Supporting Information

Mechanism of rhodium(III)-catalyzed alkenylation of *N*-phenoxyacetamide using *N*-tosylhydrazone or alkenes: a computational study†

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† Electronic supplementary information (ESI) available: Complete ref. 21, calculated imaginary frequencies of all of the transition states, and tables of Cartesian coordinates and electronic energies for all of the calculated structures.
‡ These authors contributed equally.

Complete Reference for Ref (21):

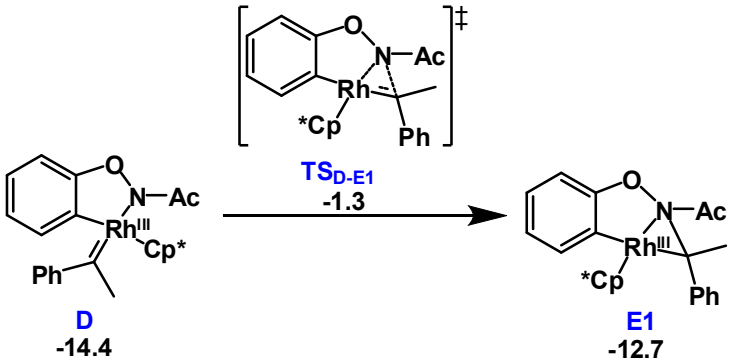
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision C.01*, Gaussian, Inc., Wallingford, CT, 2010.

Table S1. Relevant critical structures with free energies (in parentheses, kcal/mol) relative to isolated catalyst and substrate with DZVP basis set to treat the rhodium center.

	TS_{F-G}	TS_{F-L}	TS_{G-H}	TS_{G-J}	TS_{O-L}	TS_{P-Q}	TS_{M-J}
ΔG	**-15.7**	**-4.1**	**-27.6**	**-17.4**	**-2.3**	**3.5**	**10.7**

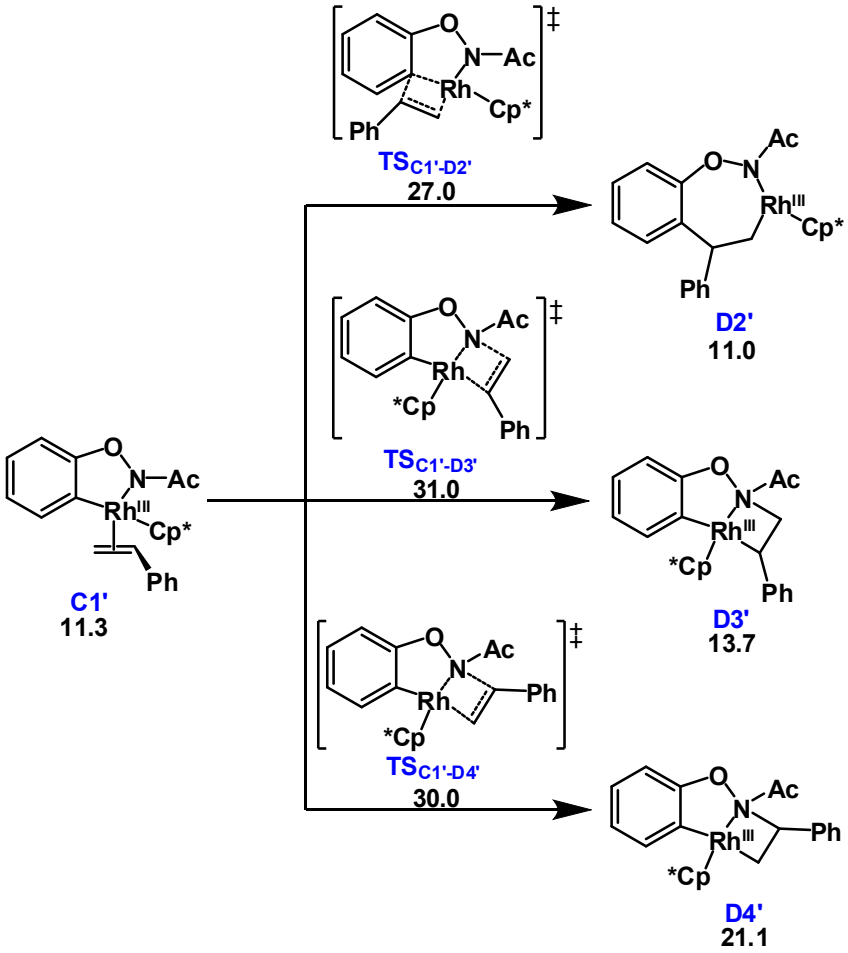
Other possible insertion of C2

Scheme S1



Other possible insertion of C1’

