ELECTRONIC SUPPORTING INFORMATION

Splitting the C-O bond in dialkylethers with bis(1,2,4-tri-t-butylcyclopentadienyl) cerium-hydride does not occur σ-bond metathesis: a joint combined experimental- DFT computational study of the mechanism.

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Coordinates, Energy (E) and Gibbs Free energy of all extrema calculated.

methane

E=-40.5086919
G=-40.483278

C	0.015187	-0.026305	-0.028305
H	-0.020397	0.035329	1.061091
H	1.055826	-0.046766	-0.357713
H	-0.487413	-0.937755	-0.357713
H	-0.486321	0.842333	-0.458359

ethane

E=-79.80958
G=-79.757631

C	-0.000023	0.000000	-0.062461
C	0.000023	0.000000	1.462461
H	1.019317	0.000000	1.862340
H	-0.509651	0.882731	1.862309
H	-0.509651	-0.882731	1.862309
H	-1.019317	0.000000	-0.462340
H	0.509651	0.882731	-0.462309
H	0.509651	-0.882731	-0.462309

propane

E=-119.112279
G=-119.033393

C	-0.025522	0.044206	-0.072237
C	-0.002489	0.004311	1.453520
H	0.990576	0.050626	-0.483133
H	-0.539131	-0.832551	-0.483133
H	-0.540099	0.935479	-0.445984
H	-1.031223	0.034015	1.835423
C	0.709082	-1.228166	2.005537
H	0.486154	0.910073	1.835422
H	0.713743	-1.236238	3.100415
H	0.221675	-2.150306	1.668751
H	1.751382	-1.267129	1.668751

butane

E=-158.414943
G=-158.310591

C	0.012252	0.021464	0.045461
C	0.028747	0.049929	1.571182
H	1.042829	0.053626	-0.334425
C	-0.695788	-1.205384	-0.528794
H	-0.475629	0.929858	-0.334277
H	-0.988578	0.054600	1.978920
H	0.540851	-0.829207	1.978754
H	0.542151	0.938300	1.953044
C	-0.712284	-1.233849	-2.054515
H	-0.207908	-2.113778	-0.149056
H	-1.726366	-1.237546	-0.148908
H	-1.225688	-2.122221	-2.436377
H	-1.224387	-0.354713	-2.462087
H	0.305042	-1.238520	-2.462253

propene

E=-117.8704352
G=-117.815511

C	0.043669	-0.009624	0.025246
H	-0.526393	-0.323346	0.908609
H	1.078195	0.139709	0.358561
H	0.033935	-0.832344	-0.695648
C	-0.520250	1.245646	-0.563616
C	-0.984307	1.371293	-1.806121
H	-0.543266	2.114702	0.095250
H	-1.381639	2.312560	-2.174716
H	-0.983544	0.534788	-2.501799

butene

E=-157.172733
G=-157.091433

C	0.081010	0.370189	0.165642
C	-0.085116	-0.288435	1.311820
C	1.296849	0.297282	-0.710193
H	-0.723560	1.015071	-0.193290
C	0.980281	-0.204039	-2.123314
H	1.748725	1.297121	-0.782492
H	2.048127	-0.349981	-0.242112
H	0.687028	-0.944801	1.707905
H	-0.994558	-0.195544	1.898576
H	1.879177	-0.217667	-2.747892
H	0.569708	-1.218213	-2.096126
H	0.242657	0.439016	-2.615873

Et-O-Et

Et2O

E=-233.586125
G=-233.479040

O	0.065119	0.000000	0.046198
C	0.022512	0.000000	1.455719
C	1.379823	0.000000	-0.464006
C	1.311180	0.000000	-1.978000
H	1.931337	0.886106	-0.102738
H	1.931337	-0.886106	-0.102738
C	-1.427841	0.000000	1.895600
H	0.547068	-0.886109	1.855115
H	0.547068	0.886109	1.855115
H	-1.498669	0.000000	2.987693
H	-1.943967	0.885798	1.514360
H	-1.943967	-0.885798	1.514360
H	2.317280	0.000000	-2.408665
H	0.779838	-0.885824	-2.337675
H	0.779838	0.885824	-2.337675

Cp2CeH

E=-419.8558335
G=-419.725269

C	0.675990	1.108596	-2.020810
C	1.525135	-0.025376	-1.918859
C	0.812095	-1.147707	-2.405643
C	-0.475511	-0.706323	-2.810803
C	-0.556420	0.688955	-2.582714
Ce	-0.471808	-0.419610	-0.000163
C	0.810397	-1.145502	2.406890
C	1.523272	-0.023111	1.920015
C	0.673455	1.110485	2.020513
C	-0.559216	0.690563	2.581605
C	-0.477776	-0.704525	2.810647
H	-2.301832	0.663752	-0.001508
H	2.549985	-0.021460	1.573296
H	0.939356	2.129208	1.762039
H	-1.409315	1.323811	2.798331
H	-1.249399	-1.318237	3.263163
H	1.200484	-2.153473	2.502765
H	2.551554	-0.024032	-1.571276
H	1.201742	-2.155942	-2.500542
H	-1.247070	-1.319924	-3.263576
H	-1.406005	1.322500	-2.800581
H	0.942208	2.127352	-1.762790

Et2O_act_CH_beta_adduct_Et2O

E=-653.4677573
G=-653.208521

C	-2.315140	2.110261	-2.554876
C	-1.339310	2.190130	-1.528110
C	-0.096337	2.500357	-2.133279
C	-0.305173	2.610392	-3.531618
C	-1.677970	2.375720	-3.791771
Ce	-0.705979	-0.146530	-2.956670
C	-0.491876	-2.456999	-1.273786
C	-1.174281	-2.920558	-2.425313
C	-2.452029	-2.310412	-2.455555
C	-2.554272	-1.458449	-1.328902
C	-1.340498	-1.545036	-0.597114
C	2.623069	-0.326680	-1.295832
C	2.810019	-1.131465	-2.563189
O	1.873588	-0.699568	-3.557229
C	2.152166	-1.258259	-4.852967
C	1.350971	-0.527777	-5.907804
H	1.914138	-2.331584	-4.839522
H	3.229299	-1.154956	-5.043066
H	0.838365	2.674050	-1.611878
H	-0.802870	-3.645419	-3.141039
H	0.445581	2.873399	-4.268441
H	-2.158222	2.398778	-4.761059
H	-3.371823	1.913363	-2.415839
H	-1.521190	2.077369	-0.465498
H	-1.129127	-1.052257	0.345177
H	-3.422697	-0.873011	-1.050126
H	-3.213116	-2.469242	-3.208136
H	0.486058	-2.784268	-0.937941
H	3.824673	-0.986700	-2.959356
H	2.671524	-2.206066	-2.376528
H	-1.681574	-0.520547	-4.822722
H	1.619649	0.532403	-5.935156
H	1.566162	-0.958818	-6.890490
H	0.265423	-0.616599	-5.747699
H	3.359614	-0.640153	-0.549754
H	2.761578	0.740861	-1.486763
H	1.630992	-0.484923	-0.858509

Et2O_act_CH_TS_beta

E=-653.3904042
G=-653.180166

C	-2.138245	2.141242	-2.367417
C	-0.957916	2.236906	-1.585092
C	0.116565	2.548757	-2.455450
C	-0.395170	2.638206	-3.772531
C	-1.790662	2.390824	-3.717843
Ce	-0.626714	-0.117893	-3.117733
C	-0.478497	-2.529804	-1.595616
C	-1.099742	-2.910609	-2.809555
C	-2.385074	-2.311672	-2.849408
C	-2.551993	-1.553381	-1.665378
C	-1.370335	-1.684906	-0.888975
C	2.805053	-0.237834	-1.034479
C	2.930802	-1.016972	-2.325440
O	1.907958	-0.612832	-3.229041
C	1.999148	-1.237751	-4.534090
C	0.886004	-0.690423	-5.399200
H	1.905424	-2.325894	-4.400469
H	3.013960	-1.036332	-4.918960
H	1.145041	2.723446	-2.161063
H	-0.687864	-3.578245	-3.557331
H	0.172255	2.888257	-4.661256
H	-2.474487	2.414897	-4.557806
H	-3.137071	1.952438	-1.991528
H	-0.901072	2.143971	-0.506309
H	-1.207903	-1.265027	0.097353
H	-3.441828	-1.004290	-1.380651
H	-3.118835	-2.434049	-3.636691
H	0.494366	-2.858860	-1.248411
H	3.906880	-0.834306	-2.797923
H	2.847408	-2.099027	-2.142944
H	-1.577981	-0.449141	-5.150519
H	1.152412	0.302943	-5.784230
H	0.762101	-1.346099	-6.268215
H	-0.651088	-0.612519	-5.298342
H	3.579810	-0.553234	-0.329249
H	2.919288	0.834968	-1.212027
H	1.832233	-0.412413	-0.562466

Et2O_act_CH_beta_adduct_H2

E=-653.4478223
G=-653.193881

C	-1.856290	2.147622	-2.251661
C	-0.526966	2.300733	-1.784672
C	0.309902	2.512030	-2.910762
C	-0.496096	2.478036	-4.071585
C	-1.837377	2.249719	-3.664126
Ce	-0.528984	-0.213627	-3.125787
C	-0.683927	-2.788273	-1.892171
C	-1.468491	-2.905810	-3.062406
C	-2.631060	-2.108944	-2.888806
C	-2.562806	-1.504008	-1.609912
C	-1.354294	-1.917193	-0.995242
C	2.701676	-0.374606	-0.681172
C	3.090471	-0.724660	-2.102783
O	1.954445	-0.661831	-2.949261
C	2.238942	-0.980130	-4.372901
C	0.962999	-0.869827	-5.155491
H	2.677335	-1.988506	-4.363275
H	3.020094	-0.268922	-4.678443
H	1.378169	2.693320	-2.885818
H	-1.239302	-3.521042	-3.924198
H	-0.155764	2.632903	-5.088347
H	-2.704143	2.220483	-4.315232
H	-2.736300	2.009180	-1.634689
H	-0.216573	2.312577	-0.745533
H	-1.030518	-1.657682	0.006846
H	-3.317357	-0.865301	-1.166037
H	-3.455478	-2.025455	-3.588373
H	0.255094	-3.295983	-1.704867
H	3.855640	-0.028086	-2.478391
H	3.517789	-1.738000	-2.150702
H	-2.214513	-0.315222	-5.449353
H	1.033788	-0.103496	-5.933892
H	0.697817	-1.820627	-5.628408
H	-1.511244	-0.486786	-5.654883
H	3.578520	-0.421640	-0.028041
H	2.293793	0.639415	-0.624273
H	1.955620	-1.075411	-0.293756

Et2O_act_CH_beta_product

E=-652.2714902
G=-652.031537

C	1.093729	0.263552	1.945595
Ce	-0.992382	1.566752	3.374851
C	-3.663970	1.186260	4.271226
H	-3.833713	1.302915	5.334793
C	-3.318505	-0.019736	3.608679
H	-3.197328	-0.991330	4.074427
C	-3.225106	0.253581	2.220826
H	-3.014467	-0.470220	1.441907
C	-3.505755	1.629248	2.027779
H	-3.557790	2.139526	1.071743
C	-3.777546	2.204143	3.295328
H	-4.050723	3.236232	3.482137
H	1.117511	0.384818	0.867706
C	1.775991	1.070531	2.893503
H	2.403463	1.925577	2.668532
C	1.536349	0.534217	4.180252
H	1.938032	0.910520	5.112651
C	0.700077	-0.601943	4.031102
H	0.366940	-1.256195	4.829308
C	0.434505	-0.773973	2.648992
H	-0.145332	-1.575532	2.206499
C	-0.274608	4.779909	0.978418
C	-0.203168	5.168789	2.441197
O	-0.451639	4.034673	3.254513
H	-0.946278	5.946985	2.672581
H	0.788717	5.578109	2.686124
H	-0.088754	5.652394	0.344644
H	0.478659	4.023376	0.735440
H	-1.264736	4.387026	0.724773
C	-0.409021	4.310640	4.723463
H	-1.138707	5.117739	4.880718
C	-0.712766	3.044405	5.467463
H	0.597029	4.712363	4.908372
H	0.110352	2.749801	6.123327
H	-1.626278	3.130417	6.062210

Et2O_act_CH_alfa_adduct_Et2O

E=-653.4429002
G=-653.211732

C	-0.641049	-0.358228	-2.871082
C	-0.347843	0.969863	-2.476083
C	0.954993	0.980160	-1.918904
C	1.470986	-0.340268	-1.976204
C	0.483366	-1.166793	-2.567635
Ce	-0.552644	-0.419808	-0.018764
C	-0.327471	0.728711	2.560544
C	-0.452988	-0.657337	2.822575
C	0.726760	-1.300483	2.368357
C	1.581193	-0.311630	1.820363
C	0.927107	0.941298	1.936715
O	-2.394538	-2.307651	-0.095593
C	-2.298524	-3.732942	-0.156716
C	-3.723329	-1.787816	-0.315441
H	-2.146853	1.018962	0.047498
H	2.577057	-0.477154	1.426115
H	1.330826	1.900751	1.634487
H	-1.056703	1.492040	2.798107
H	-1.287901	-1.135739	3.322471
H	0.964562	-2.353133	2.478193
H	2.463245	-0.650654	-1.669838
H	0.593690	-2.220162	-2.802017
H	-1.551469	-0.688070	-3.359012
H	-1.001099	1.825567	-2.584935
H	1.480506	1.852805	-1.548563
H	-3.582336	-0.709105	-0.454424
C	-0.844937	-4.140614	-0.050564
H	-2.880293	-4.175419	0.661048
H	-2.733543	-4.074223	-1.107096
C	-4.667592	-2.042426	0.844671
H	-4.108842	-2.215359	-1.251398
H	-4.868258	-3.106072	1.003456
H	-4.266997	-1.616641	1.768955
H	-5.625328	-1.554544	0.637899
H	-0.758794	-5.230389	-0.090978
H	-0.255989	-3.729629	-0.877349
H	-0.411204	-3.806944	0.897264

Et2O_act_CH_TS_alfa

E=-653.4213451
G=-653.181692

C	-0.832030	-0.471653	-2.820738
C	-0.551176	0.879148	-2.496603
C	0.760742	0.938310	-1.965341
C	1.294460	-0.376848	-1.965737
C	0.309120	-1.246746	-2.496553
Ce	-0.695168	-0.409744	0.023107
C	-0.477045	0.884750	2.540890
C	-0.644721	-0.484503	2.864757
C	0.526126	-1.176137	2.465745
C	1.417593	-0.234992	1.892569
C	0.795233	1.039437	1.936048
O	-2.001871	-2.527108	0.069403
C	-2.157788	-3.843453	-0.465598
C	-3.104567	-1.601624	-0.111723
H	-2.585081	0.871637	0.003999
H	2.416627	-0.443049	1.526715
H	1.234039	1.974138	1.606016
H	-1.186381	1.678644	2.742357
H	-1.501314	-0.920308	3.365592
H	0.722429	-2.232530	2.611326
H	2.296449	-0.656773	-1.660887
H	0.427023	-2.310716	-2.668975
H	-1.744692	-0.838180	-3.275909
H	-1.214981	1.721393	-2.650253
H	1.281557	1.836057	-1.652612
C	-2.875341	-0.056257	-0.044831
C	-0.917780	-4.654878	-0.157831
H	-3.046992	-4.303764	-0.017210
H	-2.324396	-3.767369	-1.549838
C	-4.177654	-1.789845	0.937756
H	-3.498886	-1.729416	-1.129634
H	-4.643520	-2.785093	0.914937
H	-3.780272	-1.628852	1.945706
H	-4.974693	-1.054903	0.778492
H	-1.011795	-5.659621	-0.580997
H	-0.026730	-4.188102	-0.589834
H	-0.771115	-4.749296	0.921792

Et2O_act_CH_alfa_adduct_H2

E=-653.4376721
G=-653.189379

C	-1.114155	-0.021095	-2.768043
C	-0.415274	1.123431	-2.299536
C	0.897325	0.722581	-1.949054
C	1.008625	-0.670500	-2.189010
C	-0.233813	-1.125363	-2.701325
Ce	-0.756243	-0.460125	0.025747
C	-0.328817	1.265149	2.239242
C	-1.055655	0.172371	2.784782
C	-0.208837	-0.959567	2.779774
C	1.038622	-0.575458	2.225410
C	0.966100	0.803687	1.900171
O	-1.743819	-2.700811	0.084530
C	-1.823841	-3.987421	-0.523322
C	-2.913111	-1.824044	-0.002308
H	-2.673544	1.350101	-0.008046
H	1.913972	-1.207854	2.123852
H	1.771415	1.405806	1.495651
H	-0.683427	2.286355	2.152019
H	-2.067155	0.209652	3.171803
H	-0.464783	-1.946102	3.147858
H	1.904306	-1.268379	-2.060195
H	-0.458461	-2.136951	-3.019366
H	-2.129906	-0.037554	-3.145086
H	-0.799377	2.137232	-2.271393
H	1.687726	1.372153	-1.591379
H	-3.008573	0.664261	0.003128
C	-0.501522	-4.708933	-0.364636
H	-2.634519	-4.551844	-0.045136
H	-2.081706	-3.863694	-1.585658
C	-3.914919	-2.135030	1.088522
H	-3.354763	-1.969843	-0.999863
H	-4.319807	-3.160363	1.052640
H	-3.489344	-1.986351	2.087179
H	-4.769640	-1.454364	0.996036
H	-0.554695	-5.700063	-0.825876
H	0.309545	-4.155130	-0.848915
H	-0.251641	-4.836497	0.692664

Et2O_act_CH_alfa_product

E=-652.1695176
G=-652.024675

C	-2.933194	6.694527	-3.946333
C	-3.415748	5.426767	-4.349713
C	-4.198741	4.899961	-3.290456
C	-4.207236	5.848715	-2.236167
C	-3.421861	6.956541	-2.640523
Ce	-1.575267	4.820960	-2.277777
C	-0.832860	2.269213	-1.286346
C	-2.197398	2.421412	-0.927984
C	-2.278828	3.413917	0.081111
C	-0.965875	3.881526	0.339084
C	-0.073490	3.172884	-0.505365
O	0.479878	5.520179	-3.416521
C	-0.005598	4.363619	-4.190974
C	1.077454	3.321799	-4.356750
C	1.274965	6.494266	-4.085136
C	1.631290	7.608453	-3.121878
H	-2.327750	7.364724	-4.545764
H	1.004871	3.281469	-0.526422
H	-3.238853	4.953062	-5.307427
H	-4.740336	3.960922	-3.304868
H	-4.749928	5.758246	-1.302271
H	-3.267048	7.867594	-2.071634
H	-3.180878	3.731289	0.591336
H	-3.026543	1.841952	-1.318135
H	-0.437997	1.567510	-2.010775
H	-0.687461	4.613353	1.090451
H	0.712284	6.882410	-4.946990
H	2.182282	6.010069	-4.468198
H	2.249075	8.360090	-3.623104
H	0.732029	8.109453	-2.747640
H	2.193903	7.219402	-2.267825
H	-0.334495	4.750651	-5.167063
H	1.423118	2.936024	-3.391011
H	0.669107	2.472710	-4.917171
H	1.966030	3.669892	-4.910089

Et2O_trapping_H2_TS_alfa

E=-653.4425216
G=-653.202652

C	-0.096038	-0.256378	2.489893
C	-0.076253	1.151363	2.346170
C	1.156227	1.515486	1.742875
C	1.896113	0.331263	1.512987
C	1.118975	-0.765502	1.968769
Ce	-0.261284	0.174233	-0.329911
C	0.745052	-0.262956	-2.956427
C	-0.343925	0.618548	-3.150101
C	0.012923	1.879817	-2.609604
C	1.329604	1.780107	-2.093104
C	1.781069	0.455172	-2.300993
O	-2.103908	-1.114183	-0.374368
C	-3.123555	-2.014688	-0.080060
C	-2.723385	1.107087	-0.125095
C	-3.706533	1.199857	-1.265986
H	-3.184692	0.772239	0.811380
H	1.492422	2.525596	1.537866
H	2.894771	0.275197	1.095698
H	1.424917	-1.806388	1.968215
H	-0.892025	-0.841234	2.935382
H	-0.845104	1.836432	2.685098
H	-0.592457	2.779145	-2.637579
H	1.901278	2.584393	-1.644724
H	2.763483	0.070499	-2.051257
H	0.796341	-1.293425	-3.291378
H	-1.277367	0.376191	-3.644115
H	-3.115713	2.842353	0.512439
H	-2.424299	2.489014	0.286905
H	-3.412255	-1.946454	0.984061
H	-4.030886	-1.776122	-0.664696
C	-2.710233	-3.449508	-0.391851
H	-4.751333	1.366116	-0.984137
H	-3.404949	1.950862	-2.001849
H	-3.651497	0.227424	-1.766222
H	-3.522294	-4.149799	-0.165065
H	-2.452319	-3.551577	-1.450886
H	-1.835770	-3.735589	0.202195

