Supporting Information

Origins of Ligand-Controlled Diastereoselectivity in Dirhodium-Catalyzed Direct Amination of Aliphatic C(sp^3)–H Bonds

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Table of Contents

Computational Details

All calculations were performed with Gaussian 09 by using the experimental substrates and catalysts. Geometry optimizations and frequency calculations were performed at the BP86/BS1 level in the gas phase with default convergence criteria, BS1 designating a mixed basis set of SDD for rhodium and 6-31G(d) for other atoms. Frequency outcomes were examined to confirm stationary points as minima (no imaginary frequencies) or transition states (only one imaginary frequency). Because the M06-L functional includes noncovalent interactions and gives refined energies for organotransition metal systems, we performed single-point energy calculations for all BP86/BS1-optimized structures at the M06-L/BS2 level with solvent effects simulated by the SMD solvent model. BS2 denotes a mixed basis set of SDD for rhodium and 6-31++G(d,p) for other atoms. The BP86/BS1-calculated frequencies were used to obtain zero-point energy-corrected enthalpies and free energies at 298.15 K and 1 atm. The solvation effects were considered using the SMD model with 2,2,2-TriFluoroEthanol ($\varepsilon = 26.726$) as the solvent.

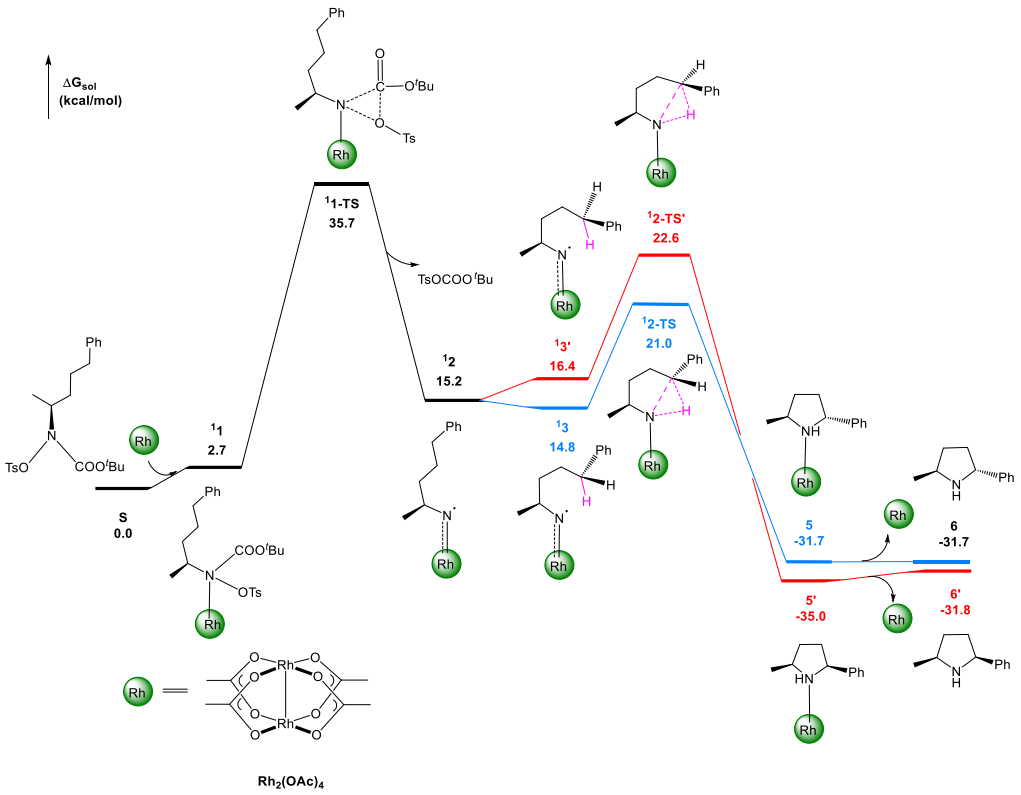

Fig. S1. Free energy profiles for dirhodium-catalyzed direct amination of aliphatic C(sp^3)-H bond on singlet leading to pyrrolidine product **1b**.

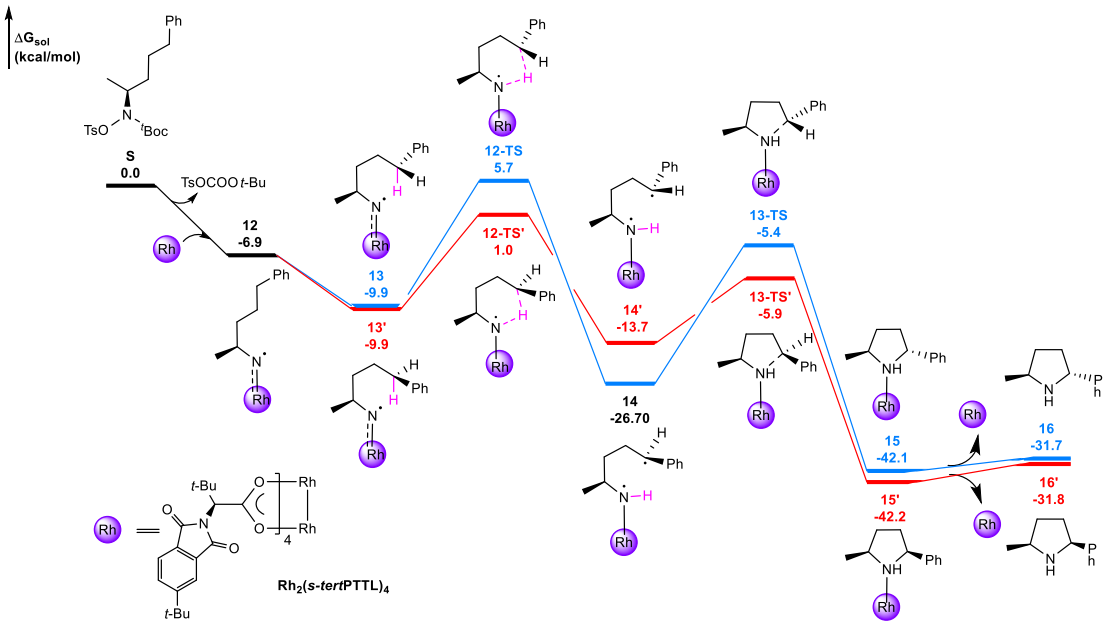

Fig. S2. Free energy profiles for dirhodium-catalyzed direct amination of aliphatic C(sp^3)-H bond on triplet leading to pyrrolidine product **2b**.

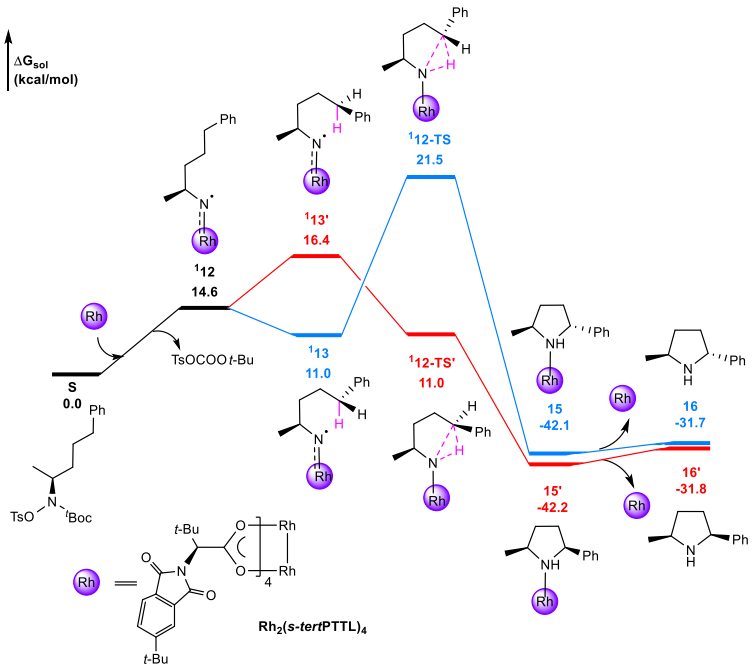

Fig. S3. Free energy profiles for dirhodium-catalyzed direct amination of aliphatic C(sp^3)-H bond on singlet leading to pyrrolidine product **2b**.

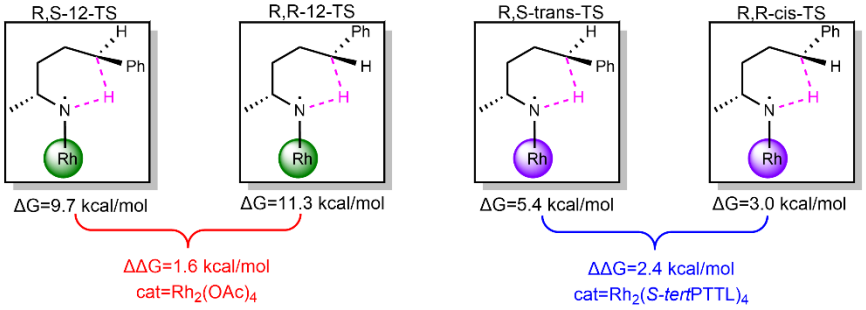

Fig. S4. Energetic differences between (R, S) and (R, R)-H-abstraction transition states.

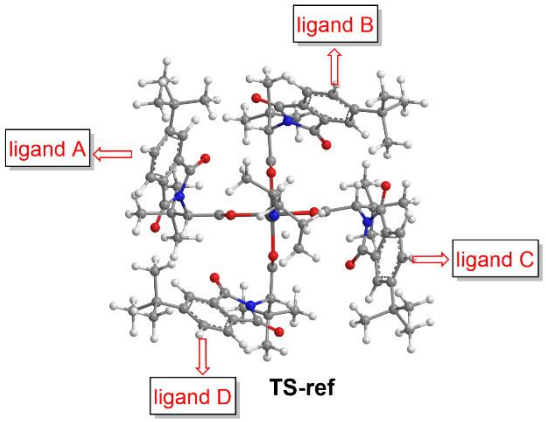

Fig. S5. The order of the four ligands of Rh_2(*S-tert*PTTL)$_4$.

Energies and Cartesian Coordinates (Å) for the Optimized Structures

a

SCF energy in CF_3CH_2OH: -1724.016574 a.u.

Free energy in CF_3CH_2OH: -1723.590845 a.u.

N	1.177388	0.542020	0.309249
C	-0.231768	0.199079	0.675747
C	-1.243722	1.182689	0.044975
C	-2.710547	0.736953	0.179752
H	-1.106842	2.178819	0.505721
H	-0.994008	1.283868	-1.029613
C	-3.685435	1.676406	-0.571937
H	-2.831093	-0.293285	-0.212370
H	-3.007485	0.698695	1.245088
H	-3.563061	2.705235	-0.180805
H	-3.398775	1.710385	-1.641056
C	1.699042	1.821611	0.611494
O	1.278345	2.462874	1.575147
O	2.693821	2.154220	-0.230034
C	3.534165	3.354672	0.041294
C	2.673446	4.623633	-0.052356
C	4.222684	3.205305	1.406219
C	4.556991	3.290642	-1.101544
H	2.163309	4.671227	-1.030513
H	1.918987	4.648435	0.748207
H	3.320409	5.514509	0.039781
H	4.774803	2.250679	1.451223
H	4.944452	4.029807	1.546199
H	3.488975	3.235412	2.225999
H	5.262958	4.135766	-1.021931
H	5.126205	2.346907	-1.058245
H	4.051880	3.346743	-2.081049
C	-5.134545	1.244990	-0.440960
C	-5.710647	0.353012	-1.368963
C	-5.928636	1.692711	0.635141
C	-7.038078	-0.080881	-1.227159
H	-5.110422	-0.000018	-2.217346
C	-7.256533	1.262126	0.782154
H	-5.499888	2.393205	1.363273
C	-7.816177	0.372231	-0.149344
H	-7.467569	-0.769754	-1.963907
H	-7.857434	1.627391	1.623111
H	-8.854166	0.038534	-0.039135
O	1.468635	0.094894	-1.020471
H	-0.368175	-0.792423	0.208299
C	-0.371628	0.030189	2.197106
H	-0.281349	0.997481	2.713384
H	-1.353527	-0.416748	2.431225
H	0.410966	-0.647007	2.579186
S	2.724321	-1.099741	-1.042269
O	2.925982	-1.265749	-2.491862
O	3.798475	-0.703437	-0.114363
C	1.908300	-2.555093	-0.378398
C	2.095555	-2.895823	0.970299
C	1.091711	-3.326815	-1.223302
C	1.444401	-4.030447	1.476182
H	2.750750	-2.287493	1.600040
C	0.452215	-4.455157	-0.696409
H	0.975158	-3.048810	-2.275137
C	0.616257	-4.825620	0.657263
H	1.586053	-4.306000	2.527828
H	-0.184019	-5.065144	-1.348661
C	-0.058777	-6.064831	1.203501
H	-0.119858	-6.041708	2.304664
H	-1.081888	-6.178192	0.803898
H	0.502081	-6.976701	0.922335

$Rh_2(OAc)_4$ (triplet)

SCF energy in CF_3CH_2OH: -1135.309797 a.u.

Free energy in CF_3CH_2OH: -1135.161019 a.u.

Rh	-0.005775	-0.000243	-1.226921
O	0.930485	-1.823856	-1.144297
C	1.202605	-2.349596	-0.001589
O	0.929037	-1.825417	1.141666
O	1.832027	0.946765	-1.153732
C	2.347658	1.202466	-0.001706
O	1.833748	0.944903	1.150565
O	-0.944357	1.821976	-1.142527
C	-1.206062	2.352429	0.000528
O	-0.942355	1.822581	1.143469
O	-1.844306	-0.946218	-1.148150
C	-2.356778	-1.205508	0.004478
O	-1.843737	-0.944283	1.156271
Rh	-0.005396	-0.000492	1.227248
C	-1.849922	3.721832	0.001094
H	-1.058104	4.492515	0.013972
H	-2.452135	3.862230	-0.909439

H	-2.470392	3.852380	0.900878
C	3.719488	1.850332	-0.001960
H	4.491713	1.059978	0.012619
H	3.859981	2.450928	-0.913557
H	3.849672	2.472271	0.896893
C	-3.711186	-1.889019	-0.002926
H	-3.652933	-2.820623	-0.590866
H	-4.039067	-2.111972	1.022672
H	-4.451014	-1.234960	-0.495941
C	1.929106	-3.677125	0.001369
H	1.788927	-4.195142	-0.959041
H	3.009139	-3.497682	0.150786
H	1.573112	-4.303371	0.834447

1

SCF energy in CF_3CH_2OH: -2859.343181

Free energy in CF_3CH_2OH: -2858.748913

Rh	-4.434257	-0.498348	-0.811635
O	-5.301545	1.234011	-0.091265
C	-4.556353	2.080190	0.526920
O	-3.295106	1.973400	0.760615
O	-4.773248	-1.408818	0.997902
C	-3.893366	-1.307544	1.930843
O	-2.772309	-0.685634	1.837041
O	-3.466279	-2.194796	-1.484476
C	-2.206856	-2.315596	-1.258901
O	-1.446454	-1.472290	-0.648303
O	-3.976978	0.458611	-2.574404
C	-2.866859	1.099873	-2.674899
O	-1.972231	1.195237	-1.756350
Rh	-2.278086	0.294292	0.084395
C	-1.538836	-3.579229	-1.770133
H	-0.994302	-4.077408	-0.950345
H	-2.286023	-4.264630	-2.195885
H	-0.798201	-3.317044	-2.545671
C	-4.220814	-1.950405	3.262902
H	-4.759252	-1.219181	3.892646
H	-4.874070	-2.824255	3.116395
H	-3.297025	-2.239802	3.786778
C	-2.609096	1.828083	-3.978445
H	-3.121943	2.806536	-3.952008
H	-1.531763	2.003032	-4.117630
H	-3.020786	1.253703	-4.823096
C	-5.231584	3.352763	1.005572
H	-5.211282	4.100813	0.192414
H	-6.284268	3.153651	1.259152
H	-4.696981	3.770109	1.872275
N	1.902979	1.389317	-0.291789
C	1.779900	-0.036594	-0.664990
C	2.210498	-0.237352	-2.125289
H	0.698069	-0.234976	-0.580964
H	1.651798	0.438730	-2.794311
H	3.289117	-0.046611	-2.257514
C	0.942456	2.067475	0.456130
O	-0.060586	1.490172	0.900793
O	1.279851	3.360770	0.604450
C	0.536333	4.254684	1.540343
C	-0.878025	4.503415	1.000282
C	0.539293	3.649882	2.951813
C	1.381912	5.535539	1.486958
H	-0.829908	4.888008	-0.034131
H	-1.490325	3.589220	1.014692
H	-1.373180	5.269545	1.625000
H	1.570473	3.406084	3.260091
H	0.128532	4.387847	3.663935
H	-0.074550	2.737386	2.997956
H	0.939690	6.300723	2.148652
H	2.416430	5.336357	1.812202
H	1.415545	5.937036	0.459781
C	2.514369	-0.957532	0.337208
H	3.609515	-0.832883	0.224630
H	2.255582	-0.622205	1.358704
O	2.990243	2.094926	-0.784088
H	2.001510	-1.275380	-2.433200
C	2.134213	-2.440858	0.177435
C	2.740499	-3.336116	1.284794
H	2.465846	-2.823489	-0.807209
H	1.031352	-2.535955	0.195097
H	3.844236	-3.244752	1.261906
H	2.412307	-2.955756	2.271703
C	2.343132	-4.793122	1.137276
C	1.149086	-5.277277	1.712291
C	3.132450	-5.688893	0.386991
C	0.754862	-6.614098	1.542358
H	0.527162	-4.597136	2.308477
C	2.743120	-7.026549	0.213561
H	4.068178	-5.331873	-0.062217
C	1.551355	-7.494093	0.790889
H	-0.173138	-6.970981	2.004086
H	3.375137	-7.706739	-0.369325
H	1.247722	-8.538962	0.660823
S	4.265337	2.455081	0.428447
O	3.813922	1.933919	1.735950
O	4.575904	3.875248	0.175657
C	5.645221	1.465413	-0.158430
C	6.290925	1.826626	-1.353967

C	6.071248	0.364320	0.599983
C	7.371913	1.054443	-1.794985
H	5.961235	2.705808	-1.915482
C	7.163474	-0.388021	0.143162
H	5.566738	0.121913	1.539691
C	7.824330	-0.064016	-1.059375
H	7.883164	1.330811	-2.724740
H	7.512875	-1.240568	0.737388
C	8.983163	-0.897775	-1.560729
H	8.656017	-1.592754	-2.357733
H	9.780353	-0.265947	-1.990355
H	9.424361	-1.505831	-0.753094

1-TS

SCF energy in CF_3CH_2OH: -2859.327513 a.u.

Free energy in CF_3CH_2OH: -2858.728760 a.u.

Rh	-2.923778	-2.517905	-1.020821
O	-4.264688	-1.046315	-0.607552
C	-3.841200	0.055643	-0.088630
O	-2.617931	0.303501	0.219004
O	-3.182615	-3.297378	0.858071
C	-2.432635	-2.871973	1.809908
O	-1.527822	-1.958771	1.716731
O	-1.545398	-3.976848	-1.419551
C	-0.320410	-3.746198	-1.112639
O	0.130536	-2.670396	-0.565685
O	-2.636807	-1.694640	-2.875931
C	-1.722998	-0.799498	-2.996830
O	-0.941581	-0.376352	-2.065443
Rh	-1.165454	-1.086363	-0.127078
C	0.695442	-4.826416	-1.420979
H	0.191756	-5.731906	-1.789205
H	1.401449	-4.460497	-2.186788
H	1.280852	-5.059805	-0.515992
C	-2.604063	-3.516903	3.169742
H	-3.568821	-4.042648	3.223561
H	-1.790374	-4.246857	3.329880
H	-2.534055	-2.757393	3.964458
C	-1.557761	-0.153369	-4.356256
H	-2.006414	-0.784978	-5.137343
H	-2.069389	0.825686	-4.349462
H	-0.491863	0.026453	-4.567252
C	-4.844154	1.142995	0.206808
H	-5.760307	0.986098	-0.382365
H	-5.100665	1.114525	1.281148
H	-4.388179	2.123430	-0.007501
N	0.447800	0.012070	0.357988
C	1.725079	-0.164110	-0.318300
C	2.836189	-0.558805	0.703160
C	4.140418	-1.029941	0.036463
H	3.026476	0.311359	1.355217
H	2.438137	-1.368873	1.343566
C	5.190988	-1.485915	1.079881
H	3.935494	-1.867486	-0.660361
H	4.579282	-0.217771	-0.573219
H	5.367934	-0.655264	1.790925
H	4.772515	-2.322757	1.672123
C	0.244154	1.495595	1.330053
O	1.382844	1.907457	1.642287
O	-0.738558	1.175338	2.226146
C	-0.427090	1.058572	3.672941
C	0.563134	-0.091778	3.916756
C	0.087516	2.390932	4.241225
C	-1.808778	0.725116	4.258346
H	0.185506	-1.026710	3.469186
H	1.548229	0.143677	3.484709
H	0.690475	-0.245054	5.004228
H	-0.596308	3.210926	3.971442
H	0.143994	2.315489	5.342974
H	1.089631	2.628026	3.852714
H	-1.733007	0.583720	5.351035
H	-2.518058	1.545599	4.056596
H	-2.201836	-0.199505	3.802667
C	6.504893	-1.907802	0.448355
C	6.769490	-3.260463	0.152000
C	7.481572	-0.947357	0.110482
C	7.971842	-3.644728	-0.463055
H	6.024491	-4.022235	0.415579
C	8.684536	-1.325203	-0.505253
H	7.296360	0.109588	0.341161
C	8.933935	-2.677131	-0.794655
H	8.159893	-4.703064	-0.678327
H	9.432243	-0.563042	-0.753799
H	9.874983	-2.974900	-1.270767
O	-0.447126	2.203128	0.167216
H	1.578828	-1.040163	-0.981859
C	2.106861	1.043467	-1.207311
H	2.376657	1.910113	-0.585044
H	2.964757	0.768524	-1.846492
H	1.260704	1.320800	-1.853930
S	-1.271016	3.626015	0.357462
O	-2.485628	3.528089	-0.485999
O	-1.390669	3.999284	1.783108
C	-0.135460	4.770702	-0.449838
C	1.200742	4.837463	-0.019082
C	-0.626698	5.627784	-1.442898

C	2.049667	5.782756	-0.605584
H	1.564923	4.140403	0.744432
C	0.242483	6.569647	-2.016251
H	-1.670429	5.548032	-1.760596
C	1.587273	6.664887	-1.608968
H	3.096217	5.837387	-0.281361
H	-0.133430	7.242324	-2.796498
C	2.521575	7.684582	-2.225246
H	3.419652	7.201917	-2.653117
H	2.026906	8.252877	-3.031113
H	2.876177	8.411195	-1.470383

$TsOCO_2{}^tBu$

SCF energy in CF_3CH_2OH: -1241.12478 a.u.

Free energy in CF_3CH_2OH: -1240.914604 a.u.

C	3.997594	0.182726	1.206608
C	2.641520	-0.166607	1.229233
C	1.977771	-0.365269	0.008588
C	2.639849	-0.231767	-1.221340
C	3.996340	0.118242	-1.218926
C	4.693936	0.336836	-0.011737
H	4.528371	0.334767	2.153744
H	2.104375	-0.297609	2.173026
H	2.101573	-0.412651	-2.156195
H	4.526043	0.219718	-2.173355
C	6.150361	0.747133	-0.022210
H	6.664907	0.395688	-0.932788
H	6.248528	1.849390	0.005888
H	6.690342	0.349868	0.854610
S	0.247275	-0.831176	0.021278
O	-0.096219	-1.425531	1.325672
O	-0.100585	-1.476156	-1.257623
O	-0.348116	0.808580	-0.008245
C	-1.710748	1.086679	-0.013926
O	-2.076885	2.245813	-0.029606
O	-2.430534	-0.043168	-0.000842
C	-3.928851	0.017743	-0.006217
C	-4.410436	0.733874	1.262725
H	-4.100680	1.790169	1.265164
H	-5.513045	0.690209	1.310316
H	-4.007846	0.237083	2.162457
C	-4.306634	-1.468603	0.009012
H	-5.405382	-1.573400	0.005124
H	-3.899705	-1.983350	-0.877663
H	-3.908070	-1.963215	0.910819
C	-4.402943	0.705109	-1.293779
H	-5.505338	0.661157	-1.346093
H	-4.092085	1.760734	-1.318760
H	-3.996230	0.187380	-2.179780

2

SCF energy in CF_3CH_2OH: -1618.201244 a.u.

Free energy in CF_3CH_2OH: -1617.840414 a.u.

Rh	2.397955	-1.223056	0.618659
O	0.792692	-2.109995	1.544058
O	3.957335	-0.290807	-0.340194
O	-0.646520	-0.564591	0.639766
O	2.546520	1.263130	-1.274947
O	2.085185	-2.399859	-1.031239
O	2.664323	0.003741	2.243482
O	1.240436	1.561354	1.338912
O	0.659722	-0.864231	-1.966250
C	2.030569	1.117632	2.257205
C	1.303291	-1.980986	-1.958674
C	-0.370092	-1.602642	1.352592
C	3.704519	0.737573	-1.064846
Rh	0.883964	0.420507	-0.363227
C	-1.033285	2.880617	-0.364203
C	-2.528460	2.894244	-0.802770
C	-4.777220	1.650650	-0.843790
C	-3.310130	1.651199	-0.352081
H	-2.562328	2.987810	-1.906221
H	-2.994253	3.811308	-0.388817
H	-2.796597	0.742986	-0.717686
H	-3.297901	1.584384	0.754003
N	-0.347878	1.789675	-0.978386
H	-4.784148	1.715108	-1.949792
H	-0.993938	2.735162	0.742025
H	-5.288523	2.560832	-0.472724
C	-5.542466	0.417866	-0.398311
C	-6.302438	0.424145	0.789252
C	-5.479506	-0.778829	-1.142764
C	-6.978238	-0.727776	1.222812
H	-6.369127	1.348040	1.378131
C	-6.153029	-1.933414	-0.714469
H	-4.898626	-0.801315	-2.073757
C	-6.905154	-1.912192	0.471861
H	-7.568119	-0.697898	2.146441
H	-6.095292	-2.850611	-1.312299
H	-7.435780	-2.811194	0.805504
C	2.204836	2.007462	3.472636
H	1.260755	2.036708	4.044760
H	3.008001	1.620841	4.116800
H	2.433265	3.038770	3.156697

C	4.878923	1.425681	-1.733274
H	4.632319	1.661546	-2.781205
H	5.085216	2.380045	-1.216935
H	5.774400	0.788849	-1.683899
C	1.127267	-2.863397	-3.177966
H	0.063762	-2.907557	-3.463291
H	1.682311	-2.426154	-4.026923
H	1.513609	-3.873633	-2.977693
C	-1.548368	-2.301561	2.001660
H	-2.309506	-1.567920	2.308883
H	-2.015006	-2.981344	1.266318
H	-1.210168	-2.895868	2.863803
C	-0.325376	4.218994	-0.702715
H	0.728740	4.185866	-0.382588
H	-0.355213	4.404998	-1.790500
H	-0.830473	5.055697	-0.186394

3

SCF energy in CF_3CH_2OH: -1618.20574 a.u.

Free energy in CF_3CH_2OH: 1617.843181 a.u.

Rh	2.332149	-1.262943	0.371002
O	0.994153	-2.033038	1.729122
O	3.618497	-0.446702	-1.004433
O	-0.591895	-0.480866	1.135852
O	2.072172	1.144986	-1.600770
O	1.566522	-2.491252	-1.080667
O	3.055638	0.016136	1.804482
O	1.481342	1.588938	1.240533
O	0.000798	-0.929226	-1.693112
C	2.473621	1.149772	1.938839
C	0.587799	-2.072644	-1.798373
C	-0.165637	-1.493343	1.812372
C	3.224651	0.572567	-1.677671
Rh	0.669252	0.404021	-0.263393
C	-0.995572	3.009052	0.075070
C	-2.480973	3.400846	-0.200390
C	-3.720959	1.227976	-0.872340
C	-3.532029	2.341862	0.185971
H	-2.582183	3.664150	-1.271848
H	-2.662224	4.331122	0.372517
H	-3.259901	1.881671	1.156483
H	-4.506138	2.843804	0.347274
N	-0.628116	1.814685	-0.610428
H	-2.741944	0.749916	-1.063028
H	-0.895102	2.818380	1.171349
H	-4.037457	1.697359	-1.824841
C	-4.739190	0.185965	-0.449540
C	-6.105812	0.331183	-0.765715
C	-4.343859	-0.939358	0.304335
C	-7.051477	-0.616493	-0.342721
H	-6.430318	1.197186	-1.357080
C	-5.285628	-1.890002	0.728723
H	-3.282044	-1.062260	0.552076
C	-6.644029	-1.731927	0.407048
H	-8.108313	-0.486114	-0.603866
H	-4.958394	-2.761478	1.308482
H	-7.379593	-2.475658	0.734325
C	2.975608	2.066191	3.037477
H	2.251259	2.065934	3.871442
H	3.949841	1.716325	3.409366
H	3.055948	3.100464	2.665702
C	4.212301	1.190390	-2.648122
H	3.697443	1.493835	-3.573534
H	4.649019	2.097757	-2.193608
H	5.022495	0.480698	-2.871996
C	0.068532	-2.990430	-2.886102
H	-1.026563	-3.089173	-2.803225
H	0.285998	-2.546740	-3.873483
H	0.546296	-3.978432	-2.815085
C	-1.145670	-2.121456	2.784473
H	-1.966858	-1.427384	3.016247
H	-1.569172	-3.034797	2.329282
H	-0.620506	-2.420306	3.705648
C	-0.040104	4.173480	-0.303081
H	1.002490	3.898239	-0.080205
H	-0.122973	4.401195	-1.380059
H	-0.304623	5.079392	0.272717

3'

SCF energy in CF_3CH_2OH: -1618.202516 a.u.

Free energy in CF_3CH_2OH: -1617.840674 a.u.

Rh	-2.685484	-0.730892	-0.346144
O	-2.334357	-0.392481	-2.340679
O	-2.970653	-1.047517	1.663021
O	-0.253764	0.471041	-1.885117
O	-0.904590	-0.171922	2.159694
O	-1.806221	-2.574082	-0.515061
O	-3.503821	1.141990	-0.163994
O	-1.435140	2.031990	0.289715
O	0.267926	-1.725190	-0.023553
C	-2.709256	2.112852	0.099532
C	-0.543273	-2.684741	-0.314634
C	-1.207170	0.118905	-2.678967
C	-2.039125	-0.698631	2.473581

Rh	-0.485448	0.188931	0.161293
C	1.651423	2.409003	0.688501
C	3.180711	2.543961	0.404863
C	3.646549	0.707772	-1.402143
C	3.628468	2.213875	-1.031168
H	3.728984	1.913019	1.129825
H	3.444937	3.595225	0.632131
H	2.976023	2.748405	-1.750712
H	4.648357	2.623059	-1.173730
N	1.212489	1.062200	0.540699
H	2.625404	0.299644	-1.296092
H	3.918676	0.625844	-2.473029
C	4.616720	-0.113215	-0.570525
C	6.001761	-0.082607	-0.840743
C	4.162846	-0.908548	0.503024
C	6.908151	-0.818397	-0.062107
H	6.372179	0.522424	-1.678834
C	5.067588	-1.645571	1.285722
H	3.087813	-0.947951	0.716969
C	6.443004	-1.602782	1.007130
H	7.979440	-0.783819	-0.293199
H	4.693949	-2.257968	2.115102
H	7.148811	-2.180339	1.615242
H	1.106586	3.032832	-0.062063
C	1.305804	2.941875	2.106394
H	0.224519	2.850985	2.294439
H	1.848249	2.362554	2.873609
H	1.598991	4.004442	2.190708
C	-2.295859	-0.897986	3.954629
H	-1.371976	-1.216348	4.462795
H	-2.612785	0.061882	4.400681
H	-3.095532	-1.638251	4.106584
C	-3.308444	3.503447	0.180153
H	-3.015455	4.080134	-0.715194
H	-4.405751	3.443501	0.225487
H	-2.917266	4.036315	1.062010
C	-0.948700	0.317921	-4.159913
H	-0.519582	1.317142	-4.339400
H	-0.210622	-0.427912	-4.504558
H	-1.880554	0.193579	-4.730852
C	0.059451	-4.072011	-0.399348
H	-0.594327	-4.736113	-0.984329
H	1.064844	-4.025541	-0.846466
H	0.161674	-4.485286	0.620227

2-TS

SCF energy in CF_3CH_2OH: -1618.180966 a.u.

Free energy in CF_3CH_2OH: -1617.821362 a.u.

Rh	-2.191695	-1.334315	-0.094091
O	-1.215714	-2.120318	-1.718674
O	-3.120861	-0.504861	1.541557
O	0.407403	-0.499970	-1.587848
O	-1.540125	1.154738	1.679936
O	-1.027429	-2.499436	1.134162
O	-3.285930	-0.107627	-1.328214
O	-1.672697	1.526759	-1.229381
O	0.570620	-0.859616	1.307076
C	-2.796002	1.036622	-1.633372
C	0.085489	-2.026017	1.562820
C	-0.136008	-1.546009	-2.107778
C	-2.612842	0.551333	2.061815
Rh	-0.485944	0.402777	0.059740
C	1.017775	3.154415	-0.287853
C	2.375909	3.793677	0.135517
C	3.453730	1.585295	0.653187
C	3.577275	2.876908	-0.153073
H	2.333747	4.016813	1.220605
H	2.482028	4.761709	-0.388447
H	3.619890	2.659733	-1.237732
H	4.521298	3.403235	0.098037
N	0.926341	1.786738	0.170409
H	2.177450	1.384315	0.468546
H	0.983503	3.136017	-1.404801
H	3.466122	1.779016	1.741569
C	4.211325	0.368911	0.296840
C	4.585074	-0.545560	1.317597
C	4.565547	0.042614	-1.038000
C	5.288028	-1.719385	1.023289
H	4.320209	-0.313052	2.356418
C	5.269244	-1.132373	-1.332332
H	4.284250	0.716569	-1.854331
C	5.636330	-2.020632	-0.306023
H	5.575006	-2.399568	1.833836
H	5.536955	-1.356219	-2.371626
H	6.190355	-2.936762	-0.539010
C	-3.612514	1.921122	-2.557506
H	-2.995231	2.237536	-3.415201
H	-4.503624	1.384005	-2.913514
H	-3.922763	2.833858	-2.019392
C	-3.353847	1.176380	3.228558
H	-2.639694	1.536005	3.986327
H	-3.930282	2.047530	2.868669
H	-4.051117	0.449225	3.670755
C	0.916074	-2.907500	2.474873
H	1.973411	-2.874297	2.165567
H	0.856581	-2.523640	3.508887

H	0.540814	-3.941284	2.452922
C	0.583704	-2.144567	-3.301427
H	0.638473	-1.399253	-4.113616
H	1.618581	-2.401569	-3.018667
H	0.057206	-3.042457	-3.656429
C	-0.167740	4.012020	0.214351
H	-1.121408	3.588718	-0.133861
H	-0.175505	4.040180	1.317721
H	-0.068344	5.044798	-0.168089

2-TS'

SCF energy in CF_3CH_2OH: -1618.179255 a.u.