Scheme S2



Calculated imaginary frequencies of all transition states species

TS_{A1-B}	-1133.92
TS_{B1-C}	-1516.78
TS_{C2-D}	-398.31
TS_{D-E}	-216.44
TS_{E-F}	-216.94
TS_{F-G}	-115.55
TS_{G-H}	-1056.47
TS_{H1-I}	-463.75
TS_{I1-A}	-305.72
TS_{G-J}	-1869.73
TS_{F-L}	-1227.98
TS_{E-M}	-662.74
TS_{M-N}	-1029.44
TS_{N-O}	-135.94
TS_{O-L}	-620.01
TS_{P-Q}	-485.58
TS_{M-J}	-1111.58
$TS_{C1'-D'}$	-274.48
$TS_{D'-D1'}$	-577.50
$TS_{D1'-E'}$	-1204.46
$TS_{E'-F'}$	-133.78
$TS_{F'-G'}$	-513.74
$TS_{G1'-H'}$	-386.08
$TS_{I'-J'}$	-570.16
$TS_{D'-K'}$	-259.15
$TS_{D1'-J}$	-1069.66
$TS_{L'-M'}$	-261.94
$TS_{M'-K}$	-1351.19
TS_{D-E1}	-252.55
$TS_{C1'-D2'}$	-277.06
$TS_{C1'-D3'}$	-387.58
$TS_{C1'-D4'}$	-357.36

Cartesian coordinates and electronic energies

AcOH

E = -228.9540758au

C	-0.092877	0.124748	0.000216
O	-0.654537	1.191915	-0.000088
O	-0.761099	-1.047705	-0.000081
H	-1.706331	-0.814984	-0.000249
C	1.387410	-0.098141	0.000045
H	1.679614	-0.680655	0.881357
H	1.679421	-0.680812	-0.881229
H	1.905180	0.863130	-0.000098

1

E = -515.0685846au

C	-3.233996	0.542852	0.303967
C	-2.974603	-0.819119	0.164415
C	-1.697797	-1.263537	-0.149205
C	-0.677082	-0.332785	-0.323787
C	-0.913159	1.028813	-0.188544
C	-2.201616	1.456007	0.125528
H	-4.236158	0.887827	0.549969
H	-3.773336	-1.546245	0.300848
H	-1.470448	-2.321591	-0.263900
H	-0.102714	1.738077	-0.332908
H	-2.392768	2.522706	0.231605
O	0.557536	-0.882487	-0.619966
N	1.556549	0.056788	-0.844169
H	1.853046	0.043655	-1.817371
C	2.597038	0.111077	0.080395
C	2.258451	-0.362174	1.463425
H	1.353730	0.129983	1.842023
H	2.061450	-1.440769	1.462613
H	3.104071	-0.141362	2.118708
O	3.662946	0.577911	-0.259980

NH_2Ac

E = -209.0789775au

N	1.019715	-0.837365	-0.009753
C	0.075335	0.150167	-0.008557
C	-1.355892	-0.333988	-0.000656
H	-1.471335	-1.378522	-0.312674
H	-1.763560	-0.226920	1.011936
H	-1.947500	0.308983	-0.659083
O	0.368403	1.330172	0.002012
H	1.990871	-0.562121	0.041707
H	0.789627	-1.818313	0.025568

A

E = -956.0633907au

Rh	-0.061807	0.181558	-0.120131
C	2.432309	-1.299498	-0.040746
O	2.040816	-1.790491	1.016170
O	1.757163	-0.515606	-0.822976
C	3.830979	-1.569481	-0.558379
H	3.806524	-1.840564	-1.619822
H	4.428002	-0.652925	-0.474682
H	4.306657	-2.362755	0.025300
C	1.306872	2.311671	0.023488
O	0.631977	2.059669	-1.019381
O	1.191817	1.562038	1.037880
C	2.264637	3.461764	0.039632
H	2.385686	3.850321	1.055274
H	3.242491	3.105765	-0.308201
H	1.929842	4.251919	-0.639150
C	-1.674017	-0.820164	-1.075336
C	-1.157800	-1.685249	-0.050208
C	-1.268318	-1.001542	1.202337
C	-2.177313	0.381061	-0.431628
C	-1.919549	0.276132	0.964969
C	-0.568772	-3.034775	-0.250328
H	0.216326	-3.223478	0.488409
H	-1.347434	-3.806001	-0.159043
H	-0.115723	-3.128387	-1.244451
C	-0.776996	-1.511165	2.509375
H	-1.319386	-2.421543	2.801828
H	0.292265	-1.749771	2.425143
H	-0.905757	-0.767895	3.303712
C	-2.190733	1.296426	2.013312
H	-3.047826	1.005359	2.636899
H	-1.319494	1.418920	2.668539
H	-2.409691	2.275670	1.573416
C	-2.760121	1.543733	-1.152319
H	-3.779267	1.319414	-1.497632
H	-2.804064	2.432712	-0.513931
H	-2.153060	1.803455	-2.028687
C	-1.733714	-1.117903	-2.531257
H	-2.651539	-1.666888	-2.788161
H	-1.715178	-0.197385	-3.126454
H	-0.877043	-1.726981	-2.843411

