-0.699441	-3.219451	5.492370
H	-0.361337	-4.860731	4.891822
H	-1.932968	-4.096081	4.555646
C	-2.597331	-1.850818	2.785725
H	-3.391244	-1.349912	2.226841
H	-2.729694	-1.659169	3.862155
H	-2.662351	-2.934783	2.621095
C	0.570631	0.398144	3.128450
H	-0.384621	0.524974	3.653454
H	0.459876	1.195422	2.358145
C	1.742002	0.757865	4.037503
H	1.616723	1.736386	4.520208
H	2.690465	0.793979	3.485460
H	1.858153	0.014490	4.838732
H	0.115150	-1.435859	4.682625

H(Et)Si(OMe)$_2$

M06L SCF energy in Solvent: -599.33375.

PBE0-D3BJ Free energy in Solvent: -599.208445.

Si	0.188074	-0.080446	0.610546
C	-0.809505	-1.249253	-0.470261
H	-0.733619	-0.930768	-1.521047
H	-0.322060	-2.234248	-0.429381
O	1.810165	-0.382371	0.530776
C	2.509984	-0.299256	-0.690779

H	2.143467	-1.037623	-1.421487
H	2.429786	0.701805	-1.137168
H	3.566067	-0.509339	-0.493219
O	-0.032888	1.494212	0.123126
C	-1.257313	1.993488	-0.351458
H	-1.636049	1.417322	-1.210915
H	-2.034904	1.994911	0.428566
H	-1.103908	3.027870	-0.677554
C	-2.276503	-1.388303	-0.067408
H	-2.806688	-2.116374	-0.693225
H	-2.376875	-1.721709	0.972991
H	-2.820346	-0.438784	-0.151651
H	-0.156097	-0.261596	2.034670

IM3

M06L SCF energy in Solvent: -6592.370096 a.u.

PBE0-D3BJ Free energy in Solvent: -6591.496593 a.u.

O	-0.517934	-0.241760	0.288195
C	-1.008062	0.625705	1.195616
C	-2.394566	0.930370	1.218725
C	-2.874477	1.704913	2.275332
H	-3.942412	1.917688	2.322450
C	-2.047690	2.235798	3.267677
C	-0.677482	2.022074	3.142868
H	0.005824	2.487600	3.857423
C	-0.137419	1.252054	2.113228
C	-2.618361	3.032291	4.401994
H	-3.133838	2.394795	5.133986
H	-3.355075	3.766866	4.053455
H	-1.836824	3.577067	4.944235
C	-3.342803	0.457281	0.084028
O	-2.787242	0.767631	-1.196853
C	-4.680180	1.228457	0.127320
C	-4.727152	2.629256	-0.188013
C	-5.855138	0.586579	0.465652
C	-3.578402	3.410617	-0.482384
C	-5.996892	3.298428	-0.171007
C	-7.098466	1.250317	0.481329
H	-5.834554	-0.467909	0.729156
C	-3.678982	4.754696	-0.759174
H	-2.607038	2.927789	-0.493083
C	-6.064368	4.680632	-0.472489
C	-7.170301	2.579844	0.159748
H	-7.996089	0.694639	0.747331
C	-4.931648	5.399988	-0.763507
H	-2.777696	5.324563	-0.979863
H	-7.042212	5.163272	-0.460396
H	-8.124035	3.108349	0.161849
H	-4.997498	6.463052	-0.990419
C	-3.607092	-1.060014	0.203671
C	-4.089429	-1.831873	-0.913093
C	-3.426057	-1.698421	1.414350
C	-4.466017	-1.270178	-2.166332
C	-4.250499	-3.251527	-0.756546
C	-3.643556	-3.081782	1.576314
H	-3.077485	-1.122953	2.269543
C	-4.898200	-2.063219	-3.205843
H	-4.412179	-0.194707	-2.291834
C	-4.676025	-4.037293	-1.855656
C	-4.017459	-3.851592	0.504970
H	-3.484434	-3.535728	2.553327
C	-4.985094	-3.461958	-3.063907
H	-5.186259	-1.598000	-4.147326
H	-4.774233	-5.114312	-1.710698
H	-4.166301	-4.927097	0.610073
H	-5.317368	-4.077103	-3.898489
H	-1.462307	-2.747297	-0.441027
Si	-0.513331	-3.372765	0.483329
O	1.060380	-2.956016	0.034601
O	-0.630898	-2.864585	2.032243
O	-0.651570	-5.012600	0.406835
C	1.711438	-3.641824	-1.043245
H	1.108913	-3.593677	-1.960267
H	2.666721	-3.135441	-1.211141
H	1.879126	-4.687232	-0.762248
C	-1.290787	-5.678774	-0.663826
H	-0.543263	-6.173173	-1.298232
H	-1.963312	-6.442823	-0.256669
H	-1.886570	-4.993645	-1.286876
C	-0.501023	-3.710401	3.156746
H	-1.008194	-4.671898	3.002665
H	0.556887	-3.904488	3.384039
H	-0.954985	-3.198947	4.012704
Zn	1.348482	-0.821198	-0.194770
O	3.172139	-0.757434	-0.728334
N	2.018722	-0.025413	1.745553
C	1.353670	1.282108	1.900010
H	1.566883	1.868680	0.998699

H	1.827860	1.824644	2.740946
C	1.827914	-0.856047	2.945338
H	2.068072	-0.255180	3.844679
H	0.781172	-1.170546	3.014182
C	2.820649	-1.981370	2.755608
H	2.391972	-2.734794	2.083817
H	3.074840	-2.478177	3.698690
C	4.020167	-1.294894	2.091361
H	4.440275	-1.906780	1.285749
H	4.828190	-1.109972	2.808608
C	3.495478	0.039770	1.525622
H	3.885880	0.893865	2.108568
C	3.844709	0.211342	0.003353
C	5.354340	0.034756	-0.200164
C	6.312972	0.418480	0.736259
H	6.005898	0.835565	1.696313
C	7.679206	0.264970	0.495481
H	8.393719	0.565968	1.257716
C	8.106436	-0.278966	-0.715983
C	7.157654	-0.663116	-1.669523
H	7.509030	-1.087043	-2.608193
C	5.806895	-0.506873	-1.409279
H	5.064174	-0.817276	-2.140921
O	9.412306	-0.481553	-1.056344
C	10.381155	-0.116756	-0.101916
H	10.343574	0.958873	0.126681
H	10.260757	-0.679930	0.835706
H	11.349918	-0.356973	-0.545118
C	3.467001	1.628314	-0.471155
C	2.550901	1.807172	-1.513386
C	3.990631	2.774703	0.128585
C	2.140290	3.072015	-1.912208
H	2.161278	0.927508	-2.022036
C	3.594961	4.052814	-0.256698
H	4.731670	2.676855	0.923310
C	2.654679	4.206863	-1.280253
H	1.424946	3.205492	-2.722039
H	4.025331	4.918766	0.240370
O	2.194335	5.406270	-1.733301
C	2.713570	6.564014	-1.119991
H	3.802481	6.641852	-1.255068
H	2.227815	7.409403	-1.611388
H	2.487423	6.590631	-0.043895
Zn	-1.299604	-0.217640	-1.568607
O	0.294818	-1.007316	-2.095484
C	0.908633	-0.980987	-3.361474
H	1.979386	-1.202244	-3.242953
H	0.826062	0.002140	-3.852228
H	0.468335	-1.732483	-4.035278

IM4

M06L SCF energy in Solvent: -6592.370179 a.u.

PBE0-D3BJ Free energy in Solvent: -6591.496804 a.u.

O	0.625534	0.449861	0.051628
C	1.201884	1.420311	-0.688292
C	2.604134	1.461670	-0.903570
C	3.115008	2.516875	-1.659899
H	4.188772	2.552837	-1.843172
C	2.314638	3.511496	-2.228438
C	0.935723	3.392075	-2.074032
H	0.273130	4.111895	-2.560732
C	0.369225	2.364926	-1.321583
C	2.922562	4.648431	-2.992106
H	3.253015	5.455639	-2.323624
H	2.209834	5.090463	-3.698366
H	3.805380	4.331884	-3.560455
C	3.505756	0.275288	-0.484185
O	3.312631	-0.062407	0.879151
C	4.998786	0.617169	-0.643965
C	5.615897	1.571325	0.232295
C	5.770657	0.015370	-1.617722
C	4.904537	2.302951	1.219967
C	7.018417	1.839558	0.086577
C	7.148695	0.279503	-1.754097
H	5.312123	-0.691287	-2.305879
C	5.539075	3.227253	2.017289
H	3.843528	2.114384	1.345396
C	7.640911	2.786866	0.935074
C	7.763925	1.167775	-0.912099
H	7.715110	-0.229709	-2.532072
C	6.920651	3.470725	1.883455
H	4.965638	3.775900	2.763137
H	8.708969	2.967744	0.810024
H	8.829329	1.381432	-1.002252
H	7.410467	4.201001	2.525846
C	3.132989	-0.945965	-1.377748
C	3.510638	-2.286424	-1.004561
C	2.434304	-0.771860	-2.559242

C	4.319872	-2.595356	0.127353
C	3.097801	-3.383752	-1.838185
C	2.034160	-1.850854	-3.372699
H	2.192268	0.238922	-2.880935
C	4.644993	-3.896622	0.438956
H	4.682800	-1.781396	0.745278
C	3.448297	-4.708619	-1.480195
C	2.350760	-3.136356	-3.014254
H	1.474772	-1.651309	-4.286369
C	4.197512	-4.968096	-0.359218
H	5.269186	-4.096719	1.308380
H	3.113672	-5.521590	-2.125026
H	2.045530	-3.983665	-3.628414
H	4.459700	-5.991588	-0.097294
Zn	-1.106157	-0.472882	-0.212483
O	-2.953240	-0.784824	-0.074307
N	-1.572770	0.913973	-1.824428
C	-1.122947	2.211186	-1.256441
H	-1.484121	2.260554	-0.220440
H	-1.614507	3.036275	-1.803355
C	-1.032712	0.651796	-3.167824
H	-1.245933	1.511124	-3.831880
H	0.054106	0.528559	-3.119307
C	-1.787799	-0.586205	-3.596260
H	-1.326620	-1.472934	-3.134836
H	-1.766476	-0.740432	-4.680360
C	-3.194275	-0.358690	-3.035237
H	-3.611967	-1.274769	-2.604998
H	-3.892173	-0.021632	-3.809775
C	-3.047118	0.724588	-1.946177
H	-3.482011	1.678133	-2.292437
C	-3.691796	0.277480	-0.591980
C	-5.128346	-0.190719	-0.862482
C	-6.015441	0.538860	-1.653199
H	-5.692153	1.467736	-2.125639
C	-7.324766	0.113888	-1.871518
H	-7.981938	0.708847	-2.500494
C	-7.770509	-1.069034	-1.278684
C	-6.893935	-1.809439	-0.480318
H	-7.257485	-2.730377	-0.028677
C	-5.593290	-1.373733	-0.279771
H	-4.905219	-1.951016	0.332701
O	-9.027841	-1.579782	-1.419461
C	-9.930272	-0.841972	-2.209582
H	-10.097619	0.166018	-1.801529
H	-9.579870	-0.747649	-3.248379
H	-10.870034	-1.398117	-2.195929
C	-3.769533	1.437190	0.419504
C	-3.478932	1.193684	1.768095
C	-4.167267	2.729903	0.072599
C	-3.550369	2.201217	2.718447
H	-3.197939	0.184410	2.062010
C	-4.237657	3.757506	1.010750
H	-4.421798	2.968208	-0.960167
C	-3.923337	3.495220	2.346080
H	-3.326618	2.008008	3.765762
H	-4.539578	4.752021	0.692149
O	-3.956957	4.421508	3.345250
C	-4.330402	5.732197	2.987241
H	-5.349372	5.766288	2.574221
H	-4.295001	6.319416	3.907047
H	-3.636145	6.165606	2.252166
O	-0.028735	-2.051521	0.662208
Si	-0.620792	-1.941234	2.599230
H	-1.133496	-0.639312	2.098881
O	-1.242358	-3.448294	2.335696
C	-2.003686	-4.165278	3.287417
H	-2.321107	-5.099054	2.810440
H	-1.415341	-4.402250	4.182387
H	-2.890915	-3.604184	3.602454
O	-1.104338	-1.762875	4.212036
C	-1.164161	-0.498218	4.813023
H	-0.381732	-0.390709	5.580298
H	-1.037100	0.324160	4.086560
H	-2.139398	-0.366236	5.301504
C	0.085066	-3.297930	-0.029263
H	0.469753	-3.112504	-1.040482
H	-0.896509	-3.778485	-0.080857
Zn	1.700908	-0.964711	1.040584
O	1.107628	-1.818417	2.795705
C	1.764119	-1.639039	4.050129
H	1.772216	-0.579524	4.333108
H	1.253703	-2.217571	4.824830
H	2.794989	-1.987858	3.937890
H	0.776855	-3.965082	0.500601

TS3

M06L SCF energy in Solvent: -6592.362851 a.u.

PBE0-D3BJ Free energy in Solvent: -6591.486074 a.u.

O	0.574832	0.473174	0.028139
C	1.153464	1.501255	-0.640197
C	2.556666	1.566994	-0.824145
C	3.070554	2.657203	-1.526594
H	4.146432	2.709615	-1.690176
C	2.271091	3.670607	-2.060841
C	0.892643	3.544268	-1.915192
H	0.231287	4.290017	-2.362550
C	0.321468	2.480946	-1.217318
C	2.881310	4.839395	-2.772866
H	3.245534	5.598466	-2.066894
H	2.159303	5.334840	-3.432497
H	3.742589	4.540748	-3.382541
C	3.466328	0.387860	-0.406597
O	3.250319	0.024267	0.946055
C	4.954429	0.770482	-0.521966
C	5.527759	1.710392	0.398648
C	5.758470	0.230672	-1.505649
C	4.777561	2.390306	1.394550
C	6.924955	2.020832	0.291318
C	7.129964	0.540757	-1.608065
H	5.330624	-0.462837	-2.226640
C	5.371678	3.298732	2.239603
H	3.719314	2.172119	1.488318
C	7.505786	2.949964	1.188846
C	7.705874	1.410331	-0.719066
H	7.724026	0.079406	-2.395250
C	6.749518	3.578740	2.146903
H	4.768477	3.805637	2.991408
H	8.571233	3.161951	1.093614
H	8.766258	1.656217	-0.780994
H	7.207562	4.294717	2.827515
C	3.141371	-0.823909	-1.325796
C	3.577423	-2.150922	-0.976135
C	2.434333	-0.659036	-2.503237
C	4.432544	-2.432610	0.126934
C	3.197136	-3.253565	-1.816660
C	2.079787	-1.741687	-3.333406
H	2.149056	0.345326	-2.810307
C	4.841230	-3.717579	0.402884
H	4.763037	-1.609983	0.752056
C	3.611870	-4.566199	-1.480555
C	2.438969	-3.019497	-2.988206
H	1.517621	-1.551974	-4.247720
C	4.414670	-4.800892	-0.391187
H	5.505259	-3.897054	1.247551
H	3.295271	-5.387460	-2.124126
H	2.162218	-3.870204	-3.611450
H	4.734616	-5.813723	-0.151995
Zn	-1.166456	-0.392788	-0.283001
O	-3.004567	-0.784336	-0.185932
N	-1.663022	1.100812	-1.763329
C	-1.173372	2.356748	-1.142479
H	-1.517511	2.365562	-0.100243
H	-1.648852	3.218889	-1.644222
C	-1.142717	0.882161	-3.123325
H	-1.321194	1.779068	-3.746098
H	-0.061147	0.709109	-3.089358
C	-1.956441	-0.297873	-3.601051
H	-1.564475	-1.222154	-3.149220
H	-1.923385	-0.427043	-4.687965
C	-3.354398	0.004105	-3.061036
H	-3.881836	-0.905082	-2.757557
H	-3.971621	0.495925	-3.822210
C	-3.147687	0.945200	-1.855963
H	-3.578781	1.940846	-2.056891
C	-3.739590	0.346692	-0.531142
C	-5.202694	-0.049422	-0.751120
C	-6.084170	0.691977	-1.536727
H	-5.734533	1.575322	-2.073251
C	-7.424202	0.330979	-1.677607
H	-8.075706	0.931947	-2.306707
C	-7.904515	-0.798405	-1.013496
C	-7.032604	-1.552148	-0.221334
H	-7.423063	-2.432162	0.286029
C	-5.704663	-1.179509	-0.095848
H	-5.022023	-1.768168	0.512194
O	-9.191173	-1.246611	-1.077851
C	-10.088981	-0.497724	-1.862790
H	-10.190413	0.533476	-1.492889
H	-9.778464	-0.464918	-2.917810
H	-11.053497	-1.004141	-1.786635
C	-3.706064	1.395177	0.597151
C	-3.137240	1.073861	1.834525
C	-4.237760	2.676997	0.444602
C	-3.060828	2.005245	2.860208
H	-2.763728	0.062664	1.987513

C	-4.169690	3.626874	1.460395
H	-4.725835	2.956007	-0.490207
C	-3.569103	3.293954	2.678279
H	-2.617708	1.752943	3.822055
H	-4.589584	4.615960	1.296216
O	-3.445378	4.142269	3.736558
C	-3.969279	5.441311	3.579457
H	-5.051335	5.421544	3.383060
H	-3.782848	5.958484	4.522830
H	-3.470840	5.984359	2.762887
O	-0.239014	-2.199553	0.229354
Si	-0.504580	-2.396569	2.027283
H	-0.527010	-0.850812	1.905931
O	-0.686477	-4.043601	1.775900
C	-1.179072	-4.947001	2.734984
H	-1.020357	-5.961667	2.349060
H	-0.665243	-4.854395	3.703277
H	-2.250584	-4.798389	2.916170
O	-1.516721	-2.351513	3.369120
C	-1.682615	-1.223537	4.185735
H	-1.213034	-1.397411	5.163551
H	-1.230720	-0.317082	3.748016
H	-2.753300	-1.034544	4.340327
C	-0.258586	-3.258085	-0.733022
H	-0.000389	-2.825619	-1.706254
H	-1.254550	-3.710302	-0.771411
Zn	1.605139	-0.816153	1.147645
O	1.191939	-2.259567	2.483329
C	2.032441	-3.406982	2.638459
H	3.043321	-3.055267	2.862062
H	1.662796	-4.013105	3.472305
H	2.047658	-4.016759	1.726892
H	0.474655	-4.027240	-0.471272

IM5

M06L SCF energy in Solvent: -6592.370096 a.u.

PBE0-D3BJ Free energy in Solvent: -6591.496593 a.u.

O	-0.437156	0.055470	0.479741
C	-0.957129	1.086931	1.179522
C	-2.356547	1.308631	1.183290
C	-2.855511	2.290169	2.042179
H	-3.932409	2.447536	2.081346
C	-2.047356	3.084835	2.856868
C	-0.673339	2.893421	2.772330
H	-0.003802	3.523072	3.363351
C	-0.112146	1.925214	1.940009
C	-2.645362	4.118039	3.763347
H	-3.188913	4.888431	3.200750
H	-1.876149	4.626575	4.355888
H	-3.365654	3.679171	4.466183
C	-3.326179	0.478667	0.296840
O	-2.843218	0.310249	-1.030760
C	-4.654117	1.256742	0.177028
C	-4.717693	2.451428	-0.613536
C	-5.781819	0.854826	0.864346
C	-3.591175	3.026330	-1.260982
C	-5.970938	3.143161	-0.723042
C	-7.007882	1.542309	0.761262
H	-5.733069	-0.026622	1.500609
C	-3.702278	4.186239	-1.991311
H	-2.631913	2.526666	-1.175789
C	-6.052242	4.324171	-1.500895
C	-7.106069	2.655419	-0.032841
H	-7.873491	1.176601	1.311364
C	-4.944217	4.839058	-2.126982
H	-2.818164	4.604272	-2.470775
H	-7.018398	4.823697	-1.579892
H	-8.050095	3.192050	-0.132123
H	-5.019218	5.751539	-2.716651
C	-3.548365	-0.925351	0.903643
C	-4.384804	-1.882998	0.226808
C	-2.933787	-1.307528	2.081105
C	-5.070225	-1.604531	-0.987552
C	-4.577130	-3.177416	0.814599
C	-3.090611	-2.598157	2.628435
H	-2.316602	-0.587997	2.615931
C	-5.908978	-2.532210	-1.563550
H	-4.914477	-0.644500	-1.467552
C	-5.439369	-4.111304	0.188393
C	-3.899972	-3.515783	2.011159
H	-2.576564	-2.851398	3.555452
C	-6.101220	-3.798331	-0.973534
H	-6.425436	-2.284138	-2.489515
H	-5.568453	-5.088086	0.655644
H	-4.046949	-4.510262	2.433445
H	-6.767200	-4.522684	-1.439716
Zn	1.365594	-0.678969	0.432019
O	3.165389	-0.851938	-0.096137

N	2.031990	0.598461	2.018829
C	1.382406	1.905119	1.787191
H	1.647623	2.222828	0.772904
H	1.830398	2.646321	2.474600
C	1.800469	0.083498	3.377922
H	2.015198	0.875632	4.119746
H	0.747006	-0.202869	3.496129
C	2.792538	-1.053893	3.479254
H	2.401994	-1.936175	2.950987
H	2.989580	-1.355700	4.513028
C	4.026765	-0.508207	2.756530
H	4.550400	-1.290673	2.198982
H	4.743390	-0.084958	3.470176
C	3.512894	0.589711	1.804153
H	3.900661	1.581537	2.094241
C	3.859172	0.288020	0.298594
C	5.363011	0.036257	0.158382
C	6.327021	0.714013	0.904232
H	6.027724	1.431294	1.669806
C	7.691694	0.492422	0.717676
H	8.409791	1.036979	1.325722
C	8.113602	-0.429743	-0.240483
C	7.159450	-1.122230	-0.993166
H	7.505530	-1.843415	-1.730671
C	5.809360	-0.889171	-0.792479
H	5.066990	-1.438683	-1.366582
O	9.416864	-0.726837	-0.508287
C	10.393527	-0.036590	0.235953
H	10.334030	1.050261	0.075957
H	10.303124	-0.240101	1.313429
H	11.359338	-0.401243	-0.119776
C	3.486202	1.498099	-0.581119
C	2.542251	1.374653	-1.607345
C	4.033316	2.763749	-0.361443
C	2.128444	2.471173	-2.351391
H	2.123162	0.393828	-1.830246
C	3.635255	3.876269	-1.097256
H	4.793303	2.896771	0.409187
C	2.666595	3.734931	-2.096030
H	1.388687	2.367949	-3.142616
H	4.083933	4.844004	-0.887961
O	2.198717	4.753724	-2.867591
C	2.730853	6.037002	-2.626861
H	3.815747	6.067192	-2.804896
H	2.231789	6.707172	-3.329425
H	2.530156	6.373558	-1.599248
O	0.587186	-2.610388	0.233917
Si	0.157689	-3.178935	-1.340873
H	0.121098	-1.369624	-1.672683
O	0.053338	-4.821030	-1.049839
C	1.212633	-5.613065	-0.941360
H	0.912961	-6.612569	-0.605397
H	1.729303	-5.698607	-1.905582
H	1.930167	-5.204088	-0.211089
O	1.353168	-3.206075	-2.471416
C	2.071370	-2.129872	-3.038139
H	2.686135	-2.539624	-3.846111
H	1.398735	-1.369845	-3.460583
H	2.720335	-1.655170	-2.289889
C	0.331998	-3.363469	1.419395
H	1.259605	-3.830339	1.773516
H	-0.414463	-4.140280	1.230172
Zn	-1.367964	-0.803482	-1.136558
O	-1.502162	-2.930994	-1.619778
C	-2.467053	-3.991800	-1.650850
H	-2.534140	-4.485817	-0.676382
H	-3.428507	-3.539008	-1.903311
H	-2.183092	-4.727665	-2.407908
H	-0.052098	-2.673985	2.181852

TS4

M06L SCF energy in Solvent: -6592.375281 a.u.

PBE0-D3BJ Free energy in Solvent: -6591.497186 a.u.

O	-0.444589	0.033569	0.519154
C	-0.955822	1.080067	1.201676
C	-2.353923	1.309984	1.193379
C	-2.852423	2.304808	2.036837
H	-3.928403	2.469773	2.067711
C	-2.043552	3.104769	2.845864
C	-0.670032	2.906360	2.769683
H	-0.000543	3.541420	3.354971
C	-0.109088	1.924586	1.953019
C	-2.640620	4.151245	3.737613
H	-3.187500	4.911462	3.164532
H	-1.870479	4.670458	4.319604
H	-3.357790	3.722321	4.449806
C	-3.318025	0.478879	0.301382
O	-2.829943	0.316605	-1.024715

C	-4.647599	1.254655	0.178985	H	2.409027	-1.945743	2.925143
C	-4.713583	2.448613	-0.612742	H	2.994125	-1.382253	4.494703
C	-5.774903	0.851118	0.865999	C	4.031793	-0.514220	2.748613
C	-3.587783	3.027285	-1.258244	H	4.560623	-1.291013	2.188106
C	-5.968803	3.136450	-0.724804	H	4.744115	-0.092277	3.467418
C	-7.002793	1.534919	0.760609	C	3.515666	0.587711	1.802012
H	-5.724482	-0.029432	1.503350	H	3.905055	1.578078	2.094937
C	-3.701405	4.186352	-1.989560	C	3.858281	0.291488	0.294597
H	-2.626904	2.531337	-1.170313	C	5.361546	0.040246	0.149058
C	-6.052703	4.316488	-1.503946	C	6.327175	0.715062	0.895504
C	-7.103451	2.646300	-0.035571	H	6.029509	1.429755	1.664097
H	-7.867980	1.167497	1.310258	C	7.691351	0.493073	0.706191
C	-4.945315	4.834677	-2.128402	H	8.410740	1.035013	1.315033
H	-2.817656	4.607203	-2.467257	C	8.111150	-0.426388	-0.255468
H	-7.020405	4.812687	-1.584989	C	7.155383	-1.115225	-1.009502
H	-8.048991	3.179850	-0.137097	H	7.499943	-1.834053	-1.750028
H	-5.022328	5.746445	-2.718945	C	5.805732	-0.881794	-0.806086
C	-3.541714	-0.926854	0.901817	H	5.062080	-1.428379	-1.381452
C	-4.378606	-1.880857	0.220910	O	9.413773	-0.724175	-0.525533
C	-2.932399	-1.312501	2.080342	C	10.391969	-0.038259	0.220774
C	-5.057687	-1.599455	-0.996267	H	10.334218	1.049251	0.064770
C	-4.579281	-3.174450	0.807909	H	10.301680	-0.245563	1.297526
C	-3.096909	-2.602378	2.627079	H	11.357000	-0.403246	-0.136713
H	-2.315012	-0.595435	2.618102	C	3.482039	1.503753	-0.580322
C	-5.898922	-2.523005	-1.575386	C	2.539216	1.382184	-1.607941
H	-4.895075	-0.640125	-1.475557	C	4.025681	2.769946	-0.354926
C	-5.444148	-4.103931	0.178784	C	2.122467	2.481128	-2.346924
C	-3.908270	-3.516294	2.006936	H	2.123327	0.401387	-1.837621
H	-2.587385	-2.857926	3.556063	C	3.624508	3.884738	-1.085451
C	-6.100194	-3.787901	-0.985572	H	4.785080	2.901458	0.416558
H	-6.410345	-2.272669	-2.503558	C	2.656429	3.745327	-2.085130
H	-5.579766	-5.080031	0.645706	H	1.383754	2.379060	-3.139266
H	-4.062013	-4.509945	2.428837	H	4.070233	4.852765	-0.871258
H	-6.768284	-4.508867	-1.454030	O	2.185868	4.766355	-2.851950
Zn	1.362399	-0.670093	0.416260	C	2.711637	6.050685	-2.602676
O	3.163710	-0.847906	-0.101476	H	3.796734	6.086947	-2.778237
N	2.035751	0.595724	2.019547	H	2.210949	6.722589	-3.302407
C	1.386011	1.903646	1.800964	H	2.507166	6.380200	-1.573537
H	1.651224	2.230950	0.789504	O	0.606566	-2.622500	0.216520
H	1.833952	2.639505	2.494440	Si	0.140799	-3.239427	-1.318942
C	1.805029	0.068252	3.373576	H	0.108452	-1.315237	-1.712060
H	2.019549	0.853233	4.123135	O	0.045033	-4.873416	-1.010586
H	0.751694	-0.219411	3.489116	C	1.211524	-5.655139	-0.887939
C	2.797779	-1.069262	3.464098	H	0.915435	-6.660512	-0.568193

H	1.746816	-5.725403	-1.843149
H	1.908477	-5.244805	-0.139133
O	1.312973	-3.236501	-2.463712
C	2.058215	-2.166275	-3.009516
H	2.724492	-2.592006	-3.766656
H	1.404970	-1.425596	-3.490140
H	2.657420	-1.669218	-2.234683
C	0.301749	-3.324552	1.424038
H	1.211933	-3.794122	1.817086
H	-0.452995	-4.096048	1.245102
Zn	-1.334483	-0.760907	-1.160622
O	-1.503206	-2.960071	-1.583434
C	-2.472123	-4.016368	-1.637673
H	-2.547336	-4.525488	-0.671622
H	-3.429774	-3.554003	-1.886679
H	-2.190726	-4.742642	-2.405472
H	-0.089522	-2.601103	2.150320

$Si(OMe)_4$

M06L SCF energy in Solvent: -749.774114 a.u.

PBE0-D3BJ Free energy in Solvent: -749.643705 a.u.

Si	0.000038	-0.000417	0.000423
O	-0.892376	1.173363	-0.720031
O	0.895864	-0.719757	-1.171499
O	-0.895606	-1.173424	0.718192
C	-1.727205	0.879464	-1.822806
H	-2.247187	1.799389	-2.108152
H	-1.144220	0.520518	-2.681283
H	-2.479099	0.118102	-1.567846
C	1.734621	-1.819000	-0.875613
H	1.155109	-2.678549	-0.513641
H	2.254449	-2.105122	-1.795439
H	2.486662	-1.559397	-0.115945
C	-1.737973	-0.878254	1.814766
H	-2.266804	-1.795681	2.091822
H	-1.159823	-0.526937	2.679679
H	-2.482402	-0.110660	1.556507
O	0.892478	0.718604	1.175216
C	1.730230	1.819277	0.881684
H	1.149314	2.680085	0.524989
H	2.252312	2.101625	1.801320
H	2.480237	1.563264	0.118861

IM6a

M06L SCF energy in Solvent: -6687.273051 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.277180 a.u.

O	-1.121391	-0.439057	-0.051520
C	-1.746170	-1.536541	-0.550090
C	-3.160949	-1.590271	-0.695159
C	-3.732952	-2.732056	-1.254438
H	-4.813497	-2.755715	-1.387139
C	-2.995159	-3.841780	-1.669583
C	-1.615230	-3.758327	-1.546538
H	-0.990401	-4.583585	-1.896735
C	-0.985771	-2.636907	-1.004736
C	-3.669573	-5.055460	-2.232059
H	-4.193041	-5.627150	-1.453581
H	-2.950350	-5.734626	-2.704672
H	-4.423697	-4.792128	-2.984472
C	-4.041321	-0.390437	-0.295160
O	-3.748062	-0.017221	1.030096
C	-5.540921	-0.760163	-0.340070
C	-6.102093	-1.635372	0.650477
C	-6.367640	-0.271086	-1.331879
C	-5.332198	-2.273822	1.659110
C	-7.506436	-1.928235	0.603287
C	-7.746234	-0.563544	-1.375331
H	-5.951934	0.370844	-2.106279
C	-5.914065	-3.123029	2.571779
H	-4.268667	-2.068796	1.706662
C	-8.073741	-2.795887	1.569088
C	-8.309059	-1.366476	-0.417951
H	-8.356848	-0.140680	-2.171770
C	-7.298447	-3.383322	2.537963
H	-5.294847	-3.599031	3.330963
H	-9.144781	-2.995023	1.516956
H	-9.374581	-1.597442	-0.433213
H	-7.746547	-4.053131	3.270589
C	-3.758227	0.799992	-1.254753
C	-4.233624	2.123218	-0.948272
C	-3.047224	0.617278	-2.425346
C	-5.023217	2.425840	0.195534
C	-3.936003	3.198575	-1.854689
C	-2.729492	1.679796	-3.295214
H	-2.724064	-0.387978	-2.688879
C	-5.465699	3.706057	0.438364
H	-5.258146	1.625790	0.889998
C	-4.417671	4.501384	-1.574408

C	-3.164039	2.950139	-3.015272
H	-2.149916	1.477864	-4.195764
C	-5.160847	4.758240	-0.448544
H	-6.066076	3.905386	1.324451
H	-4.191885	5.298593	-2.284338
H	-2.934887	3.783789	-3.681029
H	-5.523498	5.765268	-0.247043
O	2.735805	-0.028724	-0.194289
N	1.024032	-1.462850	-1.813465
C	0.511160	-2.601638	-1.017571
H	0.930529	-2.512200	-0.002644
H	0.904615	-3.549036	-1.428115
C	0.388277	-1.330617	-3.134110
H	0.447494	-2.297074	-3.669174
H	-0.671256	-1.079636	-3.024051
C	1.214881	-0.255627	-3.814940
H	0.793793	0.734103	-3.592073
H	1.210524	-0.367455	-4.904202
C	2.611823	-0.399772	-3.192844
H	2.934179	0.543928	-2.738288
H	3.381422	-0.682268	-3.918651
C	2.480218	-1.465127	-2.094777
H	2.760888	-2.458569	-2.492045
C	3.322115	-1.116379	-0.823602
C	4.736596	-0.742649	-1.304083
C	5.640126	-1.694113	-1.774603
H	5.372845	-2.750644	-1.761683
C	6.900575	-1.337226	-2.251597
H	7.576617	-2.111708	-2.604845
C	7.281261	0.006111	-2.258147
C	6.385638	0.973477	-1.793018
H	6.690693	2.018640	-1.809662
C	5.134137	0.598038	-1.328458
H	4.430644	1.349763	-0.977768
O	8.490007	0.466709	-2.691465
C	9.404980	-0.495027	-3.163073
H	9.667940	-1.223495	-2.381963
H	9.010096	-1.039391	-4.033744
H	10.299761	0.056879	-3.458075
C	3.446946	-2.296505	0.157469
C	3.552855	-1.998573	1.522122
C	3.509534	-3.641791	-0.205314
C	3.692270	-2.990001	2.478532
H	3.516842	-0.949947	1.813498
C	3.641226	-4.658886	0.741922
H	3.437534	-3.933928	-1.253291
C	3.730870	-4.334901	2.095831
H	3.777282	-2.751868	3.537939
H	3.667709	-5.693743	0.410626
O	3.860179	-5.241339	3.104650
C	3.895715	-6.601852	2.737105
H	4.748875	-6.821757	2.078682
H	4.002694	-7.164105	3.666854
H	2.969184	-6.909466	2.230491
Zn	0.816782	0.029945	-0.250849
Zn	-2.135882	0.896281	1.182883
C	1.442969	1.336932	2.465862
O	0.838912	0.389270	1.984519
O	2.190833	1.247286	3.559780
C	2.274847	-0.039394	4.227938
H	2.082962	-0.832279	3.498775
H	1.471389	-0.056723	4.973862
C	3.640541	-0.130840	4.850577
H	4.422743	-0.122397	4.082698
H	3.729981	-1.062019	5.420225
H	3.823702	0.704978	5.533644
C	1.367770	2.794888	2.006213
C	0.588326	2.919535	0.695772
O	0.560335	2.103077	-0.225902
O	0.016331	4.102811	0.586727
C	-0.803488	4.310686	-0.595248
H	-1.626627	3.585054	-0.547276
H	-0.200231	4.080358	-1.480102
C	-1.278701	5.733941	-0.558160
H	-1.906648	5.918141	0.319567
H	-1.878947	5.942879	-1.449325
H	-0.434607	6.432159	-0.541267
C	0.656149	3.541829	3.152525
H	1.297533	3.536795	4.037427
H	-0.295479	3.055166	3.390453
H	0.432533	4.572049	2.874660
C	2.760005	3.384423	1.731045
C	2.967584	4.763662	1.827222
C	3.821821	2.564592	1.339275
C	4.220778	5.309494	1.568684
H	2.148229	5.423371	2.104510
C	5.076983	3.113817	1.089401
H	3.664069	1.494229	1.195052

C	5.282798	4.485210	1.208159
H	4.365054	6.385175	1.653436
H	5.894113	2.457409	0.793400
H	6.265711	4.911227	1.014892
H	-1.491060	2.124688	1.852021

TS5a

M06L SCF energy in Solvent: -6687.264449 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.270906 a.u.

C	1.561791	1.462368	-0.952329
C	2.976688	1.588247	-0.944864
C	3.539208	2.715085	-1.543134
H	4.625299	2.799612	-1.568761
C	2.783402	3.742429	-2.112683
C	1.400264	3.615118	-2.065517
H	0.770713	4.404088	-2.484386
C	0.779517	2.505090	-1.492307
C	3.445758	4.933488	-2.736613
H	4.075301	5.472895	-2.016809
H	2.708528	5.644941	-3.126175
H	4.100812	4.649719	-3.571210
C	3.873316	0.493238	-0.321121
O	3.393603	0.145235	0.970850
C	5.310340	1.017888	-0.127058
C	5.587345	2.015939	0.866826
C	6.349460	0.555690	-0.909541
C	4.585005	2.630121	1.664355
C	6.941002	2.460207	1.042838
C	7.676797	0.996583	-0.733348
H	6.149395	-0.179873	-1.685893
C	4.901787	3.601901	2.584967
H	3.555704	2.310182	1.542659
C	7.231818	3.450894	2.012593
C	7.970081	1.922211	0.233420
H	8.462617	0.591981	-1.369423
C	6.236423	4.013979	2.772246
H	4.109250	4.057270	3.177252
H	8.269177	3.765165	2.133241
H	8.991991	2.270616	0.386275
H	6.472862	4.779596	3.509856
C	3.868250	-0.765910	-1.229270
C	4.402256	-2.015244	-0.752394
C	3.332620	-0.724703	-2.503416
C	5.031935	-2.165448	0.514342
C	4.322272	-3.174818	-1.595092
C	3.266200	-1.863723	-3.330916
H	2.950231	0.220250	-2.883501
C	5.513214	-3.385510	0.931079
H	5.116924	-1.298221	1.160094
C	4.825800	-4.415015	-1.130009
C	3.747119	-3.068499	-2.884683
H	2.830629	-1.776505	-4.325348
C	5.403753	-4.526218	0.111036
H	5.990769	-3.467017	1.906268
H	4.751304	-5.281726	-1.788166
H	3.701669	-3.959110	-3.512844
H	5.787485	-5.485193	0.455463
O	-2.754183	0.106409	0.060056
N	-1.331383	1.280817	-2.023099
C	-0.718346	2.478099	-1.413440
H	-1.050550	2.509525	-0.364544
H	-1.132625	3.383158	-1.894030
C	-0.895941	1.046820	-3.407686
H	-0.987493	1.987504	-3.981786
H	0.160821	0.756443	-3.420737
C	-1.853637	-0.023381	-3.920241
H	-1.392834	-1.017106	-3.861601
H	-2.108604	0.146038	-4.971575
C	-3.075132	0.068643	-2.990039
H	-3.159347	-0.837820	-2.375337
H	-4.024362	0.175889	-3.524016
C	-2.813533	1.262129	-2.066758
H	-3.172756	2.194462	-2.539994
C	-3.449517	1.088284	-0.641762
C	-4.903090	0.633157	-0.869672
C	-5.897910	1.514585	-1.289173
H	-5.672415	2.575020	-1.400590
C	-7.196707	1.084143	-1.557136
H	-7.943333	1.806528	-1.877566
C	-7.521233	-0.264583	-1.401735
C	-6.533257	-1.163116	-0.986785
H	-6.797977	-2.214061	-0.879814
C	-5.246783	-0.715750	-0.729897
H	-4.474047	-1.418198	-0.425663
O	-8.756839	-0.795849	-1.627124
C	-9.769651	0.095910	-2.031396
H	-9.952036	0.873697	-1.275088
H	-9.526171	0.583404	-2.987195

H	-10.672167	-0.506440	-2.154242
C	-3.473706	2.395840	0.168904
C	-3.425679	2.294013	1.565284
C	-3.592338	3.675964	-0.371747
C	-3.459188	3.411253	2.381671
H	-3.358813	1.296318	1.993517
C	-3.624778	4.817582	0.431372
H	-3.644487	3.816864	-1.451525
C	-3.551759	4.688957	1.818150
H	-3.418610	3.325403	3.466215
H	-3.703090	5.795622	-0.036375
O	-3.566407	5.730773	2.696012
C	-3.655456	7.025234	2.145488
H	-4.585451	7.159481	1.573547
H	-3.648873	7.715312	2.991560
H	-2.801330	7.246001	1.488622
Zn	-0.955248	-0.168099	-0.494219
Zn	1.898896	-0.941656	0.752145
C	-0.735657	-1.518273	2.363020
O	-0.024165	-0.595005	1.958616
O	-1.569665	-1.375912	3.372656
C	-1.667443	-0.052138	3.970536
H	-1.591771	0.691936	3.171020
H	-0.801737	0.071932	4.631642
C	-2.979038	-0.000442	4.701112
H	-3.815309	-0.150230	4.009088
H	-3.100203	0.976828	5.179641
H	-3.035591	-0.770904	5.476753
C	-0.679469	-2.948729	1.838745
C	-0.165575	-2.927800	0.376209
O	-0.690737	-2.164003	-0.491431
O	0.200681	-4.177190	0.006717
C	0.695741	-4.265121	-1.338792
H	1.454862	-3.475823	-1.469336
H	-0.124973	-4.057279	-2.035740
C	1.280066	-5.638505	-1.521159
H	2.098788	-5.809862	-0.813977
H	1.679029	-5.743424	-2.536312
H	0.522458	-6.415121	-1.370254
C	0.311343	-3.673511	2.762250
H	-0.115471	-3.790395	3.763350
H	1.249006	-3.111506	2.839492
H	0.558146	-4.657455	2.357612
C	-2.059242	-3.606098	1.820896
C	-2.212580	-4.960719	2.122332
C	-3.188180	-2.864190	1.454436
C	-3.469494	-5.558788	2.084753
H	-1.349136	-5.564876	2.390768
C	-4.444488	-3.461480	1.429873
H	-3.093957	-1.808018	1.190288
C	-4.591334	-4.809754	1.746792
H	-3.568002	-6.615604	2.327565
H	-5.314110	-2.860748	1.166243
H	-5.576163	-5.273727	1.728675
H	1.267913	-2.426922	0.654747

IM7a

M06L SCF energy in Solvent: -6592.375200 a.u.

PBE0-D3BJ Free energy in Solvent: -6591.498066 a.u.

O	-0.669708	-0.577250	-0.196802
C	-1.148164	-1.819511	-0.038891
C	-2.532587	-2.086608	-0.211495
C	-2.976963	-3.393402	-0.025777
H	-4.034672	-3.612556	-0.174248
C	-2.120809	-4.449400	0.306822
C	-0.759122	-4.170771	0.394080
H	-0.053814	-4.984081	0.583295
C	-0.259075	-2.880770	0.220034
C	-2.652951	-5.832396	0.531711
H	-3.455768	-6.080016	-0.173821
H	-3.076227	-5.950492	1.539250
H	-1.867972	-6.590343	0.423114
C	-3.456398	-0.951806	-0.719350
O	-3.404141	0.147642	0.159558
C	-4.932885	-1.384928	-0.790321
C	-5.675760	-1.624502	0.414880
C	-5.580986	-1.518492	-2.001674
C	-5.101475	-1.555675	1.711664
C	-7.061052	-1.984814	0.318272
C	-6.945686	-1.862114	-2.091311
H	-5.029232	-1.349226	-2.923776
C	-5.844824	-1.823790	2.837812
H	-4.057824	-1.270564	1.794768
C	-7.798685	-2.243079	1.499660
C	-7.674227	-2.088790	-0.953349
H	-7.411602	-1.946647	-3.071930
C	-7.208356	-2.167228	2.737249
H	-5.375046	-1.766562	3.819628

H	-8.851122	-2.512012	1.402417	H	6.932043	1.854848	-2.831227
H	-8.729451	-2.358223	-1.005223	C	5.452452	0.754683	-1.699914
H	-7.787081	-2.374654	3.636186	H	4.656767	1.480450	-1.851466
C	-2.934528	-0.552640	-2.134657	O	8.918361	0.298636	-2.657533
C	-3.039369	0.790413	-2.636830	C	9.944661	-0.653855	-2.504982
C	-2.286507	-1.488803	-2.918584	H	10.208918	-0.802401	-1.447365
C	-3.848092	1.801986	-2.037258	H	9.665265	-1.625916	-2.938148
C	-2.311206	1.147510	-3.825796	H	10.809524	-0.255951	-3.039969
C	-1.627471	-1.149140	-4.115621	C	3.953663	-0.892598	1.124622
H	-2.246358	-2.521648	-2.574755	C	4.118914	0.230786	1.950637
C	-3.865156	3.087447	-2.530152	C	4.080177	-2.146073	1.720663
H	-4.451891	1.540388	-1.174587	C	4.372299	0.108963	3.305353
C	-2.341242	2.485909	-4.288506	H	4.025009	1.217551	1.497703
C	-1.598809	0.156046	-4.538926	C	4.323002	-2.293442	3.088943
H	-1.109861	-1.924775	-4.679605	H	3.977596	-3.050952	1.121376
C	-3.088295	3.445085	-3.649480	C	4.473109	-1.160526	3.889077
H	-4.496800	3.832783	-2.047973	H	4.492127	0.984071	3.941116
H	-1.766627	2.734248	-5.181193	H	4.398098	-3.292181	3.511379
H	-1.052365	0.444808	-5.436949	O	4.714940	-1.183887	5.229359
H	-3.102795	4.468483	-4.021458	C	4.820946	-2.451941	5.835769
O	2.975950	0.498599	-0.569509	H	5.651286	-3.035890	5.412505
N	1.681603	-1.945778	-0.997125	H	5.012554	-2.266013	6.894391
C	1.223435	-2.641087	0.221935	H	3.891470	-3.030584	5.730397
H	1.529350	-2.031481	1.085028	Zn	1.118492	0.211879	-0.445898
H	1.750936	-3.610364	0.317666	Zn	-1.819867	1.121779	-0.065750
C	1.173581	-2.583911	-2.220524	C	-1.659052	3.654881	1.422282
H	1.397761	-3.668919	-2.197825	O	-2.480345	3.066553	0.716917
H	0.086975	-2.469953	-2.283075	O	-1.923567	4.836106	1.960414
C	1.935404	-1.881467	-3.318224	C	-3.237791	5.384756	1.667840
H	1.445496	-0.924460	-3.546488	H	-3.988818	4.666939	2.015506
H	1.962845	-2.460432	-4.247845	H	-3.335957	5.461955	0.579197
C	3.316820	-1.649500	-2.703256	C	-3.330873	6.713364	2.362498
H	3.687791	-0.646721	-2.933636	H	-3.207323	6.602771	3.444507
H	4.062906	-2.354961	-3.086095	H	-4.312119	7.161642	2.176316
C	3.147574	-1.834669	-1.177535	H	-2.565094	7.406043	1.999003
H	3.623697	-2.783229	-0.865290	C	-0.262850	3.129250	1.681353
C	3.763408	-0.635778	-0.379479	C	0.359986	3.052419	0.217364
C	5.169185	-0.391402	-0.952305	O	-0.052511	1.934997	-0.489550
C	6.188609	-1.326567	-0.780134	O	1.745311	3.100799	0.366357
H	6.002997	-2.224909	-0.189192	C	2.442605	3.453173	-0.828496
C	7.453646	-1.142924	-1.334831	H	1.947157	4.334145	-1.275267
H	8.221545	-1.896126	-1.178451	H	2.388641	2.626258	-1.550873
C	7.718807	0.011771	-2.074043	C	3.868369	3.752015	-0.452098
C	6.708459	0.961712	-2.250778	H	3.919384	4.566988	0.279078

H	4.449114	4.042493	-1.335092
H	4.335691	2.860637	-0.020359
C	0.547538	4.080444	2.559599
H	0.049033	4.241313	3.520920
H	0.674960	5.054022	2.073804
H	1.540389	3.664503	2.742372
C	-0.323540	1.728528	2.289549
C	0.874340	1.008358	2.426327
C	-1.514090	1.103322	2.683171
C	0.874153	-0.294267	2.914017
H	1.815587	1.470009	2.131203
C	-1.512205	-0.209447	3.159410
H	-2.471367	1.615736	2.602826
C	-0.323415	-0.915951	3.267915
H	1.822318	-0.823991	3.008952
H	-2.457960	-0.674224	3.433281
H	-0.325227	-1.946464	3.618495
H	0.036960	3.965445	-0.332422

IM6b

M06L SCF energy in Solvent: -6687.274390 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.277572 a.u.