Free energy in CF_3CH_2OH: -1617.819502 a.u.

Rh	2.513662	-1.004941	-0.029134
O	1.397839	-2.657501	0.472810
O	3.551266	0.695410	-0.531224
O	-0.539589	-1.426448	0.542348
O	1.625611	1.948965	-0.485014
O	2.169695	-1.379876	-2.018492
O	2.793410	-0.600930	1.964901
O	0.867912	0.650506	2.039610
O	0.227069	-0.154150	-1.977840
C	1.929439	0.136820	2.560572
C	1.111716	-0.892638	-2.555465
C	0.136021	-2.517635	0.662158
C	2.893416	1.788139	-0.662135
Rh	0.458988	0.307021	0.037993
C	-1.416312	2.825980	0.019721
C	-2.940959	3.129820	-0.050014
H	-0.936838	3.257899	-0.893060
C	-3.424429	0.902676	-1.214448
C	-3.626675	2.423830	-1.241465
H	-3.077764	4.225580	-0.119036
H	-3.399010	2.804196	0.903935
H	-3.120442	0.479821	-2.186939
H	-4.705071	2.680050	-1.252339
H	-3.200047	2.824776	-2.180454
N	-1.192348	1.398581	0.000743
H	-2.287300	0.865274	-0.589601
C	-0.774606	3.493645	1.257670
H	-1.218928	3.089960	2.183839
H	0.308932	3.303351	1.278713
H	-0.948537	4.584967	1.224408
C	-4.376343	0.021692	-0.502779
C	-5.271001	0.488997	0.494062
C	-4.394826	-1.366821	-0.801948
C	-6.141404	-0.388767	1.154539
H	-5.292919	1.554336	0.748145
C	-5.262459	-2.243247	-0.141510
H	-3.712282	-1.749288	-1.570872
C	-6.142590	-1.759355	0.843921
H	-6.826465	0.000793	1.916599
H	-5.260210	-3.308691	-0.400023
H	-6.824518	-2.443245	1.361380
C	-0.639393	-3.744480	1.100037
H	-1.707900	-3.630127	0.864278
H	-0.226997	-4.645212	0.618751
H	-0.533666	-3.864886	2.193373
C	2.182944	0.466383	4.019271
H	1.238336	0.440791	4.585557
H	2.909552	-0.238760	4.449574
H	2.592955	1.489564	4.094866
C	0.852472	-1.235276	-4.010505
H	0.112660	-2.054177	-4.064277
H	0.431322	-0.365870	-4.539924
H	1.782127	-1.568226	-4.495723
C	3.668675	3.019444	-1.091702
H	3.347783	3.896364	-0.506432
H	4.749166	2.852751	-0.970526
H	3.455441	3.231259	-2.154757

4

SCF energy in CF_3CH_2OH: -1618.203322 a.u.

Free energy in CF_3CH_2OH: -1617.842087 a.u.

Rh	2.283614	-1.304312	0.132153
O	1.318502	-2.035657	1.785125
O	3.206460	-0.529943	-1.528944
O	-0.305842	-0.423722	1.601549
O	1.613973	1.108920	-1.731689
O	1.117952	-2.516700	-1.056839
O	3.363704	-0.014811	1.316825
O	1.750174	1.614224	1.146297
O	-0.497094	-0.895951	-1.263727
C	2.873321	1.142297	1.570599
C	-0.001890	-2.065085	-1.489149
C	0.239453	-1.449513	2.158124
C	2.692690	0.502895	-2.090087
Rh	0.574244	0.416364	-0.082910
C	-1.150916	3.058945	0.216230
C	-2.521879	3.646930	-0.205417
C	-4.027409	1.632534	-0.690201
C	-3.760310	2.811626	0.202305
H	-2.523513	3.797213	-1.304045
H	-2.601797	4.653347	0.247824

H	-3.664463	2.502384	1.261099
H	-4.644572	3.488886	0.171402
N	-0.950884	1.711157	-0.285683
H	-1.837481	1.235387	-0.535594
H	-1.133967	3.011286	1.333144
H	-3.873379	1.800405	-1.766420
C	-4.597121	0.382111	-0.316965
C	-4.876859	-0.597212	-1.328784
C	-4.923723	0.031836	1.034484
C	-5.440866	-1.831395	-1.011221
H	-4.638785	-0.353937	-2.371578
C	-5.488290	-1.207231	1.341001
H	-4.730334	0.748336	1.839589
C	-5.753082	-2.150003	0.327222
H	-5.647188	-2.555284	-1.808258
H	-5.731128	-1.445678	2.383162
H	-6.198680	-3.119194	0.575849
C	3.689245	2.064812	2.457705
H	3.082892	2.382822	3.322877
H	4.600264	1.556682	2.805731
H	3.963624	2.974371	1.895660
C	3.433225	1.091924	-3.275016
H	2.718928	1.441304	-4.037260
H	4.021192	1.964707	-2.938283
H	4.121069	0.347437	-3.703079
C	-0.828956	-2.979189	-2.372780
H	-1.890202	-2.926693	-2.080559
H	-0.752190	-2.640447	-3.421462
H	-0.461202	-4.013582	-2.303165
C	-0.475185	-2.006379	3.374471
H	-0.552449	-1.225326	4.150254
H	-1.502176	-2.300205	3.098193
H	0.067748	-2.875393	3.773848
C	-0.002048	3.989803	-0.226131
H	0.967743	3.579527	0.093176
H	0.004399	4.089547	-1.326177
H	-0.130813	4.992502	0.220792

4’

SCF energy in CF_3CH_2OH: -1618.203287 a.u.

Free energy in CF_3CH_2OH: -1617.842157 a.u.

Rh	2.503593	-1.058001	0.386553
O	1.587597	-1.471419	2.173095
O	3.379265	-0.612062	-1.412399
O	-0.221442	-0.178105	1.612375
O	1.606168	0.725303	-1.992793
O	1.524453	-2.646737	-0.490440
O	3.378667	0.604318	1.225204
O	1.575955	1.926002	0.682745
O	-0.256939	-1.325790	-1.097947
C	2.737721	1.715456	1.204543
C	0.388821	-2.442679	-1.051072
C	0.437141	-0.955391	2.403806
C	2.756084	0.182920	-2.203429
Rh	0.603272	0.333484	-0.220722
C	-1.330629	2.796713	-0.455902
C	-2.850595	2.980087	-0.210311
C	-3.497380	0.718396	0.845064
C	-3.431029	2.208802	1.011891
H	-3.403696	2.690830	-1.126871
H	-3.032341	4.063147	-0.060192
H	-2.804773	2.448776	1.894373
H	-4.435895	2.623372	1.222382
N	-0.985646	1.425749	-0.778052
H	-1.587726	1.010849	-1.506984
H	-2.588357	0.155141	1.088608
C	-4.609502	-0.014333	0.348764
C	-5.850824	0.589828	-0.045213
C	-4.517949	-1.443044	0.224311
C	-6.911337	-0.182292	-0.521269
H	-5.968722	1.676609	0.027035
C	-5.583584	-2.204022	-0.251481
H	-3.579395	-1.929837	0.516112
C	-6.793099	-1.583003	-0.629500
H	-7.847017	0.308736	-0.814254
H	-5.480453	-3.292754	-0.331634
H	-7.630545	-2.182075	-1.003199
H	-0.783605	3.052833	0.472345
C	-0.843348	3.750100	-1.579185
H	0.235554	3.609684	-1.754250
H	-1.379625	3.545943	-2.524495
H	-1.027260	4.803330	-1.296932
C	3.441161	0.549061	-3.505718
H	2.707284	0.584665	-4.326621
H	3.888365	1.554881	-3.410768
H	4.239136	-0.173254	-3.733310
C	3.393357	2.908145	1.875109
H	2.868471	3.130078	2.821362
H	4.449874	2.693032	2.092448
H	3.308901	3.799192	1.231708
C	-0.223703	-1.278084	3.729538
H	-0.402794	-0.346192	4.292885
H	-1.205467	-1.749594	3.552908
H	0.413074	-1.952786	4.319975
C	-0.252931	-3.620681	-1.758582
H	0.027976	-4.561351	-1.260302

H	-1.347302	-3.507513	-1.786020
H	0.116885	-3.660659	-2.799233

3-TS

SCF energy in CF_3CH_2OH: -1618.194188 a.u.

Free energy in CF_3CH_2OH: -1617.832413 a.u.

Rh	-2.398067	-0.945233	0.380988
O	-1.635660	-2.567054	-0.638152
O	-3.054674	0.741350	1.364619
O	0.254150	-1.414874	-1.261472
O	-1.148461	1.909416	0.825550
O	-1.534478	-1.613100	2.100919
O	-3.339564	-0.324231	-1.323560
O	-1.505173	0.863884	-1.981045
O	0.436474	-0.555956	1.645754
C	-2.701302	0.434713	-2.142210
C	-0.318463	-1.284067	2.374690
C	-0.498256	-2.459462	-1.225678
C	-2.305153	1.784008	1.377955
Rh	-0.383617	0.288001	-0.251734
C	1.692505	2.579100	-0.919227
C	2.009828	3.168463	0.470970
C	3.203210	0.991682	0.912433
C	3.286643	2.484813	1.016336
H	1.149271	2.966415	1.134029
H	2.149323	4.265170	0.419966
H	4.169271	2.879969	0.480946
H	3.418281	2.765463	2.083362
N	1.402529	1.149201	-0.724237
H	1.879570	0.560813	-1.423976
H	2.612232	2.657682	-1.539995
H	2.415125	0.504520	1.496709
C	4.200038	0.133945	0.348076
C	4.050756	-1.285219	0.489015
C	5.346813	0.603130	-0.369788
C	4.986687	-2.169382	-0.045518
H	3.170379	-1.660897	1.022852
C	6.278503	-0.290502	-0.900936
H	5.500532	1.678769	-0.505850
C	6.110586	-1.681090	-0.744109
H	4.847835	-3.249545	0.079185
H	7.149125	0.095731	-1.443688
H	6.847074	-2.376089	-1.161823
C	-3.425775	0.857083	-3.406616
H	-3.456903	1.958266	-3.468010
H	-2.871476	0.493168	-4.288881
H	-4.448901	0.453567	-3.419639
C	-2.843591	3.006079	2.100202
H	-2.055350	3.455501	2.726093
H	-3.151688	3.763416	1.357383
H	-3.712669	2.735502	2.717794
C	0.236551	-1.792654	3.694581
H	1.285026	-2.108565	3.571763
H	0.218567	-0.972898	4.435161
H	-0.371196	-2.626656	4.076544
C	0.031069	-3.697573	-1.925981
H	0.679386	-4.258371	-1.228578
H	-0.801124	-4.351975	-2.226913
H	0.637014	-3.414960	-2.800868
C	0.567876	3.346929	-1.642856
H	0.350586	2.894804	-2.624665
H	-0.357891	3.328799	-1.046143
H	0.874623	4.397974	-1.798447

3-TS'

SCF energy in CF_3CH_2OH: -1618.195410 a.u.

Free energy in CF_3CH_2OH: -1617.831491 a.u.

Rh	2.502811	-0.884436	0.224380
O	1.684042	-1.935100	1.769709
O	3.368994	0.146425	-1.317896
O	-0.350252	-0.928042	1.525651
O	1.443701	1.305197	-1.721333
O	1.847255	-2.315512	-1.104857
O	3.045101	0.614696	1.532510
O	1.062980	1.733246	1.205227
O	-0.137433	-1.212713	-1.474328
C	2.221724	1.577018	1.745772
C	0.698992	-2.172220	-1.665145
C	0.449174	-1.749947	2.089320
C	2.671320	1.017056	-1.956066
Rh	0.399384	0.301132	-0.152175
C	-1.562917	2.659724	-0.346228
C	-2.986510	3.026560	0.129424
C	-3.203653	0.733168	1.152850
C	-3.340925	2.210408	1.397296
H	-3.709442	2.794251	-0.677708
H	-3.056905	4.114523	0.325207
H	-2.662214	2.510843	2.216450
H	-4.370809	2.466540	1.719502
N	-1.415863	1.199689	-0.378322
H	-1.953847	0.789062	-1.161123
H	-2.416317	0.190845	1.683491
C	-4.181074	-0.062670	0.472549
C	-5.376547	0.476972	-0.101606

C	-3.973392	-1.474874	0.352841
C	-6.298083	-0.346951	-0.750526
H	-5.580220	1.550007	-0.018613
C	-4.897155	-2.288627	-0.302620
H	-3.059097	-1.901190	0.781186
C	-6.067722	-1.733133	-0.859932
H	-7.209537	0.089825	-1.175158
H	-4.713134	-3.366387	-0.381264
H	-6.794644	-2.373828	-1.370884
H	-0.838925	3.023934	0.407800
C	-1.236709	3.313305	-1.706680
H	-0.219381	3.042734	-2.030887
H	-1.952601	2.977253	-2.481259
H	-1.307742	4.414675	-1.633288
C	3.361110	1.776213	-3.073612
H	2.740425	1.749901	-3.984673
H	3.476805	2.834746	-2.781235
H	4.352367	1.345748	-3.278533
C	2.642834	2.630410	2.754062
H	2.067005	2.493039	3.686704
H	3.715642	2.538894	2.979169
H	2.417356	3.638036	2.368449
C	-0.092546	-2.604791	3.222216
H	-0.691431	-1.985963	3.910251
H	-0.759018	-3.381342	2.806155
H	0.728003	-3.094432	3.767483
C	0.299660	-3.227122	-2.680692
H	0.752638	-4.196543	-2.421769
H	-0.796288	-3.313966	-2.736036
H	0.672977	-2.928908	-3.677195

5

SCF energy in CF_3CH_2OH: -1618.286468 a.u.

Free energy in CF_3CH_2OH: -1617.914237 a.u.

Rh	-2.378513	-1.042963	0.089778
O	-1.235119	-2.704812	-0.341522
O	-3.432273	0.666804	0.513140
O	0.676560	-1.442329	-0.514717
O	-1.524829	1.945306	0.405493
O	-2.004128	-1.297190	2.095020
O	-2.665865	-0.733313	-1.924481
O	-0.747056	0.521207	-2.090234
O	-0.085496	-0.039881	1.960458
C	-1.808673	-0.032161	-2.571144
C	-0.960619	-0.744669	2.595095
C	0.018993	-2.551980	-0.560035
C	-2.789870	1.775250	0.587144
Rh	-0.350744	0.291300	-0.072752
C	1.815881	2.752258	-0.596837
C	1.970270	3.269449	0.839100
C	2.626657	0.903685	0.769169
C	2.979945	2.270212	1.436523
H	0.993131	3.207973	1.352404
H	2.321780	4.314981	0.873903
H	4.011126	2.567274	1.171301
H	2.929505	2.199652	2.535930
N	1.672613	1.270864	-0.364431
H	1.936712	0.751318	-1.213745
H	2.782158	2.920858	-1.124694
H	2.045523	0.289354	1.473606
C	3.822780	0.088476	0.301264
C	4.034421	-1.202140	0.827279
C	4.739596	0.579817	-0.654343
C	5.129456	-1.979921	0.418451
H	3.323936	-1.599151	1.561813
C	5.827558	-0.199639	-1.075890
H	4.608949	1.585806	-1.072518
C	6.027939	-1.482218	-0.538481
H	5.277236	-2.978888	0.844667
H	6.525055	0.198634	-1.821716
H	6.880535	-2.088722	-0.864017
C	-2.077513	0.198539	-4.047213
H	-2.474918	1.219503	-4.190736
H	-1.141470	0.119999	-4.623572
H	-2.817853	-0.524914	-4.419779
C	-3.594205	3.020417	0.916077
H	-3.151403	3.533727	1.786541
H	-3.556682	3.722787	0.064943
H	-4.640880	2.758279	1.128844
C	-0.735106	-0.912342	4.086962
H	0.317434	-1.172734	4.286775
H	-0.943321	0.044234	4.598808
H	-1.401538	-1.688045	4.491945
C	0.808710	-3.792401	-0.934814
H	0.460108	-4.654861	-0.344454
H	0.635440	-4.024465	-2.001178
H	1.885684	-3.627862	-0.780567
C	0.695826	3.364625	-1.433898
H	0.621661	2.878349	-2.421558
H	-0.275363	3.260243	-0.926460
H	0.909095	4.437560	-1.593372

5’

SCF energy in CF_3CH_2OH: -1618.288305 a.u.

Free energy in CF_3CH_2OH: -1617.915764 a.u.

Rh	2.397542	-0.991563	0.015047
O	2.105186	-1.296653	2.028947
O	2.590515	-0.628905	-2.002198
O	0.155881	-0.080534	2.005653
O	0.637447	0.582501	-2.054106
O	1.284964	-2.677605	-0.400543
O	3.409281	0.749689	0.428543
O	1.466265	1.978087	0.394081
O	-0.667350	-1.465398	-0.455348
C	2.740355	1.838802	0.538341
C	0.018079	-2.552268	-0.561269
C	1.065863	-0.791110	2.582801
C	1.693260	0.071708	-2.592314
Rh	0.330246	0.288366	-0.027580
C	-1.509354	2.879893	-0.043385
C	-2.872630	3.336863	0.506412
C	-2.630949	0.921612	0.925368
C	-3.222732	2.240357	1.528127
H	-3.617491	3.370926	-0.313361
H	-2.827956	4.345423	0.954094
H	-2.728699	2.453526	2.493494
H	-4.304715	2.150724	1.720075
N	-1.614119	1.378734	-0.109439
H	-2.069198	0.376375	1.700207
C	-3.672959	-0.018459	0.339165
C	-4.503308	0.359710	-0.738188
C	-3.849872	-1.298195	0.901845
C	-5.476575	-0.518491	-1.240015
H	-4.397353	1.353393	-1.191693
C	-4.827532	-2.176352	0.408689
H	-3.203456	-1.608077	1.731077
C	-5.642926	-1.790036	-0.667212
H	-6.109889	-0.205913	-2.078132
H	-4.948596	-3.166446	0.863126
H	-6.403606	-2.475170	-1.057910
H	-0.720280	3.096849	0.700275
C	-1.104482	3.474311	-1.391211
H	-0.153013	3.041986	-1.740250
H	-1.880119	3.283072	-2.158314
H	-0.982739	4.568121	-1.300793
C	1.901208	0.359111	-4.068482
H	0.939285	0.326500	-4.604816
H	2.318979	1.375351	-4.186942
H	2.607847	-0.363225	-4.503726
C	3.517566	3.092877	0.897715
H	3.344898	3.337782	1.961222
H	4.594922	2.936096	0.739893
H	3.163663	3.946923	0.297472
C	0.865061	-1.079577	4.059810
H	0.337154	-0.245927	4.548772
H	0.248679	-1.990028	4.172972
H	1.835087	-1.259387	4.547907
C	-0.752920	-3.803268	-0.941022
H	-0.351673	-4.674828	-0.399449
H	-1.825278	-3.674968	-0.730439
H	-0.625673	-3.992685	-2.022239
H	-1.960802	1.111956	-1.043738

6

SCF energy in CF_3CH_2OH: -482.921387 a.u.

Free energy in CF_3CH_2OH: -482.726817 a.u.

C	-2.473513	0.541988	0.046042
C	-2.614224	-0.757381	0.860831
C	-0.474521	-0.808270	-0.313348
C	-1.149932	-1.196163	1.040164
H	-3.178020	-1.502189	0.267275
H	-3.145931	-0.603962	1.815934
H	-0.682478	-0.624385	1.863303
H	-1.027358	-2.267964	1.272566
N	-1.412212	0.179009	-0.917200
H	-0.916953	0.997044	-1.286345
H	-2.159441	1.355761	0.746553
H	-0.439288	-1.703980	-0.968954
C	0.955881	-0.306941	-0.159458
C	2.037756	-1.071902	-0.636277
C	1.233642	0.931651	0.458815
C	3.360669	-0.623858	-0.491783
H	1.836490	-2.030599	-1.131024
C	2.552310	1.385983	0.601270
H	0.404368	1.545364	0.833416
C	3.622597	0.607866	0.127242
H	4.187423	-1.235575	-0.871202
H	2.746761	2.350652	1.084446
H	4.653448	0.963108	0.236753
C	-3.747299	0.993106	-0.675840
H	-3.567509	1.906145	-1.272389
H	-4.094041	0.201853	-1.363544
H	-4.552180	1.219191	0.047664

6'

SCF energy in CF_3CH_2OH: -482.921512 a.u.

Free energy in CF_3CH_2OH: -482.726987 a.u.

C	2.704643	-0.221196	-0.357485

C	2.542961	0.189897	1.130494
C	0.482470	-0.806509	0.183284
C	1.199681	-0.457311	1.548683
H	2.481269	1.294976	1.191616
H	3.392093	-0.125502	1.763724
H	1.356649	-1.377454	2.139655
H	0.587700	0.219136	2.169439
N	1.331968	-0.253013	-0.909392
H	0.490903	-1.907884	0.064664
C	-0.957382	-0.335519	0.064873
C	-1.305119	1.009548	0.315314
C	-1.975369	-1.226097	-0.326777
C	-2.630022	1.449698	0.178402
H	-0.530113	1.722134	0.626636
C	-3.304252	-0.792376	-0.460940
H	-1.719119	-2.272722	-0.531715
C	-3.635754	0.548156	-0.209398
H	-2.879199	2.498132	0.379134
H	-4.081061	-1.503290	-0.765204
H	-4.671748	0.889943	-0.313321
H	3.084317	-1.264718	-0.392359
C	3.631743	0.669726	-1.184270
H	3.654921	0.343334	-2.238309
H	3.290921	1.723116	-1.156972
H	4.662383	0.642119	-0.788820
H	1.034713	0.721670	-1.075512

Rh_2(S-*tert*PTTL)$_4$ (triplet)

SCF energy in CF_3CH_2OH: -4440.755625 a.u.

Free energy in CF_3CH_2OH: -4439.443041 a.u.

Rh	-0.000001	-0.000006	-0.774130
O	-1.911634	0.724135	-0.858793
C	-2.473763	0.922009	-1.998039
O	-1.922084	0.723790	-3.138145
O	0.758781	1.916832	-0.849153
C	0.993374	2.445944	-1.996979
O	0.748333	1.934781	-3.146873
O	1.911633	-0.724157	-0.858699
C	2.473780	-0.922130	-1.997920
O	1.922116	-0.724017	-3.138050
O	-0.758783	-1.916851	-0.848984
C	-0.993358	-2.446066	-1.996765
O	-0.748302	-1.935009	-3.146702
Rh	0.000017	-0.000118	-3.222756
C	3.954545	-1.351749	-1.930014
H	4.478518	-0.435486	-1.588530
C	1.594797	3.873576	-1.912180
H	0.799392	4.488581	-1.444461
C	-1.594790	-3.873686	-1.911847
H	-0.799398	-4.488653	-1.444055
C	-3.954532	1.351622	-1.930189
H	-4.478504	0.435371	-1.588669
C	-1.999405	-4.604465	-3.240992
C	-3.034666	-3.825134	-4.080745
C	-0.716963	-4.850115	-4.073056
C	-2.596164	-5.980726	-2.856236
H	-3.962673	-3.639051	-3.514470
H	-2.637180	-2.852813	-4.410954
H	-3.297253	-4.417344	-4.977357
H	0.031227	-5.425430	-3.496582
H	-0.968844	-5.436405	-4.975734
H	-0.252982	-3.904491	-4.393826
H	-2.781371	-6.570789	-3.772032
H	-1.912465	-6.556850	-2.207348
H	-3.559379	-5.873563	-2.326623
C	-4.666539	1.810146	-3.255345
C	-3.951523	2.980258	-3.964635
C	-4.763959	0.594172	-4.210123
C	-6.106178	2.245099	-2.885978
H	-3.888249	3.873367	-3.321296
H	-2.927760	2.705556	-4.264880
H	-4.516693	3.254799	-4.874915
H	-5.261463	-0.262480	-3.720241
H	-5.360739	0.871908	-5.098466
H	-3.771026	0.263754	-4.551838
H	-6.672517	2.462521	-3.809489
H	-6.642738	1.454221	-2.331919
H	-6.112300	3.160375	-2.267866
C	1.999436	4.604233	-3.241385
C	3.034732	3.824837	-4.081034
C	0.717012	4.849781	-4.073507
C	2.596161	5.980541	-2.856745
H	3.962719	3.638810	-3.514710
H	2.637266	2.852485	-4.411173
H	3.297346	4.416972	-4.977688
H	-0.031203	5.425139	-3.497110
H	0.968908	5.435988	-4.976235
H	0.253055	3.904118	-4.394199
H	2.781379	6.570521	-3.772593
H	1.912435	6.556714	-2.207929
H	3.559365	5.873446	-2.327098
C	4.666580	-1.810341	-3.255133
C	3.951571	-2.980473	-3.964398
C	4.764042	-0.594407	-4.209958
C	6.106204	-2.245295	-2.885708
H	3.888271	-3.873557	-3.321026

H	2.927820	-2.705773	-4.264681	N	-4.103249	2.283761	-0.805417
H	4.516765	-3.255055	-4.874651	N	4.103233	-2.283835	-0.805193
H	5.261525	0.262265	-3.720090	N	2.651151	3.842481	-0.888628
H	5.360858	-0.872181	-5.098264	O	-1.798703	-5.575412	0.454096
H	3.771124	-0.264003	-4.551728	O	-3.825028	-1.927613	-1.576830
H	6.672568	-2.462753	-3.809195	O	-5.754646	1.076534	0.357044
H	6.642754	-1.454404	-2.331659	O	-2.365712	3.796455	-1.287120
H	6.112298	-3.160550	-2.267565	O	3.825041	1.927552	-1.576944
C	-3.628149	-2.825728	-0.759378	O	1.798663	5.575529	0.453609
C	-2.611047	-4.675627	0.262609	O	5.754717	-1.076637	0.357175
C	-4.316147	-3.079960	0.538258	O	2.365587	-3.796444	-1.286768
C	-3.722226	-4.201087	1.143678	H	-3.515518	6.144856	3.331495
C	-5.354010	-2.395177	1.167581	H	6.601069	2.346321	2.920160
C	-4.151725	-4.679849	2.377560	H	3.515482	-6.144779	3.331855
C	-5.789554	-2.880423	2.418549	H	-6.601140	-2.345963	2.920265
H	-5.795979	-1.498225	0.720927	C	5.699610	4.541053	4.408133
C	-5.216025	-4.014269	3.041676	C	6.216898	5.994842	4.236417
H	-3.659943	-5.553858	2.817733	C	4.513461	4.530676	5.409888
C	-4.974778	2.023848	0.281001	C	6.841589	3.686208	5.001370
C	-3.262068	3.399160	-0.548371	H	7.070103	6.031763	3.535540
C	-4.729035	3.118148	1.269496	H	5.432110	6.667494	3.848419
C	-3.699528	3.936627	0.773796	H	6.554301	6.396534	5.209733
C	-5.336067	3.365292	2.496984	H	4.125890	3.506318	5.554569
C	-3.250404	5.032474	1.507427	H	4.842268	4.915837	6.392729
C	-4.903933	4.476475	3.268110	H	3.676125	5.162376	5.065540
H	-6.131577	2.700106	2.849251	H	7.146287	4.104569	5.977294
C	-3.865383	5.286799	2.750799	H	6.528035	2.640320	5.172045
H	-2.442367	5.669685	1.133549	H	7.734363	3.679299	4.350219
C	2.611012	4.675728	0.262222	C	-5.569146	4.755493	4.631550
C	3.628141	2.825739	-0.759576	C	-7.089729	4.987854	4.419656
C	3.722179	4.201274	1.143353	C	-5.359496	3.528558	5.559619
C	4.316114	3.080093	0.538048	C	-4.982254	5.999977	5.333341
C	4.151658	4.680152	2.377197	H	-7.270495	5.861538	3.768154
C	5.353968	2.395370	1.167451	H	-7.580901	4.114098	3.956771
C	5.215949	4.014637	3.041393	H	-7.583652	5.175637	5.390765
H	3.659868	5.554203	2.817280	H	-4.284762	3.345498	5.738223
C	5.789491	2.880733	2.418381	H	-5.845669	3.704387	6.536932
H	5.795946	1.498378	0.720889	H	-5.791805	2.608010	5.130051
C	4.974795	-2.023911	0.281197	H	-5.493645	6.154103	6.300295
C	3.262005	-3.399183	-0.548078	H	-3.903579	5.885402	5.544011
C	4.729042	-3.118171	1.269733	H	-5.124222	6.917569	4.734089
C	3.699483	-3.936622	0.774094	C	-5.699705	-4.540551	4.408461
C	5.336110	-3.365308	2.497204	C	-6.217018	-5.994347	4.236877
C	3.250339	-5.032428	1.507773	C	-4.513561	-4.530103	5.410221
C	4.903964	-4.476458	3.268373	C	-6.841673	-3.685631	5.001613
H	6.131660	-2.700144	2.849426	H	-7.070218	-6.031317	3.535996
C	3.865358	-5.286750	2.751125	H	-5.432239	-6.667050	3.848948
H	2.442263	-5.669617	1.133942	H	-6.554437	-6.395941	5.210227
N	-2.651163	-3.842488	-0.888318	H	-4.125975	-3.505738	5.554813

H	-4.842380	-4.915171	6.393095
H	-3.676234	-5.161847	5.065934
H	-7.146398	-4.103909	5.977564
H	-6.528096	-2.639739	5.172211
H	-7.734436	-3.678751	4.350446
C	5.569218	-4.755469	4.631794
C	7.089779	-4.987932	4.419848
C	5.359681	-3.528487	5.559827
C	4.982278	-5.999891	5.333654
H	7.270464	-5.861646	3.768364
H	7.580989	-4.114220	3.956919
H	7.583726	-5.175717	5.390944
H	4.284966	-3.345367	5.738483
H	5.845899	-3.704303	6.537120
H	5.792013	-2.607978	5.130198
H	5.493717	-6.154028	6.300581
H	3.903625	-5.885234	5.544387
H	5.124144	-6.917510	4.734417

12

SCF energy in CF_3CH_2OH: -4923.659498 a.u.

Free energy in CF_3CH_2OH: -4922.130295 a.u.