Et2O_trapping_H2_TS_beta

E=-653.3362537
G=-653.085016

Ce	2.420419	0.174882	4.177503
O	3.065980	2.458174	4.835665
C	3.014320	3.780388	5.366860
C	1.593971	4.109964	5.775002
C	4.898856	-0.186274	3.478684
H	4.784549	-1.411769	3.063477
H	5.628382	-1.539564	2.819744
H	5.649015	-0.253459	4.267127
H	5.260718	0.348042	2.599721
H	3.698077	3.839008	6.225689
H	3.379005	4.478267	4.599991
H	1.548106	5.122355	6.187967
H	1.235048	3.414671	6.539793
H	0.918437	4.062384	4.915729
C	3.170013	-0.856039	6.735980
H	4.096184	-0.488643	7.162419
C	1.882886	-0.302917	6.940341
H	1.652035	0.560257	7.554440
C	0.943942	-1.101603	6.240390
H	-0.131339	-0.962432	6.230559
C	1.652616	-2.153567	5.606285
H	1.213419	-2.956069	5.024964
C	3.027695	-2.000954	5.912422
H	3.825410	-2.668607	5.607366
C	2.051085	-0.308367	1.389437
H	2.868983	-0.780523	0.857376
C	1.844850	1.085919	1.528769
H	2.479194	1.867351	1.126737
C	0.636839	1.279021	2.244078
H	0.183675	2.235288	2.480633
C	0.098120	0.004493	2.549943
H	-0.838626	-0.186834	3.061083
C	0.973930	-0.977856	2.022299
H	0.821532	-2.050585	2.057428
C	4.349077	1.971513	4.391435
H	4.710644	2.594472	3.564447
H	5.057741	1.988823	5.228496

Et2O_trapping_H2_alfa_product

E=-573.7213349
G=-573.538392

C	-0.298661	-0.747524	-2.846166
C	-0.030704	0.637804	-2.894722
C	1.208061	0.868807	-2.235156
C	1.711635	-0.380910	-1.798747
C	0.774328	-1.379188	-2.157829
Ce	-0.582413	0.119824	-0.164382
C	-0.770963	0.167026	2.670666
C	-0.195918	-1.092271	2.369834
C	1.123047	-0.871813	1.889265
C	1.355142	0.522834	1.877880
C	0.180647	1.166217	2.355871
O	-2.682104	0.607485	-0.335673
C	-4.041054	0.906798	-0.421725
H	2.280305	1.012591	1.596311
H	0.056257	2.232934	2.509811
H	-1.761814	0.335318	3.074942
H	-0.658194	-2.059106	2.539609
H	1.836977	-1.639063	1.613016
H	2.652925	-0.544841	-1.287975
H	0.890252	-2.446319	-2.000721
H	-1.158035	-1.243843	-3.282479
H	-0.650942	1.388361	-3.371180
H	1.714832	1.824099	-2.148050
H	-4.249116	1.459540	-1.353183
C	-4.905192	-0.348885	-0.385877
H	-4.337119	1.570213	0.408228
H	-5.969836	-0.097889	-0.455697
H	-4.654612	-1.011366	-1.221328
H	-4.744356	-0.899600	0.547219

Et2O_releasing_ethylene_beta

E=-652.2650468
G=-652.026258

C	-2.021560	2.058142	-2.601780
C	-0.834079	2.140223	-1.828957
C	0.225634	2.503705	-2.691636
C	-0.302961	2.644124	-4.001043
C	-1.689259	2.359699	-3.946337
Ce	-1.422898	4.827149	-2.568807
C	-2.473862	6.399851	-4.688322
C	-3.508752	5.484114	-4.378287
C	-4.023880	5.821727	-3.101613
C	-3.316585	6.958359	-2.630991
C	-2.359463	7.314349	-3.608947
O	-0.834349	5.507468	-0.368366
C	0.688366	6.242642	-0.910271
C	0.879622	6.118732	-2.315980
C	-0.978632	5.634455	1.021941
C	-2.294350	5.036213	1.491071
H	1.327114	5.651782	-0.252969
H	0.470274	7.232429	-0.508090
H	-3.495913	7.479131	-1.697496
H	1.264187	2.625668	-2.408091
H	-1.679444	8.156108	-3.557823
H	-1.905227	6.429827	-5.611287
H	-3.866537	4.685847	-5.017369
H	-4.852982	5.332973	-2.601298
H	-2.999721	1.759861	-2.240314
H	-2.370002	2.344101	-4.788875
H	0.264413	2.879481	-4.894781
H	-0.747735	1.933765	-0.768380
H	-0.932760	6.699386	1.306019
H	-0.139185	5.133270	1.532749
H	0.793236	7.029310	-2.905852
H	1.657769	5.434013	-2.648023
H	-2.397953	5.139017	2.576649
H	-3.142476	5.543887	1.020432
H	-2.346971	3.970396	1.246035

Et2O_releasing_ethylene_beta_product

E=-573.7213349
G=-573.538392

C	-0.298661	-0.747524	-2.846166
C	-0.030704	0.637804	-2.894722
C	1.208061	0.868807	-2.235156
C	1.711635	-0.380910	-1.798747
C	0.774328	-1.379188	-2.157829
Ce	-0.582413	0.119824	-0.164382
C	-0.770963	0.167026	2.670666
C	-0.195918	-1.092271	2.369834
C	1.123047	-0.871813	1.889265
C	1.355142	0.522834	1.877880
C	0.180647	1.166217	2.355871
O	-2.682104	0.607485	-0.335673
C	-4.041054	0.906798	-0.421725
H	2.280305	1.012591	1.596311
H	0.056257	2.232934	2.509811
H	-1.761814	0.335318	3.074942
H	-0.658194	-2.059106	2.539609
H	1.836977	-1.639063	1.613016
H	2.652925	-0.544841	-1.287975
H	0.890252	-2.446319	-2.000721
H	-1.158035	-1.243843	-3.282479
H	-0.650942	1.388361	-3.371180
H	1.714832	1.824099	-2.148050
H	-4.249116	1.459540	-1.353183
C	-4.905192	-0.348885	-0.385877
H	-4.337119	1.570213	0.408228
H	-5.969836	-0.097889	-0.455697
H	-4.654612	-1.011366	-1.221328
H	-4.744356	-0.899600	0.547219

Et2O_insertion_ethylene_product

E=-498.4422974
G=-498.282381

C	-0.549406	-0.669425	2.814043
C	0.684523	-1.141397	2.294042
C	1.471078	-0.016011	1.946529
C	0.722145	1.151277	2.250772
C	-0.521860	0.746935	2.794224
Ce	-0.624721	-0.000087	0.055737
C	-0.700036	0.671030	-2.702497
C	0.576175	1.088881	-2.252226
C	1.344259	-0.069973	-1.963837
C	0.538497	-1.204076	-2.228283
C	-0.727507	-0.746471	-2.680415
C	-2.754968	1.316165	0.105835
H	2.481976	-0.041258	1.556463
H	1.064688	2.173949	2.135959
H	-1.302690	1.404986	3.153837
H	-1.349379	-1.284783	3.211467
H	0.991449	-2.179152	2.219351
H	2.377886	-0.085025	-1.637697
H	0.850916	-2.239518	-2.144587
H	-1.551132	-1.371475	-3.008222
H	-1.504190	1.318839	-3.027997
H	0.924281	2.114138	-2.188391
C	-3.559039	0.029814	0.150952
H	-2.910548	1.930091	0.996271
H	-2.979915	1.909566	-0.783185
H	-4.190434	-0.130836	-0.728764
H	-2.932369	-0.923505	0.180782
H	-4.184255	-0.079788	1.043170

Et2O_act2_Cb-H_TS_beta

E=-731.9759001
G=-731.726485

C	-1.062375	-1.668342	-0.817464
C	-0.359942	-2.513991	-1.712210
C	-1.221112	-2.827919	-2.790241
C	-2.464892	-2.188823	-2.555397
C	-2.367921	-1.473380	-1.338173
Ce	-0.699415	-0.025301	-3.100271
C	-1.208173	2.723975	-3.640515
C	-2.183612	2.348203	-2.682366
C	-1.521809	2.117634	-1.451013
C	-0.136228	2.340397	-1.651085
C	0.055260	2.719853	-3.004583
O	1.840403	-0.492983	-3.377286
C	1.883220	-0.914792	-4.761233
C	0.751949	-0.230792	-5.496969
C	2.903869	-1.012255	-2.584887
C	2.869521	-0.378658	-1.211545
H	1.783038	-2.010570	-4.794205
H	2.885478	-0.661515	-5.146908
H	0.633398	2.281541	-0.889746
H	-0.987130	-3.477900	-3.625492
H	1.000979	2.982759	-3.464052
H	-1.401189	2.985812	-4.673903
H	-3.252564	2.287749	-2.852543
H	-1.994963	1.850177	-0.513639
H	-0.692965	-1.288923	0.128642
H	-3.162583	-0.906677	-0.867178
H	-3.344780	-2.259505	-3.183604
H	0.648359	-2.887082	-1.575358
H	3.854641	-0.792406	-3.091474
H	2.808141	-2.106449	-2.519259
C	-2.118882	-0.209267	-5.416763
H	0.995667	0.829407	-5.651889
H	0.673455	-0.679453	-6.494357
H	-0.666671	-0.281253	-5.315443
H	3.666496	-0.794010	-0.587425
H	3.012916	0.703273	-1.277749
H	1.914295	-0.575077	-0.714247
C	-2.405057	-1.464281	-6.240093
H	-2.929907	-0.070676	-4.678094
H	-2.166562	0.684737	-6.053311
H	-3.351127	-1.409238	-6.794092
H	-1.613467	-1.641652	-6.979629
H	-2.451713	-2.358755	-5.608186

Et2O_metathesis_TS_alfa

E=-653.2785433
G=-653.133949

C	-1.598000	2.095000	-1.763000
C	-0.291000	2.347000	-1.277000
C	0.521000	2.717000	-2.375000
C	-0.283000	2.688000	-3.544000
C	-1.592000	2.300000	-3.166000
Ce	-1.285000	4.898000	-2.091000
C	-1.720000	6.765000	-4.205000
C	-2.610000	5.701000	-4.485000
C	-3.618000	5.699000	-3.488000
C	-3.360000	6.779000	-2.603000
C	-2.188000	7.434000	-3.043000
C	-2.778000	5.387000	1.865000
C	-1.308000	5.235000	1.487000
O	-1.079000	5.541000	0.145000
C	0.570000	6.781000	0.034000
H	-3.972000	7.069000	-1.756000
H	1.578000	2.951000	-2.337000
H	-1.741000	8.314000	-2.593000
H	-0.856000	7.048000	-4.796000
H	-2.545000	5.020000	-5.326000
H	-4.471000	5.031000	-3.448000
H	-2.442000	1.750000	-1.175000
H	-2.430000	2.150000	-3.836000
H	0.055000	2.889000	-4.554000
H	0.035000	2.251000	-0.248000
H	-0.713000	5.910000	2.133000
H	-0.965000	4.214000	1.717000
H	0.599000	5.948000	-1.718000
H	-2.932000	5.158000	2.925000
H	-3.119000	6.410000	1.678000
H	-3.405000	4.707000	1.278000
H	0.656000	7.541000	-0.731000
H	-0.015000	7.143000	0.876000

C	1.817000	6.063000	0.422000
H	2.344000	6.678000	1.168000
H	1.595000	5.108000	0.906000
H	2.465000	5.874000	-0.435000

Pr-O-Pr

Pr2O

E=-312.1945499
G=-312.035092

O	0.099304	0.000000	0.070390
C	0.055708	0.000000	1.479625
C	1.413201	0.000000	-0.441090
C	1.350154	0.000000	-1.958900
H	1.966951	0.886505	-0.082131
H	1.966951	-0.886505	-0.082131
C	2.733983	0.000000	-2.601683
H	0.779383	-0.878484	-2.282040
H	0.779383	0.878484	-2.282040
H	2.661523	0.000000	-3.693249
H	3.312006	0.883932	-2.309461
H	3.312006	-0.883932	-2.309461
C	-1.396262	0.000000	1.926027
H	0.578837	-0.886512	1.881798
H	0.578837	0.886512	1.881798
C	-1.541819	0.000000	3.445065
H	-1.891079	0.878467	1.495504
H	-1.891079	-0.878467	1.495504
H	-2.595282	0.000000	3.740058
H	-1.073941	-0.883937	3.892873
H	-1.073941	0.883937	3.892873

First C-H activation of Pr2O by Cp2CeH

Pr2O_CH_act_alfa_adduct_Pr2O

E=-732.068808
G=-731.759080

C	-0.455061	-0.930777	-2.954443
C	-0.351114	0.477079	-2.830127
C	0.910459	0.770861	-2.258105
C	1.590552	-0.453178	-2.037352
C	0.745294	-1.507641	-2.464695
Ce	-0.586258	-0.515123	-0.188140
C	-1.064085	-2.753011	1.506013
C	-2.008288	-1.784601	1.932014
C	-2.960549	-1.613047	0.897606
C	-2.599072	-2.469244	-0.172114
C	-1.428480	-3.176568	0.203813
O	0.847268	0.864150	1.546565
C	0.387880	2.227782	1.724746
C	-0.628784	2.343322	2.847515
C	-0.108372	1.965702	4.231207
H	0.744963	2.587895	4.525939
C	2.194324	0.630237	1.969398
C	2.511005	-0.850463	1.873165
C	3.943863	-1.157488	2.306192
H	4.152300	-2.227765	2.227462
H	-1.973003	1.125051	-0.230838
H	0.992303	-2.563116	-2.467209
H	-1.289672	-1.470948	-3.386285
H	-1.100011	1.200470	-3.125001
H	1.301648	1.762950	-2.062397
H	2.603273	-0.561966	-1.664330
H	-0.928937	-3.939676	-0.381718
H	-0.239779	-3.143701	2.092813
H	-2.024197	-1.291611	2.897611
H	-3.815768	-0.950483	0.921314
H	-3.144445	-2.589249	-1.101162
H	-0.074611	2.529585	0.778631
H	2.878153	1.213662	1.335403
H	2.313669	0.976583	3.004011
H	1.262954	2.865000	1.903648
H	1.802446	-1.408037	2.496680
H	2.366669	-1.184516	0.835855
H	4.672596	-0.630221	1.681539
H	4.117291	-0.861555	3.346257
H	-0.979865	3.383637	2.848132
H	-1.501286	1.733742	2.583099
H	-0.887376	2.096883	4.988116
H	0.206689	0.917873	4.267201

Pr2O_CH_act_beta_adduct_Pr2O

E=-732.069675
G=-731.760703

C	-1.672457	-1.410784	-0.478566
C	-0.639147	-2.286770	-0.894145
C	-1.066109	-2.928930	-2.082215
C	-2.360036	-2.444107	-2.406755
C	-2.731936	-1.502316	-1.415539
Ce	-2.725605	-4.030461	-0.113705
C	-2.516037	-6.380584	-1.611167
C	-3.835455	-5.927954	-1.874551
C	-4.599620	-6.112949	-0.695812
C	-3.751839	-6.670133	0.294393
C	-2.466067	-6.843594	-0.273546
O	-4.532779	-3.142950	1.678700
C	-5.938206	-3.243104	1.421578
C	-6.254726	-2.744711	0.024038
C	-7.751615	-2.815459	-0.274910
H	-7.963075	-2.448796	-1.282838
C	-4.211740	-3.357184	3.064361
C	-2.799242	-2.885957	3.355736
C	-2.430877	-3.103589	4.822532
H	-3.106516	-2.562766	5.495026
H	-4.331250	-4.424960	3.301946
H	-4.933685	-2.795734	3.674369
H	-3.647722	-0.921906	-1.400640
H	-4.045253	-6.961009	1.297145
H	-1.640513	-0.755316	0.384555
H	0.309174	-2.436435	-0.395195
H	-0.488591	-3.639029	-2.662628
H	-2.937221	-2.707946	-3.285515
H	-4.205074	-5.560086	-2.824831
H	-1.698171	-6.402801	-2.321835
H	-1.600110	-7.257714	0.225484
H	-5.661426	-5.919181	-0.590422
H	-6.471434	-2.633347	2.165060
H	-6.260151	-4.287222	1.550371
H	-1.076621	-4.532831	1.152177
H	-2.723429	-1.822324	3.099814
H	-2.075727	-3.429142	2.725195
H	-5.896389	-1.713815	-0.073348
H	-5.710929	-3.347246	-0.716492
H	-2.468261	-4.165151	5.089308
H	-1.414516	-2.752149	5.017876
H	-8.125746	-3.842727	-0.210324
H	-8.328348	-2.204640	0.428025

Pr2O_CH_act_gamma_adduct_Pr2O

E=-732.0718049
G=-731.761178

C	-3.254626	-1.971843	-0.964489
C	-2.011971	-2.425423	-0.458930
C	-1.299155	-3.038886	-1.522868
C	-2.107538	-2.966219	-2.684812
C	-3.309677	-2.300334	-2.341735
Ce	-1.296111	-0.294520	-2.122185
C	-0.048166	1.689842	-0.540878
C	0.597321	1.820156	-1.794779
C	1.393092	0.665198	-2.003354
C	1.229819	-0.187841	-0.884391
C	0.337089	0.447011	0.018754
O	-1.088691	0.154310	-4.780455
C	0.122062	-0.124575	-5.492342
C	0.657587	-1.490003	-5.104718
C	1.950980	-1.822012	-5.847223
H	2.320375	-2.809820	-5.559306
C	-1.766233	1.315882	-5.287656
C	-3.174011	1.385509	-4.727149
C	-3.920347	2.616681	-5.238807
H	-4.932933	2.647917	-4.828670
H	0.530429	2.677821	-2.455098
H	2.056991	0.490347	-2.842886
H	1.738207	-1.131055	-0.720793
H	-1.678922	-2.352335	0.569759
H	-0.716910	2.410947	-0.090230
H	0.031828	0.064072	0.985628
H	-0.335906	-3.530053	-1.443752
H	-1.866287	-3.384195	-3.655822
H	-4.143838	-2.105502	-3.006324
H	-4.027735	-1.466222	-0.400889
H	-2.847545	1.044066	-1.510168
H	-3.415619	3.541472	-4.939688
H	-4.002133	2.615682	-6.331712
H	-3.151779	1.419207	-3.624609
H	-3.711647	0.472898	-5.011735
H	-1.795687	1.245910	-6.384591
H	-1.188793	2.215329	-5.025393
H	-0.094725	-0.098914	-6.570082
H	0.860754	0.662859	-5.280440
H	0.844084	-1.519921	-4.022420
H	-0.107663	-2.244343	-5.318572
H	1.798333	-1.828303	-6.931876
H	2.739560	-1.095205	-5.624780

Pr2O_TS_act_alfa

E=-732.0382034
G=-731.728819

C	-0.504567	-0.115616	-3.075601
C	-0.180988	1.174905	-2.589894
C	1.080493	1.097767	-1.947098
C	1.539262	-0.239181	-2.042959
C	0.558797	-0.992453	-2.735897
Ce	-0.693830	-0.389291	-0.288210
C	-1.664840	-2.883690	0.642569
C	-2.299662	-1.931625	1.480252
C	-3.230097	-1.208372	0.695486
C	-3.169115	-1.709122	-0.629838
C	-2.206181	-2.749875	-0.660644
O	0.986306	-0.319190	1.576614
C	0.404704	1.007544	1.728021
C	-0.160789	1.233981	3.116848
C	0.837683	1.200372	4.276346
H	1.644398	1.927860	4.129406
C	2.412212	-0.418412	1.645607
C	2.824025	-1.866559	1.456295
C	4.340080	-2.044532	1.517258
H	4.615991	-3.093173	1.375089
H	-1.576477	1.634271	0.287826
H	0.631231	-2.039843	-3.006218
H	-1.390648	-0.380319	-3.641206
H	-0.779803	2.069770	-2.709217
H	1.616003	1.927829	-1.501311
H	2.494043	-0.612610	-1.690340
H	-1.956380	-3.360416	-1.521002
H	-0.929379	-3.616740	0.954870
H	-2.127107	-1.806165	2.542692
H	-3.890987	-0.425769	1.048747
H	-3.784753	-1.385497	-1.461529
H	-0.809187	1.477076	0.877976
H	2.856687	0.219296	0.866662
H	2.748727	-0.044281	2.619922
H	1.167874	1.752246	1.464324
H	2.339306	-2.474450	2.229171
H	2.444729	-2.222646	0.489629
H	4.844808	-1.461231	0.739300
H	4.741821	-1.725332	2.485089
H	-0.659992	2.212901	3.094170
H	-0.958394	0.502418	3.303236
H	0.346384	1.437588	5.226412
H	1.289348	0.208780	4.383710