Diazo

E = -418.7943383au

C	1.380311	0.376221	0.000027
C	-0.059251	0.133305	-0.000100
C	-0.946684	1.218745	-0.000140
C	-0.594712	-1.164382	0.000082
C	-2.320722	1.009217	-0.000080
H	-0.560642	2.237004	-0.000178
C	-1.966210	-1.364828	0.000079
H	0.072419	-2.026480	0.000200
C	-2.840789	-0.280084	0.000022
H	-2.989854	1.868523	-0.000049
H	-2.357393	-2.381091	0.000209
H	-3.917290	-0.439789	0.000084
C	2.003973	1.739176	0.000152
H	3.096598	1.665705	0.000387
H	1.707519	2.315838	-0.887685
H	1.707133	2.315883	0.887867
N	2.179138	-0.650934	-0.000030
N	2.864578	-1.571896	-0.000126

Nitrogen

E = -109.4550063au

N	0.000000	0.000000	0.552560
N	0.000000	0.000000	-0.552560

A1

E = -1471.1511841au

Rh	-1.007905	-0.023258	-0.097658
C	-0.026122	-1.339478	2.474567
O	-1.045431	-1.057392	1.755872
O	1.122669	-0.879214	2.331566
C	-0.289091	-2.351924	3.562972
H	-0.402830	-3.339548	3.098049
H	0.542596	-2.381294	4.272245
H	-1.226215	-2.125386	4.082295
C	0.499733	-2.515380	-0.697596
O	0.580387	-1.220253	-0.700321
O	-0.529134	-3.184289	-0.646444
C	1.874788	-3.148668	-0.753253
H	2.403183	-2.914439	0.180593
H	1.802259	-4.232908	-0.878695
H	2.465418	-2.707593	-1.565359
C	-2.205525	-0.288701	-1.863774
C	-2.966168	-0.594709	-0.680383
C	-3.065181	0.618143	0.110236
C	-1.763756	1.073673	-1.772133
C	-2.340112	1.640531	-0.562703
C	5.491496	-0.329394	-0.563473
C	4.834436	0.057116	-1.730194
C	3.555375	0.590551	-1.669975
C	2.935789	0.747360	-0.432240
C	3.575482	0.373994	0.743804
C	4.855543	-0.170976	0.661656
H	6.490841	-0.757023	-0.612483
H	5.316457	-0.068304	-2.698503
H	3.012192	0.883013	-2.566774
H	3.089414	0.464297	1.712208
H	5.355823	-0.474247	1.579715
O	1.686666	1.330375	-0.491882
N	0.847094	1.101125	0.605014
C	0.625869	2.256240	1.396418
C	1.327768	3.511617	0.971536
H	2.416085	3.370897	0.977767
H	1.054688	3.784552	-0.055374
H	1.047664	4.312315	1.660731
O	-0.137186	2.179700	2.333717
H	1.099132	0.240090	1.205156
C	-3.728877	0.717877	1.436970
H	-3.315854	-0.038274	2.118476
H	-3.566389	1.699838	1.894411
H	-4.811656	0.552057	1.351174
C	-2.186858	3.043883	-0.090097
H	-3.136249	3.586974	-0.198078
H	-1.892422	3.086819	0.967106
H	-1.433200	3.584044	-0.675240
C	-0.889206	1.778819	-2.749096
H	-1.466497	2.222513	-3.572864
H	-0.317858	2.580210	-2.263807
H	-0.154760	1.085137	-3.176697
C	-1.889273	-1.261315	-2.940393
H	-2.718673	-1.304171	-3.661600
H	-0.980946	-0.981340	-3.485436
H	-1.735900	-2.260946	-2.518015
C	-3.540751	-1.922232	-0.339791
H	-4.377426	-2.172957	-1.007930
H	-2.761600	-2.691757	-0.434136
H	-3.907134	-1.937390	0.692169