Rh	-0.312614	0.184863	-0.796439
O	-2.366457	0.174561	-0.627898
C	-3.085617	0.397407	-1.671686
O	-2.656951	0.592243	-2.859304
O	-0.323470	2.246445	-0.528527
C	-0.500205	3.018300	-1.543431
O	-0.656408	2.656333	-2.757917
O	1.726413	0.292737	-1.170042
C	2.140116	0.586522	-2.353206
O	1.414119	0.732078	-3.394540
O	-0.374804	-1.827557	-1.285460
C	-0.571507	-2.168435	-2.510161
O	-0.643199	-1.384069	-3.516337
Rh	-0.628076	0.644239	-3.171811
C	3.653062	0.890945	-2.452975
H	3.746770	1.891588	-1.981744
C	-0.588321	4.522169	-1.182404
H	-1.495509	4.599050	-0.550618
C	-0.677899	-3.701550	-2.717252
H	0.315533	-4.100728	-2.428415
C	-4.606955	0.357836	-1.391460
H	-4.804170	-0.695002	-1.107802
C	-0.970249	-4.244879	-4.160691
C	-2.285468	-3.708735	-4.765987
C	0.225286	-3.875394	-5.072946
C	-1.049411	-5.789042	-4.071729
H	-3.157034	-3.970396	-4.143074
H	-2.263266	-2.613430	-4.876348
H	-2.435700	-4.157210	-5.765883
H	1.177247	-4.263699	-4.664627
H	0.080752	-4.327083	-6.071342
H	0.320911	-2.785712	-5.198976
H	-1.149046	-6.211272	-5.087977
H	-0.144947	-6.220284	-3.606524
H	-1.925253	-6.119635	-3.485706
C	-5.598303	0.701327	-2.559001
C	-5.382964	2.108668	-3.156426
C	-5.445233	-0.371649	-3.664935
C	-7.036299	0.608504	-1.991361
H	-5.518966	2.900175	-2.400585
H	-4.373405	2.215643	-3.583157
H	-6.121208	2.279063	-3.962285
H	-5.592469	-1.389473	-3.260946
H	-6.206070	-0.202481	-4.449031
H	-4.450175	-0.331333	-4.133830
H	-7.764970	0.736405	-2.812143
H	-7.225375	-0.369410	-1.513133
H	-7.232953	1.397718	-1.243946
C	-0.761876	5.563526	-2.346784
C	0.382369	5.523795	-3.382599
C	-2.119886	5.304501	-3.044118
C	-0.812029	6.974598	-1.709370
H	1.359151	5.749791	-2.922236
H	0.454046	4.538783	-3.869108
H	0.194127	6.284830	-4.163000
H	-2.952225	5.313636	-2.317619
H	-2.307100	6.100718	-3.787923
H	-2.132042	4.334851	-3.564696
H	-1.044709	7.721602	-2.489712
H	-1.586986	7.043423	-0.925273
H	0.156642	7.255613	-1.258651
C	4.297046	1.013092	-3.885094
C	4.055487	-0.224112	-4.777315
C	3.730838	2.278405	-4.576860
C	5.821737	1.215377	-3.701036
H	4.457236	-1.144480	-4.322577
H	2.981174	-0.379224	-4.966473
H	4.559323	-0.075241	-5.750720
H	3.885960	3.179174	-3.955604
H	4.252682	2.434866	-5.539032
H	2.653460	2.182836	-4.779603
H	6.283338	1.426080	-4.682524
H	6.043549	2.063585	-3.028674
H	6.311116	0.314329	-3.290488

C	-2.808139	-3.667647	-1.280325	C	-5.220785	-4.405085	4.244621
C	-1.115885	-5.190310	-0.726823	C	-6.764239	-3.918227	2.320542
C	-3.211165	-4.388761	-0.035640	C	-6.375416	-6.297892	3.017781
C	-2.199067	-5.304734	0.290765	H	-4.484364	-5.092714	4.697246
C	-4.350855	-4.230284	0.754741	H	-4.749566	-3.409550	4.161599
C	-2.301927	-6.099797	1.433677	H	-6.078333	-4.323902	4.937976
C	-4.486773	-5.027127	1.917504	H	-7.157865	-4.236383	1.337862
H	-5.101430	-3.483744	0.481745	H	-7.617915	-3.882397	3.021446
C	-3.451127	-5.946531	2.229081	H	-6.373906	-2.890779	2.217477
H	-1.507793	-6.800803	1.709688	H	-7.247740	-6.219399	3.692197
H	-3.540125	-6.559299	3.132813	H	-6.729535	-6.682368	2.044505
C	-5.410819	0.504953	1.003629	H	-5.687711	-7.046972	3.448238
C	-4.273647	2.369006	0.156309	C	6.627846	-4.643421	1.844412
C	-5.286303	1.515895	2.095371	C	6.264832	-4.690055	3.352618
C	-4.593734	2.627212	1.591409	C	5.885911	-5.796516	1.132975
C	-5.698764	1.486804	3.428749	C	8.156038	-4.863652	1.673837
C	-4.284839	3.733977	2.383015	H	6.780074	-3.901077	3.928885
C	-5.395618	2.602727	4.229242	H	5.177188	-4.573923	3.502350
H	-6.235761	0.624116	3.836460	H	6.563365	-5.665111	3.779343
C	-4.692561	3.734401	3.738525	H	6.127473	-5.840356	0.055413
H	-3.720817	4.565557	1.951997	H	6.192209	-6.759197	1.579299
H	-5.713491	2.589150	5.277757	H	4.790095	-5.715972	1.245613
C	0.305897	5.402479	1.022030	H	8.444179	-5.847325	2.087992
C	1.854636	4.408931	-0.432868	H	8.444259	-4.842612	0.607492
C	1.651261	5.443175	1.668424	H	8.746649	-4.092160	2.199039
C	2.576512	4.827703	0.806057	C	-4.387052	4.913448	4.685738
C	2.060958	5.934699	2.905735	C	-3.486782	4.410689	5.846510
C	3.915864	4.669816	1.148932	C	-3.657962	6.069337	3.965092
C	3.421712	5.795525	3.251085	C	-5.717940	5.464621	5.265558
H	1.350052	6.412737	3.587759	H	-3.972098	3.605424	6.425847
C	4.364116	5.167593	2.401996	H	-2.527373	4.021042	5.461946
H	4.591609	4.147149	0.463935	H	-3.266113	5.240772	6.542872
H	3.749835	6.185914	4.218540	H	-4.268601	6.487994	3.144707
C	5.200141	0.505598	-0.495224	H	-3.466830	6.885750	4.684542
C	4.233236	-1.403935	-1.453001	H	-2.685233	5.760952	3.543402
C	5.685028	-0.689802	0.254048	H	-5.512394	6.310801	5.946653
C	5.103485	-1.833573	-0.313397	H	-6.380227	5.828437	4.459601
C	6.559242	-0.801727	1.336995	H	-6.271277	4.700354	5.839237
C	5.368221	-3.115566	0.171105	C	5.846709	5.001195	2.791052
C	6.831805	-2.092001	1.823617	C	6.183703	3.486287	2.858619
H	7.018241	0.084410	1.787471	C	6.736469	5.678779	1.713935
C	6.256458	-3.263054	1.264230	C	6.174628	5.636749	4.160066
H	4.889555	-3.978553	-0.298915	H	5.573645	2.983498	3.631197
H	7.520656	-2.192740	2.669601	H	6.006336	2.975598	1.895942
N	-1.567865	-4.230002	-1.671504	H	7.249097	3.352628	3.124903
N	-4.843287	1.109264	-0.149230	H	6.514483	6.758433	1.636600
N	4.379142	0.005574	-1.534752	H	7.803487	5.566497	1.980572
N	0.515365	4.829521	-0.261595	H	6.591835	5.228270	0.717064
C	-5.704923	-4.906670	2.856987	H	7.247212	5.496217	4.383463

H	5.973718	6.723700	4.171423
H	5.602864	5.168494	4.981965
O	-0.028759	-5.762699	-0.781227
O	-3.392248	-2.759887	-1.868703
O	-5.882191	-0.629715	1.041677
O	-3.637834	3.069499	-0.628825
O	2.287657	3.809766	-1.415693
O	-0.783770	5.758410	1.465002
O	5.434748	1.696948	-0.289780
O	3.525787	-2.090927	-2.182795
N	0.076756	-0.142472	1.079348
C	1.173549	0.121209	1.951784
C	1.203529	-0.917964	3.111348
H	1.985426	-0.594799	3.827860
H	0.235414	-0.856822	3.647000
C	1.466540	-2.363940	2.664425
C	1.390019	-3.348030	3.849604
H	2.462801	-2.434358	2.185107
H	0.725990	-2.634744	1.889615
H	2.044742	-2.985411	4.667476
H	0.359519	-3.314870	4.262967
C	1.752283	-4.795084	3.543384
C	1.455833	-5.394710	2.301828
C	2.367060	-5.592714	4.532944
C	1.752838	-6.746511	2.058878
H	0.988120	-4.810116	1.503646
C	2.664373	-6.944770	4.297485
H	2.608523	-5.145742	5.506257
C	2.355935	-7.528913	3.057715
H	1.502193	-7.173732	1.081748
H	3.140479	-7.541568	5.084570
H	2.587658	-8.583857	2.870883
H	2.114596	0.018371	1.359102
C	1.096686	1.567440	2.507343
H	1.030994	2.290852	1.681134
H	0.201722	1.684119	3.143596
H	1.995506	1.787878	3.111097

13

SCF energy in CF_3CH_2OH: -4923.665357 a.u.

Free energy in CF_3CH_2OH: -4922.135012 a.u.

Rh	0.013786	0.598816	-3.194329
O	1.718369	-0.545321	-3.335642
O	-1.647508	1.786511	-2.967003
O	1.661092	-0.972818	-1.087602
O	-1.708487	1.388037	-0.713857
O	-1.205995	-1.035056	-3.465343
O	1.174812	2.258427	-2.857245
O	1.148617	1.863241	-0.600525
O	-1.305516	-1.430969	-1.211738
C	1.476063	2.535910	-1.647328
C	-1.648715	-1.644742	-2.433409
C	2.198210	-1.031534	-2.256087
C	-2.129494	1.947034	-1.794667
Rh	-0.050168	0.171059	-0.792823
C	-2.674104	-2.794525	-2.609786
C	-3.179442	-3.120616	-4.061380
N	-3.746638	-2.597847	-1.624310
C	-1.975905	-3.617724	-4.899405
C	-4.201664	-4.279872	-3.957590
C	-3.857650	-1.921888	-4.759402
C	-4.383570	-1.370953	-1.326402
C	-4.097282	-3.610210	-0.686109
H	-1.216413	-2.831818	-5.033714
H	-1.491495	-4.492945	-4.426789
H	-3.785414	-5.149571	-3.419254
H	-5.124347	-3.966360	-3.437603
H	-4.723122	-1.554628	-4.182751
H	-3.158409	-1.082754	-4.896679
O	-4.215136	-0.317773	-1.940078
C	-5.258957	-1.639931	-0.146403
O	-3.617023	-4.740891	-0.672715
C	-5.102244	-2.988553	0.221955
C	-6.098105	-0.777207	0.553890
C	-5.801173	-3.510726	1.307856
C	-6.832393	-1.283957	1.659862
C	-6.667048	-2.645603	2.007312
C	3.613739	-1.655629	-2.288292
C	4.245627	-1.998662	-3.690003
N	3.676089	-2.748396	-1.310656
C	4.522962	-0.674429	-4.445376
C	5.605630	-2.695043	-3.437416
C	3.359592	-2.920929	-4.555896
C	2.739783	-3.807749	-1.199149
C	4.605378	-2.754846	-0.240684
H	3.590255	-0.148643	-4.699159
H	5.149901	0.007636	-3.842651
H	6.262312	-2.088260	-2.788469
H	5.478962	-3.686706	-2.967877
H	3.167363	-3.889094	-4.064490
H	2.387249	-2.452758	-4.777521
O	1.783721	-3.997371	-1.944219
C	3.167954	-4.598554	-0.003150
O	5.479129	-1.907463	-0.057720
C	4.286319	-3.967360	0.568858
C	2.629026	-5.764705	0.531216

C	4.892376	-4.499475	1.705175	H	4.254217	-0.866808	-1.841185
C	3.225948	-6.334086	1.687339	H	-2.158246	-3.706072	-2.245533
C	4.349101	-5.681662	2.249212	H	6.273754	0.702468	0.553191
C	2.249496	3.842098	-1.338792	H	6.689944	3.076662	4.180270
C	2.719166	4.736083	-2.543175	H	4.852188	4.583074	3.436023
N	3.315832	3.525096	-0.379001	H	4.822850	-6.103490	3.140105
C	1.469184	5.246098	-3.301191	H	5.763068	-4.016383	2.160617
C	3.456123	5.965574	-1.956014	H	1.757093	-6.223075	0.052840
C	3.668416	4.006233	-3.518913	H	-7.217048	-3.051637	2.860467
C	4.177495	2.408309	-0.468818	H	-5.666181	-4.550171	1.621392
C	3.446790	4.187120	0.870904	H	-6.161421	0.276472	0.262500
H	0.926491	4.423029	-3.790332	H	-4.639404	4.149008	3.589521
H	0.768820	5.761060	-2.619604	H	-3.060409	5.396980	5.055535
H	2.829667	6.510446	-1.227510	H	-0.187875	5.688438	1.797694
H	4.396545	5.679228	-1.452161	C	-0.520232	6.412256	4.458849
H	4.592699	3.670503	-3.018175	C	0.810702	5.615924	4.543318
H	3.186763	3.126799	-3.973776	C	-0.242963	7.809987	3.841524
O	4.197741	1.603551	-1.398851	C	-1.061155	6.612018	5.891924
C	4.996484	2.421018	0.779861	H	0.642638	4.612520	4.974843
O	2.740321	5.118097	1.252923	H	1.287481	5.488987	3.556016
C	4.571463	3.500886	1.574174	H	1.525589	6.152531	5.194766
C	6.005010	1.553599	1.187683	H	-1.170516	8.406714	3.773462
C	5.173710	3.747230	2.805974	H	0.476957	8.364983	4.470839
C	6.640153	1.782074	2.437626	H	0.187854	7.732978	2.828315
C	6.210804	2.883129	3.216368	H	-0.315584	7.162081	6.493163
C	-3.372824	2.842862	-1.578672	H	-1.996340	7.201222	5.904978
C	-3.924112	3.679850	-2.786432	H	-1.250261	5.648873	6.400237
N	-3.142124	3.619058	-0.350005	C	-7.763638	-0.340223	2.447977
C	-4.425010	2.700110	-3.875906	C	-6.912113	0.782043	3.102229
C	-5.137737	4.493523	-2.272778	C	-8.793245	0.295537	1.475568
C	-2.887219	4.651171	-3.390045	C	-8.542504	-1.073643	3.562362
C	-1.932150	4.279352	-0.027148	H	-6.173724	0.354064	3.804431
C	-3.990359	3.507581	0.782931	H	-6.365623	1.383542	2.355692
H	-3.596920	2.118596	-4.309091	H	-7.570427	1.465244	3.671568
H	-5.165468	1.988485	-3.468170	H	-9.419789	-0.478843	0.997081
H	-5.895165	3.844509	-1.797466	H	-9.459856	0.982773	2.028402
H	-4.834458	5.259037	-1.536456	H	-8.302640	0.878860	0.677652
H	-2.530732	5.383627	-2.646705	H	-9.208989	-0.357998	4.076197
H	-2.011856	4.112106	-3.785156	H	-9.173746	-1.887093	3.160195
O	-0.987776	4.443475	-0.796924	H	-7.868530	-1.502399	4.326210
C	-2.059187	4.695930	1.400076	C	2.641875	-7.632762	2.278939
O	-5.059067	2.899220	0.801124	C	1.153628	-7.400015	2.654366
C	-3.302122	4.247666	1.881145	C	2.734888	-8.758243	1.212910
C	-1.157632	5.384320	2.206252	C	3.395885	-8.098038	3.544173
C	-3.676628	4.495565	3.199893	H	1.052708	-6.603935	3.413025
C	-1.511529	5.651311	3.555614	H	0.546111	-7.109727	1.779929
C	-2.770921	5.201356	4.019261	H	0.718773	-8.327011	3.070845
H	-4.172786	2.129817	-1.297820	H	3.785752	-8.957264	0.935688
H	1.528993	4.447869	-0.754110	H	2.301754	-9.694153	1.610959

H	2.184721	-8.499057	0.291598
H	2.936706	-9.027125	3.926223
H	4.459136	-8.316803	3.336302
H	3.346059	-7.347518	4.353937
C	7.756139	0.824324	2.900366
C	7.166695	-0.606537	3.038495
C	8.892023	0.814256	1.842087
C	8.362992	1.236731	4.259735
H	6.369503	-0.627971	3.803881
H	6.740080	-0.977328	2.090110
H	7.960563	-1.309548	3.353388
H	9.334030	1.820007	1.723443
H	9.694757	0.121932	2.155890
H	8.531027	0.482241	0.853610
H	9.159885	0.524423	4.538591
H	8.816844	2.243956	4.222300
H	7.611112	1.223589	5.069791
H	6.123145	-2.846966	-4.401755
H	5.065072	-0.894517	-5.383659
H	3.872165	-3.121278	-5.515353
H	-4.487634	-4.607501	-4.973469
H	-2.328039	-3.931031	-5.899202
H	-4.222986	-2.238921	-5.754094
H	-4.910483	3.272737	-4.687383
H	-5.616314	5.016196	-3.120750
H	-3.354871	5.211277	-4.221342
H	3.959852	4.700498	-4.329240
H	1.781515	5.967690	-4.078528
H	3.716156	6.661901	-2.773692
C	1.111842	-0.748398	1.945394
C	0.593837	-1.026480	3.392139
C	-1.690313	-2.233755	3.003092
C	-0.258372	-2.292506	3.584600
H	0.043871	-0.131188	3.742531
H	1.494501	-1.114311	4.030772
H	0.272726	-3.164787	3.153007
H	-0.334858	-2.494112	4.671765
N	0.071545	-0.242556	1.110041
H	-2.201821	-1.337644	3.405519
H	-1.641015	-2.099316	1.906696
C	-2.479256	-3.481955	3.356356
C	-2.487130	-4.604178	2.503057
C	-3.181496	-3.569375	4.577450
C	-3.174286	-5.777460	2.856550
H	-1.968915	-4.553564	1.538731
C	-3.867471	-4.739713	4.937911
H	-3.193172	-2.703139	5.251930
C	-3.864594	-5.851243	4.077892
H	-3.178429	-6.628493	2.166171
H	-4.408193	-4.783091	5.890950
H	-4.401177	-6.765866	4.355915
H	1.465757	-1.715628	1.511671
C	2.319343	0.225961	1.986717
H	2.690927	0.415157	0.969730
H	2.021330	1.186963	2.440195
H	3.133386	-0.216574	2.588445

13'

SCF energy in CF_3CH_2OH: -4923.664990 a.u.

Free energy in CF_3CH_2OH: -4922.135003 a.u.

Rh	-0.432716	0.264397	-3.244281
O	1.614606	0.400287	-3.381141
O	-2.474071	0.181879	-3.034671
O	1.847250	0.171353	-1.113790
O	-2.278297	-0.021020	-0.761161
O	-0.386628	-1.794806	-3.366683
O	-0.527706	2.307635	-3.031570
O	-0.272826	2.101632	-0.763637
O	-0.198558	-2.009864	-1.096203
C	-0.434678	2.778020	-1.847315
C	-0.340986	-2.476786	-2.287611
C	2.297247	0.381731	-2.301384
C	-2.950476	0.086514	-1.852837
Rh	-0.209181	0.028190	-0.829650
C	-0.415752	-4.023223	-2.338791
C	-0.620449	-4.716716	-3.732086
N	-1.356807	-4.456909	-1.294772
C	0.610710	-4.405217	-4.618113
C	-0.669350	-6.245640	-3.491624
C	-1.915212	-4.281692	-4.452908
C	-2.618516	-3.871053	-1.029748
C	-0.961767	-5.334949	-0.247074
H	0.687027	-3.331078	-4.848136
H	1.550089	-4.723046	-4.128312
H	0.216180	-6.603531	-2.936461
H	-1.569859	-6.540626	-2.924335
H	-2.812370	-4.511266	-3.853635
H	-1.916047	-3.201921	-4.668724
O	-3.164558	-3.020119	-1.729702
C	-3.101479	-4.492746	0.239776
O	0.133092	-5.887646	-0.171891
C	-2.118509	-5.391219	0.691101
C	-4.284260	-4.279273	0.942752
C	-2.312655	-6.121633	1.860867
C	-4.511145	-5.011820	2.139022
C	-3.517331	-5.924895	2.565578

C	3.799731	0.749127	-2.361043	C	-5.200413	1.651943	-3.550273
C	4.478722	0.910725	-3.771821	C	-4.268050	2.141843	-0.209926
N	4.534456	-0.121464	-1.436000	C	-5.425136	0.312918	0.687526
C	3.837887	2.121655	-4.495046	H	-4.187342	-0.821677	-4.334748
C	5.974977	1.235323	-3.536383	H	-5.343771	-1.849529	-3.443701
C	4.370216	-0.348193	-4.659633	H	-7.084330	-0.757469	-1.852813
C	4.433298	-1.534403	-1.386138	H	-7.129796	1.021374	-1.683335
C	5.307076	0.387533	-0.362745	H	-5.399652	2.486143	-2.856708
H	2.783327	1.932837	-4.746906	H	-4.169010	1.756006	-3.921951
H	3.885021	3.033019	-3.872279	O	-3.603773	2.806166	-1.003031
H	6.104956	2.106651	-2.869523	C	-4.668854	2.480935	1.187960
H	6.517666	0.380717	-3.094376	O	-5.884849	-0.825331	0.767314
H	4.860298	-1.221253	-4.197763	C	-5.377471	1.389203	1.720232
H	3.319389	-0.612612	-4.856843	C	-4.416342	3.631463	1.929280
O	3.751458	-2.227573	-2.134888	C	-5.865867	1.435138	3.024116
C	5.302002	-1.959618	-0.245350	C	-4.902378	3.707612	3.261968
O	5.484319	1.581934	-0.123363	C	-5.622544	2.603070	3.776683
C	5.822047	-0.807146	0.369403	H	-4.673452	-1.005687	-1.303177
C	5.603422	-3.238007	0.213716	H	-1.559360	4.383119	-1.062348
C	6.663728	-0.916628	1.474454	H	3.842987	1.746724	-1.877787
C	6.460604	-3.383254	1.336952	H	0.564815	-4.372913	-1.956565
C	6.971589	-2.210816	1.942993	H	4.394543	4.094941	0.567269
C	-0.595602	4.299031	-1.603795	H	3.102166	6.109894	4.204574
C	-0.693834	5.257459	-2.842906	H	0.784667	6.295740	3.311212
N	0.406875	4.696576	-0.603725	H	7.630966	-2.300978	2.810651
C	-1.984017	4.916229	-3.628415	H	7.073529	-0.026857	1.963509
C	-0.826721	6.703476	-2.304014	H	5.175499	-4.108503	-0.294271
C	0.530115	5.180748	-3.780700	H	-3.675997	-6.498810	3.482615
C	1.764641	4.295622	-0.621894	H	-1.552878	-6.821650	2.222875
C	0.047900	5.260554	0.649233	H	-5.006048	-3.539296	0.580972
H	-1.932248	3.912612	-4.077525	H	-6.415725	0.590898	3.452679
H	-2.874398	4.954945	-2.975053	H	-6.003992	2.643693	4.800689
H	-1.671548	6.801909	-1.598831	H	-3.833866	4.445776	1.484946
H	0.091317	7.033537	-1.785952	C	-4.628885	4.976819	4.094215
H	1.463003	5.456978	-3.261154	C	-3.094176	5.181629	4.222928
H	0.658092	4.169297	-4.197108	C	-5.250664	6.202040	3.370691
O	2.312580	3.697404	-1.545443	C	-5.231432	4.893814	5.513821
C	2.338605	4.730484	0.686275	H	-2.625488	4.324695	4.739928
O	-1.092425	5.588887	0.972784	H	-2.602323	5.299625	3.241888
C	1.312392	5.329076	1.439505	H	-2.887542	6.092567	4.815258
C	3.635852	4.600726	1.174095	H	-6.345294	6.090855	3.268802
C	1.574381	5.829536	2.712925	H	-5.051677	7.122916	3.949181
C	3.933790	5.106644	2.467959	H	-4.826435	6.342337	2.361566
C	2.890937	5.714984	3.206824	H	-5.011563	5.826934	6.062442
C	-4.483524	0.031571	-1.643420	H	-6.330079	4.774632	5.491058
C	-5.422766	0.280651	-2.876921	H	-4.802727	4.058643	6.097234
N	-4.797798	0.853807	-0.464938	C	-5.810576	-4.780557	2.936707
C	-5.200105	-0.855791	-3.905195	C	-5.835353	-3.311932	3.442430
C	-6.885444	0.195598	-2.375067	C	-7.034709	-5.028770	2.015095

C	-5.928639	-5.719996	4.157181
H	-4.969824	-3.109063	4.099067
H	-5.815728	-2.584557	2.612571
H	-6.757864	-3.134654	4.026866
H	-7.044479	-6.066909	1.636429
H	-7.970413	-4.861593	2.579670
H	-7.044360	-4.347911	1.146765
H	-6.883000	-5.526403	4.678717
H	-5.921698	-6.785346	3.862150
H	-5.115857	-5.555215	4.887686
C	6.803819	-4.798030	1.845238
C	5.491038	-5.550759	2.193148
C	7.555760	-5.564892	0.723398
C	7.699121	-4.773681	3.103429
H	4.918987	-5.021653	2.975339
H	4.833710	-5.662738	1.313833
H	5.725723	-6.565162	2.564893
H	8.505112	-5.062095	0.464766
H	7.790867	-6.591934	1.058166
H	6.951442	-5.641819	-0.197474
H	7.906546	-5.809392	3.425982
H	8.672374	-4.286854	2.910300
H	7.209545	-4.255412	3.947774
C	5.369444	4.975758	3.014991
C	5.750479	3.471655	3.091042
C	6.345631	5.705322	2.052613
C	5.525119	5.590525	4.423177
H	5.080080	2.931724	3.784185
H	5.697646	2.973495	2.107312
H	6.785343	3.367832	3.467530
H	6.103085	6.780873	1.979699
H	7.382618	5.611577	2.424118
H	6.314732	5.279014	1.035180
H	6.570196	5.475052	4.761240
H	5.292211	6.671060	4.432419
H	4.880067	5.088471	5.167184
H	6.455605	1.469566	-4.503281
H	4.388171	2.320795	-5.433229
H	4.866927	-0.153110	-5.628487
H	-0.700600	-6.769494	-4.464032
H	0.527293	-4.957571	-5.571975
H	-1.998992	-4.828552	-5.410652
H	-5.931417	-0.753186	-4.727898
H	-7.574614	0.266459	-3.235869
H	-5.891392	1.752814	-4.408109
H	0.388462	5.886549	-4.620368
H	-2.124509	5.653426	-4.440192
H	-1.000847	7.395262	-3.147835
C	0.420172	0.921896	2.090330
C	1.192857	0.231145	3.257182
C	2.225504	-1.992303	2.398480
C	2.463276	-0.528900	2.816957
H	0.498362	-0.448201	3.787302
H	1.455604	1.037071	3.969646
H	2.919361	0.003738	1.960892
H	3.218126	-0.490536	3.626001
N	0.027504	-0.020735	1.097511
H	1.423348	-2.015044	1.634708
H	3.134565	-2.358247	1.879353
C	1.888438	-2.985747	3.506049
C	2.048388	-2.702268	4.877933
C	1.434715	-4.276569	3.148958
C	1.770722	-3.670381	5.859244
H	2.394182	-1.711915	5.194234
C	1.164202	-5.247063	4.124157
H	1.296537	-4.524831	2.089126
C	1.330100	-4.948744	5.487750
H	1.901647	-3.419866	6.918826
H	0.822710	-6.242333	3.816007
H	1.116132	-5.705346	6.251492
H	1.119475	1.649566	1.610799
C	-0.810062	1.702828	2.622179
H	-1.332569	2.206944	1.794760
H	-1.514997	1.013202	3.118207
H	-0.482615	2.463690	3.354138

12-TS

SCF energy in CF_3CH_2OH: -4923.640020 a.u.

Free energy in CF_3CH_2OH: -4922.110232 a.u.

Rh	0.201657	-0.157577	-2.943644
O	1.767243	1.151476	-2.811955
O	-1.393383	-1.446332	-3.031111
O	1.604985	1.251958	-0.528848
O	-1.687494	-1.283890	-0.765584
O	1.443924	-1.775774	-2.645144
O	-1.112316	1.422337	-3.138845
O	-1.299251	1.599994	-0.862967
O	1.186034	-1.671753	-0.370949
C	-1.599194	1.926385	-2.070748
C	1.622943	-2.207080	-1.457398
C	2.117154	1.584347	-1.661535
C	-1.993392	-1.717956	-1.937285
Rh	-0.048207	-0.021952	-0.517596
C	2.473829	-3.482801	-1.222715
C	3.040062	-4.244391	-2.473064
N	1.743790	-4.336136	-0.269365

C	4.016313	-3.301695	-3.218288	H	-2.800303	1.784034	-4.747086
C	3.842577	-5.463920	-1.955728	H	-4.453690	2.048727	-4.124716
C	1.941902	-4.739892	-3.438527	H	-5.034106	4.253470	-2.876514
C	0.357648	-4.621753	-0.314648	H	-3.800574	5.543436	-2.759451
C	2.315231	-4.738142	0.967828	H	-1.404900	5.130043	-3.535843
H	3.492814	-2.437936	-3.655073	H	-0.973914	3.605469	-4.354302
H	4.801556	-2.914828	-2.543039	O	-0.370605	4.563449	-1.298348
H	4.618839	-5.166137	-1.228005	C	-1.743190	5.264182	0.614528
H	3.187859	-6.208439	-1.468393	O	-4.740283	3.516206	-0.119096
H	1.247608	-5.438681	-2.942004	C	-3.067740	4.955891	0.968596
H	1.352725	-3.902238	-3.842420	C	-0.937876	6.072189	1.411008
O	-0.398543	-4.325820	-1.237464	C	-3.619983	5.461536	2.143820
C	0.040396	-5.328066	0.963995	C	-1.469617	6.599047	2.617809
O	3.476543	-4.524960	1.309803	C	-2.806654	6.280140	2.954678
C	1.221627	-5.416839	1.720912	C	-3.175398	-2.719803	-1.959549
C	-1.171781	-5.833728	1.426391	C	-3.708176	-3.219243	-3.352729
C	1.217294	-6.035629	2.968840	N	-4.225487	-2.206692	-1.068661
C	-1.206559	-6.476291	2.693557	C	-2.593464	-4.041228	-4.045027
C	-0.003920	-6.564484	3.434813	C	-4.905990	-4.165518	-3.089772
C	3.209455	2.682257	-1.579315	C	-4.172190	-2.074578	-4.279981
C	3.645858	3.370909	-2.927840	C	-4.685894	-0.869762	-1.042317
N	4.345151	2.198201	-0.782307	C	-4.743825	-2.958920	0.015727
C	2.397802	4.012718	-3.582301	H	-1.723361	-3.415209	-4.293387
C	4.641243	4.508213	-2.586242	H	-2.246849	-4.870402	-3.402215
C	4.329635	2.405838	-3.921510	H	-4.640056	-4.981159	-2.394149
C	5.004130	0.955577	-0.938874	H	-5.772576	-3.625311	-2.668124
C	4.939147	2.983700	0.245299	H	-4.991967	-1.490153	-3.829412
H	1.687029	3.250725	-3.936896	H	-3.347396	-1.383248	-4.512523
H	1.865221	4.675385	-2.876913	O	-4.336770	0.014498	-1.821633
H	4.220696	5.221064	-1.855367	C	-5.638482	-0.787080	0.105370
H	5.589912	4.118337	-2.175600	O	-4.432259	-4.119413	0.281197
H	5.258920	1.979801	-3.504952	C	-5.688802	-2.047630	0.726967
H	3.667127	1.574069	-4.203810	C	-6.373942	0.298385	0.571249
O	4.648285	0.042999	-1.679632	C	-6.506136	-2.253266	1.836128
C	6.189237	1.010868	-0.025355	C	-7.218341	0.117710	1.699667
O	4.512725	4.061997	0.647004	C	-7.268515	-1.161728	2.302678
C	6.150123	2.224827	0.679960	H	-2.783507	-3.611132	-1.431381
C	7.229545	0.101336	0.134972	H	-3.650744	2.378401	-1.923996
C	7.166511	2.555737	1.573602	H	2.762763	3.474787	-0.948486
C	8.290124	0.416125	1.025176	H	3.352745	-3.142737	-0.639399
C	8.230294	1.642561	1.729069	H	0.091055	6.281536	1.100018
C	-2.744108	2.965724	-2.177452	H	-3.234895	6.677037	3.879432
C	-3.027918	3.636916	-3.570586	H	-4.650365	5.228028	2.431366
N	-2.620126	3.910461	-1.057861	H	9.039372	1.905581	2.416372
C	-3.561145	2.551749	-4.539310	H	7.147323	3.501758	2.124840
C	-4.146098	4.689279	-3.368741	H	7.222689	-0.831558	-0.438393
C	-1.790105	4.325630	-4.183943	H	-0.011933	-7.055615	4.411832
C	-1.428384	4.577537	-0.676402	H	2.131432	-6.107046	3.567479
C	-3.633889	4.054428	-0.077520	H	-2.077658	-5.712101	0.822510

H	-6.554098	-3.228848	2.331001
H	-7.914895	-1.319642	3.170579
H	-6.270592	1.271992	0.080466
C	-8.033520	1.314653	2.229292
C	-7.054481	2.439834	2.664618
C	-8.954277	1.846518	1.097931
C	-8.918269	0.940117	3.438441
H	-6.393724	2.091981	3.479683
H	-6.417972	2.783926	1.830774
H	-7.627959	3.309253	3.037529
H	-9.665468	1.069032	0.765505
H	-9.537688	2.712482	1.461322
H	-8.375585	2.178660	0.219150
H	-9.482393	1.829383	3.771700
H	-9.654816	0.156262	3.183805
H	-8.319237	0.588130	4.298060
C	-2.540247	-7.048416	3.215626
C	-3.566958	-5.892279	3.363503
C	-3.080346	-8.089499	2.198165
C	-2.387906	-7.743842	4.586599
H	-3.202712	-5.133961	4.080402
H	-3.772435	-5.387917	2.403744
H	-4.524816	-6.291573	3.746643
H	-2.371641	-8.927933	2.072232
H	-4.041271	-8.503502	2.555255
H	-3.258235	-7.640673	1.205901
H	-3.366555	-8.144513	4.905574
H	-1.679621	-8.591414	4.545720
H	-2.047379	-7.042846	5.370373
C	9.469726	-0.567326	1.174081
C	8.937345	-1.945073	1.651365
C	10.161198	-0.735464	-0.206561
C	10.525465	-0.077805	2.189629
H	8.461427	-1.864443	2.645223
H	8.192922	-2.365816	0.953686
H	9.771174	-2.666823	1.729107
H	10.556797	0.229048	-0.572144
H	11.005224	-1.444800	-0.124841
H	9.465984	-1.126794	-0.969583
H	11.341567	-0.818909	2.260319
H	10.977671	0.883722	1.885860
H	10.099418	0.042570	3.202351
C	-0.579806	7.487879	3.510338
C	0.675230	6.681198	3.941347
C	-0.136040	8.737020	2.701980
C	-1.310240	7.966864	4.784224
H	0.390877	5.788919	4.527548
H	1.267498	6.340994	3.074236
H	1.331888	7.310019	4.570307
H	-1.008484	9.338377	2.389128
H	0.517881	9.376899	3.322440
H	0.428155	8.461445	1.794028
H	-0.630385	8.598129	5.383654
H	-2.202355	8.574725	4.547266
H	-1.625046	7.121147	5.422418
H	4.886708	5.064440	-3.508961
H	2.712099	4.621988	-4.449775
H	4.603084	2.964107	-4.836490
H	4.340496	-5.963994	-2.806206
H	4.514283	-3.858040	-4.033634
H	2.413823	-5.275843	-4.283427
H	-2.988646	-4.477219	-4.981124
H	-5.230017	-4.619307	-4.043843
H	-4.544878	-2.503220	-5.229147
H	-2.064861	4.773071	-5.157550
H	-3.850364	3.023795	-5.496446
H	-4.458370	5.086059	-4.351527
C	-1.278507	0.677203	2.307534
C	-1.172350	0.121623	3.759265
C	1.205856	-0.628536	3.458243
C	0.255448	0.201517	4.316942
H	-1.513764	-0.932768	3.751881
H	-1.877699	0.686618	4.397131
H	0.575207	1.261071	4.342243
H	0.272708	-0.154890	5.367955
N	-0.265418	0.088343	1.456387
H	0.731983	-0.304046	2.276008
H	-1.078995	1.776548	2.349785
C	-2.710257	0.466508	1.770443
H	-2.825249	0.899801	0.767138
H	-2.937148	-0.611193	1.716335
H	-3.433953	0.946679	2.453804
H	0.932062	-1.699628	3.459733
C	2.666460	-0.430244	3.536673
C	3.535962	-1.514636	3.244130
C	3.256794	0.809573	3.896619
C	4.924918	-1.374650	3.331232
H	3.111119	-2.480205	2.947915
C	4.647169	0.947188	3.985640
H	2.620663	1.674407	4.112970
C	5.489765	-0.143757	3.709109
H	5.566853	-2.232763	3.102949
H	5.077511	1.913867	4.271093
H	6.576976	-0.028902	3.773703

12-TS'

SCF energy in CF_3CH_2OH: -4923.647221 a.u.

