Electronic Supplementary Information

Isotope Exchange Reaction in Tritium-contaminated Vacuum Pump Oil: Mechanism and HTO's Effect

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HTO:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.221459	-0.746227	0.219425
2	8	0	-1.427490	-1.077315	1.095694
3	1	0	-1.836136	-1.932500	0.948183

Zero-point Energies= -76.403385 au

H_2O:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.221459	-0.746227	0.219425
2	8	0	-1.427490	-1.077315	1.095694
3	1	0	-1.836136	-1.932500	0.948183

Zero-point Energies= -76.399270 au

CH_4:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.099261	-0.166720	0.179993
2	1	0	0.194287	0.669275	-0.453295
3	1	0	-0.912891	-0.713313	-0.294862
4	1	0	0.751341	-0.832012	0.320953
5	1	0	-0.430552	0.209276	1.146948

Zero-point Energies= -40.451869 au

$TS_{CH4\text{-}HTO}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.024503	-0.179398	0.122422
2	1	0	0.409317	1.096239	-0.407830
3	1	0	-0.682681	-0.787206	-0.498108
4	1	0	0.622674	-0.817098	0.726687
5	1	0	-0.650501	0.378659	0.827089
6	1	0	1.005031	0.301880	-0.789527
7	8	0	1.368913	1.443401	-1.134380
8	1	0	1.138119	1.701807	-2.035065

Zero-point Energies= -116.735050 au

$TS_{CH4\text{-}2HTO\text{-}1}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.052730	-0.175659	0.123296
2	1	0	-0.978396	0.088694	-0.135512
3	1	0	0.099899	-1.258472	-0.035114
4	1	0	0.184783	0.010063	1.192197
5	1	0	0.429804	1.028040	-0.648901
6	8	0	0.906960	1.886152	-1.306770
7	1	0	1.877840	1.174653	-1.350589
8	8	0	2.355254	0.084951	-1.163756
9	1	0	3.137141	0.055651	-0.606323
10	1	0	1.365136	-0.135933	-0.557405
11	1	0	1.007248	2.706660	-0.817520

Zero-point Energies= -193.175607 au

TS_{CH3T} ($TS_{CH4\text{-}2HTO\text{-}2}$):

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016807	-0.158654	0.108142
2	1	0	-0.869203	-0.449787	-0.461431
3	1	0	0.448324	-1.087410	0.499976
4	1	0	-0.306453	0.394417	0.995388
5	1	0	0.419218	1.108590	-0.534933
6	8	0	0.906753	2.029911	-1.088637
7	1	0	0.361423	2.341812	-1.815800
8	1	0	1.762471	1.246287	-1.403781
9	8	0	2.209810	0.130631	-1.355899
10	1	0	3.048379	0.050272	-0.893584
11	1	0	1.288671	-0.102769	-0.653740

Zero-point Energies= -193.176909 au

CH_3T:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.099261	-0.166720	0.179993
2	1	0	0.194287	0.669275	-0.453295
3	1	0	-0.912891	-0.713313	-0.294862
4	1	0	0.751341	-0.832012	0.320953
5	1	0	-0.430552	0.209276	1.146948

Zero-point Energies= -40.456003 au

C_2H_6:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.758675	0.073450	-0.000337
2	6	0	0.768100	0.055475	0.000361
3	1	0	-1.144144	0.934447	0.549363
4	1	0	-1.165063	-0.826287	0.465783
5	1	0	1.174488	0.955199	-0.465783
6	1	0	1.153569	-0.805537	-0.549315
7	1	0	-1.153068	0.126427	-1.017011
8	1	0	1.162492	0.002526	1.017037

Zero-point Energies= -79.722272 au

TS_{C2H5T}:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.478641	0.723861	-0.598269
2	6	0	1.035164	0.857952	-0.794668
3	1	0	-0.893919	1.646911	-0.175887
4	1	0	1.307778	1.711100	-1.420924
5	1	0	1.451912	-0.036315	-1.267412
6	1	0	-0.991644	0.631249	-1.562913
7	1	0	1.542480	0.977547	0.166048
8	1	0	-0.703584	0.159834	0.705864
9	8	0	-0.744394	-0.488323	1.733753
10	1	0	-1.495905	-0.267003	2.289631
11	1	0	-0.920234	-1.415864	0.986651
12	8	0	-1.019235	-1.827465	-0.137953
13	1	0	-0.798400	-0.670729	-0.441241
14	1	0	-0.320279	-2.429154	-0.406378

Zero-point Energies= -232.446321 au

C_2H_5T:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.758675	0.073450	-0.000337
2	6	0	0.768100	0.055475	0.000361
3	1	0	-1.144144	0.934447	0.549363
4	1	0	-1.165063	-0.826287	0.465783
5	1	0	1.174488	0.955199	-0.465783
6	1	0	1.153569	-0.805537	-0.549315
7	1	0	-1.153068	0.126427	-1.017011
8	1	0	1.162492	0.002526	1.017037

Zero-point Energies= -79.726755 au

C_3H_8:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.458518	0.175838	-0.078221
2	6	0	-0.086086	-0.493140	-0.064754
3	6	0	1.039392	0.510333	0.176698
4	1	0	-1.515548	0.929500	-0.868333
5	1	0	-2.258554	-0.547956	-0.246221
6	1	0	-1.653914	0.678589	0.872836
7	1	0	0.079839	-1.007639	-1.015960
8	1	0	-0.061621	-1.263626	0.711737
9	1	0	0.906594	1.017741	1.136046
10	1	0	2.017474	0.025127	0.186253
11	1	0	1.051142	1.275832	-0.603882

Zero-point Energies= -118.997039 au

$TS_{CH3\text{-}CH2\text{-}CH2T}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.490777	0.139264	-0.133559
2	6	0	-0.101739	-0.511459	-0.101270
3	6	0	0.981323	0.491847	0.294011
4	1	0	-1.506478	0.897607	-0.929000
5	1	0	-2.268180	-0.574957	-0.425273
6	1	0	0.148045	-0.952445	-1.071714
7	1	0	-0.101443	-1.342858	0.613913
8	1	0	0.772348	0.932622	1.273161
9	1	0	1.968809	0.027168	0.333881
10	1	0	1.025213	1.314842	-0.424831
11	1	0	-1.684024	1.327113	0.691122
12	8	0	-1.766630	2.181063	1.547491
13	1	0	-2.508350	2.777239	1.414636
14	1	0	-1.991905	1.262707	2.277935
15	8	0	-2.121635	0.068427	2.432725
16	1	0	-1.446717	-0.345167	2.977151
17	1	0	-1.859060	0.028486	1.250423