Pr2O_TS_act_beta

E=-732.0390732
G=-731.728737

C	-1.413681	-1.724238	-0.921961
C	-0.515879	-2.560276	-1.635678
C	-1.128255	-2.911836	-2.863261
C	-2.406480	-2.296183	-2.908633
C	-2.576256	-1.557316	-1.710088
Ce	-2.632958	-4.293796	-0.917203
C	-2.145263	-6.535027	-2.537484
C	-3.509619	-6.227488	-2.781971
C	-4.243211	-6.546555	-1.612442
C	-3.336272	-7.041179	-0.643617
C	-2.039664	-7.040257	-1.218720
O	-4.855749	-3.660720	0.231333
C	-6.237753	-3.679273	-0.105149
C	-6.429617	-3.142005	-1.510836
C	-7.895562	-3.158501	-1.938986
H	-8.010387	-2.764943	-2.952671
C	-4.571099	-4.104938	1.578118
C	-3.084067	-3.972676	1.824759
C	-2.702273	-4.662591	3.132123
H	-3.254309	-4.275222	4.002248
H	-4.896068	-5.153313	1.676467
H	-5.193800	-3.502525	2.266202
H	-3.435345	-0.948737	-1.452088
H	-3.591244	-7.401138	0.346235
H	-1.225661	-1.267637	0.042684
H	0.476652	-2.850045	-1.311294
H	-0.683925	-3.513341	-3.647670
H	-3.101539	-2.335054	-3.740020
H	-3.921989	-5.868153	-3.718173
H	-1.334944	-6.442755	-3.251262
H	-1.132415	-7.389595	-0.740943
H	-5.317937	-6.466402	-1.495391
H	-6.786367	-3.064074	0.623834
H	-6.620525	-4.708933	-0.025407
H	-1.031609	-4.806936	0.645518
H	-2.838925	-2.901564	1.899563
H	-1.779511	-4.558005	1.120136
H	-6.033344	-2.121143	-1.556944
H	-5.831747	-3.747301	-2.205541
H	-2.892772	-5.742871	3.083765
H	-1.635343	-4.537132	3.348918
H	-8.304960	-4.174469	-1.929460
H	-8.512231	-2.544375	-1.273824

Pr2O_TS_act_gamma

E=-732.0224738
G=-731.715088

C	-2.197266	-1.017399	-1.045232
C	-0.792714	-1.193267	-1.130066
C	-0.333012	-0.491095	-2.273034
C	-1.455088	0.114853	-2.894204
C	-2.607568	-0.209169	-2.136155
Ce	-1.115579	1.540626	-0.474783
C	1.054474	1.413897	1.338888
C	0.091981	2.216497	2.002611
C	-0.006377	3.450321	1.310522
C	0.894407	3.408845	0.217294
C	1.549464	2.150404	0.233163
C	-3.010152	3.222474	-0.793662
C	-2.276041	3.715111	-2.021848
C	-2.002776	5.211225	-2.058721
O	-1.132940	5.498806	-3.131129
C	-0.857396	6.875615	-3.271108
C	0.080095	7.073180	-4.450133
C	0.429588	8.541175	-4.679277
H	1.102533	8.656822	-5.534041
H	-4.023128	2.884745	-1.022183
H	-0.436606	1.954033	2.912439
H	-0.628590	4.290603	1.593074
H	1.080324	4.212535	-0.486266
H	-0.183668	-1.795304	-0.465240
H	1.385249	0.428365	1.646592
H	2.325507	1.826918	-0.451365
H	0.688784	-0.462792	-2.634377
H	-1.438456	0.692552	-3.811560
H	-3.625828	0.077302	-2.369542
H	-2.850971	-1.466894	-0.305877
H	-2.904408	1.049209	1.371347
H	-3.172537	1.626342	0.947392
H	-3.053346	3.985414	-0.008088
H	-1.233685	3.269150	-2.157319
H	-2.775273	3.411160	-2.948349
H	-2.956550	5.753313	-2.171041
H	-1.556302	5.531027	-1.100976
H	-1.793939	7.439459	-3.430175
H	-0.399333	7.272579	-2.347403
H	0.990390	6.488259	-4.272669
H	-0.393559	6.649874	-5.343716
H	-0.465873	9.139810	-4.881012
H	0.928069	8.975989	-3.805593

Pr2O_CH_act_alfa_adduct_H2

E=-732.0462358
G=-731.737967

C	-0.819307	0.727362	-2.843573
C	0.157682	1.490303	-2.156823
C	1.287214	0.662615	-1.933184
C	1.006907	-0.611939	-2.483987
C	-0.295290	-0.574718	-3.044380
Ce	-0.749262	-0.413718	-0.249682
C	-2.663573	-1.944130	1.212172
C	-2.857358	-0.615590	1.654127
C	-3.408672	0.128591	0.575665
C	-3.556157	-0.745530	-0.528480
C	-3.085869	-2.026101	-0.139109
O	0.874533	-1.876495	0.905100
C	1.060200	-0.565098	1.540935
C	0.911442	-0.638076	3.048872
C	1.948531	-1.473121	3.811546
H	2.969091	-1.143755	3.582847
C	2.035572	-2.612759	0.521583
C	1.618887	-3.894652	-0.178091
C	2.820394	-4.731989	-0.612058
H	2.498276	-5.648750	-1.114159
H	-0.718974	1.972249	0.864516
H	-0.784903	-1.381752	-3.578195
H	-1.781455	1.086842	-3.189990
H	0.074999	2.538533	-1.891871
H	2.214472	0.965068	-1.461498
H	1.687295	-1.455293	-2.515601
H	-3.103793	-2.923044	-0.748674
H	-2.269850	-2.760335	1.806258
H	-2.660495	-0.240409	2.651589
H	-3.718810	1.167282	0.611301
H	-3.980293	-0.488923	-1.492370
H	-0.193002	1.545888	1.218758
H	2.658438	-1.991816	-0.140678
H	2.625627	-2.837977	1.418400
H	2.058823	-0.200653	1.257904
H	0.978968	-4.472743	0.499031
H	1.005136	-3.642114	-1.052798
H	3.463026	-4.181654	-1.308121
H	3.434947	-5.023626	0.246620
H	0.953619	0.398909	3.412686
H	-0.093283	-0.998656	3.306735
H	1.808436	-1.392970	4.896036
H	1.870837	-2.534667	3.553506

Pr2O_CH_act_beta_adduct_H2

E=-732.0465085
G=-731.739903

C	-1.029595	-2.151664	-1.278180
C	-0.806476	-2.862189	-2.487719
C	-1.890536	-2.596444	-3.359698
C	-2.790486	-1.732583	-2.687450

C	-2.252259	-1.453762	-1.404564
Ce	-3.000613	-4.214203	-1.311989
C	-3.966473	-5.746731	-3.518147
C	-5.097064	-5.585916	-2.679955
C	-4.884145	-6.354746	-1.505896
C	-3.621830	-6.979233	-1.612516
C	-3.048283	-6.597878	-2.855794
O	-4.548901	-3.314790	0.498028
C	-5.569056	-2.352481	0.713824
C	-6.547216	-2.351506	-0.447414
C	-7.672783	-1.337872	-0.250555
H	-8.365548	-1.352901	-1.096592
C	-3.583884	-3.425754	1.616179
C	-2.547524	-4.456766	1.260766
C	-2.816624	-5.817644	1.904624
H	-2.867645	-5.777200	3.007140
H	-4.193601	-3.662105	2.506956
H	-3.152934	-2.423340	1.752687
H	-2.685704	-0.793039	-0.662569
H	-3.181029	-7.650699	-0.885242
H	-0.363821	-2.122047	-0.424069
H	0.069859	-3.454936	-2.725572
H	-1.997572	-2.964639	-4.373237
H	-3.698103	-1.310987	-3.105605
H	-5.992119	-5.022492	-2.919967
H	-3.837019	-5.314524	-4.503564
H	-2.104532	-6.950486	-3.257560
H	-5.576245	-6.459041	-0.678556
H	-5.114803	-1.356071	0.837822
H	-6.089882	-2.594590	1.653073
H	-0.596267	-5.662271	-1.043160
H	-1.565952	-4.083754	1.579772
H	-0.839999	-5.475775	-0.354832
H	-6.003007	-2.124678	-1.373980
H	-6.962594	-3.359806	-0.560503
H	-3.764758	-6.254759	1.565494
H	-2.034923	-6.546021	1.655361
H	-8.250650	-1.555203	0.654321
H	-7.282321	-0.318455	-0.159569

Pr2O_CH_act_gamma_adduct_H2

E=-732.030629
G=-731.724315

C	-2.197266	-1.017399	-1.045232
C	-0.792714	-1.193267	-1.130066
C	-0.333012	-0.491095	-2.273034
C	-1.455088	0.114853	-2.894204
C	-2.607568	-0.209169	-2.136155
Ce	-1.115579	1.540626	-0.474783
C	1.054474	1.413897	1.338888
C	0.091981	2.216497	2.002611
C	-0.006377	3.450321	1.310522
C	0.894407	3.408845	0.217294
C	1.549464	2.150404	0.233163
C	-3.010152	3.222474	-0.793662
C	-2.276041	3.715111	-2.021848
C	-2.002776	5.211225	-2.058721
O	-1.132940	5.498806	-3.131129
C	-0.857396	6.875615	-3.271108
C	0.080095	7.073180	-4.450133
C	0.429588	8.541175	-4.679277
H	1.102533	8.656822	-5.534041
H	-4.023128	2.884745	-1.022183
H	-0.436606	1.954033	2.912439
H	-0.628590	4.290603	1.593074
H	1.080324	4.212535	-0.486266
H	-0.183668	-1.795304	-0.465240
H	1.385249	0.428365	1.646592
H	2.325507	1.826918	-0.451365
H	0.688784	-0.462792	-2.634377
H	-1.438456	0.692552	-3.811560
H	-3.625828	0.077302	-2.369542
H	-2.850971	-1.466894	-0.305877
H	-2.904408	1.049209	1.371347
H	-3.172537	1.626342	0.947392
H	-3.053346	3.985414	-0.008088
H	-1.233685	3.269150	-2.157319
H	-2.775273	3.411160	-2.948349
H	-2.956550	5.753313	-2.171041
H	-1.556302	5.531027	-1.100976
H	-1.793939	7.439459	-3.430175
H	-0.399333	7.272579	-2.347403
H	0.990390	6.488259	-4.272669
H	-0.393559	6.649874	-5.343716
H	-0.465873	9.139810	-4.881012
H	0.928069	8.975989	-3.805593

Pr2O_CH_act_alfa_product

E=-730.8672836
G=-730.573089

C	-0.555995	0.592404	-2.669344
C	0.582485	1.109940	-2.002098
C	1.587075	0.109294	-2.007057
C	1.071141	-1.027103	-2.675130
C	-0.255798	-0.730536	-3.081412
Ce	-0.427094	-0.909994	-0.268881
C	-3.251217	-0.776762	-0.273351
C	-2.949278	-2.152458	-0.442760
C	-2.423046	-2.641300	0.780179
C	-2.385900	-1.565286	1.699270
C	-2.899469	-0.412751	1.049068
C	1.137248	-2.654298	0.648964
C	2.463091	-3.134116	0.093862
C	3.533367	-3.570241	1.103782
H	3.146270	-4.333571	1.789272
O	1.279505	-1.409653	1.437709
C	1.357398	-1.506596	2.858232
C	1.296294	-0.117837	3.472054
C	1.418083	-0.153728	4.994290
H	1.370077	0.854075	5.416651
H	-3.701633	-0.127554	-1.015198
H	-3.140000	-2.739954	-1.333980
H	-2.125368	-3.662936	0.981290
H	-2.072230	-1.623898	2.735439
H	-3.048004	0.562742	1.500459
H	-1.478303	1.127013	-2.865372
H	0.684700	2.114097	-1.603555
H	2.585587	0.207599	-1.596772
H	1.605787	-1.949443	-2.866557
H	-0.908052	-1.381599	-3.652671
H	0.527084	-2.128861	3.225571
H	2.294025	-2.006616	3.134112
H	0.692300	-3.406367	1.316863
H	2.100378	0.492380	3.043043
H	0.348318	0.359850	3.188598
H	0.611709	-0.741281	5.446705
H	2.368863	-0.599001	5.306530
H	2.223388	-3.984629	-0.560344
H	2.890534	-2.368479	-0.567394
H	4.411814	-3.990738	0.599997
H	3.881620	-2.723530	1.705068

Pr2O_CH_act_beta_product

E=-730.8701458
G=-730.575363

C	-1.810640	-1.525432	-0.779701
C	-0.640285	-2.304861	-0.968801
C	-0.706815	-2.890506	-2.257628
C	-1.913996	-2.466726	-2.867546
C	-2.595756	-1.624428	-1.952651
Ce	-0.297651	-0.120929	-2.735821
C	1.901653	0.888620	-4.248778
C	2.063487	1.462517	-2.965465
C	2.396447	0.422612	-2.061240
C	2.451242	-0.792671	-2.789182
C	2.138639	-0.506926	-4.140789
C	-2.362863	2.029846	-0.704064
H	-2.830194	3.012266	-0.513351
C	-1.228517	2.086098	-1.726422
C	-1.660153	2.626164	-3.062979
O	-1.705816	1.512940	-4.054393
C	-2.104722	1.910359	-5.355995
C	-2.126860	0.709312	-6.285922
C	-2.577024	1.080497	-7.697672
H	-2.583726	0.203062	-8.350314
H	-2.673791	3.060637	-3.073800
H	-0.963021	3.365663	-3.481924
H	1.680592	1.427880	-5.163235
H	-3.562713	-1.161058	-2.111117
H	1.972802	2.513397	-2.719851
H	2.616948	0.543399	-1.006370
H	2.714798	-1.764443	-2.388468
H	2.135521	-1.221569	-4.956823
H	0.020016	-3.570435	-2.687041
H	0.142484	-2.466964	-0.236174
H	-2.072165	-0.972415	0.114060
H	-2.277338	-2.776734	-3.841765
H	-1.411420	2.678589	-5.733866
H	-3.103931	2.368876	-5.298924
H	-0.411717	2.706774	-1.339574
H	-1.121882	0.267260	-6.324149
H	-2.797286	-0.050709	-5.865822
H	-3.171399	1.355765	-1.016011
H	-2.007655	1.660696	0.265100
H	-3.589063	1.499321	-7.695144
H	-1.909634	1.823451	-8.147471

Pr2O_CH_act_gamma_product

E=-730.8498795
G=
-730.558408

C	-2.691931	-0.233452	-1.252363
C	-1.796750	-1.297376	-1.540632
C	-1.874360	-1.573232	-2.929713
C	-2.801547	-0.669692	-3.501811
C	-3.309224	0.157326	-2.464775
Ce	-0.598148	0.951974	-2.733822
C	1.762171	2.344873	-2.004057
C	1.315403	1.718176	-0.814151
C	0.120519	2.362412	-0.398050
C	-0.175960	3.380062	-1.337221
C	0.836848	3.366440	-2.331870
C	0.863359	0.048823	-4.567581
H	1.948090	0.147788	-4.490342
C	0.260265	1.052145	-5.532526
C	-0.235833	0.478841	-6.851332
O	-0.956150	1.469559	-7.551482
C	-1.438550	1.025782	-8.800875
C	-2.192001	2.161688	-9.471470
C	-2.751072	1.766265	-10.835633
H	-3.287907	2.599850	-11.298053
H	-1.337206	-2.353028	-3.454914
H	-3.107084	-0.644284	-4.541903
H	-4.071815	0.921267	-2.573793
H	-0.442963	2.141690	0.501138
H	-1.207178	-1.846209	-0.814294
H	-2.891996	0.182800	-0.271760
H	-1.005091	4.077168	-1.279584
H	0.917358	4.052761	-3.167753
H	2.663081	2.100614	-2.552647
H	1.826383	0.922074	-0.283527
H	0.616568	-0.982177	-4.845693
H	-0.666011	1.579654	-5.125543
H	0.939018	1.888681	-5.733564
H	0.626171	0.128117	-7.442980
H	-0.875431	-0.399644	-6.656038
H	-0.600612	0.694760	-9.440047
H	-2.102152	0.152187	-8.668675
H	-3.002560	2.482185	-8.806109
H	-1.513217	3.016924	-9.570884
H	-1.953280	1.465204	-11.523925
H	-3.451375	0.927317	-10.754244

Trapping of H2

Pr2O_TS_trap_H2_alfa

E=-731.9943402
G=-731.691554

C	0.202811	-0.849556	2.008544
C	1.277390	-0.195288	1.362270
C	1.131011	1.198615	1.574252
C	-0.044685	1.405591	2.341433
C	-0.615288	0.140277	2.615371
Ce	1.789587	0.183122	4.145047
C	2.451647	1.966675	6.261919
C	2.282978	0.719794	6.907434
C	0.906171	0.383991	6.857292
C	0.222142	1.431916	6.191137
C	1.176574	2.407616	5.816844
C	2.163308	-2.392122	4.608326
C	2.876570	-2.990828	5.790759
C	3.285659	-4.461104	5.709979
H	3.882287	-4.757709	6.579389
O	3.775209	-0.836878	3.894978
C	4.989262	-1.395419	3.515504
C	6.054389	-0.328050	3.257390
C	7.400099	-0.922095	2.848345
H	8.142054	-0.139221	2.663239
H	3.066522	0.135352	7.374903
H	0.447507	-0.492454	7.301565
H	-0.847108	1.490692	6.024033
H	0.964595	3.349512	5.323352
H	3.385072	2.510136	6.162583
H	2.064884	-0.673565	0.791937
H	1.772854	1.975142	1.171504
H	-0.450831	2.365279	2.638824
H	-1.541627	-0.037675	3.150055
H	0.010311	-1.916388	2.000617
H	2.309016	-2.792201	6.708121
H	0.734242	-2.850346	4.721712
H	3.775098	-2.362993	5.870097
H	3.879882	-4.655831	4.810997
H	2.404517	-5.112493	5.675077
H	0.710781	-3.651089	4.708269
H	2.398785	-2.912680	3.670164
H	5.368918	-2.076107	4.301883
H	4.874027	-2.009467	2.603338
H	5.685932	0.347400	2.474378
H	6.165915	0.276172	4.166562
H	7.800789	-1.578271	3.629504
H	7.311744	-1.516473	1.931733

Pr2O_TS_trap_H2_beta

E=-731.9337553
G=-731.629167

C	1.212352	-1.016955	1.956767
C	2.133147	-0.088184	1.411241
C	1.669037	1.217114	1.709451
C	0.461374	1.095109	2.438869
C	0.176660	-0.285464	2.591007
Ce	-0.219272	0.174707	-0.179427
C	-2.147100	-1.930632	-0.121880
C	-1.031601	-2.488438	-0.795357
C	-0.924425	-1.856989	-2.060087
C	-1.968695	-0.906152	-2.166797
C	-2.724486	-0.952547	-0.968833
C	1.542371	0.548541	-2.084289
C	2.744687	1.484284	-2.104068
H	3.541341	1.166417	-2.783086
C	0.056553	2.465373	-1.411575
O	-1.161628	2.411912	-0.642337
C	-1.796278	3.647631	-0.323736
C	-3.024869	3.389251	0.529771
C	-3.757475	4.680145	0.890139
H	-4.636304	4.472061	1.507139
H	1.952021	-0.686515	-1.972273
H	2.398990	-0.793439	-2.726368
H	0.999568	0.520304	-3.034748
H	-1.077491	4.292022	0.204964
H	-2.070274	4.151947	-1.261747
H	-2.718565	2.864321	1.443378
H	-3.695785	2.713940	-0.014448
H	2.168101	2.144767	1.455651
H	-0.120843	1.913821	2.846904
H	-0.659679	-0.708930	3.135747
H	1.303434	-2.096748	1.930090
H	3.053621	-0.334145	0.894169
H	-0.196668	-2.093018	-2.828490
H	-2.176292	-0.279134	-3.026236
H	-3.612328	-0.368030	-0.754690
H	-2.514660	-2.227256	0.853992
H	-0.402815	-3.291572	-0.428129
H	-0.167498	2.738807	-2.449278
H	0.748567	3.184076	-0.954826
H	2.419439	2.467050	-2.454405
H	3.171167	1.610608	-1.104751
H	-3.112339	5.363429	1.453222
H	-4.100304	5.208842	-0.005912

Pr2O_TS_trap_H2_gamma

E=-731.9234529
G=-731.619531

C	-2.692767	-0.540986	-0.732452
C	-2.143917	-1.523607	0.130735
C	-1.216689	-2.292061	-0.616165
C	-1.191109	-1.781586	-1.940057
C	-2.101544	-0.699135	-2.010586
Ce	-3.742771	-3.008783	-1.678657
C	-5.476010	-5.263606	-1.490947
C	-5.615422	-4.598612	-0.245886
C	-4.397248	-4.734603	0.465021
C	-3.502833	-5.484138	-0.340833
C	-4.172354	-5.813506	-1.546734
C	-3.382259	-3.669115	-4.149974
H	-3.043793	-2.943591	-4.891073
C	-5.097539	-2.069783	-3.744365
O	-6.251895	-1.796423	-2.819326
O	-6.767339	-0.488391	-2.978891
C	-7.846330	-0.204949	-2.111959
C	-8.318571	1.217546	-2.359699
C	-9.491946	1.607007	-1.464404
H	-9.812467	2.634369	-1.661000
H	-2.313079	-4.413467	-3.958823
H	-2.203209	-4.685463	-4.782601
H	-4.102855	-4.376275	-4.562774
H	-2.289448	-0.078977	-2.878819
H	-3.404330	0.228232	-0.452443
H	-2.364418	-1.641214	1.185681
H	-0.600490	-3.096122	-0.229937
H	-0.550215	-2.126853	-2.743250
H	-3.771063	-6.417514	-2.352257
H	-6.245766	-5.371057	-2.246104
H	-6.513366	-4.112326	0.119286
H	-4.196719	-4.365701	1.464379
H	-2.502487	-5.794393	-0.060927
H	-5.452286	-2.412978	-4.716899
H	-4.522095	-1.146754	-3.887666
H	-7.050239	-2.546179	-2.947337
H	-5.982663	-1.881462	-1.716235
H	-8.672857	-0.917594	-2.282785
H	-7.533542	-0.324239	-1.057758
H	-7.473910	1.897532	-2.198215
H	-8.596978	1.311179	-3.415834
H	-10.356569	0.954322	-1.629522
H	-9.226110	1.541762	-0.403242