TS_{A1-B}

E = -1471.148671au

Rh	1.013098	-0.065086	-0.087536
C	0.186511	1.733830	2.211447
O	1.183067	1.252642	1.602224
O	-1.010903	1.359243	2.071299
C	0.459393	2.879458	3.147580
H	1.430289	2.755212	3.636256
H	0.502842	3.802476	2.554374
H	-0.338659	2.975371	3.888965
C	0.095495	2.575993	-1.066320
O	-0.305295	1.359593	-0.864361
O	1.258865	2.965797	-1.132218
C	-1.062872	3.547165	-1.185059
H	-0.725996	4.498403	-1.607267
H	-1.876096	3.123869	-1.785132
H	-1.464324	3.726547	-0.177404
C	2.282718	-0.266645	-1.819693
C	3.069108	0.049094	-0.661191
C	2.909354	-1.034268	0.291932
C	1.581581	-1.497390	-1.564214
C	2.023801	-1.993073	-0.272709
C	-5.684345	0.402955	-0.614924
C	-5.346424	-0.854326	-1.107128
C	-4.044024	-1.323840	-0.988999
C	-3.073778	-0.522420	-0.389809
C	-3.390987	0.741935	0.095162
C	-4.704507	1.188601	-0.016294
H	-6.705649	0.769336	-0.699342
H	-6.101931	-1.481780	-1.577454
H	-3.755554	-2.307069	-1.358765
H	-2.628206	1.377292	0.535103
H	-4.956602	2.177338	0.363912
O	-1.802158	-1.059691	-0.390756
N	-0.968145	-0.752533	0.704284
C	-0.924229	-1.801420	1.645104
C	-1.838895	-2.972400	1.425374
H	-2.888530	-2.651532	1.433718
H	-1.663240	-3.433834	0.445499
H	-1.665051	-3.699708	2.222856
O	-0.150239	-1.715045	2.577910
H	-1.085326	0.281808	1.271045
C	1.626169	-3.279284	0.361171
H	2.469185	-3.984237	0.340287
H	1.327320	-3.141325	1.408946
H	0.792818	-3.751003	-0.172318
C	0.618308	-2.170798	-2.476913
H	-0.157539	-2.698443	-1.908421
H	0.098861	-1.435821	-3.102649
H	1.119153	-2.894156	-3.136324
C	2.174985	0.578480	-3.036007
H	2.988710	0.336001	-3.735137
H	1.222827	0.415510	-3.553628
H	2.234006	1.638948	-2.768285
C	3.901926	1.266603	-0.481768
H	4.781137	1.240900	-1.141722
H	3.302140	2.155487	-0.718373
H	4.252505	1.356572	0.552087
C	3.518153	-1.080899	1.647804
H	4.602612	-1.249842	1.587885
H	3.347606	-0.132562	2.173697
H	3.076967	-1.877564	2.256672

B

E = -1471.158032au

Rh	0.930614	-0.137024	-0.113545
C	0.545180	1.883893	2.235256
O	1.379615	1.237564	1.602990
O	-0.748106	1.698227	2.160796
C	0.946168	3.010461	3.129846
H	1.959091	2.848689	3.506195
H	0.945851	3.933460	2.535203
H	0.236945	3.131044	3.953250
C	0.261688	2.600326	-1.078484
O	-0.262884	1.447963	-0.799376
O	1.457167	2.856795	-1.202416
C	-0.793387	3.684360	-1.206258
H	-0.361871	4.600541	-1.619724
H	-1.631401	3.342267	-1.825336
H	-1.200527	3.897051	-0.206794
C	2.109367	-0.436396	-1.916660
C	2.986271	-0.224701	-0.817106
C	2.740704	-1.278960	0.156255
C	1.273626	-1.581885	-1.614819
C	1.727896	-2.138463	-0.354869
C	-5.543426	0.620314	-0.738246
C	-5.369715	-0.747461	-0.930659