Zero-point Energies= -271.722045 au

$CH_3\text{-}CH_2\text{-}CH_2T$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.458518	0.175838	-0.078221
2	6	0	-0.086086	-0.493140	-0.064754
3	6	0	1.039392	0.510333	0.176698
4	1	0	-1.515548	0.929500	-0.868333
5	1	0	-2.258554	-0.547956	-0.246221
6	1	0	-1.653914	0.678589	0.872836
7	1	0	0.079839	-1.007639	-1.015960
8	1	0	-0.061621	-1.263626	0.711737
9	1	0	0.906594	1.017741	1.136046
10	1	0	2.017474	0.025127	0.186253
11	1	0	1.051142	1.275832	-0.603882

Zero-point Energies= -119.001507 au

$TS_{CH3\text{-}CHT\text{-}CH3}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.206890	-1.324976	-1.170052
2	6	0	-1.483550	0.361734	-0.058729
3	6	0	-0.116576	-0.319883	-0.198100
4	6	0	1.024236	0.561550	0.316497
5	1	0	-1.511854	1.295567	-0.630370
6	1	0	-2.290285	-0.278350	-0.424691
7	1	0	-1.702319	0.614547	0.983522
8	1	0	-0.150366	-1.229226	0.417991

9	1	0	0.877000	0.842964	1.364260
10	1	0	1.990570	0.056268	0.239058
11	1	0	1.091060	1.483923	-0.268186
12	8	0	0.448155	-2.068587	-2.130919
13	1	0	1.323189	-2.463988	-2.106818
14	1	0	0.382993	-1.066375	-2.759913
15	1	0	-0.596229	0.423917	-3.252435
16	8	0	0.189709	0.140658	-2.779116
17	1	0	-0.005822	-0.050442	-1.574098

Zero-point Energies= -271.719887 au

CH_3-CHT-CH_3:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.458518	0.175838	-0.078221
2	6	0	-0.086086	-0.493140	-0.064754
3	6	0	1.039392	0.510333	0.176698
4	1	0	-1.515548	0.929500	-0.868333
5	1	0	-2.258554	-0.547956	-0.246221
6	1	0	-1.653914	0.678589	0.872836
7	1	0	0.079839	-1.007639	-1.015960
8	1	0	-0.061621	-1.263626	0.711737
9	1	0	0.906594	1.017741	1.136046
10	1	0	2.017474	0.025127	0.186253
11	1	0	1.051142	1.275832	-0.603882

Zero-point Energies= -119.001744 au

C_2H_4:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.929077	0.080310	0.000000
2	6	0	0.396177	0.045190	0.000000
3	1	0	-1.472755	1.018309	0.000000
4	1	0	-1.521478	-0.827843	0.000000
5	1	0	0.988578	0.953343	0.000000
6	1	0	0.939855	-0.892809	0.000000

Zero-point Energies= -78.512292 au

TS_{C2H3T}:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.289763	0.409062	0.009034
2	6	0	0.026565	0.290036	-0.202145
3	1	0	-1.978928	-0.387632	-0.269160
4	1	0	-1.752567	1.281170	0.468538
5	1	0	0.643295	1.131975	0.117571
6	1	0	0.491895	-1.098321	-0.028569
7	8	0	0.823038	-2.217315	-0.182694
8	1	0	1.634060	-2.414107	0.293978
9	1	0	0.967990	-1.932844	-1.339053

10	8	0	0.902029	-1.131401	-2.235945
11	1	0	0.468645	-0.390133	-1.431725
12	1	0	0.256542	-1.325189	-2.921131

Zero-point Energies= -231.246474 au

C_2H_3T:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.929077	0.080310	0.000000
2	6	0	0.396177	0.045190	0.000000
3	1	0	-1.472755	1.018309	0.000000
4	1	0	-1.521478	-0.827843	0.000000
5	1	0	0.988578	0.953343	0.000000
6	1	0	0.939855	-0.892809	0.000000

Zero-point Energies= -78.516626 au

C_3H_6:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.459366	-0.253860	0.243484
2	6	0	-0.379175	0.466430	-0.035202
3	6	0	1.012743	-0.082088	-0.128790
4	1	0	-1.392775	-1.322060	0.425688
5	1	0	-0.490300	1.534283	-0.211118
6	1	0	1.672831	0.405960	0.593531
7	1	0	1.026048	-1.156227	0.063027
8	1	0	1.436415	0.096964	-1.120818
9	1	0	-2.443121	0.196499	0.299798

Zero-point Energies= -117.791794 au

$TS_{CH2T\text{-}CH=CH2}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.607532	0.200833	0.400911
2	6	0	-0.435280	0.384109	-0.213491
3	6	0	0.859030	-0.258274	0.135903
4	1	0	-1.686674	-0.415689	1.291632
5	1	0	-0.428006	1.019992	-1.100001
6	1	0	0.909435	-0.408992	1.221823
7	1	0	1.712655	0.366989	-0.136409
8	1	0	-2.514119	0.671935	0.041904
9	1	0	1.008233	-1.821821	0.230719
10	8	0	0.992248	-2.939053	0.066934
11	1	0	1.832340	-3.336041	0.314965
12	1	0	0.856825	-2.700925	-1.110515
13	1	0	-0.145577	-1.862611	-2.365712
14	8	0	0.741350	-1.897529	-1.992633
15	1	0	0.821372	-1.120624	-1.192430

Zero-point Energies= -270.520481 au

$CH_2T\text{-}CH{=}CH_2$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.459366	-0.253860	0.243484
2	6	0	-0.379175	0.466430	-0.035202
3	6	0	1.012743	-0.082088	-0.128790
4	1	0	-1.392775	-1.322060	0.425688
5	1	0	-0.490300	1.534283	-0.211118
6	1	0	1.672831	0.405960	0.593531
7	1	0	1.026048	-1.156227	0.063027
8	1	0	1.436415	0.096964	-1.120818
9	1	0	-2.443121	0.196499	0.299798