Pr2O_trap_H2_alfa_product

E=-613.0282527
G=-612.814878

C	0.038756	-0.838311	2.050530
C	1.187369	-0.356772	1.361855
C	1.271525	1.038069	1.571585
C	0.184686	1.421516	2.400475
C	-0.585242	0.263145	2.680687
Ce	1.866138	-0.103727	4.100188
C	0.138095	-0.403369	6.339316
C	1.376455	0.029840	6.888084
C	2.310635	-1.023919	6.750714
C	1.659138	-2.101721	6.100795
C	0.312252	-1.721130	5.857401
O	3.946071	0.459105	3.925457
C	5.295273	0.795014	3.840457
C	6.134702	-0.326658	3.229374
C	7.617046	0.025992	3.133545
H	8.195697	-0.791693	2.692625
H	2.028170	1.698205	1.164515
H	-0.056236	2.434708	2.705020
H	-1.500409	0.230942	3.259822
H	-0.327983	-1.858761	2.042327
H	1.855888	-0.947561	0.745025
H	3.340219	-1.010143	7.087417
H	2.094728	-3.072579	5.888526
H	-0.455049	-2.342737	5.410701

H	-0.788849	0.158736	6.335972
H	1.558602	0.980370	7.378276
H	5.424322	1.706360	3.230857
H	5.694825	1.031305	4.842298
H	6.000192	-1.231328	3.836984
H	5.735506	-0.555700	2.232621
H	7.775526	0.914956	2.512342
H	8.041812	0.235329	4.122013

Pr2O_trap_H2_beta_product

E=-652.2632923
G=-652.023175

C	1.249770	-0.672859	1.600350
C	1.986539	0.517595	1.376855
C	1.444097	1.528707	2.210016
C	0.367565	0.964019	2.942287
C	0.249910	-0.395171	2.566857
Ce	2.707621	-0.237688	4.003228
C	5.534365	-0.367670	3.775610
C	5.207113	0.969669	3.443229
C	4.748207	1.612664	4.620821
C	4.805903	0.676493	5.684723
C	5.286601	-0.547789	5.162247
C	1.436629	-0.435305	6.157358
O	1.755357	-1.768967	5.652139
C	1.335974	-2.895899	6.407664
C	1.762097	-4.177389	5.711638
C	1.343188	-5.423503	6.489299
H	1.658284	-6.334411	5.972203
H	1.777498	-2.832799	7.413574
H	0.242287	-2.859224	6.522526
H	2.852046	-4.164866	5.583575
H	1.322497	-4.197582	4.706252
H	4.544996	0.870397	6.717554
H	5.474425	-1.451502	5.731306
H	5.953717	-1.106300	3.100426
H	5.318974	1.429796	2.468372
H	4.455799	2.653504	4.704723
H	-0.267921	1.486523	3.646896
H	-0.492392	-1.093880	2.935086
H	1.392373	-1.615764	1.082435
H	2.794683	0.643748	0.665578
H	1.762913	2.564476	2.242301
H	0.345700	-0.336439	6.231373
H	1.891398	-0.314489	7.149167
H	1.790404	-5.438621	7.489144
H	0.255596	-5.471164	6.610996

Pr2O_trap_H2_gamma_product

E=-691.5469432
G=-691.283290

C	-2.640695	-0.117964	-0.987179
C	-2.453337	-1.033065	0.077625
C	-1.696444	-2.125293	-0.415646
C	-1.423074	-1.888993	-1.788380
C	-2.008435	-0.648182	-2.142304
Ce	0.110185	0.054963	-0.434778
C	1.808046	2.312177	-0.679991
C	2.677029	1.204424	-0.824737
C	2.380370	0.569623	-2.060298
C	1.323550	1.282856	-2.675586
C	0.962369	2.355089	-1.817930
C	-0.044241	0.723538	1.991947
C	0.460746	-0.609024	2.451306
O	1.553892	-0.532154	3.341384
C	2.046716	-1.794685	3.734639
C	3.197218	-1.596655	4.706675
C	3.787415	-2.918729	5.190229
H	4.609950	-2.749587	5.891440
H	1.804513	3.014565	0.144200
H	3.463525	0.921132	-0.133831
H	2.904502	-0.281143	-2.482869
H	0.890631	1.069478	-3.646034
H	0.214348	3.112030	-2.027545
H	-3.207836	0.805212	-0.939483
H	-2.841019	-0.926700	1.082828
H	-1.422673	-3.013121	0.143951
H	-0.901321	-2.560728	-2.461442
H	-2.008873	-0.202878	-3.130476
H	-0.959058	1.024220	2.506053
H	0.727781	1.485221	2.151333
H	-0.346418	-1.230291	2.874353
H	0.840589	-1.262294	1.575621
H	1.245001	-2.388987	4.208355
H	2.387430	-2.366496	2.850394
H	3.968493	-0.991425	4.215874
H	2.833372	-1.008056	5.556820
H	3.035968	-3.528926	5.703928
H	4.181260	-3.511631	4.356823

Releasing of alkene

Pr2O_TS_releasing_alkene_beta

E=-730.864382
G=-730.572552

C	-2.297303	7.383432	-3.516846
C	-2.450919	6.484710	-4.602439
C	-3.481563	5.570697	-4.271243
C	-3.961679	5.903361	-2.978252
C	-3.229160	7.021776	-2.512588
Ce	-4.828657	8.040617	-4.640961
C	-6.412281	9.038422	-6.799312
C	-5.073017	9.229424	-7.218006
C	-4.499584	7.953824	-7.450769
C	-5.485831	6.973866	-7.176027
C	-6.667987	7.645388	-6.772758
O	-6.479128	8.858217	-3.125120
C	-5.838298	10.495107	-3.194173
C	-4.541812	10.559015	-3.795679
C	-3.347368	10.859140	-2.901736
H	-3.336659	11.897416	-2.533709
C	-7.773326	8.853018	-2.579581
C	-8.306516	7.433159	-2.436251
C	-9.707856	7.395528	-1.829197
H	-10.070178	6.367561	-1.736273
H	-5.907110	10.675400	-2.118580
H	-6.675119	10.929631	-3.743394
H	-7.125001	9.821276	-6.567716
H	-3.345674	7.501877	-1.548171
H	-4.583333	10.184200	-7.370168
H	-3.497733	7.762622	-7.817731
H	-5.369191	5.902988	-7.295943
H	-7.614908	7.175853	-6.529352
H	-3.813207	4.736981	-4.879735
H	-1.857014	6.472178	-5.509116
H	-1.569398	8.183338	-3.449518
H	-4.727292	5.369256	-2.426145
H	-8.457537	9.442597	-3.214476
H	-7.759378	9.340049	-1.589457
H	-4.536003	11.095016	-4.748216
H	-8.316302	6.956209	-3.425372
H	-7.610187	6.858509	-1.813200
H	-3.325762	10.208930	-2.018915
H	-2.397368	10.705896	-3.425613
H	-9.720394	7.842579	-0.829123
H	-10.425890	7.945292	-2.447687

Pr2O_TS_releasing_alkene_gamma

E=-730.804048
G=-730.513208

C	1.021983	0.413827	-3.035487
C	0.654691	1.728482	-2.655180
C	0.302137	2.442114	-3.827578
C	0.444974	1.567063	-4.933695
C	0.891086	0.313034	-4.443305
Ce	-1.778562	0.523335	-3.532371
C	-4.286808	0.353154	-4.857797
C	-4.184406	-0.871468	-4.155208
C	-3.149691	-1.634366	-4.749959
C	-2.610636	-0.879413	-5.823560
C	-3.312619	0.351076	-5.889178
C	-1.962654	-0.795966	-1.290863
H	-0.960429	-0.938091	-0.894179
C	-2.737742	0.287472	-0.835061
C	-2.963439	2.155255	-1.835297
O	-4.167676	2.413962	-1.188160
C	-4.473126	3.792404	-1.054669
C	-5.790367	3.935613	-0.312362
C	-6.192130	5.395904	-0.120781
H	-7.143099	5.474433	0.414117
H	1.132141	-0.556055	-5.045196
H	1.377729	-0.365343	-2.371841
H	0.680219	2.129283	-1.648311
H	-3.163255	1.130178	-6.628335
H	0.286219	1.823778	-5.974901
H	0.013478	3.486463	-3.876541
H	-5.008147	1.138423	-4.662196
H	-4.806891	-1.179929	-3.323576
H	-2.849960	-2.636070	-4.463117
H	-1.830793	-1.203972	-6.502965
H	-2.139302	2.760112	-1.419168
H	-3.074615	2.484909	-2.915514
H	-3.661722	4.303818	-0.508701
H	-4.539371	4.262811	-2.050840
H	-6.565530	3.398086	-0.871006
H	-5.699401	3.434408	0.658423
H	-5.441504	5.946017	0.457688
H	-6.310717	5.908665	-1.081849
H	-3.820757	0.204246	-0.837924
H	-2.358915	0.900469	-0.021663
H	-2.474149	-1.694474	-1.630186

Pr2O_releasing_alkene_beta_product

E=-613.0282527
G=-612.814878

C	0.038756	-0.838311	2.050530
C	1.187369	-0.356772	1.361855
C	1.271525	1.038069	1.571585
C	0.184686	1.421516	2.400475
C	-0.585242	0.263145	2.680687
Ce	1.866138	-0.103727	4.100188
C	0.138095	-0.403369	6.339316
C	1.376455	0.029840	6.888084
C	2.310635	-1.023919	6.750714
C	1.659138	-2.101721	6.100795
C	0.312252	-1.721130	5.857401
O	3.946071	0.459105	3.925457
C	5.295273	0.795014	3.840457
C	6.134702	-0.326658	3.229374
C	7.617046	0.025992	3.133545
H	8.195697	-0.791693	2.692625
H	2.028170	1.698205	1.164515
H	-0.056236	2.434708	2.705020
H	-1.500409	0.230942	3.259822
H	-0.327983	-1.858761	2.042327
H	1.855888	-0.947561	0.745025
H	3.340219	-1.010143	7.087417
H	2.094728	-3.072579	5.888526
H	-0.455049	-2.342737	5.410701
H	-0.788849	0.158736	6.335972
H	1.558602	0.980370	7.378276
H	5.424322	1.706360	3.230857
H	5.694825	1.031305	4.842298
H	6.000192	-1.231328	3.836984
H	5.735506	-0.555700	2.232621
H	7.775526	0.914956	2.512342
H	8.041812	0.235329	4.122013

Pr2O_releasing_alkene_gamma_product

E=-652.2632923
G=-652.023175

C	1.249770	-0.672859	1.600350
C	1.986539	0.517595	1.376855
C	1.444097	1.528707	2.210016
C	0.367565	0.964019	2.942287
C	0.249910	-0.395171	2.566857
Ce	2.707621	-0.237688	4.003228
C	5.534365	-0.367670	3.775610
C	5.207113	0.969669	3.443229
C	4.748207	1.612664	4.620821
C	4.805903	0.676493	5.684723
C	5.286601	-0.547789	5.162247
C	1.436629	-0.435305	6.157358
O	1.755357	-1.768967	5.652139
C	1.335974	-2.895899	6.407664
C	1.762097	-4.177389	5.711638
C	1.343188	-5.423503	6.489299
H	1.658284	-6.334411	5.972203
H	1.777498	-2.832799	7.413574
H	0.242287	-2.859224	6.522526
H	2.852046	-4.164866	5.583575
H	1.322497	-4.197582	4.706252
H	4.544996	0.870397	6.717554
H	5.474425	-1.451502	5.731306
H	5.953717	-1.106300	3.100426
H	5.318974	1.429796	2.468372
H	4.455799	2.653504	4.704723
H	-0.267921	1.486523	3.646896
H	-0.492392	-1.093880	2.935086
H	1.392373	-1.615764	1.082435
H	2.794683	0.643748	0.665578
H	1.762913	2.564476	2.242301
H	0.345700	-0.336439	6.231373
H	1.891398	-0.314489	7.149167
H	1.790404	-5.438621	7.489144
H	0.255596	-5.471164	6.610996

Insertion of propene into Ce-H bond

Pr2O_TS_insertion_12_propene

E=-537.7381015
G=-537.531549

C	-0.462998	-0.811299	-2.745475
C	-0.580994	0.597035	-2.636468
C	0.640053	1.097751	-2.120762
C	1.516305	0.000200	-1.919723
C	0.835406	-1.180453	-2.306795
Ce	-0.515485	-0.363241	0.025541
C	-0.067118	-2.368805	1.976984
C	-1.156669	-1.619573	2.491652
C	-2.281774	-1.853192	1.662658
C	-1.885648	-2.741259	0.631001
C	-0.518529	-3.065094	0.828525
C	-0.207901	1.971973	1.493373
C	-1.495187	2.292833	1.151651
C	-2.641838	2.239189	2.120032
H	-1.656741	2.891728	0.258697
H	-2.285405	0.840966	-0.013712
H	1.247991	-2.182808	-2.309509
H	-1.216314	-1.484078	-3.139860
H	-1.443678	1.187039	-2.918865
H	0.881448	2.142674	-1.961496
H	2.544826	0.058243	-1.579066
H	0.066336	-3.753428	0.229351
H	0.922341	-2.440290	2.416401
H	-1.144342	-1.016936	3.392810
H	-3.274715	-1.445467	1.803955
H	-2.527996	-3.139686	-0.146334
H	0.016699	1.553456	2.474011
H	0.631394	2.326670	0.896961
H	-2.703548	3.199944	2.649058
H	-3.591569	2.065512	1.611743
H	-2.499550	1.456939	2.870785

Pr2O_TS_insertion_21_propene

E=-537.735788
G=-537.528825

C	-0.525635	-1.014492	-2.684783
C	-0.867966	0.359575	-2.732496
C	0.288824	1.108248	-2.400905
C	1.347577	0.197806	-2.157779
C	0.845385	-1.115951	-2.328615
Ce	-0.454141	-0.222537	0.005342
C	-0.072178	-2.109262	2.090939
C	-1.255990	-1.420496	2.460303
C	-2.269804	-1.756526	1.529610
C	-1.711178	-2.651464	0.581696
C	-0.354386	-2.873069	0.931014
C	-0.287081	2.008039	1.608113
C	-1.429261	2.375906	0.941859
H	-2.383718	2.390783	1.453938
H	-1.380144	2.963042	0.027998
H	-2.220876	0.974574	-0.075851
H	1.418659	-2.032784	-2.253655
H	-1.184286	-1.842563	-2.920127
H	-1.835077	0.766404	-2.998990
H	0.362414	2.189789	-2.392285
H	2.374708	0.459456	-1.927012
H	0.332715	-3.540648	0.423842
H	0.868215	-2.097718	2.631799
H	-1.379037	-0.788295	3.331935
H	-3.296291	-1.412930	1.553044
H	-2.241202	-3.119761	-0.239682
H	-0.389679	1.588979	2.608537
C	1.117263	2.210159	1.115650
H	1.732566	2.719998	1.866034
H	1.676942	1.265174	0.915291
H	1.150081	2.795166	0.191549

Pr2O_TS_insertion_12_product_propene

E=-537.767405
G=-537.557391

C	-0.331436	-0.718702	-2.828074
C	-0.431642	0.680261	-2.610595
C	0.740715	1.106540	-1.937485
C	1.560960	-0.029262	-1.730804
C	0.901361	-1.157525	-2.285190
Ce	-0.641854	-0.469373	-0.026171
C	0.151403	-2.564948	1.679940
C	-0.714756	-1.785316	2.488013
C	-2.028945	-1.929568	1.982223
C	-1.979434	-2.811035	0.869583
C	-0.632855	-3.206504	0.685287
C	-0.475657	1.618811	1.355234
C	-1.840226	2.073476	0.870825
C	-2.819895	2.554866	1.943625
H	-1.742315	2.835946	0.088157
H	-2.409553	1.244744	0.324832
H	1.290381	-2.168481	-2.323811
H	-1.048278	-1.336192	-3.358496
H	-1.238152	1.321109	-2.950232
H	0.978694	2.123616	-1.652444
H	2.543004	-0.029521	-1.270440
H	-0.269688	-3.903381	-0.061281
H	1.216765	-2.699095	1.833399
H	-0.425793	-1.201438	3.352862
H	-2.924732	-1.487528	2.404354
H	-2.829837	-3.160517	0.293693
H	-0.477738	1.420999	2.433058
H	0.307535	2.346045	1.127561
H	-2.424921	3.450185	2.433705
H	-3.805767	2.797265	1.529180
H	-2.955629	1.790038	2.715927

Pr2O_TS_insertion_21_product_propene

E=-537.7577833
G=-537.548779

C	-0.695294	-0.909822	-2.680520
C	-0.900458	0.492341	-2.630423
C	0.335214	1.108575	-2.315309
C	1.305512	0.085246	-2.164579
C	0.671081	-1.161151	-2.394853
Ce	-0.415551	-0.249473	0.083850
C	0.011388	-2.089139	2.186236
C	-1.239604	-1.500208	2.493166
C	-2.172635	-1.923453	1.512596

C	-1.499439	-2.783729	0.606215
C	-0.149177	-2.885175	1.021785
C	-0.427159	1.825498	1.461739
C	-1.527739	2.412246	0.629466
H	-2.341323	2.833549	1.228962
H	-1.194450	3.177366	-0.083734
H	-2.075856	1.659126	-0.033845
H	1.152380	-2.132439	-2.390409
H	-1.439968	-1.654452	-2.937494
H	-1.830276	1.005830	-2.848754
H	0.517465	2.174580	-2.249484
H	2.361402	0.233313	-1.966390
H	0.615436	-3.497280	0.556940
H	0.921831	-1.986961	2.766753
H	-1.452274	-0.863379	3.342528
H	-3.229143	-1.678697	1.491227
H	-1.947262	-3.302523	-0.233416
H	-0.652347	1.759577	2.523771
C	1.016372	2.090363	1.149247
H	1.607341	2.343680	2.035638
H	1.582673	1.195191	0.721913
H	1.175868	2.872266	0.395357

Second C_β-H activation of Pr-O-Pr by Cp2CePr

Pr2O_TS_C_βH_act2_beta

E=-849.9369021
G=-849.545060

C	-4.393254	0.535178	0.308143
C	-3.999574	-0.440565	1.255665
C	-4.657608	-1.655065	0.934335
C	-5.459771	-1.428201	-0.207877
C	-5.292495	-0.077048	-0.602786
Ce	-2.786383	-1.240659	-1.188924
C	-0.602704	-0.582402	-2.921722
C	-0.601769	0.423670	-1.922859
C	-1.752006	1.226815	-2.107322
C	-2.469876	0.716316	-3.219496
C	-1.750553	-0.394813	-3.727117
O	-3.731745	-2.965965	-2.846256
C	-2.769037	-4.024507	-2.660037
C	-2.302539	-4.034175	-1.215421
C	-1.236599	-5.125210	-1.076098
H	-0.288484	-4.826502	-1.541049
C	-4.335611	-2.967866	-4.137075
C	-5.426962	-1.917119	-4.211033
C	-6.087989	-1.880934	-5.587819
H	-6.875081	-1.122661	-5.621784
C	-0.774116	-2.115273	0.406798
C	-0.432928	-3.023332	1.596426
C	-1.629128	-3.394940	2.469611
H	-1.330426	-4.032594	3.309135
H	-4.582503	-2.583485	1.486940
H	-6.102772	-2.157624	-0.685990
H	-5.803283	0.418170	-1.420674
H	-2.019205	2.100279	-1.524544
H	-3.339990	-0.277761	2.099849
H	-4.093616	1.576422	0.302992
H	-3.372523	1.142697	-3.642047
H	-2.014845	-0.978215	-4.601253
H	0.163025	-1.335690	-3.066389
H	0.159298	0.567213	-1.165062
H	-1.592506	-3.002951	-0.455517
H	-3.169158	-4.312723	-0.594342
H	-1.927039	-3.863924	-3.353788
H	-3.255211	-4.972931	-2.954017
H	-6.174777	-2.127545	-3.437991
H	-4.996235	-0.935484	-3.978310
H	-5.363967	-1.641977	-6.374326
H	-6.545909	-2.844237	-5.837604
H	-1.543408	-6.072028	-1.547131
H	-1.027954	-5.347637	-0.027025
H	0.038825	-3.941838	1.226808
H	0.327874	-2.544239	2.230810
H	-2.107062	-2.502240	2.888588
H	-2.388777	-3.934755	1.893577
H	0.131105	-1.954164	-0.194998
H	-1.019399	-1.117036	0.825341
H	-3.564358	-2.784729	-4.901179
H	-4.752957	-3.968779	-4.322318