C	-4.127343	-1.332327	-0.718498
C	-3.046768	-0.543002	-0.325086
C	-3.205104	0.827112	-0.134801
C	-4.457565	1.395645	-0.342507
H	-6.517649	1.078840	-0.897849
H	-6.209957	-1.368910	-1.237164
H	-3.971197	-2.402493	-0.850355
H	-2.344897	1.442396	0.108224
H	-4.576467	2.469840	-0.203330
O	-1.854454	-1.214997	-0.198923
N	-0.946224	-0.714536	0.773380
C	-0.903165	-1.551648	1.870333
C	-2.011815	-2.561158	2.041857
H	-3.002740	-2.097874	1.961445
H	-1.957107	-3.328421	1.258515
H	-1.896675	-3.029836	3.023064
O	0.004534	-1.439790	2.688960
H	-0.938103	0.918957	1.557698
C	1.210603	-3.369165	0.301095
H	1.913331	-4.202027	0.156528
H	1.074895	-3.219727	1.379609
H	0.245962	-3.672538	-0.122808
C	0.219450	-2.149095	-2.496675
H	-0.568825	-2.631996	-1.908611
H	-0.265935	-1.359991	-3.082994
H	0.640532	-2.885887	-3.196287
C	2.023321	0.408522	-3.135703
H	2.754180	0.064564	-3.882351
H	1.027655	0.351650	-3.590456
H	2.222281	1.458109	-2.893594
C	3.964787	0.886026	-0.681531
H	4.848027	0.711004	-1.312784
H	3.494162	1.832228	-0.975810
H	4.304593	0.988663	0.354981
C	3.429153	-1.412268	1.466613
H	4.440593	-1.822885	1.333360
H	3.521647	-0.436626	1.959105
H	2.873014	-2.069141	2.142575

B1

E = -1242.1804605au

Rh	0.887557	-0.241233	-0.069322
C	-0.620797	-2.063036	-1.008197
O	-0.581230	-1.827822	0.239723
O	0.135894	-1.415578	-1.787085
C	-1.571472	-3.092303	-1.533979
H	-1.474361	-3.195612	-2.618169
H	-1.382832	-4.056701	-1.048232
H	-2.595211	-2.793594	-1.276248
C	2.470069	-1.003983	1.214933
C	3.002925	-0.798249	-0.080418
C	2.832194	0.608262	-0.419420
C	1.945657	0.267842	1.694168
C	2.238490	1.266978	0.705190
C	-5.327262	-0.715820	0.263697
C	-4.900310	-0.207988	1.489171
C	-3.652450	0.387100	1.609624
C	-2.819770	0.476689	0.494093
C	-3.231291	-0.025286	-0.738386
C	-4.486086	-0.620573	-0.840310
H	-6.307270	-1.180107	0.171003
H	-5.546088	-0.275198	2.363666
H	-3.300588	0.790711	2.557603
H	-2.561729	0.039807	-1.593943
H	-4.808590	-1.010380	-1.805773
O	-1.629041	1.121001	0.702016
N	-0.721881	1.042020	-0.373239
C	-0.621334	2.196346	-1.083663
C	-1.662062	3.264663	-0.835940
H	-2.683666	2.872213	-0.903510
H	-1.545983	3.682894	0.172727
H	-1.518846	4.055161	-1.577546
O	0.283131	2.357990	-1.905529
C	1.943971	2.720480	0.805638
H	2.792284	3.246238	1.266866
H	1.760354	3.152715	-0.184487
H	1.057343	2.908199	1.424512
C	1.285080	0.478041	3.009914
H	0.621825	1.350240	2.986815
H	0.672039	-0.390483	3.281598
H	2.026239	0.631419	3.808287
C	2.353241	-2.288239	1.954991
H	3.033766	-2.303265	2.818303
H	1.332251	-2.434153	2.330125
H	2.593545	-3.146087	1.317970
C	3.569602	-1.818987	-1.002384
H	4.649373	-1.666390	-1.140671
H	3.417137	-2.835664	-0.624259

H	3.093310	-1.758509	-1.989409
C	3.256234	1.255819	-1.688223
H	4.194974	1.811789	-1.547584
H	3.419586	0.511356	-2.475736
H	2.476423	1.943494	-2.037729