Zero-point Energies= -117.796246 au

$TS_{CH3\text{-}CT=CH2}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.480503	1.335558	-1.142149
2	6	0	-1.352105	-0.358974	0.134472
3	6	0	-0.233509	0.334788	-0.102653
4	6	0	1.120093	-0.326136	-0.001007
5	1	0	-1.347693	-1.415468	0.407968
6	1	0	1.746451	0.180443	0.739398
7	1	0	1.047078	-1.381985	0.278659
8	1	0	1.657653	-0.265272	-0.952471
9	1	0	-2.333219	0.104319	0.052351
10	8	0	-0.729498	2.317878	-1.768227
11	1	0	-0.524621	2.915171	-0.748450
12	1	0	-0.953147	3.218936	1.009989
13	8	0	-0.253471	2.914604	0.425643
14	1	0	-0.255362	1.728679	0.325029
15	1	0	-0.093746	2.472057	-2.472153

Zero-point Energies= -270.524679 au

$CH_3\text{-}CT{=}CH_2$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.459366	-0.253860	0.243484
2	6	0	-0.379175	0.466430	-0.035202
3	6	0	1.012743	-0.082088	-0.128790
4	1	0	-1.392775	-1.322060	0.425688
5	1	0	-0.490300	1.534283	-0.211118
6	1	0	1.672831	0.405960	0.593531
7	1	0	1.026048	-1.156227	0.063027
8	1	0	1.436415	0.096964	-1.120818
9	1	0	-2.443121	0.196499	0.299798

Zero-point Energies= -117.796325 au

$TS_{CH3\text{-}CH=CHT}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.425937	0.628881	0.344687
2	1	0	-0.630686	0.362368	1.641305
3	8	0	-1.204606	0.895930	2.563085
4	1	0	-1.477723	0.263924	3.233040
5	6	0	-0.167450	-0.050799	0.351346
6	6	0	0.909813	0.643497	-0.042641
7	6	0	2.070902	0.121822	-0.834374
8	1	0	-0.194847	-1.105004	0.065881
9	1	0	0.979438	1.698739	0.233662
10	1	0	3.004838	0.245921	-0.278000
11	1	0	1.941684	-0.934637	-1.072774
12	1	0	2.184066	0.681514	-1.767842
13	8	0	-2.466606	1.176111	0.627834
14	1	0	-2.539997	2.041641	0.217427
15	1	0	-2.047288	1.176491	1.756564

Zero-point Energies= -270.528399 au

CH_3-CH=CHT:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.459366	-0.253860	0.243484
2	6	0	-0.379175	0.466430	-0.035202
3	6	0	1.012743	-0.082088	-0.128790
4	1	0	-1.392775	-1.322060	0.425688
5	1	0	-0.490300	1.534283	-0.211118
6	1	0	1.672831	0.405960	0.593531
7	1	0	1.026048	-1.156227	0.063027
8	1	0	1.436415	0.096964	-1.120818
9	1	0	-2.443121	0.196499	0.299798

Zero-point Energies= -117.796271 au

CH_3CH_2OH:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.326389	0.209170	-0.141392
2	6	0	0.066947	-0.130429	0.343365
3	8	0	0.882511	-0.328724	-0.802333
4	1	0	-1.301341	1.112369	-0.753204
5	1	0	-1.998221	0.376126	0.702783
6	1	0	-1.721921	-0.606525	-0.748627
7	1	0	0.461862	0.686407	0.959872
8	1	0	0.041830	-1.037422	0.959538
9	1	0	1.769024	-0.562073	-0.519903

Zero-point Energies= -154.932147 au

$TS_{CH2T\text{-}CH2\text{-}OH}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.796845	1.389864	0.858495
2	8	0	-2.442268	1.862388	1.723554
3	1	0	-3.116958	0.884272	1.628562
4	8	0	-3.342130	-0.172330	1.075276
5	1	0	-2.422353	0.113190	0.392404
6	6	0	-1.172436	0.597086	-0.236917
7	6	0	-0.079145	-0.335603	0.232954
8	8	0	0.947983	-0.400775	-0.754756
9	1	0	-0.722728	1.567625	-0.484547
10	1	0	-1.565030	0.239656	-1.196797
11	1	0	0.342546	0.023944	1.182331
12	1	0	-0.490078	-1.337340	0.413828
13	1	0	1.622103	-1.019643	-0.463788
14	1	0	-4.166275	-0.215117	0.582928
15	1	0	-1.954985	1.941382	2.548172

Zero-point Energies= -307.658180 au

$CH_2T\text{-}CH_2\text{-}OH$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.326389	0.209170	-0.141392
2	6	0	0.066947	-0.130429	0.343365
3	8	0	0.882511	-0.328724	-0.802333
4	1	0	-1.301341	1.112369	-0.753204
5	1	0	-1.998221	0.376126	0.702783
6	1	0	-1.721921	-0.606525	-0.748627
7	1	0	0.461862	0.686407	0.959872
8	1	0	0.041830	-1.037422	0.959538
9	1	0	1.769024	-0.562073	-0.519903

Zero-point Energies= -154.936641 au

$TS_{CH3\text{-}CHT\text{-}OH}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.266802	0.280899	-0.568964
2	6	0	-0.226284	-0.135033	0.465262
3	8	0	0.929435	-0.585913	-0.257819
4	1	0	-0.912315	1.116437	-1.178488
5	1	0	-2.191497	0.586827	-0.074936
6	1	0	-1.485862	-0.554146	-1.238913
7	1	0	0.082600	1.270167	0.707220
8	1	0	-0.661484	-0.974183	1.028423
9	1	0	1.628843	-0.768117	0.376319
10	8	0	0.568341	2.341085	0.919148
11	1	0	1.015682	1.826887	1.847559
12	8	0	1.115311	0.767065	2.530641
13	1	0	0.314210	0.345427	1.691625
14	1	0	1.227802	2.554776	0.252239
15	1	0	0.785421	0.778724	3.431883

Zero-point Energies= -307.653337 au

CH_3-CHT-OH:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.326389	0.209170	-0.141392
2	6	0	0.066947	-0.130429	0.343365
3	8	0	0.882511	-0.328724	-0.802333
4	1	0	-1.301341	1.112369	-0.753204
5	1	0	-1.998221	0.376126	0.702783
6	1	0	-1.721921	-0.606525	-0.748627
7	1	0	0.461862	0.686407	0.959872
8	1	0	0.041830	-1.037422	0.959538
9	1	0	1.769024	-0.562073	-0.519903