Free energy in CF_3CH_2OH: -4922.117687 a.u.

Rh	-0.313970	0.146560	-3.204158
O	1.744091	0.161973	-3.300700
O	-2.360291	0.187614	-3.029471
O	1.916865	-0.003603	-1.022446
O	-2.220228	0.066858	-0.745040
O	-0.373823	-1.915511	-3.239012
O	-0.297970	2.200352	-3.062791
O	-0.109602	2.070686	-0.782625
O	-0.240705	-2.054369	-0.956846
C	-0.205715	2.710607	-1.895688
C	-0.386652	-2.555275	-2.133779
C	2.401580	0.139388	-2.205736
C	-2.863638	0.163978	-1.855080
Rh	-0.151469	-0.002425	-0.773544
C	-0.548934	-4.098034	-2.145636
C	-0.760631	-4.812140	-3.528704
N	-1.543745	-4.450430	-1.120781
C	0.505749	-4.591849	-4.392001
C	-0.903114	-6.330826	-3.260508
C	-2.012740	-4.322080	-4.288851
C	-2.766117	-3.773315	-0.896498
C	-1.257366	-5.369407	-0.074651
H	0.649077	-3.529318	-4.642052
H	1.413962	-4.952252	-3.873574
H	-0.054513	-6.727690	-2.675534
H	-1.833225	-6.563265	-2.712133
H	-2.934787	-4.489407	-3.706487
H	-1.948768	-3.249238	-4.527004
O	-3.228177	-2.890651	-1.617071
C	-3.331475	-4.351882	0.359280
O	-0.220901	-6.024115	0.017060
C	-2.438765	-5.329213	0.834041
C	-4.510001	-4.039592	1.031735
C	-2.724397	-6.039767	1.997125
C	-4.826837	-4.746752	2.222604
C	-3.925111	-5.740225	2.672459
C	3.923435	0.418643	-2.244601
C	4.643848	0.475831	-3.642437
N	4.588412	-0.443611	-1.259569
C	4.093021	1.687556	-4.435561
C	6.151097	0.723784	-3.384528
C	4.479278	-0.813538	-4.476310
C	4.414928	-1.845452	-1.143552
C	5.360419	0.078534	-0.192615
H	3.035152	1.549024	-4.705143
H	4.179842	2.622633	-3.853447
H	6.316360	1.614760	-2.752298
H	6.633728	-0.139990	-2.893477
H	4.902850	-1.693259	-3.963841
H	3.418650	-1.021291	-4.688787
O	3.717590	-2.542798	-1.874025
C	5.234057	-2.256221	0.039564
O	5.591690	1.273043	-0.004815
C	5.799053	-1.101688	0.609150
C	5.467037	-3.523951	0.563478
C	6.615898	-1.197227	1.733759
C	6.299202	-3.655245	1.706916
C	6.854047	-2.480635	2.267915
C	-0.278130	4.247768	-1.714927
C	-0.302413	5.159860	-2.991639
N	0.735185	4.624400	-0.717035
C	-1.602753	4.865839	-3.779385
C	-0.350500	6.632619	-2.514752
C	0.923818	4.968480	-3.910139
C	2.065793	4.141474	-0.701073
C	0.399976	5.267345	0.503899
H	-1.610692	3.840471	-4.179753
H	-2.496482	4.992957	-3.141935
H	-1.190842	6.811406	-1.820025
H	0.583612	6.929039	-2.004950
H	1.866384	5.214340	-3.392661
H	0.995367	3.932214	-4.275720
O	2.585655	3.471246	-1.590686
C	2.653764	4.600551	0.592758
O	-0.720105	5.680184	0.799372
C	1.660022	5.295801	1.305050
C	3.936899	4.417054	1.100219
C	1.942235	5.842306	2.555065
C	4.255562	4.968709	2.370132
C	3.246219	5.675334	3.067123
C	-4.402084	0.191093	-1.680723
C	-5.300578	0.424680	-2.947541
N	-4.708575	1.082666	-0.551212
C	-5.106807	-0.765672	-3.919025
C	-6.777627	0.426991	-2.481391
C	-5.001611	1.752887	-3.675805
C	-4.134281	2.359470	-0.344881
C	-5.401731	0.632204	0.602516
H	-4.084780	-0.795111	-4.326327
H	-5.303708	-1.730248	-3.417133
H	-7.034468	-0.495310	-1.930107
H	-7.001033	1.289042	-1.827868
H	-5.175636	2.626069	-3.024604
H	-3.959436	1.793031	-4.029278
O	-3.408597	2.951215	-1.141766
C	-4.576749	2.793347	1.013907
O	-5.911012	-0.480671	0.726421

C	-5.350020	1.762732	1.576448	C	7.279246	-5.918719	1.200528
C	-4.302275	3.972061	1.700521	C	7.472715	-5.019942	3.537528
C	-5.884242	1.902647	2.855671	H	4.689886	-5.136810	3.435952
C	-4.831643	4.142906	3.007375	H	4.551695	-5.832361	1.801723
C	-5.618429	3.100199	3.552551	H	5.407332	-6.737066	3.077861
H	-4.646948	-0.819346	-1.298227	H	8.251387	-5.478164	0.914747
H	-1.241311	4.412648	-1.191499	H	7.464149	-6.938071	1.586396
H	4.010228	1.434450	-1.807204	H	6.667622	-6.011662	0.286160
H	0.399004	-4.496428	-1.731183	H	7.632447	-6.048445	3.907083
H	4.667407	3.836387	0.526997	H	8.466802	-4.588670	3.319906
H	3.474239	6.107929	4.045332	H	7.012395	-4.440714	4.358504
H	1.177338	6.384139	3.121065	C	5.675979	4.776725	2.939330
H	7.495521	-2.560523	3.149897	C	5.952741	3.257859	3.111811
H	7.060525	-0.305323	2.187251	C	6.707513	5.376783	1.945772
H	5.009234	-4.397265	0.087268	C	5.863347	5.466710	4.308405
H	-4.153637	-6.296650	3.585639	H	5.240945	2.807671	3.827518
H	-2.035821	-6.800139	2.378695	H	5.874645	2.707101	2.158342
H	-5.158145	-3.242747	0.651199	H	6.974728	3.107281	3.507463
H	-6.485482	1.107340	3.308279	H	6.540247	6.459727	1.803887
H	-6.035280	3.214151	4.557214	H	7.732536	5.235987	2.335364
H	-3.667659	4.733694	1.235045	H	6.656360	4.891169	0.956178
C	-4.524301	5.441713	3.779709	H	6.896043	5.302696	4.664196
C	-2.987154	5.571394	3.964286	H	5.703542	6.558792	4.247527
C	-5.048009	6.654979	2.964570	H	5.181163	5.056752	5.075389
C	-5.187388	5.470699	5.174512	H	6.665701	0.887501	-4.348461
H	-2.590383	4.725529	4.554823	H	4.676200	1.809608	-5.366977
H	-2.448455	5.597660	3.001275	H	5.009432	-0.694043	-5.439908
H	-2.752414	6.506085	4.506861	H	-0.940664	-6.870685	-4.223964
H	-6.142115	6.596326	2.821828	H	0.411650	-5.160116	-5.335525
H	-4.821446	7.595813	3.499057	H	-2.105740	-4.885307	-5.236258
H	-4.577552	6.714757	1.968036	H	-5.815725	-0.668589	-4.761829
H	-4.937499	6.419577	5.681840	H	-7.440924	0.496759	-3.362446
H	-6.289171	5.409887	5.110529	H	-5.670477	1.845947	-4.551843
H	-4.829912	4.647334	5.819373	H	0.832218	5.640420	-4.783913
C	-6.121878	-4.402668	2.985248	H	-1.685927	5.570730	-4.627046
C	-6.051134	-2.924557	3.457959	H	-0.479485	7.297847	-3.387634
C	-7.339304	-4.582626	2.039102	C	0.213794	1.082608	2.106464
C	-6.334207	-5.302569	4.223294	C	0.846632	0.649775	3.459525
H	-5.185770	-2.767685	4.127291	C	1.863229	-1.453441	2.473904
H	-5.964505	-2.219605	2.613149	C	2.142061	-0.165085	3.253141
H	-6.969495	-2.668088	4.018942	H	0.104396	0.045638	4.016943
H	-7.420261	-5.627485	1.688622	H	1.041440	1.559543	4.058002
H	-8.273127	-4.326507	2.572536	H	2.865821	0.451577	2.688385
H	-7.271470	-3.928986	1.152748	H	2.610590	-0.383540	4.234060
H	-7.278726	-5.023030	4.723316	N	0.125164	-0.034347	1.190116
H	-6.407160	-6.371534	3.951071	H	0.915214	-1.000599	1.700606
H	-5.522316	-5.187211	4.964414	H	2.614114	-1.683991	1.699693
C	6.571944	-5.059407	2.283559	C	1.395433	-2.669124	3.177218
C	5.224081	-5.725884	2.670121	C	0.998706	-2.675592	4.539480

C	1.326433	-3.897540	2.467388
C	0.574033	-3.856775	5.163725
H	1.041593	-1.749629	5.123027
C	0.895091	-5.075377	3.087589
H	1.607980	-3.914258	1.408036
C	0.520178	-5.062547	4.444145
H	0.285262	-3.835591	6.221386
H	0.840209	-5.997996	2.500087
H	0.187965	-5.984069	4.935903
H	0.886615	1.842232	1.641852
C	-1.169321	1.737207	2.322277
H	-1.578027	2.093237	1.365196
H	-1.872959	1.008075	2.760618
H	-1.074758	2.598094	3.008955

14

SCF energy in CF_3CH_2OH: -4923.693256 a.u.

Free energy in CF_3CH_2OH: -4922.161834 a.u.

Rh	-0.504763	0.190286	-3.199747
O	1.420251	0.892723	-3.324092
O	-2.444955	-0.446973	-2.994089
O	1.725823	0.665395	-1.067082
O	-2.212115	-0.581830	-0.719836
O	0.113204	-1.776052	-3.352537
O	-1.166567	2.122708	-2.944526
O	-0.862976	1.978799	-0.677773
O	0.364198	-1.943803	-1.080941
C	-1.203107	2.592692	-1.757425
C	0.347994	-2.422104	-2.275956
C	2.088967	1.036347	-2.243916
C	-2.881669	-0.669399	-1.814908
Rh	-0.228441	0.010397	-0.788514
C	0.692602	-3.933410	-2.334557
C	0.682519	-4.652847	-3.728624
N	-0.099312	-4.608262	-1.291560
C	1.785261	-4.016313	-4.609980
C	1.048116	-6.139052	-3.492588
C	-0.681072	-4.577295	-4.448498
C	-1.474280	-4.389175	-1.028922
C	0.520148	-5.325985	-0.233908
H	1.566814	-2.961007	-4.835987
H	2.774432	-4.068261	-4.117590
H	1.997142	-6.244425	-2.936761
H	0.261041	-6.668582	-2.926724
H	-1.481802	-5.050251	-3.855330
H	-0.974609	-3.534927	-4.647126
O	-2.235290	-3.731152	-1.735030
C	-1.767247	-5.101060	0.252102
O	1.725507	-5.556855	-0.155043
C	-0.572737	-5.679559	0.716351
C	-2.964476	-5.218924	0.953431
C	-0.554368	-6.410679	1.902130
C	-2.979130	-5.965038	2.162795
C	-1.767877	-6.547570	2.606775
C	3.413251	1.833096	-2.291469
C	4.007658	2.217168	-3.699268
N	4.383597	1.215880	-1.380025
C	3.040148	3.209257	-4.392985
C	5.348445	2.955212	-3.459667
C	4.257916	1.003782	-4.621643
C	4.769033	-0.148249	-1.382299
C	4.990839	1.930593	-0.318178
H	2.086948	2.728210	-4.659936
H	2.818206	4.075359	-3.744212
H	5.225668	3.814167	-2.775594
H	6.119248	2.285989	-3.037511
H	4.984755	0.297113	-4.188324
H	3.325337	0.453020	-4.821742
O	4.325290	-1.014391	-2.129900
C	5.797117	-0.276583	-0.302141
O	4.774665	3.111062	-0.043501
C	5.918777	0.966611	0.342440
C	6.578162	-1.370147	0.057719
C	6.824753	1.134109	1.387580
C	7.527175	-1.225590	1.104441
C	7.618983	0.028126	1.754337
C	-1.768409	4.013846	-1.511847
C	-2.101792	4.920426	-2.749482
N	-0.918654	4.656861	-0.498072
C	-3.257187	4.263996	-3.544837
C	-2.603069	6.283111	-2.210111
C	-0.892603	5.162022	-3.678716
C	0.496564	4.616761	-0.495595
C	-1.428301	5.104124	0.749215
H	-2.950324	3.304916	-3.989558
H	-4.134008	4.077683	-2.898590
H	-3.443349	6.160413	-1.503289
H	-1.800764	6.840014	-1.694149
H	-0.057608	5.647009	-3.145824
H	-0.520323	4.219094	-4.109164
O	1.191950	4.192562	-1.416116
C	0.920991	5.169330	0.824416
O	-2.619847	5.131916	1.053292
C	-0.234717	5.484756	1.561281
C	2.201120	5.358881	1.336491
C	-0.127505	6.022668	2.841901

C	2.341097	5.908197	2.639218	H	-6.643004	4.912716	2.065707
C	1.167368	6.233468	3.360529	H	-6.994335	4.478135	5.761264
C	-4.339684	-1.153661	-1.625325	H	-7.918288	3.081025	5.155211
C	-5.282421	-1.218412	-2.880714	H	-6.309444	2.841216	5.908445
N	-4.910146	-0.426289	-0.481384	C	-4.297949	-6.107513	2.949589
C	-4.712627	-2.258625	-3.876543	C	-4.762570	-4.701703	3.419647
C	-6.665953	-1.722526	-2.400188	C	-5.382759	-6.725942	2.026996
C	-5.463809	0.142586	-3.587371	C	-4.147616	-7.013599	4.192078
C	-4.792209	0.967376	-0.261327	H	-4.003623	-4.236491	4.074783
C	-5.424445	-1.091814	0.660896	H	-4.952393	-4.018799	2.573773
H	-3.753833	-1.928577	-4.304299	H	-5.701616	-4.793740	3.997128
H	-4.551075	-3.236653	-3.388641	H	-5.083153	-7.730712	1.678075
H	-6.587016	-2.682404	-1.859127	H	-6.335000	-6.824743	2.579774
H	-7.158903	-0.993385	-1.732621	H	-5.576429	-6.099443	1.139535
H	-5.914400	0.895846	-2.919050	H	-5.122550	-7.098475	4.704391
H	-4.503857	0.539653	-3.952329	H	-3.824076	-8.035721	3.922809
O	-4.301382	1.772745	-1.049448	H	-3.427251	-6.600963	4.921658
C	-5.362090	1.216665	1.096531	C	8.443221	-2.412696	1.465096
O	-5.533720	-2.312162	0.774335	C	7.583556	-3.662783	1.788077
C	-5.760028	-0.017064	1.641357	C	9.355335	-2.717875	0.244912
C	-5.499485	2.412395	1.794598	C	9.343648	-2.115521	2.684580
C	-6.327336	-0.074741	2.912506	H	6.920320	-3.485051	2.652432
C	-6.075478	2.385508	3.092805	H	6.949182	-3.962796	0.936391
C	-6.482519	1.136327	3.619365	H	8.242641	-4.517510	2.028606
H	-4.234514	-2.192984	-1.257088	H	9.989300	-1.848387	-0.005896
H	-2.726833	3.836954	-0.983587	H	10.018203	-3.573320	0.471536
H	3.153902	2.788865	-1.791050	H	8.765001	-2.976536	-0.651657
H	1.730221	-4.009081	-1.950972	H	9.963555	-3.001871	2.908785
H	3.071278	5.060084	0.742276	H	10.032246	-1.271706	2.496936
H	1.256821	6.659125	4.363916	H	8.749702	-1.887346	3.588135
H	-1.018644	6.270870	3.427856	C	3.754223	6.124083	3.217125
H	8.337046	0.157644	2.568831	C	4.487155	4.756534	3.291986
H	6.925507	2.096395	1.900220	C	4.545156	7.078929	2.282121
H	6.457522	-2.317854	-0.477244	C	3.725602	6.742681	4.632203
H	-1.760584	-7.123947	3.535827	H	3.946583	4.055773	3.954073
H	0.371490	-6.859273	2.276482	H	4.588500	4.282656	2.300116
H	-3.865941	-4.722262	0.579210	H	5.503048	4.900832	3.705227
H	-6.639532	-1.028620	3.350191	H	4.047104	8.062117	2.203277
H	-6.929895	1.096270	4.616600	H	5.563183	7.241303	2.681783
H	-5.144077	3.345562	1.344805	H	4.647081	6.665116	1.264235
C	-6.227167	3.705238	3.875438	H	4.759682	6.879888	4.995609
C	-4.820400	4.323812	4.103896	H	3.237257	7.734367	4.641338
C	-7.094920	4.691508	3.047813	H	3.204340	6.091362	5.357380
C	-6.901177	3.503346	5.250359	H	5.733085	3.337271	-4.422430
H	-4.187486	3.646242	4.705411	H	3.508694	3.587914	-5.320284
H	-4.291865	4.532452	3.157520	H	4.664772	1.360051	-5.586758
H	-4.916259	5.278660	4.653639	H	1.160282	-6.649951	-4.465858
H	-8.106335	4.282136	2.873543	H	1.857601	-4.567352	-5.565421
H	-7.200718	5.648695	3.590698	H	-0.614261	-5.112598	-5.414247

H	-5.431457	-2.404315	-4.703914
H	-7.325300	-1.872559	-3.274041
H	-6.139278	0.014226	-4.453857
H	-1.197053	5.826547	-4.508817
H	-3.573075	4.940295	-4.360583
H	-2.952847	6.906090	-3.053070
C	-0.380458	0.384147	2.400396
C	-0.346405	-0.597340	3.608195
C	1.547282	-2.314351	3.285407
C	1.038856	-1.119671	4.046522
H	-1.016477	-1.451177	3.387980
H	-0.800384	-0.052157	4.457833
H	1.774399	-0.282856	4.010541
H	0.981377	-1.383940	5.125091
N	0.143036	-0.216266	1.184989
H	1.039684	-0.702353	1.348049
H	0.285918	1.242793	2.667964
C	-1.804425	0.921815	2.202358
H	-1.847166	1.629207	1.361414
H	-2.497400	0.090153	1.989274
H	-2.144937	1.436800	3.117944
H	0.955311	-2.674109	2.433702
C	2.684100	-3.082467	3.665123
C	3.048231	-4.253314	2.920841
C	3.490248	-2.753186	4.804495
C	4.126561	-5.047900	3.307818
H	2.467985	-4.525266	2.031267
C	4.567709	-3.556776	5.181721
H	3.252950	-1.859997	5.392763
C	4.893402	-4.713286	4.444279
H	4.375656	-5.939400	2.720835
H	5.161417	-3.286401	6.063182
H	5.733269	-5.346217	4.751587

14’

SCF energy in CF_3CH_2OH: -4923.673736 a.u.

Free energy in CF_3CH_2OH: -4922.141066 a.u.

Rh	-0.530716	0.146588	-3.172929
O	1.513471	0.285661	-3.310097
O	-2.571952	0.066848	-2.954264
O	1.766029	0.150133	-1.039519
O	-2.350208	-0.062112	-0.678467
O	-0.485703	-1.918330	-3.224168
O	-0.626466	2.195121	-2.999421
O	-0.349402	2.071702	-0.726799
O	-0.286856	-2.057502	-0.945857
C	-0.528099	2.707226	-1.832925
C	-0.439659	-2.560619	-2.122017
C	2.207024	0.323321	-2.236966
C	-3.035581	0.003335	-1.765240
Rh	-0.283339	0.002707	-0.761182
C	-0.523040	-4.110378	-2.141360
C	-0.750744	-4.825956	-3.521410
N	-1.453594	-4.523742	-1.079301
C	0.473404	-4.542470	-4.426474
C	-0.812564	-6.351083	-3.259516
C	-2.050295	-4.390199	-4.233282
C	-2.703801	-3.921342	-0.801906
C	-1.072379	-5.429738	-0.051809
H	0.560218	-3.472859	-4.672162
H	1.414253	-4.866228	-3.943076
H	0.073888	-6.711113	-2.707794
H	-1.711067	-6.630427	-2.681066
H	-2.941546	-4.600088	-3.617865
H	-2.042973	-3.314831	-4.468918
O	-3.250016	-3.069084	-1.499802
C	-3.177865	-4.529215	0.477938
O	-0.000802	-6.030637	-0.011072
C	-2.209282	-5.451716	0.912345
C	-4.340529	-4.282217	1.203030
C	-2.396741	-6.169841	2.091093
C	-4.560444	-5.001831	2.408577
C	-3.580674	-5.936804	2.820293
C	3.696856	0.727337	-2.332351
C	4.355001	0.815503	-3.761538
N	4.473905	-0.052615	-1.362710
C	3.688080	1.974383	-4.544418
C	5.850614	1.171632	-3.572331
C	4.249074	-0.494265	-4.573441
C	4.445454	-1.463541	-1.224012
C	5.289735	0.555023	-0.376231
H	2.630931	1.760957	-4.763275
H	3.737610	2.922280	-3.978956
H	5.980428	2.079767	-2.956854
H	6.413625	0.349346	-3.095586
H	4.748713	-1.335914	-4.065745
H	3.198444	-0.775906	-4.746599
O	3.757889	-2.230263	-1.891972
C	5.404502	-1.778140	-0.119276
O	5.427620	1.769177	-0.221086
C	5.910005	-0.566934	0.385317
C	5.819631	-3.009845	0.376932
C	6.846668	-0.566892	1.416790
C	6.782867	-3.043927	1.419977
C	7.272196	-1.813570	1.919508
C	-0.704403	4.234897	-1.646607

C	-0.842449	5.142111	-2.920778	H	0.773112	6.487979	3.128931
N	0.314859	4.686091	-0.687642	H	8.012448	-1.819829	2.724531
C	-2.142660	4.751940	-3.665844	H	7.245551	0.370533	1.818175
C	-0.986447	6.606744	-2.438003	H	5.401567	-3.930443	-0.043274
C	0.363432	5.045254	-3.879859	H	-3.734021	-6.500513	3.744611
C	1.677313	4.304596	-0.723735	H	-1.646560	-6.885065	2.443166
C	-0.019884	5.305272	0.545056	H	-5.050943	-3.526566	0.850729
H	-2.083026	3.733663	-4.079450	H	-6.410344	0.651080	3.577882
H	-3.019754	4.799803	-2.995500	H	-5.994298	2.751780	4.848476
H	-1.824913	6.723688	-1.728048	H	-3.906273	4.462512	1.433050
H	-0.066987	6.967811	-1.943582	C	-4.653682	5.071958	4.038685
H	1.302473	5.355835	-3.391698	C	-3.118949	5.297887	4.123497
H	0.497831	4.019320	-4.256676	C	-5.307647	6.265820	3.291519
O	2.209552	3.672011	-1.633524	C	-5.219868	5.028050	5.474947
C	2.279240	4.811173	0.545491	H	-2.628112	4.462811	4.655445
O	-1.156313	5.632621	0.883185	H	-2.650335	5.391214	3.128549
C	1.264447	5.432439	1.295723	H	-2.909267	6.229088	4.682218
C	3.591395	4.725516	1.001896	H	-6.403212	6.139893	3.222049
C	1.553494	6.002916	2.533366	H	-5.104100	7.207700	3.833429
C	3.917064	5.304976	2.257704	H	-4.910988	6.376297	2.267634
C	2.885324	5.935392	2.993726	H	-4.993354	5.978902	5.989398
C	-4.565584	-0.059091	-1.534459	H	-6.317856	4.900577	5.484916
C	-5.525024	0.140402	-2.761122	H	-4.769584	4.214095	6.071983
N	-4.871588	0.798205	-0.377895	C	-5.838244	-4.734119	3.229472
C	-5.302478	-1.024729	-3.756733	C	-5.828564	-3.256789	3.710029
C	-6.979296	0.053568	-2.235445	C	-7.084635	-4.975993	2.336168
C	-5.328828	1.492153	-3.480118	C	-5.947043	-5.650830	4.467734
C	-4.351480	2.100231	-0.176387	H	-4.946820	-3.057188	4.346029
C	-5.466738	0.289096	0.804682	H	-5.815240	-2.543872	2.867419
H	-4.297442	-0.989190	-4.204056	H	-6.735540	-3.054302	4.310197
H	-5.423691	-2.005257	-3.261753	H	-7.119739	-6.020016	1.975759
H	-7.157396	-0.883173	-1.677222	H	-8.006159	-4.782671	2.915517
H	-7.225370	0.899864	-1.569573	H	-7.098710	-4.309885	1.456555
H	-5.527852	2.344981	-2.809620	H	-6.885043	-5.429753	5.007624
H	-4.303967	1.596213	-3.869535	H	-5.968446	-6.720626	4.190322
O	-3.712547	2.745319	-1.004710	H	-5.114236	-5.491242	5.176594
C	-4.726517	2.480990	1.218005	C	7.262782	-4.405689	1.960379
O	-5.907297	-0.852556	0.935291	C	6.048135	-5.186289	2.529978
C	-5.412436	1.400250	1.800059	C	7.898166	-5.215351	0.797386
C	-4.471496	3.657975	1.915747	C	8.316615	-4.259801	3.079884
C	-5.876660	1.485315	3.110879	H	5.579762	-4.644193	3.369897
C	-4.931941	3.773632	3.254705	H	5.265577	-5.352568	1.770163
C	-5.631450	2.680214	3.819334	H	6.376040	-6.176396	2.897271
H	-4.739681	-1.086468	-1.158004	H	8.772408	-4.687822	0.375004
H	-1.656840	4.329582	-1.087710	H	8.236214	-6.201934	1.164218
H	3.713303	1.756413	-1.917420	H	7.179860	-5.391249	-0.022014
H	0.460898	-4.461146	-1.769583	H	8.625130	-5.261762	3.427247
H	4.339483	4.198466	0.400073	H	9.225265	-3.737092	2.728723
H	3.118435	6.387193	3.961993	H	7.916625	-3.715506	3.954572

C	5.370009	5.228178	2.768785
C	5.778020	3.737135	2.921644
C	6.306522	5.913113	1.736639
C	5.555273	5.929188	4.132431
H	5.134360	3.227567	3.661570
H	5.707946	3.185009	1.968412
H	6.823625	3.671049	3.276428
H	6.042954	6.978083	1.604985
H	7.354783	5.859519	2.083879
H	6.255814	5.424473	0.748519
H	6.611391	5.850339	4.445887
H	5.303815	7.004440	4.083035
H	4.940315	5.463494	4.924050
H	6.309539	1.358131	-4.559922
H	4.218827	2.120759	-5.503343
H	4.736504	-0.352932	-5.556438
H	-0.858546	-6.886387	-4.225084
H	0.371847	-5.107714	-5.370935
H	-2.152875	-4.954298	-5.179136
H	-6.048576	-0.958712	-4.569853
H	-7.681958	0.084493	-3.087630
H	-6.032807	1.558903	-4.330793
H	0.194538	5.714197	-4.744382
H	-2.311907	5.457134	-4.500273
H	-1.177514	7.262818	-3.306379
C	0.371910	0.859557	2.162342
C	1.333457	0.251054	3.217118
C	2.302745	-1.828283	2.066804
C	2.585022	-0.466750	2.630549
H	0.772848	-0.452679	3.864673
H	1.668063	1.084193	3.867133
H	3.010120	0.178340	1.838255
H	3.347892	-0.528612	3.430672
N	-0.132471	-0.131370	1.232179
H	-0.601223	-0.928697	1.690480
H	1.981113	-1.878365	1.019907
C	2.326100	-3.045657	2.801398
C	2.689704	-3.133228	4.187665
C	1.960249	-4.271553	2.149621
C	2.679805	-4.356956	4.860266
H	2.975153	-2.225031	4.730006
C	1.948870	-5.487123	2.831293
H	1.673595	-4.240961	1.092711
C	2.309590	-5.544183	4.194572
H	2.959236	-4.391664	5.920429
H	1.644488	-6.392704	2.295069
H	2.301139	-6.499007	4.732001
H	0.936044	1.597106	1.560180
C	-0.801703	1.594528	2.857152
H	-1.460647	2.057489	2.105528
H	-1.400420	0.888948	3.462960
H	-0.417183	2.385546	3.527266

13-TS

SCF energy in CF_3CH_2OH: -4923.658686 a.u.

Free energy in CF_3CH_2OH: -4922.127849 a.u.

Rh	-0.302535	-0.104262	-2.892257
O	0.336811	1.848110	-2.822164
O	-0.954420	-2.056803	-2.858781
O	0.589901	1.834963	-0.543936
O	-0.969696	-2.085297	-0.567648
O	1.640167	-0.731473	-3.035969
O	-2.236859	0.519305	-2.935839
O	-2.266580	0.706220	-0.666571
O	1.834242	-0.885929	-0.780062
C	-2.808763	0.779784	-1.812027
C	2.306821	-0.957164	-1.967377
C	0.656874	2.381478	-1.704439
C	-1.184774	-2.600456	-1.723736
Rh	-0.160890	-0.134245	-0.457092
C	3.822286	-1.230762	-2.097000
C	4.383574	-1.685475	-3.497954
N	4.256075	-2.067673	-0.970788
C	4.274351	-0.496503	-4.485448
C	5.885991	-2.019512	-3.324950
C	3.655842	-2.916557	-4.081174
C	3.666598	-3.291654	-0.561550
C	5.253651	-1.637990	-0.062696
H	3.225604	-0.231846	-4.686532
H	4.784904	0.400998	-4.091328
H	6.442022	-1.179207	-2.871301
H	6.041704	-2.914651	-2.696704
H	3.738743	-3.795503	-3.421070
H	2.585241	-2.710449	-4.240781
O	2.748391	-3.873378	-1.130115
C	4.397232	-3.692737	0.682719
O	5.882230	-0.582566	-0.152691
C	5.352046	-2.704041	0.975639
C	4.241911	-4.820888	1.482560
C	6.179604	-2.825803	2.089534
C	5.071044	-4.975725	2.625525
C	6.025268	-3.967928	2.902180
C	1.131249	3.860714	-1.704087
C	1.117656	4.637579	-3.072692
N	2.418387	3.937770	-0.995663
C	-0.339615	4.688844	-3.592404

C	1.581104	6.092014	-2.809437	H	0.128009	-5.436587	-3.141913
C	2.045476	4.011827	-4.137518	H	-1.815783	-6.765478	-2.050176
C	3.498328	3.042204	-1.149937	H	-3.497224	-6.195510	-2.251063
C	2.675433	4.900998	0.020847	H	-4.001387	-4.027417	-3.477977
H	-0.711811	3.689212	-3.862205	H	-2.687366	-3.063538	-4.205689
H	-1.023321	5.114866	-2.835644	O	-4.063935	-2.190255	-1.515858
H	0.977237	6.583534	-2.026717	C	-4.776460	-3.492632	0.445889
H	2.641023	6.137484	-2.501594	O	-2.123807	-5.842089	0.591913
H	3.098148	4.001793	-3.804973	C	-4.205145	-4.617109	1.066736
H	1.751317	2.978585	-4.374976	C	-5.932782	-2.888625	0.932491
O	3.521992	2.076106	-1.911050	C	-4.797233	-5.177779	2.195889
C	4.563748	3.519668	-0.214423	C	-6.564422	-3.443581	2.078110
O	1.870572	5.734198	0.424378	C	-5.980148	-4.582811	2.681695
C	4.080692	4.653143	0.461811	H	-0.963448	-4.638042	-1.143710
C	5.839274	3.010975	0.014129	H	-4.808714	0.173387	-1.534122
C	4.886589	5.326410	1.377032	H	0.428019	4.390200	-1.031967
C	6.688003	3.679918	0.937490	H	4.282779	-0.244417	-1.882776
C	6.190624	4.832111	1.593310	H	-3.347392	5.535356	1.214574
C	-4.321897	1.120555	-1.842356	H	-6.376217	4.410721	4.131473
C	-4.982527	1.536481	-3.209844	H	-6.926408	2.372860	2.810955
N	-4.610284	2.039461	-0.732210	H	6.832445	5.362526	2.302446
C	-4.999221	0.303103	-4.147165	H	4.519628	6.210462	1.908873
C	-6.452229	1.936090	-2.927893	H	6.159306	2.099326	-0.500527
C	-4.264515	2.712466	-3.906567	H	6.671550	-4.068209	3.778524
C	-3.887116	3.221290	-0.431972	H	6.923293	-2.058493	2.327770
C	-5.532571	1.717091	0.291329	H	3.485915	-5.568545	1.220334
H	-3.980533	-0.015651	-4.414065	H	-4.358164	-6.051422	2.689046
H	-5.514201	-0.552873	-3.674043	H	-6.453332	-5.023940	3.563507
H	-6.994657	1.140390	-2.386135	H	-6.320795	-1.988944	0.442992
H	-6.521141	2.864511	-2.333161	C	-7.848649	-2.785899	2.622314
H	-4.256721	3.619315	-3.279708	C	-7.523690	-1.333204	3.066269
H	-3.220148	2.457314	-4.147588	C	-8.920687	-2.750882	1.499838
O	-2.987693	3.706984	-1.110959	C	-8.436598	-3.547760	3.831071
C	-4.454649	3.724866	0.857826	H	-6.767318	-1.329976	3.872222
O	-6.239620	0.708866	0.316231	H	-7.141049	-0.718853	2.232804
C	-5.447676	2.827618	1.286158	H	-8.439101	-0.848171	3.454581
C	-4.131605	4.866202	1.584318	H	-9.177129	-3.770920	1.161191
C	-6.149413	3.063304	2.466762	H	-9.843655	-2.271365	1.874725
C	-4.827578	5.134321	2.792662	H	-8.578227	-2.175678	0.622664
C	-5.826778	4.221018	3.205075	H	-9.361068	-3.045318	4.167311
C	-1.734573	-4.053179	-1.683707	H	-8.699951	-4.590523	3.575574
C	-1.980810	-4.795957	-3.045464	H	-7.739993	-3.565175	4.689139
N	-2.885622	-4.080148	-0.768399	C	4.900921	-6.223491	3.516395
C	-0.624577	-4.935918	-3.779455	C	3.455047	-6.249890	4.081975
C	-2.499497	-6.219773	-2.724607	C	5.143021	-7.497254	2.662045
C	-3.007774	-4.086044	-3.954740	C	5.887205	-6.242844	4.704855
C	-3.927556	-3.125258	-0.729126	H	3.258461	-5.360451	4.707201
C	-2.956809	-4.978239	0.333081	H	2.697773	-6.274586	3.279141
H	-0.222806	-3.957619	-4.084751	H	3.308988	-7.148927	4.708508

H	6.167774	-7.509715	2.249374
H	5.012956	-8.401153	3.285153
H	4.437040	-7.569812	1.816462
H	5.722970	-7.156174	5.303692
H	6.939959	-6.251866	4.368722
H	5.742772	-5.376644	5.375721
C	8.102088	3.122879	1.199599
C	7.973773	1.706138	1.824435
C	8.874475	3.025837	-0.143632
C	8.919526	4.011436	2.162948
H	7.447749	1.752650	2.795460
H	7.418828	1.010241	1.171619
H	8.980022	1.282192	2.001242
H	8.980381	4.019614	-0.614976
H	9.887587	2.620526	0.033313
H	8.369762	2.358987	-0.863419
H	9.924906	3.575387	2.301372
H	9.053192	5.035558	1.768872
H	8.451425	4.080625	3.161795
C	-4.472165	6.396269	3.604530
C	-2.980739	6.320739	4.030425
C	-4.692279	7.651836	2.718126
C	-5.335605	6.544397	4.876605
H	-2.797117	5.441720	4.674146
H	-2.305256	6.248773	3.160305
H	-2.701637	7.227089	4.598698
H	-5.748179	7.736194	2.404084
H	-4.427778	8.565249	3.281855
H	-4.069433	7.629108	1.806995
H	-5.043239	7.462497	5.416797
H	-6.411266	6.629579	4.637554
H	-5.199398	5.695178	5.570706
H	1.482614	6.678232	-3.741056
H	-0.386425	5.331297	-4.491015
H	1.994589	4.614715	-5.063433
H	6.330484	-2.227579	-4.314948
H	4.755774	-0.770958	-5.442219
H	4.105430	-3.176908	-5.057688
H	-0.759335	-5.553442	-4.686381
H	-2.591766	-6.796884	-3.662497
H	-3.120441	-4.659755	-4.893795
H	-4.788594	2.953346	-4.850599
H	-5.542308	0.555625	-5.076778
H	-6.974406	2.115803	-3.885128
C	-1.186080	-0.618472	2.503712
C	-0.605008	-2.039018	2.626312
C	1.669853	-0.891982	2.563853
C	0.835258	-1.963515	3.198408
H	-0.603097	-2.503291	1.626162
H	-1.235448	-2.664773	3.285605
H	0.783907	-1.824796	4.293313
H	1.331912	-2.941122	3.027824
N	-0.393467	0.119217	1.519378
H	-1.054781	-0.105243	3.483251
C	-2.695313	-0.625337	2.179075
H	-3.086448	0.403639	2.122134
H	-2.879088	-1.108264	1.207701
H	-3.246697	-1.170895	2.966701
H	2.009881	-1.066177	1.536724
C	2.272386	0.200144	3.265205
C	3.241022	1.014209	2.593964
C	1.965878	0.531715	4.624598
C	3.871892	2.073253	3.245931
H	3.487582	0.785020	1.551240
C	2.597206	1.598271	5.266329
H	1.222614	-0.055835	5.173221
C	3.556404	2.374379	4.586413
H	4.615108	2.672705	2.710821
H	2.343366	1.830799	6.307139
H	4.051086	3.209097	5.095181
H	-0.257804	1.108491	1.774194

13-TS'

SCF energy in CF_3CH_2OH: -4923.660593 a.u.