Pr2O_TS_C_βH_act2_beta_product

E=-730.8701458
G=-730.575363

C	-1.810640	-1.525432	-0.779701
C	-0.640285	-2.304861	-0.968801
C	-0.706815	-2.890506	-2.257628
C	-1.913996	-2.466726	-2.867546
C	-2.595756	-1.624428	-1.952651
Ce	-0.297651	-0.120929	-2.735821
C	1.901653	0.888620	-4.248778
C	2.063487	1.462517	-2.965465
C	2.396447	0.422612	-2.061240
C	2.451242	-0.792671	-2.789182
C	2.138639	-0.506926	-4.140789
C	-2.362863	2.029846	-0.704064
H	-2.830194	3.012266	-0.513351
C	-1.228517	2.086098	-1.726422
C	-1.660153	2.626164	-3.062979
O	-1.705816	1.512940	-4.054393
C	-2.104722	1.910359	-5.355995
C	-2.126860	0.709312	-6.285922
C	-2.577024	1.080497	-7.697672
H	-2.583726	0.203062	-8.350314
H	-2.673791	3.060637	-3.073800
H	-0.963021	3.365663	-3.481924
H	1.680592	1.427880	-5.163235
H	-3.562713	-1.161058	-2.111117
H	1.972802	2.513397	-2.719851
H	2.616948	0.543399	-1.006370
H	2.714798	-1.764443	-2.388468
H	2.135521	-1.221569	-4.956823
H	0.020016	-3.570435	-2.687041
H	0.142484	-2.466964	-0.236174
H	-2.072165	-0.972415	0.114060
H	-2.277338	-2.776734	-3.841765
H	-1.411420	2.678589	-5.733866
H	-3.103931	2.368876	-5.298924
H	-0.411717	2.706774	-1.339574
H	-1.121882	0.267260	-6.324149
H	-2.797286	-0.050709	-5.865822
H	-3.171399	1.355765	-1.016011
H	-2.007655	1.660696	0.265100
H	-3.589063	1.499321	-7.695144
H	-1.909634	1.823451	-8.147471

Bu-O-Bu

Bu2O

E=-390.799428
G=-390.587355

O	0.136786	0.000000	0.097024
C	0.094744	0.000000	1.506683
C	1.451384	0.000000	-0.413621
C	-1.356427	0.000000	1.955088
H	0.619167	-0.886392	1.907159
H	0.619167	0.886392	1.907159
C	1.390140	0.000000	-1.931322
H	2.004161	0.886389	-0.053185
H	2.004161	-0.886389	-0.053185
C	-1.510032	0.000000	3.475668
H	-1.854134	0.878929	1.526404
H	-1.854134	-0.878929	1.526404
C	-2.968752	0.000000	3.926165
H	-0.998423	-0.877124	3.894789
H	-0.998423	0.877124	3.894789
H	-3.051052	0.000000	5.017716
H	-3.498297	0.883370	3.552478
H	-3.498297	-0.883370	3.552478
C	2.772880	0.000000	-2.581941
H	0.820165	-0.878982	-2.257751
H	0.820165	0.878982	-2.257751
C	2.712556	0.000000	-4.107446
H	3.338282	0.877140	-2.238867
H	3.338282	-0.877140	-2.238867
H	3.714507	0.000000	-4.548291
H	2.183935	-0.883369	-4.482503
H	2.183935	0.883369	-4.482503

methane

E=-40.5086919
G=-40.483278

C	0.015187	-0.026305	-0.028305
H	-0.020397	0.035329	1.061091
H	1.055826	-0.046766	-0.357713
H	-0.487413	-0.937755	-0.357713
H	-0.486321	0.842333	-0.458359

ethane

E=-79.80958
G=-79.757631

C	-0.000023	0.000000	-0.062461
C	0.000023	0.000000	1.462461
H	1.019317	0.000000	1.862340
H	-0.509651	0.882731	1.862309
H	-0.509651	-0.882731	1.862309
H	-1.019317	0.000000	-0.462340
H	0.509651	0.882731	-0.462309
H	0.509651	-0.882731	-0.462309

propane

E=-119.112279
G=-119.033393

C	-0.025522	0.044206	-0.072237
C	-0.002489	0.004311	1.453520
H	0.990576	0.050626	-0.483133
H	-0.539131	-0.832551	-0.483133
H	-0.540099	0.935479	-0.445984
H	-1.031223	0.034015	1.835423
C	0.709082	-1.228166	2.005537
H	0.486154	0.910073	1.835422
H	0.713743	-1.236238	3.100415
H	0.221675	-2.150306	1.668751
H	1.751382	-1.267129	1.668751

butane

E=-158.414943
G=-158.310591

C	0.012252	0.021464	0.045461
C	0.028747	0.049929	1.571182
H	1.042829	0.053626	-0.334425
C	-0.695788	-1.205384	-0.528794
H	-0.475629	0.929858	-0.334277
H	-0.988578	0.054600	1.978920
H	0.540851	-0.829207	1.978754
H	0.542151	0.938300	1.953044
C	-0.712284	-1.233849	-2.054515
H	-0.207908	-2.113778	-0.149056
H	-1.726366	-1.237546	-0.148908
H	-1.225688	-2.122221	-2.436377
H	-1.224387	-0.354713	-2.462087
H	0.305042	-1.238520	-2.462253

propene

E=-117.8704352
G=-117.815511

C	0.043669	-0.009624	0.025246
H	-0.526393	-0.323346	0.908609
H	1.078195	0.139709	0.358561
H	0.033935	-0.832344	-0.695648
C	-0.520250	1.245646	-0.563616
C	-0.984307	1.371293	-1.806121
H	-0.543266	2.114702	0.095250
H	-1.381639	2.312560	-2.174716
H	-0.983544	0.534788	-2.501799

butene

E=-157.172733
G=-157.091433

C	0.081010	0.370189	0.165642
C	-0.085116	-0.288435	1.311820
C	1.296849	0.297282	-0.710193
H	-0.723560	1.015071	-0.193290
C	0.980281	-0.204039	-2.123314
H	1.748725	1.297121	-0.782492
H	2.048127	-0.349981	-0.242112
H	0.687028	-0.944801	1.707905
H	-0.994558	-0.195544	1.898576
H	1.879177	-0.217667	-2.747892
H	0.569708	-1.218213	-2.096126
H	0.242657	0.439016	-2.615873

Cp2CeH

E=-419.8558335
G=-419.725269

C	0.675990	1.108596	-2.020810
C	1.525135	-0.025376	-1.918859
C	0.812095	-1.147707	-2.405643
C	-0.475511	-0.706323	-2.810803
C	-0.556420	0.688955	-2.582714
Ce	-0.471808	-0.419610	-0.000163
C	0.810397	-1.145502	2.406890
C	1.523272	-0.023111	1.920015
C	0.673455	1.110485	2.020513
C	-0.559216	0.690563	2.581605
C	-0.477776	-0.704525	2.810647
H	-2.301832	0.663752	-0.001508
H	2.549985	-0.021460	1.573296
H	0.939356	2.129208	1.762039
H	-1.409315	1.323811	2.798331
H	-1.249399	-1.318237	3.263163
H	1.200484	-2.153473	2.502765
H	2.551554	-0.024032	-1.571276
H	1.201742	-2.155942	-2.500542
H	-1.247070	-1.319924	-3.263576
H	-1.406005	1.322500	-2.800581
H	0.942208	2.127352	-1.762790

First C-H activation of Bu2O by Cp2CeH

Bu2O_CH_act_alfa_adduct_Bu2O

E=-810.673462
G=-810.309826

C	-0.493755	-0.798342	-2.955925
C	-0.259027	0.582403	-2.744512
C	1.027057	0.721249	-2.165977
C	1.591921	-0.572067	-2.028967
C	0.650471	-1.512383	-2.516242
Ce	-0.488866	-0.480984	-0.126030
C	-0.073350	0.776340	2.379993
C	-0.468631	-0.536681	2.733191
C	0.566839	-1.427327	2.351201
C	1.602113	-0.665012	1.755516
C	1.203742	0.696438	1.770681
O	-2.567959	-2.094987	0.077003
C	-2.561058	-3.483471	0.420981
C	-3.808367	-1.404725	0.374692
H	-1.881421	1.153965	-0.130692
H	2.550095	-1.048100	1.396019
H	1.790834	1.535012	1.414020
H	-0.641858	1.681179	2.550172
H	-1.384413	-0.806545	3.247377
H	0.592781	-2.495260	2.539628
H	2.584532	-0.798597	-1.657404
H	0.803273	-2.583641	-2.589818
H	-1.376099	-1.229580	-3.415695
H	-0.936246	1.390895	-2.986922
H	1.508199	1.657415	-1.906850
H	-3.543014	-0.515158	0.956453
C	-1.275026	-4.126141	-0.063700
H	-2.656850	-3.585980	1.511939
H	-3.427359	-3.973091	-0.042754
H	-4.423286	-2.057131	1.005467
C	-4.528532	-0.979989	-0.894469
C	-1.197492	-5.612197	0.296250
H	-1.197246	-4.002780	-1.151160
H	-0.415726	-3.605551	0.385481
C	0.093000	-6.270593	-0.185033
H	-1.285522	-5.727560	1.384522
H	-2.060267	-6.134578	-0.137946
H	0.121119	-7.330317	0.085731
H	0.191440	-6.202939	-1.273913
H	0.972556	-5.791043	0.258253
C	-5.020382	-2.112616	-1.799684
H	-5.378473	-0.355426	-0.585876
H	-3.855711	-0.314084	-1.448269
H	-5.354441	-1.672016	-2.746641
H	-4.176007	-2.764037	-2.060368
C	-6.161636	-2.942848	-1.212357
H	-6.483646	-3.721966	-1.910557
H	-5.877058	-3.441866	-0.279005
H	-7.032561	-2.315145	-0.992625

Bu2O_CH_act_beta_adduct_Bu2O

E=-810.674827
G=-810.309969

C	-1.446950	-1.469517	-0.436489
C	-0.597674	-2.404893	-1.078222
C	-1.276052	-2.904851	-2.217422
C	-2.552314	-2.293372	-2.273826
C	-2.656605	-1.403305	-1.177267
Ce	-0.792251	-0.153513	-2.838894
C	-2.018031	2.331099	-3.405326
C	-2.132536	2.158830	-2.004563
C	-0.837189	2.283243	-1.436460
C	0.075558	2.539009	-2.490617
C	-0.652286	2.559885	-3.705284
O	1.735067	-0.826448	-3.498592
C	1.948855	-1.452321	-4.774652
C	1.111426	-0.756577	-5.831861
C	2.704561	-1.223965	-2.522939
C	2.588679	-0.355133	-1.285308
H	1.689784	-2.519490	-4.702521
H	3.018844	-1.381495	-5.011381
H	1.138296	2.725566	-2.382424
H	-0.903811	-3.656585	-2.904637
H	-0.244273	2.749081	-4.691704
H	-2.827996	2.297477	-4.122256
H	-3.053583	1.999925	-1.456237
H	-0.600357	2.252060	-0.378977
H	-1.238119	-0.944969	0.488888
H	-3.525355	-0.807793	-0.922398
H	-3.311450	-2.474941	-3.022965
H	0.378642	-2.721917	-0.728341
H	3.705514	-1.117622	-2.965638
H	2.558436	-2.285992	-2.275521
H	-1.892972	-0.504652	-4.638093
H	1.408795	0.299273	-5.878627
C	1.241641	-1.395374	-7.220329
H	0.044818	-0.780063	-5.548893
H	2.696916	0.696452	-1.577612
H	1.586269	-0.468453	-0.847703
C	2.631513	-1.287150	-7.847624
H	0.939755	-2.449657	-7.163910
H	0.510936	-0.911893	-7.878165
H	2.630705	-1.686688	-8.866555
H	2.960276	-0.243058	-7.902181
H	3.388161	-1.844470	-7.284817
C	3.637033	-0.712898	-0.228527
C	3.540621	0.163059	1.018055
H	3.525347	-1.767974	0.054473
H	4.639539	-0.618394	-0.666875
H	4.302790	-0.110823	1.753767
H	3.680876	1.220988	0.771238

H	2.562150	0.061607	1.499972

Bu2O_CH_act_gamma_adduct_Bu2O

E=-810.675991
G=-810.312564

Ce	-3.023576	-2.001587	-0.707095
C	-0.436123	-3.217989	-0.597390
H	-0.019629	-3.624370	-1.512472
C	-1.200695	-3.929897	0.360586
H	-1.456617	-4.982931	0.317044
C	-1.509712	-3.043809	1.421934
H	-2.046766	-3.295122	2.329435
C	-0.924288	-1.785647	1.120705
H	-3.924962	-0.393426	2.180248
C	-0.257192	-1.895376	-0.123691
H	0.291948	-1.109101	-0.624349
C	-4.433163	-0.546655	1.235432
H	-0.950046	-0.905056	1.752063
C	-5.292400	-1.631032	0.919390
H	-5.566721	-2.440116	1.586964
C	-5.793187	-1.420746	-0.391045
H	-6.505801	-2.052224	-0.910106
C	-5.236015	-0.216870	-0.885546
H	-5.426046	0.227290	-1.855285
C	-4.396694	0.323884	0.118946
H	-3.834544	1.246527	0.043310
H	-2.195437	-0.567381	-2.065262
H	-2.073419	-2.700087	-5.754356
C	-3.140262	-2.447078	-5.693639
H	-3.668558	-3.193593	-6.302996
C	-3.365491	-1.054384	-6.277390
C	-3.601443	-2.553369	-4.237702
H	-3.046584	-1.808430	-3.641084
H	-4.666459	-2.298102	-4.163714
C	-3.393752	-3.949608	-3.682081
H	-3.980793	-4.678915	-4.258256
H	-2.336842	-4.249667	-3.741295
O	-3.825083	-4.008550	-2.311701
C	-3.982865	-5.353927	-1.845838
C	-4.669685	-5.367360	-0.493678
H	-4.588421	-5.904582	-2.580075
H	-2.997067	-5.839553	-1.792951
C	-4.898427	-6.791097	0.021178
H	-4.060467	-4.816938	0.237133
H	-5.628317	-4.840830	-0.575218
C	-5.585378	-6.822421	1.384134
H	-5.503372	-7.347138	-0.707458
H	-3.936053	-7.316162	0.083438
H	-5.743432	-7.850376	1.724024
H	-4.984332	-6.310448	2.143442
H	-6.563121	-6.329831	1.347133
H	-4.428240	-0.788566	-6.269539
H	-2.828805	-0.295389	-5.699207
H	-3.016290	-0.998698	-7.313103

Bu2O_CH_act_delta_adduct_Bu2O

E=-810.676106
G=-810.312424

C	-1.061826	-1.871549	-0.331941
C	-1.120821	-2.486328	-1.607693
C	-2.217623	-1.932841	-2.313728
C	-2.829287	-0.967215	-1.477387
C	-2.116665	-0.929108	-0.250629
Ce	-0.375883	0.207581	-2.140999
C	-1.044950	2.771092	-3.127565
C	-1.784976	2.609703	-1.931038
C	-0.877768	2.654251	-0.839585
C	0.423484	2.847626	-1.366844
C	0.320740	2.910008	-2.778790
C	2.201595	-1.500001	-4.043252
C	2.948917	-1.734415	-5.358889
C	2.195150	-2.672812	-6.298166
C	2.972106	-0.584579	-3.111005
O	2.241512	-0.396093	-1.886669
H	3.946431	-2.144675	-5.148358
H	3.111752	-0.770771	-5.859382
H	1.330898	2.979220	-0.787559
H	-2.534646	-2.201220	-3.312786
H	1.136870	3.077629	-3.472858
H	-1.449034	2.786480	-4.131109
H	-2.861575	2.509069	-1.858109
H	-1.142617	2.610405	0.210683
H	-0.359736	-2.110708	0.458904
H	-2.366614	-0.323342	0.612880
H	-3.710201	-0.384299	-1.720036
H	-0.466462	-3.272856	-1.966446
H	3.156421	0.395468	-3.576136
H	3.947693	-1.026725	-2.863632
H	-0.726170	-0.063642	-4.233850
H	1.206035	-2.272057	-6.542020
H	2.740981	-2.816372	-7.235828
H	2.051544	-3.658612	-5.842198
H	1.212140	-1.070528	-4.277162
H	2.030372	-2.457831	-3.535489
C	3.050152	0.167896	-0.847293
C	2.327786	0.086578	0.483843
H	3.992234	-0.396765	-0.797589
H	3.296661	1.209636	-1.100856
C	3.169678	0.650232	1.631641
H	1.381676	0.643875	0.428654
H	2.073105	-0.960800	0.685947
C	2.459017	0.567243	2.980204
H	4.121772	0.105379	1.684228
H	3.427421	1.695671	1.416332
H	3.083309	0.972831	3.782046
H	1.521546	1.133836	2.970549
H	2.217338	-0.469500	3.238370

Bu2O_CH_act_alfa_TS

E=-810.641210
G=-810.279802

C	-0.521767	-0.092063	-3.050374
C	-0.218441	1.203033	-2.561450
C	1.045365	1.145095	-1.922754
C	1.526529	-0.186092	-2.023337
C	0.556667	-0.949780	-2.719240
Ce	-0.644609	-0.345621	-0.217717
C	-0.328392	0.686483	2.396794
C	-0.885930	-0.599636	2.610080
C	0.085942	-1.563959	2.246935
C	1.242679	-0.876591	1.800968
C	0.985526	0.516246	1.896098
O	-2.138646	-2.337632	-0.511890
C	-2.285548	-3.605455	0.134376
C	-3.149114	-1.324301	-0.243282
H	-2.413335	1.085428	-0.043202
H	2.177766	-1.331628	1.494588
H	1.686163	1.309499	1.662371
H	-0.814052	1.632156	2.605164
H	-1.868793	-0.804149	3.018137
H	-0.017108	-2.639256	2.338238
H	2.485952	-0.544367	-1.667772
H	0.641869	-1.997106	-2.986512
H	-1.403092	-0.367850	-3.617601
H	-0.832226	2.088243	-2.678985
H	1.571978	1.980837	-1.476231
H	-2.781153	0.177371	-0.096430
C	-1.118789	-4.496840	-0.248129
H	-2.322697	-3.452346	1.223282
H	-3.236226	-4.055670	-0.175834
H	-3.606320	-1.535409	0.731677
C	-4.164130	-1.210477	-1.364618
C	-1.187415	-5.873057	0.416943
H	-1.102303	-4.608898	-1.339482
H	-0.180859	-3.997754	0.032209
C	-0.019800	-6.776268	0.026798
H	-1.208168	-5.751632	1.508286
H	-2.133465	-6.361255	0.147323
H	-0.091920	-7.752902	0.515234
H	0.005093	-6.946191	-1.055170
H	0.939362	-6.331152	0.313679
C	-5.117048	-2.393672	-1.599328
H	-4.762339	-0.310103	-1.158753
H	-3.625170	-0.998197	-2.297658
H	-5.715433	-2.178907	-2.494480
H	-4.533069	-3.290112	-1.845190
C	-6.057895	-2.684015	-0.431921
H	-6.736008	-3.511389	-0.664914
H	-5.512075	-2.954527	0.478601
H	-6.672848	-1.808165	-0.195077

Bu2O_CH_act_beta_TS

E=-810.642284
G=-810.279802

C	-1.413391	-1.728003	-0.922776
C	-0.523802	-2.567801	-1.638197
C	-1.137493	-2.917127	-2.865389
C	-2.415693	-2.302978	-2.905075
C	-2.585954	-1.567187	-1.707318
Ce	-0.628068	-0.124912	-3.111349
C	-1.937521	2.348000	-3.525978
C	-2.017696	2.126486	-2.129674
C	-0.712522	2.259809	-1.588132
C	0.170296	2.573595	-2.652901
C	-0.582882	2.622283	-3.849030
O	1.886739	-0.631328	-3.210656
C	1.993292	-1.242275	-4.518998
C	0.901378	-0.680821	-5.405891
C	2.911256	-1.021153	-2.302985
C	2.776912	-0.241291	-1.008784
H	1.886647	-2.333235	-4.404888
H	3.018634	-1.048157	-4.881226
H	1.232599	2.770007	-2.563821
H	-0.725620	-3.573922	-3.622587
H	-0.200414	2.859063	-4.834924
H	-2.767850	2.341170	-4.222215
H	-2.922400	1.927836	-1.566986
H	-0.450631	2.196902	-0.537742
H	-1.255026	-1.327910	0.072449
H	-3.472506	-1.014050	-1.420093
H	-3.143933	-2.402214	-3.700826
H	0.442866	-2.913114	-1.289518
H	3.887440	-0.827087	-2.772190
H	2.841939	-2.104339	-2.117304
H	-1.576866	-0.404924	-5.178168
H	1.171290	0.351748	-5.682198
C	0.738008	-1.507087	-6.685262
H	-0.674521	-0.564849	-5.287189
H	2.833608	0.831224	-1.232608
H	1.781734	-0.424585	-0.579427
C	1.960748	-1.543425	-7.608777
H	0.459240	-2.537195	-6.416055
H	-0.116055	-1.114713	-7.255084
H	1.751873	-2.106205	-8.525791
H	2.258880	-0.529801	-7.900813
H	2.825422	-2.015727	-7.128984
C	3.849431	-0.616409	0.016064
C	3.724047	0.170380	1.318330
H	3.789610	-1.691846	0.229922
H	4.842862	-0.447087	-0.420306
H	4.502796	-0.116332	2.031603
H	3.815227	1.247657	1.141561
H	2.754389	-0.005655	1.797104