Zero-point Energies= -154.936920 au

$TS_{CH3\text{-}CH2\text{-}OT}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.441382	0.189442	-0.072279
2	6	0	-0.057219	-0.222271	0.388111
3	8	0	0.795971	-0.397528	-0.742312
4	1	0	-1.402598	1.141812	-0.605890
5	1	0	-2.110810	0.302477	0.782659
6	1	0	-1.854456	-0.563694	-0.744696
7	1	0	0.373575	0.531477	1.058712
8	1	0	-0.092178	-1.171025	0.927710
9	1	0	1.911647	-0.494504	-0.444274
10	8	0	3.097816	-0.053622	-0.325277
11	1	0	2.726735	0.871250	-1.004579
12	8	0	1.893867	1.504179	-1.626063
13	1	0	1.066878	0.611328	-1.242578
14	1	0	1.762613	2.406251	-1.330534
15	1	0	3.793343	-0.581371	-0.721310

Zero-point Energies= -307.730242 au

CH_3-CH_2-OT:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.326389	0.209170	-0.141392
2	6	0	0.066947	-0.130429	0.343365
3	8	0	0.882511	-0.328724	-0.802333
4	1	0	-1.301341	1.112369	-0.753204
5	1	0	-1.998221	0.376126	0.702783
6	1	0	-1.721921	-0.606525	-0.748627
7	1	0	0.461862	0.686407	0.959872
8	1	0	0.041830	-1.037422	0.959538
9	1	0	1.769024	-0.562073	-0.519903

Zero-point Energies= -154.936937 au

CH_3CHO:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.002749	-0.103183	-0.224436
2	6	0	0.426311	-0.538454	-0.067101
3	1	0	0.989916	-0.041977	0.748732
4	8	0	0.963547	-1.363540	-0.753404
5	1	0	-1.035558	0.974857	-0.404189
6	1	0	-1.542279	-0.288897	0.708340
7	1	0	-1.476687	-0.636804	-1.046442

Zero-point Energies= -153.748587 au

$TS1_{CH2=CH-OT}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.999521	-0.292345	-0.005939
2	6	0	0.405162	-0.274340	-0.002361
3	8	0	1.097444	0.326744	-0.874980
4	1	0	-0.419200	2.775993	-0.816712
5	1	0	-1.494730	-0.750874	0.839407
6	1	0	-1.480815	-0.463217	-0.968116
7	1	0	-1.046616	1.123498	-0.401599
8	1	0	0.282111	1.273723	-1.275999
9	8	0	-0.639329	1.921810	-1.201448
10	1	0	0.953753	-0.690789	0.851956

Zero-point Energies= -230.099795 au

CH_2=CH-OT:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.965491	-0.451613	-0.004980
2	6	0	0.339064	-0.224034	0.093897
3	8	0	1.104873	0.481156	-0.775563
4	1	0	-1.469283	-1.029393	0.755760
5	1	0	-1.554388	-0.072562	-0.832975
6	1	0	0.557282	0.805822	-1.496813
7	1	0	0.937728	-0.596948	0.916314

Zero-point Energies= -153.738211 au

$TS2_{CH2T-CHO}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.968578	2.133437	0.075220
2	1	0	-1.450673	2.458009	-0.690787

3	1	0	0.036572	1.728889	-0.208307
4	6	0	-0.986730	-0.437295	0.081487
5	6	0	0.374246	-0.182819	0.319530
6	8	0	0.993756	0.811090	-0.159446
7	1	0	-1.441165	-1.264262	0.610745
8	1	0	-1.333580	-0.302455	-0.941704
9	1	0	-1.281794	1.006483	0.296313
10	1	0	0.919986	-0.792708	1.051280

Zero-point Energies= -230.101759 au

CH_2T-CHO:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.002749	-0.103183	-0.224436
2	6	0	0.426311	-0.538454	-0.067101
3	1	0	0.989916	-0.041977	0.748732
4	8	0	0.963547	-1.363540	-0.753404
5	1	0	-1.035558	0.974857	-0.404189
6	1	0	-1.542279	-0.288897	0.708340
7	1	0	-1.476687	-0.636804	-1.046442

Zero-point Energies= -153.753083 au

$TS_{CH3\text{-}CTO}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.016256	1.367935	1.939752
2	1	0	1.496368	0.216669	2.236651
3	8	0	1.517228	-0.911238	2.071957
4	1	0	0.702459	-0.817379	1.392971
5	6	0	-1.375941	-0.073653	-0.672049
6	6	0	-0.016923	-0.231523	-0.014056
7	8	0	0.905604	-0.680320	-0.688703
8	1	0	-1.355233	-0.411247	-1.711303
9	1	0	-1.682619	0.976545	-0.626814
10	1	0	-2.119363	-0.641916	-0.104390
11	1	0	0.391366	0.862686	1.207998
12	1	0	0.476069	1.823810	2.591875
13	1	0	2.257730	-1.163768	1.502911

Zero-point Energies= -306.473485 au

CH_3-CTO:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.002749	-0.103183	-0.224436
2	6	0	0.426311	-0.538454	-0.067101
3	1	0	0.989916	-0.041977	0.748732
4	8	0	0.963547	-1.363540	-0.753404
5	1	0	-1.035558	0.974857	-0.404189
6	1	0	-1.542279	-0.288897	0.708340
7	1	0	-1.476687	-0.636804	-1.046442

Zero-point Energies= -153.752981 au

CH_3COCH_3:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.016233	-0.122224	-0.232109
2	6	0	0.415808	-0.593234	-0.101943
3	6	0	1.258100	0.103770	0.944091
4	8	0	0.860562	-1.474093	-0.793480
5	1	0	2.266781	-0.303804	0.940544
6	1	0	-1.035793	0.941070	-0.485333
7	1	0	-1.534753	-0.235977	0.723352
8	1	0	-1.526949	-0.695582	-1.002879
9	1	0	0.807405	-0.026969	1.931457
10	1	0	1.288674	1.177746	0.743400