O	-0.889630	-0.549520	-0.165316
C	-1.477229	-1.656367	-0.690202
C	-2.891825	-1.786193	-0.753703
C	-3.435338	-2.906024	-1.383833
H	-4.519887	-2.980407	-1.453180
C	-2.670197	-3.931165	-1.937097
C	-1.291468	-3.796430	-1.850064
H	-0.645677	-4.570459	-2.271987
C	-0.687312	-2.697059	-1.238777
C	-3.311746	-5.124830	-2.576091
H	-4.170545	-4.842648	-3.197636
H	-3.688624	-5.834480	-1.826599
H	-2.605483	-5.672380	-3.211423
C	-3.835897	-0.693566	-0.207301
O	-3.388445	-0.230547	1.044148
C	-5.250325	-1.279033	0.003510
C	-5.488174	-2.212817	1.066828
C	-6.298608	-0.946000	-0.830841
C	-4.466180	-2.700131	1.924427
C	-6.815756	-2.722981	1.258395
C	-7.600408	-1.453521	-0.641651
H	-6.124500	-0.267111	-1.663831
C	-4.742601	-3.610175	2.918328
H	-3.455982	-2.327745	1.793162
C	-7.066054	-3.648009	2.301914
C	-7.858177	-2.315514	0.392466
H	-8.396123	-1.150147	-1.320551
C	-6.053916	-4.085096	3.120303
H	-3.936263	-3.965589	3.558523
H	-8.084994	-4.014297	2.433039
H	-8.860526	-2.712244	0.556406
H	-6.259157	-4.800460	3.915576
C	-3.885636	0.497171	-1.206753
C	-4.562295	1.718189	-0.848802
C	-3.279793	0.424112	-2.448897
C	-5.232114	1.903432	0.392000
C	-4.603913	2.797110	-1.794368
C	-3.304579	1.496019	-3.365363
H	-2.784433	-0.499258	-2.741859
C	-5.888327	3.078285	0.678862
H	-5.204825	1.099646	1.120588
C	-5.295377	3.989478	-1.465719
C	-3.962445	2.657276	-3.049717
H	-2.812043	1.384258	-4.330664
C	-5.923343	4.134729	-0.253195
H	-6.390732	3.189469	1.638412
H	-5.320813	4.792136	-2.204488
H	-4.008823	3.486874	-3.757467
H	-6.451588	5.056552	-0.014388
O	2.886430	0.011208	-0.066068
N	1.408442	-1.506471	-1.849841
C	0.810484	-2.683734	-1.184156
H	1.160704	-2.687715	-0.144073
H	1.210414	-3.603988	-1.648062
C	0.927808	-1.305121	-3.225212
H	1.039065	-2.244841	-3.798328
H	-0.136762	-1.045100	-3.214572
C	1.837137	-0.210482	-3.749207
H	1.433810	0.769286	-3.463937
H	1.914226	-0.224896	-4.841262
C	3.176646	-0.467512	-3.042677
H	3.575771	0.450396	-2.593564
H	3.944226	-0.842841	-3.728105
C	2.890702	-1.499095	-1.936739
H	3.220883	-2.509564	-2.243388
C	3.542897	-1.101951	-0.566308

C	5.022053	-0.764802	-0.809359
C	5.849012	-1.525865	-1.636827
H	5.443953	-2.379016	-2.182238
C	7.197208	-1.220152	-1.816457
H	7.801325	-1.839458	-2.474431
C	7.748814	-0.122064	-1.153976
C	6.932653	0.661232	-0.332970
H	7.373382	1.521199	0.168215
C	5.593371	0.341996	-0.171529
H	4.957671	0.961155	0.456132
O	9.052065	0.266702	-1.250976
C	9.892487	-0.517899	-2.065260
H	9.952874	-1.555933	-1.706192
H	9.553900	-0.525709	-3.111989
H	10.881874	-0.059349	-2.009746
C	3.468775	-2.273024	0.437402
C	2.827526	-2.099067	1.670175
C	3.993834	-3.536225	0.163715
C	2.717522	-3.133024	2.587971
H	2.389166	-1.127351	1.892497
C	3.888086	-4.591758	1.067186
H	4.505058	-3.722173	-0.780608
C	3.247311	-4.392170	2.292397
H	2.213869	-2.990233	3.542388
H	4.308914	-5.560128	0.808307
O	3.089186	-5.348668	3.249030
C	3.604443	-6.629382	2.964319
H	4.693170	-6.604230	2.809100
H	3.377937	-7.246512	3.835878
H	3.129920	-7.069538	2.074918
Zn	0.989608	-0.019153	-0.383772
Zn	-1.981859	0.971046	0.816610
C	1.869476	2.007525	1.576880
O	1.032169	1.116133	1.638623
O	2.891339	2.146416	2.408294
C	3.062372	1.169396	3.469842
H	2.231892	0.459133	3.426154
H	2.985469	1.746921	4.397265
C	4.402697	0.504653	3.316564
H	4.447264	-0.064685	2.382337
H	4.567594	-0.192489	4.145934
H	5.214620	1.240501	3.318374
C	1.837684	3.184848	0.588641
C	0.737842	2.960352	-0.450151
O	0.576222	1.913915	-1.083710
O	0.041478	4.043421	-0.701244
C	-1.067621	3.919451	-1.637302
H	-1.609379	2.996789	-1.397871
H	-0.645875	3.816932	-2.644768
C	-1.908065	5.150067	-1.459024
H	-2.332916	5.179455	-0.449163
H	-2.737221	5.138170	-2.173322
H	-1.321405	6.060827	-1.619766
C	3.155738	3.220942	-0.203263
H	3.140327	4.037289	-0.934569
H	3.303778	2.264763	-0.715892
H	3.996044	3.376974	0.479477
C	1.582117	4.443480	1.419864
C	2.459584	5.525790	1.437329
C	0.427929	4.494761	2.210805
C	2.184262	6.643513	2.224363
H	3.365473	5.511651	0.835070
C	0.154454	5.607782	2.994350
H	-0.274916	3.659227	2.187881
C	1.034345	6.688336	3.004964
H	2.877823	7.482764	2.224110
H	-0.750938	5.630926	3.598041
H	0.822650	7.562102	3.618616
H	-1.457991	2.403495	1.028937

TS5b

M06L SCF energy in Solvent: -6687.263120 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.266809 a.u.

O	-0.613767	-0.638911	-0.330430
C	-1.130812	-1.774342	-0.839463
C	-2.527768	-2.015516	-0.830861
C	-2.994960	-3.186625	-1.430002
H	-4.069588	-3.365796	-1.449757
C	-2.159466	-4.134533	-2.022242
C	-0.792573	-3.875681	-2.009398
H	-0.102900	-4.593596	-2.460184
C	-0.262896	-2.727812	-1.422528
C	-2.715659	-5.390492	-2.621920
H	-3.684441	-5.217034	-3.105658
H	-2.879592	-6.166455	-1.861073
H	-2.038684	-5.816718	-3.371815
C	-3.532059	-0.971067	-0.280932
O	-3.099916	-0.421997	0.956186

C	-4.888574	-1.654672	-0.003807
C	-5.015794	-2.588332	1.078695
C	-5.987304	-1.419717	-0.806506
C	-3.932628	-2.975616	1.911633
C	-6.289895	-3.205504	1.315554
C	-7.237176	-2.025691	-0.567530
H	-5.898151	-0.745766	-1.655482
C	-4.101785	-3.896219	2.920227
H	-2.960975	-2.521808	1.747768
C	-6.430199	-4.138681	2.371399
C	-7.389964	-2.893768	0.481344
H	-8.076026	-1.794933	-1.222325
C	-5.360909	-4.481190	3.162172
H	-3.250052	-4.175288	3.538815
H	-7.410176	-4.588065	2.534986
H	-8.350803	-3.368548	0.682052
H	-5.481446	-5.205187	3.966778
C	-3.705263	0.169991	-1.321842
C	-4.474039	1.345495	-0.996851
C	-3.157402	0.075564	-2.589553
C	-5.097322	1.548001	0.264935
C	-4.660440	2.356545	-1.999340
C	-3.335064	1.077504	-3.565703
H	-2.592262	-0.814533	-2.857338
C	-5.831182	2.683144	0.523530
H	-4.972245	0.791169	1.032159
C	-5.420966	3.512469	-1.695713
C	-4.083424	2.190866	-3.282082
H	-2.885900	0.949191	-4.549440
C	-5.993598	3.680434	-0.458546
H	-6.294732	2.808762	1.500649
H	-5.542799	4.268568	-2.472424
H	-4.245135	2.965202	-4.033250
H	-6.575179	4.574118	-0.238290
O	2.939414	0.290104	-0.016233
N	1.749942	-1.335035	-1.974654
C	1.231821	-2.579117	-1.361020
H	1.565308	-2.589474	-0.317248
H	1.712568	-3.443967	-1.853840
C	1.362519	-1.195239	-3.386665
H	1.635488	-2.116931	-3.934451
H	0.275671	-1.072529	-3.464840
C	2.170166	0.001594	-3.852630
H	1.616405	0.926993	-3.647675
H	2.361820	-0.026801	-4.930185
C	3.453812	-0.059922	-3.007505
H	3.643200	0.897301	-2.505752
H	4.341385	-0.282321	-3.608488
C	3.228291	-1.152143	-1.946384
H	3.700878	-2.105854	-2.247693
C	3.744703	-0.720663	-0.520760
C	5.181665	-0.192225	-0.670740
C	6.144330	-0.809899	-1.470386
H	5.884110	-1.688719	-2.061171
C	7.446886	-0.322247	-1.569011
H	8.160675	-0.831752	-2.211477
C	7.811796	0.815821	-0.848319
C	6.856654	1.458933	-0.056211
H	7.150622	2.355073	0.486617
C	5.564930	0.962037	0.021952
H	4.816497	1.478610	0.618460
O	9.055269	1.375791	-0.862802
C	10.035096	0.729485	-1.641453
H	10.202566	-0.304937	-1.306457
H	9.764733	0.715586	-2.707828
H	10.954280	1.304243	-1.510894
C	3.760964	-1.931905	0.436683
C	2.975405	-1.921477	1.595945
C	4.514450	-3.078891	0.186835
C	2.951856	-2.996775	2.470856
H	2.350956	-1.050674	1.786877
C	4.502480	-4.173587	1.048784
H	5.143291	-3.135447	-0.700842
C	3.720120	-4.134068	2.205287
H	2.334069	-2.982754	3.367146
H	5.107422	-5.045537	0.813017
O	3.637776	-5.140383	3.119941
C	4.394307	-6.301208	2.863259
H	5.471663	-6.083327	2.820994
H	4.195844	-6.981087	3.694320
H	4.093159	-6.782173	1.920960
Zn	1.147799	0.180131	-0.639647
Zn	-1.704317	0.766576	0.625766
C	1.110935	1.961276	1.820788
O	0.486922	0.903777	1.717295
O	2.045498	2.181220	2.726409
C	2.414640	1.116597	3.645895
H	1.761443	0.257443	3.469002

H	2.206897	1.522790	4.641485
C	3.869401	0.795086	3.441227
H	4.036572	0.428192	2.422863
H	4.180658	0.011361	4.140871
H	4.497188	1.677406	3.607187
C	0.889573	3.205674	0.963244
C	0.034492	2.858577	-0.280709
O	0.445782	1.989964	-1.117509
O	-0.551125	3.979491	-0.760947
C	-1.364027	3.755320	-1.922344
H	-2.027010	2.904113	-1.698977
H	-0.723797	3.460623	-2.763500
C	-2.140804	5.013465	-2.192065
H	-2.788625	5.261962	-1.344901
H	-2.773739	4.874586	-3.075741
H	-1.472103	5.861023	-2.378604
C	2.254474	3.655937	0.409720
H	2.117316	4.443659	-0.337844
H	2.758729	2.809024	-0.069644
H	2.888327	4.033634	1.217028
C	0.202721	4.256684	1.829025
C	0.506691	5.614008	1.709413
C	-0.785293	3.872811	2.742109
C	-0.162826	6.561673	2.476635
H	1.265872	5.941161	1.002403
C	-1.456138	4.818888	3.510548
H	-1.035139	2.817673	2.861450
C	-1.147274	6.169021	3.379323
H	0.088226	7.615379	2.366368
H	-2.221193	4.495506	4.214023
H	-1.668885	6.912262	3.979649
H	-1.201302	2.298556	0.408917

IM7b

M06L SCF energy in Solvent: -6687.291072 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.292686 a.u.

O	-0.641797	-0.982466	0.038261
C	-1.160095	-1.493996	1.166882
C	-2.563795	-1.638074	1.311214
C	-3.050797	-2.227582	2.475307
H	-4.127389	-2.365209	2.578709
C	-2.218353	-2.669096	3.508748
C	-0.844113	-2.526333	3.334557
H	-0.163722	-2.885180	4.110606
C	-0.301574	-1.948071	2.187467
C	-2.791027	-3.274233	4.754814
H	-3.611683	-3.967402	4.532025
H	-3.201997	-2.510090	5.429202
H	-2.032062	-3.827565	5.320224
C	-3.489337	-1.233937	0.144730
O	-3.238962	0.110185	-0.238897
C	-4.971208	-1.289161	0.546515
C	-5.500780	-0.329766	1.473889
C	-5.819392	-2.240312	0.017125
C	-4.706427	0.644548	2.137833
C	-6.900176	-0.370423	1.788042
C	-7.193233	-2.278133	0.332687
H	-5.421640	-2.982743	-0.672182
C	-5.261969	1.525261	3.038012
H	-3.643010	0.689751	1.920474
C	-7.440024	0.566166	2.703939
C	-7.726418	-1.354029	1.193333
H	-7.824342	-3.042817	-0.117215
C	-6.642536	1.498830	3.319624
H	-4.623806	2.248689	3.544186
H	-8.508223	0.520529	2.918353
H	-8.787448	-1.366467	1.443249
H	-7.068750	2.206256	4.029195
C	-3.190105	-2.176562	-1.055715
C	-3.502373	-1.784934	-2.405994
C	-2.551686	-3.386832	-0.857171
C	-4.286341	-0.640991	-2.739650
C	-3.040273	-2.607484	-3.492861
C	-2.119701	-4.197445	-1.924785
H	-2.343650	-3.712013	0.160681
C	-4.548725	-0.312243	-4.050442
H	-4.680339	-0.024978	-1.938687
C	-3.321091	-2.226960	-4.828182
C	-2.333651	-3.802058	-3.220577
H	-1.596231	-5.128717	-1.710090
C	-4.052356	-1.099056	-5.108519
H	-5.154243	0.565717	-4.268488
H	-2.951857	-2.863633	-5.632501
H	-1.984854	-4.406349	-4.057990
H	-4.262720	-0.822402	-6.140149
O	3.070426	-0.452477	-0.791816
N	1.698799	-2.319606	0.757515
C	1.188602	-1.816338	2.046829

H	1.489891	-0.759568	2.134108
H	1.689829	-2.341664	2.882697
C	1.172157	-3.643496	0.401913
H	1.342163	-4.356646	1.231912
H	0.092584	-3.586409	0.224378
C	1.981178	-4.007406	-0.822315
H	1.546175	-3.514468	-1.703839
H	1.984111	-5.084091	-1.023117
C	3.369810	-3.438175	-0.518838
H	3.806756	-2.962152	-1.402138
H	4.070467	-4.217406	-0.198275
C	3.170360	-2.406893	0.612747
H	3.605071	-2.790175	1.554618
C	3.794276	-1.015015	0.256716
C	5.241756	-1.251661	-0.201714
C	6.209146	-1.767438	0.659468
H	5.953498	-1.987133	1.695701
C	7.516463	-2.005358	0.240337
H	8.239028	-2.406529	0.946314
C	7.879376	-1.717383	-1.077116
C	6.920375	-1.206457	-1.955634
H	7.217244	-0.991296	-2.980272
C	5.622518	-0.983646	-1.521321
H	4.872591	-0.598539	-2.207880
O	9.128407	-1.899442	-1.594026
C	10.111769	-2.404408	-0.721322
H	10.274939	-1.736464	0.137380
H	9.848348	-3.404309	-0.345256
H	11.031290	-2.470221	-1.306716
C	3.825321	-0.055155	1.461352
C	3.593592	1.310652	1.240663
C	4.115914	-0.449474	2.769750
C	3.641750	2.231041	2.276953
H	3.358514	1.642181	0.229544
C	4.159968	0.459931	3.825476
H	4.291672	-1.499799	3.002148
C	3.923792	1.813866	3.580884
H	3.470491	3.291637	2.098288
H	4.375424	0.101835	4.829048
O	3.944196	2.788775	4.532487
C	4.232560	2.386315	5.852071
H	5.227742	1.923831	5.927188
H	4.210285	3.294581	6.457534
H	3.483477	1.676678	6.233546
Zn	1.208976	-0.545815	-0.570350
Zn	-1.693514	0.223185	-1.264309
C	-1.683832	2.956746	-1.015939
O	-2.264267	2.333817	-1.906108
O	-2.322377	3.671645	-0.105288
C	-3.778288	3.558662	-0.125779
H	-4.026432	2.491755	-0.047209
H	-4.130761	3.921595	-1.097775
C	-4.295932	4.371637	1.025130
H	-3.873160	4.017224	1.970885
H	-5.384276	4.269324	1.089142
H	-4.050308	5.433003	0.912228
C	-0.177642	2.915460	-0.796736
C	0.463207	2.013528	-1.903274
O	0.100414	0.658007	-1.829143
O	1.836875	2.151376	-1.732522
C	2.616888	1.762342	-2.862163
H	2.200807	2.256157	-3.758123
H	2.549294	0.674242	-3.008074
C	4.035291	2.190656	-2.600272
H	4.085510	3.270489	-2.417103
H	4.675879	1.952106	-3.456968
H	4.429230	1.663796	-1.724361
C	0.066591	2.310453	0.593179
H	1.117050	2.010844	0.703999
H	-0.556145	1.422082	0.766430
H	-0.174371	3.031821	1.379898
C	0.399797	4.314534	-0.953089
C	1.389707	4.802746	-0.099021
C	-0.007900	5.109551	-2.029057
C	1.954485	6.056387	-0.310964
H	1.735010	4.194102	0.734639
C	0.556002	6.363399	-2.243785
H	-0.776921	4.741507	-2.711668
C	1.540452	6.841736	-1.383502
H	2.726770	6.418769	0.365762
H	0.224047	6.967774	-3.086309
H	1.982877	7.822545	-1.547801
H	0.161802	2.401776	-2.895222

TS6a

M06L SCF energy in Solvent: -7322.524825 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.398938 a.u.

O	-0.588796	-0.969397	-0.433521

C	-1.047836	-2.186492	-0.825682
C	-2.428532	-2.520598	-0.804265
C	-2.810501	-3.769683	-1.300062
H	-3.873851	-4.011412	-1.297469
C	-1.918557	-4.718682	-1.796196
C	-0.570190	-4.384976	-1.766675
H	0.172990	-5.102578	-2.122462
C	-0.124526	-3.156783	-1.280879
C	-2.396502	-6.042902	-2.309683
H	-3.201715	-5.929599	-3.046918
H	-2.798096	-6.671416	-1.503490
H	-1.586328	-6.605134	-2.788286
C	-3.538346	-1.567238	-0.286513
O	-3.091370	-0.785530	0.785936
C	-4.720684	-2.406677	0.260026
C	-4.542484	-3.207139	1.438624
C	-5.953800	-2.411091	-0.360545
C	-3.305169	-3.329392	2.125264
C	-5.656957	-3.958456	1.942173
C	-7.048085	-3.144121	0.143568
H	-6.099869	-1.835035	-1.271529
C	-3.179343	-4.134460	3.233814
H	-2.452221	-2.761145	1.769510
C	-5.494198	-4.766879	3.093689
C	-6.905808	-3.898293	1.277932
H	-8.003057	-3.103629	-0.378424
C	-4.281259	-4.858935	3.730631
H	-2.214587	-4.211314	3.733646
H	-6.357835	-5.324391	3.458056
H	-7.741411	-4.471283	1.681119
H	-4.168501	-5.489484	4.611510
C	-4.029539	-0.656731	-1.445207
C	-4.863483	0.488965	-1.175548
C	-3.720110	-0.944919	-2.762098
C	-5.298410	0.857982	0.127909
C	-5.331139	1.284443	-2.277665
C	-4.199576	-0.171068	-3.839482
H	-3.101289	-1.811995	-2.982632
C	-6.098109	1.960445	0.328315
H	-4.969564	0.259902	0.970832
C	-6.136147	2.423787	-2.030112
C	-4.993043	0.921317	-3.603793
H	-3.932961	-0.450199	-4.858146
C	-6.511702	2.763889	-0.753259
H	-6.413036	2.213049	1.340127
H	-6.463552	3.018300	-2.883624
H	-5.368090	1.532274	-4.425772
H	-7.135784	3.639521	-0.577336
O	2.972296	-0.233689	0.034990
N	1.831780	-1.751172	-1.939819
C	1.354136	-2.933806	-1.197633
H	1.666045	-2.799471	-0.151933
H	1.888913	-3.828825	-1.564687
C	1.398623	-1.696347	-3.341622
H	1.658138	-2.640418	-3.856724
H	0.310179	-1.574208	-3.394498
C	2.196881	-0.523027	-3.873786
H	1.689919	0.413188	-3.599248
H	2.290110	-0.532974	-4.964323
C	3.545167	-0.644818	-3.148836
H	3.924720	0.324797	-2.812639
H	4.316680	-1.054657	-3.810338
C	3.305995	-1.605075	-1.962998
H	3.737269	-2.594328	-2.202197
C	3.843925	-1.142772	-0.553365
C	5.221769	-0.481804	-0.721611
C	6.192431	-0.971566	-1.596199
H	5.974642	-1.835807	-2.225141
C	7.447515	-0.377641	-1.713508
H	8.168611	-0.785871	-2.416984
C	7.757224	0.735526	-0.929775
C	6.800854	1.234849	-0.040687
H	7.058398	2.101940	0.564183
C	5.556191	0.631699	0.057197
H	4.808352	1.025637	0.743722
O	8.948036	1.398141	-0.961663
C	9.929445	0.906442	-1.844890
H	10.211974	-0.128859	-1.603288
H	9.592404	0.945449	-2.891424
H	10.798884	1.555552	-1.722487
C	4.049956	-2.369152	0.367771
C	3.515032	-2.363688	1.659163
C	4.792355	-3.489011	-0.008235
C	3.702025	-3.420932	2.535087
H	2.918784	-1.507600	1.957547
C	4.990832	-4.567231	0.853018
H	5.249052	-3.536896	-0.996910
C	4.445003	-4.536155	2.137994

H	3.275999	-3.407927	3.536977
H	5.575006	-5.418918	0.514199
O	4.579766	-5.527963	3.062233
C	5.315151	-6.665936	2.674053
H	6.354960	-6.411420	2.420960
H	5.307534	-7.338704	3.533809
H	4.854933	-7.171696	1.812426
Zn	1.189423	-0.175520	-0.633295
Zn	-1.824961	0.500260	0.303271
C	0.366519	1.856756	2.282779
O	0.220023	1.032144	1.379084
O	1.274837	1.723258	3.229844
C	2.168065	0.577345	3.111644
H	1.567251	-0.323930	3.287876
H	2.542262	0.535957	2.080703
C	3.266679	0.751090	4.119876
H	2.879248	0.790701	5.143309
H	3.960540	-0.093946	4.046228
H	3.830908	1.669988	3.927583
C	-0.421093	3.155526	2.450288
C	-1.573609	3.175749	1.417789
O	-2.315229	2.155191	1.300593
O	-2.148887	4.409114	1.360061
C	-3.248146	4.480077	0.434921
H	-2.867063	4.187469	-0.561111
H	-4.011437	3.745915	0.717643
C	-3.769087	5.889784	0.438347
H	-2.997096	6.604829	0.132850
H	-4.610369	5.974467	-0.258164
H	-4.122823	6.174694	1.435258
C	-1.081198	3.133696	3.841976
H	-1.756693	3.985882	3.954797
H	-1.676876	2.223179	3.964089
H	-0.320189	3.173749	4.625847
C	0.531694	4.332222	2.268685
C	1.699443	4.192024	1.513373
C	0.237061	5.587546	2.809623
C	2.553011	5.270410	1.305526
H	1.948772	3.228746	1.061596
C	1.089120	6.667297	2.604107
H	-0.675032	5.730628	3.384735
C	2.252017	6.512793	1.853078
H	3.451853	5.135575	0.705879
H	0.840361	7.636258	3.033666
H	2.918929	7.358279	1.693997
H	-1.038016	1.533971	-0.928623
H	-0.773637	3.221555	0.169140
Si	-0.187194	2.834868	-1.297228
O	1.200658	1.815526	-1.337458
O	-1.046554	3.059477	-2.705439
O	0.663737	4.286072	-1.348765
C	2.508546	2.330529	-1.666610
H	3.240111	1.634184	-1.247987
H	2.610738	2.397963	-2.756180
H	2.634013	3.325874	-1.238547
C	-0.001092	5.507318	-1.147483
H	-0.419659	5.576356	-0.129806
H	0.727976	6.317113	-1.268591
H	-0.811536	5.654342	-1.878634
C	-1.968384	2.108688	-3.188270
H	-2.464229	2.533058	-4.067703
H	-1.473569	1.169142	-3.483662
H	-2.737401	1.862389	-2.442838

TS6b

M06L SCF energy in Solvent: -7322.522157 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.395939 a.u.

O	0.133723	0.756134	-0.818808
C	0.447101	2.026086	-1.182463
C	1.795751	2.462063	-1.300052
C	2.019631	3.745738	-1.805413
H	3.050967	4.072281	-1.931614
C	1.008095	4.636709	-2.160754
C	-0.298839	4.209051	-1.971025
H	-1.129610	4.880435	-2.201206
C	-0.590746	2.938539	-1.478486
C	1.328085	5.999043	-2.696542
H	1.873176	6.607308	-1.962627
H	0.419116	6.548838	-2.966621
H	1.961590	5.949277	-3.591804
C	3.032439	1.584741	-0.950166
O	2.838413	0.800056	0.200025
C	4.222983	2.520692	-0.628226
C	4.238795	3.265905	0.597852
C	5.271787	2.679034	-1.511969
C	3.171737	3.259416	1.536635
C	5.370956	4.098488	0.889178
C	6.376486	3.507037	-1.226811

H	5.255169	2.146316	-2.460946
C	3.233432	3.998863	2.695419
H	2.298352	2.650677	1.331047
C	5.406852	4.834991	2.099021
C	6.432994	4.193120	-0.041371
H	7.183312	3.590551	-1.953407
C	4.364024	4.786967	2.990961
H	2.395129	3.974054	3.390707
H	6.283117	5.451965	2.301049
H	7.285073	4.829393	0.199362
H	4.402292	5.363133	3.914435
C	3.374977	0.648864	-2.134499
C	4.426248	-0.326387	-2.004051
C	2.691368	0.722624	-3.333893
C	5.231328	-0.459608	-0.839826
C	4.729728	-1.176150	-3.119857
C	2.988040	-0.122997	-4.423487
H	1.910330	1.471468	-3.451682
C	6.269156	-1.361887	-0.789092
H	5.009433	0.162309	0.021386
C	5.780761	-2.121903	-3.017046
C	3.989469	-1.053713	-4.320995
H	2.419750	-0.023966	-5.347566
C	6.544349	-2.213121	-1.879180
H	6.883887	-1.420426	0.109100
H	5.983787	-2.762826	-3.875860
H	4.235681	-1.709508	-5.157072
H	7.362910	-2.930117	-1.820629
O	-3.326077	-0.362635	-0.025982
N	-2.530125	1.433121	-1.947480
C	-2.023215	2.604165	-1.205841
H	-2.170373	2.390829	-0.136904
H	-2.661075	3.477628	-1.434420
C	-2.318204	1.492501	-3.398828
H	-2.700582	2.451125	-3.798060
H	-1.247097	1.439107	-3.626526
C	-3.134467	0.313304	-3.890911
H	-2.549452	-0.609562	-3.770029
H	-3.395767	0.393010	-4.950945
C	-4.356183	0.301921	-2.960024
H	-4.610600	-0.710652	-2.630114
H	-5.251990	0.691993	-3.455969
C	-3.983672	1.199138	-1.764209
H	-4.492765	2.173130	-1.868417
C	-4.283788	0.591729	-0.346144
C	-5.664689	-0.084789	-0.401814
C	-6.808584	0.605667	-0.801671
H	-6.741719	1.661151	-1.068084
C	-8.054514	-0.013299	-0.875233
H	-8.919028	0.563709	-1.193367
C	-8.173691	-1.362760	-0.533887
C	-7.038756	-2.068292	-0.126846
H	-7.147890	-3.118264	0.137992
C	-5.805922	-1.434718	-0.065489
H	-4.921431	-1.986649	0.244334
O	-9.338784	-2.070722	-0.567513
C	-10.494538	-1.380705	-0.982491
H	-10.731683	-0.541429	-0.311966
H	-10.392721	-0.995376	-2.008019
H	-11.308838	-2.107600	-0.950181
C	-4.344670	1.684537	0.743038
C	-3.830205	1.391748	2.012500
C	-4.922888	2.943071	0.567228
C	-3.870251	2.310492	3.047533
H	-3.381804	0.414202	2.170106
C	-4.971328	3.885430	1.594836
H	-5.344641	3.231065	-0.395641
C	-4.440453	3.570881	2.846297
H	-3.460240	2.075583	4.027579
H	-5.421254	4.856619	1.405215
O	-4.430573	4.411271	3.918852
C	-4.994976	5.688813	3.733566
H	-6.060992	5.628169	3.468433
H	-4.889970	6.207286	4.688695
H	-4.468121	6.256367	2.952199
Zn	-1.609243	-0.153967	-0.823860
Zn	1.488269	-0.470433	0.123674
C	0.199638	-2.315899	1.874887
O	0.219966	-1.087582	1.512731
O	-0.909791	-2.785748	2.494167
C	-2.132702	-2.178071	2.050963
H	-2.073134	-1.095989	2.208178
H	-2.215814	-2.341753	0.966302
C	-3.273946	-2.807370	2.797770
H	-3.152066	-2.683235	3.879456
H	-4.211847	-2.323088	2.503588
H	-3.350877	-3.878457	2.580349
C	1.460290	-2.997714	2.495623

C	2.570680	-3.041955	1.454514
O	2.672894	-2.292134	0.486091
O	3.476192	-3.975129	1.703902
C	4.604153	-4.004696	0.785703
H	4.214279	-4.132499	-0.231281
H	5.088539	-3.023301	0.821555
C	5.508267	-5.123355	1.214873
H	4.999152	-6.091549	1.166540
H	6.378725	-5.162397	0.550976
H	5.867101	-4.973478	2.238423
C	1.117329	-4.427421	2.917723
H	0.292265	-4.434472	3.630255
H	0.793825	-5.005136	2.043827
H	1.985608	-4.918600	3.363344
C	1.946152	-2.105507	3.645759
C	1.617982	-2.399784	4.970846
C	2.679977	-0.941669	3.377400
C	2.015473	-1.554460	6.003332
H	1.043124	-3.292310	5.206332
C	3.074394	-0.097044	4.409467
H	2.956818	-0.675015	2.356744
C	2.743828	-0.401391	5.727339
H	1.750297	-1.801938	7.029798
H	3.639338	0.802656	4.172600
H	3.052207	0.258178	6.536629
H	0.616679	-1.750853	-0.930624
H	0.169963	-3.027221	0.628268
Si	-0.113438	-3.127523	-0.972007
O	-1.491311	-2.191153	-1.475385
O	0.889146	-3.758865	-2.141162
O	-0.873883	-4.574975	-0.544093
C	-2.744639	-2.819396	-1.782342
H	-3.532676	-2.075329	-1.647989
H	-2.727592	-3.182214	-2.817851
H	-2.925920	-3.656047	-1.100471
C	-1.043689	-5.652359	-1.436716
H	-0.080237	-6.036039	-1.794513
H	-1.573357	-6.451273	-0.904300
H	-1.641668	-5.374896	-2.320461
C	1.881374	-3.035432	-2.827981
H	2.840587	-3.562647	-2.743778
H	1.616498	-2.953238	-3.890080
H	2.016334	-2.018219	-2.428128

TS6c

M06L SCF energy in Solvent: -7322.527250 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.401149 a.u.

O	-0.323383	-1.238088	-0.160832
C	-0.693529	-2.541557	-0.135775
C	-2.061415	-2.908371	-0.222899
C	-2.373616	-4.268401	-0.220959
H	-3.417943	-4.563583	-0.309273
C	-1.415077	-5.280789	-0.131357
C	-0.081911	-4.892970	-0.079523
H	0.702838	-5.652238	-0.037010
C	0.292200	-3.549347	-0.079944
C	-1.819566	-6.723280	-0.095935
H	-0.968149	-7.387132	-0.286267
H	-2.592452	-6.948852	-0.841238
H	-2.236688	-7.004114	0.880898
C	-3.162378	-1.837682	-0.414790
O	-3.084554	-0.837235	0.578960
C	-4.557005	-2.493165	-0.280857
C	-5.041048	-2.915082	1.003012
C	-5.345803	-2.723390	-1.390362
C	-4.272364	-2.837453	2.195425
C	-6.347113	-3.504054	1.093947
C	-6.627535	-3.302455	-1.296682
H	-4.977979	-2.442236	-2.374915
C	-4.770263	-3.284696	3.397650
H	-3.276664	-2.411419	2.142803
C	-6.833960	-3.936866	2.351836
C	-7.126988	-3.671846	-0.075180
H	-7.215311	-3.447563	-2.201888
C	-6.066430	-3.830530	3.485362
H	-4.151672	-3.218566	4.291626
H	-7.833357	-4.371281	2.395947
H	-8.119003	-4.115110	0.016305
H	-6.450653	-4.175565	4.444181
C	-3.014923	-1.184862	-1.815099
C	-3.839569	-0.064882	-2.184767
C	-2.117302	-1.668151	-2.748872
C	-4.825818	0.495817	-1.328087
C	-3.713844	0.490141	-3.502439
C	-1.964360	-1.089920	-4.025288
H	-1.515927	-2.540064	-2.500915
C	-5.630270	1.531041	-1.748079
H	-4.927991	0.094139	-0.324691

C	-4.546950	1.567320	-3.893479
C	-2.754146	-0.034069	-4.400953
H	-1.230801	-1.505040	-4.716249
C	-5.490954	2.081416	-3.038122
H	-6.390168	1.927218	-1.073863
H	-4.422936	1.977619	-4.896604
H	-2.662356	0.414430	-5.390767
H	-6.131280	2.903667	-3.354735
O	3.041533	-0.115475	-0.210965
N	2.186094	-2.492053	-1.277667
C	1.748711	-3.199756	-0.049600
H	1.981663	-2.538379	0.795509
H	2.361670	-4.109274	0.078359
C	1.911704	-3.222861	-2.523031
H	2.332767	-4.242986	-2.451203
H	0.831610	-3.321687	-2.677939
C	2.631590	-2.387821	-3.568842
H	1.958866	-1.601860	-3.941007
H	2.932202	-2.983785	-4.436385
C	3.822004	-1.774421	-2.809303
H	3.831859	-0.680748	-2.888958
H	4.788202	-2.117625	-3.191738
C	3.639261	-2.179751	-1.340450
H	4.190418	-3.115431	-1.135126
C	4.034549	-1.078858	-0.292191
C	5.340216	-0.396422	-0.737182
C	6.458669	-1.108144	-1.169744
H	6.423748	-2.196895	-1.233671
C	7.638921	-0.468058	-1.544613
H	8.485737	-1.060695	-1.881320
C	7.714624	0.924640	-1.479647
C	6.601635	1.653240	-1.050575
H	6.675812	2.738333	-1.013390
C	5.434079	0.999292	-0.686914
H	4.559687	1.563751	-0.365880
O	8.815711	1.656752	-1.816164
C	9.947109	0.942397	-2.254728
H	10.322629	0.257215	-1.479993
H	9.735197	0.362296	-3.165514
H	10.711662	1.690622	-2.474063
C	4.294966	-1.720422	1.089078
C	3.719913	-1.144145	2.224777
C	5.107541	-2.837547	1.283367
C	3.936596	-1.651266	3.495707
H	3.067630	-0.290419	2.074439
C	5.336903	-3.370150	2.551865
H	5.591143	-3.324122	0.436190
C	4.751296	-2.773688	3.670141
H	3.478533	-1.195917	4.372572
H	5.973737	-4.245282	2.653987
O	4.910150	-3.208387	4.952605
C	5.731800	-4.336101	5.146327
H	6.759853	-4.154165	4.799610
H	5.741224	-4.522954	6.222150
H	5.336027	-5.221958	4.627668
Zn	1.344225	-0.575531	-0.926724
Zn	-1.596910	0.275971	0.469536
C	-0.275345	2.420564	1.938982
O	-0.515931	1.177902	1.903151
O	0.896035	2.854206	2.446341
C	1.978822	1.904884	2.361226
H	1.744299	1.062681	3.024950
H	2.034442	1.514039	1.333600
C	3.250662	2.606931	2.745104
H	3.195277	3.013347	3.761264
H	4.085258	1.897796	2.701740
H	3.468661	3.429462	2.055160
C	-1.390049	3.451474	2.244265
C	-2.646581	3.069297	1.474772
O	-2.719216	2.243521	0.574231
O	-3.695036	3.789225	1.857545
C	-4.913817	3.549896	1.104374
H	-4.696698	3.738986	0.044987
H	-5.167668	2.487388	1.196243
C	-5.972254	4.459550	1.658455
H	-5.681027	5.510722	1.564355
H	-6.908734	4.313793	1.109352
H	-6.163168	4.248832	2.715706
C	-1.683041	3.339689	3.751405
H	-2.434493	4.076498	4.047685
H	-2.053693	2.337654	3.993114
H	-0.770988	3.504680	4.330985
C	-0.980980	4.859873	1.820996
C	-0.242235	5.691968	2.665529
C	-1.286617	5.316651	0.534653
C	0.177036	6.947268	2.233642
H	0.029221	5.354419	3.663374
C	-0.871155	6.571302	0.102831

H	-1.831327	4.678323	-0.160868
C	-0.136827	7.393113	0.952550
H	0.756606	7.578686	2.904890
H	-1.111420	6.894305	-0.908776
H	0.194539	8.374331	0.617284
H	-0.674601	1.239446	-0.746861
H	-0.048094	2.812281	0.414000
Si	0.331260	2.393135	-1.094342
O	0.996376	1.091578	-2.100016
O	-0.548428	3.407062	-2.068541
O	1.836531	3.118012	-0.938241
C	2.067577	1.390724	-3.003889
H	3.026842	1.391992	-2.473637
H	2.066041	0.621708	-3.786736
H	1.902097	2.370881	-3.461775
C	1.993450	4.387326	-0.348264
H	1.563868	5.178319	-0.980159
H	1.522060	4.446317	0.644309
H	3.068952	4.574028	-0.235921
C	-1.738707	2.972222	-2.693638
H	-2.173417	3.823655	-3.230750
H	-1.534523	2.166699	-3.412772
H	-2.480277	2.602237	-1.968211

TS6d

M06L SCF energy in Solvent: -7322.527369 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.403081 a.u.

O	0.234993	0.896270	-0.574538
C	0.505205	2.169078	-0.970184
C	1.824905	2.692862	-0.972996
C	2.018885	3.983280	-1.471761
H	3.038266	4.370309	-1.491001
C	0.995109	4.797759	-1.951309
C	-0.293092	4.281816	-1.890327
H	-1.137328	4.891928	-2.219900
C	-0.554527	3.005157	-1.395699
C	1.275431	6.169944	-2.484196
H	0.356378	6.668271	-2.813714
H	1.961684	6.145845	-3.341144
H	1.744492	6.812261	-1.727548
C	3.074094	1.901625	-0.498207
O	2.779608	1.029883	0.557026
C	4.116530	2.900554	0.060218
C	3.823700	3.624551	1.264542
C	5.322266	3.127373	-0.571885
C	2.595426	3.508806	1.967982
C	4.798336	4.542796	1.778622
C	6.281301	4.025291	-0.057388
H	5.548517	2.604518	-1.499414
C	2.349482	4.244494	3.103929
H	1.850669	2.808795	1.604884
C	4.515356	5.277006	2.956760
C	6.027338	4.716585	1.098423
H	7.222264	4.163116	-0.588231
C	3.316080	5.136010	3.610525
H	1.395219	4.134524	3.617473
H	5.274286	5.965398	3.330308
H	6.757930	5.415292	1.506928
H	3.109576	5.710825	4.512323
C	3.666286	1.112979	-1.701304
C	4.670083	0.098355	-1.493763
C	3.274465	1.386111	-3.000238
C	5.223337	-0.211400	-0.220126
C	5.193200	-0.608706	-2.631012
C	3.817296	0.712184	-4.113746
H	2.529976	2.158649	-3.178827
C	6.196284	-1.175093	-0.079177
H	4.849717	0.319942	0.648873
C	6.173798	-1.614335	-2.443264
C	4.753265	-0.273161	-3.934269
H	3.479539	0.977525	-5.115144
C	6.670034	-1.896441	-1.193842
H	6.599970	-1.384456	0.910395
H	6.543193	-2.144130	-3.322220
H	5.175340	-0.810712	-4.784258
H	7.430715	-2.665701	-1.064361
O	-3.165583	-0.290170	0.069129
N	-2.364110	1.367221	-1.953917
C	-1.989244	2.604158	-1.242452
H	-2.225609	2.441006	-0.181410
H	-2.645843	3.426869	-1.579700
C	-2.047362	1.363918	-3.387145
H	-2.472601	2.264738	-3.868439
H	-0.960476	1.390535	-3.531622
C	-2.725158	0.092879	-3.865957
H	-2.064662	-0.767624	-3.690257
H	-2.945284	0.114728	-4.937876
C	-3.986690	-0.005997	-2.990522

H	-4.119867	-1.011463	-2.576216
H	-4.896959	0.208720	-3.560517
C	-3.804656	1.029210	-1.863897
H	-4.378147	1.943749	-2.102014
C	-4.174243	0.530325	-0.420731
C	-5.487557	-0.267171	-0.474099
C	-6.590013	0.138812	-1.226076
H	-6.528136	1.034553	-1.846291
C	-7.786905	-0.575986	-1.221925
H	-8.618848	-0.229153	-1.829345
C	-7.899384	-1.727253	-0.439511
C	-6.806349	-2.145387	0.324599
H	-6.908698	-3.043854	0.929979
C	-5.623767	-1.422732	0.302151
H	-4.771446	-1.751534	0.892835
O	-9.018272	-2.501843	-0.358791
C	-10.134378	-2.089752	-1.113588
H	-10.482139	-1.090496	-0.812636
H	-9.914035	-2.077625	-2.191285
H	-10.920980	-2.820462	-0.915403
C	-4.415284	1.712883	0.542819
C	-3.851953	1.676838	1.823853
C	-5.210730	2.813333	0.222878
C	-4.051645	2.701218	2.735034
H	-3.227869	0.825211	2.085679
C	-5.420571	3.857678	1.122401
H	-5.694763	2.876438	-0.752200
C	-4.835124	3.806145	2.389049
H	-3.604398	2.672230	3.726657
H	-6.040760	4.699707	0.826221
O	-4.969510	4.767313	3.345148
C	-5.739146	5.898950	3.008932
H	-6.780515	5.629321	2.778844
H	-5.720542	6.549078	3.885808
H	-5.314429	6.436676	2.148475
Zn	-1.438214	-0.095881	-0.709035
Zn	1.695435	-0.413663	0.085011
C	-0.074792	-2.366566	1.868021
O	-0.004987	-1.287089	1.270760
O	-1.122016	-2.691606	2.600163
C	-2.173461	-1.688135	2.725695
H	-1.711177	-0.783731	3.140924
H	-2.550936	-1.441668	1.726038
C	-3.236425	-2.259682	3.618662
H	-2.846520	-2.496904	4.614041
H	-4.044426	-1.527871	3.729890
H	-3.665467	-3.171747	3.188999
C	0.998591	-3.458335	1.908554
C	2.036301	-3.193773	0.786707
O	2.609056	-2.062531	0.692517
O	2.792525	-4.312561	0.564869
C	3.781159	-4.120053	-0.459750
H	3.257393	-3.790007	-1.377207
H	4.456959	-3.308427	-0.167125
C	4.497196	-5.425034	-0.669576
H	3.809588	-6.214684	-0.993857
H	5.267748	-5.305477	-1.439166
H	4.985411	-5.756214	0.253273
C	0.331350	-4.816390	1.687155
H	-0.405422	-5.026813	2.466042
H	-0.175525	-4.831141	0.714438
H	1.084316	-5.607932	1.682516
C	1.698192	-3.334608	3.268272
C	1.828786	-4.432677	4.120246
C	2.211356	-2.097500	3.680205
C	2.459729	-4.301105	5.354744
H	1.437215	-5.403081	3.825484
C	2.839430	-1.968101	4.914363
H	2.136096	-1.229201	3.027290
C	2.964631	-3.069101	5.757403
H	2.551717	-5.169914	6.004334
H	3.232079	-0.998583	5.214979
H	3.453658	-2.966125	6.724434
H	0.937356	-1.464002	-1.241849
H	1.156647	-3.262837	-0.327316
Si	0.274083	-2.829862	-1.646774
O	-1.257353	-2.106650	-1.341854
O	0.941619	-2.792580	-3.170693
O	-0.325601	-4.408557	-1.708560
C	-2.468833	-2.892365	-1.328310
H	-3.280978	-2.219351	-1.046698
H	-2.634047	-3.337230	-2.313847
H	-2.380695	-3.695680	-0.590159
C	0.564463	-5.480183	-1.914545
H	1.280312	-5.574548	-1.081031
H	-0.021720	-6.404792	-1.966661
H	1.127326	-5.365857	-2.852058
C	1.731718	-1.701997	-3.598352

H	2.138036	-1.944148	-4.586034
H	1.143868	-0.773363	-3.676461
H	2.572306	-1.509062	-2.916024

IM8a

M06L SCF energy in Solvent: -7322.588339 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.452437 a.u.