Free energy in CF_3CH_2OH: -4922.128649 a.u.

Rh	-0.440642	-0.018798	-3.062376
O	1.592137	-0.050478	-3.246592
O	-2.483823	0.079262	-2.922187
O	1.918059	-0.165852	-0.996474
O	-2.386706	0.068482	-0.646156
O	-0.550952	-2.085599	-3.034781
O	-0.369934	2.037436	-2.954444
O	-0.144181	1.990393	-0.671861
O	-0.448931	-2.156483	-0.745541
C	-0.240781	2.586909	-1.806665
C	-0.602277	-2.685284	-1.906964
C	2.333381	-0.063777	-2.196104
C	-3.016402	0.129588	-1.759161
Rh	-0.265125	-0.091617	-0.626807
C	-0.824333	-4.222576	-1.878203
C	-1.050744	-4.968980	-3.241233
N	-1.838365	-4.508275	-0.851046
C	0.236876	-4.832637	-4.090594
C	-1.264947	-6.471368	-2.931355
C	-2.268203	-4.446948	-4.035787
C	-3.035406	-3.780349	-0.655231

C	-1.590683	-5.404970	0.224394	H	1.822473	4.991038	-3.524017
H	0.438169	-3.784538	-4.360844	H	0.893403	3.676593	-4.293412
H	1.117828	-5.228568	-3.551037	O	2.583326	3.267204	-1.718097
H	-0.443684	-6.887422	-2.321189	C	2.834676	4.513040	0.387355
H	-2.212883	-6.646524	-2.392157	O	-0.488063	5.701655	0.763993
H	-3.204486	-4.547694	-3.460780	C	1.910803	5.271958	1.127963
H	-2.148388	-3.387999	-4.311103	C	4.148775	4.328758	0.807701
O	-3.465127	-2.906841	-1.405966	C	2.295796	5.880541	2.320514
C	-3.624291	-4.292974	0.619228	C	4.571556	4.943757	2.016814
O	-0.586756	-6.103403	0.339957	C	3.630326	5.710169	2.745238
C	-2.768225	-5.283555	1.131948	C	-4.556181	0.213816	-1.623961
C	-4.792913	-3.916345	1.276187	C	-5.421817	0.422853	-2.917051
C	-3.077327	-5.937776	2.321917	N	-4.852759	1.160945	-0.536851
C	-5.135659	-4.567310	2.491799	C	-5.252470	-0.816916	-3.829443
C	-4.267372	-5.571029	2.983793	C	-6.906248	0.499143	-2.481379
C	3.851620	0.180377	-2.388512	C	-5.060864	1.704127	-3.699398
C	4.455886	0.045471	-3.837879	C	-4.238518	2.426645	-0.373050
N	4.594957	-0.559828	-1.360303	C	-5.566114	0.775526	0.627278
C	3.909785	1.204268	-4.709222	H	-4.221677	-0.906578	-4.204839
C	5.992469	0.215232	-3.738404	H	-5.503984	-1.749162	-3.292020
C	4.142732	-1.310143	-4.509199	H	-7.204197	-0.383792	-1.887788
C	4.445932	-1.934560	-1.049322	H	-7.111809	1.401436	-1.878259
C	5.492868	0.081587	-0.470335	H	-5.202798	2.611599	-3.088817
H	2.820046	1.132643	-4.842958	H	-4.014915	1.685766	-4.043888
H	4.137546	2.186559	-4.256538	O	-3.492076	2.967279	-1.185723
H	6.268718	1.151053	-3.220034	C	-4.672099	2.921571	0.967623
H	6.468704	-0.627240	-3.205494	O	-6.108148	-0.317011	0.790581
H	4.539933	-2.158597	-3.927540	C	-5.483865	1.938488	1.560509
H	3.057653	-1.457718	-4.628905	C	-4.358048	4.111300	1.617004
O	3.682305	-2.718765	-1.606525	C	-6.018122	2.140269	2.831410
C	5.394156	-2.198847	0.078999	C	-4.883897	4.343774	2.915455
O	5.746073	1.286665	-0.466085	C	-5.711282	3.349571	3.490484
C	6.027672	-0.990942	0.416718	H	-4.842961	-0.771251	-1.205854
C	5.685876	-3.389132	0.737815	H	-1.177901	4.359447	-1.128822
C	6.982421	-0.951674	1.430479	H	3.983058	1.241167	-2.090516
C	6.660805	-3.384652	1.770997	H	0.103857	-4.645111	-1.443641
C	7.288320	-2.158093	2.093464	H	4.824288	3.705064	0.212367
C	-0.254991	4.133567	-1.698753	H	3.938772	6.190743	3.677984
C	-0.324668	4.987555	-3.014395	H	1.586334	6.472766	2.907988
N	0.829588	4.519848	-0.784331	H	8.042516	-2.134519	2.885051
C	-1.665637	4.686225	-3.727081	H	7.482090	-0.015637	1.700625
C	-0.322803	6.480757	-2.602963	H	5.163322	-4.307169	0.450685
C	0.852371	4.731368	-3.980471	H	-4.515683	-6.083074	3.917630
C	2.144839	3.999049	-0.833696	H	-2.415215	-6.707680	2.731394
C	0.596717	5.237657	0.417931	H	-5.414930	-3.114603	0.863694
H	-1.707268	3.647122	-4.087608	H	-6.649646	1.382554	3.306689
H	-2.525804	4.849154	-3.053372	H	-6.127545	3.511848	4.488795
H	-1.131152	6.708874	-1.884990	H	-3.697391	4.836004	1.129588
H	0.636491	6.778056	-2.142680	C	-4.526267	5.653872	3.645607

C	-2.985787	5.725425	3.833785
C	-4.995700	6.859994	2.787632
C	-5.192691	5.758064	5.035205
H	-2.626165	4.884142	4.453817
H	-2.441587	5.697552	2.874033
H	-2.714001	6.667034	4.346081
H	-6.090321	6.840285	2.638571
H	-4.734823	7.807932	3.293109
H	-4.516821	6.869172	1.793372
H	-4.904043	6.712329	5.510617
H	-6.295894	5.741576	4.968450
H	-4.872369	4.943108	5.709648
C	-6.425587	-4.155051	3.229686
C	-6.324923	-2.657549	3.630249
C	-7.640911	-4.353640	2.284229
C	-6.666129	-4.987141	4.509094
H	-5.464231	-2.488158	4.302763
H	-6.212739	-1.995721	2.754133
H	-7.242862	-2.352733	4.167082
H	-7.742475	-5.412019	1.983364
H	-8.572200	-4.052087	2.797972
H	-7.553102	-3.744915	1.368048
H	-7.605441	-4.658934	4.988654
H	-6.765261	-6.066001	4.289575
H	-5.854621	-4.855166	5.247861
C	6.995667	-4.701757	2.499943
C	5.723774	-5.210965	3.229772
C	7.454125	-5.760098	1.460251
C	8.121871	-4.532492	3.543133
H	5.390753	-4.491202	3.998243
H	4.879868	-5.364616	2.535738
H	5.934073	-6.175468	3.728181
H	8.360308	-5.424948	0.924314
H	7.689233	-6.713077	1.968886
H	6.673204	-5.967830	0.708558
H	8.325444	-5.505332	4.024809
H	9.064872	-4.186656	3.081701
H	7.842445	-3.821403	4.341591
C	6.029934	4.762361	2.484476
C	6.324379	3.248633	2.668178
C	6.982007	5.340560	1.402112
C	6.317887	5.481399	3.820578
H	5.664816	2.809065	3.438373
H	6.186263	2.680839	1.731625
H	7.371497	3.110004	2.996954
H	6.799947	6.419373	1.247476
H	8.034273	5.211501	1.716204
H	6.856210	4.830436	0.431668
H	7.370410	5.312118	4.109828
H	6.167969	6.573933	3.745183
H	5.683641	5.098781	4.641034
H	6.423544	0.249008	-4.755376
H	4.387357	1.170975	-5.705923
H	4.608162	-1.336703	-5.512247
H	-1.311781	-7.037603	-3.879141
H	0.126752	-5.415995	-5.023058
H	-2.377043	-5.039385	-4.963506
H	-5.932778	-0.728958	-4.696485
H	-7.551191	0.543961	-3.377595
H	-5.717529	1.785958	-4.585742
H	0.725341	5.358847	-4.882554
H	-1.777891	5.361242	-4.595515
H	-0.471972	7.110295	-3.498871
C	-0.110709	0.899722	2.287981
C	0.817754	0.717812	3.511012
C	2.195802	-0.941034	2.209415
C	2.237826	0.308675	3.043625
H	0.403239	-0.073180	4.167266
H	0.850197	1.650720	4.107364
H	2.673026	1.132764	2.450202
H	2.885519	0.171581	3.933754
N	0.050826	-0.232242	1.373804
H	-0.349917	-1.098983	1.770645
H	2.455487	-0.858697	1.150271
C	2.038756	-2.260100	2.745308
C	1.910596	-2.527664	4.146286
C	1.985692	-3.379981	1.853270
C	1.733951	-3.830803	4.616266
H	1.965779	-1.700548	4.862573
C	1.790528	-4.676885	2.330721
H	2.078340	-3.196251	0.776815
C	1.663786	-4.913014	3.715963
H	1.645001	-4.010124	5.694366
H	1.708561	-5.508586	1.623491
H	1.508912	-5.931397	4.089060
H	0.216045	1.796893	1.729055
C	-1.579718	1.090830	2.718637
H	-2.225902	1.216071	1.835840
H	-1.936693	0.211521	3.288254
H	-1.685807	1.983540	3.361971

15

SCF energy in CF_3CH_2OH: -4923.751392 a.u.

Free energy in CF_3CH_2OH: -4922.209620 a.u.

Rh	0.426656	0.168136	-3.130490
O	-1.632045	0.099436	-3.228080

O	2.469882	0.179223	-2.930658	C	-5.488501	2.099734	0.044576
O	-1.851189	0.085702	-0.948034	O	-5.564573	-1.439313	-0.186946
O	2.289166	0.119728	-0.645237	C	-6.014803	0.879790	0.502328
O	0.432556	2.228837	-3.042056	C	-5.895749	3.319760	0.574430
O	0.466590	-1.896736	-3.098233	C	-6.966322	0.857436	1.519269
O	0.201643	-1.929229	-0.821458	C	-6.874539	3.331602	1.603456
O	0.251872	2.207045	-0.758168	C	-7.385476	2.092294	2.055738
C	0.353629	-2.487144	-1.971439	C	0.477184	-4.030746	-1.902303
C	0.402120	2.790146	-1.895187	C	0.572040	-4.844667	-3.241766
C	-2.310546	0.007640	-2.149892	N	-0.551538	-4.517605	-0.970089
C	2.952269	0.140531	-1.747746	C	1.884830	-4.453172	-3.963841
Rh	0.205683	0.132416	-0.708472	C	0.654400	-6.347153	-2.875351
C	0.506881	4.336369	-1.801556	C	-0.631614	-4.620850	-4.182553
C	0.717780	5.151828	-3.126846	C	-1.897749	-4.084477	-0.960420
N	1.467105	4.658992	-0.732418	C	-0.232234	-5.254251	0.200336
C	-0.524767	4.945256	-4.027728	H	1.869874	-3.401505	-4.288277
C	0.797822	6.653420	-2.755298	H	2.763064	-4.597406	-3.308915
C	1.999801	4.759497	-3.893701	H	1.484347	-6.552896	-2.175540
C	2.719350	4.032153	-0.534591	H	-0.280962	-6.708474	-2.411609
C	1.119778	5.490050	0.368888	H	-1.581563	-4.928600	-3.713877
H	-0.627703	3.895998	-4.344631	H	-0.721451	-3.562727	-4.473756
H	-1.453450	5.244016	-3.506285	O	-2.416412	-3.364071	-1.810731
H	-0.078703	6.979362	-2.167442	C	-2.509112	-4.669196	0.270307
H	1.705721	6.883183	-2.169474	O	0.890967	-5.658374	0.495346
H	2.904932	4.917897	-3.283027	C	-1.514824	-5.390412	0.955108
H	1.978390	3.703932	-4.205432	C	-3.813773	-4.571061	0.745196
O	3.238036	3.220020	-1.297886	C	-1.817607	-6.049430	2.144674
C	3.239878	4.553920	0.766527	C	-4.154107	-5.240758	1.951003
O	0.048821	6.076611	0.497707	C	-3.142775	-5.969031	2.622359
C	2.292809	5.450779	1.291679	C	4.490059	0.184785	-1.557065
C	4.424690	4.256512	1.434803	C	5.415023	0.119652	-2.824739
C	2.524893	6.091515	2.506773	N	4.843013	-0.786452	-0.508737
C	4.690045	4.895599	2.675784	C	5.160912	1.380766	-3.686700
C	3.731320	5.807120	3.179522	C	6.885284	0.159947	-2.338678
C	-3.812658	-0.347680	-2.256973	C	5.202518	-1.150459	-3.676507
C	-4.481119	-0.345825	-3.684575	C	4.359777	-2.115073	-0.435687
N	-4.566442	0.406951	-1.248548	C	5.504486	-0.407365	0.686930
C	-3.845074	-1.476946	-4.530985	H	4.141140	1.388617	-4.100491
C	-5.983760	-0.677991	-3.507092	H	5.298610	2.304925	-3.096913
C	-4.349565	1.001171	-4.428917	H	7.076929	1.029019	-1.683839
C	-4.516341	1.810032	-1.056236	H	7.159921	-0.754381	-1.782775
C	-5.401961	-0.223477	-0.294177	H	5.424957	-2.068453	-3.106855
H	-2.783052	-1.278027	-4.738695	H	4.166364	-1.219134	-4.042623
H	-3.917868	-2.452511	-4.017842	O	3.673312	-2.671980	-1.289296
H	-6.131282	-1.617567	-2.945119	C	4.834817	-2.651735	0.875359
H	-6.526425	0.127161	-2.979917	O	5.930164	0.721388	0.930591
H	-4.832750	1.826332	-3.879703	C	5.535463	-1.631817	1.542063
H	-3.293528	1.269508	-4.588489	C	4.639561	-3.907066	1.442294
O	-3.806601	2.593152	-1.680159	C	6.075641	-1.859768	2.806014

C	5.176613	-4.169512	2.730615	H	-5.356936	5.638326	2.008737
C	5.891154	-3.135113	3.381180	H	-6.452220	6.413449	3.183986
H	4.673021	1.168822	-1.082416	H	-8.854942	5.018085	0.603144
H	1.428331	-4.205015	-1.360393	H	-8.304203	6.507995	1.427354
H	-3.859271	-1.394604	-1.893299	H	-7.255841	5.713541	0.221816
H	-0.462913	4.671598	-1.382032	H	-8.706784	5.507205	3.668146
H	-4.544844	-3.968289	0.196019	H	-9.315480	4.006618	2.927329
H	-3.387138	-6.491609	3.551387	H	-8.009546	3.940911	4.153182
H	-1.052752	-6.612321	2.689934	C	-5.600646	-5.153514	2.478463
H	-8.137352	2.080818	2.849792	C	-5.956036	-3.666867	2.754292
H	-7.380799	-0.087713	1.884863	C	-6.567508	-5.718952	1.402497
H	-5.462670	4.247939	0.186394	C	-5.803421	-5.955902	3.782609
H	3.920749	6.310727	4.131623	H	-5.288667	-3.239449	3.524786
H	1.793082	6.789926	2.926111	H	-5.876213	-3.041236	1.848436
H	5.118524	3.523466	1.009423	H	-6.995181	-3.595152	3.126652
H	6.621509	-1.073753	3.338200	H	-6.343247	-6.778351	1.182934
H	6.314155	-3.318884	4.372934	H	-7.610985	-5.656444	1.762585
H	4.058832	-4.660697	0.900143	H	-6.505303	-5.153580	0.456922
C	4.949424	-5.553768	3.370643	H	-6.853814	-5.863585	4.111686
C	3.423154	-5.783038	3.549963	H	-5.592959	-7.032226	3.644354
C	5.528636	-6.650816	2.436988	H	-5.165840	-5.579563	4.603387
C	5.628714	-5.685799	4.751691	H	-6.451627	-0.795726	-4.501161
H	2.988579	-5.023492	4.224999	H	-4.380581	-1.556439	-5.495215
H	2.874895	-5.739267	2.593124	H	-4.840397	0.919556	-5.417156
H	3.242791	-6.779022	3.995499	H	0.837456	7.258217	-3.679330
H	6.616698	-6.519944	2.296269	H	-0.432375	5.573568	-4.932503
H	5.357290	-7.650279	2.877227	H	2.088740	5.390340	-4.797879
H	5.053006	-6.639025	1.441189	H	5.879211	1.401950	-4.527152
H	5.443377	-6.696202	5.157447	H	7.559472	0.233224	-3.211167
H	6.723840	-5.549547	4.688864	H	5.880675	-1.122749	-4.550118
H	5.228281	-4.958806	5.481614	H	-0.495400	-5.224819	-5.099218
C	5.995122	4.569235	3.429487	H	2.016150	-5.092205	-4.856480
C	6.001830	3.060776	3.801062	H	0.823003	-6.941371	-3.791652
C	7.208726	4.877272	2.511497	C	0.737618	-0.406133	2.499919
C	6.149585	5.392916	4.727261	C	1.592801	0.863517	2.644316
H	5.149455	2.816017	4.460815	C	-0.755320	1.374088	2.010369
H	5.946949	2.408859	2.912141	C	0.568579	2.026784	2.538231
H	6.934026	2.814294	4.343106	H	2.322259	0.905384	1.817992
H	7.235555	5.945960	2.231873	H	2.148277	0.868610	3.597435
H	8.150283	4.636876	3.038546	H	0.392559	2.510652	3.512901
H	7.185534	4.281507	1.582997	H	0.916208	2.798331	1.834998
H	7.103847	5.130563	5.217955	N	-0.287088	0.048234	1.497172
H	6.167325	6.480052	4.528083	H	-1.070841	-0.617456	1.429165
H	5.339681	5.184140	5.449889	H	0.208554	-0.578743	3.462478
C	-7.348629	4.681630	2.179201	C	1.473922	-1.680049	2.104473
C	-6.130243	5.439819	2.770865	H	0.786841	-2.539248	2.014975
C	-7.975723	5.526943	1.037471	H	1.988410	-1.553732	1.140638
C	-8.404114	4.513115	3.293931	H	2.221613	-1.924593	2.879844
H	-5.660451	4.857424	3.583493	H	-1.150097	1.944381	1.153167

C	-1.851257	1.309805	3.083294
C	-2.335967	2.532178	3.600545
C	-2.409371	0.116262	3.579674
C	-3.327467	2.559441	4.590704
H	-1.927005	3.475686	3.218271
C	-3.405092	0.139258	4.572222
H	-2.070707	-0.856824	3.204560
C	-3.865753	1.359332	5.085773
H	-3.678709	3.522403	4.979459
H	-3.816931	-0.805947	4.944049
H	-4.638140	1.377016	5.862768

15'

SCF energy in CF_3CH_2OH: -4923.752458 a.u.

Free energy in CF_3CH_2OH: -4922.209815 a.u**.**

Rh	-0.350178	0.000429	-3.210089
O	1.708981	-0.080520	-3.309865
O	-2.390393	0.146699	-2.993802
O	1.893643	-0.170551	-1.028687
O	-2.227593	0.079829	-0.706901
O	-0.506020	-2.066636	-3.176927
O	-0.231199	2.054246	-3.099744
O	-0.034488	1.989783	-0.815787
O	-0.348518	-2.125332	-0.891813
C	-0.105614	2.595352	-1.949258
C	-0.530815	-2.661784	-2.049053
C	2.375877	-0.102528	-2.221141
C	-2.877232	0.184214	-1.813530
Rh	-0.159598	-0.074194	-0.783369
C	-0.753695	-4.196572	-1.992294
C	-0.997039	-4.970151	-3.335352
N	-1.753347	-4.465464	-0.943537
C	0.276440	-4.838973	-4.206743
C	-1.194106	-6.467330	-2.991124
C	-2.228881	-4.471654	-4.122749
C	-2.963570	-3.752683	-0.757590
C	-1.467165	-5.298695	0.170008
H	0.461555	-3.794412	-4.501424
H	1.169897	-5.213174	-3.672615
H	-0.357365	-6.864362	-2.388648
H	-2.130254	-6.638454	-2.430211
H	-3.158104	-4.574624	-3.536934
H	-2.122723	-3.414943	-4.412393
O	-3.416755	-2.909309	-1.527525
C	-3.528864	-4.234450	0.540464
O	-0.430280	-5.943984	0.317482
C	-2.642331	-5.182447	1.080629
C	-4.701906	-3.866956	1.194966
C	-2.925460	-5.804957	2.293996
C	-5.019053	-4.485945	2.434083
C	-4.121009	-5.449700	2.951809
C	3.911718	0.077456	-2.291876
C	4.613882	-0.009853	-3.698406
N	4.537279	-0.756585	-1.256883
C	4.149861	1.192690	-4.558267
C	6.140498	0.128240	-3.475915
C	4.332945	-1.329539	-4.450268
C	4.286403	-2.135537	-1.043474
C	5.363420	-0.212390	-0.243438
H	3.077549	1.130312	-4.797283
H	4.331787	2.151326	-4.039371
H	6.391086	1.044567	-2.911701
H	6.558146	-0.736521	-2.929779
H	4.688944	-2.208832	-3.888191
H	3.256611	-1.461446	-4.643151
O	3.542297	-2.841162	-1.717646
C	5.097897	-2.511725	0.156340
O	5.672610	0.975442	-0.143926
C	5.744518	-1.358563	0.633412
C	5.255816	-3.749761	0.770475
C	6.572423	-1.424932	1.751950
C	6.095287	-3.851286	1.911235
C	6.735703	-2.678604	2.376981
C	-0.094839	4.140182	-1.825911
C	-0.094845	5.008628	-3.132506
N	0.957654	4.498165	-0.860884
C	-1.418260	4.749074	-3.893371
C	-0.067585	6.497695	-2.707388
C	1.107669	4.727341	-4.059218
C	2.263483	3.949584	-0.855985
C	0.681753	5.192469	0.344200
H	-1.476466	3.712855	-4.259862
H	-2.296013	4.935089	-3.248402
H	-0.889296	6.738992	-2.009043
H	0.885991	6.767128	-2.218807
H	2.067409	4.958301	-3.566837
H	1.131881	3.673277	-4.376665
O	2.733271	3.228275	-1.732631
C	2.901995	4.421428	0.409392
O	-0.411006	5.666932	0.652767
C	1.959667	5.187931	1.117814
C	4.187684	4.196198	0.893036
C	2.298250	5.766431	2.339116
C	4.563796	4.779526	2.132769
C	3.606024	5.557979	2.826006
C	-4.411047	0.314441	-1.631005

C	-5.307298	0.550861	-2.898601	H	-4.406608	5.039278	5.713896
N	-4.649108	1.272825	-0.538137	C	-6.311525	-4.081037	3.171670
C	-5.197929	-0.690067	-3.818635	C	-6.224815	-2.578184	3.555312
C	-6.776438	0.666545	-2.421919	C	-7.529577	-4.304306	2.235574
C	-4.934588	1.824772	-3.687593	C	-6.537125	-4.901242	4.461606
C	-3.987191	2.515796	-0.386702	H	-5.368637	-2.395233	4.230037
C	-5.363723	0.919248	0.634250	H	-6.112616	-1.924132	2.673407
H	-4.182594	-0.802329	-4.228033	H	-7.147296	-2.274454	4.084859
H	-5.452951	-1.617751	-3.274933	H	-7.620274	-5.366864	1.946252
H	-7.083420	-0.210425	-1.824218	H	-8.461026	-4.008810	2.752315
H	-6.939764	1.571349	-1.809469	H	-7.456592	-3.704203	1.312428
H	-5.039739	2.734128	-3.072002	H	-7.481618	-4.583048	4.937701
H	-3.898629	1.780866	-4.058065	H	-6.617673	-5.984236	4.255257
O	-3.241468	3.032765	-1.214889	H	-5.728302	-4.745958	5.198727
C	-4.374975	3.025128	0.963072	C	6.281227	-5.223408	2.590043
O	-5.943917	-0.151962	0.809114	C	4.896590	-5.763472	3.038628
C	-5.222688	2.078892	1.565138	C	6.912708	-6.209152	1.569539
C	-3.994471	4.196226	1.611575	C	7.201370	-5.151075	3.828533
C	-5.727398	2.299471	2.844862	H	4.411723	-5.076557	3.754428
C	-4.491346	4.448206	2.918428	H	4.208680	-5.894043	2.185684
C	-5.355459	3.491153	3.502944	H	5.016252	-6.747814	3.527896
H	-4.721616	-0.658937	-1.203091	H	7.911006	-5.862666	1.246927
H	-1.036766	4.374399	-1.291236	H	7.027426	-7.208618	2.028078
H	4.072143	1.112471	-1.926657	H	6.286119	-6.323277	0.667861
H	0.180468	-4.609897	-1.561726	H	7.301770	-6.157935	4.271484
H	4.876197	3.562183	0.324442	H	8.217285	-4.801351	3.569314
H	3.878874	6.016674	3.780569	H	6.791351	-4.484629	4.608988
H	1.574126	6.365400	2.901277	C	5.989010	4.544993	2.673882
H	7.384751	-2.736040	3.255215	C	6.205921	3.022447	2.891677
H	7.080911	-0.533180	2.132945	C	7.019144	5.066270	1.635265
H	4.732117	-4.622583	0.367032	C	6.240516	5.271066	4.013586
H	-4.350010	-5.938097	3.903026	H	5.495326	2.628230	3.640911
H	-2.240959	-6.543633	2.723631	H	6.078694	2.443926	1.960200
H	-5.349404	-3.097856	0.760685	H	7.231007	2.841693	3.266225
H	-6.385572	1.569363	3.327201	H	6.892262	6.149536	1.458299
H	-5.750241	3.669467	4.507185	H	8.047097	4.897251	2.005459
H	-3.305219	4.889995	1.118226	H	6.923249	4.548297	0.665679
C	-4.071346	5.741912	3.645198	H	7.272251	5.069594	4.352683
C	-2.526279	5.759291	3.805871	H	6.131051	6.366948	3.918812
C	-4.512338	6.965765	2.796995	H	5.557251	4.920362	4.808538
C	-4.708343	5.867268	5.046695	H	6.649969	0.179254	-4.455159
H	-2.184740	4.902855	4.415556	H	4.718438	1.205457	-5.506557
H	-2.000062	5.721494	2.836231	H	4.859731	-1.311968	-5.422875
H	-2.215577	6.687938	4.320037	H	-1.254216	-7.054740	-3.925144
H	-5.609295	6.984445	2.666160	H	0.157851	-5.442753	-5.125052
H	-4.210266	7.902809	3.299946	H	-2.340810	-5.076901	-5.041799
H	-4.049339	6.959883	1.795301	H	-5.905114	-0.583342	-4.661781
H	-4.375655	6.808989	5.518270	H	-7.444019	0.734611	-3.299902
H	-5.812402	5.892302	5.000159	H	-5.611779	1.924887	-4.556509

H	1.029555	5.362460	-4.961571
H	-1.482542	5.430491	-4.761731
H	-0.177394	7.138949	-3.600703
C	-0.656971	0.880407	2.204099
C	0.405810	1.271150	3.255511
C	1.344540	-0.563953	1.981934
C	1.726312	0.771621	2.644276
H	0.197382	0.753927	4.211268
H	0.406423	2.356958	3.451883
H	2.066542	1.467523	1.857432
H	2.548480	0.668241	3.371704
N	-0.043901	-0.273019	1.424770
H	-0.626171	-1.113221	1.554605
H	1.998941	-0.771076	1.119831
C	1.322339	-1.804630	2.879121
C	1.583085	-1.777671	4.263579
C	1.029775	-3.050249	2.277383
C	1.542503	-2.957357	5.026585
H	1.825600	-0.832208	4.760984
C	0.980670	-4.228798	3.036691
H	0.838161	-3.094363	1.197794
C	1.236714	-4.184734	4.418112
H	1.748407	-2.912548	6.102553
H	0.743053	-5.175438	2.538752
H	1.200445	-5.102400	5.016521
H	-0.785746	1.706280	1.483406
C	-2.018113	0.494944	2.786487
H	-2.708788	0.173828	1.988886
H	-1.915962	-0.326259	3.521309
H	-2.472977	1.359912	3.300791

Rh2(OAc)4(singlet)

SCF energy in CF_3CH_2OH: -1135.335386 a.u.

Free energy in CF_3CH_2OH: -1135.184571 a.u**.**

Rh	-0.006259	-0.001823	-1.195059
O	1.427991	-1.473624	-1.148834
C	1.837849	-1.888753	-0.000776
O	1.428536	-1.473716	1.147583
O	1.463907	1.434066	-1.149855
C	1.887110	1.836053	-0.001872
O	1.464726	1.434805	1.146564
O	-1.441772	1.468318	-1.147989
C	-1.842686	1.891643	0.000249
O	-1.441295	1.468534	1.148475
O	-1.477468	-1.437048	-1.144244
C	-1.895190	-1.842571	0.004488
O	-1.475833	-1.435992	1.152168
Rh	-0.005889	-0.001676	1.195409
C	-2.859648	3.014324	0.000842
H	-2.328331	3.983211	0.017576
H	-3.474662	2.975112	-0.911192
H	-3.493785	2.956086	0.898797
C	3.008761	2.854327	-0.002128
H	3.978238	2.324673	0.027919
H	2.976100	3.460902	-0.919996
H	2.942811	3.496604	0.889568
C	-2.981313	-2.898721	-0.002028
H	-2.618803	-3.799086	-0.527154
H	-3.273447	-3.159870	1.025424
H	-3.858405	-2.524789	-0.557402
C	2.925760	-2.943052	0.000658
H	2.900533	-3.522147	-0.934829
H	3.910594	-2.447599	0.077037
H	2.811637	-3.607863	0.870934

^{1}1

SCF energy in CF_3CH_2OH: -2859.373926 a.u.