Zero-point Energies= -193.035356 au

$TS1_{CH2=COT-CH3}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.295026	-0.375996	-1.447156
2	6	0	-0.594086	0.296826	-0.638126
3	6	0	0.040828	-0.197803	0.629391
4	8	0	-0.591102	-1.093816	1.277253
5	1	0	-0.251161	1.299526	-0.890290
6	1	0	-1.680199	0.266130	-0.556495
7	6	0	1.228885	0.369026	1.143910
8	1	0	1.666874	1.196449	0.601126
9	1	0	1.951056	-0.342575	1.542385
10	1	0	-0.495688	0.189999	3.854887
11	1	0	0.710440	0.396263	2.501973
12	1	0	-0.268753	-0.876216	2.478904
13	8	0	0.187579	-0.274191	3.362114

Zero-point Energies= -269.386986 au

CH_2=COT-CH_3:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.326284	0.631828	-1.228254
2	6	0	-0.486441	0.278118	-0.596841
3	6	0	-0.012993	0.041408	0.800350
4	8	0	-1.036089	-0.405696	1.584819
5	1	0	-1.291164	1.016789	-0.594159
6	1	0	-0.890302	-0.648342	-1.011372
7	6	0	1.229904	0.233681	1.239300
8	1	0	1.995969	0.590023	0.566721
9	1	0	-0.714685	-0.554315	2.479147
10	1	0	1.506816	0.041205	2.269689

Zero-point Energies= -193.022146 au

$TS2_{CH3COCH2T}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.906784	2.198099	-0.104965
2	1	0	-1.387077	2.447502	-0.899280
3	1	0	0.081387	1.656794	-0.343445
4	6	0	-1.081734	-0.330943	0.262279
5	6	0	0.309518	-0.162140	0.446260
6	8	0	0.951921	0.734369	-0.189803
7	1	0	-1.588733	-1.046169	0.896816
8	1	0	-1.418973	-0.328085	-0.772927
9	6	0	1.074558	-0.945005	1.474249
10	1	0	1.826386	-0.313666	1.946693
11	1	0	0.410644	-1.382983	2.218514
12	1	0	1.591274	-1.759100	0.957255
13	1	0	-1.288389	1.125227	0.272155

Zero-point Energies= -269.388932 au

CH_3COCH_2T:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.016233	-0.122224	-0.232109
2	6	0	0.415808	-0.593234	-0.101943
3	6	0	1.258100	0.103770	0.944091
4	8	0	0.860562	-1.474093	-0.793480
5	1	0	2.266781	-0.303804	0.940544
6	1	0	-1.035793	0.941070	-0.485333
7	1	0	-1.534753	-0.235977	0.723352
8	1	0	-1.526949	-0.695582	-1.002879
9	1	0	0.807405	-0.026969	1.931457
10	1	0	1.288674	1.177746	0.743400

Zero-point Energies= -193.039780 au

CH_3COOH:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.951219	-0.101509	-0.182994
2	6	0	0.464803	-0.587143	-0.077509
3	8	0	1.147956	0.083426	0.873941
4	8	0	0.965225	-1.456345	-0.734211
5	1	0	2.045036	-0.275709	0.890422
6	1	0	-0.953049	0.962308	-0.424531
7	1	0	-1.449528	-0.223398	0.779667
8	1	0	-1.470424	-0.665030	-0.952985

Zero-point Energies= -229.002259 au

$TS_{CH2T\text{-}COOH}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.049300	0.743468	-1.474895
2	6	0	-1.038368	-0.345117	-0.104396
3	6	0	0.386022	-0.598644	-0.086103
4	8	0	1.046007	0.242793	0.818687
5	8	0	1.054324	-1.323580	-0.783425
6	1	0	1.976574	-0.009490	0.771337
7	1	0	-1.443506	-0.247353	0.906466
8	1	0	-1.572506	-1.121806	-0.645851
9	1	0	-1.002595	1.397311	0.287559
10	8	0	-0.662908	2.371824	0.181310
11	1	0	-0.700767	2.287178	-0.958399
12	8	0	-0.854206	1.616413	-2.034731
13	1	0	-1.588175	1.811705	-2.624748
14	1	0	0.251003	2.300498	0.501791

Zero-point Energies= -381.742206 au

$TS1_{CH2=C(OT)(OH)}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.004716	-0.282852	0.014473
2	6	0	0.401407	-0.283138	0.005668
3	8	0	1.065556	-0.825691	1.026048
4	8	0	1.096556	0.332594	-0.867423
5	1	0	1.995595	-0.582153	0.928140
6	1	0	-0.455326	2.788892	-0.808392
7	1	0	-1.479530	-0.739832	0.871637
8	1	0	-1.451979	-0.521717	-0.947314
9	1	0	-1.050594	1.154982	-0.441145
10	1	0	0.339638	1.251635	-1.229332
11	8	0	-0.623771	1.929118	-1.205030

Zero-point Energies= -305.347903 au

CH_2=C(OT)(OH):

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.978038	-0.458847	0.011319
2	6	0	0.334780	-0.263714	0.096867
3	8	0	1.094255	-0.769375	1.083811
4	8	0	1.101842	0.452097	-0.766671
5	1	0	2.003828	-0.488404	0.941323
6	1	0	-1.477439	-1.047310	0.763980
7	1	0	-1.547873	-0.034074	-0.801387
8	1	0	0.552826	0.810762	-1.469178

Zero-point Energies= -228.966046 au

$TS2_{CH2T-COOH}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.977686	2.137587	0.075798
2	1	0	-1.441716	2.483026	-0.691608
3	1	0	0.080977	1.688996	-0.177185
4	6	0	-0.996170	-0.438959	0.104017
5	6	0	0.370198	-0.189387	0.329115
6	8	0	1.047399	-0.963132	1.174917
7	8	0	0.981364	0.829748	-0.132170
8	1	0	1.896415	-0.532985	1.344224
9	1	0	-1.425721	-1.272127	0.643290
10	1	0	-1.290505	-0.362980	-0.939581
11	1	0	-1.304154	1.037713	0.274982

Zero-point Energies= -305.350374 au

CH_2T-COOH:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.951219	-0.101509	-0.182994
2	6	0	0.464803	-0.587143	-0.077509
3	8	0	1.147956	0.083426	0.873941
4	8	0	0.965225	-1.456345	-0.734211
5	1	0	2.045036	-0.275709	0.890422
6	1	0	-0.953049	0.962308	-0.424531
7	1	0	-1.449528	-0.223398	0.779667
8	1	0	-1.470424	-0.665030	-0.952985