Bu2O_CH_act_gamma_TS

E=-810.616042
G=-810.255195

Ce	-2.297784	-1.291882	-1.221534
C	0.353488	-2.091279	-1.843046
H	0.559536	-2.390373	-2.863786
C	-0.041345	-2.947643	-0.785677
H	-0.176600	-4.021739	-0.853033
C	-0.165349	-2.166263	0.391856
H	-0.412257	-2.535562	1.380823
C	0.152523	-0.824332	0.059506
H	-2.769127	0.623447	1.594791
C	0.474217	-0.778980	-1.321140
H	0.792476	0.097530	-1.873115
C	-3.451098	0.170874	0.884281
H	0.188330	0.010857	0.749377
C	-4.027830	-1.121098	0.989896
H	-3.874124	-1.821809	1.803066
C	-4.902809	-1.300211	-0.114007
H	-5.512600	-2.175481	-0.309050
C	-4.858555	-0.127395	-0.903380
H	-5.431339	0.057303	-1.804485
C	-3.959590	0.783215	-0.288314
H	-3.737528	1.786837	-0.631764
H	-2.169522	0.196257	-2.961309
H	-2.463632	-0.578889	-3.306182
C	-2.910217	-2.101466	-3.780888
H	-2.032818	-2.768700	-3.848659
C	-3.108855	-1.457973	-5.153482
C	-4.142879	-2.942110	-3.406212
H	-4.949748	-2.318942	-2.997076
H	-4.575472	-3.429997	-4.295480
C	-3.835728	-4.052480	-2.410034
H	-3.113233	-4.762738	-2.848709
H	-3.334952	-3.673382	-1.482432
O	-5.019030	-4.701296	-2.039984
C	-4.809364	-5.832935	-1.216681
C	-6.151244	-6.472397	-0.907540
H	-4.146931	-6.553525	-1.726628
H	-4.302159	-5.533284	-0.282026
C	-6.025774	-7.712907	-0.022667
H	-6.792201	-5.726631	-0.420865
H	-6.639401	-6.732871	-1.854909
C	-7.374095	-8.358907	0.287543
H	-5.372775	-8.447439	-0.513369
H	-5.525408	-7.442912	0.917361
H	-7.256064	-9.244104	0.920391
H	-8.036575	-7.661099	0.811475
H	-7.884005	-8.671353	-0.630382
H	-3.333639	-2.202651	-5.932000
H	-3.945157	-0.745930	-5.142181
H	-2.221405	-0.901760	-5.477846

Bu2O_CH_act_delta_TS

E=-810.619238
G=-810.258556

C	-2.209914	-1.542924	-1.169097
C	-1.128810	-2.347082	-1.610460
C	-1.467675	-2.886418	-2.876446
C	-2.764182	-2.422951	-3.215486
C	-3.222129	-1.590852	-2.162681
Ce	-1.175978	-0.106361	-3.355762
C	-1.951411	2.369719	-4.477838
C	-2.897862	2.112313	-3.452239
C	-2.236007	2.238174	-2.204231
C	-0.879351	2.558546	-2.458978
C	-0.705048	2.642491	-3.865343
C	1.967686	-0.479871	-2.863486
C	1.893475	-1.222516	-4.203780
C	0.829648	-0.655723	-5.157217
C	3.204794	-0.808982	-2.043813
O	3.099003	-0.162009	-0.797364
H	1.701200	-2.286246	-4.008838
H	2.891701	-1.184102	-4.671520
H	-0.120204	2.754322	-1.709371
H	-0.862427	-3.565438	-3.465083
H	0.211592	2.907157	-4.379523
H	-2.154345	2.378546	-5.542086
H	-3.952591	1.907514	-3.596618
H	-2.694919	2.138795	-1.227348
H	-2.273334	-1.026230	-0.218246
H	-4.192182	-1.110458	-2.106381
H	-3.318181	-2.683075	-4.109251
H	-0.222949	-2.552909	-1.051202
H	4.108917	-0.477967	-2.583787
H	3.290477	-1.901679	-1.909322
H	-1.643433	-0.679193	-5.497033
H	1.078355	0.388741	-5.407058
H	0.891550	-1.200326	-6.107954
H	-0.718556	-0.765551	-5.423420
H	1.942329	0.607049	-3.024616
H	1.120366	-0.748040	-2.206244
C	4.212225	-0.387354	0.043390
C	3.983560	0.324867	1.365156
H	4.350920	-1.470195	0.210361
H	5.134309	-0.016703	-0.437894
C	5.144134	0.144774	2.343747
H	3.822393	1.391566	1.164422
H	3.054428	-0.053200	1.810107
C	4.911872	0.852742	3.676689
H	5.308245	-0.926474	2.523321
H	6.069478	0.520628	1.886513
H	5.756188	0.708676	4.358230
H	4.779040	1.931045	3.534767
H	4.013237	0.472826	4.175181

Bu2O_CH_act_alfa_adduct_H2

E=-810.64935
G=-810.288050

C	-0.838257	0.667698	-2.860199
C	0.100470	1.490066	-2.179566
C	1.262689	0.718174	-1.937494
C	1.039502	-0.583671	-2.454747
C	-0.255813	-0.608369	-3.032055
Ce	-0.708847	-0.396061	-0.222203
C	-0.371151	0.743258	2.358109
C	-0.993780	-0.505381	2.614716
C	-0.059415	-1.526069	2.313963
C	1.138571	-0.911404	1.868102
C	0.945943	0.492950	1.899710
O	-2.034877	-2.452759	-0.566702
C	-2.190775	-3.697024	0.114273
C	-3.046373	-1.408969	-0.353061
H	-2.333652	1.659828	0.029925
H	2.058102	-1.421040	1.601939
H	1.687291	1.243294	1.650201
H	-0.809000	1.720091	2.531150
H	-1.991358	-0.649207	3.012007
H	-0.215017	-2.590469	2.446827
H	1.756204	-1.397724	-2.461082
H	-0.714699	-1.455860	-3.527308
H	-1.813087	0.976563	-3.219239
H	-0.026437	2.540946	-1.943184
H	2.173646	1.068611	-1.466250
H	-2.765687	1.034333	-0.045922
C	-0.986260	-4.581912	-0.154646
H	-2.303166	-3.508274	1.192876
H	-3.110604	-4.181125	-0.236874
H	-3.537211	-1.614051	0.608320
C	-4.035385	-1.335246	-1.500726
C	-1.081332	-5.935262	0.552106
H	-0.890736	-4.731303	-1.237628
H	-0.076381	-4.059710	0.172582
C	0.129311	-6.828079	0.289732
H	-1.190827	-5.776204	1.633407
H	-1.994382	-6.451925	0.227550
H	0.035748	-7.788251	0.806589
H	0.244403	-7.035708	-0.779804
H	1.054454	-6.353510	0.635495
C	-4.987777	-2.526191	-1.724492
H	-4.643461	-0.432684	-1.333636
H	-3.487795	-1.151292	-2.434556
H	-5.565893	-2.342325	-2.640457
H	-4.397152	-3.429587	-1.926483
C	-5.954755	-2.782915	-0.570969
H	-6.619616	-3.626071	-0.786227
H	-5.425872	-3.010607	0.360911
H	-6.583760	-1.904934	-0.382353

Bu2O_CH_act_beta_adduct_H2

E=-810.6507118
G=-810.291953

C	-1.099866	-2.102631	-1.262790
C	-0.795401	-2.856975	-2.425759
C	-1.834208	-2.657616	-3.361991
C	-2.786234	-1.777420	-2.780325
C	-2.335813	-1.445075	-1.479109
Ce	-0.520569	-0.131135	-3.238035
C	-1.746615	2.387317	-3.697286
C	-1.809970	2.217156	-2.292938
C	-0.491871	2.314073	-1.781252
C	0.382958	2.557984	-2.871284
C	-0.388824	2.599900	-4.055285
O	1.965333	-0.562027	-3.108223

C	2.262730	-0.532946	-4.564034
C	0.976448	-0.669563	-5.332600
C	3.107593	-0.383227	-2.285305
C	2.724235	-0.480214	-0.819570
H	2.986154	-1.349747	-4.723867
H	2.780731	0.419860	-4.743337
H	1.452912	2.718377	-2.805132
H	-1.904235	-3.117586	-4.340562
H	-0.016171	2.798343	-5.052918
H	-2.594113	2.410279	-4.373293
H	-2.710979	2.070293	-1.709052
H	-0.212768	2.272036	-0.734081
H	-0.519796	-2.079564	-0.346937
H	-2.857032	-0.817751	-0.765414
H	-3.725093	-1.468329	-3.226793
H	0.072606	-3.490416	-2.565590
H	3.563883	0.596055	-2.502154
H	3.850894	-1.154551	-2.539642
H	-2.247802	-0.097623	-5.515416
H	0.916787	0.141898	-6.071466
C	0.822565	-2.017260	-6.045574
H	-1.548731	-0.237707	-5.754236
H	1.970929	0.287217	-0.593015
H	2.252652	-1.454526	-0.638570
C	1.763319	-2.228763	-7.239728
H	0.972874	-2.836413	-5.326453
H	-0.210337	-2.141011	-6.402847
H	1.622261	-3.210651	-7.708530
H	1.592286	-1.464260	-8.006834
H	2.815550	-2.157212	-6.939088
C	3.923540	-0.303881	0.114177
C	3.544159	-0.396820	1.590116
H	4.679719	-1.065293	-0.118823
H	4.398206	0.666935	-0.081569
H	4.418743	-0.264428	2.234451
H	2.812819	0.372819	1.860923
H	3.102118	-1.371093	1.825944

Bu2O_CH_act_gamma_adduct_H2

E=-810.629762
G=-810.270382

Ce	-2.345867	-0.899257	-1.258366
C	0.395486	-1.566648	-0.925630
H	1.106678	-1.155726	-1.633609
C	-0.261353	-2.816969	-1.038760
H	-0.147120	-3.524792	-1.850794
C	-1.053004	-3.000397	0.123016
H	-1.647866	-3.876225	0.357046
C	-0.883554	-1.863733	0.954782
H	-2.233115	2.312991	0.033864
C	0.012163	-0.976658	0.306198
H	0.375084	-0.035442	0.703532
C	-3.036281	1.679570	-0.325830
H	-1.326933	-1.717741	1.933211
C	-3.811316	0.790463	0.461486
H	-3.697165	0.619203	1.525848
C	-4.791174	0.202844	-0.377731
H	-5.562840	-0.492045	-0.065512
C	-4.626763	0.733386	-1.683697
H	-5.245814	0.511536	-2.544423
C	-3.544925	1.645764	-1.650030
H	-3.193170	2.245691	-2.481984
H	-1.088249	0.160489	-3.272154
H	-1.529118	-0.406897	-3.539216
C	-3.017402	-2.197643	-3.384778
H	-2.172590	-2.854974	-3.638744
C	-3.650243	-1.650940	-4.660475
C	-3.989269	-2.951138	-2.496080
H	-3.851882	-2.775738	-1.380184
H	-5.018878	-2.613172	-2.666343
C	-3.936097	-4.468353	-2.603026
H	-4.250553	-4.773097	-3.615525
H	-2.897357	-4.815889	-2.465601
O	-4.781827	-5.032754	-1.625543
C	-4.851653	-6.441007	-1.694096
C	-5.781789	-6.941573	-0.602465
H	-5.221330	-6.756308	-2.686045
H	-3.846193	-6.882248	-1.573219
C	-5.942104	-8.461758	-0.608065
H	-5.394161	-6.607677	0.368454
H	-6.759459	-6.459770	-0.729812
C	-6.872726	-8.965308	0.492875
H	-6.325030	-8.784767	-1.585732
H	-4.956575	-8.934471	-0.497854
H	-6.973456	-10.054966	0.464174
H	-6.496807	-8.692039	1.485110
H	-7.875482	-8.535658	0.390863
H	-4.112405	-2.430665	-5.288820
H	-4.435841	-0.915735	-4.444879
H	-2.910637	-1.143393	-5.292010

Bu2O_CH_act_delta_adduct_H2

E=-810.626674
G=-810.268178

C	-2.073420	-1.886222	-1.332162
C	-1.136612	-2.665368	-2.062408
C	-1.696026	-2.958890	-3.327298
C	-2.982871	-2.360195	-3.382590
C	-3.218273	-1.706027	-2.146939
Ce	-1.208269	-0.161232	-3.397082
C	-1.679914	2.458365	-4.404380
C	-2.801574	2.177026	-3.576868
C	-2.356606	2.162252	-2.231618
C	-0.961710	2.408287	-2.228351
C	-0.546458	2.599562	-3.574345
C	2.023835	-0.431150	-2.770524
C	1.869069	-1.255749	-4.055979
C	0.746889	-0.725206	-4.965217
C	3.202396	-0.836901	-1.902690
O	3.169358	-0.080019	-0.713671
H	1.660441	-2.298196	-3.774121
H	2.850524	-1.280154	-4.561097
H	-0.331595	2.495361	-1.349800
H	-1.235672	-3.556682	-4.104348
H	0.457232	2.839617	-3.904088
H	-1.696356	2.575557	-5.482034
H	-3.828157	2.067103	-3.909030
H	-2.978260	2.006457	-1.357406
H	-1.957138	-1.540232	-0.311019
H	-4.125493	-1.184652	-1.864284
H	-3.688794	-2.444159	-4.201672
H	-0.174011	-3.006811	-1.698806
H	4.145487	-0.664771	-2.450231
H	3.154385	-1.916772	-1.675972
H	-2.322803	-0.409548	-5.895393
H	1.090188	0.204336	-5.449233
H	0.581050	-1.441730	-5.782536
H	-1.586548	-0.562314	-5.963601
H	2.115074	0.635492	-3.012367
H	1.137902	-0.535331	-2.112792
C	4.232681	-0.379726	0.165451
C	4.111685	0.493573	1.402259
H	4.208263	-1.447888	0.446028
H	5.202114	-0.203218	-0.333611
C	5.227192	0.242135	2.416747
H	4.117633	1.545215	1.088933
H	3.133747	0.311685	1.865957
C	5.113164	1.125413	3.657069
H	5.216459	-0.814256	2.717957
H	6.201177	0.410196	1.937243
H	5.923770	0.926842	4.365396
H	5.155663	2.187556	3.391526
H	4.165479	0.954496	4.179893

Bu2O_CH_act_alfa_product

E=-809.470338
G=-809.122495

C	-0.544009	0.588037	-2.662102
C	0.599077	1.096698	-1.994061
C	1.593304	0.089321	-2.003952
C	1.069173	-1.040315	-2.684566
C	-0.250266	-0.730360	-3.095388
Ce	-0.451356	-0.914518	-0.282987
C	-2.166806	-3.093232	0.365127
C	-2.272567	-2.221402	1.478323
C	-2.950955	-1.052518	1.057385
C	-3.262351	-1.199430	-0.319244
C	-2.781873	-2.463206	-0.745876
O	1.139030	-0.591998	1.569123
C	0.328827	0.646349	1.532248
C	-0.325302	0.939245	2.867037
C	0.569277	1.309955	4.066022
C	1.376295	2.592396	3.877594
C	2.549017	-0.489981	1.755259
C	3.190857	-1.849221	1.533682
C	4.703608	-1.835406	1.762353
C	5.350100	-3.199593	1.533405
H	-0.908422	-1.373483	-3.667991
H	-1.462200	1.130850	-2.856949
H	0.700664	2.089047	-1.572592
H	2.596643	0.181548	-1.603919
H	1.603064	-1.959700	-2.901589
H	-2.899797	-2.888554	-1.735920
H	-1.737496	-4.089822	0.374479
H	-1.923629	-2.427462	2.483678
H	-3.212142	-0.208538	1.684238
H	-3.818040	-0.492838	-0.925577
H	2.954927	0.251207	1.050355
H	2.753123	-0.129699	2.771312
H	0.994041	1.457726	1.207100
H	2.719515	-2.576173	2.207902
H	2.980844	-2.184552	0.507545
H	5.166960	-1.094155	1.097562
H	4.911774	-1.497979	2.786288
H	6.430066	-3.162507	1.706562
H	4.930878	-3.954926	2.207242
H	5.190379	-3.547096	0.506625
H	-1.026857	1.768299	2.688112
H	-0.950302	0.083984	3.155815
H	-0.067938	1.417151	4.954723
H	1.244419	0.473150	4.289519
H	1.974660	2.823421	4.765312
H	2.063175	2.519676	3.027422
H	0.716551	3.447930	3.690852

Bu2O_CH_act_beta_product

E=-809.474422
G=-809.128052

C	-1.903312	-1.511190	-0.925125
C	-0.750185	-2.316347	-1.091063
C	-0.783001	-2.867826	-2.397237
C	-1.961284	-2.408942	-3.036217
C	-2.653063	-1.569186	-2.124950
Ce	-2.880052	-4.194705	-1.032051
C	-1.555140	-6.589951	-1.732087
C	-2.463218	-6.372641	-2.798630
C	-3.774592	-6.583916	-2.304728
C	-3.676127	-6.938495	-0.935291
C	-2.306466	-6.943581	-0.581347
O	-5.024583	-3.591651	0.146787
C	-6.378231	-3.190430	0.011208
C	-6.801445	-3.269100	-1.445495
C	-8.254373	-2.841479	-1.663284
C	-8.682242	-2.919182	-3.126813
C	-4.501829	-3.530825	1.541014
C	-3.050965	-3.934334	1.549795
C	-2.734622	-5.085822	2.506726
C	-2.893276	-4.755075	3.997754
H	-5.143866	-4.210555	2.121861
H	-4.701553	-2.501303	1.872920
H	-3.569085	-1.025260	-2.328825
H	-4.502425	-7.189639	-0.280386
H	-2.153592	-0.934307	-0.042952
H	0.038519	-2.454436	-0.360040
H	-0.022536	-3.498794	-2.842565
H	-2.255632	-2.623624	-4.057643
H	-2.198226	-6.124946	-3.820142
H	-0.473811	-6.547146	-1.798878
H	-1.903308	-7.196626	0.391526
H	-4.688356	-6.536326	-2.887680
H	-6.490798	-2.162893	0.390878
H	-7.011297	-3.842051	0.633116
H	-2.435063	-3.065606	1.820659
H	-6.138941	-2.628518	-2.044561
H	-6.664534	-4.298752	-1.802765
H	-3.367569	-5.953839	2.268192
H	-1.702668	-5.427096	2.343592
H	-2.646494	-5.610613	4.638890
H	-2.237150	-3.923878	4.281907
H	-3.920961	-4.453607	4.234797
H	-8.913609	-3.474020	-1.054234
H	-8.389771	-1.815857	-1.295163
H	-9.723041	-2.605829	-3.253395
H	-8.061862	-2.272095	-3.756779
H	-8.593921	-3.940651	-3.512839

Bu2O_CH_act_gamma_product

E=-809.445086
G=-809.099952

C	-2.524091	-0.622323	-1.089682
C	-1.271508	-1.288225	-1.030581
C	-1.139900	-2.073684	-2.200555
C	-2.313037	-1.897057	-2.981505
C	-3.171583	-1.008376	-2.290196
Ce	-0.994031	0.611400	-3.086531
C	0.092992	2.503819	-1.335770
C	-0.155371	3.252029	-2.515539
C	0.757205	2.818981	-3.505400
C	1.580613	1.811594	-2.936799
C	1.173114	1.619340	-1.594856
C	-2.211562	0.556953	-6.355775
O	-2.666125	-0.379122	-7.293451
C	-1.693780	-0.734228	-8.254217
C	-2.298763	-1.737407	-9.220591
C	-1.318635	-2.181516	-10.306489
C	-1.927428	-3.189957	-11.278149
C	-3.341308	0.986655	-5.432090
C	-2.847707	1.886089	-4.291206
C	-4.017624	2.470755	-3.503234
H	-0.901428	4.027853	-2.634152
H	0.840703	3.218461	-4.510064
H	2.410937	1.313877	-3.427059
H	-0.556718	-1.229505	-0.218319
H	-0.410672	2.628854	-0.383763
H	1.628391	0.943199	-0.880473
H	-0.308560	-2.729902	-2.435840
H	-2.536845	-2.394777	-3.918836
H	-4.157139	-0.696628	-2.611457
H	-2.938003	0.022029	-0.322089
H	-2.306799	2.732689	-4.755613
H	-3.822331	0.079640	-5.039046
H	-4.106148	1.478754	-6.058883
H	-1.772978	1.436681	-6.859034
H	-1.365235	0.097367	-5.777399
H	-1.348503	0.163443	-8.796616
H	-0.807101	-1.169215	-7.756673
H	-2.647857	-2.606906	-8.649592
H	-3.188776	-1.286932	-9.677337
H	-0.967919	-1.302740	-10.864603
H	-0.426231	-2.618885	-9.838081
H	-1.206803	-3.491341	-12.044947
H	-2.255603	-4.095099	-10.755272
H	-2.800833	-2.769609	-11.788785
H	-4.734985	3.019457	-4.138818
H	-4.595827	1.690548	-2.990652
H	-3.680462	3.173746	-2.730896