O	0.545046	-0.198027	-0.730105
C	0.982177	0.588475	-1.723906
C	2.374670	0.721706	-1.993462
C	2.761044	1.558641	-3.039285
H	3.822822	1.657285	-3.264534
C	1.850133	2.263149	-3.832685
C	0.495558	2.071802	-3.577807
H	-0.245994	2.578246	-4.201459
C	0.046850	1.247759	-2.546293
C	2.324244	3.175085	-4.924111
H	3.115304	2.713734	-5.528699
H	2.743289	4.109509	-4.524912
H	1.507823	3.451816	-5.601606
C	3.417260	-0.090182	-1.186242
O	3.293072	0.159841	0.204598
C	4.860274	0.317341	-1.562215
C	5.416481	1.553117	-1.091988
C	5.651503	-0.502607	-2.342373
C	4.667684	2.520308	-0.372652
C	6.785758	1.863056	-1.385668
C	6.991331	-0.185971	-2.646537
H	5.238821	-1.433390	-2.726270
C	5.236114	3.692883	0.067672
H	3.626084	2.303691	-0.173811
C	7.345196	3.074419	-0.907145
C	7.555837	0.966074	-2.162853
H	7.575653	-0.871895	-3.257829
C	6.594386	3.972522	-0.188770
H	4.626959	4.413379	0.615591
H	8.391037	3.283440	-1.134297
H	8.595265	1.215270	-2.377339
H	7.038547	4.900624	0.167960
C	3.216353	-1.604144	-1.441347
C	3.838302	-2.577174	-0.583433
C	2.437142	-2.054520	-2.489555
C	4.739908	-2.242781	0.466528
C	3.572582	-3.971573	-0.807466
C	2.180957	-3.422654	-2.706294
H	1.991211	-1.327827	-3.166162
C	5.310558	-3.215727	1.255539
H	4.964356	-1.196688	0.645310
C	4.171520	-4.943940	0.033610
C	2.729674	-4.365488	-1.874743
H	1.536914	-3.722683	-3.532336
C	5.020154	-4.579492	1.049861
H	5.998803	-2.925103	2.047920
H	3.957214	-5.995844	-0.161887
H	2.536328	-5.428026	-2.025815
H	5.476887	-5.337799	1.684068
H	1.115500	-2.656004	-0.130360
Si	0.154047	-3.568966	0.487029
O	-1.303798	-2.758910	0.381757
O	-0.158653	-4.987378	-0.283469
O	0.643121	-3.949962	2.011554
C	-2.515317	-3.452347	0.705406
H	-2.427790	-3.941429	1.684988
H	-3.311409	-2.702456	0.735847
H	-2.729916	-4.208978	-0.057997
C	1.626083	-3.203270	2.701230
H	2.219430	-3.893013	3.311671
H	2.322048	-2.689287	2.013968
H	1.161682	-2.448902	3.347947
C	0.543055	-6.184947	-0.016496
H	1.577197	-6.002240	0.307406
H	0.033368	-6.757141	0.769327
H	0.561341	-6.783451	-0.934354
O	-3.171232	-0.309268	0.450399
N	-1.908479	-0.233822	-2.027880
C	-1.430376	1.132408	-2.297962
H	-1.727555	1.753118	-1.438493
H	-1.972163	1.540940	-3.173962
C	-1.445493	-1.198626	-3.035361
H	-1.588576	-0.773977	-4.047902
H	-0.373026	-1.385205	-2.900342
C	-2.317819	-2.421417	-2.815378
H	-1.836262	-3.109520	-2.110298
H	-2.473843	-2.976338	-3.746703
C	-3.620623	-1.861057	-2.228029
H	-3.884874	-2.364811	-1.292441
H	-4.477389	-1.998761	-2.896581

C	-3.379347	-0.362821	-1.973512
H	-3.814649	0.219590	-2.806976
C	-3.968193	0.126791	-0.601401
C	-5.376798	-0.482743	-0.473076
C	-6.359092	-0.250855	-1.435607
H	-6.137351	0.393143	-2.289056
C	-7.629168	-0.814675	-1.338135
H	-8.365125	-0.614327	-2.112844
C	-7.942099	-1.621689	-0.240773
C	-6.974917	-1.848621	0.740871
H	-7.237466	-2.470529	1.594470
C	-5.712098	-1.285911	0.618984
H	-4.957282	-1.458340	1.382580
O	-9.151761	-2.221198	-0.040718
C	-10.141389	-1.998823	-1.017509
H	-10.392516	-0.931532	-1.107774
H	-9.830939	-2.372712	-2.004777
H	-11.024198	-2.549584	-0.686165
C	-4.181180	1.650656	-0.503095
C	-4.354133	2.188305	0.782257
C	-4.338819	2.519056	-1.580898
C	-4.652698	3.524578	0.981537
H	-4.239416	1.520848	1.635221
C	-4.622596	3.876259	-1.404076
H	-4.232247	2.155004	-2.602736
C	-4.785373	4.385043	-0.115912
H	-4.783383	3.934180	1.981366
H	-4.720221	4.517975	-2.276212
O	-5.068141	5.686212	0.175319
C	-5.201473	6.567702	-0.915539
H	-6.026495	6.270354	-1.579608
H	-5.417219	7.548948	-0.487820
H	-4.275379	6.624722	-1.506760
Zn	-1.300411	-0.507550	0.121633
Zn	1.676181	-0.325218	0.947631
C	1.900792	1.106766	3.444808
O	2.468999	0.095574	3.036676
O	2.555455	2.085518	4.055632
C	4.006926	1.974443	4.041794
H	4.315642	1.708732	3.022670
H	4.290898	1.147438	4.702101
C	4.553805	3.300234	4.487771
H	4.227572	4.101023	3.815343
H	5.648153	3.272395	4.476962
H	4.226019	3.549250	5.502490
C	0.420429	1.393670	3.229273
C	-0.269498	-0.000892	3.049417
O	-0.036241	-0.594208	1.810442
O	-1.635160	0.166346	3.280429
C	-2.323925	-1.075923	3.380177
H	-1.786089	-1.722135	4.100399
H	-2.309574	-1.582193	2.406842
C	-3.734849	-0.798429	3.820680
H	-3.757394	-0.292260	4.792436
H	-4.301184	-1.733676	3.905103
H	-4.238024	-0.163722	3.082952
C	-0.161777	2.118633	4.447337
H	0.384662	3.045183	4.642482
H	-0.106788	1.486964	5.343037
H	-1.213032	2.354616	4.271284
C	0.279457	2.253159	1.968941
C	-1.002164	2.594023	1.515328
C	1.384620	2.704619	1.235422
C	-1.163940	3.381226	0.378982
H	-1.878843	2.226526	2.046060
C	1.218839	3.475420	0.084480
H	2.400490	2.454008	1.543543
C	-0.055967	3.823597	-0.340472
H	-2.168525	3.639823	0.047802
H	2.091970	3.791157	-0.485216
H	-0.189085	4.418637	-1.242738
H	0.136668	-0.672551	3.839565

IM9a

M06L SCF energy in Solvent: -7322.585617 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.455255 a.u.

O	0.403641	0.619433	-0.717896
C	0.755188	1.866112	-1.066668
C	2.129259	2.224768	-1.128361
C	2.446202	3.530998	-1.500742
H	3.494330	3.817945	-1.573196
C	1.478473	4.490517	-1.814124
C	0.144068	4.096907	-1.778839
H	-0.635634	4.815763	-2.043107
C	-0.236240	2.806998	-1.409098
C	1.873961	5.889426	-2.179816
H	2.746917	5.906508	-2.844001
H	2.143647	6.481814	-1.294389

H	1.059550	6.420439	-2.686317
C	3.224726	1.153490	-0.900522
O	3.107620	0.506602	0.363805
C	4.619767	1.815873	-0.892984
C	5.039322	2.616652	0.222662
C	5.474699	1.682591	-1.968856
C	4.211476	2.907045	1.340360
C	6.348255	3.206444	0.199779
C	6.759225	2.262359	-1.985807
H	5.155914	1.105981	-2.834663
C	4.649860	3.707034	2.369464
H	3.219594	2.469949	1.375965
C	6.773758	4.010164	1.286267
C	7.194342	2.999950	-0.915919
H	7.400133	2.114605	-2.853595
C	5.946169	4.259852	2.353010
H	3.984987	3.914386	3.207352
H	7.775822	4.438705	1.247809
H	8.187071	3.450971	-0.910848
H	6.283862	4.886072	3.177499
C	3.137623	0.091617	-2.028987
C	3.891975	-1.130322	-1.953643
C	2.348663	0.299561	-3.144692
C	4.822126	-1.413521	-0.916634
C	3.758158	-2.102198	-3.004951
C	2.200930	-0.664390	-4.161207
H	1.808367	1.238176	-3.246127
C	5.563969	-2.574532	-0.917247
H	4.934868	-0.695941	-0.109819
C	4.523885	-3.294810	-2.960695
C	2.885550	-1.849876	-4.091054
H	1.539980	-0.457218	-5.002286
C	5.413557	-3.531956	-1.940836
H	6.279623	-2.751820	-0.114375
H	4.405103	-4.013882	-3.773221
H	2.788577	-2.601978	-4.874863
H	6.007065	-4.444826	-1.928090
H	1.190806	-1.741502	-1.620844
Si	0.253951	-2.865483	-1.665285
O	-1.234258	-2.255300	-1.230744
O	0.039903	-3.506681	-3.168299
O	0.695239	-4.037710	-0.582764
C	-2.225590	-3.140828	-0.663378
H	-1.832119	-3.598023	0.249992
H	-3.092367	-2.522276	-0.412057
H	-2.494611	-3.905307	-1.401165
C	2.056260	-4.428753	-0.501785
H	2.307715	-5.164043	-1.279262
H	2.740887	-3.570458	-0.604664
H	2.223877	-4.890495	0.478576
C	0.780006	-4.604247	-3.657854
H	1.865758	-4.425449	-3.611452
H	0.551781	-5.521065	-3.096238
H	0.502467	-4.757960	-4.705650
O	-3.210923	-0.247135	0.245923
N	-2.082454	1.165030	-1.857247
C	-1.700884	2.479800	-1.313062
H	-2.031386	2.502339	-0.263843
H	-2.285157	3.269425	-1.824218
C	-1.609317	0.958340	-3.232149
H	-1.819354	1.861692	-3.835204
H	-0.521772	0.811949	-3.221908
C	-2.398218	-0.247494	-3.731837
H	-1.800627	-1.164663	-3.670754
H	-2.678298	-0.122392	-4.783428
C	-3.622708	-0.326787	-2.804027
H	-3.596549	-1.239990	-2.194894
H	-4.572810	-0.341406	-3.346994
C	-3.533407	0.887697	-1.873717
H	-4.054991	1.753750	-2.323282
C	-4.079156	0.599539	-0.428756
C	-5.455075	-0.074834	-0.559563
C	-6.444905	0.417685	-1.409793
H	-6.247629	1.298973	-2.022109
C	-7.693865	-0.190674	-1.516366
H	-8.433001	0.220471	-2.199323
C	-7.975387	-1.318713	-0.742849
C	-6.998993	-1.817976	0.123400
H	-7.237174	-2.694726	0.722465
C	-5.758613	-1.202661	0.209201
H	-4.996829	-1.588120	0.883633
O	-9.160940	-1.994924	-0.762538
C	-10.164103	-1.498760	-1.616463
H	-10.451335	-0.469710	-1.353334
H	-9.849517	-1.517191	-2.670824
H	-11.025473	-2.157603	-1.486879
C	-4.287081	1.903030	0.371338
C	-3.937038	1.925922	1.726517

C	-4.834996	3.067915	-0.166986
C	-4.084882	3.068174	2.498082
H	-3.530867	1.014368	2.160477
C	-4.990015	4.228991	0.589695
H	-5.146524	3.099078	-1.211025
C	-4.606208	4.235447	1.931924
H	-3.808144	3.080753	3.551029
H	-5.409337	5.117057	0.123446
O	-4.703741	5.313554	2.761806
C	-5.226276	6.498302	2.207042
H	-6.256352	6.359033	1.846679
H	-5.221888	7.237194	3.010933
H	-4.607726	6.863612	1.373695
Zn	1.478487	-0.243502	0.768977
Zn	-1.396081	-0.269930	-0.341747
C	-0.580126	-3.062550	3.214134
O	-1.713083	-3.161331	2.790893
O	0.184982	-4.116511	3.546053
C	-0.379298	-5.404560	3.225688
H	-0.541002	-5.441026	2.139505
H	-1.361378	-5.491035	3.705098
C	0.597054	-6.446831	3.696709
H	1.572917	-6.315482	3.216237
H	0.227842	-7.449287	3.455826
H	0.744390	-6.387774	4.780180
C	0.105783	-1.727474	3.509230
C	-0.467310	-0.728278	2.470341
O	-0.232618	-1.140438	1.177637
O	0.227587	0.520466	2.680586
C	-0.574465	1.672724	2.396010
H	-1.321634	1.786380	3.197762
H	-1.135367	1.511879	1.458050
C	0.314734	2.879716	2.282808
H	0.886019	3.037635	3.204913
H	-0.291752	3.772226	2.088857
H	1.023194	2.771553	1.450854
C	-0.353914	-1.298707	4.906492
H	0.088284	-1.932321	5.683372
H	-1.445020	-1.370292	4.980371
H	-0.072136	-0.258611	5.099517
C	1.615981	-1.770468	3.356222
C	2.464229	-1.025885	4.180397
C	2.193751	-2.483928	2.291842
C	3.839256	-0.997758	3.957967
H	2.050096	-0.447431	5.003177
C	3.570004	-2.468242	2.078555
H	1.548982	-3.078644	1.647178
C	4.398308	-1.718590	2.907964
H	4.475218	-0.400284	4.608569
H	3.991962	-3.031689	1.248236
H	5.472324	-1.689795	2.730668
H	-1.546636	-0.584878	2.645423

TS7a

M06L SCF energy in Solvent: -7322.554985 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.435275 a.u.

O	0.540695	0.717872	-0.562010
C	1.014358	1.915519	-0.970914
C	2.412466	2.149058	-1.022028
C	2.848950	3.381141	-1.513007
H	3.920498	3.560553	-1.591775
C	1.981817	4.391988	-1.933234
C	0.616160	4.141144	-1.849425
H	-0.094892	4.909910	-2.161822
C	0.119307	2.932119	-1.365210
C	2.512044	5.698717	-2.441671
H	3.296450	5.556090	-3.195781
H	2.958617	6.298150	-1.636725
H	1.720329	6.304807	-2.897059
C	3.428685	1.034151	-0.666889
O	3.179045	0.413798	0.585520
C	4.842200	1.647448	-0.525021
C	5.142050	2.510965	0.582450
C	5.833586	1.396921	-1.452275
C	4.178540	2.931938	1.537314
C	6.473595	3.027426	0.721600
C	7.137832	1.915681	-1.317257
H	5.612623	0.771950	-2.314697
C	4.510463	3.771305	2.574886
H	3.155746	2.584887	1.434272
C	6.786347	3.876595	1.812391
C	7.457892	2.702910	-0.241858
H	7.886765	1.678668	-2.071341
C	5.830171	4.241436	2.726961
H	3.742300	4.078858	3.283660
H	7.808843	4.245416	1.900620
H	8.464326	3.103496	-0.117854
H	6.084115	4.898350	3.557515

C	3.407247	-0.030927	-1.791508
C	4.083007	-1.289230	-1.632662
C	2.783992	0.225946	-2.999459
C	4.901413	-1.603938	-0.513546
C	4.012021	-2.256559	-2.693502
C	2.712799	-0.727241	-4.033249
H	2.316638	1.194265	-3.161421
C	5.599056	-2.788790	-0.449890
H	4.966445	-0.886971	0.298585
C	4.702757	-3.488611	-2.567213
C	3.291307	-1.959997	-3.873835
H	2.169569	-0.488434	-4.946327
C	5.489081	-3.752879	-1.472769
H	6.239540	-2.988387	0.408908
H	4.616795	-4.212254	-3.379321
H	3.220597	-2.718291	-4.654112
H	6.035507	-4.692356	-1.400422
H	1.139252	-1.611509	-1.897251
Si	0.099951	-2.536843	-2.325178
O	-1.390095	-1.894982	-1.893708
O	0.162923	-2.673712	-3.970522
O	0.169388	-4.017797	-1.597669
C	-2.466742	-2.747139	-1.439553
H	-2.104386	-3.448127	-0.683913
H	-3.223591	-2.090550	-0.999712
H	-2.883157	-3.290974	-2.296213
C	1.361132	-4.777756	-1.709567
H	1.509411	-5.141189	-2.737913
H	2.248230	-4.192518	-1.422228
H	1.276161	-5.640112	-1.040042
C	-0.825271	-3.409456	-4.665551
H	-0.946722	-4.423253	-4.255027
H	-1.800013	-2.900504	-4.631461
H	-0.514684	-3.492508	-5.711631
O	-3.047732	-0.017871	0.022479
N	-1.910789	1.591039	-1.934637
C	-1.362583	2.757810	-1.212357
H	-1.620861	2.632903	-0.151519
H	-1.885921	3.670478	-1.553183
C	-1.576734	1.598842	-3.366247
H	-1.795423	2.598508	-3.786889
H	-0.503346	1.414877	-3.501737
C	-2.478266	0.526966	-3.962482
H	-1.944716	-0.428327	-4.019917
H	-2.785616	0.787376	-4.980796
C	-3.663548	0.431198	-2.986405
H	-3.730765	-0.571160	-2.543954
H	-4.627593	0.622459	-3.467590
C	-3.388008	1.452356	-1.875636
H	-3.834310	2.431446	-2.133584
C	-3.872064	0.988482	-0.452089
C	-5.309014	0.449436	-0.569441
C	-6.298592	1.078519	-1.324674
H	-6.061981	1.977306	-1.895771
C	-7.599073	0.581081	-1.396046
H	-8.336727	1.097633	-2.005197
C	-7.933110	-0.573671	-0.686308
C	-6.955170	-1.214818	0.079141
H	-7.231270	-2.113971	0.626442
C	-5.666264	-0.706980	0.132287
H	-4.901513	-1.207553	0.722310
O	-9.170999	-1.148230	-0.681724
C	-10.174488	-0.502524	-1.429085
H	-10.349914	0.523599	-1.073077
H	-9.925602	-0.466039	-2.500316
H	-11.083059	-1.092308	-1.290773
C	-3.904186	2.175827	0.534104
C	-3.306816	2.051088	1.794196
C	-4.525743	3.389055	0.236744
C	-3.314356	3.095639	2.706130
H	-2.809787	1.113897	2.042036
C	-4.541305	4.452753	1.136949
H	-5.020353	3.529604	-0.724478
C	-3.929832	4.308226	2.383845
H	-2.843627	2.997140	3.682752
H	-5.033013	5.381778	0.858786
O	-3.881262	5.278795	3.340622
C	-4.492682	6.509347	3.031084
H	-5.570101	6.392056	2.841738
H	-4.347786	7.148044	3.904871
H	-4.029547	6.984572	2.153498
Zn	-1.282064	-0.057850	-0.696415
Zn	1.461261	0.059130	1.138056
C	-1.193197	-3.772689	2.633452
O	-1.939739	-3.978763	1.697788
O	-0.882877	-4.690168	3.560788
C	-1.474120	-5.991660	3.354358
H	-1.156690	-6.359759	2.371110

H	-2.564053	-5.877424	3.321521
C	-1.015639	-6.875563	4.480580
H	0.075847	-6.958769	4.495862
H	-1.434665	-7.880535	4.364565
H	-1.340790	-6.480446	5.448640
C	-0.498249	-2.437902	2.929288
C	-0.983187	-1.494627	1.827419
O	-0.462389	-1.488687	0.700094
O	0.169579	0.194662	2.511056
C	-0.001046	1.419386	3.175938
H	-0.875445	1.327878	3.845694
H	-0.252059	2.229431	2.462258
C	1.226518	1.792989	3.984124
H	1.416251	1.053304	4.771993
H	1.118983	2.778582	4.454778
H	2.120177	1.820100	3.342815
C	-0.993770	-1.938096	4.286845
H	-0.696003	-2.623097	5.085787
H	-2.088143	-1.862817	4.291203
H	-0.588265	-0.943478	4.489302
C	1.009258	-2.617126	2.837492
C	1.875983	-2.045973	3.771362
C	1.554317	-3.317332	1.752304
C	3.255608	-2.162317	3.623645
H	1.473707	-1.487417	4.613055
C	2.932945	-3.439653	1.609046
H	0.888678	-3.751892	1.005825
C	3.787034	-2.857966	2.542488
H	3.915604	-1.696798	4.353549
H	3.345931	-3.978353	0.757106
H	4.865362	-2.939256	2.420245
H	-1.958213	-1.000188	1.986205

IM10

M06L SCF energy in Solvent: -6631.659759 a.u.

PBE0-D3BJ Free energy in Solvent: -6630.756992 a.u.

O	-0.512819	-0.251944	0.394064
C	-1.008322	0.618744	1.294197
C	-2.393295	0.929402	1.296695
C	-2.887974	1.703461	2.346502
H	-3.955750	1.920231	2.376413
C	-2.075015	2.227556	3.353790
C	-0.703801	2.010349	3.248541
H	-0.030010	2.473409	3.973755
C	-0.149709	1.242108	2.224640
C	-2.660232	3.020028	4.483469
H	-3.172650	2.378321	5.214010
H	-3.402796	3.746095	4.129685
H	-1.887467	3.573904	5.029188
C	-3.320058	0.458638	0.144951
O	-2.740544	0.775106	-1.123800
C	-4.660099	1.224582	0.169365
C	-4.706429	2.625947	-0.143257
C	-5.837386	0.578528	0.491201
C	-3.555805	3.410540	-0.422422
C	-5.978047	3.291795	-0.140011
C	-7.082558	1.238959	0.492832
H	-5.817024	-0.476456	0.753009
C	-3.656789	4.755068	-0.697044
H	-2.583198	2.929613	-0.424283
C	-6.045332	4.674638	-0.438505
C	-7.153636	2.569280	0.174291
H	-7.982029	0.680447	0.746447
C	-4.910946	5.397338	-0.714265
H	-2.754405	5.327524	-0.906307
H	-7.024464	5.154859	-0.437149
H	-8.108665	3.095426	0.166204
H	-4.976766	6.460846	-0.939261
C	-3.579662	-1.060698	0.255763
C	-4.038699	-1.830861	-0.871609
C	-3.412926	-1.702965	1.466860
C	-4.391122	-1.266713	-2.131559
C	-4.200355	-3.251170	-0.720798
C	-3.629729	-3.087017	1.622046
H	-3.079021	-1.128442	2.328262
C	-4.799609	-2.058365	-3.181579
H	-4.337287	-0.190630	-2.253179
C	-4.604191	-4.034664	-1.829972
C	-3.987551	-3.854105	0.542815
H	-3.477106	-3.543137	2.598681
C	-4.888431	-3.457525	-3.043414
H	-5.068148	-1.591733	-4.128172
H	-4.704600	-5.112027	-1.689032
H	-4.133554	-4.930610	0.641847
H	-5.203213	-4.071552	-3.885529
H	-1.423568	-2.744972	-0.305607
Si	-0.485336	-3.433455	0.579246
O	1.104942	-3.005391	0.198040
O	-0.630752	-3.008338	2.154544

O	-0.614988	-5.066590	0.401728
C	1.801364	-3.672871	-0.864221
H	1.218889	-3.639472	-1.794188
H	2.746230	-3.140391	-1.010254
H	1.987247	-4.714067	-0.579515
C	-1.237022	-5.669106	-0.715650
H	-0.478331	-6.075813	-1.397800
H	-1.869474	-6.493414	-0.366344
H	-1.870334	-4.961458	-1.272694
C	-0.181724	-3.861336	3.191258
H	-0.852405	-4.723109	3.305590
H	0.836708	-4.234241	3.009062
H	-0.179942	-3.284721	4.122206
Zn	1.342622	-0.867536	-0.057718
O	3.154575	-0.757487	-0.626913
N	2.026953	-0.009253	1.850358
C	1.342753	1.285711	2.027567
H	1.559707	1.895777	1.143385
H	1.803701	1.811704	2.886121
C	1.869245	-0.854533	3.044537
H	2.088349	-0.252885	3.948470
H	0.832670	-1.204635	3.114794
C	2.902748	-1.942409	2.847010
H	2.505458	-2.705666	2.167379
H	3.171507	-2.439157	3.786177
C	4.077244	-1.207030	2.192208
H	4.539978	-1.807863	1.401970
H	4.862741	-0.975786	2.921205
C	3.497749	0.095797	1.605324
H	3.870962	0.975845	2.159909
C	3.809795	0.246687	0.070522
C	5.319118	0.115753	-0.163085
C	6.285909	0.541138	0.746670
H	5.987560	0.960623	1.708403
C	7.650649	0.426475	0.477382
H	8.371528	0.760448	1.219432
C	8.067948	-0.121495	-0.735691
C	7.110777	-0.548464	-1.662316
H	7.454514	-0.975603	-2.602381
C	5.761950	-0.429632	-1.374344
H	5.013478	-0.773945	-2.084637
O	9.371675	-0.289183	-1.102117
C	10.349358	0.120264	-0.175215
H	10.284084	1.198024	0.036438
H	10.265844	-0.430111	0.773909
H	11.315247	-0.098492	-0.635490
C	3.369858	1.642746	-0.415453
C	2.378966	1.782542	-1.393923
C	3.902530	2.812424	0.129021
C	1.907690	3.030476	-1.779396
H	1.969928	0.886751	-1.859518
C	3.449969	4.074139	-0.246970
H	4.698437	2.745788	0.871964
C	2.437057	4.188265	-1.203926
H	1.131768	3.136651	-2.535701
H	3.891973	4.958559	0.205293
O	1.917475	5.368105	-1.643134
C	2.445196	6.547697	-1.080486
H	3.521208	6.649189	-1.285268
H	1.908912	7.373410	-1.552220
H	2.286518	6.585522	0.007324
Zn	-1.275430	-0.255073	-1.475890
O	0.285999	-1.144355	-1.954168
C	0.880978	-1.144599	-3.235895
H	1.964117	-0.981766	-3.106830
H	0.756797	-2.141532	-3.694460
C	0.290761	-0.089106	-4.142859
H	0.740288	-0.108040	-5.143248
H	-0.792136	-0.245642	-4.263815
H	0.444852	0.915957	-3.726844

IM11

M06L SCF energy in Solvent: -6631.658363 a.u.

PBE0-D3BJ Free energy in Solvent: -6630.754612 a.u.

O	0.631260	0.465718	-0.013255
C	1.197168	1.404568	-0.795237
C	2.600927	1.450178	-0.999942
C	3.105726	2.477313	-1.798268
H	4.180219	2.521649	-1.974377
C	2.297615	3.435242	-2.417360
C	0.918483	3.304874	-2.272868
H	0.253210	3.993435	-2.799555
C	0.356423	2.306198	-1.479957
C	2.898818	4.545465	-3.224476
H	3.790708	4.215832	-3.770820
H	3.213043	5.385338	-2.589183
H	2.187353	4.947470	-3.955565
C	3.510688	0.290691	-0.520284

O	3.322042	0.009522	0.858619
C	4.998754	0.643135	-0.701058
C	5.615745	1.630867	0.137053
C	5.762973	0.026326	-1.671575
C	4.909435	2.385218	1.111363
C	7.012664	1.911895	-0.037709
C	7.134667	0.304448	-1.837810
H	5.301771	-0.703632	-2.333238
C	5.544386	3.340285	1.871420
H	3.852303	2.189886	1.257294
C	7.635895	2.891157	0.773054
C	7.751380	1.222235	-1.029204
H	7.695353	-0.217570	-2.611418
C	6.921227	3.594735	1.711204
H	4.974692	3.905664	2.607651
H	8.699608	3.081164	0.626364
H	8.812364	1.446913	-1.141994
H	7.411472	4.349755	2.324008
C	3.149171	-0.979653	-1.342736
C	3.583668	-2.284361	-0.913290
C	2.401306	-0.893057	-2.503224
C	4.472452	-2.497437	0.179654
C	3.155369	-3.440567	-1.652863
C	1.982972	-2.029599	-3.224185
H	2.128678	0.090918	-2.878899
C	4.879786	-3.764698	0.531191
H	4.830512	-1.635925	0.733076
C	3.583982	-4.729330	-1.249121
C	2.335460	-3.284060	-2.796045
H	1.383819	-1.900447	-4.125239
C	4.426628	-4.895317	-0.178123
H	5.569677	-3.891665	1.363990
H	3.238691	-5.589877	-1.822933
H	2.018227	-4.174141	-3.339724
H	4.752918	-5.891414	0.116267
Zn	-1.105297	-0.465758	-0.202618
O	-2.951211	-0.780714	-0.053453
N	-1.572938	0.806779	-1.905261
C	-1.136445	2.141248	-1.419002
H	-1.511904	2.257021	-0.392601
H	-1.627127	2.925760	-2.023437
C	-1.020525	0.464341	-3.225253
H	-1.243232	1.273882	-3.946346
H	0.067382	0.361118	-3.165305
C	-1.754339	-0.811269	-3.572389
H	-1.288616	-1.654683	-3.039199
H	-1.717003	-1.045290	-4.641646
C	-3.169795	-0.558819	-3.046990
H	-3.588880	-1.448961	-2.567180
H	-3.856518	-0.277082	-3.853216
C	-3.045240	0.593526	-2.028084
H	-3.486131	1.517712	-2.439889
C	-3.700236	0.228326	-0.653989
C	-5.123933	-0.288539	-0.905242
C	-6.024091	0.367941	-1.743608
H	-5.721868	1.274309	-2.270586
C	-7.320310	-0.105063	-1.942777
H	-7.989041	0.432138	-2.610462
C	-7.739131	-1.260583	-1.280371
C	-6.849352	-1.926973	-0.433229
H	-7.191533	-2.827452	0.073066
C	-5.561922	-1.445525	-0.253424
H	-4.862799	-1.965652	0.396962
O	-8.981808	-1.812393	-1.396636
C	-9.893276	-1.155340	-2.245296
H	-10.091813	-0.126177	-1.910780
H	-9.533262	-1.124464	-3.284651
H	-10.818719	-1.733434	-2.202807
C	-3.818586	1.452231	0.274288
C	-3.586507	1.298690	1.647659
C	-4.218323	2.713953	-0.170593
C	-3.716702	2.362353	2.527525
H	-3.307653	0.314566	2.019779
C	-4.348067	3.797089	0.696365
H	-4.433504	2.882121	-1.226169
C	-4.092945	3.623924	2.058261
H	-3.539997	2.238271	3.594172
H	-4.651764	4.763370	0.301577
O	-4.189710	4.607593	2.996105
C	-4.589600	5.881458	2.545675
H	-5.588233	5.854066	2.085272
H	-4.617276	6.520468	3.430569
H	-3.876483	6.298438	1.819126
O	-0.038022	-1.932036	0.861309
Si	-0.671618	-1.463784	2.752490
H	-1.088994	-0.234889	2.029767
O	-1.409118	-2.942025	2.703811
C	-2.352282	-3.375498	3.665854

H	-2.748724	-4.335978	3.319356
H	-1.892295	-3.509685	4.652223
H	-3.180027	-2.663686	3.770712
O	-1.184768	-0.991676	4.295485
C	-1.189861	0.358073	4.674325
H	-0.325651	0.598270	5.313887
H	-1.168263	1.040774	3.806523
H	-2.102233	0.570147	5.247458
C	0.046944	-3.275263	0.351647
H	0.335526	-3.197015	-0.708575
H	-0.955519	-3.715391	0.409601
Zn	1.703456	-0.861636	1.097776
O	1.051260	-1.409843	2.973987
C	1.705036	-1.088171	4.200521
H	2.662622	-1.617373	4.217026
H	1.892641	-0.009431	4.263631
H	1.089406	-1.403931	5.046798
C	1.052299	-4.100922	1.113218
H	0.742456	-4.230414	2.154560
H	1.163297	-5.090239	0.654029
H	2.046673	-3.628037	1.102321

TS8

M06L SCF energy in Solvent: -6631.644986 a.u.

PBE0-D3BJ Free energy in Solvent: -6630.738982 a.u.

O	0.589126	0.417551	-0.106297
C	1.138875	1.447320	-0.783722
C	2.545779	1.547965	-0.910741
C	3.057565	2.637083	-1.615629
H	4.136986	2.720923	-1.736026
C	2.249669	3.609349	-2.211931
C	0.870576	3.440667	-2.128414
H	0.209328	4.154180	-2.625930
C	0.299009	2.380328	-1.425368
C	2.854146	4.779373	-2.927176
H	3.737160	4.489800	-3.509751
H	3.184048	5.557432	-2.224969
H	2.139318	5.248191	-3.613506
C	3.462374	0.383703	-0.458904
O	3.227013	-0.001105	0.885196
C	4.942505	0.812017	-0.516166
C	5.447559	1.766771	0.429193
C	5.800491	0.308876	-1.473438
C	4.637008	2.411143	1.401116
C	6.834938	2.128158	0.376724
C	7.162442	0.671183	-1.523566
H	5.423343	-0.392406	-2.214989
C	5.166189	3.330292	2.277555
H	3.584321	2.155573	1.453798
C	7.348370	3.068386	1.303598
C	7.673563	1.554897	-0.608617
H	7.802035	0.238898	-2.291442
C	6.535809	3.659160	2.239574
H	4.517129	3.807080	3.010637
H	8.408288	3.319037	1.250386
H	8.725705	1.839485	-0.630448
H	6.943419	4.382528	2.944046
C	3.203951	-0.823396	-1.405044
C	3.693082	-2.136744	-1.079899
C	2.510018	-0.663797	-2.591501
C	4.482287	-2.422477	0.070346
C	3.404611	-3.228446	-1.971145
C	2.212245	-1.740973	-3.450199
H	2.181687	0.331525	-2.883335
C	4.922894	-3.700182	0.334539
H	4.727163	-1.610935	0.747789
C	3.879592	-4.527789	-1.665903
C	2.643379	-3.005253	-3.141931
H	1.645428	-1.555158	-4.362413
C	4.615982	-4.768469	-0.532825
H	5.526058	-3.883723	1.222761
H	3.641632	-5.337972	-2.356195
H	2.424227	-3.851115	-3.794049
H	4.970927	-5.773237	-0.309381
Zn	-1.173653	-0.384641	-0.229539
O	-3.000626	-0.763433	-0.051868
N	-1.670357	0.920987	-1.868916
C	-1.198497	2.241167	-1.384673
H	-1.571389	2.369809	-0.360360
H	-1.664816	3.038682	-1.991152
C	-1.131442	0.563952	-3.190338
H	-1.329893	1.378713	-3.912201
H	-0.045993	0.428465	-3.127931
C	-1.901916	-0.690260	-3.533928
H	-1.465297	-1.545361	-2.994977
H	-1.870718	-0.931605	-4.601520
C	-3.310190	-0.391094	-3.014539
H	-3.778571	-1.276109	-2.571957

H	-3.966013	-0.048817	-3.823380
C	-3.147764	0.718693	-1.953664
H	-3.603209	1.663768	-2.297261
C	-3.747535	0.296860	-0.565292
C	-5.199421	-0.157070	-0.733243
C	-6.071813	0.376199	-1.680101
H	-5.720286	1.123362	-2.393183
C	-7.403515	-0.032919	-1.763063
H	-8.049616	0.399839	-2.522753
C	-7.884287	-0.994083	-0.873327
C	-7.021743	-1.535563	0.085687
H	-7.413098	-2.284882	0.770596
C	-5.702949	-1.120286	0.149880
H	-5.026936	-1.545830	0.888152
O	-9.162988	-1.467841	-0.862116
C	-10.049899	-0.927868	-1.813582
H	-10.171720	0.158021	-1.685896
H	-9.713822	-1.126360	-2.842248
H	-11.010286	-1.420231	-1.647327
C	-3.741389	1.495929	0.399313
C	-3.121069	1.396232	1.649480
C	-4.335621	2.713857	0.065912
C	-3.057902	2.481726	2.512023
H	-2.695599	0.437442	1.946126
C	-4.279880	3.815494	0.914829
H	-4.862692	2.817708	-0.883656
C	-3.627779	3.704375	2.146908
H	-2.575247	2.404211	3.484756
H	-4.749370	4.748381	0.612788
O	-3.507794	4.714218	3.052166
C	-4.085709	5.953869	2.710784
H	-5.173451	5.870147	2.571166
H	-3.880027	6.623242	3.548374
H	-3.641531	6.371095	1.795023
O	-0.254002	-2.080840	0.625060
Si	-0.443508	-2.011881	2.463189
H	-0.224824	-0.499549	2.113277
O	-0.812514	-3.647889	2.550148
C	-2.117733	-4.124964	2.777904
H	-2.107587	-5.213000	2.637763
H	-2.460738	-3.895259	3.794160
H	-2.844180	-3.692857	2.069773
O	-1.534637	-1.583091	3.663811
C	-1.625448	-0.315616	4.258116
H	-1.191847	-0.345621	5.266662
H	-1.094981	0.459618	3.679608
H	-2.681280	-0.026367	4.338502
C	-0.237541	-3.294023	-0.159634
H	-0.176712	-2.967353	-1.208465
H	-1.196466	-3.807468	-0.018523
Zn	1.577530	-0.775094	1.208506
O	1.248107	-2.056634	2.829325
C	2.006040	-3.180947	3.277523
H	2.676882	-3.519381	2.477851
H	2.602806	-2.872704	4.141451
H	1.329572	-3.994326	3.555431
C	0.928919	-4.183562	0.185097
H	0.792328	-4.645254	1.166049
H	1.040532	-4.974335	-0.566180
H	1.866744	-3.611420	0.188265

IM12

M06L SCF energy in Solvent: -6631.665200 a.u.

PBE0-D3BJ Free energy in Solvent: -6630.762267 a.u.

O	-0.544189	0.038054	0.390214
C	-1.029486	1.113683	1.057407
C	-2.422561	1.374527	1.101853
C	-2.862479	2.412180	1.926703
H	-3.933215	2.599251	1.996421
C	-2.006259	3.229530	2.665620
C	-0.642010	2.998506	2.538808
H	0.066864	3.640551	3.067236
C	-0.139829	1.971311	1.741074
C	-2.544317	4.326933	3.532837
H	-3.085336	5.080709	2.945886
H	-1.741877	4.844335	4.070949
H	-3.252269	3.947507	4.281252
C	-3.451664	0.539357	0.293756
O	-3.018245	0.314262	-1.040524
C	-4.767855	1.340453	0.183310
C	-4.826850	2.515194	-0.637945
C	-5.890899	0.973244	0.897671
C	-3.705791	3.048792	-1.328426
C	-6.068279	3.229171	-0.737024
C	-7.105787	1.681810	0.802337
H	-5.848107	0.105199	1.552436
C	-3.810840	4.191927	-2.085845
H	-2.755411	2.530864	-1.256347

C	-6.143937	4.392779	-1.541213
C	-7.197838	2.780395	-0.012119
H	-7.967263	1.344851	1.376577
C	-5.041311	4.868650	-2.206480
H	-2.931056	4.577339	-2.599350
H	-7.101352	4.910394	-1.609748
H	-8.132451	3.334669	-0.103070
H	-5.111677	5.767929	-2.816546
C	-3.692596	-0.825119	0.979018
C	-4.515082	-1.821815	0.343749
C	-3.135752	-1.118715	2.209146
C	-5.179661	-1.613635	-0.896645
C	-4.723121	-3.078098	1.005177
C	-3.332911	-2.360791	2.847372
H	-2.532295	-0.364706	2.711345
C	-5.994810	-2.580530	-1.441024
H	-5.029088	-0.675466	-1.420017
C	-5.555399	-4.056308	0.406527
C	-4.107266	-3.325164	2.256311
H	-2.864789	-2.544556	3.813979
C	-6.184824	-3.816924	-0.790931
H	-6.495080	-2.386512	-2.388489
H	-5.693577	-5.004736	0.926718
H	-4.273550	-4.287555	2.741261
H	-6.829074	-4.574211	-1.234810
Zn	1.296081	-0.614396	0.249021
O	3.093281	-0.657514	-0.314282
N	1.942496	0.578621	1.908185
C	1.345082	1.882768	1.547563
H	1.593107	2.072632	0.494940
H	1.845678	2.677685	2.130307
C	1.660404	0.195767	3.298588
H	1.900580	1.044472	3.966324
H	0.591791	-0.021972	3.418381
C	2.584265	-0.983623	3.540287
H	2.083331	-1.919605	3.258318
H	2.854495	-1.078918	4.596964
C	3.792859	-0.714047	2.628092
H	3.999442	-1.566199	1.968697
H	4.710809	-0.525806	3.194126
C	3.423158	0.506976	1.770727
H	3.845375	1.432793	2.202515
C	3.860872	0.344298	0.271339
C	5.339088	-0.063103	0.225871
C	6.300478	0.493140	1.069353
H	6.009636	1.216257	1.832695
C	7.647170	0.142541	0.983435
H	8.361050	0.594217	1.667273
C	8.054780	-0.785648	0.024249
C	7.103278	-1.352653	-0.829528
H	7.438210	-2.077177	-1.569090
C	5.768757	-0.994235	-0.725811
H	5.027814	-1.441069	-1.384544
O	9.341364	-1.201859	-0.152550
C	10.314510	-0.640510	0.697052
H	10.372907	0.452059	0.582643
H	10.115186	-0.874159	1.753608
H	11.267176	-1.085345	0.402527
C	3.721048	1.669888	-0.503467
C	3.035594	1.696284	-1.723643
C	4.260900	2.871160	-0.042009
C	2.868438	2.874373	-2.436137
H	2.625348	0.764938	-2.109476
C	4.101116	4.065953	-0.740073
H	4.827724	2.893151	0.889284
C	3.394439	4.072458	-1.945453
H	2.330487	2.891324	-3.381790
H	4.531357	4.980392	-0.339672
O	3.174137	5.180363	-2.706440
C	3.700904	6.397840	-2.230591
H	4.796809	6.360604	-2.144525
H	3.422337	7.155449	-2.965668
H	3.277739	6.668739	-1.252109
O	0.793123	-2.593847	-0.124508
Si	0.120561	-3.021808	-1.655156
H	-0.061232	-1.302857	-1.808020
O	0.124741	-4.693796	-1.538392
C	1.268616	-5.449144	-1.862528
H	1.103619	-6.479008	-1.522992
H	1.451643	-5.452209	-2.944052
H	2.178202	-5.063219	-1.373923
O	1.141459	-2.902405	-2.955846
C	1.812296	-1.733661	-3.375534
H	2.371998	-1.983430	-4.282663
H	1.109376	-0.920959	-3.611950
H	2.513612	-1.378619	-2.605423
C	1.012386	-3.498814	0.971775
H	2.012126	-3.268125	1.369173

H	1.022816	-4.524689	0.591991
Zn	-1.577373	-0.839109	-1.148022
O	-1.596074	-2.888911	-1.605196
C	-2.500970	-3.991486	-1.466482
H	-2.427272	-4.426438	-0.463172
H	-3.509331	-3.603857	-1.627321
H	-2.263241	-4.757713	-2.207102
C	-0.069407	-3.305205	2.004039
H	-1.053053	-3.562403	1.592168
H	0.108448	-3.930814	2.887286
H	-0.122742	-2.256602	2.330834

TS9

M06L SCF energy in Solvent: -6631.664144 a.u.

PBE0-D3BJ Free energy in Solvent: -6630.760583 a.u.