Zero-point Energies= -229.006853 au

$TS_{CH3\text{-}COOT}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.659070	-0.543243	-0.910379
2	6	0	-0.509973	-0.292678	0.017784
3	8	0	-0.279405	-1.128171	0.942553
4	8	0	0.182392	0.757956	-0.134946
5	1	0	0.704138	-0.627374	1.563362
6	1	0	-1.482931	-0.058149	-1.867890
7	1	0	-2.554642	-0.109249	-0.459520
8	1	0	-1.818824	-1.612990	-1.028587
9	1	0	2.396011	-0.071291	1.651318
10	8	0	1.484482	0.212690	1.756962
11	1	0	1.029265	0.700518	0.804313

Zero-point Energies= -305.403435 au

CH_3-COOT:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.951219	-0.101509	-0.182994
2	6	0	0.464803	-0.587143	-0.077509

3	8	0	1.147956	0.083426	0.873941
4	8	0	0.965225	-1.456345	-0.734211
5	1	0	2.045036	-0.275709	0.890422
6	1	0	-0.953049	0.962308	-0.424531
7	1	0	-1.449528	-0.223398	0.779667
8	1	0	-1.470424	-0.665030	-0.952985

Zero-point Energies= -229.007290 au

$TS_{CH2OH-CH2T}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.728513	0.245404	0.211621
2	6	0	0.595523	-0.209989	-0.031761
3	1	0	-0.990633	1.283526	0.028024
4	1	0	-1.566510	-0.439488	0.153003
5	1	0	1.310953	0.496994	-0.434714
6	1	0	0.735555	-1.245460	-0.315384
7	8	0	-0.577647	0.252913	1.991714
8	1	0	-0.588588	1.120510	2.421375
9	1	0	0.442361	-0.058112	1.426822

Zero-point Energies= -154.828930 au

CH_2OH-CH2T:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.555908	0.427455	0.457857
2	6	0	0.746975	-0.170809	-0.028672
3	1	0	-0.590163	1.498174	0.222583
4	1	0	-1.403500	-0.056281	-0.042815
5	1	0	0.850611	-0.041536	-1.107842
6	1	0	0.779781	-1.236928	0.201482
7	8	0	-0.623889	0.223297	1.861729
8	1	0	-1.436606	0.607561	2.196265
9	1	0	1.590126	0.314122	0.465787

Zero-point Energies= -154.936644 au

$TS_{CH2=CHT}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.728501	0.245392	0.211641
2	6	0	0.595540	-0.209985	-0.031744
3	1	0	-0.990634	1.283510	0.028048
4	1	0	-1.566489	-0.439511	0.153023
5	1	0	1.310962	0.497010	-0.434691
6	1	0	0.735585	-1.245452	-0.315374
7	8	0	-0.577634	0.252899	1.991734
8	1	0	-0.588580	1.120494	2.421397
9	1	0	0.442374	-0.058119	1.426841

Zero-point Energies= -154.830705 au

$TS_{CH3\text{-}CHOH\text{-}CH2T}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.713134	0.263922	0.137296
2	6	0	0.613670	-0.216694	-0.026910
3	6	0	-1.073131	1.678094	-0.208301
4	1	0	-1.532799	-0.447020	0.116807
5	1	0	1.344441	0.468266	-0.444757
6	1	0	0.756604	-1.267014	-0.248006
7	1	0	-1.241806	1.730367	-1.287942
8	1	0	-1.979058	2.010770	0.297724
9	1	0	-0.249051	2.352613	0.032611
10	8	0	-0.593265	0.266511	1.985638
11	1	0	-0.645434	1.110650	2.455187
12	1	0	0.441262	-0.025463	1.374751

Zero-point Energies= -194.111183 au

CH_3-CHOH-CH_2T:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.759378	0.307487	0.303008
2	6	0	0.667169	-0.138760	0.012432
3	6	0	-1.017951	1.736252	-0.156591
4	1	0	-1.456965	-0.365262	-0.202690
5	1	0	0.878059	-0.106964	-1.058908
6	1	0	0.826794	-1.156000	0.372634
7	1	0	-0.860017	1.837626	-1.232748
8	1	0	-2.041691	2.031194	0.078286
9	1	0	-0.334670	2.426894	0.349458
10	8	0	-1.065762	0.157212	1.684280
11	1	0	-0.479134	0.731782	2.185159
12	1	0	1.381314	0.522221	0.515179

Zero-point Energies= -194.217939 au

$TS_{CH3\text{-}CH=CHT}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.641443	0.292899	0.326740
2	6	0	0.639735	-0.258831	0.057670
3	6	0	-1.149723	1.479376	-0.436341
4	1	0	-1.402831	-0.344288	0.764999
5	1	0	0.775736	0.456878	1.282684
6	1	0	1.218490	0.190633	-0.742726
7	1	0	-1.556215	1.120867	-1.386755
8	1	0	-1.938788	2.009392	0.096695
9	1	0	-0.333213	2.168040	-0.663031
10	8	0	-0.110016	0.994549	1.956632
11	1	0	-0.103714	1.954572	2.075744

12	1	0	0.788327	-1.318568	0.223153

Zero-point Energies= -194.113057 au

$TS_{CH2=CH-CH2T}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.862175	0.386087	0.246704
2	6	0	0.527796	-0.166323	0.140731
3	6	0	-1.246705	1.550028	-0.471763
4	1	0	-1.628624	-0.325324	0.537167
5	1	0	1.255196	0.642049	0.043100
6	1	0	0.581213	-0.774201	-0.767350
7	1	0	-0.506118	2.001117	-1.124317
8	1	0	-2.280535	1.646446	-0.778875
9	1	0	-1.091215	1.965068	0.882741
10	8	0	-0.879845	1.263214	1.878267
11	1	0	-0.050265	1.364325	2.365352
12	1	0	0.790544	-0.795016	0.991206