TS_{B1-C}

E = -1242.1511381au

Rh	-0.367213	-0.270734	0.112088
C	-0.517768	1.865411	2.251322
O	-1.222283	1.041345	1.604820
O	0.742057	1.910529	2.230107
C	-1.253640	2.880713	3.085931
H	-0.583513	3.349650	3.811289
H	-1.653023	3.652348	2.416193
H	-2.104895	2.413507	3.591214
C	-2.300858	-1.117506	-0.474106
C	-1.407840	-1.185809	-1.581383
C	-0.252569	-1.961395	-1.188870
C	-1.733481	-1.912308	0.599603
C	-0.502545	-2.466354	0.145921
C	3.848749	-1.133438	1.028702
C	4.418257	-0.422148	-0.038824
C	3.682912	0.501870	-0.760176
C	2.342415	0.710155	-0.416439
C	1.729987	0.030866	0.663089
C	2.529308	-0.895259	1.367693
H	4.451184	-1.840254	1.596480
H	5.459702	-0.596435	-0.306914
H	4.113976	1.049184	-1.596039
H	2.092595	-1.402767	2.229810
O	1.641651	1.578099	-1.153797
N	0.238247	1.398445	-0.964002
C	-0.511780	2.423930	-1.421834
C	0.209179	3.612908	-2.014144
H	0.895207	4.059552	-1.284683
H	0.812562	3.319520	-2.881682
H	-0.541890	4.346196	-2.319283
O	-1.744996	2.367367	-1.368963
H	1.160837	0.885627	1.432697
C	0.364214	-3.424574	0.883927
H	0.245784	-3.328613	1.970000
H	0.103115	-4.457914	0.612378
H	1.425062	-3.276848	0.650783
C	-2.360002	-2.091317	1.937188
H	-1.662116	-2.538700	2.653796
H	-2.680593	-1.123972	2.343778
H	-3.243818	-2.742148	1.874383
C	-3.553622	-0.314842	-0.428835
H	-4.309454	-0.716813	-1.118985
H	-3.983049	-0.304280	0.578722
H	-3.331141	0.723968	-0.713913
C	-1.622148	-0.515620	-2.891046
H	-2.295769	-1.122189	-3.514249
H	-2.070504	0.475223	-2.749006
H	-0.681907	-0.388404	-3.439122
C	0.922790	-2.277975	-2.048099
H	0.730915	-3.144792	-2.697161
H	1.174990	-1.423032	-2.688412
H	1.811818	-2.496298	-1.443068

C

E = -1242.1730285au

Rh	0.431598	-0.220990	-0.064247
C	-0.717198	2.077024	-1.935983
O	0.197768	1.264100	-1.877628
O	-1.970401	1.775997	-1.636491
C	-0.511405	3.510301	-2.284773
H	-1.429143	3.979185	-2.648772
H	-0.194535	4.002273	-1.353722
H	0.297484	3.608272	-3.013700
C	2.273832	-0.132527	1.218116
C	1.532384	-1.394350	1.277268
C	1.653062	-2.041742	-0.014812
C	2.690431	0.055015	-0.105345
C	2.268288	-1.109536	-0.887085
C	-3.087318	-2.637325	-1.064773
C	-4.004356	-2.141144	-0.138481
C	-3.657106	-1.099423	0.712074
C	-2.371643	-0.560293	0.629159
C	-1.414166	-1.055177	-0.274700
C	-1.803826	-2.096718	-1.121286
H	-3.372303	-3.442589	-1.740380
H	-5.007437	-2.561920	-0.084422
H	-4.364168	-0.689917	1.431639
H	-1.085418	-2.493063	-1.842790
O	-2.050852	0.468567	1.448971
N	-0.776554	0.987875	1.076899

C	-0.641979	2.314871	1.278803
C	-1.792043	3.048430	1.927863
H	-2.676335	3.017656	1.278334
H	-2.082222	2.590707	2.880430
H	-1.488476	4.086632	2.088213
O	0.389035	2.901041	0.920266
H	-1.988115	0.843111	-1.316175
C	3.343652	1.261286	-0.682411
H	3.575749	1.998003	0.093468
H	4.277521	1.002805	-1.202145
H	2.674186	1.746306	-1.407162
C	2.452086	0.814311	2.354252
H	2.308633	1.850876	2.029324
H	1.719033	0.623859	3.146569
H	3.453816	0.709188	2.795452
C	0.945933	-1.994583	2.507808
H	0.217234	-2.774838	2.257530
H	1.722337	-2.442930	3.145517
H	0.418327	-1.234904	3.098245
C	1.198572	-3.422454	-0.335785
H	1.125541	-3.584344	-1.417878
H	1.910140	-4.161535	0.060382
H	0.214040	-3.639170	0.096634
C	2.543775	-1.281278	-2.339745
H	2.402195	-0.336416	-2.878280
H	3.579730	-1.610207	-2.511725
H	1.875894	-2.023377	-2.793703