Bu2O_CH_act_delta_product

E=-809.449557
G=-809.103026

C	-1.974819	-1.516792	-1.479258
C	-1.022376	-2.506912	-1.142895
C	-0.837917	-3.338679	-2.277412
C	-1.668864	-2.851629	-3.319975
C	-2.373492	-1.727274	-2.825134
Ce	-3.426695	-3.966531	-1.420728
C	-3.440647	-6.250895	-3.052829
C	-4.813983	-6.017405	-2.805843
C	-5.065694	-6.291654	-1.434884
C	-3.849403	-6.697628	-0.836376
C	-2.840797	-6.661374	-1.832586
C	-5.705570	-3.091870	0.774393
C	-7.105987	-2.924033	1.338041
O	-7.882649	-2.211186	0.401323
C	-9.206358	-1.979495	0.835616
C	-9.950514	-1.214501	-0.245155
C	-11.399696	-0.907908	0.132737
C	-12.146402	-0.137715	-0.953925
C	-4.761478	-3.949642	1.630031
C	-3.316452	-3.910810	1.108110
H	-5.140640	-4.981649	1.629689
H	-4.845788	-3.605460	2.675599
H	-3.059292	-1.105961	-3.391917
H	-3.714442	-6.995070	0.195563
H	-2.312682	-0.715054	-0.832259
H	-0.516124	-2.605518	-0.190716
H	-0.141993	-4.166360	-2.353599
H	-1.725763	-3.248555	-4.327021
H	-5.553194	-5.726625	-3.544830
H	-2.940412	-6.160866	-4.009986
H	-1.804961	-6.952957	-1.700330
H	-6.031578	-6.246222	-0.944287
H	-7.059887	-2.384857	2.299907
H	-7.554223	-3.912213	1.542128
H	-2.865734	-2.943107	1.383320
H	-2.710445	-4.679844	1.605091
H	-5.274407	-2.091173	0.623296
H	-5.853586	-3.546916	-0.224560
H	-9.713618	-2.937708	1.046340
H	-9.203667	-1.405213	1.778929
H	-9.409244	-0.281621	-0.447799
H	-9.920032	-1.800638	-1.172546
H	-11.928946	-1.846957	0.344400
H	-11.419513	-0.331863	1.067870
H	-13.179930	0.069421	-0.658802
H	-11.661403	0.822225	-1.163190
H	-12.175412	-0.703554	-1.891771

Trapping of H2

Bu2O_TS_trap_H2_alfa

E=-810.598562
G=-810.243744

C	0.126028	-0.866005	2.067408
H	0.964787	-0.422466	1.544103
C	-0.875371	-0.165205	2.787655
H	-0.949408	0.911699	2.891893
C	-1.805300	-1.113394	3.281764
H	-2.704841	-0.891439	3.843974
C	-1.371010	-2.400261	2.882780
H	-1.889266	-3.333854	3.071548
C	-0.177300	-2.245325	2.127950
H	0.382504	-3.041089	1.648744
Ce	0.581647	-1.595802	4.793280
C	0.915245	-2.295289	7.543694
H	1.935469	-2.425037	7.885093
C	0.081766	-3.307975	7.007616
H	0.345430	-4.353804	6.890192
C	-1.182156	-2.730287	6.718793
H	-2.048720	-3.253530	6.331569
C	-1.124570	-1.359643	7.064929
H	-1.942335	-0.651080	6.996834
C	0.173518	-1.090691	7.573848
H	0.518534	-0.140758	7.966110
C	2.164765	0.506948	5.021875
C	2.842068	1.251495	3.905543
H	2.092790	1.738561	3.267861
H	1.204167	1.491355	5.645469
H	3.256400	0.439146	3.290360
C	3.964128	2.230222	4.265472
C	4.656913	2.822806	3.040752
H	4.698245	1.714972	4.898523
H	3.545319	3.039929	4.879656
H	1.606970	2.129116	5.913840
C	2.817173	0.385406	5.897718
O	2.804308	-1.702253	4.507815
C	4.176537	-1.918469	4.490388
C	4.528776	-3.318662	3.984820
H	4.679421	-1.179832	3.836465
H	4.609548	-1.784614	5.498750
C	6.034167	-3.581287	3.936810
H	4.041792	-4.057613	4.635862
H	4.093932	-3.447113	2.984433
C	6.383198	-4.982614	3.440086

H	6.512860	-2.834454	3.288530
H	6.462085	-3.431461	4.937519
H	7.466256	-5.141019	3.413876
H	5.950454	-5.752138	4.089193
H	5.997970	-5.151444	2.428183
H	5.441894	3.528557	3.329606
H	5.121215	2.039824	2.430964
H	3.946116	3.360192	2.403082

Bu2O_TS_trap_H2_beta

E=-810.538256
G=-810.179521

C	1.161724	-1.003884	2.017051
C	2.133819	-0.139590	1.450544
C	1.736373	1.194337	1.702551
C	0.514443	1.157319	2.422060
C	0.156706	-0.200196	2.610111
Ce	2.446392	0.168957	4.281111
C	2.950435	-2.005193	6.053580
C	3.141659	-0.855927	6.861238
C	1.881041	-0.240248	7.049458
C	0.909643	-1.004785	6.355056
C	1.571627	-2.098181	5.741378
O	3.072589	2.480222	4.878789
C	4.376058	1.896929	4.676948
C	4.909956	-0.301506	3.502546
C	3.007564	3.743358	5.535662
C	1.561881	4.191601	5.651690
H	4.545637	-1.428240	2.884881
H	5.237132	-1.611295	2.400819
C	6.159995	-0.613477	4.314506
H	5.097340	0.350350	2.641956
H	3.474745	3.652111	6.527952
H	3.596163	4.468217	4.954733
C	1.424273	5.555073	6.332353
H	0.996280	3.437912	6.215546
H	1.122443	4.231472	4.646854
H	4.082044	-0.525071	7.285973
H	1.687043	0.642019	7.649124
H	-0.157846	-0.815579	6.335164
H	1.098427	-2.886553	5.167386
H	3.717543	-2.713356	5.761994
H	3.006875	-0.447797	0.886388
H	2.256600	2.087617	1.376657
H	-0.068652	2.017655	2.731612
H	-0.741800	-0.561449	3.097135
H	1.157822	-2.086457	1.956898
H	4.942978	2.498148	3.955952
H	4.906296	1.844689	5.637784
C	7.500253	-0.493317	3.589334
H	6.146949	0.078045	5.162429
H	6.057343	-1.612342	4.755932
H	8.340575	-0.670910	4.269959
H	7.573314	-1.218782	2.770670
H	7.624921	0.505875	3.157578
C	-0.026783	6.016550	6.446214
H	1.874465	5.510785	7.333090
H	2.002436	6.301532	5.771398
H	-0.096610	6.993843	6.933906
H	-0.493328	6.103208	5.458763
H	-0.623351	5.308943	7.032497

Bu2O_TS_trap_H2_gamma

E=-810.521379
G=-810.165208

C	-2.788054	-0.437370	-0.946100
C	-2.378464	-1.319831	0.083470
C	-1.374735	-2.171044	-0.444032
C	-1.171373	-1.816734	-1.802366
C	-2.041185	-0.744027	-2.112976
Ce	-0.133202	0.367430	-0.302704
C	0.069532	0.729955	2.502242
C	0.912867	-0.375022	2.227962
C	2.040266	0.102026	1.511965
C	1.897364	1.503361	1.351228
C	0.680189	1.890979	1.960804
C	1.690338	0.021726	-2.149683
C	3.053044	0.679133	-2.283362
C	0.423321	2.245557	-2.051337
C	-0.929475	2.848064	-1.796131
O	-0.862909	4.240235	-1.551026
C	-2.121626	4.818451	-1.271541
C	-1.935112	6.304048	-1.016166
C	-3.246572	7.023699	-0.700939
H	3.657436	0.321640	-3.122922
H	1.886605	-1.253376	-1.737463
H	2.352025	-1.593468	-2.364268
H	1.198630	-0.151460	-3.112662
H	2.607423	2.166945	0.872424
H	0.301453	2.904509	2.034335
H	-0.855189	0.700013	3.067665
H	0.743414	-1.398287	2.543264
H	2.889473	-0.492638	1.194182
H	-0.499642	-2.311598	-2.494457
H	-2.150717	-0.272423	-3.082469
H	-3.571563	0.308488	-0.869104
H	-2.784148	-1.360366	1.087882
H	-0.888803	-2.984142	0.083707
H	0.672947	2.254868	-3.112672
H	1.180773	2.807113	-1.491549
H	2.883929	1.745742	-2.451115
H	3.635819	0.585791	-1.362493
H	-1.626053	2.631061	-2.622889
H	-1.457853	2.409059	-0.886028
H	-2.813060	4.658252	-2.117920
H	-2.578151	4.333262	-0.388793
H	-1.228435	6.429875	-0.186146
H	-1.461867	6.752911	-1.898466
C	-3.057153	8.516773	-0.443087
H	-3.950532	6.882916	-1.532475
H	-3.717360	6.558795	0.176134
H	-4.009273	9.007792	-0.217901
H	-2.384795	8.689733	0.404598
H	-2.622576	9.017399	-1.315432

Bu2O_TS_trap_H2_delta

E=-810.527990
G=-810.171527

C	0.673839	-0.268899	2.221129
C	1.893135	-0.084567	1.519902
C	2.026228	1.295896	1.226796
C	0.888292	1.963130	1.739673
C	0.050232	0.996230	2.353997
Ce	-0.133383	0.393909	-0.408491
C	-2.657072	-0.839505	-0.015358
C	-1.789742	-1.903265	-0.372036
C	-1.448590	-1.748990	-1.739877
C	-2.097397	-0.588301	-2.226648
C	-2.845421	-0.026743	-1.160404
C	1.650488	-0.216081	-2.172727
H	2.632706	0.258130	-2.179471
C	0.822817	2.032204	-2.247889
H	1.907256	-1.421747	-1.728338
H	2.477833	-1.669778	-2.350081
H	1.273963	-0.400234	-3.179969
H	2.865246	1.761922	0.724013
H	0.707712	3.031952	1.707638
H	-0.879716	1.196572	2.874243
H	0.302123	-1.206180	2.619374
H	2.621916	-0.855678	1.296416
H	-0.832823	-2.424991	-2.322013
H	-2.062708	-0.218317	-3.244602
H	-3.483153	0.848300	-1.221521
H	-3.122749	-0.694925	0.952875
H	-1.484332	-2.718839	0.273843
H	0.987231	1.915825	-3.320717
H	1.702462	2.515253	-1.805262
C	-0.434723	2.847638	-1.984303
C	-0.253753	4.359736	-2.071358
H	-1.245154	2.550395	-2.659987
H	-0.864893	2.712604	-0.953142
O	-1.451615	4.984083	-1.666623
H	0.586182	4.672198	-1.426862
H	0.006863	4.639852	-3.105875
C	-1.399313	6.393155	-1.737867
C	-2.722744	6.958272	-1.251360
H	-0.568225	6.777915	-1.120299
H	-1.202566	6.716570	-2.775454
C	-2.773791	8.485166	-1.303929
H	-3.529051	6.533506	-1.862585
H	-2.894259	6.611174	-0.224496
C	-4.101269	9.051980	-0.805563
H	-1.951768	8.899819	-0.704607
H	-2.596883	8.821789	-2.334554
H	-4.113773	10.145399	-0.856267
H	-4.939999	8.681313	-1.405296
H	-4.288434	8.764939	0.235131

Bu2O_trap_H2_alfa_product

E=-652.330193
G=-769.833486

C	1.068304	-1.229046	2.106532
C	1.630466	-0.098496	1.466110
C	0.799713	1.015008	1.740270
C	-0.291373	0.567385	2.533825
C	-0.125501	-0.818237	2.760077
Ce	1.981662	0.396413	4.240801
C	1.734155	1.715600	6.735564
C	2.277055	0.452388	7.061160
C	1.275963	-0.526974	6.827463
C	0.105541	0.138416	6.380531
C	0.389862	1.521962	6.310435
O	4.117912	0.565664	3.950685
C	5.492406	0.697064	3.764270
C	5.890474	2.124058	3.388424
C	7.394618	2.298054	3.178070
C	7.788007	3.724248	2.799146
H	3.278000	0.266852	7.432319
H	1.366695	-1.589809	7.026176
H	-0.844682	-0.328972	6.151459
H	-0.312391	2.303119	6.040814
H	2.241090	2.669203	6.835375
H	2.535497	-0.087371	0.870959
H	0.938816	2.020652	1.357410
H	-1.124295	1.172770	2.872533
H	-0.809171	-1.461854	3.301515
H	1.449560	-2.243503	2.055218
H	6.031497	0.407538	4.683046
H	5.837038	0.010959	2.971140
H	5.350901	2.407785	2.474109
H	5.544128	2.803246	4.179969
H	7.926214	2.003433	4.093281
H	7.734523	1.605588	2.395738
H	8.869236	3.818048	2.653937
H	7.299571	4.035521	1.868842
H	7.494698	4.436532	3.578660

Bu2O_trap_H2_beta_product

E=-691.565277
G=-691.298193

C	0.783123	-1.119239	2.223652
C	1.823760	-0.759767	1.329651
C	1.988655	0.647986	1.389366
C	1.042353	1.159014	2.308956
C	0.296300	0.067133	2.825410
Ce	-0.511405	0.242674	0.108384
C	-2.108857	-2.063467	-0.244120
C	-0.987785	-2.265637	-1.087922
C	-1.081609	-1.350865	-2.168796
C	-2.258130	-0.584657	-1.992260
C	-2.892893	-1.021734	-0.803111
C	0.271966	2.067235	-1.423728
O	-0.854681	2.547184	-0.625870
C	-1.322352	3.870362	-0.846248
C	-2.494174	4.169172	0.073050
C	-3.045293	5.583633	-0.117171
C	-4.222741	5.891799	0.804777
H	-0.494660	4.572365	-0.666153
H	-1.617952	3.969594	-1.901432
H	-2.173711	4.034803	1.115066
H	-3.289921	3.435166	-0.113043
H	2.721517	1.226708	0.841214
H	0.933906	2.198424	2.597708
H	-0.474155	0.123547	3.587407
H	0.442281	-2.126558	2.432859
H	2.424534	-1.446330	0.743505
H	-0.390317	-1.271391	-2.999372
H	-2.619217	0.188115	-2.660667
H	-3.840074	-0.660147	-0.416368
H	-2.347901	-2.635764	0.645135
H	-0.220406	-3.019833	-0.955566
H	0.001930	2.123576	-2.486501
H	1.143108	2.704616	-1.224515
H	-2.242821	6.312794	0.056857
H	-3.354421	5.715506	-1.162625
H	-4.598118	6.907418	0.645406
H	-5.053950	5.199310	0.631440
H	-3.935019	5.805601	1.858494

Bu2O_trap_H2_gamma_product

E=-730.848177
G=-730.555403

C	-2.568121	-0.667489	-1.875590
C	-2.578150	-1.290247	-0.602754
C	-1.522087	-2.239284	-0.566534
C	-0.868940	-2.212040	-1.821580
C	-1.519387	-1.243674	-2.632858
Ce	-3.418607	-3.321259	-2.331423
C	-4.807795	-5.793890	-2.368827
C	-5.527496	-4.980247	-1.461863
C	-4.708441	-4.767351	-0.323727
C	-3.488542	-5.467596	-0.520844
C	-3.548989	-6.099664	-1.785485
C	-5.362442	-2.065109	-3.319935
C	-6.362569	-1.242615	-2.554506
O	-7.322161	-0.640662	-3.422710
C	-8.260796	0.150647	-2.737206
C	-9.231954	0.748044	-3.742659
C	-10.291429	1.641004	-3.098072
C	-11.265787	2.237295	-4.111534
H	-1.226998	-0.953183	-3.636477
H	-3.237412	0.116311	-2.206662
H	-3.241623	-1.046226	0.219281
H	-1.243271	-2.849752	0.284218
H	0.005051	-2.793171	-2.096320
H	-2.787520	-6.745125	-2.210832
H	-5.176106	-6.162354	-3.320246
H	-6.529937	-4.598345	-1.607289
H	-4.987578	-4.216623	0.567487
H	-2.671228	-5.535577	0.187364
H	-5.905644	-2.836264	-3.894979
H	-4.868249	-1.413103	-4.064321
H	-6.896831	-1.868338	-1.815288
H	-5.855576	-0.444025	-1.981699
H	-8.811214	-0.453015	-1.990786
H	-7.754523	0.957575	-2.173840
H	-8.657376	1.319973	-4.482524
H	-9.713377	-0.071768	-4.291062
H	-10.851615	1.062910	-2.350218
H	-9.798627	2.452494	-2.545061
H	-12.014943	2.870027	-3.624365
H	-10.740699	2.852610	-4.850771
H	-11.798742	1.450940	-4.657866

Bu2O_trap_H2_delta_product

E=-770.151810
G=-769.833486

C	1.331777	-1.643542	2.073312
C	1.749681	-0.406147	1.527769
C	1.017761	0.625605	2.172601
C	0.135745	0.021739	3.105290
C	0.336073	-1.378069	3.050667
Ce	2.738231	-0.347168	4.170877
C	5.201327	0.528750	3.110692
C	4.756702	1.592158	3.940128
C	4.854138	1.167630	5.289826
C	5.342092	-0.161294	5.293609
C	5.560411	-0.555501	3.947331
C	1.610327	0.113450	6.368082
C	1.878322	-1.317006	6.796937
C	0.678686	-2.073723	7.347170
O	1.010541	-3.437392	7.491768
C	-0.044213	-4.210570	8.022323
C	0.405226	-5.658086	8.122321
C	-0.674482	-6.576502	8.694749
C	-0.225221	-8.032380	8.795303
H	5.557112	-0.757115	6.173782
H	5.974855	-1.502826	3.618909
H	5.286550	0.556336	2.030499
H	4.454420	2.577464	3.602417
H	4.617856	1.761918	6.163473
H	-0.580055	0.538737	3.732140
H	-0.208451	-2.121672	3.621798
H	1.676541	-2.624794	1.764515
H	2.475261	-0.271316	0.733968
H	1.076140	1.684114	1.943789
H	0.537618	0.312515	6.264986
H	2.044938	0.841206	7.056426
H	2.230202	-1.991732	5.947036
H	2.706834	-1.384310	7.511048
H	0.385134	-1.635944	8.315851
H	-0.179722	-1.955145	6.663054
H	-0.333750	-3.830465	9.018201
H	-0.939022	-4.131411	7.379103
H	0.701058	-6.002900	7.123278
H	1.306624	-5.701819	8.746633
H	-0.970724	-6.216192	9.689320
H	-1.575885	-6.514678	8.069835
H	-1.015336	-8.667200	9.208877
H	0.042625	-8.433287	7.811361
H	0.653891	-8.131596	9.441732

Releasing of alkene

Bu2O_TS_releasing_alkene_beta

E=-809.469049
G=-809.124157

C	-2.252049	7.226125	-3.728631
C	-2.631351	6.231761	-4.667944
C	-3.695402	5.483665	-4.107083
C	-3.962114	6.003416	-2.815907
C	-3.073133	7.085090	-2.586118
Ce	-1.430289	4.747042	-2.580114
C	-1.625938	2.432403	-4.212048
C	-2.294572	2.083119	-3.012613
C	-1.320507	1.965765	-1.987107
C	-0.054292	2.248547	-2.551152
C	-0.242585	2.541005	-3.925932
O	-0.759403	5.412666	-0.389598
C	-1.029706	5.746215	0.947697
C	-2.189341	4.925165	1.496676
C	0.623449	6.312656	-0.994473
C	0.910020	6.027234	-2.367133
H	1.325490	5.937779	-0.245362
H	0.240006	7.303430	-0.745117
H	-3.048113	7.711775	-1.702263
H	0.895157	2.219874	-2.030327
H	-1.491833	7.983540	-3.877396
H	-2.216979	6.103094	-5.661826
H	-4.228322	4.672857	-4.589297
H	-4.746882	5.668568	-2.146109
H	-3.356422	1.888984	-2.909579
H	-2.088050	2.562921	-5.183546
H	0.540593	2.764656	-4.641454
H	-1.508107	1.672623	-0.960151
H	-1.264424	6.821644	1.031526
H	-0.130268	5.568629	1.561788
H	0.734317	6.877700	-3.032727
C	2.175369	5.242531	-2.691742
C	-2.499500	5.238665	2.961600
H	-3.081619	5.114248	0.883388
H	-1.948988	3.859274	1.387995
C	3.456132	6.086426	-2.650574
H	2.277149	4.405244	-1.987053
H	2.100760	4.777792	-3.684138

H	4.345336	5.494037	-2.898604
H	3.397483	6.916115	-3.364359
H	3.608800	6.521903	-1.656260
C	-3.663680	4.418715	3.512817
H	-1.602807	5.055667	3.568773
H	-2.723753	6.308842	3.065257
H	-3.861719	4.661923	4.561448
H	-4.583963	4.607173	2.948720
H	-3.454833	3.344722	3.454541