Zero-point Energies= -194.113168 au

$TS_{CH3-CHT-CH2OH}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.602570	0.304393	-0.015298
2	6	0	0.571804	-0.250354	-0.580720
3	1	0	-0.748057	1.379779	0.005220
4	1	0	-1.516548	-0.278147	0.040931
5	1	0	1.267357	0.457721	-1.022705
6	6	0	0.551623	-1.646931	-1.169176
7	1	0	0.217221	-1.659213	-2.211694
8	1	0	-0.116561	-2.296143	-0.596984
9	1	0	1.544159	-2.100473	-1.139438
10	8	0	-0.086818	0.027690	1.717132
11	1	0	0.061786	0.801269	2.279920
12	1	0	0.748238	-0.249622	0.850684

Zero-point Energies= -194.101807 au

CH_3-CHT-CH_2OH:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.592717	-0.006511	0.326205
2	6	0	0.725018	-0.558994	-0.197256
3	1	0	-1.112092	0.539792	-0.472824
4	1	0	-1.243923	-0.826370	0.638284
5	1	0	1.373459	0.276451	-0.486764
6	6	0	0.517353	-1.488221	-1.390367
7	1	0	0.018181	-0.968176	-2.212132
8	1	0	-0.101472	-2.345529	-1.113523
9	1	0	1.467575	-1.870754	-1.765833
10	8	0	-0.431024	0.811903	1.471401

11	1	0	0.150458	1.541479	1.243918
12	1	0	1.229534	-1.085703	0.617503

Zero-point Energies= -194.211069 au

$TS_{CH3-CT=CH2}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.633362	0.668975	0.451698
2	6	0	0.779199	0.650944	0.555946
3	1	0	-1.232573	1.188442	1.192782
4	1	0	-1.118378	0.532450	-0.509518
5	6	0	1.636317	0.500553	-0.684845
6	1	0	0.300766	-0.611796	1.061078
7	1	0	1.825479	1.457149	-1.182755
8	1	0	1.155089	-0.162360	-1.408866
9	1	0	2.606137	0.061995	-0.442303
10	8	0	-0.851939	-1.053188	1.026113
11	1	0	-1.323719	-1.206527	1.857453
12	1	0	1.202846	1.222840	1.376814

Zero-point Energies= -194.103786 au

$TS_{CH3-CHT(OOH)}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.033390	-0.120332	-0.239873
2	6	0	0.391983	-0.484970	0.137164
3	1	0	0.890352	0.098643	0.924048
4	8	0	0.721183	-1.744791	0.117355
5	1	0	-1.120512	0.951339	-0.423480
6	1	0	-1.720356	-0.391121	0.564796
7	1	0	-1.321195	-0.663049	-1.141148
8	8	0	1.686915	-1.457837	-1.430053
9	1	0	2.235027	-1.983411	-2.045793
10	1	0	1.120411	-0.239186	-0.869532

Zero-point Energies= -229.967206 au

CH_3-CHT(OOH):

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.116849	-0.005871	-0.270542
2	6	0	0.166025	-0.693273	0.148929
3	1	0	0.636781	-0.185240	0.995884
4	8	0	1.036427	-0.626789	-0.969637
5	1	0	-0.920838	1.030576	-0.547819
6	1	0	-1.827206	-0.016763	0.557573
7	1	0	-1.569149	-0.515941	-1.122240
8	8	0	2.277005	-1.193458	-0.560429
9	1	0	2.383691	-1.903053	-1.204648
10	1	0	-0.004386	-1.741588	0.417028

Zero-point Energies= -230.058631 au

$TS_{CH3\text{-}CHOH(OT)}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.966836	-0.094388	-0.239552
2	6	0	0.514655	-0.333693	-0.235350
3	1	0	1.026436	-0.002732	0.681949
4	8	0	1.176977	-0.277842	-1.356617
5	1	0	-1.124511	0.976550	-0.391714
6	1	0	-1.428242	-0.393795	0.701455
7	1	0	-1.418183	-0.633204	-1.072479
8	8	0	0.691250	-2.030499	-0.141275
9	1	0	1.321138	-2.313164	0.533728
10	1	0	1.208596	-1.558734	-1.070581

Zero-point Energies= -230.094450 au

CH_3-CHOH(OT):

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.002411	-0.111919	-0.383923
2	6	0	0.493328	-0.248376	-0.148789
3	1	0	1.044635	0.514260	-0.708572
4	8	0	0.989461	-1.467822	-0.600919
5	1	0	-1.364878	0.867157	-0.059248
6	1	0	-1.535766	-0.885991	0.174259
7	1	0	-1.220669	-0.226235	-1.446094
8	8	0	0.803283	-0.161789	1.230277
9	1	0	0.309980	0.564103	1.620452
10	1	0	0.674138	-2.150188	0.001655

Zero-point Energies= -230.161980 au

$TS_{CH2=CH(OT)}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.014880	-0.338865	-0.471322
2	6	0	0.407549	-0.277896	-0.468032
3	1	0	0.969418	0.433414	-1.058240
4	8	0	1.164335	-1.287928	-0.053127
5	1	0	-0.804750	0.425836	0.641207
6	1	0	-1.451498	-1.313553	-0.268510
7	1	0	-1.515911	0.242190	-1.235572
8	8	0	0.283144	0.968275	1.019972
9	1	0	0.743183	0.940251	1.868727
10	1	0	0.609513	-1.954529	0.368214

Zero-point Energies= -230.061231 au

$TS_{CH3\text{-}CT(OOH)\text{-}CH3}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.096593	-0.071366	-0.111805
2	6	0	0.411318	-0.302173	-0.059782
3	6	0	1.158304	0.138334	1.196157
4	8	0	0.836184	-1.404825	-0.616002
5	1	0	2.230185	0.001266	1.053277
6	1	0	-1.335928	0.974122	0.087366
7	1	0	-1.591200	-0.687517	0.644045
8	1	0	-1.476755	-0.348701	-1.094945
9	1	0	0.836648	-0.465377	2.049171
10	1	0	0.954314	1.186196	1.420734
11	8	0	1.559029	-0.427739	-2.013741
12	1	0	2.044955	-0.607437	-2.842815
13	1	0	0.890239	0.388516	-0.996659

Zero-point Energies= -269.247868 au

CH_3-CT(OOH)-CH_3:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.075859	-0.064344	-0.086891
2	6	0	0.427239	-0.213094	-0.240413
3	6	0	1.188604	0.153250	1.022736
4	8	0	0.612556	-1.586797	-0.581674
5	1	0	2.259622	0.000352	0.887214
6	1	0	-1.322391	0.974180	0.140733
7	1	0	-1.435450	-0.693463	0.730548
8	1	0	-1.587642	-0.355512	-1.004505
9	1	0	0.842000	-0.458921	1.859648
10	1	0	1.022631	1.204026	1.269736
11	8	0	1.972096	-1.753142	-0.974442
12	1	0	2.263826	-2.440495	-0.364668
13	1	0	0.782969	0.387661	-1.085322