C1

E = -1013.204986au

Rh	0.220225	-0.097724	0.025027
C	2.422149	-0.006325	0.626019
C	1.739268	-1.181956	1.140535
C	1.329592	-1.996277	0.037752
C	2.333472	-0.043346	-0.775375
C	1.618508	-1.257571	-1.150187
C	-3.709359	-2.036722	-0.029598
C	-4.536404	-0.906378	0.000398
C	-3.986119	0.361018	0.035818
C	-2.592142	0.481399	0.041206
C	-1.722511	-0.623487	0.021599
C	-2.330782	-1.889071	-0.019298
H	-4.151937	-3.031540	-0.062420
H	-5.619133	-1.022646	-0.007486
H	-4.604381	1.256738	0.053124
H	-1.710400	-2.784920	-0.043915
O	-2.078337	1.726992	0.058014
N	-0.677736	1.671601	0.034872
C	-0.130480	2.936084	-0.000176
C	-1.068616	4.114846	0.026179
H	-1.750140	4.092875	-0.831958
H	-1.693681	4.102029	0.926462
H	-0.466828	5.026810	0.002060
O	1.085974	3.073409	-0.053806
C	1.589613	-1.530222	2.578301
H	2.477973	-2.063664	2.949606
H	1.458272	-0.632525	3.193934
H	0.716685	-2.172288	2.743161
C	0.786381	-3.379507	0.123600
H	1.603113	-4.109859	0.220935
H	0.127986	-3.508119	0.992015
H	0.213631	-3.650236	-0.771653
C	1.335511	-1.691415	-2.544385
H	2.182867	-2.255200	-2.963408
H	0.446119	-2.331870	-2.588588
H	1.154173	-0.830599	-3.198791
C	2.839968	0.981323	-1.726736
H	3.790537	0.664518	-2.181712
H	2.122239	1.150602	-2.539945
H	2.987148	1.942685	-1.225532
C	3.052513	1.067442	1.442563
H	4.133073	1.121404	1.247999
H	2.612215	2.042322	1.197243
H	2.920016	0.887643	2.515568

C2

E = -1432.0094525au

Rh	0.336531	-0.339877	0.211117
C	0.905276	-2.442290	1.012115
C	1.320396	-1.313296	1.835095
C	0.131472	-0.703587	2.378074
C	-0.491589	-2.418981	0.933482
C	-0.984920	-1.309968	1.742925
C	0.431550	3.893620	1.336699
C	1.634893	4.279931	0.750187
C	2.383982	3.365921	0.020311
C	1.917423	2.057506	-0.110747
C	0.712744	1.636261	0.470611

C	-0.015741	2.578652	1.197613
H	-0.158818	4.612188	1.903956
H	1.991169	5.303807	0.853917
H	3.322725	3.646430	-0.454617
H	-0.953417	2.285267	1.675540
O	2.673930	1.177851	-0.803169
N	1.890319	0.027901	-1.130924
C	2.609996	-0.866703	-1.851444
C	4.027268	-0.501868	-2.228083
H	4.060957	0.432775	-2.799456
H	4.642650	-0.342441	-1.333409
H	4.440453	-1.318935	-2.825458
O	2.103199	-1.932656	-2.223147
C	-1.338629	-3.415842	0.224891
H	-0.793068	-3.888100	-0.602293
H	-1.652251	-4.218092	0.910511
H	-2.257522	-2.967290	-0.176218
C	1.806856	-3.449255	0.388618
H	1.640869	-3.524333	-0.692280
H	2.861427	-3.182432	0.526010
H	1.651949	-4.437700	0.845909
C	2.723552	-1.000102	2.225739
H	2.810182	0.023504	2.609633
H	3.085206	-1.687363	3.005729
H	3.399342	-1.084281	1.365389
C	0.096182	0.312724	3.464735
H	-0.872790	0.822856	3.514655
H	0.257133	-0.177994	4.436213
H	0.868244	1.080939	3.341808
C	-2.419001	-1.023071	2.026712
H	-3.062309	-1.304852	1.184069
H	-2.765713	-1.579335	2.910941
H	-2.592248	0.044743	2.212792
C	-1.157396	0.020127	-1.661088
C	-2.536888	0.307671	-1.170196
C	-3.552886	-0.640699	-1.331828
C	-2.852733	1.523140	-0.548229
C	-4.840674	-0.388233	-0.864412
H	-3.347010	-1.581532	-1.839354
C	-4.139126	1.773948	-0.093326
H	-2.074577	2.274434	-0.410059
C	-5.141547	0.816840	-0.242024
H	-5.614915	-1.141633	-1.002355
H	-4.360176	2.727993	0.383059
H	-6.149638	1.014734	0.117267
C	-0.933855	-1.177443	-2.566234
H	0.125018	-1.291830	-2.820363
H	-1.211265	-2.086985	-2.023982
H	-1.549833	-1.118086	-3.477321
N	-0.573590	1.132672	-2.173207
N	-0.014204	2.054630	-2.506035