O	-0.500797	0.016419	0.548783
C	-1.003787	1.097624	1.188687
C	-2.399943	1.342838	1.170795
C	-2.888991	2.372764	1.977035
H	-3.963642	2.546884	2.001742
C	-2.073778	3.196810	2.754044
C	-0.702134	2.988752	2.677264
H	-0.025430	3.644140	3.231025
C	-0.150690	1.972158	1.897683
C	-2.661461	4.278519	3.608893
H	-3.217599	5.012751	3.011441
H	-1.885058	4.822680	4.158831
H	-3.368375	3.878174	4.347575
C	-3.374676	0.497341	0.305503
O	-2.893339	0.305298	-1.017161
C	-4.702272	1.277061	0.163799
C	-4.760514	2.459644	-0.646351
C	-5.836338	0.885731	0.846986
C	-3.630639	3.023564	-1.297774
C	-6.011642	3.152660	-0.771376
C	-7.060886	1.573073	0.726190
H	-5.794520	0.013165	1.495520
C	-3.735988	4.173976	-2.044040
H	-2.672641	2.523571	-1.202783
C	-6.086955	4.323877	-1.564566
C	-7.152019	2.676575	-0.081664
H	-7.930675	1.215341	1.274973
C	-4.975419	4.828461	-2.192689
H	-2.848936	4.583086	-2.525841
H	-7.051838	4.824154	-1.653980
H	-8.094141	3.214169	-0.193395
H	-5.045791	5.733579	-2.794156
C	-3.614764	-0.882997	0.954937
C	-4.424782	-1.868927	0.289184
C	-3.071223	-1.200998	2.183924
C	-5.068357	-1.641048	-0.958341
C	-4.640064	-3.137667	0.924341
C	-3.270780	-2.456661	2.794188
H	-2.473574	-0.457520	2.707838
C	-5.875603	-2.597978	-1.531625
H	-4.905130	-0.696782	-1.466629
C	-5.462963	-4.105350	0.296378
C	-4.037507	-3.410072	2.176524
H	-2.812023	-2.658465	3.761873
C	-6.075849	-3.845147	-0.905107
H	-6.359101	-2.388950	-2.484651
H	-5.606441	-5.063603	0.796899
H	-4.208328	-4.382128	2.640141
H	-6.712883	-4.594915	-1.371770
Zn	1.327058	-0.607400	0.357733
O	3.146617	-0.765803	-0.113812
N	1.992749	0.651538	2.001167
C	1.341911	1.948413	1.731508
H	1.595550	2.234726	0.704473
H	1.795871	2.714730	2.387418
C	1.747986	0.186379	3.374049
H	1.951251	1.008383	4.086546
H	0.693588	-0.096607	3.490788
C	2.738358	-0.945842	3.535285
H	2.332029	-1.857746	3.075496
H	2.944923	-1.180080	4.584646
C	3.970175	-0.459960	2.763985
H	4.441859	-1.271358	2.199744
H	4.732005	-0.059177	3.442438
C	3.472686	0.644678	1.810521
H	3.857104	1.633525	2.118223
C	3.845444	0.359718	0.309531
C	5.348457	0.092897	0.193918
C	6.303956	0.734517	0.980941
H	5.996106	1.432120	1.761179
C	7.669542	0.500152	0.817229
H	8.380942	1.015507	1.457693
C	8.100273	-0.397701	-0.159747

C	7.154233	-1.051504	-0.956445
H	7.507704	-1.752478	-1.709817
C	5.803269	-0.806197	-0.777933
H	5.065889	-1.323259	-1.388142
O	9.405122	-0.705873	-0.407103
C	10.373492	-0.056841	0.383761
H	10.338017	1.035224	0.255582
H	10.249200	-0.290790	1.451592
H	11.341921	-0.428858	0.043154
C	3.506305	1.584620	-0.563425
C	2.591114	1.479675	-1.617149
C	4.055735	2.843349	-0.313293
C	2.204208	2.587623	-2.358526
H	2.171202	0.504803	-1.861483
C	3.682939	3.967813	-1.044762
H	4.796889	2.961106	0.478157
C	2.740660	3.845251	-2.070764
H	1.486730	2.498285	-3.171789
H	4.130669	4.930306	-0.810532
O	2.298230	4.876707	-2.840595
C	2.818936	6.156443	-2.559351
H	3.908488	6.193423	-2.704393
H	2.338921	6.838938	-3.263311
H	2.586598	6.471871	-1.531662
O	0.875617	-2.640310	-0.067771
Si	0.200176	-3.184415	-1.533796
H	0.083188	-1.159305	-1.774718
O	0.181005	-4.839692	-1.377972
C	1.308213	-5.625542	-1.699656
H	1.080594	-6.664792	-1.438101
H	1.543919	-5.565988	-2.768876
H	2.204735	-5.314866	-1.139268
O	1.174737	-3.014067	-2.841810
C	1.989414	-1.912976	-3.191943
H	2.656371	-2.246919	-3.993351
H	1.385248	-1.073097	-3.561328
H	2.591852	-1.570625	-2.337759
C	1.111671	-3.501332	1.065985
H	2.129644	-3.272082	1.412708
H	1.087653	-4.544507	0.736869
Zn	-1.361188	-0.706572	-1.186496
O	-1.462888	-2.914595	-1.549369
C	-2.418740	-3.984711	-1.532368
H	-2.390796	-4.511368	-0.572132
H	-3.401456	-3.533357	-1.680048
H	-2.203519	-4.695515	-2.334738
C	0.067694	-3.237363	2.120013
H	-0.935724	-3.468315	1.741458
H	0.251055	-3.843424	3.015637
H	0.060248	-2.179102	2.420227

EtOSi(OMe)$_3$

M06L SCF energy in Solvent: -789.061851 a.u.

PBE0-D3BJ Free energy in Solvent: -788.902548 a.u.

Si	0.361738	0.052601	-0.003649
O	0.765674	-0.835113	-1.323255
O	0.652694	1.628071	-0.362396
O	1.248646	-0.308833	1.329424
C	2.046887	-0.729370	-1.911330
H	2.119182	-1.480948	-2.703980
H	2.203893	0.264871	-2.350201
H	2.845391	-0.917602	-1.178336
C	0.449308	2.637548	0.606394
H	1.105464	2.496181	1.475230
H	0.678125	3.602770	0.143568
H	-0.593644	2.656519	0.955837
C	1.173272	-1.583882	1.934931
H	1.911428	-1.619876	2.742639
H	0.176442	-1.767269	2.357617
H	1.401555	-2.386374	1.217848
O	-1.208514	-0.274216	0.341834
C	-2.227215	-0.102018	-0.640193
H	-1.992695	-0.711983	-1.525291
H	-2.249953	0.950126	-0.967823
C	-3.552427	-0.502710	-0.044758
H	-4.359441	-0.377892	-0.775432
H	-3.532534	-1.551295	0.270862
H	-3.784489	0.109677	0.833416

3a'

M06L SCF energy in Solvent: -690.884657 a.u.

PBE0-D3BJ Free energy in Solvent: -690.687611 a.u.

C	-1.256454	0.604978	-0.362688
O	-1.505565	1.108772	-1.439599
O	-1.973382	-0.381620	0.195077
C	-3.079445	-0.862258	-0.601438
H	-2.685857	-1.201696	-1.566780
H	-3.753237	-0.021190	-0.802984

C	-3.743081	-1.966417	0.173430
H	-3.042749	-2.785259	0.367826
H	-4.589205	-2.367871	-0.393891
H	-4.119532	-1.603241	1.135472
C	-0.054291	0.996296	0.490485
C	-0.442931	1.116715	1.966649
H	-0.853250	0.174996	2.340870
H	-1.209320	1.889121	2.103108
H	0.427359	1.390615	2.573328
C	1.048601	-0.013082	0.218260
C	1.553675	-0.855599	1.209326
C	1.561228	-0.118722	-1.080360
C	2.556917	-1.776024	0.913933
H	1.169698	-0.797564	2.225837
C	2.560211	-1.037698	-1.375328
H	1.172816	0.531734	-1.862659
C	3.063558	-1.870026	-0.377704
H	2.941456	-2.422773	1.700913
H	2.950611	-1.101862	-2.389513
H	3.848409	-2.588647	-0.607084
C	0.332405	2.410915	0.035593
O	1.437573	2.773578	-0.275080
H	-0.528565	3.123326	0.071427

***ent*-3a'**

M06L SCF energy in Solvent: -690.884657 a.u.

PBE0-D3BJ Free energy in Solvent: -690.687611 a.u.

C	1.256454	0.604978	-0.362688
O	1.505565	1.108772	-1.439599
O	1.973382	-0.381620	0.195077
C	3.079445	-0.862258	-0.601438
H	2.685857	-1.201696	-1.566780
H	3.753237	-0.021190	-0.802984
C	3.743081	-1.966417	0.173430
H	3.042749	-2.785259	0.367826
H	4.589205	-2.367871	-0.393891
H	4.119532	-1.603241	1.135472
C	0.054291	0.996296	0.490485
C	0.442931	1.116715	1.966649
H	0.853250	0.174996	2.340870
H	1.209320	1.889121	2.103108
H	-0.427359	1.390615	2.573328
C	-1.048601	-0.013082	0.218260
C	-1.553675	-0.855599	1.209326
C	-1.561228	-0.118722	-1.080360
C	-2.556917	-1.776024	0.913933
H	-1.169698	-0.797564	2.225837
C	-2.560211	-1.037698	-1.375328
H	-1.172816	0.531734	-1.862659
C	-3.063558	-1.870026	-0.377704
H	-2.941456	-2.422773	1.700913
H	-2.950611	-1.101862	-2.389513
H	-3.848409	-2.588647	-0.607084
C	-0.332405	2.410915	0.035593
O	-1.437573	2.773578	-0.275080
H	0.528565	3.123326	0.071427

IM13a

M06L SCF energy in Solvent: -6533.518194 a.u.

PBE0-D3BJ Free energy in Solvent: -6532.581813 a.u.

O	0.961685	-0.562148	0.070188
C	1.713964	-1.204677	0.995994
C	3.100950	-0.949580	1.092925
C	3.820220	-1.591402	2.099061
H	4.884721	-1.377438	2.195550
C	3.234784	-2.487865	2.998938
C	1.871218	-2.733527	2.868540
H	1.381889	-3.435442	3.548664
C	1.104798	-2.116693	1.878987
C	4.056878	-3.163547	4.054777
H	4.633729	-2.442773	4.648690
H	4.785116	-3.860754	3.619123
H	3.430196	-3.737002	4.747606
C	3.739693	0.069678	0.130241
O	3.449834	-0.270177	-1.202833
C	5.281525	0.057147	0.261064
C	6.036717	-1.074278	-0.202315
C	5.964061	1.115749	0.827455
C	5.443802	-2.252085	-0.731117
C	7.467563	-1.047679	-0.090504
C	7.370089	1.138428	0.930470
H	5.410506	1.970860	1.208426
C	6.210685	-3.321236	-1.133560
H	4.364738	-2.292487	-0.826774
C	8.226099	-2.161244	-0.527346
C	8.110226	0.081239	0.471614
H	7.858133	2.004267	1.375694
C	7.615883	-3.279212	-1.039852

H	5.723408	-4.209905	-1.532659
H	9.311779	-2.111607	-0.437570
H	9.198415	0.083815	0.540925
H	8.211234	-4.130650	-1.366436
C	3.201709	1.482692	0.481068
C	3.328351	2.579039	-0.439732
C	2.654668	1.733688	1.726735
C	3.977041	2.475023	-1.702097
C	2.835563	3.872948	-0.054560
C	2.187711	3.006801	2.106018
H	2.588183	0.922678	2.449842
C	4.086985	3.560747	-2.541318
H	4.381758	1.512128	-1.995864
C	2.963229	4.965881	-0.947219
C	2.254260	4.055948	1.224919
H	1.764311	3.144061	3.101010
C	3.568198	4.817143	-2.171971
H	4.590231	3.446022	-3.499990
H	2.584632	5.938721	-0.627971
H	1.907526	5.052797	1.505074
H	3.663226	5.667773	-2.845245
O	-2.585741	-0.109558	-0.127237
N	-1.245643	-1.305613	2.024388
C	-0.347548	-2.450474	1.722997
H	-0.548897	-2.763018	0.693722
H	-0.621652	-3.292925	2.384076
C	-1.138100	-0.899692	3.438379
H	-1.162469	-1.804927	4.074520
H	-0.176024	-0.402454	3.612742
C	-2.353393	-0.024352	3.672788
H	-2.123080	1.014889	3.414892
H	-2.662153	-0.035671	4.723286
C	-3.419626	-0.593820	2.727285
H	-3.897857	0.199510	2.139975
H	-4.220179	-1.108052	3.270222
C	-2.696997	-1.572671	1.785185
H	-2.896407	-2.619726	2.076513
C	-3.085778	-1.341222	0.279382
C	-4.615466	-1.333561	0.152907
C	-5.450922	-2.169248	0.895316
H	-5.028921	-2.850720	1.634445
C	-6.837000	-2.154677	0.741158
H	-7.448999	-2.816556	1.348311
C	-7.417770	-1.284518	-0.182370
C	-6.596872	-0.440860	-0.937698
H	-7.062400	0.232854	-1.654829
C	-5.221338	-0.471205	-0.768383
H	-4.587136	0.192366	-1.352332
O	-8.757447	-1.181091	-0.414083
C	-9.600381	-2.029944	0.330338
H	-9.380618	-3.090636	0.138807
H	-9.517056	-1.841181	1.411043
H	-10.618484	-1.807840	0.004159
C	-2.530187	-2.476134	-0.601912
C	-1.636489	-2.197635	-1.642258
C	-2.852823	-3.814462	-0.371765
C	-1.065317	-3.210032	-2.399501
H	-1.366495	-1.164056	-1.853331
C	-2.292744	-4.846567	-1.120197
H	-3.559397	-4.074553	0.417265
C	-1.385951	-4.545584	-2.140889
H	-0.361987	-2.980808	-3.197891
H	-2.568540	-5.874992	-0.901364
O	-0.775248	-5.473184	-2.929756
C	-1.076202	-6.826046	-2.676806
H	-2.145698	-7.038947	-2.822921
H	-0.492107	-7.405205	-3.394862
H	-0.792668	-7.121882	-1.655867
Zn	-0.796692	0.144883	0.504248
Zn	1.707551	-0.292440	-1.846940
C	-1.136147	2.666563	-1.181972
O	-0.435258	1.668495	-1.060651
O	-1.687182	3.048117	-2.318790
C	-1.549945	2.118115	-3.441872
H	-0.555845	1.661931	-3.393715
H	-1.618102	2.766456	-4.318795
C	-2.648830	1.091957	-3.374250
H	-2.616503	0.554654	-2.417127
H	-2.525716	0.358470	-4.178951
H	-3.634757	1.559727	-3.478287
C	-1.399324	3.666613	-0.065203
C	-0.936427	3.154776	1.283520
O	-0.801909	1.995229	1.643994
C	-0.650908	4.956765	-0.415070
H	-1.156216	5.471383	-1.237410
H	0.378392	4.739594	-0.716532
H	-0.611426	5.631217	0.449055
C	-2.900993	3.893779	0.165884

C	-3.424316	5.171797	0.381869
C	-3.755702	2.784227	0.212475
C	-4.787408	5.340655	0.612234
H	-2.778896	6.047019	0.356946
C	-5.116158	2.961225	0.439729
H	-3.369550	1.768475	0.066788
C	-5.636241	4.238298	0.639718
H	-5.184784	6.341937	0.768233
H	-5.767459	2.087767	0.458410
H	-6.701383	4.374647	0.818545
H	0.777851	-0.325100	-3.076050
H	-0.807719	3.964673	2.034197

TS10a

M06L SCF energy in Solvent: -6533.505947 a.u.

PBE0-D3BJ Free energy in Solvent: -6532.56688 a.u.

O	1.046067	0.413425	0.051070
C	1.701783	1.408993	-0.593877
C	3.115579	1.404458	-0.752079
C	3.711033	2.460229	-1.442232
H	4.791682	2.444106	-1.578832
C	2.993341	3.525258	-1.988243
C	1.610264	3.485915	-1.859196
H	1.003532	4.277485	-2.305532
C	0.958180	2.457675	-1.179078
C	3.689062	4.654977	-2.684481
H	4.536724	4.304052	-3.285580
H	4.093363	5.385076	-1.969579
H	3.009618	5.200566	-3.349964
C	3.963545	0.204825	-0.282699
O	3.673766	-0.093660	1.077047
C	5.470898	0.502982	-0.364507
C	6.078610	1.429236	0.547268
C	6.262885	-0.108300	-1.315765
C	5.348171	2.175394	1.510233
C	7.493749	1.655269	0.462713
C	7.652029	0.116764	-1.394438
H	5.808864	-0.794489	-2.027720
C	5.977154	3.071091	2.343625
H	4.277417	2.018683	1.586381
C	8.108921	2.573560	1.347931
C	8.258830	0.973934	-0.514303
H	8.234274	-0.398367	-2.156805
C	7.370473	3.270416	2.272311
H	5.389498	3.631684	3.069267
H	9.186479	2.721799	1.270249
H	9.333022	1.156132	-0.558131
H	7.855068	3.978155	2.943312
C	3.598748	-1.026803	-1.167536
C	3.939160	-2.360597	-0.744025
C	2.884855	-0.878445	-2.343540
C	4.765414	-2.638528	0.381058
C	3.424251	-3.479032	-1.484185
C	2.419304	-1.978819	-3.089583
H	2.658557	0.125501	-2.698349
C	5.016030	-3.931909	0.777470
H	5.186899	-1.807833	0.936863
C	3.693150	-4.796474	-1.036129
C	2.659312	-3.256430	-2.653530
H	1.845744	-1.802937	-3.999033
C	4.462199	-5.024079	0.078467
H	5.653826	-4.112476	1.641224
H	3.282215	-5.629264	-1.607952
H	2.276534	-4.117888	-3.201373
H	4.662765	-6.041871	0.409592
O	-2.748799	0.045705	0.238909
N	-1.167408	1.274768	-1.682125
C	-0.539094	2.488161	-1.111250
H	-0.884706	2.578132	-0.073577
H	-0.921001	3.377428	-1.644711
C	-0.674868	0.929758	-3.026019
H	-0.753950	1.812052	-3.688587
H	0.381741	0.643959	-2.973981
C	-1.605555	-0.188557	-3.452114
H	-1.231550	-1.145560	-3.065447
H	-1.669286	-0.280756	-4.541263
C	-2.945950	0.172014	-2.793697
H	-3.367858	-0.684672	-2.253319
H	-3.700579	0.485143	-3.522958
C	-2.647009	1.314328	-1.805101
H	-2.928463	2.293141	-2.236553
C	-3.350399	1.107566	-0.417431
C	-4.830981	0.785408	-0.682041
C	-5.590969	1.467766	-1.633596
H	-5.133237	2.246394	-2.244262
C	-6.932767	1.168968	-1.863719
H	-7.479552	1.721680	-2.623368
C	-7.549391	0.158957	-1.124320

C	-6.803490	-0.541695	-0.171800
H	-7.292745	-1.334308	0.391760
C	-5.468192	-0.230150	0.038267
H	-4.890331	-0.793625	0.767074
O	-8.852248	-0.218936	-1.262922
C	-9.617216	0.469278	-2.225312
H	-9.683282	1.543985	-2.000045
H	-9.204437	0.345349	-3.237638
H	-10.616688	0.031087	-2.187241
C	-3.271889	2.389055	0.439218
C	-2.690991	2.347039	1.712940
C	-3.738735	3.624459	-0.010565
C	-2.579050	3.484828	2.497907
H	-2.297073	1.399043	2.073832
C	-3.632600	4.780709	0.760301
H	-4.203520	3.708817	-0.992510
C	-3.049774	4.713642	2.027559
H	-2.120043	3.447260	3.484044
H	-4.008425	5.721357	0.365948
O	-2.896511	5.776502	2.866927
C	-3.349374	7.027072	2.402198
H	-4.431189	7.020389	2.202781
H	-3.134758	7.742048	3.199093
H	-2.822960	7.335012	1.486686
Zn	-0.877620	-0.165193	-0.142910
Zn	2.069982	-1.039297	1.020595
C	-1.177219	-2.037614	2.280719
O	-0.750176	-0.913873	2.029783
O	-1.960482	-2.312688	3.312662
C	-2.483435	-1.183525	4.069892
H	-1.714072	-0.405970	4.109871
H	-2.637842	-1.593416	5.071486
C	-3.755734	-0.700588	3.426466
H	-3.558195	-0.350562	2.405018
H	-4.176759	0.134422	3.997844
H	-4.500776	-1.503551	3.385128
C	-0.830089	-3.297975	1.499532
C	-0.014905	-2.955449	0.243286
O	-0.366918	-2.095569	-0.599965
C	-0.015654	-4.210777	2.420338
H	-0.651696	-4.651434	3.192790
H	0.792701	-3.656370	2.907252
H	0.449263	-5.019187	1.843175
C	-2.107257	-3.966877	0.979670
C	-2.274115	-5.352758	1.014881
C	-3.113996	-3.176531	0.409629
C	-3.432158	-5.937804	0.506259
H	-1.506195	-5.991239	1.446840
C	-4.269636	-3.763599	-0.092363
H	-3.006160	-2.089727	0.352174
C	-4.433712	-5.146885	-0.046188
H	-3.547431	-7.019636	0.546363
H	-5.043142	-3.128493	-0.524130
H	-5.339022	-5.605473	-0.440443
H	1.304034	-2.431000	1.127561
H	0.582100	-3.814455	-0.119643

IM14a

M06L SCF energy in Solvent: -6533.560070 a.u.

PBE0-D3BJ Free energy in Solvent: -6532.618286 a.u.

O	-0.326663	-1.094566	0.240278
C	-0.924307	-2.262596	-0.061930
C	-2.324063	-2.367456	-0.265746
C	-2.843398	-3.629422	-0.558755
H	-3.915812	-3.725515	-0.727089
C	-2.054333	-4.777225	-0.679085
C	-0.675320	-4.626044	-0.554583
H	-0.019873	-5.488213	-0.702033
C	-0.103655	-3.392205	-0.254194
C	-2.676218	-6.114165	-0.947712
H	-3.527022	-6.037286	-1.635691
H	-3.058842	-6.576994	-0.027216
H	-1.955771	-6.816741	-1.383150
C	-3.209387	-1.101146	-0.337704
O	-2.990104	-0.242082	0.769365
C	-4.700836	-1.483922	-0.336264
C	-5.311968	-1.994358	0.856790
C	-5.467827	-1.373020	-1.478716
C	-4.598007	-2.224980	2.062364
C	-6.706410	-2.333203	0.830825
C	-6.837654	-1.705210	-1.499022
H	-5.009414	-1.014530	-2.398356
C	-5.224643	-2.740964	3.173074
H	-3.543695	-1.971933	2.097316
C	-7.320695	-2.849631	1.998010
C	-7.448930	-2.167602	-0.362723
H	-7.401729	-1.589922	-2.423365
C	-6.599356	-3.051179	3.148828

H	-4.650074	-2.911256	4.082487
H	-8.382682	-3.094019	1.957462
H	-8.507771	-2.427349	-0.360647
H	-7.082934	-3.454811	4.037447
C	-2.845387	-0.310066	-1.629234
C	-3.337774	1.032497	-1.814209
C	-2.008890	-0.835446	-2.597908
C	-4.253445	1.660776	-0.922333
C	-2.930363	1.773818	-2.974425
C	-1.581191	-0.088314	-3.714626
H	-1.668365	-1.864401	-2.497209
C	-4.724309	2.931981	-1.162781
H	-4.573501	1.117044	-0.039237
C	-3.435982	3.081438	-3.185945
C	-2.026595	1.195479	-3.897394
H	-0.902633	-0.545682	-4.434436
C	-4.312331	3.657266	-2.299241
H	-5.439922	3.375391	-0.470331
H	-3.106531	3.623662	-4.072827
H	-1.709840	1.783021	-4.759177
H	-4.694573	4.661865	-2.475780
O	3.079507	0.169067	-0.739490
N	1.881792	-2.315644	-1.266299
C	1.384676	-3.223398	-0.199197
H	1.692328	-2.799319	0.762929
H	1.886540	-4.202639	-0.306414
C	1.479943	-2.759112	-2.612613
H	1.712588	-3.834062	-2.738753
H	0.397777	-2.640544	-2.742446
C	2.331604	-1.900540	-3.518190
H	1.911184	-0.885303	-3.567795
H	2.385523	-2.284927	-4.542265
C	3.681346	-1.881919	-2.800006
H	4.198652	-0.925855	-2.923554
H	4.343623	-2.663758	-3.191432
C	3.367742	-2.145369	-1.313444
H	3.824312	-3.090704	-0.973198
C	3.825236	-0.953302	-0.403360
C	5.311117	-0.660324	-0.633227
C	6.260944	-1.645852	-0.898186
H	5.957355	-2.688706	-1.002681
C	7.613069	-1.338242	-1.057296
H	8.319789	-2.135600	-1.272543
C	8.034261	-0.013341	-0.944595
C	7.093326	0.986812	-0.678243
H	7.438872	2.015589	-0.598735
C	5.755881	0.662218	-0.526713
H	5.018015	1.436888	-0.332819
O	9.326648	0.402767	-1.083195
C	10.288749	-0.588340	-1.356084
H	10.340061	-1.338883	-0.553194
H	10.085264	-1.103457	-2.306984
H	11.247329	-0.069859	-1.426149
C	3.641679	-1.318400	1.083562
C	2.882827	-0.500185	1.927218
C	4.199473	-2.471826	1.639340
C	2.648072	-0.839947	3.252443
H	2.485636	0.434956	1.531748
C	3.975204	-2.833650	2.964497
H	4.824426	-3.120290	1.023863
C	3.183509	-2.017514	3.778863
H	2.052017	-0.203071	3.902629
H	4.418591	-3.747346	3.352490
O	2.893433	-2.276518	5.084414
C	3.421843	-3.461848	5.633824
H	4.521637	-3.464469	5.613650
H	3.080556	-3.492884	6.670408
H	3.055878	-4.353623	5.104191
Zn	1.244290	-0.290126	-0.683136
Zn	-1.373468	0.646086	0.482876
C	0.807498	2.516865	0.044271
O	0.142707	1.409408	-0.510348
C	-0.071644	3.783355	0.067655
C	-0.553340	4.093377	-1.348680
H	0.307570	4.238722	-2.011451
H	-1.125292	3.246811	-1.739017
H	-1.184592	4.987128	-1.380152
C	0.738072	4.909925	0.702086
C	1.099572	4.812201	2.052094
C	1.171311	6.020280	-0.023907
C	1.876447	5.793234	2.657492
H	0.766445	3.953889	2.638413
C	1.952495	7.002797	0.580159
H	0.899659	6.125855	-1.071878
C	2.308290	6.893359	1.920472
H	2.146190	5.697192	3.707766
H	2.281897	7.860286	-0.004116
H	2.918089	7.662627	2.390686

C	-1.287860	3.528812	0.945763
O	-1.508870	2.484331	1.569321
O	-2.112589	4.559231	0.998967
C	-3.308524	4.392874	1.808227
H	-3.788466	3.451766	1.517818
H	-2.993136	4.299419	2.853813
C	-4.173461	5.595905	1.563104
H	-4.438817	5.673502	0.503164
H	-5.098660	5.515252	2.143085
H	-3.663725	6.519351	1.856411
H	1.706640	2.746241	-0.548510
H	1.152988	2.311050	1.074118

IM13c

M06L SCF energy in Solvent: -6533.512659 a.u.

PBE0-D3BJ Free energy in Solvent: -6532.574476 a.u.

O	0.791706	-0.764953	0.058177
C	1.520663	-1.581758	0.860725
C	2.918890	-1.406462	0.973005
C	3.615106	-2.234148	1.852338
H	4.688995	-2.089557	1.967781
C	2.996074	-3.237289	2.605201
C	1.620779	-3.394427	2.464263
H	1.103257	-4.167434	3.038116
C	0.875172	-2.590743	1.600804
C	3.796596	-4.112248	3.522215
H	4.445429	-3.524775	4.184350
H	4.455286	-4.791000	2.963788
H	3.150661	-4.732366	4.154497
C	3.601692	-0.289231	0.160075
O	3.287637	-0.425137	-1.204878
C	5.141766	-0.399991	0.278633
C	5.845269	-1.472960	-0.367226
C	5.868896	0.512555	1.017864
C	5.201750	-2.525243	-1.072052
C	7.276454	-1.526722	-0.263161
C	7.273811	0.454693	1.117203
H	5.351215	1.314040	1.539805
C	5.921081	-3.545560	-1.650107
H	4.121466	-2.507113	-1.156885
C	7.985892	-2.582641	-0.886213
C	7.967663	-0.538300	0.477152
H	7.798941	1.209586	1.700584
C	7.327325	-3.575679	-1.568500
H	5.394755	-4.338462	-2.179553
H	9.073015	-2.593490	-0.800340
H	9.054896	-0.594285	0.537595
H	7.884812	-4.384441	-2.038750
C	3.143468	1.090980	0.696477
C	3.410596	2.293598	-0.043949
C	2.542622	1.206340	1.936471
C	4.089524	2.312111	-1.294326
C	3.036694	3.558676	0.523531
C	2.170111	2.450340	2.484940
H	2.358710	0.306595	2.522211
C	4.346961	3.493778	-1.951492
H	4.397535	1.367120	-1.729309
C	3.325171	4.754624	-0.178751
C	2.404160	3.607898	1.789871
H	1.689987	2.478310	3.462699
C	3.958390	4.729794	-1.397568
H	4.868543	3.471283	-2.907068
H	3.043616	5.701511	0.285065
H	2.127273	4.580914	2.200016
H	4.176806	5.658186	-1.924299
O	-2.748937	0.089822	0.275153
N	-1.381289	-1.644342	1.990049
C	-0.603638	-2.795827	1.464994
H	-0.878225	-2.926407	0.412641
H	-0.915306	-3.707811	2.006028
C	-1.141576	-1.437401	3.430865
H	-1.216237	-2.407922	3.957102
H	-0.127398	-1.051618	3.591317
C	-2.250345	-0.496032	3.844874
H	-1.975332	0.534055	3.587254
H	-2.438469	-0.524409	4.923288
C	-3.446406	-0.958799	3.009277
H	-4.043741	-0.112988	2.652245
H	-4.119140	-1.596769	3.594418
C	-2.865660	-1.750949	1.821718
H	-3.136049	-2.819274	1.890892
C	-3.319282	-1.165948	0.431449
C	-4.846690	-1.039293	0.406451
C	-5.706946	-1.959524	1.005659
H	-5.304334	-2.805271	1.564503
C	-7.093869	-1.827339	0.935866
H	-7.724731	-2.565094	1.425273
C	-7.649688	-0.748105	0.247510

C	-6.802929	0.189096	-0.352801
H	-7.250814	1.030250	-0.878548
C	-5.428031	0.041966	-0.267804
H	-4.770930	0.781884	-0.719427
O	-8.987020	-0.517946	0.115329
C	-9.855975	-1.453366	0.711231
H	-9.722060	-2.459436	0.286953
H	-9.710743	-1.506877	1.800427
H	-10.868640	-1.104288	0.499464
C	-2.880553	-2.119719	-0.699629
C	-1.963040	-1.706292	-1.672452
C	-3.329044	-3.440543	-0.766283
C	-1.495945	-2.570873	-2.652386
H	-1.592291	-0.681204	-1.665873
C	-2.873804	-4.326987	-1.738993
H	-4.056834	-3.802640	-0.039706
C	-1.945122	-3.893063	-2.690038
H	-0.773871	-2.231549	-3.392740
H	-3.248640	-5.347348	-1.748665
O	-1.432933	-4.675128	-3.679735
C	-1.865242	-6.015852	-3.723721
H	-2.950315	-6.087674	-3.889745
H	-1.340680	-6.475418	-4.563620
H	-1.612019	-6.554788	-2.798789
Zn	-0.873900	-0.014271	0.683911
Zn	1.541706	-0.272867	-1.820464
C	-1.621737	2.334516	-0.850368
O	-0.608001	1.644707	-0.883236
O	-2.484486	2.472041	-1.839285
C	-2.251458	1.717124	-3.067892
H	-1.353853	1.102042	-2.940618
H	-2.050032	2.477693	-3.829819
C	-3.479101	0.906395	-3.376245
H	-3.656294	0.156276	-2.598322
H	-3.338287	0.378562	-4.326068
H	-4.369082	1.540002	-3.462941
C	-1.964704	3.246496	0.325437
C	-1.185743	2.874607	1.569717
O	-0.758424	1.774932	1.882552
C	-3.439984	3.113236	0.739029
H	-3.668393	3.771598	1.585852
H	-3.651511	2.071330	1.001381
H	-4.081808	3.393636	-0.101539
C	-1.568343	4.663706	-0.089277
C	-2.495055	5.703633	-0.182316
C	-0.227492	4.915768	-0.405782
C	-2.089648	6.972685	-0.586521
H	-3.542093	5.529398	0.054975
C	0.173058	6.183231	-0.815354
H	0.509318	4.112129	-0.345657
C	-0.756921	7.215403	-0.906459
H	-2.823783	7.773248	-0.657507
H	1.216560	6.353342	-1.074133
H	-0.444330	8.206365	-1.230482
H	0.599323	-0.124971	-3.030407
H	-1.065601	3.711522	2.290853

3a

M06L SCF energy in Solvent: -692.101253 a.u.

PBE0-D3BJ Free energy in Solvent: -691.880882 a.u.

C	-1.314412	0.560980	-0.150945
O	-1.820415	1.209359	-1.052154
O	-1.800758	-0.617359	0.260846
C	-2.951185	-1.100547	-0.466938
H	-2.686604	-1.157815	-1.529544
H	-3.756762	-0.362511	-0.372818
C	-3.320621	-2.438382	0.110509
H	-2.495282	-3.150939	0.012108
H	-4.189898	-2.847251	-0.415306
H	-3.573372	-2.354260	1.172643
C	-0.069035	0.964644	0.630087
C	0.290645	2.424088	0.256290
O	0.517758	2.654280	-1.105107
C	-0.396681	0.940274	2.124117
H	-0.593658	-0.074621	2.481409
H	-1.281655	1.552616	2.333987
H	0.433204	1.358615	2.706186
C	1.064130	0.018659	0.251077
C	1.906005	-0.552693	1.208621
C	1.303538	-0.269307	-1.098684
C	2.958704	-1.382844	0.830472
H	1.744673	-0.355220	2.266583
C	2.352332	-1.099003	-1.477261
H	0.665922	0.174922	-1.860735
C	3.186465	-1.659933	-0.513252
H	3.601849	-1.816173	1.594980
H	2.519896	-1.306782	-2.532891
H	4.008492	-2.309848	-0.808268

H	-0.508495	3.079083	0.651084
H	-0.338191	2.476826	-1.533434
H	1.217895	2.687488	0.780789

***ent*-3a**

M06L SCF energy in Solvent: -692.101249 a.u.

PBE0-D3BJ Free energy in Solvent: -691.880878 a.u.

C	1.314283	0.560955	-0.151185
O	1.819738	1.209447	-1.052617
O	1.801082	-0.617264	0.260438
C	2.951334	-1.100214	-0.467786
H	2.686273	-1.157777	-1.530265
H	3.756701	-0.361873	-0.374249
C	3.321501	-2.437782	0.109766
H	2.496371	-3.150663	0.011919
H	4.190679	-2.846494	-0.416338
H	3.574711	-2.353360	1.171770
C	0.069055	0.964251	0.630325
C	-0.290786	2.423916	0.257589
O	-0.518040	2.655151	-1.103613
C	0.397160	0.938926	2.124241
H	0.594122	-0.076226	2.480825
H	1.282275	1.551036	2.334209
H	-0.432491	1.357008	2.706816
C	-1.064179	0.018429	0.251149
C	-1.905382	-0.553986	1.208637
C	-1.304381	-0.268267	-1.098752
C	-2.958165	-1.383962	0.830328
H	-1.743449	-0.357489	2.266691
C	-2.353270	-1.097757	-1.477502
H	-0.667333	0.176856	-1.860763
C	-3.186712	-1.659775	-0.513522
H	-3.600757	-1.818142	1.594815
H	-2.521475	-1.304492	-2.533233
H	-4.008807	-2.309547	-0.808663
H	0.508244	3.078768	0.652848
H	0.338000	2.478500	-1.532077
H	-1.218050	2.686815	0.782317

IM15

M06L SCF energy in Solvent: -6577.137479 a.u.

PBE0-D3BJ Free energy in Solvent: -6576.301821 a.u.

O	-0.401352	-0.402916	0.354119
C	-0.890273	0.465021	1.267995
C	-2.256035	0.843710	1.234354
C	-2.759771	1.570251	2.315553
H	-3.818311	1.829134	2.318600
C	-1.970034	1.992306	3.384691
C	-0.604315	1.731262	3.309351
H	0.061238	2.128136	4.079900
C	-0.042476	1.003628	2.260935
C	-2.567243	2.720840	4.550120
H	-2.965992	2.028530	5.305331
H	-3.399285	3.365183	4.242407
H	-1.826722	3.350875	5.057087
C	-3.182652	0.497903	0.035344
O	-2.536967	0.752171	-1.216324
C	-4.402753	1.437528	0.018604
C	-4.227313	2.839863	-0.238036
C	-5.675638	0.953517	0.240041
C	-2.960952	3.455434	-0.425273
C	-5.386944	3.683167	-0.278806
C	-6.811549	1.787764	0.195363
H	-5.815894	-0.103967	0.454987
C	-2.847636	4.807353	-0.652057
H	-2.067689	2.840692	-0.397148
C	-5.234712	5.070543	-0.521504
C	-6.670785	3.125657	-0.066013
H	-7.796858	1.357797	0.367332
C	-3.992652	5.627118	-0.706157
H	-1.858971	5.240517	-0.797200
H	-6.131596	5.689811	-0.552053
H	-7.539646	3.782974	-0.106072
H	-3.891466	6.695859	-0.889871
C	-3.616871	-0.983279	0.113198
C	-4.132373	-1.675179	-1.040494
C	-3.500166	-1.678000	1.300256
C	-4.424568	-1.041807	-2.281996
C	-4.404457	-3.082699	-0.938271
C	-3.815002	-3.048475	1.405788
H	-3.111622	-1.166534	2.177718
C	-4.895623	-1.761509	-3.357245
H	-4.267953	0.027656	-2.372345
C	-4.868510	-3.792610	-2.072839
C	-4.230541	-3.746256	0.301269
H	-3.686111	-3.551041	2.363203
C	-5.103360	-3.151931	-3.264782
H	-5.115277	-1.244539	-4.290018

H	-5.053548	-4.862982	-1.969816
H	-4.449948	-4.813292	0.359695
H	-5.465389	-3.709096	-4.127253
H	-1.539405	-2.758348	-0.502372
Si	-0.631899	-3.477805	0.394518
O	0.984067	-3.117604	0.044664
O	-0.797820	-3.062969	1.970235
O	-0.819766	-5.100628	0.190829
C	1.684195	-3.814875	-1.003680
H	1.176778	-3.672307	-1.964408
H	2.684831	-3.377592	-1.061376
H	1.742153	-4.878999	-0.753927
C	-1.490350	-5.664306	-0.919896
H	-0.762430	-6.061409	-1.639815
H	-2.121270	-6.488357	-0.568381
H	-2.132266	-4.932323	-1.433204
C	-0.350698	-3.930642	2.997380
H	-0.920888	-4.868967	2.998600
H	0.718072	-4.169516	2.890983
H	-0.501372	-3.419708	3.953696
Zn	1.434558	-1.042553	-0.066255
O	3.231251	-0.982021	-0.676574
N	2.157401	-0.213967	1.808359
C	1.456651	1.043303	2.117948
H	1.699922	1.748308	1.315198
H	1.890388	1.468319	3.043590
C	2.060860	-1.195017	2.903812
H	2.256663	-0.693807	3.871394
H	1.045881	-1.610073	2.936952
C	3.151698	-2.187957	2.570030
H	2.814284	-2.849601	1.760989
H	3.428295	-2.816583	3.423738
C	4.290588	-1.293522	2.080928
H	4.908072	-1.787311	1.324198
H	4.951395	-1.018841	2.912867
C	3.615472	-0.035251	1.505010
H	3.959488	0.875097	2.024682
C	3.835810	0.100032	-0.048222
C	5.329595	0.111897	-0.373180
C	6.304268	0.627554	0.479451
H	6.030522	1.001910	1.466758
C	7.651451	0.669957	0.115714
H	8.380326	1.072439	0.814444
C	8.041035	0.190048	-1.134539
C	7.075495	-0.334040	-2.000950
H	7.398258	-0.707810	-2.970625
C	5.744874	-0.370521	-1.620935
H	4.992349	-0.784462	-2.288256
O	9.324428	0.186218	-1.597686
C	10.308079	0.731834	-0.750606
H	10.102159	1.786852	-0.515904
H	10.390861	0.171049	0.192506
H	11.251639	0.660899	-1.295818
C	3.224305	1.434423	-0.523887
C	2.168038	1.450797	-1.442829
C	3.634126	2.659967	0.005952
C	1.487001	2.624183	-1.744866
H	1.885415	0.524752	-1.943330
C	2.971698	3.848384	-0.289651
H	4.484490	2.691255	0.689034
C	1.869691	3.829711	-1.151844
H	0.655300	2.632570	-2.448383
H	3.314415	4.778499	0.157111
O	1.129536	4.923245	-1.485319
C	1.490002	6.148747	-0.888342
H	2.506291	6.456896	-1.174327
H	0.773438	6.885647	-1.257108
H	1.428434	6.098218	0.208618
Zn	-1.146221	-0.374538	-1.511785
F	0.336013	-1.275725	-2.081982

IM16

M06L SCF energy in Solvent: -6577.139753 a.u.

PBE0-D3BJ Free energy in Solvent: -6576.301188 a.u.

O	0.608835	0.098770	-0.510906
C	1.293082	-0.367895	-1.574954
C	2.691171	-0.600502	-1.537215
C	3.299067	-1.064331	-2.704171
H	4.370877	-1.262330	-2.689156
C	2.596078	-1.322020	-3.885695
C	1.212349	-1.157336	-3.864654
H	0.623451	-1.408977	-4.750172
C	0.555144	-0.689588	-2.729054
C	3.311260	-1.773607	-5.122943
H	3.680209	-0.922731	-5.712698
H	2.657238	-2.357724	-5.781419
H	4.185073	-2.391496	-4.884336
C	3.463208	-0.507846	-0.198774

O	3.239376	0.747934	0.423871
C	4.979792	-0.646108	-0.408112
C	5.719646	0.401952	-1.049688
C	5.656182	-1.772617	0.015160
C	5.115729	1.572824	-1.579487
C	7.138524	0.254792	-1.204886
C	7.051203	-1.911219	-0.135690
H	5.102345	-2.581810	0.486906
C	5.866071	2.539547	-2.208167
H	4.044161	1.699944	-1.467516
C	7.880401	1.276039	-1.847137
C	7.780480	-0.913498	-0.728125
H	7.540281	-2.815371	0.223567
C	7.262239	2.398658	-2.340408
H	5.374422	3.425770	-2.607504
H	8.958351	1.145694	-1.947293
H	8.860015	-1.004671	-0.850454
H	7.844049	3.174504	-2.835892
C	2.926753	-1.635854	0.733633
C	3.111664	-1.558634	2.158982
C	2.200693	-2.699338	0.227124
C	3.948453	-0.594818	2.793579
C	2.440940	-2.510219	3.000980
C	1.567232	-3.646702	1.056522
H	2.106648	-2.804274	-0.852313
C	4.067958	-0.547973	4.164422
H	4.497735	0.106629	2.174511
C	2.580287	-2.420982	4.407607
C	1.661987	-3.538596	2.421058
H	0.997074	-4.457393	0.602960
C	3.367280	-1.455276	4.984791
H	4.725119	0.192792	4.617823
H	2.051995	-3.148522	5.024135
H	1.156757	-4.247077	3.077332
H	3.466240	-1.400897	6.067572
Zn	-1.000479	-0.711866	0.324659
O	-2.826773	-0.940281	0.730761
N	-1.507828	-1.537368	-1.664839
C	-0.941312	-0.602498	-2.668170
H	-1.257599	0.410114	-2.389139
H	-1.376741	-0.828817	-3.659271
C	-1.019981	-2.918383	-1.858086
H	-1.076757	-3.193976	-2.928280
H	0.031726	-2.987479	-1.557225
C	-1.977397	-3.738591	-1.031153
H	-1.752719	-3.615807	0.038104
H	-1.935351	-4.807687	-1.265043
C	-3.316005	-3.094864	-1.364875
H	-4.061421	-3.242647	-0.579461
H	-3.725418	-3.531791	-2.284787
C	-3.006314	-1.599051	-1.591618
H	-3.418937	-1.270104	-2.559377
C	-3.572497	-0.702475	-0.429384
C	-5.036217	-1.086076	-0.191557
C	-5.986324	-0.953025	-1.203169
H	-5.687503	-0.556723	-2.175782
C	-7.321167	-1.296710	-1.002427
H	-8.034089	-1.178152	-1.814458
C	-7.725923	-1.776050	0.246017
C	-6.785376	-1.904882	1.271748
H	-7.121487	-2.275265	2.238112
C	-5.458557	-1.565151	1.051104
H	-4.720257	-1.667860	1.843071
O	-9.004234	-2.134758	0.558788
C	-9.969721	-2.010971	-0.459154
H	-10.071703	-0.969819	-0.799543
H	-9.730901	-2.643907	-1.326926
H	-10.914514	-2.341443	-0.022609
C	-3.574934	0.806536	-0.732870
C	-3.765925	1.663469	0.364660
C	-3.475035	1.396854	-1.990389
C	-3.791523	3.037889	0.225146
H	-3.885084	1.216921	1.350376
C	-3.480644	2.786289	-2.155838
H	-3.383956	0.778855	-2.883381
C	-3.626931	3.612917	-1.042911
H	-3.911063	3.692745	1.086057
H	-3.375135	3.202520	-3.154391
O	-3.627383	4.975229	-1.082068
C	-3.455236	5.575926	-2.345438
H	-4.263555	5.302334	-3.038817
H	-3.476394	6.654132	-2.173604
H	-2.491483	5.297397	-2.798695
Si	-0.811778	2.728779	1.665879
H	-0.989948	1.859302	0.499094
O	-1.746756	2.470471	2.968210
C	-2.058246	1.210250	3.550312
H	-1.199846	0.813839	4.104389

H	-2.890288	1.376364	4.241552
H	-2.354881	0.473366	2.792190
O	-1.017413	4.321991	1.334949
C	-0.523688	4.870501	0.126955
H	0.557862	5.057979	0.190354
H	-0.714738	4.209594	-0.732895
H	-1.044323	5.816566	-0.048110
Zn	1.542972	0.674638	1.193790
O	0.842187	2.465233	1.978647
C	1.548169	3.169956	3.004336
H	2.618796	3.039984	2.822812
H	1.295553	4.235268	2.964903
H	1.288078	2.767454	3.990305
F	0.021073	-0.260087	1.998542

TS11

M06L SCF energy in Solvent: -6577.116757 a.u.

PBE0-D3BJ Free energy in Solvent: -6576.280306 a.u.