Free energy in CF_3CH_2OH: -2858.771149 a.u.

Rh	3.716722	1.281573	-1.277251
O	4.782346	-0.001179	-0.078634
C	4.128024	-0.792413	0.696187
O	2.850894	-0.846834	0.835227
O	3.775084	2.723562	0.179424
C	2.848485	2.715674	1.070425
O	1.865955	1.887903	1.143509
O	2.594570	2.539767	-2.449439
C	1.320470	2.530890	-2.295945
O	0.655829	1.776592	-1.491079
O	3.600875	-0.178256	-2.717548
C	2.610003	-0.995031	-2.674835
O	1.653564	-0.994057	-1.813724
Rh	1.677453	0.419104	-0.297119
C	0.512374	3.494143	-3.144400
H	-0.113466	4.129096	-2.494508
H	1.178653	4.123667	-3.752011
H	-0.166353	2.928105	-3.805841
C	2.920899	3.774301	2.153971
H	3.177403	3.297418	3.116399
H	3.685251	4.525888	1.907446
H	1.936327	4.255106	2.275431
C	2.575959	-2.089808	-3.724988
H	2.938771	-3.032802	-3.277722
H	1.542511	-2.256961	-4.068552
H	3.225535	-1.828908	-4.573819

C	4.944979	-1.783455	1.503621
H	5.170685	-2.662917	0.873831
H	5.901635	-1.330771	1.808499
H	4.379268	-2.124715	2.383477
N	-0.482373	-0.420556	0.644749
C	-1.600663	0.226985	-0.157569
C	-1.638505	-0.379701	-1.564394
H	-1.243048	1.267308	-0.233131
H	-0.635425	-0.435881	-2.010968
H	-2.078709	-1.391090	-1.553339
C	-0.351341	0.019143	2.028211
O	-0.767389	1.119440	2.363438
O	0.295743	-0.898039	2.751325
C	0.522293	-0.686348	4.217078
C	1.440964	0.525639	4.419138
C	-0.829185	-0.533936	4.930199
C	1.219441	-1.991441	4.621525
H	2.372716	0.395838	3.843544
H	0.949146	1.453994	4.092535
H	1.697165	0.610927	5.490779
H	-1.488591	-1.384786	4.690876
H	-0.660775	-0.516875	6.021836
H	-1.330857	0.401098	4.638077
H	1.433574	-1.977878	5.704570
H	0.583073	-2.861798	4.392233
H	2.169994	-2.107062	4.074108
C	-2.998158	0.243533	0.509850
H	-3.530505	-0.702511	0.297474
H	-2.899772	0.322216	1.603867
O	-0.287529	-1.814344	0.418679
H	-2.271470	0.259898	-2.202968
C	-3.831544	1.438130	0.004276
C	-5.242775	1.503019	0.635945
H	-3.938228	1.405216	-1.097635
H	-3.293353	2.378194	0.236128
H	-5.793457	0.572837	0.394152
H	-5.140206	1.531970	1.738110
C	-6.032790	2.707889	0.158472
C	-5.909535	3.954009	0.807776
C	-6.869960	2.625902	-0.973194
C	-6.598327	5.084112	0.340491
H	-5.266793	4.035700	1.693629
C	-7.561343	3.752957	-1.445287
H	-6.983303	1.663028	-1.487973
C	-7.426853	4.987556	-0.789655
H	-6.490838	6.041816	0.862973
H	-8.209818	3.665488	-2.324895
H	-7.967718	5.868128	-1.154434
S	-1.264298	-3.002658	1.295271
O	-2.256295	-2.310181	2.147601
O	-0.267184	-3.947963	1.831480
C	-2.114247	-3.805505	-0.069609
C	-1.371653	-4.578790	-0.979412
C	-3.505048	-3.669232	-0.188010
C	-2.044551	-5.207918	-2.032556
H	-0.289619	-4.684550	-0.859019
C	-4.158759	-4.316664	-1.247495
H	-4.059887	-3.078225	0.546088
C	-3.444834	-5.088831	-2.185645
H	-1.473146	-5.808282	-2.750419
H	-5.246480	-4.220589	-1.344860
C	-4.155911	-5.792503	-3.321058
H	-3.653804	-5.606670	-4.287551
H	-4.163918	-6.888102	-3.166998
H	-5.203836	-5.460756	-3.411115

^{1}1-TS

SCF energy in CF_3CH_2OH: -2859.322767 a.u.

Free energy in CF_3CH_2OH: -2858.718446 a.u**.**

Rh	0.625954	-3.803848	-0.843678
O	-1.381639	-4.078046	-0.617113
C	-2.080401	-3.060608	-0.246975
O	-1.627720	-1.884269	0.010024
O	0.925227	-4.320708	1.108374
C	0.901189	-3.398281	1.998557
O	0.705278	-2.141854	1.780156
O	2.646901	-3.483842	-1.058157
C	3.124358	-2.327899	-0.783271
O	2.450253	-1.300364	-0.384202
O	0.318614	-3.259061	-2.789825
C	0.151028	-2.013136	-3.040624
O	0.166291	-1.057266	-2.174769
Rh	0.387401	-1.475005	-0.155092
C	4.620484	-2.132552	-0.924562
H	5.083685	-3.033101	-1.353108
H	4.827564	-1.259494	-1.565809
H	5.060952	-1.927775	0.066782
C	1.099373	-3.812465	3.441168
H	1.715843	-3.070656	3.972983
H	0.116735	-3.855375	3.943913
H	1.565679	-4.807757	3.488484
C	-0.111690	-1.609752	-4.475435
H	0.130432	-2.440185	-5.154807
H	-1.179583	-1.349922	-4.584797
H	0.477326	-0.715361	-4.735105
C	-3.570154	-3.248808	-0.077050

H	-3.893745	-4.179632	-0.566440
H	-3.805660	-3.304254	1.000698
H	-4.098469	-2.372062	-0.486483
N	0.092130	0.411582	0.208705
C	0.951136	1.348811	-0.472943
C	1.921008	1.952738	0.621146
C	3.110731	2.698271	-0.004436
H	1.317354	2.611818	1.266489
H	2.296974	1.120822	1.244156
C	4.069461	3.246043	1.085331
H	3.674527	2.021395	-0.675561
H	2.760884	3.543052	-0.626374
H	3.502211	3.922804	1.752798
H	4.420917	2.403831	1.712181
C	-1.257928	1.142956	1.229572
O	-0.959855	2.298750	1.563095
O	-1.584982	0.126682	2.074584
C	-1.471978	0.321378	3.543808
C	-0.003628	0.548515	3.937599
C	-2.382310	1.461770	4.028939
C	-1.981561	-1.027308	4.074151
H	0.628533	-0.255216	3.522837
H	0.355383	1.520296	3.564518
H	0.091514	0.542154	5.039102
H	-3.410348	1.311197	3.662784
H	-2.393589	1.468125	5.134674
H	-2.018747	2.437676	3.674478
H	-1.942278	-1.040266	5.177742
H	-3.023880	-1.193228	3.753923
H	-1.358429	-1.849146	3.683376
C	5.257859	3.979986	0.492855
C	6.465152	3.303546	0.221606
C	5.170322	5.349034	0.163930
C	7.553784	3.972530	-0.359400
H	6.553491	2.240241	0.479021
C	6.255379	6.022585	-0.417754
H	4.240819	5.893246	0.374445
C	7.451833	5.335609	-0.682116
H	8.485769	3.429575	-0.554961
H	6.168529	7.088129	-0.659737
H	8.301552	5.860927	-1.132452
O	-2.162716	1.006381	-0.016253
H	1.588668	0.778006	-1.175926
C	0.196473	2.441089	-1.270185
H	-0.349308	3.116746	-0.597025
H	0.931374	3.013600	-1.863175
H	-0.519920	1.969671	-1.959853
S	-3.813255	0.947260	0.018842
O	-4.232245	-0.019406	-1.023409
O	-4.324982	0.803647	1.399013
C	-4.206388	2.603336	-0.582092
C	-3.584287	3.722862	-0.005139
C	-5.189403	2.743344	-1.571596
C	-3.964850	4.999945	-0.435395
H	-2.794356	3.587830	0.743150
C	-5.555994	4.032889	-1.986372
H	-5.645869	1.852840	-2.013651
C	-4.957202	5.178228	-1.425075
H	-3.476481	5.879665	0.001550
H	-6.320016	4.150181	-2.764424
C	-5.373213	6.568099	-1.858256
H	-6.053267	7.029566	-1.116637
H	-4.501571	7.239316	-1.958027
H	-5.903892	6.550191	-2.825532

^{1}2

SCF energy in CF_3CH_2OH: -1618.198363 a.u.

Free energy in CF_3CH_2OH: -1617.836607 a.u.

Rh	2.448469	-1.186803	0.626087
O	0.999332	-1.742773	1.968357
O	3.852482	-0.588963	-0.742677
O	-0.473921	-0.209437	1.105096
O	2.389241	0.913693	-1.676457
O	1.768332	-2.584500	-0.717150
O	3.069070	0.279503	1.929516
O	1.602722	1.805194	1.034683
O	0.273928	-1.093334	-1.626368
C	2.531618	1.438397	1.855065
C	0.841473	-2.246951	-1.537225
C	-0.129337	-1.138793	1.933436
C	3.521418	0.302462	-1.603086
Rh	0.870693	0.427049	-0.337640
C	-0.975874	2.645809	-0.423039
C	-2.474398	2.740466	-0.836587
C	-4.784582	1.631742	-0.840188
C	-3.300186	1.513806	-0.420145
H	-2.519937	2.878170	-1.934187
H	-2.892907	3.656633	-0.371726
H	-2.858979	0.603361	-0.868472
H	-3.240419	1.377816	0.677155
N	-0.330843	1.627079	-1.184901
H	-4.837562	1.732984	-1.942217
H	-0.898584	2.495012	0.678288
H	-5.207935	2.564996	-0.419025
C	-5.620749	0.447191	-0.391888
C	-6.380808	0.502243	0.794100

C	-5.629811	-0.751927	-1.135301
C	-7.127795	-0.604978	1.227282
H	-6.390904	1.429519	1.381285
C	-6.373792	-1.862056	-0.706676
H	-5.050355	-0.810899	-2.065551
C	-7.126132	-1.792429	0.477759
H	-7.717001	-0.537309	2.149322
H	-6.371630	-2.782081	-1.302808
H	-7.712182	-2.656368	0.811180
C	3.039411	2.508845	2.801911
H	2.195651	3.083218	3.217225
H	3.628291	2.053094	3.611438
H	3.681563	3.213715	2.244122
C	4.544947	0.662847	-2.661706
H	4.325630	0.093194	-3.582662
H	4.485215	1.734941	-2.905877
H	5.556221	0.398861	-2.317438
C	0.335642	-3.310306	-2.493290
H	-0.667640	-3.641374	-2.171223
H	0.237875	-2.891620	-3.507962
H	1.015986	-4.174643	-2.497867
C	-1.177665	-1.537674	2.952646
H	-1.456009	-0.661145	3.562551
H	-2.089379	-1.880757	2.434683
H	-0.792577	-2.336276	3.603171
C	-0.234449	3.974477	-0.787087
H	0.823932	3.913984	-0.490922
H	-0.297171	4.163095	-1.871738
H	-0.718687	4.805163	-0.242433

^{1}3

SCF energy in CF_3CH_2OH: -1618.201157 a.u.

Free energy in CF_3CH_2OH: -1617.837284 a.u**.**

Rh	2.224489	-1.310689	0.432672
O	0.827888	-1.924468	1.806767
O	3.579443	-0.661907	-0.957778
O	-0.625399	-0.262696	1.181787
O	2.145935	0.998364	-1.633171
O	1.385043	-2.539204	-0.982697
O	3.005055	-0.001987	1.819909
O	1.551557	1.659715	1.183505
O	-0.092516	-0.905435	-1.643324
C	2.514192	1.176422	1.898683
C	0.428435	-2.083371	-1.706662
C	-0.270550	-1.274926	1.904316
C	3.247478	0.333103	-1.695573
Rh	0.668896	0.454768	-0.263684
C	-0.832130	2.912039	-0.075561
C	-2.309822	3.357790	-0.298498
C	-3.548746	1.168573	-0.890191
C	-3.370301	2.324927	0.119361
H	-2.440031	3.630880	-1.363683
H	-2.441498	4.283927	0.295492
H	-3.118271	1.909498	1.115061
H	-4.341477	2.844360	0.240890
N	-0.472630	1.828785	-0.929207
H	-2.578433	0.654007	-1.032107
H	-0.674871	2.695799	1.005989
H	-3.814645	1.601140	-1.875304
C	-4.612596	0.176807	-0.457841
C	-5.982464	0.480648	-0.607488
C	-4.263802	-1.055349	0.132184
C	-6.973737	-0.414018	-0.176266
H	-6.273730	1.430908	-1.073608
C	-5.252130	-1.956207	0.562570
H	-3.201620	-1.304903	0.244754
C	-6.611391	-1.637391	0.411951
H	-8.032030	-0.157993	-0.304785
H	-4.960056	-2.913076	1.011503
H	-7.384095	-2.339476	0.745265
C	3.110926	2.117158	2.928274
H	2.321187	2.477422	3.609214
H	3.895208	1.604048	3.503526
H	3.538634	2.999694	2.422146
C	4.231533	0.774862	-2.760901
H	3.808297	0.565250	-3.758846
H	4.397434	1.862829	-2.694519
H	5.184005	0.236881	-2.646660
C	-0.157795	-3.008193	-2.756246
H	-1.250861	-3.076831	-2.626266
H	0.027652	-2.588576	-3.760199
H	0.295260	-4.007611	-2.683370
C	-1.246854	-1.700874	2.982015
H	-2.282366	-1.487863	2.674663
H	-1.119216	-2.771103	3.205398
H	-1.038085	-1.127976	3.903726
C	0.123156	4.088123	-0.475319
H	1.171680	3.803176	-0.302885
H	-0.012955	4.346230	-1.538632
H	-0.125506	4.964512	0.150372

^{1}3'

SCF energy in CF_3CH_2OH: -1618.198647 a.u.

Free energy in CF_3CH_2OH: -1617.834731 a.u**.**

Rh	2.605487	-0.756397	0.556850
O	2.261497	0.200162	2.343949
O	2.875503	-1.682320	-1.250740
O	0.323716	1.147935	1.555440
O	0.914823	-0.798568	-2.059610
O	1.543473	-2.380167	1.222949
O	3.598170	0.903949	-0.138623
O	1.650544	1.826774	-0.930826
O	-0.426995	-1.490728	0.448379
C	2.924578	1.827703	-0.713149
C	0.277970	-2.408767	1.017094
C	1.220657	0.935094	2.462814
C	1.985098	-1.509494	-2.158500
Rh	0.514677	0.214026	-0.282128
C	-1.439427	2.250701	-0.891305
C	-2.934743	2.493508	-0.510611
C	-3.403787	0.580051	1.192586
C	-3.305545	2.103814	0.930286
H	-3.576817	1.954908	-1.232317
H	-3.117321	3.576817	-0.654605
H	-2.563020	2.538862	1.628012
H	-4.280206	2.570685	1.175737
N	-1.135728	0.862061	-0.979982
H	-2.449476	0.101527	0.899623
H	-3.515351	0.425469	2.283764
C	-4.553264	-0.097098	0.466753
C	-5.858126	-0.069719	1.003765
C	-4.349787	-0.754145	-0.765531
C	-6.930380	-0.676145	0.331356
H	-6.032366	0.427476	1.967191
C	-5.421314	-1.361438	-1.441432
H	-3.337758	-0.784073	-1.187443
C	-6.714901	-1.324520	-0.896499
H	-7.935105	-0.647888	0.769518
H	-5.242451	-1.869507	-2.396582
H	-7.550121	-1.802248	-1.421614
H	-0.781890	2.803758	-0.180678
C	-1.182950	2.813706	-2.332223
H	-0.132268	2.662633	-2.621450
H	-1.838982	2.308741	-3.060359
H	-1.408596	3.895562	-2.324348
C	2.206922	-2.191886	-3.494511
H	1.290715	-2.721536	-3.803269
H	2.424165	-1.430148	-4.263865
H	3.050447	-2.894679	-3.429266
C	3.675044	3.061964	-1.174597
H	3.427731	3.910034	-0.511561
H	4.759649	2.882820	-1.140613
H	3.364671	3.336959	-2.195840
C	0.990084	1.618780	3.796136
H	0.742604	2.681681	3.640226
H	0.130407	1.148605	4.305402
H	1.883123	1.525090	4.431085
C	-0.472435	-3.651124	1.454071
H	0.094883	-4.184330	2.231700
H	-1.477069	-3.385727	1.818322
H	-0.594919	-4.321428	0.584314

^{1}2-TS

SCF energy in CF_3CH_2OH: -1618.189605 a.u.

Free energy in CF_3CH_2OH: -1617.827406 a.u**.**

Rh	1.885388	-1.423709	0.464949
O	0.945807	-1.326341	2.294574
O	2.772739	-1.443317	-1.382452
O	-0.380774	0.424766	1.624587
O	1.467726	0.313911	-2.087866
O	0.437294	-2.703429	-0.234258
O	3.283567	-0.075006	1.126755
O	1.959195	1.692700	0.492364
O	-0.869597	-0.959105	-0.958715
C	3.023151	1.173694	1.005545
C	-0.597109	-2.211614	-0.811134
C	0.040969	-0.442201	2.485458
C	2.380692	-0.579669	-2.248211
Rh	0.472262	0.441478	-0.261648
C	-0.639441	3.168042	-0.239286
C	-2.032240	3.853235	-0.272303
C	-3.169341	1.680015	-0.738560
C	-3.122207	2.879110	0.195437
H	-2.247415	4.183431	-1.308055
H	-2.002801	4.757889	0.362928
H	-2.919586	2.560880	1.235128
H	-4.109988	3.385067	0.204034
N	-0.645238	1.914003	-0.980571
H	-1.895859	1.509821	-0.992878
H	-0.345441	3.017315	0.825045
H	-3.445603	1.975999	-1.768379
C	-3.825575	0.419643	-0.334505
C	-4.555819	-0.324236	-1.296533
C	-3.771753	-0.081400	0.990819
C	-5.224397	-1.504381	-0.947617
H	-4.604326	0.045752	-2.327902
C	-4.436203	-1.263720	1.338680
H	-3.181062	0.451291	1.742721
C	-5.169604	-1.980131	0.374729
H	-5.794644	-2.052171	-1.706556

H	-4.384835	-1.633084	2.369488
H	-5.692353	-2.902156	0.652506
C	4.065584	2.155698	1.508497
H	4.437615	2.765413	0.666844
H	3.609496	2.845381	2.238888
H	4.904927	1.618758	1.973898
C	3.071040	-0.588719	-3.599878
H	2.321843	-0.535896	-4.406710
H	3.715373	0.304058	-3.687146
H	3.688409	-1.492457	-3.709555
C	-1.596895	-3.185471	-1.401728
H	-1.383249	-4.207047	-1.054027
H	-2.622318	-2.889213	-1.127509
H	-1.523571	-3.156294	-2.503648
C	-0.624605	-0.410245	3.848879
H	-0.693935	0.626735	4.216572
H	-1.652279	-0.806573	3.765706
H	-0.060353	-1.028982	4.562024
C	0.413824	4.092500	-0.909286
H	1.410555	3.629774	-0.872578
H	0.140499	4.278683	-1.962245
H	0.445246	5.055675	-0.367099

^{1}2-TS'

SCF energy in CF_3CH_2OH: -1618.186690 a.u.

Free energy in CF_3CH_2OH: -1617.824817 a.u.

Rh	-2.566878	-0.951347	-0.192201
O	-1.477568	-2.425545	-1.120247
O	-3.575984	0.565265	0.753981
O	0.489512	-1.277841	-0.829909
O	-1.629206	1.747990	1.040517
O	-2.769412	0.045884	-1.985870
O	-2.280695	-1.899849	1.604611
O	-0.298444	-0.780629	1.932465
O	-0.806582	1.202209	-1.683689
C	-1.217697	-1.616308	2.267386
C	-1.876728	0.891533	-2.339311
C	-0.210296	-2.283951	-1.236815
C	-2.903347	1.576901	1.158269
Rh	-0.467689	0.276569	0.141199
C	1.245645	2.651863	0.429337
C	1.937616	2.941187	-0.950471
H	0.211989	3.050380	0.341091
C	3.209236	0.773898	-0.788194
C	3.320189	2.279491	-1.030142
H	1.281271	2.543533	-1.744048
H	2.009857	4.036641	-1.088669
H	2.695386	0.264904	-1.621787
H	4.014387	2.745863	-0.307571
H	3.753754	2.461339	-2.035075
N	1.160361	1.222860	0.686813
H	2.356433	0.711809	0.101461
C	1.950667	3.358461	1.609990
H	2.979915	2.984400	1.749923
H	1.397779	3.167675	2.544831
H	1.991820	4.451598	1.442663
C	4.393217	0.002731	-0.314476
C	4.635263	-1.297932	-0.820046
C	5.281234	0.508204	0.666771
C	5.731770	-2.053303	-0.384773
H	3.949730	-1.708992	-1.570548
C	6.376333	-0.247114	1.105523
H	5.106389	1.500354	1.098181
C	6.609578	-1.529972	0.579957
H	5.903634	-3.053225	-0.799407
H	7.050008	0.164820	1.865592
H	7.466686	-2.119259	0.924494
C	-1.027252	-2.316894	3.600362
H	0.022346	-2.631275	3.716528
H	-1.700007	-3.184004	3.677061
H	-1.256613	-1.610886	4.418401
C	-3.661325	2.682008	1.868796
H	-3.311138	3.668400	1.524028
H	-3.465271	2.618566	2.954069
H	-4.742198	2.576641	1.693769
C	-2.085503	1.624004	-3.651970
H	-2.917032	1.173174	-4.213072
H	-1.161758	1.596086	-4.253419
H	-2.317334	2.684555	-3.448735
C	0.560310	-3.396770	-1.921354
H	-0.120653	-4.209791	-2.212168
H	1.337370	-3.784577	-1.240772
H	1.069794	-3.001825	-2.817333

Rh_2(S-*tert*PTTL)$_4$(singlet)

SCF energy in CF_3CH_2OH: -4440.780450 a.u.

Free energy in CF_3CH_2OH: -4439.466314 a.u.

Rh	0.000049	-0.000062	-0.805563
O	-1.915528	0.730369	-0.853436
C	-2.468847	0.923558	-1.997836
O	-1.925763	0.725384	-3.143126
O	0.756095	1.903199	-0.852298
C	0.987196	2.442951	-1.996211
O	0.739899	1.922811	-3.142224

O	1.915621	-0.730497	-0.853447	H	0.923881	5.432390	-4.970192
C	2.468890	-0.923714	-1.997872	H	0.225251	3.892356	-4.389217
O	1.925760	-0.725544	-3.143137	H	2.732242	6.581280	-3.773005
O	-0.756019	-1.903306	-0.852211	H	1.865601	6.559540	-2.207158
C	-0.987138	-2.443085	-1.996111	H	3.518508	5.891333	-2.328533
O	-0.739865	-1.922977	-3.142138	C	4.664228	-1.817342	-3.255706
Rh	0.000005	-0.000067	-3.192535	C	3.946581	-2.985106	-3.966264
C	3.951383	-1.355731	-1.932036	C	4.767617	-0.602224	-4.210962
H	4.478103	-0.440884	-1.591748	C	6.102078	-2.257223	-2.884868
C	1.576345	3.872611	-1.910725	H	3.878221	-3.877469	-3.322387
H	0.777523	4.480301	-1.438897	H	2.924642	-2.705687	-4.268104
C	-1.576296	-3.872734	-1.910578	H	4.512720	-3.262558	-4.875156
H	-0.777473	-4.480441	-1.438778	H	5.270165	0.251770	-3.721452
C	-3.951360	1.355501	-1.931937	H	5.362401	-0.883072	-5.099762
H	-4.478003	0.440670	-1.591488	H	3.775668	-0.267070	-4.550555
C	-1.969082	-4.608264	-3.240494	H	6.669321	-2.475448	-3.807713
C	-3.009284	-3.839387	-4.083833	H	6.640209	-1.468475	-2.329199
C	-0.681231	-4.841826	-4.067772	H	6.104613	-3.173047	-2.267517
C	-2.553574	-5.989883	-2.856654	C	-3.620198	-2.835397	-0.766705
H	-3.942533	-3.666215	-3.522149	C	-2.594215	-4.677528	0.262150
H	-2.622868	-2.861100	-4.409643	C	-4.308932	-3.090486	0.530273
H	-3.259766	-4.432436	-4.983327	C	-3.710380	-4.207307	1.139242
H	0.071182	-5.407832	-3.487762	C	-5.351004	-2.409200	1.156483
H	-0.923974	-5.432422	-4.970140	C	-4.139792	-4.685582	2.373392
H	-0.225369	-3.892401	-4.389134	C	-5.786375	-2.893991	2.407666
H	-2.732105	-6.581531	-3.772726	H	-5.795842	-1.514816	0.707549
H	-1.865406	-6.559654	-2.206919	C	-5.208658	-4.023939	3.034076
H	-3.518375	-5.891574	-2.328256	H	-3.644431	-5.556147	2.816370
C	-4.664329	1.816905	-3.255609	C	-4.969093	2.022121	0.281580
C	-3.946842	2.984692	-3.966295	C	-3.260451	3.401618	-0.546522
C	-4.767640	0.601694	-4.210750	C	-4.723016	3.113266	1.273714
C	-6.102213	2.256666	-2.884765	C	-3.695476	3.934352	0.778735
H	-3.878595	3.877134	-3.322512	C	-5.328244	3.355952	2.502980
H	-2.924873	2.705390	-4.268129	C	-3.246535	5.028618	1.514788
H	-4.513038	3.261985	-4.875201	C	-4.896236	4.465379	3.276704
H	-5.270047	-0.252313	-3.721116	H	-6.122490	2.688776	2.854421
H	-5.362531	0.882395	-5.099525	C	-3.859593	5.278533	2.760048
H	-3.775682	0.266621	-4.550393	H	-2.440129	5.668124	1.141243
H	-6.669490	2.474772	-3.807617	C	2.594329	4.677438	0.261959
H	-6.640251	1.467903	-2.329030	C	3.620300	2.835303	-0.766900
H	-6.104833	3.172536	-2.267484	C	3.710524	4.207242	1.139024
C	1.969067	4.608106	-3.240664	C	4.309064	3.090412	0.530061
C	3.009148	3.839108	-4.084039	C	4.139953	4.685538	2.373160
C	0.681177	4.841748	-4.067847	C	5.351151	2.409140	1.156259
C	2.553694	5.989689	-2.856900	C	5.208835	4.023907	3.033834
H	3.942457	3.665997	-3.522435	H	3.644590	5.556104	2.816131
H	2.622676	2.860795	-4.409703	C	5.786544	2.893955	2.407426
H	3.259562	4.432047	-4.983626	H	5.795973	1.514740	0.707341
H	-0.071181	5.407742	-3.487751	C	4.969145	-2.022092	0.281552

C	3.260470	-3.401656	-0.546366
C	4.722971	-3.113041	1.273878
C	3.695429	-3.934186	0.778993
C	5.328096	-3.355512	2.503234
C	3.246382	-5.028285	1.515228
C	4.895994	-4.464778	3.277137
H	6.122333	-2.688302	2.854629
C	3.859349	-5.277988	2.760579
H	2.439977	-5.667826	1.141743
N	-2.636086	-3.846943	-0.890497
N	-4.101254	2.287069	-0.806087
N	4.101300	-2.287164	-0.806080
N	2.636174	3.846838	-0.890677
O	-1.776840	-5.571882	0.457748
O	-3.820336	-1.941482	-1.587394
O	-5.747414	1.073306	0.357281
O	-2.365973	3.804255	-1.284899
O	3.820405	1.941367	-1.587571
O	1.776959	5.571796	0.457562
O	5.747449	-1.073257	0.357156
O	2.365936	-3.804322	-1.284659
H	-3.509870	6.135418	3.342596
H	6.601375	2.362181	2.906724
H	3.509544	-6.134731	3.343285
H	-6.601196	-2.362209	2.906971
C	5.692640	4.549887	4.400688
C	6.202872	6.006392	4.230756
C	4.508491	4.532154	5.404684
C	6.839705	3.699179	4.990071
H	7.054395	6.048576	3.528135
H	5.414172	6.676214	3.845805
H	6.540562	6.407679	5.204131
H	4.125901	3.505753	5.548178
H	4.837447	4.916931	6.387612
H	3.667628	5.160721	5.063181
H	7.144541	4.117254	5.966071
H	6.531248	2.651597	5.159626
H	7.731141	3.697407	4.337066
C	-5.559616	4.739545	4.642035
C	-7.080971	4.969866	4.433539
C	-5.346361	3.510471	5.566443
C	-4.973683	5.983108	5.346291
H	-7.264363	5.845006	3.784738
H	-7.571375	4.096555	3.969013
H	-7.573560	5.154056	5.406032
H	-4.271008	3.329032	5.743058
H	-5.831540	3.682509	6.544944
H	-5.777406	2.590316	5.134758
H	-5.483650	6.133710	6.314566
H	-3.894431	5.869844	5.554730
H	-5.118225	6.902066	4.749754
C	-5.692444	-4.549923	4.400936
C	-6.202723	-6.006409	4.230994
C	-4.508266	-4.532239	5.404900
C	-6.839468	-3.699191	4.990365
H	-7.054269	-6.048552	3.528399
H	-5.414057	-6.676248	3.846004
H	-6.540395	-6.407704	5.204372
H	-4.125658	-3.505848	5.548413
H	-4.837207	-4.917043	6.387822
H	-3.667423	-5.160809	5.063352
H	-7.144297	-4.117280	5.966361
H	-6.530972	-2.651625	5.159938
H	-7.730919	-3.697376	4.337380
C	5.559291	-4.738717	4.642559
C	7.080552	-4.969707	4.434063
C	5.346566	-3.509277	5.566583
C	4.972898	-5.981814	5.347253
H	7.263562	-5.845160	3.785577
H	7.571252	-4.096755	3.969175
H	7.573131	-5.153728	5.406594
H	4.271292	-3.327277	5.743105
H	5.831623	-3.681266	6.545151
H	5.778065	-2.589437	5.134679
H	5.482730	-6.132193	6.315632
H	3.893660	-5.868120	5.555536
H	5.117211	-6.901056	4.751099

^{1}12

SCF energy in CF_3CH_2OH: -4923.652050 a.u.