Bu2O_TS_releasing_alkene_gamma

E=-809.404295
G=-809.059763

C	1.065822	0.378699	-3.070611
C	0.697699	1.678282	-2.642484
C	0.297008	2.418892	-3.785063
C	0.408912	1.571535	-4.915266
C	0.884042	0.309468	-4.472643
Ce	-1.753539	0.524716	-3.442697
C	-4.594811	0.723465	-3.219314
C	-4.278154	1.429951	-4.405929
C	-3.578666	2.607982	-4.041989
C	-3.465857	2.629661	-2.628772
C	-4.093850	1.464600	-2.120539
C	-2.141718	-1.718571	-4.768521
O	-1.512803	-2.831565	-5.317250
C	-2.075794	-3.274774	-6.541493
C	-1.337981	-4.519941	-7.001981
C	-1.890639	-5.080082	-8.312557
C	-1.152862	-6.332222	-8.781436
H	-3.016408	3.420907	-2.039030
H	-4.209631	1.207024	-1.074735
H	-5.158546	-0.200433	-3.159164
H	0.208777	1.853452	-5.943193
H	-3.227919	3.376516	-4.721357
H	-4.559060	1.143236	-5.413478
H	1.100486	-0.546773	-5.100737
H	1.450464	-0.414101	-2.440227
H	0.761466	2.058019	-1.628560
H	-0.006555	3.459293	-3.796154
H	-3.239389	-1.834082	-4.754992
H	-1.927713	-0.835113	-5.446709
H	-3.149029	-3.489504	-6.401238
H	-2.001890	-2.478360	-7.301615
H	-0.273997	-4.277212	-7.115885
H	-1.402889	-5.277863	-6.211224
H	-2.958007	-5.309244	-8.190451
H	-1.833752	-4.308787	-9.092640
H	-1.568628	-6.713347	-9.719564
H	-0.089630	-6.126676	-8.948011
H	-1.220742	-7.133781	-8.037542
C	-1.552828	-2.252631	-2.830428
C	-1.645291	-1.430789	-1.683317
C	-2.803765	-1.587181	-0.717756
H	-2.907867	-0.727464	-0.047160
H	-3.758513	-1.700511	-1.244317
H	-2.686339	-2.474687	-0.077379
H	-0.569507	-2.525044	-3.206354
H	-2.285192	-3.046852	-2.963035
H	-0.690145	-1.153656	-1.232111

Bu2O_TS_releasing_alkene_delta

E=-809.410501
G=-809.065570

C	0.935371	0.334604	-2.997184
C	0.552003	1.540290	-2.356103
C	0.177950	2.468411	-3.356977
C	0.322667	1.836911	-4.618783
C	0.796343	0.518840	-4.394797
Ce	-1.873703	0.498226	-3.450125
C	-4.337593	-0.535827	-4.447894
C	-3.421457	-1.607680	-4.579022
C	-2.474322	-1.257096	-5.573499
C	-2.811438	0.030590	-6.065045
C	-3.962543	0.475103	-5.368494
C	-2.017013	-1.054526	-1.327311
H	-0.975338	-1.118846	-1.023189
C	-2.838904	-0.075599	-0.760567
C	-3.291375	1.867358	-1.769185
C	-4.400261	2.252758	-0.826642
O	-4.742245	3.614469	-1.015035
C	-5.792218	4.038036	-0.171647
C	-6.087597	5.501648	-0.450757
C	-7.222471	6.054252	0.411605
H	1.043477	-0.206724	-5.161283
H	1.311408	-0.556162	-2.507274
H	0.579319	1.730799	-1.289242
H	-4.488548	1.408194	-5.538731
H	0.154109	2.297731	-5.585408
H	-0.132243	3.494304	-3.190960
H	-5.197921	-0.508871	-3.789337
H	-3.461056	-2.548994	-4.043847
H	-1.666318	-1.883810	-5.933725
H	-2.302540	0.561537	-6.861250
H	-2.429625	2.531646	-1.602084
H	-3.689844	2.063128	-2.790200
H	-6.695858	3.426126	-0.345812
H	-5.514008	3.898985	0.888791
H	-5.171053	6.081574	-0.284084
H	-6.335944	5.610782	-1.514074
C	-7.522205	7.524698	0.129683
H	-8.130402	5.458327	0.245940
H	-6.968743	5.930032	1.473252
H	-3.906436	-0.260541	-0.691155
H	-2.439507	0.555190	0.027696
H	-2.464094	-1.958690	-1.731654
H	-5.288455	1.618876	-1.002876
H	-4.095429	2.089415	0.222123
H	-8.337689	7.894776	0.759300
H	-6.643992	8.151596	0.320234
H	-7.814024	7.675976	-0.915573

Bu2O_releasing_alkene_beta_product

E=-652.330193
G=-769.833486

C	1.068304	-1.229046	2.106532
C	1.630466	-0.098496	1.466110
C	0.799713	1.015008	1.740270
C	-0.291373	0.567385	2.533825
C	-0.125501	-0.818237	2.760077
Ce	1.981662	0.396413	4.240801
C	1.734155	1.715600	6.735564
C	2.277055	0.452388	7.061160
C	1.275963	-0.526974	6.827463
C	0.105541	0.138416	6.380531
C	0.389862	1.521962	6.310435
O	4.117912	0.565664	3.950685
C	5.492406	0.697064	3.764270
C	5.890474	2.124058	3.388424
C	7.394618	2.298054	3.178070
C	7.788007	3.724248	2.799146
H	3.278000	0.266852	7.432319
H	1.366695	-1.589809	7.026176
H	-0.844682	-0.328972	6.151459
H	-0.312391	2.303119	6.040814
H	2.241090	2.669203	6.835375
H	2.535497	-0.087371	0.870959
H	0.938816	2.020652	1.357410
H	-1.124295	1.172770	2.872533
H	-0.809171	-1.461854	3.301515
H	1.449560	-2.243503	2.055218
H	6.031497	0.407538	4.683046
H	5.837038	0.010959	2.971140
H	5.350901	2.407785	2.474109
H	5.544128	2.803246	4.179969
H	7.926214	2.003433	4.093281
H	7.734523	1.605588	2.395738
H	8.869236	3.818048	2.653937
H	7.299571	4.035521	1.868842
H	7.494698	4.436532	3.578660

Bu2O_releasing_alkene_gamma_product

E=-691.565277
G=-691.298193

C	0.783123	-1.119239	2.223652
C	1.823760	-0.759767	1.329651
C	1.988655	0.647986	1.389366
C	1.042353	1.159014	2.308956
C	0.296300	0.067133	2.825410
Ce	-0.511405	0.242674	0.108384
C	-2.108857	-2.063467	-0.244120
C	-0.987785	-2.265637	-1.087922
C	-1.081609	-1.350865	-2.168796
C	-2.258130	-0.584657	-1.992260
C	-2.892893	-1.021734	-0.803111
C	0.271966	2.067235	-1.423728
O	-0.854681	2.547184	-0.625870
C	-1.322352	3.870362	-0.846248
C	-2.494174	4.169172	0.073050
C	-3.045293	5.583633	-0.117171
C	-4.222741	5.891799	0.804777
H	-0.494660	4.572365	-0.666153
H	-1.617952	3.969594	-1.901432
H	-2.173711	4.034803	1.115066
H	-3.289921	3.435166	-0.113043
H	2.721517	1.226708	0.841214
H	0.933906	2.198424	2.597708
H	-0.474155	0.123547	3.587407
H	0.442281	-2.126558	2.432859
H	2.424534	-1.446330	0.743505
H	-0.390317	-1.271391	-2.999372
H	-2.619217	0.188115	-2.660667
H	-3.840074	-0.660147	-0.416368
H	-2.347901	-2.635764	0.645135
H	-0.220406	-3.019833	-0.955566
H	0.001930	2.123576	-2.486501
H	1.143108	2.704616	-1.224515
H	-2.242821	6.312794	0.056857
H	-3.354421	5.715506	-1.162625
H	-4.598118	6.907418	0.645406
H	-5.053950	5.199310	0.631440
H	-3.935019	5.805601	1.858494

Bu2O_releasing_alkene_delta_product

E=-730.848177
G=-730.555403

C	-2.568121	-0.667489	-1.875590
C	-2.578150	-1.290247	-0.602754
C	-1.522087	-2.239284	-0.566534
C	-0.868940	-2.212040	-1.821580
C	-1.519387	-1.243674	-2.632858
Ce	-3.418607	-3.321259	-2.331423
C	-4.807795	-5.793890	-2.368827
C	-5.527496	-4.980247	-1.461863
C	-4.708441	-4.767351	-0.323727
C	-3.488542	-5.467596	-0.520844
C	-3.548989	-6.099664	-1.785485
C	-5.362442	-2.065109	-3.319935
C	-6.362569	-1.242615	-2.554506
O	-7.322161	-0.640662	-3.422710
C	-8.260796	0.150647	-2.737206
C	-9.231954	0.748044	-3.742659
C	-10.291429	1.641004	-3.098072
C	-11.265787	2.237295	-4.111534
H	-1.226998	-0.953183	-3.636477
H	-3.237412	0.116311	-2.206662
H	-3.241623	-1.046226	0.219281
H	-1.243271	-2.849752	0.284218
H	0.005051	-2.793171	-2.096320
H	-2.787520	-6.745125	-2.210832
H	-5.176106	-6.162354	-3.320246
H	-6.529937	-4.598345	-1.607289
H	-4.987578	-4.216623	0.567487
H	-2.671228	-5.535577	0.187364
H	-5.905644	-2.836264	-3.894979
H	-4.868249	-1.413103	-4.064321
H	-6.896831	-1.868338	-1.815288
H	-5.855576	-0.444025	-1.981699
H	-8.811214	-0.453015	-1.990786
H	-7.754523	0.957575	-2.173840
H	-8.657376	1.319973	-4.482524
H	-9.713377	-0.071768	-4.291062
H	-10.851615	1.062910	-2.350218
H	-9.798627	2.452494	-2.545061
H	-12.014943	2.870027	-3.624365
H	-10.740699	2.852610	-4.850771
H	-11.798742	1.450940	-4.657866

Insertion of butene into Ce-H bond

Bu2O_TS_insertion_12_butene

E=-577.039895
G=-576.806988

C	-0.508251	-3.082325	0.817962
C	-0.061714	-2.387364	1.969144
C	-1.154857	-1.643079	2.483277
C	-2.277418	-1.878494	1.651338
C	-1.876099	-2.762690	0.618359
Ce	-0.513065	-0.378702	0.021483
C	0.837244	-1.185621	-2.314598
C	-0.463369	-0.820578	-2.750258
C	-0.586620	0.587062	-2.638160
C	0.633365	1.091390	-2.123481
C	1.514265	-0.003141	-1.926376
C	-0.194601	1.954769	1.493815
C	-1.479075	2.282984	1.149615
C	-2.628250	2.252884	2.123435
H	-1.636479	2.882146	0.255020
H	-2.283703	0.822817	-0.011729
H	1.253702	-2.186360	-2.320031
H	-1.214761	-1.495467	-3.144701
H	-1.452118	1.174324	-2.917604
H	0.870815	2.136893	-1.962118
H	2.543126	0.058151	-1.587308
H	0.080145	-3.767395	0.218483
H	0.927120	-2.456460	2.410368
H	-1.146664	-1.041849	3.385408
H	-3.271910	-1.474226	1.791508
H	-2.515405	-3.161494	-0.161291
H	0.024083	1.532838	2.474610
H	0.650235	2.300646	0.899764
C	-2.758387	3.595175	2.856602
H	-3.555640	2.027606	1.590139
H	-2.474944	1.447929	2.851449
H	-3.609252	3.575157	3.545079
H	-1.857232	3.822466	3.434247
H	-2.920283	4.418464	2.152378

Bu2O_TS_insertion_21_butene

E=-577.038227
G=-576.804561

C	-0.352198	-2.873900	0.923529
C	-0.071455	-2.109121	2.083154
C	-1.257393	-1.424842	2.453949
C	-2.271009	-1.764574	1.524390
C	-1.710202	-2.657437	0.575894
Ce	-0.462605	-0.223978	-0.002937
C	0.842808	-1.116245	-2.334302
C	-0.528637	-1.023665	-2.691030
C	-0.878947	0.348274	-2.742299
C	0.273519	1.104449	-2.412522
C	1.337420	0.200785	-2.166892
C	-0.306970	2.005890	1.606749
C	1.106188	2.198511	1.130780
C	-1.442463	2.376448	0.930907
H	-2.401851	2.396075	1.433602
H	-1.383927	2.956358	0.012839
H	-2.235195	0.966447	-0.086763
H	1.421253	-2.029576	-2.256444
H	-1.182457	-1.856189	-2.924151
H	-1.848440	0.748762	-3.009743
H	0.340809	2.186448	-2.406040
H	2.362791	0.468909	-1.935886
H	0.336859	-3.538698	0.415358
H	0.869517	-2.094270	2.622866
H	-1.381733	-0.793009	3.325651
H	-3.298736	-1.424794	1.548928
H	-2.239323	-3.127592	-0.245007
H	-0.417599	1.590629	2.609165
C	1.991245	2.922915	2.151309
H	1.620975	1.225736	0.918545
H	1.111149	2.738015	0.175679
H	3.020254	3.014470	1.789774
H	1.602570	3.926378	2.346803
H	2.014592	2.381732	3.102854

Bu2O_TS_insertion_12_product_butene

E=-577.070126
G=-576.833664

C	-0.625140	-3.215787	0.679801
C	0.161108	-2.577020	1.674694
C	-0.703262	-1.798972	2.486109
C	-2.018385	-1.941350	1.982218
C	-1.971191	-2.820099	0.867292
Ce	-0.633865	-0.476852	-0.025478
C	0.906735	-1.159646	-2.288150
C	-0.326628	-0.719063	-2.828386
C	-0.426208	0.679320	-2.607074
C	0.747058	1.103501	-1.934232
C	1.567332	-0.033011	-1.731675
C	-0.461993	1.606121	1.362592
C	-1.824708	2.063458	0.877364
C	-2.807392	2.569267	1.940959
H	-1.726270	2.815183	0.082854
H	-2.404703	1.230706	0.346799
H	1.295425	-2.170609	-2.329907
H	-1.044297	-1.334989	-3.359513
H	-1.233179	1.321229	-2.943578
H	0.985554	2.119709	-1.646532
H	2.549896	-0.034732	-1.272429
H	-0.263544	-3.910846	-0.069227
H	1.226697	-2.711950	1.825898
H	-0.412574	-1.217432	3.351949
H	-2.913208	-1.500224	2.407309
H	-2.822709	-3.167718	0.291915
H	-0.467653	1.402455	2.439494
H	0.321420	2.335191	1.141849
H	-2.359874	3.449296	2.418957
C	-4.189704	2.916685	1.395237
H	-2.895901	1.808817	2.727986
H	-4.855677	3.275145	2.186893
H	-4.131124	3.701190	0.631999
H	-4.667691	2.043567	0.934097

Bu2O_TS_insertion_21_product_butene

E=-577.060216
G=-576.824017

C	-0.167102	-2.903383	1.005769
C	-0.006040	-2.112592	2.173642
C	-1.255183	-1.518925	2.479154
C	-2.187554	-1.934247	1.494493
C	-1.515863	-2.794295	0.587016
Ce	-0.418066	-0.262737	0.075941
C	0.674667	-1.156164	-2.402453
C	-0.693313	-0.911128	-2.687102
C	-0.906027	0.489570	-2.632514
C	0.326782	1.111336	-2.315676
C	1.302646	0.092806	-2.169231
C	-0.427045	1.811444	1.462959
C	1.017439	2.072363	1.158685
C	-1.535604	2.393960	0.641248
H	-2.348561	2.809589	1.245619
H	-1.210942	3.161365	-0.073295
H	-2.084377	1.637987	-0.020359
H	1.160899	-2.125007	-2.401058
H	-1.434209	-1.659034	-2.945474
H	-1.838692	0.998729	-2.848726
H	0.503776	2.178096	-2.247583
H	2.357561	0.245866	-1.970023
H	0.595905	-3.517364	0.540763
H	0.903229	-2.017482	2.757094
H	-1.467899	-0.885437	3.331068
H	-3.242885	-1.684745	1.471321
H	-1.963715	-3.307775	-0.255867

H	-0.648826	1.713034	2.524899
C	1.862261	2.517314	2.354238
H	1.560022	1.142663	0.756436
H	1.133989	2.783407	0.328136
H	2.925361	2.592346	2.100224
H	1.522628	3.493495	2.713977
H	1.764751	1.807232	3.182598

Second C_β-H activation of Bu-O-Bu by Cp2CeBu

Bu2O_TS_C_βH_act2_beta

E=-967.840935
G=-967.370380

C	-4.408068	0.529066	0.294050
C	-3.996341	-0.431764	1.247660
C	-4.641774	-1.657530	0.942145
C	-5.462694	-1.444427	-0.194021
C	-5.311769	-0.097790	-0.600637
Ce	-2.764910	-1.282373	-1.153144
C	-0.023249	-1.028946	-0.438004
C	-0.003157	-1.934386	-1.529571
C	-0.599198	-3.143933	-1.104750
C	-0.998629	-2.987655	0.246600
C	-0.633982	-1.680495	0.660592
O	-3.793570	-3.173765	-2.563764
C	-4.619906	-4.315550	-2.349807
C	-4.130395	-5.104890	-1.151208
C	-4.995097	-6.337605	-0.877762
C	-4.512344	-7.142062	0.326679
H	-5.144666	-8.018628	0.497655
C	-4.138704	-2.433555	-3.752948
C	-3.124024	-1.320339	-3.957298
C	-3.480042	-0.552051	-5.241810
H	0.422455	-1.741707	-2.506761
H	-0.714871	-4.038571	-1.705045
H	-1.451071	-3.749223	0.871548
H	-3.332485	-0.254390	2.085422
H	0.391981	-0.028026	-0.433192
H	-0.767398	-1.267304	1.653262
H	-4.567694	-2.573503	1.516953
H	-6.119360	-2.175283	-0.651321
H	-5.822385	0.380306	-1.428257
H	-4.103550	1.568606	0.266864
C	-2.359422	1.079916	-2.425062
H	-2.789665	-0.163400	-3.112620
H	-2.151413	-1.811923	-4.130645
H	-5.161088	-2.043925	-3.632835
H	-4.156495	-3.147405	-4.597507
H	-3.090884	-5.409320	-1.323666
H	-4.128794	-4.452786	-0.267980
H	-6.035521	-6.025352	-0.716453
H	-5.004324	-6.980943	-1.767845
H	-3.485547	-7.495402	0.182119
H	-4.529021	-6.537331	1.240047
H	-3.635769	-1.262068	-6.072238
C	-4.708664	0.354638	-5.140881
H	-2.617200	0.053437	-5.539343
C	-1.529175	1.792653	-3.500458
H	-2.117457	1.871950	-4.424661
H	-1.328974	2.832740	-3.198098
C	-0.192851	1.124035	-3.823940
C	0.614432	1.875631	-4.880320
H	0.400696	1.038750	-2.903536
H	-0.374068	0.095086	-4.162312
H	1.568761	1.380522	-5.088487
H	0.063599	1.944458	-5.825651
H	0.835328	2.898890	-4.555494
H	-3.305137	1.619979	-2.283114
H	-1.815112	1.204398	-1.465972
H	-4.882900	0.883929	-6.083899
H	-5.621009	-0.209057	-4.916861
H	-4.584144	1.106493	-4.354908
H	-5.660970	-3.988603	-2.203474

Bu2O_TS_C_βH_act2_beta_product

E=-809.474422
G=-809.128052

C	-1.903312	-1.511190	-0.925125
C	-0.750185	-2.316347	-1.091063
C	-0.783001	-2.867826	-2.397237
C	-1.961284	-2.408942	-3.036217
C	-2.653063	-1.569186	-2.124950
Ce	-2.880052	-4.194705	-1.032051
C	-1.555140	-6.589951	-1.732087
C	-2.463218	-6.372641	-2.798630
C	-3.774592	-6.583916	-2.304728
C	-3.676127	-6.938495	-0.935291
C	-2.306466	-6.943581	-0.581347
O	-5.024583	-3.591651	0.146787
C	-6.378231	-3.190430	0.011208
C	-6.801445	-3.269100	-1.445495
C	-8.254373	-2.841479	-1.663284
C	-8.682242	-2.919182	-3.126813
C	-4.501829	-3.530825	1.541014
C	-3.050965	-3.934334	1.549795
C	-2.734622	-5.085822	2.506726
C	-2.893276	-4.755075	3.997754
H	-5.143866	-4.210555	2.121861
H	-4.701553	-2.501303	1.872920
H	-3.569085	-1.025260	-2.328825
H	-4.502425	-7.189639	-0.280386
H	-2.153592	-0.934307	-0.042952
H	0.038519	-2.454436	-0.360040
H	-0.022536	-3.498794	-2.842565
H	-2.255632	-2.623624	-4.057643
H	-2.198226	-6.124946	-3.820142
H	-0.473811	-6.547146	-1.798878
H	-1.903308	-7.196626	0.391526
H	-4.688356	-6.536326	-2.887680
H	-6.490798	-2.162893	0.390878
H	-7.011297	-3.842051	0.633116
H	-2.435063	-3.065606	1.820659
H	-6.138941	-2.628518	-2.044561
H	-6.664534	-4.298752	-1.802765
H	-3.367569	-5.953839	2.268192
H	-1.702668	-5.427096	2.343592
H	-2.646494	-5.610613	4.638890
H	-2.237150	-3.923878	4.281907
H	-3.920961	-4.453607	4.234797
H	-8.913609	-3.474020	-1.054234
H	-8.389771	-1.815857	-1.295163
H	-9.723041	-2.605829	-3.253395
H	-8.061862	-2.272095	-3.756779
H	-8.593921	-3.940651	-3.512839