O	-0.473020	-0.625437	0.207082
C	-1.155130	-1.747525	-0.141383
C	-2.553213	-1.712411	-0.350770
C	-3.182236	-2.910317	-0.692544
H	-4.256157	-2.904931	-0.873776
C	-2.494043	-4.117886	-0.843243
C	-1.108563	-4.096862	-0.703579
H	-0.533378	-5.009361	-0.877581
C	-0.427763	-2.929394	-0.363045
C	-3.228757	-5.383896	-1.164576
H	-3.696306	-5.817448	-0.269841
H	-2.559818	-6.146639	-1.579650
H	-4.035455	-5.214857	-1.887956
C	-3.311781	-0.364907	-0.342658
O	-3.133357	0.317440	0.897872
C	-4.827278	-0.593911	-0.498643
C	-5.597252	-1.140611	0.581952
C	-5.466638	-0.303218	-1.687484
C	-5.031165	-1.578809	1.808643
C	-7.012922	-1.304788	0.409269
C	-6.855758	-0.472611	-1.853951
H	-4.888212	0.081683	-2.524883
C	-5.812611	-2.115945	2.805064
H	-3.961872	-1.475085	1.954420
C	-7.789139	-1.844403	1.464153
C	-7.618074	-0.948534	-0.819388
H	-7.314770	-0.214728	-2.807001
C	-7.206803	-2.241953	2.642265
H	-5.346707	-2.446221	3.732380
H	-8.863970	-1.947474	1.312521
H	-8.695380	-1.075214	-0.928357
H	-7.814718	-2.660189	3.443135
C	-2.771843	0.528451	-1.492955
C	-3.144454	1.914867	-1.576309
C	-1.927159	0.021635	-2.465897
C	-4.073999	2.533825	-0.694218
C	-2.605560	2.718684	-2.639686
C	-1.366296	0.824134	-3.479920
H	-1.694867	-1.041512	-2.460956
C	-4.449498	3.847041	-0.859700
H	-4.494769	1.949940	0.117152
C	-3.010811	4.070844	-2.772797
C	-1.691971	2.154439	-3.560051
H	-0.694926	0.372568	-4.210149
C	-3.918347	4.627898	-1.905981
H	-5.171023	4.285416	-0.172321
H	-2.587625	4.656815	-3.588961
H	-1.277096	2.788266	-4.343573
H	-4.226988	5.665497	-2.024256
Zn	1.063018	0.063321	-0.736230
O	2.852285	0.485201	-1.064362
N	1.599766	-1.996453	-1.393750
C	1.072114	-2.888492	-0.334064
H	1.439540	-2.515453	0.629588
H	1.484084	-3.904889	-0.474315
C	1.146597	-2.391986	-2.740004
H	1.286639	-3.481269	-2.879551
H	0.076592	-2.183282	-2.857546
C	2.054738	-1.601925	-3.651620
H	1.741666	-0.548521	-3.669163
H	2.049711	-1.971268	-4.682473
C	3.409594	-1.731887	-2.962561
H	4.052793	-0.867156	-3.148645
H	3.941988	-2.620787	-3.323892
C	3.093260	-1.877138	-1.462000
H	3.526140	-2.805439	-1.054738
C	3.577651	-0.633290	-0.641595
C	5.064975	-0.370523	-0.877901
C	6.005260	-1.388367	-1.027712
H	5.688449	-2.432299	-1.039719

C	7.364182	-1.112184	-1.180379
H	8.065796	-1.933073	-1.303827
C	7.800867	0.213328	-1.178813
C	6.868039	1.244719	-1.028490
H	7.225878	2.272241	-1.033755
C	5.522823	0.952114	-0.879379
H	4.791273	1.749376	-0.770462
O	9.101239	0.599089	-1.320437
C	10.057797	-0.424892	-1.463387
H	10.073024	-1.091978	-0.588650
H	9.875518	-1.028787	-2.364722
H	11.024992	0.073698	-1.554042
C	3.386500	-0.879186	0.869126
C	2.769307	0.095578	1.662032
C	3.827593	-2.039566	1.509892
C	2.546021	-0.094382	3.019374
H	2.498861	1.042774	1.194889
C	3.613037	-2.253620	2.868577
H	4.350072	-2.811502	0.943016
C	2.956737	-1.281031	3.631338
H	2.071592	0.680192	3.620084
H	3.962366	-3.176904	3.323664
O	2.691456	-1.394151	4.961273
C	3.108718	-2.579158	5.601416
H	4.199916	-2.705736	5.550163
H	2.805726	-2.480569	6.645597
H	2.626750	-3.466688	5.165698
Si	0.458825	2.855478	1.569673
H	-0.200298	1.488597	2.130895
O	1.871402	3.253943	0.815381
C	3.006633	3.773871	1.481549
H	3.686149	4.152376	0.711101
H	2.747262	4.584717	2.171673
H	3.520533	2.988196	2.052007
O	0.959876	3.093267	3.157387
C	0.069717	2.958272	4.234191
H	-0.634559	3.800440	4.278949
H	-0.519314	2.025133	4.167966
H	0.650346	2.925286	5.162816
Zn	-1.407831	0.926450	1.085536
O	-0.853907	3.842146	1.389716
C	-1.113680	4.582809	0.208972
H	-1.998315	5.199175	0.392450
H	-0.266150	5.234356	-0.042282
H	-1.315594	3.922309	-0.641582
F	0.084757	1.948019	-0.059772

$FSi(OMe)_3$

M06L SCF energy in Solvent: -734.542700 a.u.

PBE0-D3BJ Free energy in Solvent: -734.447258 a.u.

Si	-0.073787	-0.032357	0.323733
O	1.159824	-1.079966	0.532028
O	-1.400137	-0.832181	-0.182381
O	0.239639	1.141601	-0.778108
C	1.620451	-1.877196	-0.543003
H	2.466754	-2.469198	-0.182377
H	0.836848	-2.559247	-0.898181
H	1.958210	-1.259921	-1.388375
C	-2.558942	-0.153621	-0.633650
H	-2.319553	0.559181	-1.432857
H	-3.255477	-0.902781	-1.021010
H	-3.048252	0.385482	0.188847
C	1.305374	2.052097	-0.580992
H	1.350169	2.713510	-1.451106
H	1.148956	2.662539	0.318433
H	2.268574	1.530343	-0.485721
F	-0.285457	0.647753	1.754849

TS10b

M06L SCF energy in Solvent: -6533.49219 a.u.

PBE0-D3BJ Free energy in Solvent: --6532.556347 a.u.

O	-0.514800	-0.540275	-0.320656
C	-1.023547	-1.681170	-0.829904
C	-2.421268	-1.918352	-0.841148
C	-2.883230	-3.080462	-1.459702
H	-3.958096	-3.255138	-1.497428
C	-2.041151	-4.027311	-2.046461
C	-0.673609	-3.781414	-1.996735
H	0.020947	-4.504568	-2.431152
C	-0.149046	-2.639961	-1.391272
C	-2.596286	-5.265555	-2.682963
H	-3.423995	-5.038726	-3.366862
H	-2.992774	-5.965447	-1.934882
H	-1.830635	-5.802295	-3.255045
C	-3.425127	-0.883627	-0.272511
O	-3.000186	-0.379692	0.986037
C	-4.787997	-1.567460	-0.033405
C	-4.935511	-2.528030	1.022559

C	-5.871576	-1.309513	-0.849454	H	3.873211	0.913783	-2.385152
C	-3.866950	-2.938950	1.863211	H	4.571668	-0.308389	-3.439801
C	-6.214403	-3.147797	1.222428	C	3.379857	-1.113134	-1.798518
C	-7.126467	-1.918910	-0.647299	H	3.855127	-2.076673	-2.056096
H	-5.764682	-0.614248	-1.679382	C	3.812730	-0.655033	-0.357491
C	-4.055090	-3.883068	2.846436	C	5.262035	-0.149942	-0.407715
H	-2.891787	-2.483475	1.727765	C	6.247069	-0.727212	-1.208035
C	-6.374479	-4.105840	2.253067	H	5.998485	-1.556575	-1.871605
C	-7.298902	-2.812797	0.377103	C	7.563315	-0.266126	-1.205030
H	-7.953712	-1.670577	-1.310437	H	8.296043	-0.738278	-1.854597
C	-5.319525	-4.469792	3.053434	C	7.916693	0.797683	-0.374332
H	-3.214354	-4.178637	3.472312	C	6.944053	1.381271	0.444007
H	-7.358115	-4.556181	2.389900	H	7.237079	2.208033	1.088086
H	-8.264074	-3.289984	0.549045	C	5.641361	0.910470	0.423018
H	-5.455295	-5.211939	3.838767	H	4.883926	1.363477	1.059566
C	-3.575037	0.294169	-1.274269	O	9.167885	1.334150	-0.292415
C	-4.337968	1.464069	-0.918417	C	10.165302	0.749616	-1.097149
C	-2.996524	0.246650	-2.530433	H	10.318612	-0.311088	-0.848498
C	-4.987190	1.621377	0.336774	H	9.923657	0.829612	-2.167531
C	-4.487735	2.518938	-1.880843	H	11.083427	1.304171	-0.892339
C	-3.134054	1.293165	-3.465410	C	3.775126	-1.834981	0.631477
H	-2.433248	-0.637465	-2.821285	C	3.065170	-1.729119	1.832727
C	-5.714979	2.753329	0.625769	C	4.446145	-3.032066	0.380439
H	-4.887525	0.832120	1.074839	C	3.008858	-2.783016	2.732521
C	-5.244584	3.668978	-1.547159	H	2.532987	-0.804316	2.043923
C	-3.875749	2.403399	-3.153048	C	4.398758	-4.103623	1.268741
H	-2.659455	1.202059	-4.441374	H	5.035144	-3.145443	-0.530528
C	-5.845227	3.791443	-0.318075	C	3.672550	-3.981346	2.456073
H	-6.199928	2.843871	1.596457	H	2.448097	-2.702623	3.661430
H	-5.343147	4.456935	-2.294945	H	4.933440	-5.019861	1.031111
H	-4.005901	3.212682	-3.873098	O	3.555132	-4.961163	3.396138
H	-6.424617	4.680651	-0.075166	C	4.205176	-6.182401	3.130751
O	2.983902	0.380205	0.062569	H	5.293888	-6.052958	3.040094
N	1.901679	-1.289650	-1.908421	H	3.988737	-6.831256	3.981772
C	1.343630	-2.508683	-1.278267	H	3.827108	-6.651883	2.210493
H	1.639252	-2.486643	-0.222349	Zn	1.237350	0.257040	-0.671156
H	1.832485	-3.393820	-1.723692	Zn	-1.602648	0.818790	0.718154
C	1.601664	-1.180176	-3.343411	C	1.238501	1.822255	1.920052
H	1.926175	-2.102768	-3.859809	O	0.468851	0.872788	1.935150
H	0.520328	-1.075784	-3.491929	C	1.079286	3.111372	1.134414
C	2.421988	0.024369	-3.764524	C	0.202177	2.926906	-0.119904
H	1.856317	0.944181	-3.562002	O	0.559082	2.108137	-1.028343
H	2.652827	0.017496	-4.834516	O	-0.356508	4.098748	-0.487893
C	3.672471	-0.048456	-2.871947	C	-1.214552	3.995685	-1.636084

H	-1.925191	3.176484	-1.439037
H	-0.616859	3.710978	-2.510756
C	-1.913797	5.314422	-1.810470
H	-2.518941	5.556922	-0.930755
H	-2.579081	5.267926	-2.679676
H	-1.196116	6.126156	-1.972304
C	2.477615	3.511890	0.639766
H	2.420786	4.408749	0.015151
H	2.920731	2.698142	0.056217
H	3.133680	3.725516	1.492227
C	0.486557	4.115381	2.124777
C	1.000106	5.411081	2.238653
C	-0.596750	3.754132	2.935689
C	0.433970	6.324453	3.121178
H	1.843064	5.718663	1.624791
C	-1.163397	4.668282	3.818672
H	-1.005016	2.746379	2.882106
C	-0.649940	5.957405	3.914665
H	0.845707	7.329900	3.189413
H	-2.006364	4.365404	4.436638
H	-1.087345	6.671973	4.609271
H	-1.080766	2.342275	0.536613
H	2.141310	1.800743	2.568247

TS5c

M06L SCF energy in Solvent: -6687.257757 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.260870 a.u.

O	-1.067146	-0.631093	0.001066
C	-1.775420	-1.708921	-0.412034
C	-3.178088	-1.644609	-0.624738
C	-3.828270	-2.790470	-1.079766
H	-4.900613	-2.739547	-1.265711
C	-3.167200	-3.995579	-1.328430
C	-1.787053	-4.016522	-1.152462
H	-1.228416	-4.926501	-1.383776
C	-1.081149	-2.900426	-0.704466
C	-3.920511	-5.210547	-1.777800
H	-3.253457	-5.958566	-2.221999
H	-4.688091	-4.963135	-2.521392
H	-4.440776	-5.698387	-0.941924
C	-3.930015	-0.306268	-0.454584
O	-3.718242	0.198375	0.861711
C	-5.449851	-0.464401	-0.620664
C	-6.220896	-1.164666	0.367292
C	-6.098940	0.063024	-1.719192
C	-5.651325	-1.797617	1.504195
C	-7.640338	-1.274330	0.185773
C	-7.494661	-0.041384	-1.887973
H	-5.523132	0.579957	-2.484067
C	-6.433579	-2.482582	2.405050
H	-4.580415	-1.722733	1.661399
C	-8.415116	-1.977726	1.140083
C	-8.252407	-0.692061	-0.950106
H	-7.960847	0.399657	-2.767644
C	-7.829055	-2.572707	2.230064
H	-5.966458	-2.960148	3.265204
H	-9.492357	-2.041963	0.983520
H	-9.332859	-0.781169	-1.065260
H	-8.435916	-3.115008	2.953689
C	-3.361975	0.697891	-1.502901
C	-3.460104	2.121023	-1.309257
C	-2.705252	0.238792	-2.630418
C	-4.250574	2.726703	-0.288172
C	-2.757500	2.995680	-2.209909
C	-2.046832	1.100958	-3.527584
H	-2.675954	-0.832740	-2.819750
C	-4.291079	4.093802	-0.134766
H	-4.827825	2.087101	0.371008
C	-2.814562	4.397358	-2.009010
C	-2.042309	2.453870	-3.302673
H	-1.520520	0.679226	-4.383403
C	-3.555381	4.941083	-0.988164
H	-4.911561	4.524745	0.649221
H	-2.264333	5.038848	-2.698226
H	-1.508847	3.132869	-3.968477
H	-3.591071	6.020364	-0.849128
O	2.797459	-0.025243	-0.388906
N	1.068623	-1.912924	-1.434293
C	0.418220	-2.963555	-0.616234
H	0.761782	-2.843567	0.420968
H	0.765175	-3.959690	-0.948520
C	0.474475	-1.780349	-2.776102
H	0.408485	-2.771651	-3.264005
H	-0.539651	-1.375847	-2.699319
C	1.445690	-0.869277	-3.485350
H	1.276408	0.161737	-3.142825
H	1.327070	-0.885499	-4.574571
C	2.801980	-1.384492	-3.010881

H	3.546418	-0.584382	-2.927847
H	3.206275	-2.125186	-3.711774
C	2.543200	-2.040311	-1.638127
H	2.798835	-3.114137	-1.663374
C	3.323090	-1.303650	-0.495478
C	4.807922	-1.213551	-0.865008
C	5.538565	-2.301763	-1.340614
H	5.051897	-3.266966	-1.485264
C	6.892484	-2.197708	-1.656869
H	7.422527	-3.071592	-2.027276
C	7.544954	-0.973866	-1.495601
C	6.825095	0.130311	-1.029798
H	7.345159	1.079907	-0.915463
C	5.478877	0.006432	-0.722509
H	4.915117	0.867664	-0.369429
O	8.864597	-0.758110	-1.766933
C	9.609548	-1.862240	-2.224681
H	9.615399	-2.681491	-1.490559
H	9.222355	-2.247948	-3.179763
H	10.629663	-1.500335	-2.369511
C	3.186959	-2.071425	0.834799
C	2.808213	-1.383895	1.995298
C	3.409791	-3.446087	0.947419
C	2.627253	-2.043046	3.203010
H	2.645646	-0.309285	1.948292
C	3.236829	-4.124873	2.151258
H	3.714581	-4.026086	0.076252
C	2.836677	-3.420968	3.290756
H	2.325776	-1.500343	4.096881
H	3.413214	-5.197024	2.189710
O	2.632545	-3.983868	4.514984
C	2.852246	-5.370968	4.625831
H	3.892434	-5.638029	4.387344
H	2.643130	-5.628196	5.666292
H	2.180936	-5.943928	3.968989
Zn	0.894110	-0.137393	-0.132106
Zn	-1.992417	0.891267	0.830034
C	0.169801	2.159012	1.615322
O	0.605314	0.938605	1.612540
O	-0.140383	2.702079	2.856197
C	-0.820571	1.782353	3.687884
H	-0.174459	0.922662	3.904996
H	-1.691193	1.378111	3.108758
C	-1.288849	2.498157	4.925063
H	-0.434351	2.893768	5.483915
H	-1.837008	1.811744	5.578323
H	-1.947862	3.335033	4.671623
C	0.948228	3.246391	0.805418
C	0.062458	4.479460	0.596999
H	-0.292285	4.855286	1.561154
H	-0.818718	4.224382	-0.005727
H	0.613909	5.275266	0.084927
C	2.246781	3.537889	1.546712
C	2.440899	4.726949	2.249647
C	3.259471	2.570195	1.564110
C	3.625947	4.953704	2.946254
H	1.665271	5.489984	2.260148
C	4.439428	2.796380	2.263063
H	3.128424	1.634925	1.015532
C	4.629370	3.990494	2.956060
H	3.761590	5.891271	3.483492
H	5.214547	2.030228	2.261812
H	5.555573	4.169412	3.499977
C	1.212688	2.666209	-0.577352
O	0.505321	1.802881	-1.105269
O	2.245557	3.218522	-1.182336
C	2.679924	2.583576	-2.419232
H	1.886482	2.710389	-3.166973
H	2.793226	1.514869	-2.194862
C	3.976576	3.230698	-2.813607
H	3.850867	4.297466	-3.027649
H	4.374468	2.743255	-3.710327
H	4.717883	3.124972	-2.014334
H	-0.991542	2.239712	1.055389

TS5d

M06L SCF energy in Solvent: -6687.255955 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.260197 a.u.

O	-0.814914	-0.776873	-0.100218
C	-1.386479	-1.923283	-0.525731
C	-2.783785	-1.990137	-0.764614
C	-3.316896	-3.188517	-1.234028
H	-4.385012	-3.239593	-1.442776
C	-2.537213	-4.322859	-1.478318
C	-1.163830	-4.211206	-1.285058
H	-0.519132	-5.062233	-1.516865
C	-0.570500	-3.037661	-0.817962
C	-3.162546	-5.602142	-1.945284
H	-3.929730	-5.427155	-2.709664

H	-3.657803	-6.136391	-1.122665
H	-2.417685	-6.285265	-2.369907
C	-3.644414	-0.716516	-0.609743
O	-3.512047	-0.201176	0.710383
C	-5.142256	-0.999931	-0.819828
C	-5.886183	-1.750009	0.152367
C	-5.798271	-0.536053	-1.942777
C	-5.302619	-2.335100	1.307546
C	-7.289387	-1.962222	-0.063263
C	-7.176331	-0.747906	-2.149429
H	-5.242445	0.016768	-2.696935
C	-6.057428	-3.064189	2.197202
H	-4.242960	-2.188915	1.486780
C	-8.037223	-2.707700	0.880558
C	-7.910868	-1.439829	-1.222743
H	-7.648065	-0.353891	-3.048267
C	-7.439231	-3.249368	1.991561
H	-5.579334	-3.502965	3.071959
H	-9.102977	-2.849248	0.698032
H	-8.978552	-1.608924	-1.365302
H	-8.025446	-3.824631	2.706671
C	-3.138401	0.336767	-1.640587
C	-3.399452	1.742168	-1.468199
C	-2.404375	-0.056810	-2.744427
C	-4.285854	2.264474	-0.481239
C	-2.789510	2.679406	-2.374223
C	-1.817088	0.863986	-3.633012
H	-2.256876	-1.120340	-2.923064
C	-4.528804	3.615440	-0.382910
H	-4.781737	1.572435	0.191046
C	-3.050097	4.064669	-2.227325
C	-1.979512	2.211122	-3.434208
H	-1.224953	0.495106	-4.469972
C	-3.904735	4.528227	-1.257139
H	-5.223996	3.980093	0.371255
H	-2.576461	4.755117	-2.925857
H	-1.521832	2.938638	-4.105008
H	-4.116182	5.593689	-1.174780
O	2.957711	0.144148	-0.143989
N	1.503270	-1.825621	-1.443275
C	0.932513	-2.977482	-0.707598
H	1.256297	-2.900420	0.341755
H	1.363664	-3.920075	-1.094543
C	0.942697	-1.676017	-2.796185
H	1.014762	-2.633935	-3.346239
H	-0.114290	-1.399503	-2.738330
C	1.819651	-0.611178	-3.406692
H	1.514021	0.367964	-3.009384
H	1.741899	-0.568198	-4.498762
C	3.210988	-0.991303	-2.908174
H	3.851147	-0.117061	-2.746193
H	3.725843	-1.628790	-3.637595
C	2.989752	-1.767447	-1.592648
H	3.372052	-2.799032	-1.684129
C	3.648618	-1.038438	-0.364905
C	5.109191	-0.702404	-0.690673
C	6.001421	-1.622008	-1.241071
H	5.669721	-2.634378	-1.474969
C	7.324024	-1.283128	-1.526202
H	7.984941	-2.029569	-1.959244
C	7.777573	0.009057	-1.255840
C	6.893918	0.945834	-0.712844
H	7.261547	1.950929	-0.513407
C	5.582409	0.590051	-0.437415
H	4.888293	1.318739	-0.023626
O	9.048073	0.448574	-1.489993
C	9.957313	-0.487498	-2.019441
H	10.083712	-1.352887	-1.352215
H	9.640358	-0.849155	-3.009135
H	10.910727	0.036116	-2.116175
C	3.604862	-1.953288	0.874919
C	3.111254	-1.459300	2.088642
C	4.023071	-3.286267	0.849045
C	3.009549	-2.265529	3.213754
H	2.789284	-0.422159	2.144162
C	3.932064	-4.110647	1.968004
H	4.428248	-3.717602	-0.066132
C	3.415647	-3.600519	3.162080
H	2.616711	-1.875156	4.150475
H	4.263093	-5.143835	1.898820
O	3.275707	-4.317932	4.312558
C	3.688515	-5.664608	4.279224
H	4.760210	-5.755797	4.048249
H	3.500447	-6.064052	5.277821
H	3.116961	-6.247283	3.541692
Zn	1.089584	-0.220729	0.001298
Zn	-1.865639	0.658185	0.800411
C	0.206335	1.756858	2.022862

O	0.598384	0.540310	1.877929
O	-0.172997	2.149939	3.286978
C	-0.907548	1.148947	3.979576
H	-0.276828	0.264856	4.132611
H	-1.747129	0.829787	3.319953
C	-1.419496	1.738203	5.265357
H	-0.587995	2.053569	5.904526
H	-2.009430	0.996500	5.813399
H	-2.051631	2.610969	5.073150
C	1.063443	2.892965	1.390539
C	2.444996	2.788247	2.055154
H	3.089008	3.611562	1.733351
H	2.919007	1.841851	1.771112
H	2.340994	2.815151	3.144189
C	0.397948	4.251578	1.551148
C	0.839795	5.170814	2.505036
C	-0.705504	4.587218	0.756456
C	0.196911	6.393886	2.664344
H	1.691536	4.930718	3.137136
C	-1.348635	5.810540	0.917260
H	-1.068483	3.890466	-0.002763
C	-0.899952	6.719145	1.871427
H	0.558001	7.096759	3.413354
H	-2.204030	6.048013	0.287166
H	-1.400664	7.677940	1.994573
C	1.224073	2.598802	-0.094415
O	0.515285	1.814960	-0.732617
O	2.217021	3.276077	-0.638491
C	2.561213	2.913633	-2.004434
H	1.678513	3.075355	-2.635535
H	2.792261	1.841603	-1.987188
C	3.738503	3.755124	-2.405676
H	3.499255	4.823282	-2.373274
H	4.040631	3.502358	-3.427461
H	4.593510	3.570799	-1.746762
H	-0.986984	1.950780	1.385408

TS4'

M06L SCF energy in Solvent: -6556.424852 a.u.

PBE0-D3BJ Free energy in Solvent: -6558.644628 a.u.

O	0.505043	0.457034	-0.103315
C	1.109002	1.458010	-0.778682
C	2.516808	1.488213	-0.950011
C	3.055579	2.562086	-1.661689
H	4.133034	2.595870	-1.818307
C	2.281021	3.586253	-2.211889
C	0.898602	3.492693	-2.075355
H	0.256585	4.248018	-2.534990
C	0.303755	2.448916	-1.370414
C	2.921882	4.735653	-2.929054
H	3.285877	5.499002	-2.227404
H	2.218757	5.233204	-3.607309
H	3.788449	4.415762	-3.520155
C	3.411855	0.299465	-0.513718
O	3.186793	-0.069759	0.844817
C	4.899895	0.679404	-0.616473
C	5.470979	1.609426	0.314642
C	5.702981	0.153961	-1.608425
C	4.717967	2.281005	1.314028
C	6.868830	1.919016	0.214246
C	7.074069	0.466323	-1.706675
H	5.273544	-0.530695	-2.337393
C	5.311309	3.177790	2.171896
H	3.658160	2.066652	1.399128
C	7.448804	2.835575	1.125309
C	7.649995	1.322007	-0.803819
H	7.668503	0.016988	-2.500482
C	6.690575	3.454099	2.088453
H	4.706259	3.679020	2.926017
H	8.514926	3.046749	1.036139
H	8.710645	1.567748	-0.861341
H	7.147964	4.160589	2.779355
C	3.087332	-0.925595	-1.413037
C	3.569606	-2.236769	-1.061839
C	2.314403	-0.797467	-2.552963
C	4.480272	-2.478714	0.005062
C	3.164328	-3.363382	-1.856415
C	1.931090	-1.904874	-3.337069
H	1.996725	0.195829	-2.863642
C	4.925946	-3.749341	0.287237
H	4.815482	-1.640493	0.606139
C	3.622327	-4.660801	-1.516421
C	2.333231	-3.168335	-2.985803
H	1.315831	-1.745349	-4.222377
C	4.483584	-4.856305	-0.464885
H	5.627424	-3.899298	1.106628
H	3.289266	-5.501451	-2.125617
H	2.038472	-4.036589	-3.575541

H	4.834647	-5.857744	-0.221021
Zn	-1.191414	-0.511166	-0.366742
O	-3.027912	-0.914478	-0.400442
N	-1.701484	1.079515	-1.855669
C	-1.190383	2.345985	-1.284540
H	-1.523554	2.400329	-0.241114
H	-1.655513	3.196544	-1.816805
C	-1.203243	0.822731	-3.217082
H	-1.335423	1.722037	-3.848574
H	-0.131917	0.592827	-3.188307
C	-2.080305	-0.314321	-3.684897
H	-1.752143	-1.252640	-3.212011
H	-2.048179	-0.461695	-4.769689
C	-3.456797	0.086518	-3.160098
H	-4.072436	-0.783387	-2.912362
H	-4.003157	0.670328	-3.911154
C	-3.186536	0.949954	-1.911008
H	-3.617568	1.959692	-2.024850
C	-3.728181	0.270923	-0.603298
C	-5.216329	-0.046918	-0.781017
C	-6.116066	0.842774	-1.369466
H	-5.770015	1.799431	-1.761067
C	-7.470171	0.539225	-1.503716
H	-8.133831	1.260440	-1.973621
C	-7.950135	-0.687075	-1.041490
C	-7.059660	-1.596825	-0.463689
H	-7.445706	-2.555014	-0.122144
C	-5.716612	-1.277794	-0.340780
H	-5.017719	-1.995358	0.081457
O	-9.250764	-1.089242	-1.120419
C	-10.164077	-0.185207	-1.697000
H	-10.214289	0.757926	-1.132740
H	-9.907781	0.042221	-2.742527
H	-11.138545	-0.676859	-1.664149
C	-3.547339	1.231351	0.591112
C	-2.781324	0.852940	1.701281
C	-4.078660	2.523171	0.598972
C	-2.522883	1.725580	2.749735
H	-2.399694	-0.165595	1.759118
C	-3.834073	3.415951	1.638429
H	-4.698145	2.861265	-0.231341
C	-3.042474	3.021364	2.722263
H	-1.929054	1.412036	3.606471
H	-4.262628	4.414083	1.595303
O	-2.736290	3.814469	3.784998
C	-3.262007	5.122626	3.782459
H	-4.361828	5.118469	3.775945
H	-2.908500	5.590848	4.703060
H	-2.904171	5.702998	2.919455
O	-0.031251	-2.096329	0.521419
Si	-0.516151	-2.197763	2.601627
H	0.357036	-0.909915	2.405828
C	0.615337	-3.682988	2.820858
H	0.550615	-3.982341	3.876096
H	0.201790	-4.525438	2.249821
O	-2.015456	-2.516131	1.980035
C	-3.263460	-2.415435	2.637232
H	-3.677916	-3.422189	2.777686
H	-3.180414	-1.922903	3.612123
H	-3.937288	-1.838792	1.991458
O	-0.966308	-1.676804	4.151274
C	-0.008481	-1.127066	5.011345
H	0.688503	-1.889576	5.399229
H	0.593520	-0.344104	4.515198
H	-0.520980	-0.669065	5.865484
C	-0.129711	-3.264325	-0.286291
H	0.124422	-3.029649	-1.329689
H	0.569421	-4.037305	0.064377
H	-1.155463	-3.649578	-0.229807
C	2.071041	-3.457866	2.432762
H	2.715945	-4.305386	2.698078
H	2.192391	-3.323422	1.347562
H	2.506063	-2.572212	2.922934
Zn	1.531688	-0.885579	0.970660

IM8b

M06L SCF energy in Solvent: -7322.584185 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.454166 a.u.

O	0.596778	-0.600280	-0.871933
C	1.068973	-0.138698	-2.039985
C	2.464750	-0.058303	-2.294838
C	2.881470	0.322350	-3.569640
H	3.950815	0.352114	-3.779523
C	1.994736	0.667847	-4.592748
C	0.634540	0.625671	-4.301724
H	-0.090129	0.900087	-5.072349
C	0.160512	0.239795	-3.048921
C	2.498688	1.088438	-5.940406

H	3.223666	0.373082	-6.349662
H	3.009302	2.060523	-5.900387
H	1.681302	1.181287	-6.664834
C	3.484872	-0.410412	-1.189222
O	3.187998	0.303934	0.003287
C	4.909238	0.024576	-1.577009
C	5.240221	1.419950	-1.650582
C	5.895001	-0.906009	-1.835215
C	4.289262	2.465598	-1.494112
C	6.594272	1.794969	-1.941879
C	7.223510	-0.531735	-2.123007
H	5.648263	-1.965572	-1.808162
C	4.654966	3.786865	-1.612147
H	3.255959	2.211154	-1.278192
C	6.939908	3.166525	-2.025626
C	7.570555	0.793449	-2.161453
H	7.968676	-1.303943	-2.306588
C	5.993297	4.148762	-1.866934
H	3.897120	4.562392	-1.506285
H	7.978104	3.423983	-2.237103
H	8.594880	1.098966	-2.375941
H	6.269989	5.199127	-1.944946
C	3.425859	-1.929435	-0.892928
C	3.973434	-2.468057	0.324702
C	2.808845	-2.795268	-1.776557
C	4.714146	-1.699701	1.268852
C	3.793956	-3.866811	0.607414
C	2.656899	-4.168870	-1.505305
H	2.408423	-2.398043	-2.707352
C	5.196645	-2.263559	2.428383
H	4.883559	-0.647556	1.064960
C	4.296444	-4.407630	1.817672
C	3.129657	-4.694549	-0.329379
H	2.148313	-4.804835	-2.228585
C	4.977117	-3.625261	2.718287
H	5.758268	-1.646496	3.127876
H	4.146136	-5.471500	2.007798
H	3.010274	-5.754004	-0.100727
H	5.358788	-4.055403	3.642910
H	1.177938	-2.718012	0.516070
Si	0.192089	-3.458493	1.310315
O	-1.267693	-2.791050	0.853495
O	0.001533	-5.054178	0.967848
O	0.568091	-3.350018	2.905736
C	-2.498293	-3.381717	1.293869
H	-2.463486	-3.576554	2.373387
H	-3.290844	-2.660475	1.071949
H	-2.671797	-4.323616	0.760652
C	1.491840	-2.412155	3.421058
H	2.059611	-2.894081	4.224455
H	2.221804	-2.079120	2.659788
H	0.975019	-1.528048	3.811897
C	0.695862	-6.085212	1.640777
H	1.638486	-5.738033	2.086551
H	0.070237	-6.497528	2.442383
H	0.916502	-6.880419	0.919785
O	-3.161168	-0.477589	0.211529
N	-1.849766	-0.966032	-2.180987
C	-1.312996	0.274271	-2.771500
H	-1.555926	1.096874	-2.079269
H	-1.858437	0.499117	-3.708730
C	-1.407899	-2.173892	-2.891113
H	-1.536558	-2.037058	-3.981993
H	-0.341561	-2.345469	-2.699687
C	-2.315333	-3.263851	-2.351734
H	-1.869286	-3.705455	-1.451881
H	-2.451065	-4.075296	-3.074562
C	-3.623427	-2.535506	-2.012747
H	-3.963090	-2.771777	-0.998231
H	-4.442880	-2.815104	-2.683859
C	-3.326133	-1.030978	-2.132574
H	-3.726840	-0.646208	-3.089564
C	-3.894886	-0.198300	-0.930809
C	-5.356478	-0.632484	-0.715519
C	-6.308376	-0.558441	-1.732429
H	-6.028958	-0.175291	-2.714332
C	-7.627533	-0.962507	-1.537843
H	-8.336202	-0.887522	-2.358867
C	-8.021618	-1.450685	-0.290115
C	-7.080848	-1.535771	0.738801
H	-7.402255	-1.919332	1.705302
C	-5.770417	-1.135232	0.521484
H	-5.037204	-1.204869	1.321398
O	-9.285590	-1.863999	0.016322
C	-10.250662	-1.775235	-1.005351
H	-10.384668	-0.739141	-1.350260
H	-9.988927	-2.403315	-1.870232
H	-11.186179	-2.134103	-0.571061

C	-3.900433	1.319154	-1.210264
C	-3.617544	2.197930	-0.154660
C	-4.228306	1.887005	-2.442954
C	-3.655194	3.573546	-0.327579
H	-3.343518	1.778402	0.812981
C	-4.258199	3.267367	-2.638865
H	-4.453467	1.252833	-3.300334
C	-3.972876	4.122011	-1.573298
H	-3.447623	4.253051	0.498148
H	-4.505300	3.660279	-3.621975
O	-3.977722	5.483624	-1.647686
C	-4.293696	6.051544	-2.897647
H	-5.305495	5.772330	-3.227010
H	-4.245034	7.133660	-2.759916
H	-3.574134	5.751681	-3.673876
Zn	-1.283891	-0.731505	-0.014500
Zn	1.668002	-0.338260	0.840717
C	1.778784	1.919274	2.404145
O	2.322420	0.868023	2.743921
O	2.450693	3.022798	2.118840
C	3.903701	2.894500	2.129966
H	4.167887	2.181551	1.338425
H	4.197933	2.462464	3.093051
C	4.470756	4.266808	1.909557
H	4.113928	4.688352	0.964810
H	5.563215	4.209759	1.855052
H	4.197216	4.948713	2.721932
C	0.272054	2.069140	2.222142
C	-0.386560	0.694414	2.562274
O	-0.075105	-0.330289	1.661157
O	-1.758582	0.920282	2.578932
C	-2.506465	-0.105675	3.220955
H	-2.030524	-0.332943	4.192616
H	-2.484712	-1.023903	2.613656
C	-3.912339	0.401970	3.394280
H	-3.920517	1.322662	3.989192
H	-4.537566	-0.344930	3.897275
H	-4.353367	0.614493	2.414492
C	-0.008591	2.446457	0.761162
H	-1.076707	2.333123	0.537450
H	0.543496	1.807207	0.058616
H	0.287335	3.481321	0.563205
C	-0.253653	3.099340	3.212282
C	-1.297677	3.963484	2.878682
C	0.257411	3.139667	4.513005
C	-1.813753	4.849889	3.817855
H	-1.719470	3.936824	1.875808
C	-0.254515	4.028090	5.454374
H	1.070759	2.467543	4.794973
C	-1.293392	4.887456	5.109084
H	-2.630715	5.513262	3.537369
H	0.161881	4.048193	6.460301
H	-1.695658	5.583919	5.842487
H	-0.046926	0.391581	3.574999

IM9b

M06L SCF energy in Solvent: -7322.586303 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.457732 a.u.

O	-0.762116	-0.883615	-0.676370
C	-1.382876	-1.998587	-1.091146
C	-2.797398	-2.100037	-1.081514
C	-3.365987	-3.254575	-1.619433
H	-4.453132	-3.334619	-1.645269
C	-2.609430	-4.316540	-2.125346
C	-1.222016	-4.209949	-2.062061
H	-0.600329	-5.036218	-2.415962
C	-0.600026	-3.076637	-1.541842
C	-3.277713	-5.530188	-2.698471
H	-3.878276	-5.288606	-3.585942
H	-3.961475	-5.998191	-1.978339
H	-2.544852	-6.288481	-2.997497
C	-3.672176	-0.952012	-0.516466
O	-3.214946	-0.558328	0.770964
C	-5.125712	-1.418606	-0.298914
C	-5.424204	-2.383934	0.721585
C	-6.162601	-0.907204	-1.052282
C	-4.432783	-3.027171	1.509748
C	-6.792384	-2.753082	0.946376
C	-7.505422	-1.275123	-0.827728
H	-5.947874	-0.190696	-1.842296
C	-4.770694	-3.955897	2.466346
H	-3.391143	-2.771492	1.348588
C	-7.104832	-3.705048	1.947870
C	-7.816277	-2.173015	0.159161
H	-8.289232	-0.835098	-1.442389
C	-6.118544	-4.296472	2.698159
H	-3.984645	-4.433020	3.050515
H	-8.152742	-3.963216	2.104613

H	-8.850072	-2.462578	0.349660
H	-6.372886	-5.029359	3.462521
C	-3.626908	0.249487	-1.493875
C	-3.958015	1.581982	-1.061844
C	-3.282105	0.055745	-2.820046
C	-4.466316	1.896386	0.232871
C	-3.827407	2.666531	-1.998210
C	-3.197485	1.116133	-3.741507
H	-3.052637	-0.952708	-3.159400
C	-4.754612	3.193344	0.593012
H	-4.626098	1.086822	0.936800
C	-4.120728	3.990094	-1.582949
C	-3.444753	2.402760	-3.334230
H	-2.900556	0.912944	-4.768886
C	-4.561693	4.257756	-0.310633
H	-5.145362	3.395636	1.589378
H	-4.006388	4.793631	-2.312106
H	-3.348464	3.237484	-4.029525
H	-4.787841	5.279614	-0.009465
H	-1.128228	1.492929	-1.922058
Si	-0.066076	2.397490	-2.331743
O	1.367954	1.574456	-2.083266
O	-0.288509	2.702655	-3.942661
O	0.082824	3.828601	-1.519218
C	2.642644	2.239260	-2.032207
H	2.524668	3.266238	-1.675374
H	3.270041	1.682252	-1.330665
H	3.091842	2.228996	-3.033780
C	-0.723315	4.955822	-1.800498
H	-0.075685	5.809137	-2.046022
H	-1.402521	4.784684	-2.648148
H	-1.321216	5.210757	-0.915773
C	0.663406	3.423864	-4.696388
H	1.091432	4.269023	-4.134327
H	1.487365	2.770834	-5.018205
H	0.168372	3.821154	-5.588884
O	2.921226	-0.298223	-0.133781
N	1.572537	-1.895798	-2.001183
C	0.887158	-3.035537	-1.355150
H	1.121111	-2.984431	-0.282695
H	1.336161	-3.976510	-1.727483
C	1.266418	-1.812952	-3.437391
H	1.318691	-2.824860	-3.883036
H	0.240059	-1.447954	-3.578008
C	2.339886	-0.897714	-4.006789
H	1.978976	0.136919	-4.032530
H	2.595114	-1.176646	-5.034642
C	3.524683	-1.039105	-3.038398
H	3.819526	-0.069814	-2.619993
H	4.417625	-1.452792	-3.518329
C	3.051987	-1.953459	-1.900235
H	3.370898	-2.994744	-2.093980
C	3.563500	-1.473840	-0.493132
C	5.073530	-1.201876	-0.603596
C	5.959054	-2.124645	-1.159837
H	5.587688	-3.079053	-1.535902
C	7.323799	-1.862540	-1.263175
H	7.979649	-2.605664	-1.709631
C	7.828116	-0.649416	-0.789816
C	6.955361	0.281295	-0.219684
H	7.365574	1.219763	0.147943
C	5.598967	0.004957	-0.131235
H	4.913687	0.726951	0.308295
O	9.142927	-0.285230	-0.841964
C	10.038747	-1.214307	-1.404190
H	10.055234	-2.158362	-0.839206
H	9.791762	-1.436319	-2.453349
H	11.026231	-0.750217	-1.357488
C	3.364059	-2.547437	0.594831
C	2.935030	-2.143577	1.864511
C	3.622591	-3.906491	0.410456
C	2.742563	-3.051954	2.893508
H	2.761225	-1.080543	2.023192
C	3.425925	-4.839255	1.427820
H	3.971220	-4.275292	-0.554346
C	2.978788	-4.413214	2.680112
H	2.415095	-2.729696	3.880940
H	3.624404	-5.890318	1.233642
O	2.751813	-5.235670	3.743670
C	2.990365	-6.610475	3.548583
H	4.039018	-6.807133	3.280854
H	2.764632	-7.095226	4.500786
H	2.340789	-7.028326	2.765241
Zn	1.122734	-0.141199	-0.715598
Zn	-1.596694	0.322163	0.683731
C	1.227422	3.856381	1.300058
O	2.285309	3.409344	0.904440
O	0.851599	5.137122	1.136810

C	1.785429	5.954094	0.406275
H	1.876675	5.539574	-0.606500
H	2.770502	5.873555	0.881169
C	1.254307	7.361433	0.412259
H	0.259994	7.412070	-0.045634
H	1.922948	8.021669	-0.150494
H	1.174132	7.747517	1.433812
C	0.201614	3.063764	2.105101
C	0.425824	1.576518	1.739497
O	0.103460	1.321794	0.434023
O	-0.510705	0.784362	2.531966
C	0.004830	-0.219370	3.426211
H	-0.101701	0.156922	4.453706
H	1.078188	-0.349429	3.227361
C	-0.751645	-1.506095	3.210648
H	-1.830870	-1.356971	3.333121
H	-0.427238	-2.269973	3.926277
H	-0.575225	-1.900633	2.199239
C	-1.222250	3.467047	1.732225
H	-1.955517	2.842435	2.256515
H	-1.375780	3.339830	0.654282
H	-1.421981	4.514100	1.980037
C	0.530389	3.231902	3.585951
C	-0.447782	3.515188	4.542128
C	1.844689	3.014300	4.020735
C	-0.122000	3.577756	5.895213
H	-1.478017	3.682822	4.235398
C	2.170264	3.077864	5.371289
H	2.621406	2.798100	3.287208
C	1.186169	3.358381	6.315840
H	-0.900194	3.797181	6.624641
H	3.198451	2.906089	5.685792
H	1.437943	3.406317	7.373799
H	1.452752	1.263667	1.991069

TS7b

M06L SCF energy in Solvent: -7322.560260 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.434209 a.u.

O	-0.684790	-0.950788	-0.557980
C	-1.414002	-1.964398	-1.083847
C	-2.830554	-1.945627	-1.080069
C	-3.498264	-2.979088	-1.739534
H	-4.588104	-2.955784	-1.764501
C	-2.843252	-4.043518	-2.362956
C	-1.454724	-4.078482	-2.274636
H	-0.906688	-4.923947	-2.698128
C	-0.735515	-3.072314	-1.631900
C	-3.614094	-5.110907	-3.079354
H	-4.017314	-4.753379	-4.037106
H	-4.471290	-5.458263	-2.489514
H	-2.986574	-5.982324	-3.299491
C	-3.615167	-0.822653	-0.359343
O	-3.093189	-0.609785	0.933632
C	-5.089652	-1.235140	-0.132527
C	-5.407310	-2.304006	0.774374
C	-6.125903	-0.579190	-0.767148
C	-4.428482	-3.085784	1.444285
C	-6.785425	-2.633860	1.002868
C	-7.478244	-0.905603	-0.534982
H	-5.906298	0.220204	-1.470806
C	-4.785349	-4.111633	2.288543
H	-3.380302	-2.853845	1.291053
C	-7.116738	-3.690429	1.886193
C	-7.803536	-1.909315	0.337937
H	-8.257395	-0.350418	-1.054939
C	-6.140744	-4.418428	2.520778
H	-4.007898	-4.690589	2.784936
H	-8.171693	-3.915899	2.046382
H	-8.844084	-2.172052	0.530580
H	-6.409842	-5.230689	3.194590
C	-3.559181	0.463338	-1.221657
C	-3.733655	1.770531	-0.652421
C	-3.411062	0.359525	-2.594005
C	-4.089448	2.004671	0.707696
C	-3.621676	2.921146	-1.509483
C	-3.365251	1.485076	-3.436982
H	-3.314787	-0.629582	-3.037688
C	-4.248505	3.280969	1.197745
H	-4.250208	1.150190	1.355344
C	-3.768039	4.220691	-0.961025
C	-3.431416	2.747145	-2.901110
H	-3.229411	1.349926	-4.508090
C	-4.064657	4.404925	0.367435
H	-4.527570	3.420494	2.241940
H	-3.672753	5.075424	-1.632741
H	-3.372334	3.629649	-3.539783
H	-4.185323	5.409347	0.771083
H	-1.047478	1.370595	-2.021201

Si	-0.006099	2.158650	-2.653679	C	9.977017	-2.478074	-0.266090
O	1.399814	1.256309	-2.504198	H	9.732108	-3.405898	0.272481
O	-0.403979	2.341275	-4.249021	H	9.900175	-2.668139	-1.347271
O	0.346381	3.633839	-1.993914	H	10.999813	-2.180698	-0.025059
C	2.717021	1.846868	-2.508937	C	2.931510	-2.513730	0.776081
H	2.683153	2.864709	-2.110074	C	2.067906	-1.906755	1.695714
H	3.349604	1.224384	-1.867890	C	3.221643	-3.865783	0.964920
H	3.102144	1.852893	-3.536777	C	1.487754	-2.626092	2.730787
C	-0.412218	4.796485	-2.266154	H	1.838614	-0.846757	1.594818
H	0.276101	5.617111	-2.507719	C	2.654607	-4.605534	2.000011
H	-1.096039	4.657940	-3.115964	H	3.906356	-4.373426	0.284955
H	-0.998227	5.077284	-1.379886	C	1.772271	-3.984839	2.888851
C	0.558697	2.758494	-5.195027	H	0.811535	-2.147637	3.437039
H	1.096184	3.664198	-4.871850	H	2.905930	-5.658099	2.104368
H	1.297321	1.965873	-5.383952	O	1.154863	-4.609666	3.930728
H	0.042074	2.981803	-6.133869	C	1.439171	-5.977065	4.116289
O	2.996187	-0.414358	-0.404329	H	2.508943	-6.147324	4.309027
N	1.592272	-2.216901	-2.042236	H	0.861361	-6.290127	4.988155
C	0.736037	-3.242397	-1.402905	H	1.136863	-6.577997	3.245804
H	0.937962	-3.215663	-0.327128	Zn	1.185911	-0.356587	-1.001082
H	1.057109	-4.236487	-1.766410	Zn	-1.352131	0.009138	1.071101
C	1.442603	-2.240692	-3.508933	C	1.657774	4.075167	0.692191
H	1.467904	-3.290876	-3.857483	O	2.733222	3.654874	0.312826
H	0.467800	-1.824852	-3.793598	O	1.222664	5.325114	0.477720
C	2.638075	-1.460740	-4.017470	C	2.132561	6.157359	-0.271487
H	2.400885	-0.391097	-4.034349	H	2.300612	5.685184	-1.248318
H	2.908771	-1.750201	-5.038429	H	3.097166	6.175075	0.249341
C	3.742307	-1.759686	-2.994063	C	1.507981	7.520925	-0.380399
H	4.271484	-0.849067	-2.689611	H	0.535020	7.472798	-0.882471
H	4.499425	-2.440795	-3.398022	H	2.156762	8.189019	-0.956599
C	3.052041	-2.396651	-1.775217	H	1.354925	7.963606	0.609206
H	3.252851	-3.482663	-1.736068	C	0.672106	3.255104	1.532899
C	3.477749	-1.711611	-0.422495	C	1.001069	1.815441	1.136447
C	5.008640	-1.682994	-0.334865	O	0.497803	1.345371	0.096415
C	5.824725	-2.731215	-0.759751	O	-0.217114	0.717843	2.395562
H	5.387548	-3.615502	-1.225898	C	-0.529284	0.638971	3.770731
C	7.212711	-2.684543	-0.626089	H	0.186109	1.270119	4.319618
H	7.811488	-3.521746	-0.975841	H	-0.373367	-0.394144	4.130344
C	7.809842	-1.562755	-0.050172	C	-1.950659	1.072531	4.062832
C	7.007175	-0.498415	0.371725	H	-2.112762	2.111989	3.748058
H	7.490084	0.372539	0.810558	H	-2.179959	1.002031	5.133767
C	5.630745	-0.562292	0.228068	H	-2.672423	0.442812	3.522361
H	5.003185	0.268018	0.544756	C	-0.772640	3.580150	1.183468
O	9.153265	-1.409473	0.136045	H	-1.448443	2.954889	1.776360

H	-0.968858	3.377142	0.126085
H	-1.001032	4.632301	1.375750
C	1.027944	3.498414	2.995913
C	0.098205	4.001937	3.908773
C	2.316925	3.194199	3.451629
C	0.438021	4.169065	5.248999
H	-0.907648	4.254310	3.579833
C	2.655720	3.360501	4.790259
H	3.066354	2.832573	2.748082
C	1.715059	3.844197	5.696117
H	-0.303822	4.554876	5.946302
H	3.661186	3.111391	5.125148
H	1.978542	3.972926	6.744483
H	1.899736	1.357051	1.575485

TS5e

M06L SCF energy in Solvent: -7322.541862 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.413814 a.u.