Free energy in CF_3CH_2OH: -4922.119263 a.u**.**

Rh	0.337129	-0.143316	-0.774877
O	2.344897	0.353209	-0.619313
C	3.088771	0.310124	-1.667724
O	2.723244	0.036559	-2.860818
O	0.815069	-2.150221	-0.582980
C	1.163079	-2.846421	-1.610160
O	1.236726	-2.427163	-2.812196
O	-1.632905	-0.706791	-1.102251
C	-1.970664	-1.063906	-2.295860
O	-1.238406	-1.016110	-3.338556
O	-0.086291	1.822860	-1.278203
C	0.034711	2.226626	-2.494101
O	0.306510	1.499400	-3.506916
Rh	0.749383	-0.471390	-3.173613
C	-3.376633	-1.702330	-2.395210

H	-3.247895	-2.690235	-1.906614	C	-5.397546	-2.560147	-3.634907
C	1.583353	-4.295431	-1.266257	H	-4.686907	0.051238	-4.282252
H	2.503112	-4.174666	-0.659276	H	-3.048704	-0.299906	-4.894232
C	-0.233964	3.741650	-2.673882	H	-4.476316	-1.011019	-5.702165
H	-1.286998	3.887479	-2.359113	H	-3.020699	-3.976923	-3.883812
C	4.563715	0.688867	-1.382135	H	-3.592274	-3.371305	-5.465845
H	4.517564	1.754346	-1.081841	H	-2.097474	-2.710391	-4.740379
C	-0.114457	4.352961	-4.114273	H	-5.800640	-2.870295	-4.615800
C	1.283412	4.176997	-4.746461	H	-5.399259	-3.442108	-2.969516
C	-1.192127	3.698193	-5.013168	H	-6.090729	-1.810767	-3.213316
C	-0.429899	5.865584	-4.007177	C	1.875010	4.195251	-1.280033
H	2.068316	4.662604	-4.142445	C	-0.113876	5.276820	-0.674560
H	1.548154	3.114278	-4.858407	C	2.127461	4.987197	-0.039088
H	1.289719	4.645627	-5.748243	C	0.936735	5.638550	0.319265
H	-2.204140	3.824025	-4.584744	C	3.292619	5.099420	0.720743
H	-1.187045	4.183000	-6.006450	C	0.879527	6.430677	1.467727
H	-1.007500	2.622003	-5.155394	C	3.268658	5.903250	1.886366
H	-0.453547	6.308184	-5.019452	H	4.189511	4.550632	0.421555
H	-1.408515	6.048576	-3.528443	C	2.053784	6.551443	2.231652
H	0.340088	6.403080	-3.425769	H	-0.049785	6.924049	1.769751
C	5.610220	0.597889	-2.547424	H	2.019251	7.166920	3.137272
C	5.730008	-0.814721	-3.159409	C	5.373351	0.697368	1.012533
C	5.217223	1.616939	-3.645039	C	4.688003	-1.365992	0.142216
C	6.985901	1.016535	-1.971721	C	5.469878	-0.324512	2.096492
H	6.046176	-1.560642	-2.410751	C	5.047805	-1.558326	1.578948
H	4.773596	-1.148828	-3.591282	C	5.853777	-0.213310	3.433830
H	6.489425	-0.800006	-3.963603	C	4.987911	-2.712088	2.361812
H	5.114959	2.635761	-3.229752	C	5.799914	-1.374118	4.225657
H	6.004118	1.641506	-4.421240	H	6.179696	0.745149	3.850887
H	4.264092	1.347499	-4.125159	C	5.371557	-2.630517	3.722041
H	7.729202	1.056952	-2.788470	H	4.629507	-3.646216	1.920668
H	6.944036	2.012371	-1.494994	H	6.096107	-1.297526	5.277734
H	7.353203	0.294253	-1.221164	C	0.963780	-5.342246	0.958898
C	1.946815	-5.266252	-2.446726	C	-0.804744	-4.715966	-0.449296
C	0.802067	-5.451366	-3.466916	C	-0.321524	-5.662226	1.647593
C	3.209494	-4.723319	-3.160160	C	-1.382695	-5.265873	0.813565
C	2.298094	-6.643481	-1.831321	C	-0.578845	-6.215328	2.899972
H	-0.104522	-5.866487	-2.995293	C	-2.714030	-5.391884	1.199359
H	0.530501	-4.499212	-3.949067	C	-1.926642	-6.362508	3.289389
H	1.127592	-6.158130	-4.252824	H	0.238148	-6.524348	3.560291
H	4.043659	-4.581605	-2.449398	C	-3.007103	-5.959282	2.468815
H	3.536152	-5.447745	-3.928706	H	-3.506732	-5.033760	0.533966
H	3.014417	-3.759409	-3.654241	H	-2.133677	-6.801313	4.269443
H	2.664934	-7.316782	-2.626993	C	-4.977205	-1.631532	-0.441647
H	3.085900	-6.561048	-1.061452	C	-4.447663	0.424709	-1.435770
H	1.417344	-7.124309	-1.369442	C	-5.717281	-0.557501	0.282842
C	-3.971099	-1.986802	-3.824629	C	-5.398355	0.674869	-0.307432
C	-4.047189	-0.732043	-4.721554	C	-6.601641	-0.618635	1.361576
C	-3.111186	-3.074796	-4.515521	C	-5.943759	1.876138	0.148001

C	-7.156906	0.589316	1.818874	C	-5.138781	-4.705847	2.959439
H	-6.856401	-1.574623	1.830623	C	-5.227000	-6.990621	1.866691
C	-6.852259	1.846242	1.233728	C	-4.620471	-6.772634	4.292909
H	-5.664847	2.813689	-0.339605	H	-4.633832	-4.064057	3.704428
H	-7.857323	0.552770	2.660505	H	-5.105924	-4.190021	1.984180
N	0.528606	4.454625	-1.638414	H	-6.199576	-4.804190	3.257637
N	4.963377	-0.008181	-0.149368	H	-4.781077	-7.999734	1.805316
N	-4.286544	-0.983964	-1.494690	H	-6.286946	-7.101275	2.160748
N	0.598758	-4.837805	-0.318969	H	-5.204614	-6.545446	0.857219
C	4.507578	6.077037	2.789142	H	-5.691377	-6.862542	4.548248
C	4.194148	5.491428	4.192931	H	-4.188147	-7.789700	4.313579
C	5.750006	5.353677	2.223891	H	-4.141017	-6.173847	5.088762
C	4.841421	7.587230	2.923388	O	-1.306387	5.576674	-0.700403
H	3.332864	5.994431	4.667401	O	2.637909	3.448689	-1.889420
H	3.964004	4.413159	4.127333	O	5.578847	1.908206	1.062734
H	5.067279	5.617393	4.859707	O	4.231282	-2.186089	-0.652189
H	6.032859	5.746331	1.230069	O	-1.385206	-4.232838	-1.419816
H	6.608050	5.519617	2.900106	O	2.117215	-5.452977	1.368291
H	5.601558	4.263511	2.133187	O	-4.939882	-2.840363	-0.209540
H	5.727630	7.720636	3.570719	O	-3.896101	1.236103	-2.172679
H	5.067629	8.032350	1.937907	N	0.172791	0.163879	1.095565
H	4.011407	8.161219	3.371929	C	-0.931733	-0.346186	1.841838
C	-7.527396	3.122367	1.777373	C	-1.281256	0.612082	3.014435
C	-7.182847	3.294219	3.281109	H	-2.014940	0.091664	3.663960
C	-7.067849	4.391929	1.026953	H	-0.362869	0.761781	3.615261
C	-9.065859	2.985967	1.612888	C	-1.847232	1.973831	2.581573
H	-7.510667	2.427927	3.882820	C	-2.138890	2.864221	3.805371
H	-6.096744	3.426832	3.429073	H	-2.773843	1.829346	1.991965
H	-7.690436	4.190802	3.681649	H	-1.118218	2.464582	1.909564
H	-7.317191	4.348225	-0.048975	H	-2.768039	2.297178	4.521476
H	-7.581791	5.273496	1.449457	H	-1.181843	3.042637	4.340321
H	-5.981839	4.563646	1.130575	C	-2.804542	4.207527	3.536923
H	-9.568197	3.891913	1.999089	C	-2.686355	4.876713	2.302199
H	-9.343455	2.867043	0.550132	C	-3.534296	4.841901	4.566744
H	-9.466107	2.118190	2.166666	C	-3.266356	6.142283	2.104718
C	5.320664	-3.851647	4.663664	H	-2.136780	4.419442	1.474104
C	4.297655	-3.571626	5.797779	C	-4.114426	6.105673	4.376346
C	4.895382	-5.142158	3.928125	H	-3.640674	4.336798	5.535856
C	6.724196	-4.087855	5.283897	C	-3.980735	6.763462	3.141685
H	4.570182	-2.679429	6.389162	H	-3.144452	6.631970	1.132380
H	3.285899	-3.408917	5.385559	H	-4.674046	6.575949	5.193644
H	4.253209	-4.433454	6.489041	H	-4.432467	7.750591	2.989728
H	5.604487	-5.404878	3.122226	H	-1.830902	-0.539974	1.214249
H	4.883517	-5.983509	4.644352	C	-0.453115	-1.719999	2.423144
H	3.886984	-5.068298	3.484389	H	-0.190290	-2.412405	1.610993
H	6.692794	-4.956350	5.967262	H	0.429420	-1.573213	3.068270
H	7.474283	-4.296498	4.500157	H	-1.277838	-2.147794	3.020119
H	7.075895	-3.218145	5.866354				
C	-4.478338	-6.110843	2.904537				

^{1}13

SCF energy in CF_3CH_2OH: -4923.659785 a.u.
Free energy in CF_3CH_2OH: -4922.124984 a.u.

Rh	0.566702	-0.208330	-3.095669
O	1.061236	1.780219	-3.158358
O	0.147387	-2.211132	-2.972017
O	0.818745	1.974671	-0.894688
O	-0.167331	-2.050214	-0.713248
O	2.549829	-0.666956	-2.808191
O	-1.451944	0.180676	-3.262566
O	-1.728555	0.347366	-0.995270
O	2.306538	-0.507304	-0.532684
C	-2.162936	0.302280	-2.209445
C	2.976624	-0.739288	-1.605988
C	1.156040	2.416316	-2.055760
C	-0.109449	-2.702099	-1.824716
Rh	0.286865	-0.028050	-0.662885
C	4.462865	-1.086559	-1.338176
C	5.370863	-1.515962	-2.544240
N	4.501958	-2.004990	-0.189387
C	5.494638	-0.319113	-3.519030
C	6.780076	-1.825528	-1.980504
C	4.848984	-2.757613	-3.299093
C	3.653446	-3.124163	-0.019280
C	5.173784	-1.676527	1.016972
H	4.526652	-0.071299	-3.980562
H	5.867886	0.583078	-3.001887
H	7.181869	-0.978648	-1.395615
H	6.774670	-2.718168	-1.329852
H	4.780170	-3.638817	-2.639361
H	3.852536	-2.577123	-3.732110
O	2.891622	-3.572911	-0.874005
C	3.876745	-3.602258	1.377097
O	5.896827	-0.693677	1.173456
C	4.801689	-2.741632	1.994113
C	3.308933	-4.681641	2.047221
C	5.189558	-2.955477	3.314864
C	3.687881	-4.927225	3.393872
C	4.626104	-4.054899	3.995718
C	1.672540	3.879867	-2.060503
C	2.101367	4.498334	-3.441443
N	2.678072	4.012583	-0.996508
C	0.854204	4.567603	-4.357084
C	2.585945	5.946653	-3.183069
C	3.233686	3.714245	-4.139908
C	3.704319	3.086767	-0.705736
C	2.590113	5.029281	0.000755
H	0.474778	3.565165	-4.609166
H	0.037222	5.141577	-3.880357
H	1.833017	6.543894	-2.639601
H	3.522461	5.966554	-2.597895
H	4.135561	3.655356	-3.507559
H	2.924872	2.687632	-4.389125
O	3.985298	2.102277	-1.388502
C	4.341749	3.562843	0.559503
O	1.755198	5.926515	0.011515
C	3.689359	4.740506	0.965136
C	5.390359	3.012297	1.292015
C	4.089369	5.411060	2.118485
C	5.823868	3.676267	2.470968
C	5.162652	4.867854	2.853924
C	-3.701456	0.271907	-2.370268
C	-4.295786	0.568452	-3.803109
N	-4.334591	1.035495	-1.288776
C	-3.944932	-0.612693	-4.742927
C	-5.838567	0.626177	-3.679375
C	-3.788779	1.894140	-4.412016
C	-4.019929	2.362932	-0.905278
C	-5.318386	0.465824	-0.441687
H	-2.860808	-0.690146	-4.913292
H	-4.299280	-1.573601	-4.326827
H	-6.245752	-0.285442	-3.206764
H	-6.175145	1.499360	-3.092560
H	-4.038727	2.760331	-3.777467
H	-2.696198	1.879116	-4.553116
O	-3.175955	3.077149	-1.441115
C	-4.922483	2.675808	0.249123
O	-5.733108	-0.691203	-0.517192
C	-5.711238	1.541422	0.510523
C	-5.059431	3.848092	0.988274
C	-6.670954	1.561179	1.520113
C	-6.033078	3.901180	2.022323
C	-6.821371	2.750752	2.261286
C	-0.303161	-4.228623	-1.663652
C	-0.310433	-5.123594	-2.954595
N	-1.451307	-4.447210	-0.773728
C	1.078355	-5.028693	-3.633278
C	-0.524255	-6.590641	-2.505125
C	-1.416588	-4.742477	-3.962566
C	-2.693420	-3.777683	-0.878872
C	-1.359358	-5.195846	0.429248
H	1.270641	-4.019516	-4.028294
H	1.889433	-5.280366	-2.926876
H	0.221108	-6.901645	-1.751402
H	-1.530431	-6.746577	-2.076732
H	-2.424681	-4.859582	-3.529957
H	-1.310142	-3.701612	-4.305737
O	-2.997007	-2.992763	-1.775089

C	-3.493855	-4.215353	0.303772	C	6.981012	3.074271	3.294699
O	-0.352505	-5.785900	0.817233	C	6.537429	1.693058	3.850554
C	-2.698595	-5.079423	1.078390	C	8.221987	2.886301	2.381108
C	-4.794645	-3.881220	0.667750	C	7.390045	3.971825	4.483416
C	-3.204093	-5.643047	2.247777	H	5.650603	1.799191	4.501685
C	-5.341105	-4.451107	1.849419	H	6.290164	0.980006	3.045205
C	-4.528756	-5.323135	2.612652	H	7.354193	1.253721	4.453895
H	0.571084	-4.547163	-1.060914	H	8.560582	3.852260	1.964696
H	-3.964741	-0.780350	-2.132733	H	9.055944	2.453165	2.963495
H	0.827611	4.494975	-1.689996	H	8.015836	2.204138	1.538747
H	4.888933	-0.144290	-0.941472	H	8.235145	3.505759	5.020702
H	-4.410531	4.703422	0.775506	H	7.718747	4.973816	4.151745
H	-7.579623	2.775383	3.049046	H	6.567409	4.098235	5.210645
H	-7.292547	0.683912	1.727021	C	-6.187715	5.191423	2.851971
H	5.485569	5.391345	3.757992	C	-4.877468	5.431442	3.650174
H	3.582409	6.325619	2.442965	C	-6.438903	6.392946	1.901959
H	5.848495	2.071865	0.968134	C	-7.363150	5.113880	3.851209
H	4.928618	-4.228340	5.032147	H	-4.681673	4.596521	4.346899
H	5.904726	-2.290328	3.809707	H	-4.000885	5.536004	2.988508
H	2.570256	-5.308926	1.536768	H	-4.963510	6.359883	4.244606
H	-2.594112	-6.313638	2.861940	H	-7.358610	6.246598	1.307287
H	-4.933330	-5.769865	3.525272	H	-6.556210	7.320036	2.492455
H	-5.362266	-3.175451	0.051939	H	-5.600238	6.550192	1.202212
C	-6.788352	-4.104732	2.251616	H	-7.441170	6.069030	4.400281
C	-6.898122	-2.572496	2.480449	H	-8.329494	4.942517	3.342395
C	-7.746506	-4.521118	1.102712	H	-7.218052	4.315737	4.601864
C	-7.234433	-4.827441	3.541688	H	2.788960	6.440735	-4.150432
H	-6.235026	-2.249065	3.303404	H	1.116314	5.082914	-5.299141
H	-6.627296	-2.000000	1.576065	H	3.510493	4.233437	-5.076466
H	-7.936998	-2.309743	2.755180	H	7.474723	-2.025756	-2.816284
H	-7.688100	-5.607482	0.909797	H	6.210276	-0.572573	-4.322754
H	-8.790107	-4.276710	1.373697	H	5.546246	-3.004245	-4.121678
H	-7.512284	-3.994287	0.161796	H	1.123154	-5.744687	-4.474534
H	-8.277951	-4.551080	3.775900	H	-0.427856	-7.259446	-3.379379
H	-7.199777	-5.926949	3.433416	H	-1.349460	-5.407616	-4.843732
H	-6.614627	-4.543869	4.411836	H	-4.260885	2.046358	-5.400663
C	3.069899	-6.124139	4.145104	H	-4.441009	-0.463009	-5.719683
C	1.527148	-5.952606	4.199487	H	-6.281126	0.715399	-4.687776
C	3.414779	-7.432857	3.383511	C	-0.950292	-0.286387	1.945182
C	3.597221	-6.250622	5.591343	C	-1.242555	0.642783	3.164321
H	1.252604	-5.025254	4.734188	C	-0.461088	2.984770	2.378025
H	1.072482	-5.914436	3.194464	C	-1.637706	2.092013	2.834259
H	1.075649	-6.805030	4.740628	H	-0.353254	0.635698	3.824653
H	4.507769	-7.586260	3.331237	H	-2.067834	0.158351	3.723627
H	2.970749	-8.301434	3.903718	H	-2.433001	2.101781	2.063501
H	3.022079	-7.423834	2.352185	H	-2.088445	2.541974	3.741361
H	3.128134	-7.123888	6.078636	N	0.215702	0.122173	1.236828
H	4.691589	-6.402921	5.621852	H	-0.041654	2.585973	1.433649
H	3.352766	-5.360995	6.200021	H	-1.856112	-0.357016	1.299430

C	-0.623392	-1.722268	2.484746
H	-0.402150	-2.406391	1.653551
H	0.245036	-1.682095	3.163104
H	-1.506196	-2.089032	3.038745
H	0.348651	2.912660	3.130026
C	-0.862638	4.438563	2.202281
C	-0.661370	5.371848	3.240471
C	-1.472913	4.886335	1.011169
C	-1.052094	6.713209	3.097427
H	-0.183036	5.041269	4.171702
C	-1.861975	6.228170	0.862570
H	-1.644013	4.180491	0.189628
C	-1.653318	7.147469	1.904909
H	-0.878245	7.421929	3.915897
H	-2.313182	6.558185	-0.080890
H	-1.946328	8.196747	1.784172

^{1}13’

SCF energy in CF_3CH_2OH: -4923.649723 a.u.

Free energy in CF_3CH_2OH: -4922.116495 a.u**.**

Rh	-0.467043	0.198055	-3.194193
O	1.578798	0.329364	-3.315600
O	-2.506009	0.131421	-3.008303
O	1.808473	0.195558	-1.043628
O	-2.320386	-0.034196	-0.731875
O	-0.434821	-1.863948	-3.279409
O	-0.550902	2.249346	-2.991704
O	-0.308711	2.094008	-0.717412
O	-0.238680	-2.036124	-1.002200
C	-0.467784	2.745537	-1.819688
C	-0.393425	-2.520043	-2.185021
C	2.261463	0.370539	-2.239315
C	-2.987667	0.053088	-1.827812
Rh	-0.239633	0.023107	-0.759099
C	-0.488540	-4.068066	-2.212306
C	-0.693294	-4.778120	-3.597863
N	-1.441995	-4.476459	-1.169669
C	0.546493	-4.492845	-4.480635
C	-0.761297	-6.303439	-3.338828
C	-1.979089	-4.338934	-4.332225
C	-2.696802	-3.871502	-0.916853
C	-1.071866	-5.362531	-0.121133
H	0.637179	-3.422570	-4.722758
H	1.478994	-4.817103	-3.981712
H	0.115975	-6.664940	-2.773240
H	-1.669008	-6.581354	-2.774372
H	-2.881814	-4.549225	-3.734074
H	-1.966063	-3.262842	-4.564684
O	-3.226747	-3.019128	-1.627288
C	-3.196971	-4.478648	0.353104
O	0.009165	-5.942939	-0.044986
C	-2.231672	-5.391437	0.813973
C	-4.379585	-4.241724	1.048580
C	-2.442488	-6.110454	1.987896
C	-4.624172	-4.963469	2.247993
C	-3.647014	-5.889097	2.685617
C	3.753019	0.775169	-2.316729
C	4.407688	0.926675	-3.742081
N	4.528692	-0.056282	-1.389693
C	3.723783	2.103821	-4.481619
C	5.897746	1.298038	-3.537625
C	4.323956	-0.353605	-4.602114
C	4.482106	-1.471052	-1.318058
C	5.353135	0.494645	-0.376239
H	2.672194	1.880785	-4.717296
H	3.752973	3.028997	-3.878679
H	6.014248	2.188176	-2.893877
H	6.471691	0.469153	-3.085856
H	4.846695	-1.202185	-4.130268
H	3.279236	-0.652818	-4.780092
O	3.781695	-2.197209	-2.016789
C	5.433030	-1.849810	-0.226698
O	5.507143	1.697535	-0.165636
C	5.952941	-0.671297	0.336780
C	5.807688	-3.109880	0.229073
C	6.870781	-0.734943	1.383172
C	6.742574	-3.208628	1.293700
C	7.254312	-2.010641	1.846637
C	-0.638540	4.270216	-1.605719
C	-0.745681	5.203459	-2.863096
N	0.361229	4.694744	-0.613937
C	-2.032178	4.834134	-3.641895
C	-0.892867	6.657982	-2.351672
C	0.478430	5.120720	-3.800085
C	1.722864	4.309255	-0.629793
C	-0.001059	5.270911	0.632653
H	-1.968916	3.823446	-4.073277
H	-2.922955	4.874268	-2.989303
H	-1.741942	6.762481	-1.652400
H	0.019932	7.005213	-1.835512
H	1.408381	5.420854	-3.288576
H	0.618267	4.101545	-4.193128
O	2.273848	3.701294	-1.545430
C	2.296280	4.770735	0.669317
O	-1.144487	5.588587	0.955575
C	1.264897	5.366119	1.417881

C	3.596616	4.663772	1.154274	H	-6.377867	6.117788	3.213845
C	1.524494	5.886510	2.683855	H	-5.084424	7.152520	3.890422
C	3.891919	5.189628	2.440796	H	-4.852817	6.353615	2.312922
C	2.843769	5.794309	3.175148	H	-5.061863	5.880085	6.018230
C	-4.521367	-0.000131	-1.622428	H	-6.380838	4.826412	5.450416
C	-5.455426	0.235889	-2.862571	H	-4.859852	4.111554	6.073769
N	-4.839558	0.835981	-0.454491	C	-5.924383	-4.707551	3.036588
C	-5.229200	-0.911056	-3.878333	C	-5.932294	-3.234217	3.528911
C	-6.920005	0.156095	-2.365299	C	-7.146552	-4.947365	2.110146
C	-5.230283	1.600156	-3.549006	C	-6.061696	-5.634649	4.264560
C	-4.306208	2.124730	-0.211505	H	-5.066874	-3.036425	4.187209
C	-5.471301	0.309302	0.702069	H	-5.899577	-2.515470	2.691943
H	-4.215419	-0.880890	-4.305753	H	-6.854990	-3.039671	4.107612
H	-5.373819	-1.899899	-3.406809	H	-7.168820	-5.988893	1.741428
H	-7.120775	-0.791466	-1.833895	H	-8.083209	-4.761412	2.667243
H	-7.167098	0.989030	-1.683201	H	-7.140695	-4.274866	1.235330
H	-5.431011	2.441328	-2.864318	H	-7.015779	-5.423432	4.779817
H	-4.197817	1.699854	-3.918979	H	-6.068400	-6.702445	3.978519
O	-3.639316	2.779172	-1.010751	H	-5.250128	-5.475470	4.997689
C	-4.707258	2.479185	1.182510	C	7.160872	-4.602144	1.803247
O	-5.936817	-0.825759	0.792454	C	5.900294	-5.363010	2.296836
C	-5.421298	1.395611	1.724135	C	7.817417	-5.391611	0.638397
C	-4.453304	3.636861	1.912312	C	8.172065	-4.526353	2.968271
C	-5.914136	1.457273	3.025634	H	5.402868	-4.824760	3.122535
C	-4.944008	3.729049	3.242341	H	5.156586	-5.499797	1.492658
C	-5.669458	2.632419	3.766360	H	6.185368	-6.366817	2.661963
H	-4.711079	-1.033806	-1.271597	H	8.722361	-4.876697	0.268652
H	-1.602693	4.357608	-1.065672	H	8.112463	-6.399460	0.983589
H	3.775112	1.782985	-1.853621	H	7.127006	-5.518486	-0.213507
H	0.484597	-4.426123	-1.819526	H	8.433970	-5.548397	3.294885
H	4.359843	4.160931	0.550611	H	9.110398	-4.023813	2.670089
H	3.052995	6.204310	4.167213	H	7.755094	-3.996470	3.843801
H	0.730945	6.350766	3.278577	C	5.330871	5.084611	2.984780
H	7.975271	-2.065781	2.667105	C	5.736526	3.587368	3.068369
H	7.282149	0.175838	1.830494	C	6.292299	5.823874	2.014976
H	5.377663	-4.002475	-0.237142	C	5.480357	5.710185	4.388830
H	-3.818946	-6.453967	3.605916	H	5.073822	3.039199	3.762477
H	-1.694931	-6.818388	2.359600	H	5.694093	3.084872	2.086398
H	-5.086860	-3.491663	0.678870	H	6.772181	3.502262	3.447251
H	-6.468539	0.619751	3.461398	H	6.033359	6.895283	1.937730
H	-6.054661	2.685455	4.788392	H	7.332112	5.747614	2.382603
H	-3.867600	4.444951	1.460882	H	6.263293	5.391887	0.999875
C	-4.670595	5.006661	4.061748	H	6.527712	5.612286	4.725347
C	-3.135951	5.207050	4.197466	H	5.231649	6.787196	4.391730
C	-5.283445	6.226015	3.321010	H	4.844113	5.203395	5.137208
C	-5.281918	4.941765	5.478584	H	6.355818	1.521776	-4.517803
H	-2.673886	4.354476	4.727482	H	4.257483	2.297943	-5.430329
H	-2.637888	5.312194	3.218094	H	4.802292	-0.163877	-5.581196
H	-2.929349	6.123933	4.780550	H	-0.792461	-6.838308	-4.305262

H	0.461595	-5.055667	-5.428240
H	-2.064475	-4.900166	-5.281518
H	-5.958493	-0.817224	-4.703887
H	-7.605806	0.217913	-3.229497
H	-5.918707	1.692883	-4.409815
H	0.326990	5.805067	-4.655649
H	-2.180430	5.555426	-4.466443
H	-1.068736	7.332795	-3.208773
C	0.521616	0.788312	1.909815
C	1.431873	0.126700	2.992503
C	2.172055	-2.151569	2.017206
C	2.579101	-0.718839	2.402355
H	0.799487	-0.485741	3.662258
H	1.840131	0.961397	3.595700
H	2.963037	-0.209188	1.499032
H	3.425006	-0.747226	3.116270
N	-0.152602	-0.195000	1.130158
H	1.227740	-2.103482	1.432868
H	2.924433	-2.559776	1.313837
C	2.000845	-3.154710	3.153099
C	2.270629	-2.856208	4.504408
C	1.584177	-4.469188	2.839197
C	2.134760	-3.833184	5.507072
H	2.594978	-1.849091	4.788761
C	1.452529	-5.446731	3.835002
H	1.363459	-4.731208	1.797204
C	1.727226	-5.133858	5.177908
H	2.351054	-3.571530	6.549887
H	1.136692	-6.459381	3.557600
H	1.623966	-5.896765	5.958244
H	1.136309	1.489201	1.299660
C	-0.605814	1.613112	2.614574
H	-1.238577	2.118032	1.869492
H	-1.233001	0.950187	3.233557
H	-0.126900	2.373290	3.257660

^{1}12-TS

SCF energy in CF_3CH_2OH: -4923.641557 a.u.

Free energy in CF_3CH_2OH: -4922.108329 a.u.

Rh	-0.379902	-0.263440	-3.045217
O	-0.325727	-2.309841	-2.887373
O	-0.495996	1.793835	-3.115590
O	-0.211472	-2.247836	-0.600692
O	-0.322324	1.894793	-0.835496
O	-2.428169	-0.330110	-2.936185
O	1.676685	-0.117153	-3.075780
O	1.833468	-0.035710	-0.791668
O	-2.322239	-0.231208	-0.646990
C	2.317086	0.053194	-1.984456
C	-2.946047	-0.280517	-1.767590
C	-0.329276	-2.851983	-1.731282
C	-0.465405	2.416988	-2.003843
Rh	-0.223966	-0.167630	-0.597506
C	-4.487866	-0.335916	-1.612610
C	-5.383561	-0.289552	-2.900663
N	-4.865548	0.640163	-0.577759
C	-5.099665	-1.557799	-3.742631
C	-6.863468	-0.335404	-2.445638
C	-5.160632	0.972447	-3.761373
C	-4.378081	1.966367	-0.499408
C	-5.521784	0.258193	0.619498
H	-4.069268	-1.563202	-4.129522
H	-5.247076	-2.476750	-3.146846
H	-7.062358	-1.199240	-1.785993
H	-7.154576	0.582153	-1.903702
H	-5.403241	1.894536	-3.206902
H	-4.116514	1.044960	-4.103458
O	-3.695605	2.524692	-1.355958
C	-4.852699	2.502054	0.811032
O	-5.951990	-0.869964	0.858481
C	-5.553130	1.480707	1.476126
C	-4.675809	3.763978	1.370412
C	-6.108694	1.711810	2.732495
C	-5.236217	4.031405	2.647996
C	-5.944895	2.993577	3.299013
C	-0.433543	-4.399984	-1.629343
C	-0.572948	-5.213350	-2.967545
N	-1.454022	-4.723856	-0.617245
C	0.712430	-5.002692	-3.805094
C	-0.667467	-6.717444	-2.608838
C	-1.820071	-4.824615	-3.791627
C	-2.699753	-4.068419	-0.463335
C	-1.199035	-5.614948	0.458231
H	0.828846	-3.954287	-4.119545
H	1.614408	-5.298452	-3.236757
H	0.176332	-7.045856	-1.977213
H	-1.604773	-6.953372	-2.074152
H	-2.749139	-4.975843	-3.215809
H	-1.784813	-3.772698	-4.113299
O	-3.165655	-3.242511	-1.244382
C	-3.288121	-4.593343	0.806717
O	-0.173339	-6.278215	0.596530
C	-2.398950	-5.542288	1.341339
C	-4.482221	-4.262373	1.442154
C	-2.699425	-6.203499	2.530191
C	-4.814387	-4.917643	2.659035

C	-3.913603	-5.881833	3.171151	H	-0.657265	-7.314237	-3.538856
C	3.782940	0.540902	-2.067819	H	-1.874456	-5.465178	-4.691689
C	4.467211	0.602279	-3.489690	H	0.668764	-5.632974	-4.712157
N	4.601779	-0.119651	-1.043847	H	4.944441	-0.601967	-5.235745
C	3.746625	1.680215	-4.338367	H	6.396961	1.237098	-4.279523
C	5.932753	1.064325	-3.291907	H	4.283453	1.807087	-5.296754
C	4.463936	-0.743340	-4.249258	H	0.354686	5.144879	-5.146352
C	4.787082	-1.518123	-0.894907	H	-1.163972	6.784227	-3.948735
C	5.354708	0.613377	-0.095259	H	-2.153255	4.844117	-5.026748
H	2.707332	1.394221	-4.559543	H	-5.817186	0.929783	-4.650758
H	3.731908	2.655913	-3.821451	H	-5.795439	-1.592849	-4.601327
H	5.991699	2.007053	-2.718652	H	-7.519182	-0.421845	-3.331000
H	6.542006	0.304272	-2.770320	H	-5.130547	-3.489614	1.015171
H	5.021931	-1.525886	-3.709966	H	-4.155051	-6.397708	4.104630
H	3.438175	-1.108267	-4.414030	H	-2.013099	-6.943936	2.954264
O	4.198491	-2.389709	-1.525309	H	6.211832	-3.791456	0.201419
C	5.834940	-1.672297	0.165932	H	8.570962	-1.278875	2.860094
O	5.337502	1.837661	0.034450	H	7.387800	0.750085	2.030745
C	6.158320	-0.395792	0.655936	H	4.204883	4.281654	0.355001
C	6.483963	-2.816905	0.619415	H	2.725594	6.809928	3.578526
C	7.131910	-0.240405	1.640362	H	0.433969	6.755725	2.605080
C	7.504342	-2.689710	1.599914	H	-6.653685	0.924700	3.263853
C	7.794028	-1.397616	2.099971	H	-6.383037	3.180876	4.283462
C	-0.697160	3.948869	-1.975310	H	-4.095889	4.519638	0.829730
C	-0.780165	4.725342	-3.338050	C	-6.127618	-4.550826	3.379158
N	0.245904	4.527297	-1.006675	C	-6.086325	-3.048522	3.772681
C	-2.018064	4.223337	-4.121887	C	-7.323720	-4.797970	2.420795
C	-0.995686	6.223933	-3.011294	C	-6.352473	-5.385542	4.659797
C	0.487712	4.576994	-4.206443	H	-5.239881	-2.844002	4.453529
C	1.616548	4.189833	-0.923105	H	-5.989437	-2.388640	2.893395
C	-0.176767	5.275549	0.123125	H	-7.020652	-2.775666	4.298344
H	-1.902618	3.174669	-4.435301	H	-7.383981	-5.860827	2.124515
H	-2.937388	4.300898	-3.514079	H	-8.270684	-4.527741	2.923146
H	-1.872468	6.378388	-2.357132	H	-7.248009	-4.190304	1.502927
H	-0.114874	6.666354	-2.512632	H	-7.309514	-5.090836	5.125902
H	1.382272	4.973609	-3.696988	H	-6.408354	-6.468408	4.444719
H	0.679062	3.523120	-4.462242	H	-5.556387	-5.219332	5.408366
O	2.220001	3.481366	-1.726420	C	8.284218	-3.942816	2.050951
C	2.128182	4.850278	0.313797	C	7.299736	-5.007866	2.601378
O	-1.337355	5.611868	0.352366	C	9.034119	-4.527954	0.822345
C	1.056377	5.520389	0.930285	C	9.323785	-3.630105	3.150473
C	3.411600	4.850947	0.851200	H	6.759564	-4.630785	3.488398
C	1.258409	6.229829	2.112346	H	6.551319	-5.306319	1.846815
C	3.648475	5.570829	2.052886	H	7.853510	-5.916514	2.900736
C	2.561240	6.248980	2.654081	H	9.750013	-3.795609	0.408111
H	-1.686111	4.059713	-1.486871	H	9.598648	-5.431755	1.117029
H	3.719701	1.589894	-1.711633	H	8.337272	-4.813278	0.014910
H	0.512802	-4.729570	-1.155878	H	9.843873	-4.560390	3.440684
H	-4.671607	-1.317176	-1.133591	H	10.093021	-2.917406	2.802091

H	8.851670	-3.216277	4.060094
C	-5.051342	5.429002	3.272612
C	-3.534624	5.704675	3.464343
C	-5.651091	6.496494	2.317644
C	-5.749561	5.560351	4.644263
H	-3.084278	4.961972	4.147560
H	-2.978086	5.672796	2.511774
H	-3.389754	6.708257	3.906273
H	-6.733813	6.333850	2.168614
H	-5.511237	7.506614	2.744736
H	-5.165099	6.482447	1.326959
H	-5.596685	6.580749	5.038556
H	-6.839803	5.393335	4.571168
H	-5.337848	4.853823	5.387909
C	5.069292	5.587290	2.651424
C	5.501271	4.131561	2.977564
C	6.049914	6.192356	1.610331
C	5.156799	6.425601	3.945467
H	4.825089	3.679187	3.725633
H	5.503028	3.484786	2.082939
H	6.523923	4.132093	3.399310
H	5.767846	7.229299	1.353421
H	7.075951	6.207817	2.021948
H	6.072032	5.603566	0.677295
H	6.193058	6.406052	4.327654
H	4.887771	7.483795	3.772983
H	4.503338	6.026039	4.742409
C	0.158645	1.260004	1.958254
C	1.162876	0.899475	3.099438
C	0.302250	-1.465330	3.258157
C	0.590129	-0.179542	4.033170
H	1.409490	1.825068	3.653271
H	2.097536	0.537588	2.633755
H	-0.658962	-1.940347	3.525598
H	1.300349	-0.376118	4.860849
H	-0.341738	0.188715	4.498228
N	-0.432901	0.068240	1.348455
H	-0.102910	-0.956837	2.142396
C	1.369166	-2.472810	3.066548
C	2.744527	-2.198294	3.274910
C	1.009746	-3.790111	2.685111
C	3.708892	-3.201477	3.119780
H	3.063376	-1.195085	3.575843
C	1.971717	-4.791346	2.517870
H	-0.049761	-4.021327	2.527075
C	3.329039	-4.500491	2.739246
H	4.764894	-2.965359	3.291481
H	1.654851	-5.791727	2.207082
H	4.086736	-5.282412	2.616861
H	0.738248	1.833089	1.206010
C	-0.994069	2.158670	2.470316
H	-1.675614	2.402492	1.640588
H	-1.581146	1.653402	3.257057
H	-0.585440	3.103600	2.875807

^{1}12-TS'

SCF energy in CF_3CH_2OH: -4923.655404 a.u.