Zero-point Energies= -269.340275 au

$TS_{CH3\text{-}COT(OH)\text{-}CH3}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.144829	-0.219447	0.029968
2	6	0	0.349919	-0.398001	-0.042282
3	6	0	1.116205	-0.083047	1.221866
4	8	0	0.813246	-1.352181	-0.810471
5	1	0	2.188755	-0.113204	1.026870
6	1	0	-1.422694	0.735606	0.475505
7	1	0	-1.539293	-1.031773	0.646692
8	1	0	-1.568685	-0.307209	-0.969108
9	1	0	0.887990	-0.873648	1.941625
10	1	0	0.826672	0.875403	1.654604
11	8	0	0.825205	0.806385	-1.208638
12	1	0	1.605626	1.306432	-0.939622
13	1	0	1.083039	-0.302217	-1.506069

Zero-point Energies= -269.380704 au

CH_3-COT(OH)-CH_3:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.173607	-0.208793	0.089440
2	6	0	0.336192	-0.185624	-0.072947
3	6	0	1.064217	-0.011682	1.257040
4	8	0	0.693720	-1.394183	-0.682891
5	1	0	2.143572	-0.004430	1.089141
6	1	0	-1.521722	0.717459	0.551765
7	1	0	-1.471491	-1.050379	0.716510
8	1	0	-1.630904	-0.314853	-0.894178
9	1	0	0.815906	-0.837633	1.924576
10	1	0	0.779412	0.925475	1.743045
11	8	0	0.732854	0.836042	-0.981256
12	1	0	0.682898	1.688004	-0.539837
13	1	0	1.595252	-1.297804	-1.006808

Zero-point Energies= -269.446164 au

$TS_{CH2=COT-CH3}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.216729	-0.138062	0.098820
2	6	0	0.220540	-0.504421	0.192293
3	6	0	1.057846	-0.127358	1.287997
4	8	0	0.588820	-1.423469	-0.674165
5	1	0	1.442733	0.857272	0.608438
6	1	0	-1.376812	0.831175	0.563990
7	1	0	-1.797234	-0.899944	0.630541
8	1	0	-1.528565	-0.109935	-0.942817
9	1	0	1.879282	-0.806121	1.504455
10	1	0	0.524361	0.228844	2.163048
11	8	0	1.072367	1.258359	-0.657939
12	1	0	1.167563	1.889787	-1.378568
13	1	0	1.536206	-1.589760	-0.594438

Zero-point Energies= -269.348444 au

$TS_{CH3-CT(OOH)-OH}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.183482	-0.686858	0.075611
2	8	0	1.027803	-0.318448	-0.824909
3	8	0	0.960849	-2.035076	-1.581958
4	1	0	1.363924	-2.497394	-2.342904
5	6	0	0.596297	-0.548165	1.538601
6	1	0	1.605555	-0.933658	1.666460
7	1	0	0.298430	-1.892105	-0.210286
8	1	0	-0.101062	-1.100306	2.165216
9	1	0	0.563735	0.507620	1.810828
10	8	0	-1.149409	-0.331497	-0.110413

11	1	0	-1.301005	-0.261814	-1.059746

Zero-point Energies= -305.193379 au

CH_3-CT(OOH)-OH:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.300672	-0.841999	0.003870
2	8	0	1.061545	0.118131	-0.710870
3	8	0	0.871081	-0.176484	-2.094399
4	1	0	0.613583	0.689172	-2.432447
5	6	0	0.588348	-0.580086	1.473207
6	1	0	1.063579	-1.441019	1.940659
7	1	0	0.636393	-1.829331	-0.332352
8	1	0	-0.349307	-0.366581	1.983916
9	1	0	1.250662	0.280268	1.573406
10	8	0	-1.064379	-0.692587	-0.241125
11	1	0	-1.228676	-0.950084	-1.153565

Zero-point Energies= -305.284183 au

$TS_{CH3\text{-}COT(OH)2}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.716954	-1.259901	-0.229827
2	6	0	0.534666	-1.356855	0.586524
3	8	0	1.807871	-1.106786	-0.604147
4	8	0	1.065171	-2.509372	0.894256
5	1	0	2.408965	-0.391668	-0.366382
6	1	0	-0.889012	-0.233846	-0.549487
7	1	0	-1.544454	-1.585946	0.403868
8	1	0	-0.637452	-1.919006	-1.090516
9	1	0	1.884293	-2.126420	0.047488
10	8	0	0.631115	-0.373649	1.506092
11	1	0	1.231590	-0.696204	2.190924

Zero-point Energies= -305.341949 au

CH_3-COT$(OH)_2$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.751889	-1.279889	-0.219556
2	6	0	0.574988	-1.318748	0.495912
3	8	0	1.566003	-0.936060	-0.418511
4	8	0	0.782621	-2.630421	0.943980
5	1	0	2.432117	-0.939331	0.000486
6	1	0	-0.933493	-0.266254	-0.572064
7	1	0	-1.536283	-1.579130	0.473121
8	1	0	-0.719035	-1.966531	-1.063352
9	1	0	1.623617	-2.700117	1.406317
10	8	0	0.508317	-0.422918	1.571520
11	1	0	1.341737	-0.410202	2.052246

Zero-point Energies= -305.391573 au

$TS2_{CH3COOT}$:

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.978090	2.138169	0.075191
2	1	0	-1.440287	2.483627	-0.693352
3	1	0	0.078962	1.690904	-0.175539
4	6	0	-0.995979	-0.439694	0.104723
5	6	0	0.370288	-0.189484	0.329655
6	8	0	1.048074	-0.964494	1.174057
7	8	0	0.981228	0.830160	-0.130565
8	1	0	1.897297	-0.534660	1.343070
9	1	0	-1.424806	-1.273223	0.644025
10	1	0	-1.290333	-0.364473	-0.938944
11	1	0	-1.305953	1.040667	0.273476

Zero-point Energies= -305.348550 au