O	1.062949	0.266104	-0.552367
C	1.601194	1.334111	-1.198534
C	3.003109	1.577153	-1.188459
C	3.503202	2.605241	-1.985089
H	4.581224	2.762668	-2.006463
C	2.695123	3.451147	-2.747470
C	1.323934	3.245990	-2.675037
H	0.649210	3.905095	-3.226858
C	0.767101	2.218951	-1.910507
C	3.290799	4.546956	-3.577836
H	4.002217	4.159626	-4.319324
H	3.845042	5.267621	-2.961793
H	2.519397	5.103906	-4.122165
C	3.940602	0.749602	-0.278726
O	3.454370	0.811940	1.042770
C	5.367603	1.348405	-0.225596
C	5.599849	2.614974	0.413974
C	6.446809	0.677754	-0.767079
C	4.566437	3.422769	0.960316
C	6.939236	3.127542	0.473319
C	7.761678	1.181840	-0.696018
H	6.292159	-0.275391	-1.266987
C	4.838824	4.644986	1.530524
H	3.547894	3.052305	0.932638
C	7.183923	4.384959	1.077899
C	8.005882	2.382340	-0.083789
H	8.576987	0.607362	-1.133236
C	6.158201	5.134936	1.597536
H	4.021806	5.239759	1.937149
H	8.211913	4.747308	1.113625
H	9.016239	2.787675	-0.021375
H	6.359559	6.102577	2.055095
C	4.014121	-0.700754	-0.823987
C	4.332251	-1.829434	0.006565
C	3.847507	-0.911072	-2.181081
C	4.661734	-1.733726	1.389567
C	4.376274	-3.138671	-0.590014
C	3.961066	-2.183656	-2.769556
H	3.628744	-0.057381	-2.820462
C	4.926109	-2.854698	2.143844
H	4.705038	-0.748332	1.840915
C	4.642860	-4.269847	0.222242
C	4.196327	-3.284426	-1.985495
H	3.825058	-2.289488	-3.843553
C	4.898205	-4.139601	1.565705
H	5.174169	-2.742667	3.198336
H	4.667618	-5.251470	-0.255031
H	4.270464	-4.281365	-2.422940
H	5.105484	-5.018913	2.174320
H	1.578304	-2.310029	-1.035643
Si	0.606612	-2.969117	-1.901004
O	-0.925818	-2.332378	-1.681320
O	1.057328	-2.680261	-3.458027
O	0.402629	-4.582538	-1.599765
C	-2.014217	-3.121059	-1.174812
H	-1.684572	-3.772923	-0.360981
H	-2.766953	-2.422204	-0.795387
H	-2.434114	-3.724562	-1.988798
C	1.498896	-5.456397	-1.427028
H	2.022488	-5.637291	-2.377516
H	2.226086	-5.058593	-0.702505
H	1.114995	-6.411555	-1.052481
C	0.501868	-3.389906	-4.546195
H	1.106746	-4.278960	-4.772687
H	-0.532294	-3.716703	-4.358820
H	0.501588	-2.733178	-5.423145
O	-2.689392	0.033924	-0.122123
N	-1.269866	0.838884	-2.308099
C	-0.725272	2.124246	-1.834942
H	-1.079661	2.260764	-0.799145

H	-1.169505	2.946156	-2.426566
C	-0.760687	0.447772	-3.634815
H	-0.701656	1.342575	-4.280935
H	0.257215	0.047759	-3.540071
C	-1.777471	-0.560893	-4.168876
H	-1.380315	-1.578495	-4.124483
H	-2.015142	-0.350048	-5.217711
C	-3.002795	-0.420214	-3.259086
H	-3.104237	-1.286239	-2.594563
H	-3.944255	-0.339461	-3.811159
C	-2.744785	0.825836	-2.416560
H	-3.059665	1.715122	-2.993032
C	-3.432468	0.803793	-1.007726
C	-4.832960	0.184676	-1.184250
C	-5.791052	0.771933	-2.010096
H	-5.554929	1.702000	-2.531450
C	-7.053021	0.208201	-2.184596
H	-7.771240	0.694100	-2.840446
C	-7.382506	-0.966701	-1.502963
C	-6.438472	-1.558422	-0.659941
H	-6.711764	-2.469309	-0.129683
C	-5.182049	-0.987092	-0.510606
H	-4.445240	-1.442748	0.147745
O	-8.588538	-1.598987	-1.590360
C	-9.556267	-1.012397	-2.428716
H	-9.816069	0.005355	-2.101582
H	-9.218317	-0.970814	-3.474959
H	-10.441138	-1.648805	-2.362274
C	-3.680509	2.206166	-0.412818
C	-4.009671	2.272361	0.950446
C	-3.730503	3.398441	-1.133257
C	-4.358739	3.466138	1.557528
H	-3.998507	1.351736	1.535682
C	-4.054699	4.618554	-0.534265
H	-3.506690	3.411820	-2.198818
C	-4.371458	4.656481	0.821460
H	-4.636927	3.507572	2.608508
H	-4.060382	5.521918	-1.138654
O	-4.705964	5.781907	1.515043
C	-4.747079	6.988597	0.787925
H	-5.490007	6.949391	-0.022211
H	-5.033257	7.763294	1.502258
H	-3.766289	7.237155	0.356434
Zn	-0.863329	-0.376905	-0.534487
Zn	1.870581	-0.138576	1.261943
C	-0.695703	0.384271	2.886538
O	0.045915	0.903455	2.052290
O	-1.527179	1.096502	3.624970
C	-1.497916	2.536107	3.415858
H	-1.800763	2.729965	2.381066
H	-0.463292	2.876302	3.536119
C	-2.437530	3.138303	4.420578
H	-3.429319	2.680605	4.343248
H	-2.543091	4.212627	4.235346
H	-2.075862	2.995160	5.444295
C	-0.666900	-1.083577	3.301794
C	-0.091348	-1.934282	2.144098
O	-0.525869	-1.835304	0.963257
O	0.271560	-3.150943	2.628638
C	0.923730	-4.004750	1.683649
H	1.735912	-3.423044	1.206617
H	0.213575	-4.295111	0.898315
C	1.463467	-5.189524	2.438048
H	2.168015	-4.866124	3.212124
H	1.996788	-5.861291	1.755877
H	0.656596	-5.753686	2.918262
C	0.258714	-1.121575	4.526712
H	-0.201599	-0.593768	5.367881
H	1.220076	-0.649764	4.295402
H	0.463518	-2.154501	4.815985
C	-2.067490	-1.617452	3.605693
C	-2.322408	-2.397328	4.735084
C	-3.118555	-1.348630	2.720150
C	-3.603043	-2.883880	4.987879
H	-1.523071	-2.629150	5.435597
C	-4.398893	-1.824908	2.982923
H	-2.943330	-0.759388	1.816605
C	-4.648058	-2.593678	4.117411
H	-3.781487	-3.486769	5.876914
H	-5.209534	-1.582154	2.295726
H	-5.651595	-2.963519	4.321599
H	1.394302	-1.377446	2.162582

TS5f

M06L SCF energy in Solvent: -7322.537626 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.408802 a.u.

O	0.856913	-0.086836	-0.813122
C	1.287447	0.734631	-1.802252

C	2.676308	0.977197	-1.995288
C	3.077335	1.701830	-3.114549
H	4.144006	1.848519	-3.282162
C	2.178468	2.265092	-4.023987
C	0.825411	2.093370	-3.763167
H	0.086758	2.546407	-4.429169
C	0.365952	1.355966	-2.669213
C	2.664870	3.043435	-5.208475
H	3.291159	2.432374	-5.872136
H	3.278121	3.902835	-4.906262
H	1.831048	3.427810	-5.807358
C	3.692840	0.505671	-0.933503
O	3.309483	1.046619	0.312589
C	5.117021	1.051681	-1.208470
C	5.406268	2.452889	-1.058429
C	6.145188	0.206665	-1.579603
C	4.425334	3.433548	-0.748624
C	6.749858	2.909977	-1.273880
C	7.462852	0.662003	-1.786463
H	5.948353	-0.853474	-1.716092
C	4.752438	4.766166	-0.644639
H	3.403624	3.110692	-0.583249
C	7.052392	4.288025	-1.145431
C	7.763787	1.988300	-1.628298
H	8.235062	-0.052209	-2.068577
C	6.077735	5.203794	-0.836597
H	3.974280	5.491698	-0.410670
H	8.082942	4.605672	-1.308006
H	8.777858	2.359067	-1.780466
H	6.323509	6.261043	-0.746694
C	3.744786	-1.042749	-0.922266
C	4.177768	-1.794699	0.223365
C	3.468923	-1.726449	-2.092649
C	4.591513	-1.205495	1.453450
C	4.252301	-3.228360	0.123588
C	3.594353	-3.123245	-2.199645
H	3.163210	-1.159266	-2.970383
C	4.974794	-1.978383	2.526423
H	4.598338	-0.123186	1.526926
C	4.651287	-3.989370	1.251105
C	3.963939	-3.866962	-1.106089
H	3.382316	-3.605813	-3.152588
C	4.991672	-3.384626	2.436506
H	5.279917	-1.492962	3.452278
H	4.698427	-5.074957	1.147598
H	4.068747	-4.951993	-1.170211
H	5.294461	-3.984319	3.293865
H	1.414678	-2.672799	-0.333300
Si	0.402173	-3.623423	-0.788915
O	-1.101585	-2.893897	-0.736022
O	0.610744	-4.056973	-2.367147
O	0.291971	-4.950547	0.188696
C	-2.163153	-3.473030	0.038673
H	-1.794956	-3.809624	1.012814
H	-2.915121	-2.691365	0.181653
H	-2.595032	-4.321192	-0.506240
C	1.409073	-5.554629	0.805119
H	1.929325	-6.231065	0.110035
H	2.132384	-4.809939	1.169647
H	1.052426	-6.144143	1.657469
C	1.018148	-5.337609	-2.789591
H	2.087890	-5.506849	-2.589208
H	0.443417	-6.134830	-2.298217
H	0.857281	-5.405420	-3.870598
O	-2.889484	-0.279348	0.056365
N	-1.643883	-0.090851	-2.392752
C	-1.114007	1.283735	-2.438583
H	-1.399167	1.774805	-1.493073
H	-1.623459	1.838198	-3.248867
C	-1.183951	-0.901291	-3.538319
H	-1.179269	-0.273407	-4.447360
H	-0.149748	-1.227575	-3.365799
C	-2.180588	-2.051085	-3.652317
H	-1.736405	-2.990056	-3.306913
H	-2.477840	-2.197352	-4.696892
C	-3.363739	-1.641092	-2.770663
H	-3.404394	-2.252313	-1.862078
H	-4.332383	-1.761813	-3.264691
C	-3.123186	-0.183056	-2.368623
H	-3.531913	0.489298	-3.147078
C	-3.730308	0.163945	-0.955866
C	-5.094201	-0.550300	-0.861546
C	-6.099627	-0.314856	-1.799146
H	-5.925154	0.399199	-2.607106
C	-7.329943	-0.964005	-1.734581
H	-8.085005	-0.759942	-2.489704
C	-7.579106	-1.863054	-0.693471
C	-6.593524	-2.086487	0.270453

H	-6.810301	-2.776292	1.083827
C	-5.370038	-1.436370	0.181458
H	-4.603917	-1.600378	0.937053
O	-8.744344	-2.554655	-0.531262
C	-9.750094	-2.340557	-1.493388
H	-10.078650	-1.290855	-1.512999
H	-9.414986	-2.623395	-2.502549
H	-10.589773	-2.974781	-1.201399
C	-4.052899	1.652383	-0.723355
C	-4.544800	1.978050	0.553432
C	-3.987788	2.680055	-1.658121
C	-4.950662	3.258072	0.875241
H	-4.620452	1.184762	1.296387
C	-4.353207	3.994506	-1.341490
H	-3.643375	2.482718	-2.672148
C	-4.839942	4.287512	-0.070248
H	-5.356678	3.493543	1.857526
H	-4.263709	4.767230	-2.100666
O	-5.224906	5.526387	0.352343
C	-5.092238	6.581310	-0.572339
H	-5.711903	6.419547	-1.466304
H	-5.430672	7.482003	-0.056215
H	-4.045943	6.712756	-0.887852
Zn	-1.058503	-0.668055	-0.396007
Zn	1.728777	0.326457	0.979450
C	-0.924533	1.443107	2.134344
O	-0.187542	1.530957	1.151914
O	-1.759330	2.408448	2.472490
C	-1.697117	3.619238	1.662876
H	-2.221621	3.413723	0.721127
H	-0.644409	3.816354	1.434284
C	-2.333631	4.723619	2.456584
H	-3.367564	4.480452	2.718527
H	-2.349868	5.642265	1.859601
H	-1.776925	4.920149	3.379369
C	-0.935693	0.293549	3.141557
C	-0.164711	-0.918339	2.563401
O	-0.492921	-1.421247	1.452310
O	0.235194	-1.751980	3.557244
C	0.978509	-2.885407	3.087604
H	1.762467	-2.510890	2.401864
H	0.316444	-3.540189	2.503771
C	1.572494	-3.575563	4.284532
H	2.236325	-2.898589	4.832870
H	2.160358	-4.442966	3.963644
H	0.792309	-3.922462	4.970838
C	-2.389122	-0.186075	3.317577
H	-2.412324	-1.104806	3.912662
H	-2.829528	-0.392404	2.334991
H	-2.982350	0.581159	3.824149
C	-0.305013	0.800641	4.434898
C	-0.736780	0.342182	5.681123
C	0.745583	1.724102	4.393562
C	-0.136594	0.793373	6.852129
H	-1.546587	-0.381604	5.741170
C	1.346367	2.178678	5.563360
H	1.101417	2.102019	3.433879
C	0.906012	1.714405	6.798919
H	-0.489665	0.422422	7.812871
H	2.160339	2.898965	5.504482
H	1.370680	2.070856	7.716542
H	1.263166	-0.252023	2.408497

TS5g

M06L SCF energy in Solvent: -7322.529382 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.405038 a.u.

O	0.670151	-0.503694	-0.545184
C	1.151115	-0.420867	-1.819269
C	2.549243	-0.469159	-2.067635
C	2.988534	-0.398935	-3.390023
H	4.059610	-0.462132	-3.579830
C	2.129986	-0.279053	-4.482808
C	0.766891	-0.254289	-4.214536
H	0.055169	-0.180236	-5.040142
C	0.266884	-0.313549	-2.913856
C	2.662656	-0.179948	-5.879640
H	3.450696	-0.919120	-6.070139
H	3.105895	0.806172	-6.074202
H	1.873627	-0.333299	-6.624917
C	3.564420	-0.725800	-0.929812
O	3.377028	0.128701	0.167696
C	5.014251	-0.448461	-1.402227
C	5.418446	0.890204	-1.734712
C	5.955229	-1.455926	-1.475900
C	4.528930	1.997055	-1.768658
C	6.785099	1.133609	-2.100142
C	7.298881	-1.209634	-1.827238
H	5.664945	-2.478777	-1.249520

C	4.958645	3.252266	-2.135696
H	3.486221	1.847903	-1.502711
C	7.197374	2.442794	-2.450313
C	7.709796	0.062023	-2.125830
H	8.002606	-2.040178	-1.856283
C	6.306696	3.487120	-2.471656
H	4.244446	4.074800	-2.170739
H	8.243517	2.599219	-2.715846
H	8.744985	0.270537	-2.396991
H	6.633919	4.486817	-2.753810
C	3.422630	-2.217546	-0.509035
C	3.899288	-2.692726	0.759919
C	2.863284	-3.137033	-1.380575
C	4.636082	-1.889417	1.674547
C	3.678113	-4.068906	1.118553
C	2.678347	-4.491249	-1.040024
H	2.537893	-2.807001	-2.364910
C	5.072604	-2.395145	2.877706
H	4.836393	-0.857637	1.406965
C	4.122393	-4.546046	2.377207
C	3.054321	-4.946265	0.197966
H	2.224043	-5.168028	-1.762854
C	4.799537	-3.728106	3.247187
H	5.639445	-1.754919	3.552336
H	3.931472	-5.590442	2.629063
H	2.915556	-5.991221	0.478961
H	5.143370	-4.110570	4.207084
H	1.114847	-2.878483	0.492755
Si	0.352165	-3.219767	1.679286
O	-1.104865	-2.416976	1.363529
O	-0.083072	-4.785109	1.887597
O	1.003916	-2.713796	3.099353
C	-2.224848	-2.629808	2.234858
H	-2.000994	-2.239236	3.235783
H	-3.076166	-2.095086	1.802524
H	-2.438445	-3.702042	2.297594
C	1.508673	-1.396096	3.240240
H	2.109766	-1.356374	4.153713
H	2.162387	-1.117826	2.397387
H	0.685652	-0.669484	3.317394
C	0.592378	-5.707739	2.720778
H	1.376936	-6.229751	2.156213
H	1.051235	-5.216377	3.588004
H	-0.137120	-6.445629	3.070991
O	-3.047885	-0.335976	0.173629
N	-1.740728	-1.433343	-1.987440
C	-1.219355	-0.265417	-2.728113
H	-1.517591	0.636757	-2.169962
H	-1.717684	-0.198485	-3.712256
C	-1.285120	-2.729736	-2.511261
H	-1.453544	-2.765535	-3.603938
H	-0.208437	-2.845962	-2.340424
C	-2.149230	-3.744946	-1.773509
H	-1.625862	-4.124712	-0.886864
H	-2.370187	-4.611764	-2.404919
C	-3.411070	-2.962369	-1.372395
H	-3.518610	-2.919192	-0.280780
H	-4.335019	-3.403792	-1.759138
C	-3.215335	-1.539322	-1.907342
H	-3.628923	-1.458740	-2.929556
C	-3.826004	-0.442647	-0.972589
C	-5.248814	-0.887165	-0.588853
C	-6.217445	-1.164868	-1.553662
H	-5.975496	-1.056666	-2.611960
C	-7.502133	-1.577998	-1.208865
H	-8.224528	-1.787149	-1.993691
C	-7.846756	-1.707248	0.139019
C	-6.892216	-1.422951	1.118924
H	-7.175004	-1.522271	2.165513
C	-5.615383	-1.023622	0.752177
H	-4.873556	-0.807086	1.517139
O	-9.072162	-2.097395	0.591411
C	-10.046164	-2.396814	-0.381915
H	-10.275812	-1.523620	-1.010190
H	-9.729979	-3.226377	-1.031664
H	-10.942509	-2.690881	0.167820
C	-3.953720	0.930187	-1.659397
C	-3.800571	2.083289	-0.877412
C	-4.282782	1.108717	-3.003280
C	-3.956028	3.350881	-1.413878
H	-3.549381	1.964139	0.175966
C	-4.433381	2.376734	-3.565506
H	-4.419828	0.248381	-3.658779
C	-4.271003	3.509156	-2.767340
H	-3.839515	4.242807	-0.800930
H	-4.676081	2.465629	-4.621434
O	-4.399729	4.792784	-3.205068
C	-4.720010	4.973985	-4.565366

H	-5.683184	4.508050	-4.820985
H	-4.789252	6.052741	-4.718796
H	-3.941564	4.562452	-5.224705
Zn	-1.203770	-0.796054	-0.013718
Zn	1.701323	0.809907	0.639201
C	0.885879	2.998435	1.061088
O	0.788004	2.547045	-0.129524
O	1.735100	4.025348	1.336531
C	2.935582	3.984275	0.555951
H	2.674761	4.084470	-0.504650
H	3.389726	2.983976	0.686139
C	3.849358	5.078077	1.034190
H	3.389914	6.063969	0.902112
H	4.784428	5.053730	0.463667
H	4.089723	4.953094	2.095152
C	-0.393325	3.151354	1.911295
C	-1.297322	4.112072	1.122718
H	-2.231574	4.300087	1.660869
H	-1.521498	3.682291	0.141251
H	-0.779437	5.062000	0.957258
C	-0.088595	3.621718	3.328147
C	-0.254618	4.950041	3.721880
C	0.387107	2.702139	4.270487
C	0.048612	5.349240	5.020544
H	-0.622063	5.687414	3.011756
C	0.691593	3.098576	5.568098
H	0.524076	1.659038	3.980039
C	0.522149	4.426776	5.948772
H	-0.088423	6.390809	5.306970
H	1.061254	2.365948	6.283528
H	0.755779	4.740382	6.964706
C	-1.110276	1.809910	2.022906
O	-0.673179	0.718168	1.656773
O	-2.265073	1.959554	2.650932
C	-2.973629	0.759503	3.057636
H	-2.356163	0.272940	3.826381
H	-3.057431	0.105793	2.184874
C	-4.314867	1.191993	3.579472
H	-4.217445	1.903959	4.405745
H	-4.870209	0.319147	3.941653
H	-4.907608	1.657891	2.784183
H	1.608099	1.886082	1.943201

TS5h

M06L SCF energy in Solvent: -7322.530395 a.u.

PBE0-D3BJ Free energy in Solvent: -7321.407954 a.u.

O	0.670151	-0.503694	-0.545184
C	1.151115	-0.420867	-1.819269
C	2.549243	-0.469159	-2.067635
C	2.988534	-0.398935	-3.390023
H	4.059610	-0.462132	-3.579830
C	2.129986	-0.279053	-4.482808
C	0.766891	-0.254289	-4.214536
H	0.055169	-0.180236	-5.040142
C	0.266884	-0.313549	-2.913856
C	2.662656	-0.179948	-5.879640
H	3.450696	-0.919120	-6.070139
H	3.105895	0.806172	-6.074202
H	1.873627	-0.333299	-6.624917
C	3.564420	-0.725800	-0.929812
O	3.377028	0.128701	0.167696
C	5.014251	-0.448461	-1.402227
C	5.418446	0.890204	-1.734712
C	5.955229	-1.455926	-1.475900
C	4.528930	1.997055	-1.768658
C	6.785099	1.133609	-2.100142
C	7.298881	-1.209634	-1.827238
H	5.664945	-2.478777	-1.249520
C	4.958645	3.252266	-2.135696
H	3.486221	1.847903	-1.502711
C	7.197374	2.442794	-2.450313
C	7.709796	0.062023	-2.125830
H	8.002606	-2.040178	-1.856283
C	6.306696	3.487120	-2.471656
H	4.244446	4.074800	-2.170739
H	8.243517	2.599219	-2.715846
H	8.744985	0.270537	-2.396991
H	6.633919	4.486817	-2.753810
C	3.422630	-2.217546	-0.509035
C	3.899288	-2.692726	0.759919
C	2.863284	-3.137033	-1.380575
C	4.636082	-1.889417	1.674547
C	3.678113	-4.068906	1.118553
C	2.678347	-4.491249	-1.040024
H	2.537893	-2.807001	-2.364910
C	5.072604	-2.395145	2.877706
H	4.836393	-0.857637	1.406965
C	4.122393	-4.546046	2.377207

C	3.054321	-4.946265	0.197966
H	2.224043	-5.168028	-1.762854
C	4.799537	-3.728106	3.247187
H	5.639445	-1.754919	3.552336
H	3.931472	-5.590442	2.629063
H	2.915556	-5.991221	0.478961
H	5.143370	-4.110570	4.207084
H	1.114847	-2.878483	0.492755
Si	0.352165	-3.219767	1.679286
O	-1.104865	-2.416976	1.363529
O	-0.083072	-4.785109	1.887597
O	1.003916	-2.713796	3.099353
C	-2.224848	-2.629808	2.234858
H	-2.000994	-2.239236	3.235783
H	-3.076166	-2.095086	1.802524
H	-2.438445	-3.702042	2.297594
C	1.508673	-1.396096	3.240240
H	2.109766	-1.356374	4.153713
H	2.162387	-1.117826	2.397387
H	0.685652	-0.669484	3.317394
C	0.592378	-5.707739	2.720778
H	1.376936	-6.229751	2.156213
H	1.051235	-5.216377	3.588004
H	-0.137120	-6.445629	3.070991
O	-3.047885	-0.335976	0.173629
N	-1.740728	-1.433343	-1.987440
C	-1.219355	-0.265417	-2.728113
H	-1.517591	0.636757	-2.169962
H	-1.717684	-0.198485	-3.712256
C	-1.285120	-2.729736	-2.511261
H	-1.453544	-2.765535	-3.603938
H	-0.208437	-2.845962	-2.340424
C	-2.149230	-3.744946	-1.773509
H	-1.625862	-4.124712	-0.886864
H	-2.370187	-4.611764	-2.404919
C	-3.411070	-2.962369	-1.372395
H	-3.518610	-2.919192	-0.280780
H	-4.335019	-3.403792	-1.759138
C	-3.215335	-1.539322	-1.907342
H	-3.628923	-1.458740	-2.929556
C	-3.826004	-0.442647	-0.972589
C	-5.248814	-0.887165	-0.588853
C	-6.217445	-1.164868	-1.553662
H	-5.975496	-1.056666	-2.611960
C	-7.502133	-1.577998	-1.208865
H	-8.224528	-1.787149	-1.993691
C	-7.846756	-1.707248	0.139019
C	-6.892216	-1.422951	1.118924
H	-7.175004	-1.522271	2.165513
C	-5.615383	-1.023622	0.752177
H	-4.873556	-0.807086	1.517139
O	-9.072162	-2.097395	0.591411
C	-10.046164	-2.396814	-0.381915
H	-10.275812	-1.523620	-1.010190
H	-9.729979	-3.226377	-1.031664
H	-10.942509	-2.690881	0.167820
C	-3.953720	0.930187	-1.659397
C	-3.800571	2.083289	-0.877412
C	-4.282782	1.108717	-3.003280
C	-3.956028	3.350881	-1.413878
H	-3.549381	1.964139	0.175966
C	-4.433381	2.376734	-3.565506
H	-4.419828	0.248381	-3.658779
C	-4.271003	3.509156	-2.767340
H	-3.839515	4.242807	-0.800930
H	-4.676081	2.465629	-4.621434
O	-4.399729	4.792784	-3.205068
C	-4.720010	4.973985	-4.565366
H	-5.683184	4.508050	-4.820985
H	-4.789252	6.052741	-4.718796
H	-3.941564	4.562452	-5.224705
Zn	-1.203770	-0.796054	-0.013718
Zn	1.701323	0.809907	0.639201
C	0.885879	2.998435	1.061088
O	0.788004	2.547045	-0.129524
O	1.735100	4.025348	1.336531
C	2.935582	3.984275	0.555951
H	2.674761	4.084470	-0.504650
H	3.389726	2.983976	0.686139
C	3.849358	5.078077	1.034190
H	3.389914	6.063969	0.902112
H	4.784428	5.053730	0.463667
H	4.089723	4.953094	2.095152
C	-0.393325	3.151354	1.911295
C	-1.297322	4.112072	1.122718
H	-2.231574	4.300087	1.660869
H	-1.521498	3.682291	0.141251
H	-0.779437	5.062000	0.957258

C	-0.088595	3.621718	3.328147
C	-0.254618	4.950041	3.721880
C	0.387107	2.702139	4.270487
C	0.048612	5.349240	5.020544
H	-0.622063	5.687414	3.011756
C	0.691593	3.098576	5.568098
H	0.524076	1.659038	3.980039
C	0.522149	4.426776	5.948772
H	-0.088423	6.390809	5.306970
H	1.061254	2.365948	6.283528
H	0.755779	4.740382	6.964706
C	-1.110276	1.809910	2.022906
O	-0.673179	0.718168	1.656773
O	-2.265073	1.959554	2.650932
C	-2.973629	0.759503	3.057636
H	-2.356163	0.272940	3.826381
H	-3.057431	0.105793	2.184874
C	-4.314867	1.191993	3.579472
H	-4.217445	1.903959	4.405745
H	-4.870209	0.319147	3.941653
H	-4.907608	1.657891	2.784183
H	1.608099	1.886082	1.943201

TS6e

M06L SCF energy in Solvent: -7957.811715 a.u.

PBE0-D3BJ Free energy in Solvent: -7956.552418 a.u.

O	0.340107	-0.344259	-1.165604
C	0.689201	0.541271	-2.124357
C	2.056200	0.781240	-2.426038
C	2.365387	1.643513	-3.477801
H	3.414853	1.805475	-3.722480
C	1.401638	2.299933	-4.244259
C	0.070787	2.050970	-3.931403
H	-0.718924	2.536694	-4.509798
C	-0.302181	1.198264	-2.891321
C	1.793795	3.231051	-5.350996
H	2.530360	2.777529	-6.026486
H	2.251587	4.152339	-4.965334
H	0.928045	3.526452	-5.955019
C	3.186597	0.039276	-1.678313
O	3.018443	0.066244	-0.285317
C	4.533447	0.758463	-1.919716
C	4.746964	2.064007	-1.360399
C	5.550289	0.177244	-2.647807
C	3.741048	2.797448	-0.676106
C	6.022824	2.695632	-1.532719
C	6.804235	0.801775	-2.815085
H	5.390435	-0.800127	-3.099273
C	3.977900	4.060395	-0.184203
H	2.768594	2.339155	-0.533905
C	6.243618	3.985643	-0.988621
C	7.042156	2.030943	-2.256798
H	7.581208	0.295068	-3.385356
C	5.246192	4.660466	-0.326981
H	3.176004	4.592331	0.330052
H	7.226162	4.439656	-1.121524
H	8.008816	2.521815	-2.372402
H	5.428748	5.655487	0.077505
C	3.229123	-1.431664	-2.164394
C	4.005230	-2.413230	-1.455497
C	2.475520	-1.850698	-3.245000
C	4.892260	-2.092656	-0.391072
C	3.919707	-3.791568	-1.851685
C	2.386474	-3.205002	-3.624513
H	1.905135	-1.119656	-3.813594
C	5.636108	-3.066509	0.237567
H	4.963858	-1.058923	-0.067365
C	4.686781	-4.768759	-1.169398
C	3.083154	-4.162630	-2.932137
H	1.754716	-3.482056	-4.468399
C	5.532528	-4.419078	-0.145329
H	6.311678	-2.785097	1.045001
H	4.597923	-5.808548	-1.487367
H	3.029686	-5.214288	-3.215856
H	6.122165	-5.178748	0.365871
H	1.335542	-2.701612	-0.931346
Si	0.315314	-3.655259	-0.510037
O	-0.954558	-2.718785	0.094535
O	-0.426331	-4.543801	-1.679384
O	0.923776	-4.714556	0.582081
C	-1.955360	-3.400462	0.882501
H	-1.544087	-3.585483	1.880373
H	-2.833551	-2.748555	0.926208
H	-2.228837	-4.345969	0.399323
C	2.136793	-4.474169	1.282670
H	2.735941	-5.391622	1.258956
H	2.730469	-3.669282	0.819584
H	1.914326	-4.198142	2.319272

C	0.106318	-5.742280	-2.208253
H	0.372662	-5.593305	-3.262399
H	0.998097	-6.078464	-1.661447
H	-0.657828	-6.525444	-2.143155
O	-3.304690	-0.644949	0.087639
N	-2.240409	-0.314139	-2.434429
C	-1.767814	1.072942	-2.592668
H	-2.011365	1.614066	-1.663854
H	-2.350448	1.572760	-3.389950
C	-1.849692	-1.202112	-3.538749
H	-2.076398	-0.714498	-4.505767
H	-0.767502	-1.383369	-3.501855
C	-2.688523	-2.452057	-3.317556
H	-2.128172	-3.181740	-2.721577
H	-2.935236	-2.939061	-4.267203
C	-3.930361	-1.962558	-2.557038
H	-4.044473	-2.493065	-1.603253
H	-4.861032	-2.114878	-3.113586
C	-3.704888	-0.471404	-2.275805
H	-4.206916	0.148876	-3.041728
C	-4.163289	-0.061001	-0.836692
C	-5.588087	-0.584052	-0.602257
C	-6.602680	-0.422684	-1.545698
H	-6.389030	0.064204	-2.498147
C	-7.900709	-0.874359	-1.316441
H	-8.658790	-0.733791	-2.082410
C	-8.206411	-1.500805	-0.106900
C	-7.202805	-1.667251	0.851499
H	-7.457524	-2.158242	1.788779
C	-5.915959	-1.215309	0.601338
H	-5.134946	-1.348597	1.347191
O	-9.439998	-1.979560	0.226886
C	-10.467349	-1.806723	-0.720838
H	-10.644603	-0.742988	-0.939351
H	-10.244368	-2.327852	-1.664008
H	-11.366587	-2.237746	-0.275675
C	-4.202666	1.468408	-0.655663
C	-3.695678	2.036205	0.519530
C	-4.751547	2.335085	-1.601940
C	-3.720051	3.404398	0.732350
H	-3.261815	1.383781	1.273912
C	-4.761295	3.717287	-1.417972
H	-5.177796	1.942267	-2.525181
C	-4.238274	4.259560	-0.242905
H	-3.318882	3.835635	1.646092
H	-5.181187	4.355643	-2.191458
O	-4.186772	5.594763	0.040076
C	-4.671388	6.471649	-0.948888
H	-5.739635	6.306314	-1.154014
H	-4.533640	7.481105	-0.554840
H	-4.112349	6.368929	-1.891584
Zn	-1.480292	-0.698540	-0.444493
Zn	1.461875	-0.489182	0.594913
C	1.776709	1.856382	2.680634
O	2.307078	0.851139	2.228420
O	2.481579	2.893809	3.112716
C	3.927705	2.742115	3.028875
H	4.182420	2.439663	2.006956
H	4.212965	1.926896	3.705030
C	4.534906	4.060318	3.413575
H	4.194073	4.856188	2.742843
H	5.625449	3.999315	3.334832
H	4.277262	4.339944	4.440666
C	0.272631	2.073795	2.830908
C	-0.483189	0.761068	2.465331
O	-0.406434	0.290221	1.276763
O	-1.631603	0.682351	3.168073
C	-2.351523	-0.563627	3.058580
H	-1.610557	-1.376048	3.104636
H	-2.854639	-0.602562	2.084840
C	-3.317096	-0.629346	4.209055
H	-2.793228	-0.548110	5.168394
H	-3.852113	-1.586289	4.187352
H	-4.060245	0.174036	4.148177
C	-0.003681	2.431166	4.293425
H	0.581476	3.304027	4.593411
H	0.264072	1.583779	4.935613
H	-1.065123	2.638528	4.445826
C	-0.109739	3.175626	1.833623
C	-0.690625	4.374747	2.249520
C	0.183290	3.012186	0.472283
C	-0.996356	5.371887	1.325301
H	-0.915235	4.537441	3.301414
C	-0.118945	4.007243	-0.450510
H	0.656542	2.095461	0.120171
C	-0.719623	5.190223	-0.025553
H	-1.474354	6.289345	1.664909
H	0.126679	3.848740	-1.501003

H	-0.973342	5.968083	-0.744346
H	1.238618	-1.586815	1.913990
H	0.332283	-0.210446	3.187176
Si	1.120840	-1.533323	3.600178
O	0.219541	-2.939594	3.430931
O	2.764438	-1.690209	3.781699
O	0.769024	-1.028503	5.179855
C	-0.424037	-3.586102	4.507633
H	-1.272156	-4.157881	4.107946
H	0.257407	-4.291175	5.005563
H	-0.796800	-2.871166	5.253202
C	1.492120	-1.483678	6.298784
H	2.548760	-1.191070	6.244677
H	1.045220	-1.041217	7.197748
H	1.453867	-2.580722	6.405641
C	3.753069	-1.849477	2.802322
H	4.122652	-2.885835	2.792489
H	3.400252	-1.604823	1.788670
H	4.591821	-1.176886	3.026290

TS6f

M06L SCF energy in Solvent: -7957.813383 a.u.

PBE0-D3BJ Free energy in Solvent: -7956.557467 a.u.

O	0.500400	-0.442532	-0.795883
C	0.876819	-0.103664	-2.058041
C	2.244815	-0.076566	-2.446406
C	2.541453	0.318396	-3.752384
H	3.585989	0.329104	-4.060512
C	1.576494	0.664910	-4.698484
C	0.246245	0.556475	-4.312182
H	-0.545725	0.765408	-5.035671
C	-0.119794	0.180501	-3.019237
C	1.966328	1.117829	-6.072175
H	1.143064	1.002407	-6.787042
H	2.825889	0.556078	-6.457258
H	2.255321	2.177758	-6.081822
C	3.391818	-0.623833	-1.551571
O	3.348371	-0.178914	-0.226541
C	4.762743	-0.149825	-2.088556
C	5.130756	1.233563	-1.975102
C	5.665896	-1.033297	-2.642933
C	4.254298	2.243779	-1.496468
C	6.441037	1.638949	-2.397104
C	6.951475	-0.628935	-3.059744
H	5.387501	-2.080000	-2.752325
C	4.650350	3.560281	-1.425353
H	3.255775	1.973481	-1.169893
C	6.821434	2.999797	-2.291439
C	7.337041	0.679386	-2.927466
H	7.634253	-1.366254	-3.479135
C	5.948425	3.947169	-1.815153
H	3.944990	4.309401	-1.064870
H	7.826227	3.280126	-2.609598
H	8.330293	1.005800	-3.237187
H	6.251502	4.991059	-1.747818
C	3.302168	-2.174477	-1.553545
C	4.002521	-2.938632	-0.556631
C	2.513297	-2.853153	-2.464623
C	4.963568	-2.382507	0.333891
C	3.754591	-4.350096	-0.460727
C	2.297370	-4.244432	-2.386787
H	2.008359	-2.297218	-3.252143
C	5.599874	-3.159769	1.274983
H	5.189171	-1.324132	0.262746
C	4.403881	-5.112127	0.543035
C	2.880475	-4.976362	-1.383494
H	1.645418	-4.725806	-3.116574
C	5.308017	-4.533357	1.398938
H	6.340220	-2.704585	1.932215
H	4.178155	-6.177425	0.607545
H	2.714839	-6.051132	-1.298844
H	5.807584	-5.132138	2.159218
H	1.280945	-2.843644	-0.185718
Si	0.415635	-3.549687	0.741513
O	-0.708211	-2.365274	1.179796
O	-0.517486	-4.761687	0.147009
O	1.199944	-4.126146	2.062333
C	-1.618421	-2.676158	2.250969
H	-1.180152	-2.329279	3.192596
H	-2.559735	-2.157263	2.043038
H	-1.802257	-3.755828	2.293169
C	2.166228	-3.291979	2.696164
H	2.842581	-3.933524	3.269344
H	2.766170	-2.733257	1.958979
H	1.673600	-2.575841	3.368668
C	-0.118790	-6.113830	0.035181
H	0.213242	-6.325872	-0.990062
H	0.692711	-6.364245	0.731661

H	-0.984259	-6.745990	0.261982
Zn	-1.322538	-0.781480	-0.081396
O	-3.162700	-0.574574	0.334312
N	-1.975654	-1.202320	-2.089789
C	-1.587504	0.079397	-2.710351
H	-1.912325	0.880877	-2.027729
H	-2.161353	0.231014	-3.643647
C	-1.412660	-2.394575	-2.767843
H	-1.280434	-2.188307	-3.842273
H	-0.412046	-2.601356	-2.359216
C	-2.415995	-3.523795	-2.515807
H	-1.938570	-4.405663	-2.076086
H	-2.874672	-3.836967	-3.461765
C	-3.466268	-2.914191	-1.592136
H	-3.194537	-3.050258	-0.533891
H	-4.463703	-3.343298	-1.726420
C	-3.430638	-1.423702	-1.909192
H	-3.958543	-1.230423	-2.862176
C	-4.022495	-0.538271	-0.757109
C	-5.376518	-1.151464	-0.361625
C	-6.442557	-1.203948	-1.258916
H	-6.333762	-0.764506	-2.251369
C	-7.656821	-1.798348	-0.923223
H	-8.462060	-1.820468	-1.653327
C	-7.825017	-2.347855	0.350313
C	-6.771230	-2.290765	1.265870
H	-6.921194	-2.717596	2.255508
C	-5.566750	-1.703157	0.908000
H	-4.744226	-1.664501	1.619577
O	-8.967523	-2.950275	0.788788
C	-10.036844	-3.028220	-0.125007
H	-10.380473	-2.030690	-0.436542
H	-9.763251	-3.602821	-1.022605
H	-10.846212	-3.541115	0.398438
C	-4.285541	0.922324	-1.172209
C	-4.233746	1.911913	-0.178043
C	-4.653104	1.328668	-2.454415
C	-4.526836	3.236296	-0.450612
H	-3.955159	1.619964	0.833002
C	-4.942036	2.661801	-2.754198
H	-4.711053	0.604818	-3.267580
C	-4.882890	3.623236	-1.746088
H	-4.463907	3.999760	0.322412
H	-5.210417	2.932882	-3.772292
O	-5.141058	4.950825	-1.923315
C	-5.502932	5.361076	-3.220723
H	-6.428181	4.871953	-3.559557
H	-5.665341	6.439603	-3.164091
H	-4.706912	5.151927	-3.951532
Zn	1.742825	0.189407	0.655443
C	-1.083640	1.732486	2.069091
O	-0.727034	0.707640	1.486787
O	-2.083244	1.763087	2.930857
C	-2.746356	0.494754	3.215218
H	-3.140481	0.102901	2.269229
H	-1.971751	-0.188326	3.582055
C	-3.816250	0.772093	4.231755
H	-4.564548	1.469491	3.839344
H	-4.330647	-0.162249	4.483683
H	-3.401545	1.193206	5.154457
C	-0.397395	3.088921	1.900277
C	1.134663	2.792215	1.779800
O	1.579048	2.149892	0.773845
O	1.863894	3.874872	2.207627
C	3.280733	3.650324	2.146870
H	3.514703	2.802332	2.817329
H	3.562326	3.347962	1.131312
C	3.971790	4.912549	2.582189
H	3.708675	5.183326	3.611338
H	5.057795	4.781229	2.528640
H	3.698290	5.749445	1.930008
C	-0.656931	3.957704	3.126486
H	-1.725332	4.148452	3.257020
H	-0.294008	3.444558	4.024615
H	-0.129817	4.910077	3.040367
C	-0.896622	3.706944	0.587081
C	-0.791960	2.997972	-0.619034
C	-1.456168	4.987095	0.557535
C	-1.215431	3.564449	-1.815998
H	-0.353561	2.002247	-0.624811
C	-1.889047	5.549069	-0.641706
H	-1.555278	5.560772	1.476105
C	-1.764660	4.842707	-1.832905
H	-1.111096	2.997702	-2.741648
H	-2.331878	6.543865	-0.639147
H	-2.103374	5.283675	-2.769331
H	1.652611	-0.041240	2.348193
H	1.264481	1.923678	2.856848

Si	1.603278	0.602609	3.843050
O	0.450568	-0.564054	4.172461
O	3.220451	0.331099	4.101928
O	1.290688	1.597173	5.167247
C	-0.113317	-0.718237	5.463543
H	-0.782603	-1.588095	5.430351
H	0.655065	-0.894546	6.226634
H	-0.688324	0.168260	5.759730
C	2.083864	2.732041	5.425498
H	1.775024	3.150393	6.390494
H	3.152076	2.476983	5.477451
H	1.941988	3.505177	4.653639
C	4.121104	-0.375278	3.281049
H	3.777620	-0.473409	2.238848
H	5.079148	0.159017	3.269864
H	4.287961	-1.384032	3.685149

TS6g

M06L SCF energy in Solvent: -7957.805665 a.u.

PBE0-D3BJ Free energy in Solvent: -7956.547141 a.u.