Free energy in CF_3CH_2OH: -4922.125071 a.u**.**

Rh	-0.410616	0.191374	-3.175560
O	1.633160	-0.042151	-3.300149
O	-2.425156	0.486007	-2.962062
O	1.850664	-0.196196	-1.027329
O	-2.239420	0.321018	-0.682837
O	-0.733575	-1.843962	-3.207737
O	-0.128439	2.224820	-3.022041
O	0.091361	2.077449	-0.745329
O	-0.520848	-2.020460	-0.931875
C	0.050018	2.720627	-1.860957
C	-0.778453	-2.484434	-2.104995
C	2.318265	-0.128937	-2.227814
C	-2.894514	0.506254	-1.773258
Rh	-0.181841	0.018354	-0.739100
C	-1.132367	-3.996707	-2.125608
C	-1.442291	-4.664387	-3.513847
N	-2.154885	-4.236729	-1.095232
C	-0.166345	-4.589949	-4.388201
C	-1.764096	-6.158554	-3.262342
C	-2.633847	-4.017693	-4.253336
C	-3.284582	-3.419600	-0.847813
C	-1.983541	-5.209577	-0.075050
H	0.105250	-3.550163	-4.627064
H	0.694507	-5.068282	-3.884153
H	-0.961330	-6.662961	-2.696014
H	-2.707884	-6.285483	-2.702660
H	-3.559602	-4.069989	-3.655518
H	-2.439518	-2.960453	-4.489293
O	-3.641532	-2.475653	-1.549060
C	-3.909872	-3.950852	0.400639
O	-1.038100	-5.993845	-0.007046
C	-3.143675	-5.042558	0.845564
C	-5.038025	-3.512774	1.088811
C	-3.507457	-5.739403	1.994968
C	-5.435065	-4.205510	2.264116
C	-4.659329	-5.311378	2.686248
C	3.860158	-0.038831	-2.321457
C	4.525288	-0.149779	-3.745275

N	4.456985	-0.924100	-1.312753	C	-5.273158	1.241147	0.765309
C	4.121307	1.091475	-4.580178	H	-4.296788	-0.300827	-4.197930
C	6.062050	-0.111289	-3.555639	H	-5.600692	-1.078676	-3.258839
C	4.145016	-1.439791	-4.504948	H	-7.111678	0.356051	-1.709731
C	4.118759	-2.284025	-1.103402	H	-6.863457	2.124411	-1.626873
C	5.368083	-0.454509	-0.333911	H	-4.924542	3.228194	-2.879956
H	3.042980	1.101706	-4.798963	H	-3.860935	2.254200	-3.930334
H	4.375527	2.029258	-4.053678	O	-3.095957	3.339059	-1.037687
H	6.382563	0.776900	-2.982122	C	-4.185900	3.285498	1.162788
H	6.437058	-1.010882	-3.035437	O	-5.905605	0.194586	0.899408
H	4.457885	-2.346574	-3.960838	C	-5.049733	2.343188	1.747755
H	3.058673	-1.501539	-4.675657	C	-3.753302	4.417135	1.847188
O	3.295099	-2.924434	-1.750388	C	-5.512669	2.525871	3.048994
C	4.952527	-2.733824	0.055796	C	-4.208857	4.631060	3.175162
O	5.765292	0.706491	-0.235065	C	-5.085429	3.676760	3.744466
C	5.706046	-1.637597	0.510297	H	-4.765671	-0.264530	-1.170247
C	5.043909	-3.986048	0.655386	H	-0.746003	4.539311	-1.135904
C	6.580690	-1.778079	1.585656	H	4.088080	0.980256	-1.947063
C	5.928981	-4.163106	1.751948	H	-0.238030	-4.513978	-1.724160
C	6.680660	-3.047684	2.191620	H	5.118396	3.299232	0.384229
C	0.172055	4.255757	-1.688765	H	4.316788	5.717310	3.916267
C	0.220389	5.159887	-2.970477	H	2.034842	6.246553	3.069357
N	1.255800	4.511316	-0.727100	H	7.368341	-3.164438	3.033722
C	-1.124512	5.018226	-3.725339	H	7.172379	-0.930726	1.947230
C	0.355865	6.630221	-2.502409	H	4.434861	-4.812953	0.276084
C	1.393601	4.822911	-3.915871	H	-4.950979	-5.856898	3.587909
C	2.522092	3.879595	-0.750790	H	-2.916162	-6.588400	2.352456
C	1.041804	5.202692	0.494726	H	-5.584389	-2.632441	0.734003
H	-1.256748	4.003980	-4.131909	H	-6.181914	1.797717	3.518821
H	-1.982109	5.237819	-3.063877	H	-5.446618	3.824293	4.766165
H	-0.439452	6.907154	-1.787159	H	-3.058151	5.110929	1.362597
H	1.331198	6.818979	-2.019314	C	-3.732647	5.882727	3.939867
H	2.369939	4.962899	-3.421852	C	-2.184172	5.850259	4.058573
H	1.337183	3.782652	-4.272636	C	-4.161382	7.151277	3.153505
O	2.931397	3.143409	-1.646372	C	-4.328025	5.968358	5.362479
C	3.206177	4.283994	0.514104	H	-1.852389	4.960300	4.623628
O	-0.011290	5.746325	0.822567	H	-1.684925	5.834356	3.074108
C	2.324586	5.094321	1.251461	H	-1.832230	6.748737	4.599164
C	4.478398	3.961269	0.977298	H	-5.260541	7.205676	3.055068
C	2.712078	5.616006	2.483828	H	-3.818440	8.058923	3.683455
C	4.903329	4.483885	2.228330	H	-3.727424	7.172362	2.138956
C	4.005928	5.305202	2.952137	H	-3.957318	6.880995	5.862204
C	-4.414121	0.712946	-1.554978	H	-5.431837	6.024263	5.347109
C	-5.316585	1.058098	-2.792507	H	-4.031850	5.105850	5.986935
N	-4.579688	1.624694	-0.411917	C	-6.679096	-3.724807	3.038475
C	-5.297381	-0.145378	-3.766802	C	-6.426470	-2.281441	3.554676
C	-6.766522	1.237915	-2.278769	C	-7.906567	-3.722375	2.087562
C	-4.885136	2.341710	-3.535214	C	-7.006595	-4.626753	4.249183
C	-3.852344	2.822908	-0.217358	H	-5.554988	-2.254211	4.233742

H	-6.243194	-1.569091	2.731869
H	-7.310442	-1.927391	4.117976
H	-8.115511	-4.737326	1.703627
H	-8.802828	-3.369311	2.630162
H	-7.755913	-3.053616	1.223075
H	-7.911288	-4.245960	4.755693
H	-7.209652	-5.670309	3.946147
H	-6.189578	-4.632534	4.993496
C	6.034582	-5.549401	2.418746
C	4.644882	-5.944642	2.987641
C	6.473792	-6.593629	1.356742
C	7.059635	-5.574596	3.573888
H	4.310454	-5.229221	3.759337
H	3.867911	-5.973340	2.204576
H	4.697009	-6.948661	3.447673
H	7.461824	-6.339233	0.932694
H	6.546516	-7.594822	1.819724
H	5.754859	-6.663638	0.521921
H	7.096489	-6.588528	4.010351
H	8.079534	-5.325447	3.228275
H	6.785936	-4.876553	4.385835
C	6.315902	4.145833	2.746887
C	6.453466	2.605517	2.890922
C	7.365326	4.661583	1.724839
C	6.613400	4.792252	4.117476
H	5.721877	2.212201	3.620053
H	6.299456	2.079565	1.932637
H	7.467061	2.355314	3.256682
H	7.296234	5.757653	1.603244
H	8.385486	4.419031	2.075116
H	7.232582	4.199185	0.731695
H	7.633409	4.517616	4.440554
H	6.566093	5.895769	4.074853
H	5.913767	4.444003	4.899181
H	6.551363	-0.073656	-4.545615
H	4.670569	1.080427	-5.539736
H	4.650600	-1.443839	-5.488706
H	-1.880749	-6.675918	-4.231828
H	-0.338923	-5.129437	-5.337311
H	-2.813162	-4.561104	-5.200023
H	-6.008491	0.039834	-4.592969
H	-7.446241	1.379582	-3.138516
H	-5.571758	2.518039	-4.384374
H	1.360030	5.494982	-4.793851
H	-1.150752	5.736049	-4.565872
H	0.280903	7.302889	-3.375897
C	0.545241	0.919578	1.945139
C	1.361655	0.380576	3.145932
C	1.667693	-1.841025	1.988976
C	2.384503	-0.664412	2.651669
H	0.669571	-0.076162	3.879618
H	1.863460	1.231260	3.644400
H	3.054041	-0.182910	1.916489
H	3.020784	-1.008554	3.490238
N	-0.114538	-0.153651	1.220394
H	0.634660	-1.306976	1.558884
H	2.134104	-2.176571	1.048915
C	1.219670	-2.993372	2.821743
C	1.156895	-2.946062	4.236226
C	0.833835	-4.197506	2.181332
C	0.747921	-4.063915	4.977223
H	1.447565	-2.032356	4.765413
C	0.418484	-5.312674	2.919453
H	0.855476	-4.251021	1.087235
C	0.377525	-5.251791	4.323917
H	0.718551	-4.006784	6.071686
H	0.118522	-6.220852	2.386498
H	0.057199	-6.123377	4.906298
H	1.228888	1.507546	1.293688
C	-0.583968	1.868253	2.436862
H	-1.141394	2.274801	1.580205
H	-1.282709	1.324466	3.095211
H	-0.130212	2.706521	2.996125

R, S-12-TS

SCF energy in CF_3CH_2OH: -1618.182084 a.u.

Free energy in CF_3CH_2OH: -1617.821831 a.u**.**

Rh	-2.149354	-1.313048	0.349664
O	-0.800447	-2.154095	1.653098
O	-3.443294	-0.428586	-0.976957
O	0.768031	-0.556974	1.141062
O	-1.896632	1.182290	-1.517444
O	-2.860568	-0.096166	1.846562
O	-1.380134	-2.463532	-1.164917
O	0.187834	-0.871775	-1.697082
O	-1.304275	1.515645	1.341519
C	-0.390887	-2.013703	-1.848077
C	-2.290053	1.037458	2.023000
C	0.354460	-1.606040	1.764017
C	-3.049099	0.612821	-1.613946
Rh	-0.493365	0.389984	-0.207426
C	0.946449	3.135884	-0.012043
C	2.326089	3.787785	-0.325432
C	3.448063	1.585709	-0.772323
C	3.504091	2.871727	0.049471
H	2.386218	4.750045	0.216205

H	2.368203	4.022989	-1.407858
H	4.463934	3.401910	-0.120530
H	3.459019	2.646441	1.132352
N	0.884316	1.781209	-0.517126
H	2.156993	1.382284	-0.699482
H	3.546609	1.786405	-1.855128
C	4.177704	0.367959	-0.365786
C	4.584132	-0.564615	-1.357144
C	4.476927	0.058189	0.986666
C	5.261543	-1.741423	-1.018925
H	4.362894	-0.345408	-2.409042
C	5.159479	-1.118035	1.324916
H	4.171717	0.746641	1.781737
C	5.555839	-2.026207	0.326730
H	5.569914	-2.437219	-1.807902
H	5.390525	-1.325673	2.376524
H	6.091806	-2.943591	0.594446
C	-4.036242	1.262283	-2.565354
H	-3.529998	1.543775	-3.502836
H	-4.874195	0.580196	-2.771643
H	-4.430636	2.187250	-2.107903
C	0.176721	-2.913364	-2.928380
H	-0.537735	-3.712775	-3.174709
H	0.418326	-2.322453	-3.826447
H	1.114398	-3.369911	-2.564368
C	1.329091	-2.230331	2.743708
H	1.242558	-1.716983	3.718601
H	1.090428	-3.294812	2.889861
H	2.361691	-2.107836	2.381334
C	-2.801576	1.906002	3.156862
H	-2.058928	1.914976	3.974411
H	-2.929419	2.945351	2.812594
H	-3.754111	1.511715	3.540268
C	-0.210943	4.001212	-0.561630
H	-0.137651	4.084391	-1.660127
H	-1.182198	3.549364	-0.310305
H	-0.160453	5.015389	-0.123759
H	0.837389	3.082630	1.098208

R, R-12-TS

SCF energy in CF_3CH_2OH: -1618.178333 a.u.

Free energy in CF_3CH_2OH: -1617.819268 a.u.

Rh	2.590096	-0.948536	0.065399
O	2.948749	-0.125976	1.914355
O	2.168712	-1.734607	-1.783175
O	0.963449	1.027253	1.848339
O	0.166446	-0.610462	-1.880605
O	1.592863	-2.512105	0.949369
O	3.507781	0.663394	-0.823345
O	1.527886	1.822944	-0.901791
O	-0.405815	-1.383110	0.869413
C	2.795581	1.690921	-1.102654
C	0.329557	-2.403565	1.148907
C	2.070762	0.668805	2.404226
C	1.067338	-1.402883	-2.351973
Rh	0.472143	0.263961	-0.020534
C	-1.324107	2.777155	-0.027548
C	-2.408899	3.276804	-1.030800
C	-3.577475	1.034544	-1.035587
C	-3.752659	2.542686	-0.851167
H	-2.033594	3.110510	-2.058881
H	-2.540641	4.367949	-0.903645
H	-4.169580	2.770730	0.146602
H	-4.486779	2.933425	-1.585634
N	-1.185505	1.340331	-0.123855
H	-2.391168	0.887197	-0.499786
H	-3.328880	0.774072	-2.080786
C	-4.514648	0.067581	-0.427371
C	-4.766135	-1.168883	-1.079453
C	-5.158101	0.294006	0.817455
C	-5.628109	-2.122966	-0.526991
H	-4.276314	-1.367442	-2.040807
C	-6.020028	-0.661089	1.370603
H	-4.978480	1.228053	1.361483
C	-6.263427	-1.874326	0.702734
H	-5.810252	-3.063673	-1.059486
H	-6.506432	-0.457876	2.331793
H	-6.940273	-2.618435	1.137049
C	3.503829	2.885796	-1.712734
H	3.608074	3.678037	-0.949916
H	4.504502	2.596630	-2.066211
H	2.908448	3.298280	-2.543378
C	0.787673	-1.987366	-3.723900
H	-0.206731	-2.464340	-3.732897
H	0.772511	-1.177346	-4.473931
H	1.560745	-2.721926	-3.992787
C	-0.385529	-3.598945	1.747919
H	-1.176959	-3.264624	2.436991
H	-0.866284	-4.175961	0.937559
H	0.331320	-4.251842	2.268122
C	2.340877	1.243344	3.782111
H	2.221886	2.339569	3.764490
H	1.603391	0.841458	4.498850
H	3.355213	0.978815	4.114874
C	-1.605397	3.210266	1.435337
H	-0.796651	2.849419	2.090023

H	-1.658904	4.313238	1.499862
H	-2.557104	2.790087	1.804468
H	-0.350434	3.219607	-0.331120

R, S-trans-TS

SCF energy in CF_3CH_2OH: -4923.639955 a.u.
Free energy in CF_3CH_2OH: -4922.110653 a.u.

Rh	-0.414120	0.100371	-3.171116
O	1.576736	-0.410070	-3.315184
O	-2.375814	0.675585	-2.908306
O	1.803996	-0.578897	-1.042734
O	-2.152625	0.563002	-0.629135
O	-1.000479	-1.867812	-3.191286
O	0.118741	2.081489	-3.083797
O	0.362208	1.951666	-0.810539
O	-0.820324	-2.025582	-0.915169
C	0.373227	2.577302	-1.935791
C	-1.144062	-2.473929	-2.075294
C	2.258739	-0.575140	-2.244923
C	-2.805566	0.804220	-1.713683
Rh	-0.182719	-0.051886	-0.744998
C	-1.722270	-3.915698	-2.069983
C	-2.150478	-4.538021	-3.449465
N	-2.758750	-3.987004	-1.028311
C	-0.889520	-4.675603	-4.337856
C	-2.703414	-5.960118	-3.183482
C	-3.234107	-3.716244	-4.181397
C	-3.740577	-3.003690	-0.774025
C	-2.758112	-4.998458	-0.025031
H	-0.456483	-3.694852	-4.588009
H	-0.111957	-5.283834	-3.838230
H	-1.988129	-6.582514	-2.617793
H	-3.651490	-5.931770	-2.617431
H	-4.144938	-3.610175	-3.567942
H	-2.876297	-2.707555	-4.437704
O	-3.948280	-2.009354	-1.468332
C	-4.442596	-3.435317	0.472477
O	-1.976862	-5.943604	0.017324
C	-3.870389	-4.644651	0.903922
C	-5.484544	-2.823046	1.163888
C	-4.350370	-5.285255	2.043804
C	-5.995850	-3.453601	2.329690
C	-5.416665	-4.678605	2.738888
C	3.798781	-0.654458	-2.377537
C	4.399712	-1.021399	-3.790286
N	4.355883	-1.440647	-1.268857
C	4.151217	0.162057	-4.759389
C	5.931664	-1.187197	-3.634323
C	3.809683	-2.319330	-4.384185
C	3.949491	-2.738938	-0.872164
C	5.345721	-0.915867	-0.399726
H	3.077903	0.317393	-4.945178
H	4.572540	1.102315	-4.358677
H	6.394197	-0.299611	-3.166671
H	6.193143	-2.072441	-3.027580
H	3.982287	-3.187727	-3.727223
H	2.724181	-2.227453	-4.549044
O	3.071382	-3.413468	-1.403012
C	4.807716	-3.089578	0.304616
O	5.833931	0.211324	-0.479557
C	5.647578	-1.997791	0.580916
C	4.865624	-4.265264	1.047411
C	6.575940	-2.063712	1.617938
C	5.802723	-4.365879	2.110130
C	6.639991	-3.254979	2.369477
C	0.661620	4.093466	-1.805502
C	0.781724	4.952565	-3.115285
N	1.787513	4.256823	-0.875488
C	-0.581788	4.933392	-3.849766
C	1.075937	6.413360	-2.691471
C	1.899023	4.470519	-4.065207
C	2.980465	3.494871	-0.914879
C	1.693566	5.019521	0.316396
H	-0.821609	3.930272	-4.234186
H	-1.402834	5.250264	-3.181699
H	0.320446	6.793635	-1.980751
H	2.069705	6.512668	-2.219498
H	2.890994	4.511734	-3.584704
H	1.725083	3.435952	-4.399839
O	3.269531	2.683147	-1.790854
C	3.753242	3.884315	0.302444
O	0.714890	5.685132	0.653344
C	2.988192	4.812990	1.030844
C	5.004969	3.456045	0.733622
C	3.475583	5.347360	2.221401
C	5.531226	3.990863	1.940294
C	4.750827	4.929582	2.656206
C	-4.272753	1.235955	-1.468550
C	-5.149145	1.674087	-2.694827
N	-4.273714	2.191746	-0.349304
C	-5.322091	0.457951	-3.637882
C	-6.546932	2.066783	-2.154597
C	-4.560180	2.867414	-3.477328
C	-3.375533	3.276984	-0.209765
C	-4.980668	1.944964	0.855465

H	-4.364539	0.155696	-4.088499	H	-7.475410	-0.925519	4.218864
H	-5.735699	-0.413313	-3.098936	H	-8.721068	-3.528260	1.754430
H	-6.993525	1.258140	-1.548420	H	-9.185097	-2.087695	2.708636
H	-6.505300	2.977910	-1.531362	H	-8.097249	-1.914434	1.307478
H	-4.462222	3.764167	-2.842661	H	-8.456811	-3.124328	4.815668
H	-3.566274	2.629419	-3.887647	H	-7.990400	-4.631148	3.986919
O	-2.581720	3.656670	-1.067823	H	-6.822314	-3.788309	5.053407
C	-3.594303	3.817496	1.165122	C	5.869976	-5.662719	2.941643
O	-5.751474	1.003799	1.038906	C	4.527140	-5.841997	3.700748
C	-4.570940	3.028102	1.798213	C	6.096335	-6.873248	1.996720
C	-2.980909	4.890711	1.804606	C	7.016409	-5.641629	3.977154
C	-4.966902	3.311619	3.103637	H	4.358493	-5.010053	4.407688
C	-3.366615	5.205998	3.135016	H	3.662240	-5.876394	3.016000
C	-4.357879	4.406187	3.752705	H	4.541916	-6.784838	4.278265
H	-4.750727	0.330294	-1.046270	H	7.044934	-6.771539	1.439460
H	-0.210089	4.488123	-1.246378	H	6.143223	-7.807377	2.585777
H	4.130144	0.381003	-2.152674	H	5.281349	-6.985509	1.260842
H	-0.912824	-4.558989	-1.670730	H	7.029488	-6.597539	4.530430
H	5.547824	2.704408	0.150390	H	8.004892	-5.521419	3.497333
H	5.140804	5.350995	3.587067	H	6.889691	-4.834193	4.721007
H	2.888096	6.067636	2.800224	C	6.922504	3.533648	2.421490
H	7.371934	-3.314072	3.179906	C	6.901097	1.996861	2.644629
H	7.238907	-1.220812	1.838590	C	7.973783	3.877803	1.331615
H	4.192998	-5.093114	0.801222	C	7.347353	4.215399	3.740628
H	-5.800335	-5.179004	3.632415	H	6.164332	1.721814	3.421145
H	-3.910798	-6.226465	2.389040	H	6.645451	1.450618	1.719886
H	-5.878724	-1.862088	0.816495	H	7.897627	1.654171	2.981546
H	-5.723909	2.703735	3.609983	H	8.014324	4.966540	1.147666
H	-4.667688	4.634990	4.776220	H	8.977691	3.546811	1.655861
H	-2.202534	5.459062	1.284101	H	7.749331	3.378278	0.373477
C	-2.699604	6.397828	3.850880	H	8.348719	3.854615	4.036196
C	-1.167534	6.154859	3.931653	H	7.409205	5.314231	3.637955
C	-2.972246	7.692565	3.037594	H	6.654095	3.982017	4.569337
C	-3.237036	6.603438	5.284231	H	6.386321	-1.323834	-4.632083
H	-0.944668	5.240054	4.510472	H	4.646244	-0.046183	-5.725934
H	-0.703254	6.050142	2.935876	H	4.289785	-2.526404	-5.358896
H	-0.681212	7.007068	4.441971	H	-2.908445	-6.457433	-4.148853
H	-4.055765	7.898849	2.970722	H	-1.156198	-5.186367	-5.281280
H	-2.488255	8.556512	3.528971	H	-3.515546	-4.236593	-5.115995
H	-2.573766	7.625126	2.010755	H	-6.023556	0.721192	-4.450864
H	-2.728800	7.468138	5.746855	H	-7.224034	2.274098	-3.002893
H	-4.322098	6.813883	5.294316	H	-5.232794	3.120457	-4.318297
H	-3.046284	5.724889	5.927347	H	1.927784	5.125375	-4.956281
C	-7.146630	-2.785340	3.109576	H	-0.547364	5.634437	-4.703987
C	-6.661583	-1.411571	3.648601	H	1.066013	7.064003	-3.584561
C	-8.354493	-2.567550	2.158928	C	-0.658825	0.623409	2.272988
C	-7.622626	-3.638649	4.305888	C	-0.693073	-0.180596	3.609249
H	-5.798528	-1.539360	4.327364	C	1.158479	-1.744534	2.875526
H	-6.362045	-0.725478	2.837660	C	0.694564	-0.770457	3.959943

H	-1.426224	-1.002871	3.510691
H	-1.053250	0.487025	4.414660
H	1.429958	0.049211	4.053843
H	0.650281	-1.259811	4.953824
N	-0.046181	-0.165009	1.225742
H	0.642784	-1.137399	1.839772
H	2.226861	-1.660890	2.611806
C	0.685489	-3.149767	2.884987
C	-0.225051	-3.653445	3.847576
C	1.145362	-4.045624	1.882362
C	-0.632233	-4.995515	3.827325
H	-0.604268	-2.994883	4.636612
C	0.725880	-5.379624	1.854044
H	1.814684	-3.671920	1.099234
C	-0.161013	-5.866809	2.832467
H	-1.324276	-5.360884	4.595319
H	1.072422	-6.041403	1.052850
H	-0.492295	-6.910075	2.804117
C	0.045575	1.995313	2.435406
H	-0.484035	2.596112	3.197296
H	1.096072	1.869694	2.750679
H	0.038466	2.541184	1.480533
H	-1.709930	0.820625	1.962724

R, R-cis-TS

SCF energy in CF_3CH_2OH: -4923.640799 a.u.
Free energy in CF_3CH_2OH: -4922.114494 a.u**.**

Rh	0.013873	0.046090	-3.159956
O	1.127099	1.766355	-3.050986
O	-1.095307	-1.691399	-3.182418
O	1.120738	1.748626	-0.759225
O	-1.255808	-1.632504	-0.897882
O	1.725866	-1.091329	-3.020874
O	-1.733558	1.139908	-3.194317
O	-1.807026	1.195590	-0.903207
O	1.624233	-1.100918	-0.729613
C	-2.272715	1.445638	-2.076803
C	2.134691	-1.438551	-1.862811
C	1.469906	2.217720	-1.905264
C	-1.495616	-2.140292	-2.056401
Rh	-0.079047	0.064884	-0.717777
C	3.400731	-2.321115	-1.727169
C	4.073672	-2.883633	-3.028839
N	3.118322	-3.339080	-0.702002
C	4.578049	-1.693842	-3.882138
C	5.302234	-3.720632	-2.594281
C	3.133535	-3.772534	-3.871699
C	1.919177	-4.087599	-0.614461
C	3.883683	-3.443570	0.490111
H	3.742966	-1.091338	-4.270342
H	5.234379	-1.025722	-3.296262
H	5.995350	-3.134302	-1.964463
H	5.005511	-4.620813	-2.027054
H	2.796990	-4.660739	-3.310712
H	2.241027	-3.217740	-4.201013
O	1.030023	-4.108396	-1.462740
C	1.975886	-4.802162	0.696094
O	4.911084	-2.811331	0.726233
C	3.164071	-4.430591	1.349741
C	1.064101	-5.686397	1.265628
C	3.472970	-4.955929	2.602906
C	1.354729	-6.243449	2.539704
C	2.560325	-5.865017	3.177896
C	2.352421	3.489374	-1.823216
C	2.727036	4.213078	-3.167654
N	3.508495	3.198705	-0.961933
C	1.419436	4.690982	-3.844948
C	3.570024	5.465187	-2.819217
C	3.536752	3.325787	-4.138931
C	4.317014	2.042285	-1.023740
C	3.874738	4.038406	0.129277
H	0.791929	3.844950	-4.164571
H	0.821545	5.325012	-3.164427
H	3.054564	6.120407	-2.095157
H	4.553643	5.195525	-2.394808
H	4.483245	2.983194	-3.686658
H	2.966015	2.437788	-4.450383
O	4.167465	1.105733	-1.806600
C	5.352395	2.211920	0.041452
O	3.280924	5.059059	0.461472
C	5.090269	3.409563	0.727894
C	6.440365	1.405031	0.358383
C	5.924789	3.826655	1.762159
C	7.320966	1.811187	1.395552
C	7.037945	3.018939	2.077377
C	-3.674992	2.103702	-2.067749
C	-4.279093	2.618125	-3.424793
N	-3.713930	3.086137	-0.975223
C	-4.545434	1.396588	-4.338974
C	-5.640348	3.286282	-3.109088
C	-3.377198	3.634771	-4.158035
C	-2.726131	4.074030	-0.729888
C	-4.634236	2.990239	0.098017
H	-3.609240	0.894224	-4.626378
H	-5.195013	0.654856	-3.839612

H	-6.305159	2.611651	-2.540010	H	-6.177767	-0.552424	0.486102
H	-5.514896	4.215923	-2.525925	C	-7.535144	-0.962890	2.873720
H	-3.184336	4.530342	-3.544569	C	-6.903614	0.424403	3.173418
H	-2.405810	3.190179	-4.426626	C	-8.722729	-0.783602	1.889565
O	-1.764517	4.317250	-1.452430	C	-8.084839	-1.545618	4.194185
C	-3.107617	4.713642	0.566753	H	-6.062015	0.326766	3.883431
O	-5.538689	2.159057	0.181952	H	-6.528082	0.919662	2.261054
C	-4.256650	4.069717	1.057791	H	-7.661077	1.087205	3.632365
C	-2.496230	5.755508	1.256267	H	-9.194930	-1.754289	1.653827
C	-4.825852	4.467772	2.265937	H	-9.490745	-0.128951	2.340951
C	-3.050010	6.181875	2.492323	H	-8.404358	-0.319037	0.940601
C	-4.210094	5.525178	2.967413	H	-8.846739	-0.861685	4.608603
C	-2.298465	-3.463748	-1.996154	H	-8.568893	-2.527916	4.043498
C	-2.783043	-4.118548	-3.338209	H	-7.294074	-1.659980	4.957941
N	-3.357725	-3.294196	-0.989105	C	0.355035	-7.229263	3.177597
C	-1.540745	-4.545948	-4.158333	C	-1.005014	-6.509773	3.391336
C	-3.580069	-5.396288	-2.974514	C	0.152637	-8.437969	2.223916
C	-3.678437	-3.191307	-4.187780	C	0.842303	-7.766913	4.541320
C	-4.193978	-2.156730	-0.881289	H	-0.890365	-5.649919	4.076212
C	-3.446658	-4.115725	0.164441	H	-1.439215	-6.139186	2.446635
H	-0.958443	-3.675101	-4.496178	H	-1.731004	-7.211083	3.843504
H	-0.873026	-5.198709	-3.567343	H	1.103802	-8.973642	2.052938
H	-2.990152	-6.078887	-2.336714	H	-0.567688	-9.150752	2.665959
H	-4.519396	-5.158738	-2.443783	H	-0.245147	-8.126779	1.242717
H	-4.587383	-2.887009	-3.642455	H	0.094599	-8.471685	4.946666
H	-3.141023	-2.278930	-4.491137	H	1.798959	-8.313682	4.453331
O	-4.253065	-1.240367	-1.698103	H	0.969820	-6.958432	5.284042
C	-4.940385	-2.316032	0.402732	C	8.549708	0.937838	1.722008
O	-2.751008	-5.107634	0.378057	C	8.079075	-0.480797	2.142513
C	-4.508918	-3.504988	1.017895	C	9.440292	0.828800	0.454202
C	-5.898322	-1.488300	0.981432	C	9.406378	1.524708	2.865712
C	-5.050074	-3.902940	2.238694	H	7.486179	-0.441163	3.074146
C	-6.470933	-1.870745	2.224191	H	7.455826	-0.965308	1.371720
C	-6.033948	-3.077125	2.822213	H	8.955579	-1.129483	2.325637
H	-1.598698	-4.184192	-1.527427	H	9.800183	1.823346	0.134572
H	-4.344339	1.291772	-1.717100	H	10.321723	0.195124	0.663674
H	1.760455	4.212608	-1.228571	H	8.896483	0.376975	-0.393436
H	4.148842	-1.660711	-1.245763	H	10.268383	0.861342	3.057898
H	-1.597833	6.223679	0.840868	H	9.806844	2.523387	2.612949
H	-4.652138	5.840768	3.916572	H	8.835985	1.607203	3.808862
H	-5.719847	3.973592	2.660164	C	-2.373964	7.332468	3.265356
H	7.704369	3.350593	2.878789	C	-0.907004	6.937198	3.586749
H	5.727608	4.755976	2.306404	C	-2.381548	8.609849	2.382354
H	6.604710	0.476539	-0.197984	C	-3.092187	7.656455	4.593731
H	2.800829	-6.284957	4.158519	H	-0.868269	6.030299	4.216375
H	4.392972	-4.671388	3.124130	H	-0.320826	6.737034	2.673256
H	0.135389	-5.924372	0.736177	H	-0.405892	7.756897	4.133710
H	-4.722068	-4.825436	2.728932	H	-3.414282	8.921408	2.143477
H	-6.466701	-3.387084	3.777457	H	-1.886403	9.441961	2.915694

H	-1.845141	8.455238	1.430126
H	-2.565575	8.481607	5.105476
H	-4.136206	7.981082	4.431811
H	-3.099122	6.791436	5.281670
H	3.755845	6.047219	-3.740005
H	1.666432	5.294619	-4.737477
H	3.790552	3.913225	-5.041226
H	5.853252	-4.057191	-3.490999
H	5.159152	-2.080391	-4.739871
H	3.675090	-4.125317	-4.769390
H	-1.867963	-5.111502	-5.050128
H	-3.848656	-5.937228	-3.899812
H	-3.994591	-3.728057	-5.101806
H	-3.878282	3.960425	-5.088897
H	-5.057055	1.733046	-5.259553
H	-6.148007	3.551236	-4.054221
C	-1.497075	-0.385976	1.965065
C	-1.219289	-1.577491	2.930684
C	1.187301	-0.820991	3.225578
C	-0.095935	-1.256602	3.936983
H	-0.933507	-2.452907	2.318299
H	-2.154070	-1.839682	3.461676
H	-0.440264	-0.474956	4.637846
H	0.105357	-2.153860	4.557666
N	-0.285300	-0.052893	1.247373
H	0.688913	-0.251835	2.153225
H	1.696481	-1.667773	2.731409
C	2.141155	0.104073	3.872852
C	3.521797	0.028088	3.547614
C	1.736964	1.109633	4.790031
C	4.450401	0.902218	4.123508
H	3.859612	-0.734278	2.834943
C	2.668082	1.981752	5.366781
H	0.678590	1.212084	5.054065
C	4.031570	1.882901	5.039893
H	5.508371	0.822630	3.851281
H	2.327607	2.746249	6.075012
H	4.759186	2.566671	5.491249
C	-2.066002	0.863640	2.681935
H	-2.289371	1.647336	1.941333
H	-2.997813	0.603797	3.217577
H	-1.344414	1.278267	3.406923
H	-2.246093	-0.723460	1.218943