O	-0.803839	-0.754742	0.555042
C	-1.226073	-0.648478	1.848596
C	-2.611922	-0.563748	2.165551
C	-2.982813	-0.502899	3.509181
H	-4.046065	-0.471982	3.745203
C	-2.072352	-0.490963	4.566660
C	-0.725995	-0.557229	4.233802
H	0.030149	-0.554406	5.023043
C	-0.296134	-0.631533	2.908170
C	-2.536869	-0.403814	5.988227
H	-3.000112	0.568129	6.205340
H	-1.707647	-0.536288	6.692673
H	-3.292427	-1.165815	6.218360
C	-3.699360	-0.594078	1.065816
O	-3.436877	0.347639	0.070816
C	-5.083510	-0.180655	1.629955
C	-5.301403	1.172532	2.067727
C	-6.140760	-1.066109	1.674370
C	-4.284233	2.164481	2.115700
C	-6.609576	1.552199	2.518727
C	-7.426342	-0.684219	2.111633
H	-5.991708	-2.095152	1.355914
C	-4.543056	3.438384	2.565231
H	-3.284335	1.909322	1.780175
C	-6.843548	2.876580	2.964532
C	-7.659010	0.601210	2.521818
H	-8.228768	-1.420549	2.116501
C	-5.834805	3.807244	2.989180
H	-3.737517	4.171692	2.590095
H	-7.849681	3.138170	3.294115
H	-8.647068	0.914132	2.860514
H	-6.027976	4.821226	3.336494
C	-3.771199	-2.044370	0.513475
C	-4.240668	-2.341707	-0.810516
C	-3.430324	-3.101990	1.340353
C	-4.754878	-1.364539	-1.709883
C	-4.242651	-3.710170	-1.255965
C	-3.471731	-4.443109	0.914310
H	-3.106562	-2.893191	2.358300
C	-5.186469	-1.711016	-2.970767
H	-4.796722	-0.332828	-1.378157
C	-4.669359	-4.023078	-2.570546
C	-3.849625	-4.742545	-0.371016
H	-3.184499	-5.235683	1.605275
C	-5.128569	-3.046262	-3.419135
H	-5.579699	-0.938263	-3.631214
H	-4.629552	-5.065750	-2.888486
H	-3.885272	-5.773797	-0.724002
H	-5.459014	-3.301280	-4.425314
H	-1.513443	-2.998446	-0.397978
Si	-0.686165	-3.906428	-1.173130
O	0.812971	-3.133385	-1.094237
O	-0.404984	-5.407572	-0.577338
O	-1.167367	-4.086157	-2.736442
C	1.929195	-3.752564	-1.747702
H	1.785479	-3.730904	-2.835034
H	2.824400	-3.185430	-1.476724
H	2.028288	-4.791163	-1.409819
C	-1.542647	-2.915921	-3.449365
H	-0.658475	-2.329782	-3.743428
H	-2.086451	-3.225838	-4.347176
H	-2.208635	-2.273211	-2.851143
C	-1.066109	-6.587957	-0.986889
H	-1.760979	-6.915371	-0.203029
H	-1.623448	-6.444893	-1.922009
H	-0.315280	-7.371568	-1.140030
Zn	1.034076	-1.219590	-0.090325
O	2.911568	-0.970159	-0.272147

N	1.591887	-1.910307	1.945747
C	1.172224	-0.689821	2.647943
H	1.485858	0.155910	2.020190
H	1.726181	-0.596874	3.602662
C	1.079347	-3.154476	2.536903
H	1.205512	-3.122679	3.635920
H	0.004334	-3.254242	2.335122
C	1.935336	-4.244821	1.904775
H	1.431208	-4.665039	1.027211
H	2.096664	-5.073010	2.602951
C	3.242157	-3.539000	1.508922
H	3.432325	-3.624134	0.433871
H	4.122205	-3.958596	2.007525
C	3.058758	-2.065351	1.883826
H	3.463193	-1.894960	2.899429
C	3.695667	-1.055184	0.868791
C	5.087994	-1.588063	0.486628
C	6.050119	-1.881753	1.452688
H	5.825323	-1.718079	2.508131
C	7.303844	-2.383964	1.112359
H	8.023557	-2.603514	1.896932
C	7.619134	-2.591350	-0.232783
C	6.671521	-2.288707	-1.213912
H	6.936213	-2.448359	-2.257409
C	5.425846	-1.795218	-0.853199
H	4.688402	-1.551727	-1.615327
O	8.812671	-3.075887	-0.681945
C	9.780614	-3.389109	0.292168
H	10.066937	-2.505078	0.881209
H	9.427563	-4.171972	0.980071
H	10.652280	-3.755605	-0.253852
C	3.920233	0.349278	1.473038
C	3.854240	1.454347	0.613040
C	4.274126	0.596911	2.800361
C	4.112493	2.743727	1.052931
H	3.587693	1.270471	-0.425752
C	4.534231	1.887067	3.267789
H	4.350931	-0.221358	3.516544
C	4.457313	2.969022	2.390314
H	4.044135	3.595456	0.377235
H	4.795383	2.031482	4.313492
O	4.679308	4.269587	2.743905
C	5.094779	4.506759	4.070000
H	6.036267	3.986320	4.298515
H	5.246713	5.584873	4.151265
H	4.332287	4.193003	4.799408
Zn	-1.730135	0.715173	-0.569145
C	0.355597	2.974394	0.338241
O	0.319134	1.752768	0.214647
O	0.711593	3.581031	1.460694
C	1.003764	2.727641	2.598556
H	0.132871	2.081041	2.771553
H	1.857884	2.095406	2.334696
C	1.309886	3.625421	3.762487
H	0.450521	4.250870	4.026668
H	1.570403	3.013154	4.633723
H	2.160261	4.276749	3.532591
C	0.017899	3.965350	-0.767166
C	-1.017915	3.289218	-1.710896
O	-1.978107	2.632465	-1.194810
O	-1.277463	4.162172	-2.736369
C	-2.269578	3.718430	-3.665471
H	-1.888919	2.801485	-4.145387
H	-3.187151	3.458811	-3.122786
C	-2.482005	4.817743	-4.670669
H	-1.550713	5.058526	-5.195423
H	-3.225156	4.511387	-5.414546
H	-2.843485	5.729570	-4.183181
C	-0.700354	5.181146	-0.164149
H	-1.057724	5.842397	-0.957051
H	-1.570386	4.849473	0.411845
H	-0.033639	5.738159	0.499221
C	1.308685	4.329056	-1.495263
C	1.590399	5.643036	-1.880789
C	2.230645	3.328003	-1.819202
C	2.758877	5.944797	-2.573455
H	0.891646	6.442588	-1.645800
C	3.399454	3.628511	-2.511291
H	2.032092	2.295721	-1.533863
C	3.669165	4.939497	-2.890430
H	2.958320	6.974549	-2.865350
H	4.098163	2.828742	-2.754175
H	4.583950	5.178168	-3.430117
H	-0.991205	0.397061	-2.052385
H	-0.232356	2.296854	-2.394554
Si	0.065678	0.848037	-3.153554
O	1.066712	-0.329062	-2.452621
O	-1.005037	0.461608	-4.378763

O	1.246520	1.563774	-4.110990
C	2.314158	-0.635628	-3.086281
H	2.749950	-1.483385	-2.561536
H	2.155975	-0.879234	-4.143867
H	3.004546	0.211675	-3.019266
C	0.964970	2.711076	-4.872068
H	1.868157	2.976670	-5.434051
H	0.145393	2.533965	-5.585983
H	0.701898	3.567710	-4.230369
C	-2.362229	0.125279	-4.259411
H	-2.983296	0.911790	-4.712936
H	-2.558965	-0.813051	-4.795283
H	-2.687817	-0.002336	-3.213634

TS6h

M06L SCF energy in Solvent: -7957.807955 a.u.

PBE0-D3BJ Free energy in Solvent: -7956.549130 a.u.

O	-0.055309	-0.980130	0.507227
C	-0.391256	-1.496126	1.727458
C	-1.713899	-1.936725	2.015270
C	-1.962117	-2.505660	3.266115
H	-2.966767	-2.874460	3.469919
C	-0.998363	-2.645436	4.263709
C	0.280679	-2.196094	3.964348
H	1.075613	-2.289441	4.707724
C	0.592957	-1.625792	2.731097
C	-1.339701	-3.240402	5.595393
H	-1.910373	-2.538628	6.219000
H	-0.440113	-3.515070	6.158243
H	-1.958169	-4.140820	5.493793
C	-2.862925	-1.861227	0.976838
O	-2.955842	-0.587861	0.417117
C	-4.243986	-2.073625	1.650965
C	-4.732710	-1.106798	2.598440
C	-5.049656	-3.147684	1.331489
C	-3.993930	0.036114	3.010820
C	-6.021024	-1.309790	3.196564
C	-6.330261	-3.323029	1.897677
H	-4.694768	-3.892941	0.623585
C	-4.487750	0.906651	3.956579
H	-3.023636	0.225434	2.562564
C	-6.498157	-0.393997	4.166738
C	-6.806224	-2.425348	2.816539
H	-6.929617	-4.183362	1.604080
C	-5.749234	0.692971	4.547975
H	-3.892408	1.769101	4.252909
H	-7.479272	-0.574697	4.607096
H	-7.787636	-2.555141	3.273362
H	-6.127206	1.387439	5.296725
C	-2.622926	-2.965347	-0.088776
C	-3.108306	-2.864721	-1.438998
C	-1.972298	-4.128445	0.288626
C	-3.888429	-1.779977	-1.935129
C	-2.833728	-3.941482	-2.355368
C	-1.726958	-5.187591	-0.604741
H	-1.627347	-4.226819	1.316338
C	-4.336704	-1.752901	-3.236849
H	-4.114940	-0.957417	-1.267426
C	-3.295480	-3.866903	-3.693188
C	-2.134032	-5.088819	-1.912010
H	-1.205114	-6.077352	-0.252691
C	-4.034054	-2.796435	-4.133709
H	-4.929690	-0.901955	-3.573140
H	-3.055424	-4.692070	-4.365123
H	-1.958198	-5.897500	-2.622199
H	-4.386855	-2.756168	-5.163357
H	-0.282018	-2.898589	-1.264186
Si	0.677730	-3.160537	-2.325018
O	1.891868	-2.051453	-1.940359
O	1.435722	-4.614609	-2.336078
O	0.109915	-2.905091	-3.843785
C	3.014065	-1.911785	-2.827321
H	2.686715	-1.468485	-3.774543
H	3.736661	-1.254800	-2.334236
H	3.462257	-2.895052	-3.011352
C	-0.658709	-1.738240	-4.101991
H	-1.455524	-1.606716	-3.353759
H	-0.027418	-0.837146	-4.106756
H	-1.128558	-1.856064	-5.083208
C	1.015042	-5.745846	-3.073278
H	0.437429	-6.423433	-2.430132
H	0.400152	-5.465241	-3.938628
H	1.906685	-6.273307	-3.428830
Zn	1.767475	-0.764971	-0.244241
O	3.444642	0.119778	-0.303220
N	2.634072	-1.904386	1.371835
C	2.004203	-1.188390	2.499546
H	2.060009	-0.110246	2.280413

H	2.601821	-1.348880	3.415454
C	2.482135	-3.367453	1.440509
H	2.701423	-3.711411	2.468382
H	1.443556	-3.647334	1.219894
C	3.498378	-3.900179	0.436005
H	3.015552	-4.125808	-0.520740
H	3.946046	-4.833905	0.792566
C	4.530355	-2.773233	0.281231
H	4.550827	-2.389586	-0.745364
H	5.552035	-3.094186	0.506923
C	4.084254	-1.656406	1.227368
H	4.553082	-1.799017	2.218404
C	4.360286	-0.209632	0.693012
C	5.779307	-0.172405	0.099362
C	6.878646	-0.692297	0.782613
H	6.742051	-1.151292	1.762783
C	8.163851	-0.655524	0.246944
H	8.990064	-1.081524	0.810461
C	8.370082	-0.071485	-1.005163
C	7.282399	0.468383	-1.696530
H	7.460277	0.927740	-2.666787
C	6.009392	0.415902	-1.147611
H	5.163731	0.843570	-1.681857
O	9.581085	0.021029	-1.626149
C	10.691185	-0.507906	-0.939423
H	10.851515	-0.003534	0.025163
H	10.581123	-1.587707	-0.758529
H	11.555923	-0.336743	-1.583811
C	4.329634	0.835337	1.827468
C	3.776614	2.094744	1.568915
C	4.885561	0.627934	3.090482
C	3.757580	3.091332	2.531941
H	3.353881	2.267462	0.580420
C	4.873475	1.615728	4.075038
H	5.349924	-0.325988	3.340283
C	4.303443	2.858527	3.797655
H	3.323817	4.069564	2.330284
H	5.311314	1.404191	5.047226
O	4.234428	3.895693	4.679367
C	4.788515	3.683313	5.957199
H	5.863825	3.457682	5.901452
H	4.643204	4.614394	6.508717
H	4.282614	2.863430	6.488521
Zn	-1.465589	0.260808	-0.308707
C	-3.560123	2.472365	-0.367917
O	-3.288577	1.655214	-1.239091
O	-4.694651	2.461488	0.315353
C	-5.571266	1.327064	0.045147
H	-4.984261	0.421053	0.241033
H	-5.830642	1.350741	-1.021433
C	-6.764609	1.455811	0.946078
H	-6.455250	1.465920	1.997015
H	-7.424746	0.592983	0.801862
H	-7.335842	2.367597	0.738250
C	-2.637308	3.629778	0.001091
C	-1.180905	3.068892	-0.036137
O	-0.945403	1.976235	0.592233
O	-0.297790	4.101781	0.086162
C	1.064482	3.696855	0.284276
H	1.280125	2.836727	-0.368355
H	1.185497	3.348794	1.319280
C	1.941998	4.872162	-0.049830
H	1.800555	5.166019	-1.095004
H	2.997518	4.610310	0.089132
H	1.716212	5.733170	0.589868
C	-2.877241	4.067037	1.453332
H	-2.124525	4.796065	1.764840
H	-2.801159	3.201939	2.119594
H	-3.871936	4.506500	1.565636
C	-2.833266	4.770776	-0.994194
C	-2.409808	6.065658	-0.669926
C	-3.383103	4.557214	-2.263364
C	-2.526796	7.106905	-1.583416
H	-1.957251	6.257981	0.299389
C	-3.508055	5.601957	-3.176040
H	-3.710125	3.561628	-2.555628
C	-3.078159	6.881046	-2.842834
H	-2.182465	8.102480	-1.307717
H	-3.938656	5.406728	-4.157045
H	-3.171805	7.697255	-3.556993
H	-0.887277	0.685664	-1.836220
H	-1.023429	2.742213	-1.391421
Si	-0.160761	1.958108	-2.562341
O	-1.017284	1.738304	-3.967971
O	1.248495	1.065935	-2.239826
O	0.627191	3.397798	-2.927013
C	-2.220334	1.027996	-4.120327
H	-2.163564	0.416428	-5.031451

H	-3.058806	1.731130	-4.226762
H	-2.439918	0.372366	-3.266595
C	-0.076684	4.542304	-3.348891
H	-0.591657	5.027426	-2.506185
H	-0.817123	4.305024	-4.125894
H	0.649991	5.251765	-3.763763
C	2.512017	1.562862	-2.689526
H	2.853592	2.393150	-2.058406
H	2.451894	1.913238	-3.725517
H	3.232039	0.749344	-2.602843

TS7a'

M06L SCF energy in Solvent: -6687.266972 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.273264 a.u.

O	-0.421311	-0.720265	-0.332875
C	-0.893070	-1.928655	-0.704460
C	-2.287935	-2.143608	-0.825089
C	-2.706558	-3.404599	-1.258368
H	-3.771915	-3.589384	-1.382426
C	-1.829573	-4.447026	-1.565879
C	-0.466936	-4.194754	-1.455589
H	0.252196	-4.976913	-1.710518
C	0.014025	-2.958484	-1.029301
C	-2.349559	-5.783427	-2.001829
H	-1.552655	-6.410565	-2.418062
H	-3.131384	-5.687735	-2.765628
H	-2.796337	-6.338533	-1.165806
C	-3.316419	-0.999786	-0.602081
O	-3.134130	-0.297980	0.626198
C	-4.723073	-1.633526	-0.528113
C	-5.124673	-2.375832	0.631676
C	-5.589681	-1.562429	-1.600512
C	-4.268048	-2.640290	1.733986
C	-6.443908	-2.941052	0.671075
C	-6.879870	-2.126981	-1.561797
H	-5.276901	-1.042554	-2.504014
C	-4.693561	-3.379810	2.812382
H	-3.259439	-2.242492	1.713176
C	-6.856792	-3.677887	1.808758
C	-7.308547	-2.785668	-0.438305
H	-7.532435	-2.027964	-2.427757
C	-6.004571	-3.894363	2.863077
H	-4.006967	-3.569665	3.636413
H	-7.868558	-4.084650	1.819365
H	-8.308401	-3.217485	-0.387374
H	-6.332265	-4.470207	3.727189
C	-3.220973	0.042021	-1.740800
C	-4.092182	1.186768	-1.752848
C	-2.292772	-0.081582	-2.756315
C	-5.120630	1.397498	-0.795428
C	-3.973193	2.141728	-2.817195
C	-2.136246	0.892024	-3.763070
H	-1.664655	-0.968096	-2.794710
C	-6.016075	2.434850	-0.922679
H	-5.189424	0.729497	0.056829
C	-4.890998	3.219205	-2.898030
C	-2.960803	1.986602	-3.794502
H	-1.370827	0.752272	-4.526185
C	-5.908511	3.356145	-1.984004
H	-6.806527	2.553663	-0.182596
H	-4.781259	3.929649	-3.717983
H	-2.870282	2.736608	-4.580448
H	-6.620369	4.175601	-2.071594
O	3.151034	0.408761	-0.269984
N	1.966564	-1.619380	-1.788066
C	1.494002	-2.735035	-0.937873
H	1.792102	-2.501093	0.094427
H	2.035192	-3.657915	-1.215425
C	1.558330	-1.735950	-3.196260
H	1.856136	-2.726857	-3.588015
H	0.468206	-1.659330	-3.282184
C	2.328445	-0.613417	-3.861278
H	1.778808	0.330856	-3.741546
H	2.457234	-0.774980	-4.936271
C	3.653513	-0.564445	-3.086803
H	3.915666	0.460815	-2.803960
H	4.491791	-0.957825	-3.671554
C	3.440400	-1.413963	-1.820043
H	3.918365	-2.403381	-1.932967
C	3.960900	-0.691236	-0.529349
C	5.396019	-0.215811	-0.799516
C	6.377893	-1.077083	-1.287950
H	6.135861	-2.119355	-1.499091
C	7.681376	-0.646741	-1.525505
H	8.415077	-1.349306	-1.912242
C	8.023715	0.681327	-1.261620
C	7.050602	1.556649	-0.771747
H	7.333433	2.588900	-0.575580

C	5.756503	1.111750	-0.547867
H	4.995069	1.794293	-0.178845
O	9.265850	1.212398	-1.450642
C	10.263904	0.343992	-1.933093
H	10.439204	-0.496438	-1.245087
H	10.009294	-0.059124	-2.924715
H	11.174329	0.942026	-2.010385
C	4.002708	-1.629217	0.692489
C	3.606628	-1.132779	1.940309
C	4.457199	-2.948296	0.644596
C	3.640247	-1.919026	3.082007
H	3.268738	-0.099088	1.996447
C	4.490265	-3.758851	1.777889
H	4.785936	-3.384141	-0.299016
C	4.076323	-3.244543	3.008907
H	3.329219	-1.526095	4.048789
H	4.838638	-4.784770	1.689562
O	4.063323	-3.946356	4.176775
C	4.516496	-5.279947	4.125433
H	5.561381	-5.340513	3.787462
H	4.443742	-5.663735	5.145076
H	3.892996	-5.895971	3.460695
Zn	1.332326	0.072806	-0.620262
Zn	-1.480062	0.413865	0.987411
C	1.018409	4.698279	0.895349
O	1.906198	4.597586	0.075623
O	0.476615	5.862262	1.285752
C	1.014677	7.034952	0.636322
H	0.892198	6.916771	-0.446773
H	2.091930	7.080661	0.837336
C	0.271842	8.225168	1.176321
H	-0.800846	8.143359	0.972961
H	0.640720	9.143748	0.707954
H	0.406281	8.316910	2.259153
C	0.419809	3.524948	1.683123
C	0.940746	2.269395	0.982523
O	0.481130	1.894124	-0.119924
O	-0.079166	0.924187	2.153989
C	0.330159	0.094666	3.215728
H	-0.213338	0.366111	4.140735
H	1.399069	0.292862	3.412122
C	0.134599	-1.375203	2.908100
H	-0.922651	-1.593309	2.688078
H	0.436233	-2.009055	3.751150
H	0.726933	-1.669279	2.031423
C	1.025173	3.600302	3.086987
H	0.704100	4.512429	3.598671
H	2.120433	3.605977	3.029745
H	0.722392	2.734083	3.681448
H	1.927807	1.905341	1.320686
C	-1.097135	3.567726	1.660468
C	-1.861601	3.441826	2.822869
C	-1.759360	3.713457	0.434087
C	-3.252787	3.472135	2.764687
H	-1.372548	3.306877	3.785290
C	-3.148420	3.746826	0.376899
H	-1.179492	3.802520	-0.484194
C	-3.899471	3.627144	1.542984
H	-3.830746	3.368879	3.681672
H	-3.645929	3.865464	-0.583625
H	-4.986610	3.642963	1.491817

TS7b'

M06L SCF energy in Solvent: -6687.277593 a.u.

PBE0-D3BJ Free energy in Solvent: -6686.282479 a.u.

O	-0.843600	-0.899210	-0.141642
C	-1.574470	-1.870906	-0.725526
C	-2.981151	-1.763662	-0.831683
C	-3.664570	-2.797544	-1.471640
H	-4.746086	-2.719807	-1.578335
C	-3.026149	-3.921375	-2.005208
C	-1.638175	-3.982461	-1.909966
H	-1.104049	-4.834842	-2.337219
C	-0.903343	-2.980033	-1.278566
C	-3.815714	-5.019961	-2.650400
H	-3.188506	-5.642764	-3.298881
H	-4.639606	-4.627215	-3.258576
H	-4.268353	-5.687095	-1.903841
C	-3.700187	-0.477361	-0.367590
O	-3.347926	-0.147210	0.973863
C	-5.226996	-0.680373	-0.373389
C	-5.845854	-1.538869	0.596130
C	-6.022275	-0.067043	-1.320328
C	-5.119850	-2.291770	1.557649
C	-7.273396	-1.689434	0.575241
C	-7.423441	-0.219394	-1.336856
H	-5.561594	0.563012	-2.078436
C	-5.762029	-3.120143	2.448555

H	-4.039603	-2.197129	1.587158
C	-7.901463	-2.538766	1.518768
C	-8.039455	-1.005706	-0.398910
H	-8.007318	0.295876	-2.097801
C	-7.165894	-3.242303	2.440141
H	-5.176339	-3.687320	3.170680
H	-8.987698	-2.628990	1.488107
H	-9.122699	-1.129704	-0.394033
H	-7.661024	-3.896799	3.155985
C	-3.296958	0.693177	-1.303353
C	-3.618736	2.052875	-0.955300
C	-2.633720	0.461713	-2.495010
C	-4.364786	2.416623	0.201737
C	-3.216149	3.110549	-1.840212
C	-2.226541	1.504903	-3.349249
H	-2.419529	-0.563208	-2.791163
C	-4.659683	3.732613	0.477778
H	-4.706330	1.635332	0.871478
C	-3.538472	4.452955	-1.521706
C	-2.505995	2.807544	-3.025507
H	-1.691672	1.264876	-4.267670
C	-4.239383	4.765874	-0.383263
H	-5.236155	3.974413	1.369268
H	-3.212741	5.236268	-2.207198
H	-2.199182	3.627121	-3.675945
H	-4.479461	5.802274	-0.151611
O	2.642193	-0.462318	0.009438
N	1.297044	-1.998125	-1.913875
C	0.591318	-3.078315	-1.176062
H	0.909822	-3.007713	-0.127879
H	0.941642	-4.054716	-1.554816
C	0.999008	-1.986669	-3.355193
H	1.183302	-2.995118	-3.769937
H	-0.058024	-1.750300	-3.521663
C	1.976536	-0.962370	-3.907765
H	1.522053	0.037512	-3.894948
H	2.243377	-1.176531	-4.947544
C	3.177313	-1.024805	-2.946719
H	3.371345	-0.043489	-2.494561
H	4.106216	-1.331883	-3.437182
C	2.791738	-2.015807	-1.839978
H	3.135581	-3.033032	-2.097445
C	3.333366	-1.584478	-0.428541
C	4.819573	-1.219614	-0.608132
C	5.784894	-2.165183	-0.950250
H	5.508615	-3.215085	-1.048819
C	7.116853	-1.811558	-1.160695
H	7.838118	-2.581200	-1.423974
C	7.504100	-0.477692	-1.019381
C	6.548403	0.481403	-0.672602
H	6.865811	1.517085	-0.568317
C	5.226832	0.112165	-0.474283
H	4.479166	0.859517	-0.216252
O	8.777050	-0.018637	-1.196947
C	9.755433	-0.970100	-1.543031
H	9.865197	-1.743214	-0.767772
H	9.526194	-1.461870	-2.500434
H	10.693881	-0.419533	-1.637601
C	3.221462	-2.719867	0.605543
C	2.905907	-2.386713	1.929399
C	3.441147	-4.068938	0.322786
C	2.799865	-3.351671	2.917614
H	2.735179	-1.338355	2.165225
C	3.338354	-5.057091	1.302571
H	3.679882	-4.390206	-0.691281
C	3.014704	-4.699184	2.611765
H	2.550814	-3.086186	3.943356
H	3.507150	-6.096071	1.030916
O	2.882191	-5.577128	3.645664
C	3.104655	-6.938332	3.358412
H	4.125517	-7.113508	2.987709
H	2.965322	-7.473286	4.300144
H	2.388783	-7.319129	2.614832
Zn	0.918907	-0.294723	-0.750874
Zn	-1.633701	0.508247	1.076493
C	1.877791	4.350116	-0.303149
O	2.872085	3.799360	-0.732843
O	1.593262	5.645621	-0.499057
C	2.580842	6.376976	-1.258838
H	2.696146	5.891394	-2.235097
H	3.543787	6.294661	-0.740855
C	2.100779	7.797272	-1.369038
H	1.134748	7.848300	-1.882234
H	2.820980	8.394886	-1.937701
H	1.985056	8.251622	-0.379643
C	0.824709	3.666434	0.576721
C	1.011663	2.178035	0.284579
O	0.499530	1.678949	-0.751689

O	-0.137104	1.427818	1.746973
C	0.555939	0.876371	2.857198
H	0.497743	1.581437	3.702500
H	1.623255	0.786611	2.587638
C	0.015257	-0.483034	3.241091
H	-1.050970	-0.424692	3.510328
H	0.543007	-0.896277	4.109734
H	0.128615	-1.197151	2.412793
C	-0.580317	4.104235	0.189103
H	-1.330999	3.549481	0.765465
H	-0.759588	3.898924	-0.869558
H	-0.725306	5.173992	0.362815
H	1.891343	1.703067	0.750847
C	1.206434	3.953802	2.025906
C	0.280583	4.431986	2.955020
C	2.514031	3.693844	2.453659
C	0.651648	4.640835	4.280722
H	-0.744101	4.632240	2.649453
C	2.884030	3.900208	3.779179
H	3.251979	3.327600	1.739207
C	1.953135	4.375264	4.698500
H	-0.084282	5.013695	4.991236
H	3.905459	3.689638	4.091568
H	2.240308	4.540279	5.735530

TS10c

M06L SCF energy in Solvent: -7168.782557 a.u.

PBE0-D3BJ Free energy in Solvent: -7167.715972 a.u.

O	1.133285	-0.409558	-0.493556
C	1.653074	0.402113	-1.458556
C	3.056961	0.633586	-1.544403
C	3.556046	1.286365	-2.670189
H	4.634437	1.410937	-2.756660
C	2.749821	1.813499	-3.678650
C	1.378967	1.694098	-3.505631
H	0.703137	2.139057	-4.240057
C	0.817824	1.019922	-2.417363
C	3.345553	2.510341	-4.863393
H	3.982598	1.840164	-5.455975
H	3.978263	3.355377	-4.561583
H	2.570154	2.900928	-5.532559
C	4.014313	0.265790	-0.385224
O	3.489627	0.771800	0.824029
C	5.380690	0.969919	-0.568079
C	5.491382	2.392497	-0.401294
C	6.515508	0.252766	-0.891331
C	4.380278	3.248867	-0.172153
C	6.783974	3.005774	-0.517642
C	7.781565	0.861718	-1.011796
H	6.442300	-0.821155	-1.049802
C	4.540107	4.608566	-0.039263
H	3.391309	2.810242	-0.095339
C	6.913135	4.407618	-0.358009
C	7.916859	2.210606	-0.812709
H	8.647593	0.248927	-1.256556
C	5.817111	5.199498	-0.120698
H	3.666320	5.236248	0.131961
H	7.908338	4.845656	-0.441466
H	8.890295	2.695245	-0.893089
H	5.930156	6.276586	-0.005743
C	4.212862	-1.261443	-0.294610
C	4.844881	-1.858912	0.851098
C	3.819130	-2.082784	-1.333347
C	5.341456	-1.110541	1.953463
C	5.020954	-3.283699	0.882854
C	4.002031	-3.480147	-1.299356
H	3.349277	-1.636428	-2.208597
C	5.938549	-1.732701	3.026267
H	5.231656	-0.031364	1.938715
C	5.631481	-3.889425	2.008654
C	4.587750	-4.071530	-0.209889
H	3.670660	-4.084694	-2.143553
C	6.079214	-3.134397	3.064757
H	6.309638	-1.130938	3.854631
H	5.745557	-4.974089	2.011919
H	4.722567	-5.152531	-0.163617
H	6.550169	-3.612941	3.922222
H	1.130612	-3.037475	-1.925349
Si	0.406505	-3.908000	-1.007550
O	-0.885715	-2.950773	-0.503492
O	-0.141444	-5.220019	-1.824003
O	1.206866	-4.471120	0.307909
C	-1.946903	-3.564703	0.242103
H	-1.553043	-4.073762	1.130297
H	-2.628557	-2.766478	0.550969
H	-2.478049	-4.279290	-0.399588
C	1.645037	-3.581600	1.328171
H	2.331045	-4.126536	1.983054

H	2.190900	-2.724040	0.904186
H	0.791744	-3.208805	1.909571
C	-0.329432	-6.500357	-1.249585
H	-0.465120	-7.215893	-2.065985
H	0.535149	-6.800886	-0.646225
H	-1.225083	-6.524328	-0.612540
O	-2.665483	-0.259093	0.016884
N	-1.286603	-0.306402	-2.336491
C	-0.679669	1.033229	-2.315866
H	-1.018064	1.527598	-1.389201
H	-1.079403	1.630602	-3.155591
C	-0.830914	-1.112675	-3.479828
H	-0.846986	-0.487694	-4.392598
H	0.209685	-1.422967	-3.326535
C	-1.833494	-2.260802	-3.576903
H	-1.420173	-3.200246	-3.189759
H	-2.104223	-2.447380	-4.621880
C	-3.033248	-1.799359	-2.741039
H	-3.099098	-2.364161	-1.802616
H	-3.992851	-1.927877	-3.250545
C	-2.767322	-0.330749	-2.403783
H	-3.093195	0.305991	-3.249244
C	-3.442597	0.129654	-1.065482
C	-4.827056	-0.543382	-0.983092
C	-5.800522	-0.321739	-1.956940
H	-5.581369	0.343946	-2.794721
C	-7.055901	-0.921074	-1.888417
H	-7.785722	-0.727977	-2.670667
C	-7.364060	-1.752059	-0.807031
C	-6.406814	-1.966601	0.187516
H	-6.666247	-2.606423	1.029062
C	-5.156685	-1.370011	0.092733
H	-4.411188	-1.530737	0.869960
O	-8.560079	-2.384694	-0.633755
C	-9.541267	-2.175124	-1.622579
H	-9.819399	-1.113819	-1.702116
H	-9.206465	-2.527613	-2.609614
H	-10.413646	-2.753327	-1.311398
C	-3.727181	1.641921	-0.963235
C	-4.292491	2.079656	0.248242
C	-3.536763	2.600284	-1.953225
C	-4.634181	3.399880	0.462821
H	-4.469746	1.348880	1.035905
C	-3.847883	3.950915	-1.748380
H	-3.129959	2.319676	-2.923553
C	-4.399589	4.355486	-0.535267
H	-5.081434	3.723145	1.401124
H	-3.664888	4.665823	-2.546800
O	-4.732596	5.639616	-0.218602
C	-4.484057	6.619964	-1.199983
H	-5.060091	6.431705	-2.117752
H	-4.797897	7.571224	-0.765654
H	-3.415672	6.672303	-1.459533
Zn	-0.837497	-0.794915	-0.251996
Zn	1.904093	-0.004646	1.381669
C	-0.685302	1.563792	2.144531
O	0.140757	1.435537	1.240560
O	-1.491903	2.602251	2.232938
C	-1.334014	3.625664	1.202564
H	-1.877695	3.274928	0.316706
H	-0.270667	3.691334	0.950883
C	-1.884618	4.909331	1.754054
H	-2.935941	4.803759	2.038273
H	-1.823317	5.690581	0.988348
H	-1.315768	5.241156	2.629339
C	-0.747306	0.610386	3.327521
C	-0.393268	-0.819635	2.880442
O	-0.808747	-1.344922	1.830276
C	0.279443	1.138046	4.335873
H	-0.081662	2.058106	4.806743
H	1.238222	1.345454	3.852047
H	0.463264	0.393366	5.119424
C	-2.143698	0.467812	3.938531
C	-2.368170	0.614942	5.309742
C	-3.216790	0.112202	3.111526
C	-3.643398	0.435816	5.841977
H	-1.552730	0.877843	5.979488
C	-4.489432	-0.057140	3.645800
H	-3.049314	-0.030413	2.040425
C	-4.709107	0.103696	5.012871
H	-3.799000	0.559563	6.912403
H	-5.315056	-0.321665	2.984042
H	-5.705470	-0.032790	5.429811
H	1.370358	-0.661147	2.739689
H	-0.167425	-1.468791	3.751001

IM14b

M06L SCF energy in Solvent: -6533.562064 a.u.

PBE0-D3BJ Free energy in Solvent: -6532.619196 a.u.

O	-0.537373	-1.075430	0.272649
C	-1.165723	-2.152069	-0.243078
C	-2.563436	-2.185158	-0.501118
C	-3.109470	-3.371830	-0.991984
H	-4.179312	-3.400842	-1.199943
C	-2.351629	-4.512257	-1.273773
C	-0.972914	-4.418403	-1.106507
H	-0.335878	-5.263486	-1.379703
C	-0.375554	-3.264198	-0.604120
C	-3.001709	-5.771872	-1.759824
H	-2.276691	-6.445077	-2.232562
H	-3.794322	-5.567740	-2.490419
H	-3.471100	-6.330862	-0.938368
C	-3.419355	-0.895800	-0.442030
O	-3.203248	-0.188554	0.761040
C	-4.923146	-1.212235	-0.505958
C	-5.560151	-1.870877	0.597912
C	-5.685361	-0.866878	-1.603676
C	-4.859442	-2.313443	1.750741
C	-6.969598	-2.131133	0.530645
C	-7.072126	-1.118110	-1.662036
H	-5.208662	-0.384694	-2.455055
C	-5.511441	-2.963529	2.773454
H	-3.795183	-2.113369	1.822421
C	-7.608604	-2.793903	1.606673
C	-7.703720	-1.733926	-0.612874
H	-7.632944	-0.820382	-2.546692
C	-6.898514	-3.204507	2.708408
H	-4.947462	-3.292183	3.645159
H	-8.681436	-2.977041	1.536402
H	-8.774696	-1.936602	-0.643758
H	-7.402283	-3.716637	3.526880
C	-2.984347	0.000483	-1.647837
C	-3.224622	1.421636	-1.637016
C	-2.283900	-0.529354	-2.717411
C	-4.042010	2.075339	-0.669704
C	-2.622809	2.239821	-2.653636
C	-1.734909	0.274166	-3.737222
H	-2.134841	-1.606548	-2.766996
C	-4.194780	3.444333	-0.671204
H	-4.539576	1.472904	0.082481
C	-2.794830	3.646356	-2.615579
C	-1.873129	1.637648	-3.691249
H	-1.183433	-0.198706	-4.549680
C	-3.553547	4.244847	-1.638345
H	-4.837187	3.909815	0.075430
H	-2.316225	4.244361	-3.391872
H	-1.425351	2.275604	-4.453475
H	-3.681132	5.326663	-1.626240
O	2.957881	0.124687	-0.323801
N	1.649000	-2.102399	-1.425852
C	1.117378	-3.158290	-0.521081
H	1.438267	-2.909303	0.496250
H	1.587458	-4.121704	-0.788939
C	1.218336	-2.272403	-2.825433
H	1.436778	-3.303366	-3.162580
H	0.137156	-2.115185	-2.908234
C	2.067293	-1.256460	-3.554739
H	1.646587	-0.250856	-3.399837
H	2.106693	-1.429963	-4.635390
C	3.426884	-1.380840	-2.863891
H	3.929362	-0.413254	-2.767141
H	4.097296	-2.038715	-3.429381
C	3.138751	-1.982530	-1.472913
H	3.558473	-3.000016	-1.388699
C	3.673413	-1.068010	-0.316953
C	5.159460	-0.766797	-0.542550
C	6.060293	-1.693804	-1.065848
H	5.714750	-2.677608	-1.386164
C	7.415915	-1.399498	-1.213835
H	8.081610	-2.148038	-1.635699
C	7.894762	-0.148598	-0.823569
C	7.005143	0.792121	-0.295115
H	7.394521	1.763746	0.002440
C	5.662238	0.482034	-0.159605
H	4.967096	1.214981	0.243035
O	9.196507	0.248284	-0.921214
C	10.110732	-0.688536	-1.440239
H	10.155285	-1.598763	-0.823783
H	9.859917	-0.973875	-2.472847
H	11.086448	-0.198161	-1.429453
C	3.548116	-1.786777	1.040637
C	2.883506	-1.170740	2.105509
C	4.077109	-3.059772	1.261941
C	2.712130	-1.811188	3.324503
H	2.503759	-0.160850	1.960933
C	3.915379	-3.721950	2.475793

H	4.631050	-3.563523	0.468904
C	3.219875	-3.098298	3.515981
H	2.187874	-1.330400	4.147736
H	4.335579	-4.716464	2.602140
O	2.997967	-3.654754	4.739990
C	3.498973	-4.954672	4.951246
H	4.594379	-4.988935	4.856214
H	3.216820	-5.225589	5.970671
H	3.060131	-5.678202	4.248514
Zn	1.106476	-0.227721	-0.518170
Zn	-1.557019	0.674409	0.596093
C	-0.707778	3.317374	1.712498
O	-1.394359	2.301100	1.883815
O	-1.004718	4.440957	2.338265
C	-2.184222	4.423879	3.189226
H	-2.021425	3.680051	3.977006
H	-3.032347	4.083938	2.585850
C	-2.358926	5.818099	3.720044
H	-1.490489	6.129786	4.308749
H	-3.243274	5.862729	4.363623
H	-2.492267	6.534955	2.903240
C	0.555623	3.365852	0.869984
C	0.294155	2.716246	-0.527334
O	-0.068262	1.377720	-0.492084
C	1.578949	2.505733	1.622290
H	2.462579	2.319509	1.000891
H	1.143079	1.528420	1.858422
H	1.890504	2.972867	2.564021
C	1.020895	4.786102	0.601186
C	2.325727	5.205319	0.866555
C	0.144490	5.692975	-0.011621
C	2.739767	6.496851	0.545584
H	3.035913	4.522072	1.327355
C	0.554319	6.981134	-0.330789
H	-0.880656	5.387279	-0.229341
C	1.857081	7.389614	-0.050988
H	3.761395	6.802113	0.765260
H	-0.146422	7.670050	-0.799583
H	2.180685	8.398729	-0.299859
H	-0.482438	3.300341	-1.052388
H	1.233794	2.844202	-1.090684

TS10d

M06L SCF energy in Solvent: -7168.782557 a.u.

PBE0-D3BJ Free energy in Solvent: -7167.715972 a.u.

O	1.133285	-0.409558	-0.493556
C	1.653074	0.402113	-1.458556
C	3.056961	0.633586	-1.544403
C	3.556046	1.286365	-2.670189
H	4.634437	1.410937	-2.756660
C	2.749821	1.813499	-3.678650
C	1.378967	1.694098	-3.505631
H	0.703137	2.139057	-4.240057
C	0.817824	1.019922	-2.417363
C	3.345553	2.510341	-4.863393
H	3.982598	1.840164	-5.455975
H	3.978263	3.355377	-4.561583
H	2.570154	2.900928	-5.532559
C	4.014313	0.265790	-0.385224
O	3.489627	0.771800	0.824029
C	5.380690	0.969919	-0.568079
C	5.491382	2.392497	-0.401294
C	6.515508	0.252766	-0.891331
C	4.380278	3.248867	-0.172153
C	6.783974	3.005774	-0.517642
C	7.781565	0.861718	-1.011796
H	6.442300	-0.821155	-1.049802
C	4.540107	4.608566	-0.039263
H	3.391309	2.810242	-0.095339
C	6.913135	4.407618	-0.358009
C	7.916859	2.210606	-0.812709
H	8.647593	0.248927	-1.256556
C	5.817111	5.199498	-0.120698
H	3.666320	5.236248	0.131961
H	7.908338	4.845656	-0.441466
H	8.890295	2.695245	-0.893089
H	5.930156	6.276586	-0.005743
C	4.212862	-1.261443	-0.294610
C	4.844881	-1.858912	0.851098
C	3.819130	-2.082784	-1.333347
C	5.341456	-1.110541	1.953463
C	5.020954	-3.283699	0.882854
C	4.002031	-3.480147	-1.299356
H	3.349277	-1.636428	-2.208597
C	5.938549	-1.732701	3.026267
H	5.231656	-0.031364	1.938715
C	5.631481	-3.889425	2.008654
C	4.587750	-4.071530	-0.209889

H	3.670660	-4.084694	-2.143553
C	6.079214	-3.134397	3.064757
H	6.309638	-1.130938	3.854631
H	5.745557	-4.974089	2.011919
H	4.722567	-5.152531	-0.163617
H	6.550169	-3.612941	3.922222
H	1.130612	-3.037475	-1.925349
Si	0.406505	-3.908000	-1.007550
O	-0.885715	-2.950773	-0.503492
O	-0.141444	-5.220019	-1.824003
O	1.206866	-4.471120	0.307909
C	-1.946903	-3.564703	0.242103
H	-1.553043	-4.073762	1.130297
H	-2.628557	-2.766478	0.550969
H	-2.478049	-4.279290	-0.399588
C	1.645037	-3.581600	1.328171
H	2.331045	-4.126536	1.983054
H	2.190900	-2.724040	0.904186
H	0.791744	-3.208805	1.909571
C	-0.329432	-6.500357	-1.249585
H	-0.465120	-7.215893	-2.065985
H	0.535149	-6.800886	-0.646225
H	-1.225083	-6.524328	-0.612540
O	-2.665483	-0.259093	0.016884
N	-1.286603	-0.306402	-2.336491
C	-0.679669	1.033229	-2.315866
H	-1.018064	1.527598	-1.389201
H	-1.079403	1.630602	-3.155591
C	-0.830914	-1.112675	-3.479828
H	-0.846986	-0.487694	-4.392598
H	0.209685	-1.422967	-3.326535
C	-1.833494	-2.260802	-3.576903
H	-1.420173	-3.200246	-3.189759
H	-2.104223	-2.447380	-4.621880
C	-3.033248	-1.799359	-2.741039
H	-3.099098	-2.364161	-1.802616
H	-3.992851	-1.927877	-3.250545
C	-2.767322	-0.330749	-2.403783
H	-3.093195	0.305991	-3.249244
C	-3.442597	0.129654	-1.065482
C	-4.827056	-0.543382	-0.983092
C	-5.800522	-0.321739	-1.956940
H	-5.581369	0.343946	-2.794721
C	-7.055901	-0.921074	-1.888417
H	-7.785722	-0.727977	-2.670667
C	-7.364060	-1.752059	-0.807031
C	-6.406814	-1.966601	0.187516
H	-6.666247	-2.606423	1.029062
C	-5.156685	-1.370011	0.092733
H	-4.411188	-1.530737	0.869960
O	-8.560079	-2.384694	-0.633755
C	-9.541267	-2.175124	-1.622579
H	-9.819399	-1.113819	-1.702116
H	-9.206465	-2.527613	-2.609614
H	-10.413646	-2.753327	-1.311398
C	-3.727181	1.641921	-0.963235
C	-4.292491	2.079656	0.248242
C	-3.536763	2.600284	-1.953225
C	-4.634181	3.399880	0.462821
H	-4.469746	1.348880	1.035905
C	-3.847883	3.950915	-1.748380
H	-3.129959	2.319676	-2.923553
C	-4.399589	4.355486	-0.535267
H	-5.081434	3.723145	1.401124
H	-3.664888	4.665823	-2.546800
O	-4.732596	5.639616	-0.218602
C	-4.484057	6.619964	-1.199983
H	-5.060091	6.431705	-2.117752
H	-4.797897	7.571224	-0.765654
H	-3.415672	6.672303	-1.459533
Zn	-0.837497	-0.794915	-0.251996
Zn	1.904093	-0.004646	1.381669
C	-0.685302	1.563792	2.144531
O	0.140757	1.435537	1.240560
O	-1.491903	2.602251	2.232938
C	-1.334014	3.625664	1.202564
H	-1.877695	3.274928	0.316706
H	-0.270667	3.691334	0.950883
C	-1.884618	4.909331	1.754054
H	-2.935941	4.803759	2.038273
H	-1.823317	5.690581	0.988348
H	-1.315768	5.241156	2.629339
C	-0.747306	0.610386	3.327521
C	-0.393268	-0.819635	2.880442
O	-0.808747	-1.344922	1.830276
C	0.279443	1.138046	4.335873
H	-0.081662	2.058106	4.806743
H	1.238222	1.345454	3.852047

H	0.463264	0.393366	5.119424
C	-2.143698	0.467812	3.938531
C	-2.368170	0.614942	5.309742
C	-3.216790	0.112202	3.111526
C	-3.643398	0.435816	5.841977
H	-1.552730	0.877843	5.979488
C	-4.489432	-0.057140	3.645800
H	-3.049314	-0.030413	2.040425
C	-4.709107	0.103696	5.012871
H	-3.799000	0.559563	6.912403
H	-5.315056	-0.321665	2.984042
H	-5.705470	-0.032790	5.429811
H	1.370358	-0.661147	2.739689
H	-0.167425	-1.468791	3.751001

TS10e

M06L SCF energy in Solvent: -7168.780218 a.u.

PBE0-D3BJ Free energy in Solvent: -7167.715972 a.u.

O	0.860068	-0.599386	-0.549052
C	1.303777	-0.002981	-1.689178
C	2.697570	0.176640	-1.923927
C	3.114690	0.579509	-3.191336
H	4.184835	0.665491	-3.376775
C	2.236637	0.910420	-4.223281
C	0.882959	0.874886	-3.922605
H	0.157327	1.195112	-4.674524
C	0.401068	0.449524	-2.681307
C	2.741528	1.326841	-5.570782
H	1.931180	1.704826	-6.205124
H	3.213205	0.492860	-6.108490
H	3.499526	2.116932	-5.494244
C	3.729169	0.039604	-0.779714
O	3.276095	0.776204	0.334513
C	5.077309	0.683186	-1.187869
C	5.193932	2.109160	-1.317073
C	6.190296	-0.094753	-1.438933
C	4.098118	3.005108	-1.186926
C	6.472538	2.673024	-1.645217
C	7.443028	0.464438	-1.763961
H	6.110441	-1.177771	-1.377590
C	4.260500	4.361950	-1.346681
H	3.120256	2.598649	-0.951030
C	6.605988	4.076712	-1.783670
C	7.586341	1.824212	-1.850832
H	8.292354	-0.194379	-1.938344
C	5.525691	4.910899	-1.636794
H	3.398076	5.020262	-1.247667
H	7.590904	4.479239	-2.023232
H	8.549808	2.274081	-2.092732
H	5.641363	5.987660	-1.752620
C	3.953521	-1.441137	-0.408098
C	4.647869	-1.805425	0.798142
C	3.541647	-2.446515	-1.260917
C	5.175284	-0.858912	1.718979
C	4.862871	-3.197271	1.081493
C	3.762701	-3.810341	-0.981174
H	3.030428	-2.175249	-2.183337
C	5.834368	-1.262820	2.857689
H	5.036834	0.197622	1.514490
C	5.536839	-3.574653	2.269344
C	4.407731	-4.180331	0.170831
H	3.412714	-4.565161	-1.685293
C	6.011112	-2.630404	3.146600
H	6.226825	-0.512783	3.542614
H	5.679879	-4.638119	2.465225
H	4.576947	-5.231634	0.406010
H	6.531445	-2.934280	4.053778
H	0.819354	-3.357174	-1.636489
Si	0.132694	-4.098249	-0.584989
O	-1.136924	-3.082511	-0.132668
O	-0.459569	-5.489190	-1.216649
O	0.987360	-4.507067	0.751639
C	-2.140492	-3.611743	0.743461
H	-1.684177	-4.037630	1.645856
H	-2.799101	-2.783889	1.025816
H	-2.720155	-4.380189	0.215828
C	1.501858	-3.511734	1.630136
H	2.236997	-3.986400	2.286125
H	2.011996	-2.708817	1.073630
H	0.694016	-3.072496	2.228580
C	-0.655469	-6.697009	-0.505918
H	-0.533844	-7.527647	-1.208455
H	0.066448	-6.810594	0.311543
H	-1.671791	-6.739442	-0.090337
O	-2.820797	-0.176790	0.271208
N	-1.748073	-0.715615	-2.187110
C	-1.080335	0.567142	-2.459784
H	-1.310767	1.237382	-1.614682

H	-1.529585	1.026483	-3.359640
C	-1.460829	-1.723099	-3.220775
H	-1.535397	-1.248645	-4.216804
H	-0.429219	-2.078747	-3.113331
C	-2.528428	-2.799677	-3.036854
H	-2.120242	-3.699187	-2.560668
H	-2.929877	-3.112088	-4.007090
C	-3.595785	-2.140153	-2.156247
H	-3.578520	-2.552311	-1.139626
H	-4.614405	-2.282925	-2.528983
C	-3.225815	-0.656478	-2.083577
H	-3.623507	-0.135332	-2.975544
C	-3.718813	0.046413	-0.764057
C	-5.089991	-0.561526	-0.404569
C	-6.185944	-0.436794	-1.257693
H	-6.080064	0.122845	-2.189676
C	-7.421223	-1.002879	-0.951436
H	-8.250478	-0.887243	-1.644821
C	-7.579111	-1.699211	0.250679
C	-6.496307	-1.812967	1.126090
H	-6.641990	-2.346135	2.063822
C	-5.270896	-1.251122	0.795878
H	-4.424177	-1.329148	1.476371
O	-8.740225	-2.289820	0.656209
C	-9.847736	-2.180030	-0.207165
H	-10.135244	-1.130607	-0.369259
H	-9.650269	-2.646185	-1.184072
H	-10.668276	-2.706881	0.284294
C	-3.962858	1.562719	-0.893550
C	-4.431799	2.208628	0.264735
C	-3.810727	2.343977	-2.034083
C	-4.721812	3.558032	0.284241
H	-4.577998	1.614526	1.166330
C	-4.067755	3.721373	-2.030633
H	-3.478170	1.898290	-2.969851
C	-4.525553	4.333888	-0.866991
H	-5.098612	4.044261	1.182683
H	-3.915796	4.292477	-2.943174
O	-4.798673	5.663773	-0.739674
C	-4.574009	6.469556	-1.873959
H	-5.207994	6.167099	-2.720263
H	-4.828974	7.488931	-1.577736
H	-3.521102	6.434833	-2.192751
Zn	-1.085769	-0.908658	-0.138420
Zn	1.770663	0.112493	1.190190
C	-0.815337	1.752031	1.809524
O	-0.027513	1.493363	0.903115
O	-1.558327	2.843423	1.819664
C	-1.366361	3.760152	0.703017
H	-1.945165	3.363584	-0.139743
H	-0.306396	3.743932	0.428794
C	-1.830446	5.117448	1.148518
H	-2.872529	5.092535	1.480691
H	-1.765606	5.820566	0.310474
H	-1.210528	5.498850	1.967339
C	-0.965540	0.930425	3.080699
C	-0.514614	-0.525539	2.898531
O	-0.895831	-1.260040	1.977153
C	-2.467475	0.801666	3.417749
H	-2.627773	0.093293	4.237863
H	-2.995966	0.431871	2.531852
H	-2.872132	1.774236	3.712784
C	-0.161297	1.586295	4.198363
C	-0.458663	1.304791	5.534941
C	0.930426	2.417347	3.921783
C	0.308693	1.840823	6.565308
H	-1.302348	0.662388	5.781626
C	1.693619	2.959677	4.949957
H	1.201087	2.644120	2.889652
C	1.386258	2.672117	6.276947
H	0.057927	1.607605	7.598530
H	2.537899	3.602289	4.708308
H	1.984815	3.093976	7.082162
H	1.330560	-0.252944	2.673038
H	-0.187696	-0.983665	3.854321

TS10f

M06L SCF energy in Solvent: -7168.771855 a.u.

PBE0-D3BJ Free energy in Solvent: -7167.705658 a.u.

O	0.929886	0.354125	-0.399153
C	1.531651	1.418429	-0.995478
C	2.942282	1.589049	-0.975204
C	3.493365	2.615266	-1.741801
H	4.578212	2.717794	-1.756461
C	2.729882	3.528943	-2.470221
C	1.348730	3.412057	-2.374323
H	0.707616	4.143787	-2.872234

C	0.742976	2.390734	-1.641680
C	3.378626	4.602835	-3.289276
H	2.652786	5.360859	-3.605950
H	3.843634	4.200426	-4.200143
H	4.173545	5.114732	-2.732570
C	3.841344	0.706668	-0.077173
O	3.310384	0.700394	1.230678
C	5.263960	1.301468	0.061876
C	5.465962	2.540217	0.763525
C	6.366103	0.653316	-0.459979
C	4.409155	3.323299	1.300823
C	6.801042	3.047679	0.904704
C	7.676105	1.153554	-0.310736
H	6.234680	-0.277813	-1.005976
C	4.655739	4.517161	1.938685
H	3.392372	2.957436	1.213000
C	7.018458	4.275948	1.575857
C	7.891701	2.326363	0.362404
H	8.510225	0.597950	-0.736730
C	5.970435	5.001915	2.085108
H	3.821274	5.092280	2.337652
H	8.043528	4.635598	1.672052
H	8.897820	2.728263	0.485461
H	6.151209	5.947093	2.595240
C	3.936230	-0.713251	-0.693709
C	4.224326	-1.881541	0.093320
C	3.816206	-0.858689	-2.063597
C	4.508401	-1.853256	1.488973
C	4.283747	-3.161524	-0.560756
C	3.958847	-2.102614	-2.707980
H	3.604796	0.020454	-2.669412
C	4.738161	-3.010705	2.198377
H	4.546302	-0.891397	1.988280
C	4.507050	-4.333036	0.205774
C	4.167646	-3.238443	-1.968770
H	3.874424	-2.154687	-3.791706
C	4.715394	-4.267538	1.562197
H	4.954602	-2.949314	3.263801
H	4.535104	-5.291859	-0.315695
H	4.269559	-4.212741	-2.448600
H	4.890438	-5.176463	2.136536
H	1.408878	-2.203199	-1.130077
Si	0.493483	-2.560254	-2.208225
O	-1.061099	-1.969122	-1.980537
O	1.054355	-1.857229	-3.584989
O	0.251940	-4.189755	-2.345352
C	-2.151942	-2.828638	-1.608896
H	-1.817466	-3.635484	-0.950918
H	-2.884603	-2.211967	-1.077077
H	-2.597379	-3.250021	-2.518155
C	1.316270	-5.116737	-2.295844
H	1.915017	-5.087548	-3.218358
H	1.987488	-4.923687	-1.444341
H	0.887815	-6.118816	-2.186615
C	0.488480	-2.135772	-4.850031
H	0.383022	-1.195977	-5.404793
H	1.151343	-2.805008	-5.414797
H	-0.502231	-2.609343	-4.779998
O	-2.799348	0.065471	0.010224
N	-1.432201	1.243738	-2.069682
C	-0.744951	2.409319	-1.483286
H	-1.016504	2.442870	-0.417077
H	-1.145837	3.332434	-1.941569
C	-1.062321	1.026855	-3.482406
H	-0.960290	2.007153	-3.982106
H	-0.084016	0.532247	-3.538725
C	-2.210408	0.216171	-4.084741
H	-1.907975	-0.815013	-4.294244
H	-2.529617	0.655145	-5.036967
C	-3.323961	0.258246	-3.035555
H	-3.393349	-0.696420	-2.500052
H	-4.314447	0.454208	-3.457722
C	-2.912231	1.339353	-2.040213
H	-3.213613	2.331125	-2.426946
C	-3.495619	1.101328	-0.603897
C	-4.971169	0.699239	-0.780051
C	-5.921684	1.610831	-1.237560
H	-5.627121	2.644135	-1.428589
C	-7.249620	1.244092	-1.445386
H	-7.959037	1.985922	-1.803118
C	-7.651561	-0.067127	-1.177692
C	-6.712950	-0.989873	-0.708122
H	-7.042809	-2.006175	-0.498862
C	-5.392969	-0.606717	-0.517712
H	-4.661381	-1.324792	-0.151479
O	-8.923459	-0.534131	-1.335407
C	-9.889919	0.387744	-1.783223
H	-9.996869	1.233861	-1.088520

H	-9.647169	0.779923	-2.782084
H	-10.832675	-0.161290	-1.831377
C	-3.488840	2.347716	0.299267
C	-3.655444	2.134622	1.676196
C	-3.424617	3.669901	-0.133691
C	-3.710789	3.181592	2.577552
H	-3.757393	1.108879	2.030390
C	-3.472855	4.744601	0.758042
H	-3.318140	3.899296	-1.193520
C	-3.609677	4.502475	2.123728
H	-3.841684	3.007173	3.644027
H	-3.400969	5.758828	0.373585
O	-3.666046	5.468793	3.082697
C	-3.572847	6.805034	2.645358
H	-4.393998	7.065979	1.961428
H	-3.639422	7.423148	3.542888
H	-2.615703	7.000293	2.139663
Zn	-0.994671	-0.250941	-0.543683
Zn	1.736822	-0.276669	1.349995
C	-1.049226	-0.023280	2.788751
O	-0.187237	0.656844	2.253575
C	-0.911475	-1.508398	3.091475
C	-0.269640	-2.206262	1.870762
O	-0.661951	-1.950749	0.699888
O	0.100955	-3.468817	2.205424
C	0.795399	-4.178027	1.172827
H	1.673908	-3.570735	0.883787
H	0.145420	-4.268957	0.291099
C	1.199568	-5.517141	1.725069
H	1.847677	-5.398086	2.599801
H	1.754185	-6.083061	0.967963
H	0.322763	-6.103403	2.020386
C	-0.010597	-1.586825	4.332554
H	-0.515130	-1.166923	5.210002
H	0.920919	-1.036936	4.165769
H	0.249620	-2.627065	4.543602
C	-2.279116	-2.139412	3.319708
C	-2.491648	-3.091286	4.321474
C	-3.349598	-1.780171	2.491970
C	-3.748672	-3.659749	4.503681
H	-1.673975	-3.400192	4.969325
C	-4.609420	-2.342698	2.685066
H	-3.198648	-1.062911	1.679430
C	-4.814134	-3.283212	3.690529
H	-3.894346	-4.398747	5.289884
H	-5.435060	-2.034258	2.044022
H	-5.799173	-3.722009	3.840178
H	1.191361	-1.627104	2.013166
H	-1.978469	0.466585	3.148469

TS10g

M06L SCF energy in Solvent: -7168.771134 a.u.

PBE0-D3BJ Free energy in Solvent: -7167.703089 a.u.

O	0.697839	0.354600	-0.610901
C	1.162941	1.470087	-1.229895
C	2.554883	1.739226	-1.316902
C	2.972374	2.814645	-2.098316
H	4.042847	2.995592	-2.196338
C	2.089264	3.684491	-2.742397
C	0.731044	3.461905	-2.551706
H	0.003874	4.151314	-2.987671
C	0.256095	2.387350	-1.797987
C	2.596574	4.831572	-3.562281
H	3.250471	5.490268	-2.975720
H	1.773990	5.443749	-3.949812
H	3.187286	4.492553	-4.423896
C	3.568823	0.897049	-0.509739
O	3.156938	0.865615	0.839548
C	4.971539	1.552395	-0.491408
C	5.181883	2.796567	0.198538
C	6.051925	0.949950	-1.105728
C	4.143828	3.535476	0.826923
C	6.503142	3.356687	0.231063
C	7.349536	1.499841	-1.059525
H	5.912755	0.015530	-1.644153
C	4.394486	4.738198	1.446671
H	3.138534	3.129763	0.823664
C	6.726349	4.592491	0.886641
C	7.573368	2.679141	-0.400223
H	8.167516	0.977335	-1.553014
C	5.696225	5.275742	1.484300
H	3.574131	5.278012	1.917515
H	7.740996	4.992210	0.900023
H	8.570255	3.118717	-0.355036
H	5.880992	6.227065	1.981442
C	3.668352	-0.515675	-1.141934
C	4.067980	-1.676121	-0.393304
C	3.446551	-0.656510	-2.499944

C	4.450305	-1.648109	0.979209
C	4.139983	-2.945993	-1.066693
C	3.589132	-1.887276	-3.167573
H	3.157402	0.219559	-3.077569
C	4.790674	-2.798931	1.654341
H	4.472088	-0.690496	1.487516
C	4.485030	-4.110456	-0.335629
C	3.910342	-3.018198	-2.461009
H	3.409053	-1.936498	-4.239524
C	4.792091	-4.047628	1.002327
H	5.074543	-2.738122	2.703748
H	4.525943	-5.060997	-0.871294
H	4.014046	-3.983558	-2.958561
H	5.057727	-4.951138	1.549783
H	1.262144	-2.168294	-1.410192
Si	0.253028	-2.686565	-2.324766
O	-1.296581	-2.151239	-1.964168
O	0.616609	-2.106322	-3.821718
O	0.093259	-4.332390	-2.284976
C	-2.305168	-3.038795	-1.454105
H	-1.865637	-3.823870	-0.832489
H	-2.994742	-2.437403	-0.851088
H	-2.839204	-3.494193	-2.297215
C	1.202630	-5.198811	-2.400894
H	1.658174	-5.136161	-3.400439
H	1.976928	-4.970599	-1.652049
H	0.849674	-6.222922	-2.240751
C	-0.080905	-2.520265	-4.978646
H	-0.321700	-1.638090	-5.583638
H	0.552879	-3.190681	-5.574512
H	-1.019081	-3.047388	-4.747861
O	-2.948696	-0.169529	0.161453
N	-1.847541	1.062833	-2.055104
C	-1.215246	2.289948	-1.531069
H	-1.409134	2.317526	-0.447605
H	-1.724511	3.170535	-1.965174
C	-1.573480	0.858915	-3.489476
H	-1.630456	1.833572	-4.007420
H	-0.551535	0.481931	-3.620515
C	-2.663205	-0.094476	-3.976936
H	-2.265595	-1.101153	-4.137625
H	-3.073676	0.248262	-4.933437
C	-3.717485	-0.099805	-2.865000
H	-3.701904	-1.047049	-2.312203
H	-4.738950	0.028388	-3.236018
C	-3.324525	1.028702	-1.913702
H	-3.733260	1.984164	-2.291757
C	-3.775246	0.779355	-0.432227
C	-5.221491	0.252985	-0.479706
C	-6.253877	1.011629	-1.030818
H	-6.044596	2.015016	-1.406852
C	-7.557411	0.527596	-1.112487
H	-8.333226	1.148198	-1.553981
C	-7.850578	-0.744836	-0.615057
C	-6.831434	-1.508901	-0.041581
H	-7.079325	-2.493919	0.349447
C	-5.536995	-1.012275	0.019597
H	-4.741116	-1.604982	0.466172
O	-9.088404	-1.318877	-0.641796
C	-10.127020	-0.564108	-1.220602
H	-10.293317	0.380829	-0.682166
H	-9.923493	-0.335928	-2.277627
H	-11.025371	-1.181067	-1.152328
C	-3.806350	2.060152	0.422644
C	-3.739799	1.903491	1.813693
C	-3.980658	3.355154	-0.061434
C	-3.796315	2.982518	2.677031
H	-3.649246	0.890507	2.203114
C	-4.037318	4.461394	0.789249
H	-4.061436	3.540387	-1.132243
C	-3.935983	4.278947	2.167590
H	-3.741364	2.851932	3.756458
H	-4.155804	5.454419	0.363465
O	-3.970549	5.282297	3.088888
C	-4.107333	6.594664	2.594494
H	-5.049834	6.723737	2.041927
H	-4.108291	7.249236	3.468420
H	-3.270595	6.868204	1.935011
Zn	-1.188258	-0.368326	-0.579121
Zn	1.634923	-0.166280	1.112710
C	-1.007163	0.058921	2.754669
O	-0.248320	0.741667	2.085490
C	-0.964447	-1.444520	2.948791
C	-0.196898	-2.142354	1.815223
O	-0.550507	-1.972549	0.614537
O	0.249296	-3.358595	2.209555
C	1.021327	-4.051592	1.217568
H	1.829644	-3.372166	0.887489

H	0.387835	-4.267687	0.345996
C	1.566829	-5.300589	1.852841
H	2.198642	-5.054927	2.713145
H	2.177053	-5.851439	1.128326
H	0.758444	-5.956521	2.194334
C	-2.420772	-1.931593	2.857704
H	-2.464641	-3.024958	2.898866
H	-2.865473	-1.593015	1.914714
H	-3.010150	-1.530860	3.691445
C	-0.338308	-1.674069	4.322446
C	-0.841271	-2.635576	5.204067
C	0.777009	-0.925167	4.718316
C	-0.233792	-2.856263	6.435471
H	-1.707848	-3.230738	4.924542
C	1.382221	-1.142395	5.952562
H	1.184736	-0.162817	4.056173
C	0.879746	-2.110440	6.815254
H	-0.636585	-3.615428	7.103817
H	2.247502	-0.547313	6.237756
H	1.349030	-2.280567	7.782512
H	1.229274	-1.436840	2.010763
H	-1.805956	0.561396	3.339964

TSa

M06L SCF energy in Solvent: -7173.942687 a.u.

PBE0-D3BJ Free energy in Solvent: -7172.838421 a.u.

O	0.822607	0.158905	-0.430254
C	1.282507	1.104579	-1.290988
C	2.668632	1.403616	-1.400798
C	3.080143	2.271536	-2.411007
H	4.147439	2.466583	-2.515608
C	2.198262	2.920450	-3.276956
C	0.842297	2.693745	-3.078942
H	0.110490	3.221463	-3.695773
C	0.372675	1.816264	-2.100422
C	2.700241	3.842473	-4.346159
H	3.389782	4.595126	-3.942636
H	1.877179	4.375653	-4.836125
H	3.250158	3.303257	-5.129813
C	3.694323	0.830115	-0.392595
O	3.229194	1.064571	0.916346
C	5.051493	1.569966	-0.478507
C	5.145858	2.953331	-0.096604
C	6.198502	0.922365	-0.892546
C	4.030957	3.736064	0.305786
C	6.423060	3.604580	-0.159718
C	7.453789	1.563627	-0.935363
H	6.148013	-0.119381	-1.199392
C	4.168197	5.068259	0.621355
H	3.058855	3.260550	0.375565
C	6.529125	4.975006	0.183457
C	7.565939	2.879901	-0.574401
H	8.328378	1.001664	-1.259497
C	5.426642	5.699428	0.564233
H	3.291349	5.640413	0.921272
H	7.511928	5.444687	0.129081
H	8.527813	3.392607	-0.606705
H	5.521745	6.754059	0.819410
C	3.908369	-0.676950	-0.697089
C	4.341436	-1.618091	0.300564
C	3.747031	-1.125056	-1.994851
C	4.668384	-1.265353	1.641502
C	4.501376	-2.998445	-0.071923
C	3.985899	-2.460833	-2.370190
H	3.422187	-0.420753	-2.758165
C	5.032594	-2.219264	2.565186
H	4.618563	-0.218661	1.923067
C	4.863928	-3.953867	0.910249
C	4.337277	-3.387135	-1.422820
H	3.858306	-2.753500	-3.410979
C	5.110616	-3.580264	2.209360
H	5.273100	-1.913599	3.582367
H	4.965589	-4.996385	0.602193
H	4.515875	-4.429188	-1.691649
H	5.390823	-4.325996	2.952495
H	1.574487	-2.414172	-0.612456
Si	0.629277	-3.095375	-1.489805
O	-0.957847	-2.607448	-1.252620
O	1.037596	-2.707508	-3.034629
O	0.543735	-4.729103	-1.240070
C	-1.921523	-3.466535	-0.627399
H	-1.473073	-4.038825	0.190819
H	-2.717204	-2.828376	-0.225669
H	-2.332614	-4.154513	-1.376328
C	1.696720	-5.533017	-1.109564
H	2.238671	-5.616840	-2.063742
H	2.390811	-5.130822	-0.354726
H	1.378398	-6.533591	-0.797677

C	0.543991	-3.415064	-4.153177
H	-0.300938	-4.074444	-3.903861
H	0.211082	-2.696106	-4.911193
H	1.346129	-4.031388	-4.581703
O	-2.862450	-0.226710	0.263272
N	-1.652211	0.363560	-2.137112
C	-1.107145	1.711237	-1.893345
H	-1.376752	1.988068	-0.860481
H	-1.618825	2.435398	-2.554795
C	-1.264344	-0.173819	-3.454201
H	-1.303876	0.640981	-4.200265
H	-0.229092	-0.534319	-3.421911
C	-2.296335	-1.258819	-3.767647
H	-1.863182	-2.260755	-3.687378
H	-2.669110	-1.149379	-4.792778
C	-3.406884	-1.062825	-2.731434
H	-3.357002	-1.831238	-1.951757
H	-4.414433	-1.110456	-3.155841
C	-3.128454	0.294737	-2.095223
H	-3.539307	1.086177	-2.749613
C	-3.685147	0.437562	-0.638141
C	-5.087340	-0.202368	-0.627613
C	-6.123758	0.317606	-1.402170
H	-5.952653	1.219417	-1.993190
C	-7.382098	-0.277845	-1.440611
H	-8.162220	0.158171	-2.059732
C	-7.624739	-1.419767	-0.672394
C	-6.600900	-1.943456	0.121198
H	-6.811182	-2.827728	0.719927
C	-5.350869	-1.340669	0.137984
H	-4.551396	-1.744114	0.756499
O	-8.816191	-2.084117	-0.627409
C	-9.864221	-1.568215	-1.413775
H	-10.129581	-0.542480	-1.117188
H	-9.609380	-1.569815	-2.484224
H	-10.720490	-2.224985	-1.246102
C	-3.893305	1.901308	-0.198906
C	-4.035005	2.142651	1.175481
C	-4.078631	2.987057	-1.054016
C	-4.339638	3.401150	1.665587
H	-3.907061	1.305226	1.862078
C	-4.365283	4.269296	-0.579214
H	-3.997123	2.862409	-2.132858
C	-4.500965	4.480945	0.790880
H	-4.468783	3.580088	2.731494
H	-4.484978	5.084945	-1.287853
O	-4.787905	5.681210	1.370771
C	-4.967927	6.778673	0.505121
H	-5.806143	6.615906	-0.188371
H	-5.190089	7.635746	1.144064
H	-4.060537	6.987240	-0.080743
Zn	-1.052696	-0.573307	-0.239389
Zn	1.774064	-0.010918	1.359694
C	-0.699422	0.394109	3.127215
O	-0.045814	0.933634	2.234446
O	-1.555046	1.073790	3.874468
C	-1.595238	2.512147	3.661276
H	-1.921319	2.696599	2.632708
H	-0.573617	2.894824	3.766159
C	-2.539386	3.074837	4.684842
H	-3.531879	2.619923	4.593451
H	-2.645287	4.154946	4.539767
H	-2.176475	2.898102	5.702986
C	-0.522506	-1.036175	3.609405
C	0.035406	-1.899893	2.469961
O	-0.460264	-1.890036	1.310410
O	0.500797	-3.066921	2.991492
C	1.160184	-3.929178	2.059221
H	1.934119	-3.334274	1.539482
H	0.439729	-4.276669	1.305281
C	1.765856	-5.065569	2.837277
H	2.483111	-4.688982	3.574406
H	2.300788	-5.742803	2.161833
H	0.996384	-5.641170	3.363398
C	0.458485	-0.952676	4.789890
H	0.042474	-0.319091	5.580736
H	1.426212	-0.542132	4.479270
H	0.629972	-1.953569	5.195347
H	1.501991	-1.239307	2.362605
C	-1.841381	-1.665455	4.115494
H	-2.222225	-1.011062	4.908627
H	-1.568138	-2.611898	4.601237
C	-2.916220	-1.902101	3.070326
H	-2.645800	-2.720578	2.393070
H	-3.862811	-2.169360	3.554703
H	-3.089297	-1.022092	2.438681

TSb

M06L SCF energy in Solvent: -7173.943423 a.u.

PBE0-D3BJ Free energy in Solvent: -7172.835583 a.u.

O	0.797739	-0.081146	-0.643580
C	1.253632	0.793285	-1.573343
C	2.641605	1.071038	-1.712586
C	3.057631	1.824162	-2.808429
H	4.125862	1.999145	-2.937498
C	2.174750	2.395273	-3.728189
C	0.817011	2.225564	-3.487054
H	0.087468	2.712712	-4.139103
C	0.343994	1.456481	-2.422201
C	2.679417	3.191144	-4.893123
H	1.861489	3.696721	-5.419565
H	3.198186	2.560544	-5.628378
H	3.397658	3.959664	-4.579342
C	3.643389	0.649709	-0.610911
O	3.136185	1.079464	0.634817
C	5.001008	1.373900	-0.771379
C	5.093449	2.793858	-0.565429
C	6.152018	0.676992	-1.081967
C	3.973122	3.625616	-0.297360
C	6.376714	3.427991	-0.670395
C	7.410487	1.305885	-1.180783
H	6.101056	-0.395471	-1.254808
C	4.113298	4.984354	-0.133227
H	2.993454	3.168729	-0.212174
C	6.485252	4.828149	-0.484481
C	7.523074	2.654818	-0.972369
H	8.287829	0.707973	-1.422286
C	5.379170	5.597540	-0.220264
H	3.232635	5.592698	0.068814
H	7.473051	5.283073	-0.565455
H	8.488824	3.155997	-1.043988
H	5.476680	6.673729	-0.084271
C	3.860073	-0.882278	-0.656254
C	4.259349	-1.640762	0.499337
C	3.723348	-1.542815	-1.862336
C	4.555685	-1.068825	1.771332
C	4.410533	-3.065374	0.371536
C	3.960025	-2.923918	-1.998740
H	3.419459	-0.973659	-2.739113
C	4.877973	-1.856182	2.854547
H	4.521419	0.010869	1.871423
C	4.730384	-3.843511	1.512030
C	4.278327	-3.676653	-0.897808
H	3.852415	-3.390045	-2.976043
C	4.944974	-3.258421	2.736738
H	5.096138	-1.383518	3.811278
H	4.825957	-4.923888	1.387954
H	4.448048	-4.750950	-0.980515
H	5.191895	-3.870145	3.603433
H	1.510453	-2.586743	-0.297302
Si	0.570612	-3.368227	-1.096441
O	-1.017330	-2.836769	-1.040543
O	1.042756	-3.234508	-2.668739
O	0.451389	-4.935177	-0.574034
C	-2.045319	-3.583862	-0.370359
H	-1.641315	-4.143370	0.477655
H	-2.791354	-2.864805	-0.015029
H	-2.499505	-4.282087	-1.084477
C	1.590527	-5.701401	-0.247546
H	2.151580	-5.989250	-1.149436
H	2.272906	-5.154787	0.422220
H	1.253819	-6.611671	0.260548
C	0.413688	-3.975389	-3.694401
H	0.177657	-3.303144	-4.528210
H	1.094483	-4.757728	-4.055860
H	-0.519400	-4.456834	-3.365146
O	-2.952954	-0.469739	0.207499
N	-1.737528	0.089905	-2.218413
C	-1.131602	1.431593	-2.157903
H	-1.353175	1.846050	-1.161236
H	-1.636137	2.087852	-2.892572
C	-1.378677	-0.612918	-3.466850
H	-1.364873	0.114884	-4.297942
H	-0.365085	-1.024260	-3.377870
C	-2.461797	-1.668896	-3.672634
H	-2.079314	-2.674293	-3.468764
H	-2.812782	-1.662634	-4.710882
C	-3.571967	-1.299999	-2.685640
H	-3.598998	-2.006736	-1.847036
H	-4.570893	-1.307690	-3.132534
C	-3.217569	0.081438	-2.133944
H	-3.620037	0.869196	-2.800125
C	-3.742723	0.264614	-0.664052
C	-5.187978	-0.266601	-0.639930
C	-6.189120	0.334754	-1.401733

H	-5.952428	1.216284	-2.000815
C	-7.493941	-0.151834	-1.412725
H	-8.246600	0.344088	-2.020739
C	-7.818698	-1.263091	-0.630178
C	-6.829721	-1.866605	0.151075
H	-7.103748	-2.725415	0.760723
C	-5.533253	-1.371481	0.141362
H	-4.760035	-1.835233	0.751665
O	-9.061985	-1.821743	-0.558832
C	-10.077228	-1.215976	-1.323845
H	-10.244590	-0.170789	-1.023756
H	-9.847133	-1.241062	-2.399559
H	-10.984310	-1.794257	-1.135710
C	-3.837462	1.718226	-0.167782
C	-4.090589	1.882702	1.204191
C	-3.809051	2.867644	-0.951698
C	-4.299063	3.129313	1.762095
H	-4.137149	0.992549	1.830037
C	-3.975799	4.143266	-0.401011
H	-3.643872	2.796929	-2.026678
C	-4.221897	4.278177	0.963642
H	-4.519771	3.243193	2.822124
H	-3.919347	5.014113	-1.049148
O	-4.391917	5.466546	1.613009
C	-4.310747	6.634553	0.828462
H	-5.083003	6.652568	0.045713
H	-4.469766	7.471090	1.512040
H	-3.323827	6.734607	0.352320
Zn	-1.112305	-0.699782	-0.278233
Zn	1.678867	0.059642	1.176493
C	-0.807437	0.943583	2.701737
O	-0.263685	1.150361	1.616914
O	-1.345645	1.929840	3.405041
C	-1.153481	3.264685	2.850970
H	-1.647334	3.299821	1.873843
H	-0.077691	3.402872	2.691701
C	-1.726205	4.248486	3.829650
H	-2.792045	4.066137	3.998966
H	-1.625874	5.262793	3.428760
H	-1.207248	4.203206	4.793065
C	-0.917729	-0.403304	3.403217
C	-0.184485	-1.485829	2.582163
O	-0.569631	-1.793470	1.417297
O	0.256857	-2.479724	3.403788
C	1.012465	-3.496912	2.735832
H	1.813422	-2.994769	2.159455
H	0.369210	-4.024435	2.017400
C	1.578458	-4.411877	3.787273
H	2.221983	-3.855917	4.478385
H	2.182201	-5.197187	3.318624
H	0.781854	-4.890831	4.367055
C	-2.403186	-0.815428	3.435572
H	-2.492981	-1.790541	3.928610
H	-2.815775	-0.885306	2.421935
H	-2.979757	-0.083248	4.011785
H	1.222293	-0.829522	2.438537
C	-0.393722	-0.275998	4.847979
H	-0.556464	-1.241945	5.340089
H	-1.041195	0.447239	5.359463
C	1.060400	0.139214	4.998624
H	1.301704	0.304269	6.054868
H	1.743538	-0.626415	4.614395
H	1.282508	1.076314	4.467598

TS(3a-Si)

M06L SCF energy in Solvent: -7168.842861 a.u.

PBE0-D3BJ Free energy in Solvent: -7167.769332 a.u.

O	0.516369	0.228745	-0.758792
C	0.835517	1.409215	-1.324921
C	2.190554	1.831695	-1.404462
C	2.468960	3.043759	-2.035280
H	3.508083	3.361045	-2.116307
C	1.484303	3.865748	-2.586425
C	0.170014	3.421857	-2.507889
H	-0.628028	4.031529	-2.938873
C	-0.177702	2.218697	-1.890790
C	1.840267	5.167650	-3.237887
H	2.635038	5.047974	-3.985496
H	2.207854	5.902041	-2.508392
H	0.976167	5.614860	-3.742871
C	3.347714	0.931889	-0.901908
O	3.110638	0.456904	0.415622
C	4.653196	1.740932	-0.812700
C	4.790884	2.756380	0.191632
C	5.698114	1.521557	-1.686100
C	3.749472	3.116832	1.088439
C	6.025470	3.480696	0.280237
C	6.909384	2.238544	-1.596887

H	5.591184	0.772615	-2.468775
C	3.925725	4.108663	2.026103
H	2.804713	2.585005	1.043260
C	6.174790	4.488671	1.264894
C	7.074604	3.192746	-0.625930
H	7.710001	2.025181	-2.303400
C	5.150534	4.799878	2.125564
H	3.102661	4.356466	2.697411
H	7.125733	5.019862	1.318983
H	8.007156	3.751609	-0.542403
H	5.280112	5.579133	2.875158
C	3.494758	-0.283084	-1.861153
C	4.291135	-1.423595	-1.486373
C	2.833314	-0.316840	-3.075482
C	5.077792	-1.477916	-0.301622
C	4.325054	-2.565998	-2.356378
C	2.874623	-1.438654	-3.927527
H	2.249919	0.547354	-3.384675
C	5.815793	-2.596013	0.014158
H	5.080622	-0.620409	0.362736
C	5.091166	-3.701157	-1.993589
C	3.599235	-2.547498	-3.571606
H	2.322658	-1.416567	-4.866320
C	5.818469	-3.724864	-0.828997
H	6.409186	-2.603765	0.926895
H	5.093691	-4.558110	-2.668465
H	3.636390	-3.425722	-4.217419
H	6.403752	-4.603621	-0.563454
O	-3.035306	-0.492822	0.226117
N	-2.032620	0.536053	-2.159531
C	-1.646408	1.904049	-1.780995
H	-1.987116	2.038730	-0.746828
H	-2.216291	2.625632	-2.395995
C	-1.656241	0.160927	-3.527823
H	-1.974006	0.958169	-4.225539
H	-0.565690	0.073233	-3.603253
C	-2.413586	-1.142093	-3.775785
H	-1.754590	-2.007766	-3.638870
H	-2.789570	-1.187373	-4.803409
C	-3.544193	-1.142667	-2.733362
H	-3.374309	-1.920590	-1.975527
H	-4.533084	-1.329680	-3.162476
C	-3.481237	0.223159	-2.045353
H	-4.055756	0.967172	-2.627063
C	-3.968578	0.178894	-0.552236
C	-5.299164	-0.598189	-0.551747
C	-6.443612	-0.095286	-1.168346
H	-6.423184	0.898282	-1.618592
C	-7.630544	-0.824014	-1.217150
H	-8.501853	-0.395667	-1.706300
C	-7.685920	-2.087337	-0.624105
C	-6.549420	-2.600588	0.006869
H	-6.612925	-3.584900	0.466880
C	-5.374809	-1.863493	0.036101
H	-4.482561	-2.258259	0.517826
O	-8.792872	-2.886243	-0.606509
C	-9.944129	-2.392220	-1.249133
H	-10.303740	-1.461818	-0.784694
H	-9.764087	-2.204406	-2.318400
H	-10.707302	-3.165917	-1.142106
C	-4.252457	1.572461	0.042381
C	-4.159202	1.716798	1.434154
C	-4.666923	2.686009	-0.687219
C	-4.455420	2.914336	2.061287
H	-3.835405	0.856241	2.016301
C	-4.954669	3.909303	-0.076259
H	-4.763491	2.630702	-1.771835
C	-4.850482	4.026595	1.309048
H	-4.395791	3.018583	3.143683
H	-5.260619	4.752736	-0.689862
O	-5.108078	5.165073	2.015212
C	-5.526750	6.289435	1.277186
H	-6.464859	6.094336	0.736556
H	-5.688456	7.087202	2.005096
H	-4.762570	6.608435	0.552660
Zn	-1.286468	-0.577212	-0.518858
Zn	1.813489	-0.865605	0.345744
C	-0.317859	-3.211725	1.735127
C	0.049494	-3.121154	0.226934
O	-0.719751	-2.504903	-0.583289
O	0.607263	-4.286605	-0.205656
C	1.044888	-4.252148	-1.569694
H	1.615343	-3.318954	-1.719893
H	0.170171	-4.215261	-2.231142
C	1.901660	-5.465877	-1.804445
H	2.771186	-5.461168	-1.137334
H	2.264850	-5.475307	-2.838362
H	1.337106	-6.389366	-1.633166

C	-1.416443	-4.281122	1.857485
H	-1.030932	-5.275656	1.617545
H	-2.242194	-4.058857	1.170837
H	-1.810716	-4.305469	2.880494
C	0.887359	-3.566790	2.598277
C	1.513270	-4.815362	2.475966
C	1.408073	-2.672037	3.541206
C	2.617913	-5.146804	3.252206
H	1.137904	-5.535805	1.754636
C	2.519378	-2.998973	4.316170
H	0.941073	-1.701390	3.691650
C	3.132332	-4.237864	4.173712
H	3.080883	-6.125197	3.133862
H	2.900515	-2.276254	5.036623
H	3.999692	-4.496795	4.778151
H	1.299937	-2.388677	0.350066
Si	-0.284693	0.766998	2.418558
O	-1.064586	1.792259	1.417130
C	-0.726123	3.169879	1.312701
H	-1.424136	3.627154	0.603242
H	-0.835438	3.680154	2.279976
H	0.300874	3.300607	0.947942
O	1.208588	1.405143	2.604383
C	2.276874	0.796424	3.308827
H	3.144641	1.457397	3.230520
H	2.014939	0.645072	4.367090
H	2.552688	-0.171115	2.864352
O	-1.070354	0.497129	3.837420
C	-1.563596	1.588995	4.594578
H	-2.279067	2.183622	4.008985
H	-2.073542	1.187087	5.474586
H	-0.746803	2.245092	4.930416
C	-0.976338	-1.896648	2.152442
O	-0.175404	-0.755204	1.746823
H	-1.961132	-1.790246	1.680084
H	-1.117799	-1.869820	3.238879

TS(3a)

M06L SCF energy in Solvent: -6534.705321 a.u.

PBE0-D3BJ Free energy in Solvent: -6533.744562 a.u.

O	0.431872	0.460187	-0.355966
C	0.810179	1.619133	-0.924096
C	2.179218	1.988909	-0.992015
C	2.506157	3.169578	-1.658198
H	3.557658	3.446293	-1.734889
C	1.555677	4.012283	-2.240205
C	0.220436	3.637591	-2.136110
H	-0.553826	4.278043	-2.565950
C	-0.169672	2.468880	-1.482087
C	1.966688	5.277893	-2.930181
H	1.123597	5.743045	-3.454123
H	2.760137	5.104025	-3.668421
H	2.358467	6.019645	-2.221022
C	3.288965	1.073260	-0.418007
O	2.953654	0.612416	0.885462
C	4.609911	1.853215	-0.281740
C	4.735895	2.887011	0.704971
C	5.682349	1.592247	-1.110674
C	3.672307	3.291060	1.554520
C	5.984466	3.584193	0.823019
C	6.907931	2.278947	-0.989879
H	5.587386	0.832317	-1.883952
C	3.836851	4.304616	2.470315
H	2.721440	2.774124	1.480898
C	6.122030	4.612659	1.787091
C	7.060313	3.249632	-0.033766
H	7.729172	2.028839	-1.659808
C	5.072717	4.969948	2.597853
H	3.000641	4.594098	3.105135
H	7.083329	5.121777	1.864970
H	8.003053	3.786742	0.075211
H	5.191366	5.765569	3.332003
C	3.465561	-0.154338	-1.358084
C	4.217025	-1.306149	-0.926794
C	2.866011	-0.191172	-2.604072
C	4.941085	-1.358064	0.297372
C	4.261309	-2.464782	-1.773762
C	2.932948	-1.323554	-3.440983
H	2.316905	0.681400	-2.951722
C	5.634157	-2.488308	0.667086
H	4.926751	-0.489426	0.947703
C	4.975840	-3.613733	-1.352284

C	3.608231	-2.444365	-3.029546
H	2.439311	-1.300133	-4.411851
C	5.646242	-3.633312	-0.154190
H	6.180612	-2.494366	1.609062
H	4.993685	-4.480621	-2.014365
H	3.662028	-3.332284	-3.660920
H	6.195009	-4.521760	0.154992
O	-2.930543	-0.157071	0.600141
N	-2.083913	0.874413	-1.801159
C	-1.635759	2.191688	-1.306378
H	-1.905285	2.224531	-0.240667
H	-2.224922	2.983332	-1.803088
C	-1.808855	0.629555	-3.222036
H	-2.171064	1.486301	-3.819615
H	-0.727201	0.548690	-3.384881
C	-2.594126	-0.646609	-3.524833
H	-1.934649	-1.523222	-3.502597
H	-3.037585	-0.608630	-4.525282
C	-3.653936	-0.728546	-2.411395
H	-3.444222	-1.568863	-1.733542
H	-4.670772	-0.881402	-2.785693
C	-3.531638	0.582334	-1.630923
H	-4.116485	1.369544	-2.138740
C	-3.941234	0.476599	-0.115905
C	-5.228423	-0.369412	-0.068067
C	-6.457120	0.123432	-0.504282
H	-6.539419	1.161429	-0.828538
C	-7.601613	-0.672656	-0.525096
H	-8.541364	-0.248470	-0.869385
C	-7.526442	-1.998090	-0.092675
C	-6.301897	-2.506653	0.350376
H	-6.261145	-3.541463	0.684754
C	-5.173737	-1.700825	0.355990
H	-4.215741	-2.098473	0.686695
O	-8.579856	-2.864472	-0.063072
C	-9.823846	-2.369138	-0.500098
H	-10.164919	-1.524764	0.117020
H	-9.787111	-2.045435	-1.551030
H	-10.530866	-3.195601	-0.402377
C	-4.241059	1.849616	0.513473
C	-4.065270	1.984441	1.898425
C	-4.729394	2.959641	-0.174872
C	-4.342413	3.168789	2.557842
H	-3.703445	1.123602	2.456661
C	-5.008131	4.167212	0.468629
H	-4.899519	2.915792	-1.250441
C	-4.811971	4.277157	1.844332
H	-4.204124	3.264353	3.632836
H	-5.373447	5.008838	-0.114414
O	-5.049106	5.402642	2.574748
C	-5.522062	6.528709	1.872204
H	-6.488030	6.327501	1.385465
H	-5.649944	7.318166	2.615572
H	-4.804179	6.861229	1.107876
Zn	-1.301762	-0.475950	-0.376906
Zn	1.715736	-0.760847	0.654091
C	-1.195737	-2.115994	2.251391
O	-0.616317	-0.846624	1.920065
C	-0.362847	-3.279719	1.716697
C	-0.173515	-3.096669	0.185875
O	-1.000993	-2.450630	-0.527443
O	0.431872	-4.171124	-0.353060
C	0.695184	-4.080200	-1.763708
H	1.172078	-3.105779	-1.955736
H	-0.258543	-4.103868	-2.305167
C	1.600276	-5.226269	-2.122180
H	2.542512	-5.161616	-1.565322
H	1.831387	-5.203983	-3.192803
H	1.129754	-6.189587	-1.895674
C	-1.234770	-4.533903	1.907911
H	-0.707704	-5.440797	1.602201
H	-2.154711	-4.458642	1.314641
H	-1.513471	-4.639848	2.963000
C	0.981598	-3.433880	2.421622
C	1.787964	-4.551810	2.173893
C	1.485112	-2.440341	3.273407
C	3.053763	-4.663799	2.739026
H	1.436355	-5.333636	1.506031

C	2.752548	-2.555616	3.844930
H	0.891157	-1.555904	3.493547
C	3.544293	-3.665820	3.576307
H	3.663767	-5.537876	2.515606
H	3.118565	-1.762971	4.495103
H	4.537950	-3.752012	4.012638
H	1.136051	-2.191098	0.272616
H	-2.205448	-2.156928	1.823354
H	-1.278866	-2.213424	3.344964
H	-1.333202	-0.184948	2.004421