$TS_{C2\text{-}D}$

E = -1431.9459712au

N	1.832547	0.349328	-1.071176
C	1.442766	2.303612	0.015123
C	1.717807	3.642835	0.287283
H	2.653155	4.077805	-0.061562
C	0.784889	4.389029	0.996262
C	-0.406836	3.802406	1.417079
H	-1.142005	4.388505	1.967367
C	-0.658883	2.459126	1.133954
H	-1.598116	2.013668	1.469042
C	0.259975	1.680955	0.431646
C	0.918524	-2.495019	0.886043
C	1.642772	-1.441798	1.568659
C	0.719871	-0.667072	2.330069
C	-0.600747	-1.148078	2.021138
C	-0.447294	-2.318367	1.186669
Rh	0.311579	-0.334634	0.150464
C	-1.569975	-3.232423	0.842076
H	-1.805501	-3.872250	1.706020
H	-2.487631	-2.681207	0.600257
H	-1.332017	-3.898503	0.003509
C	1.545246	-3.580250	0.079590
H	2.194160	-4.214051	0.702013
H	0.786627	-4.231164	-0.372331
H	2.146437	-3.163256	-0.739654
C	3.125368	-1.272970	1.545940
H	3.581123	-1.663848	2.467800
H	3.567731	-1.811280	0.698767
H	3.413442	-0.217094	1.458264
C	1.071574	0.417317	3.288025
H	1.152801	0.017936	4.309944
H	2.032525	0.881105	3.032405
H	0.323974	1.219087	3.297838
C	-1.878353	-0.708798	2.652826
H	-2.134002	-1.331012	3.524824

H	-1.814054	0.328775	3.002819
H	-2.719813	-0.764618	1.947309
C	-1.059162	-0.385980	-1.411503
N	0.456607	1.248158	-2.921365
O	2.387763	1.583903	-0.646591
C	2.729583	-0.379645	-1.799407
O	2.446122	-1.522984	-2.163403
C	4.032420	0.275837	-2.179016
H	4.619891	0.533982	-1.288970
H	4.594330	-0.420148	-2.807202
H	3.852669	1.211421	-2.722161
C	-0.861947	-1.620915	-2.267250
H	-1.500779	-1.626669	-3.163915
H	0.192893	-1.741481	-2.541273
H	-1.133855	-2.496850	-1.664067
C	-2.474255	-0.011694	-1.142836
C	-2.849647	1.310978	-0.869833
C	-3.472320	-0.995538	-1.105770
C	-4.155986	1.628241	-0.529431
H	-2.099711	2.097498	-0.923243
C	-4.779260	-0.680920	-0.741595
H	-3.232906	-2.024370	-1.366661
C	-5.126241	0.630916	-0.445263
H	-4.418121	2.665140	-0.324286
H	-5.530657	-1.468376	-0.707211
H	-6.148697	0.880330	-0.166978
N	-0.516738	0.807483	-2.576892
H	0.987728	5.436628	1.213543

D

E = -1322.5757728au

Rh	-0.197737	-0.227705	0.168912
C	0.332285	-1.127733	2.211580
C	-0.897424	-1.743793	1.760640
C	-0.606702	-2.472666	0.584077
C	1.376573	-1.505520	1.327391
C	0.790995	-2.288560	0.274121
C	-3.105863	-0.548924	-3.086566
C	-4.126287	0.244128	-2.570669
C	-3.963509	0.908677	-1.358158
C	-2.765916	0.762925	-0.662167
C	-1.742274	-0.063432	-1.144086
C	-1.914616	-0.692063	-2.369984
H	-3.232132	-1.053471	-4.043394
H	-5.059274	0.360641	-3.120180
H	-4.743474	1.550653	-0.951724
H	-1.109377	-1.312221	-2.773060
O	-2.608153	1.437836	0.508645
N	-1.255630	1.325561	0.957152
C	-0.716668	2.486413	1.400644
C	-1.651317	3.652827	1.610843
H	-2.030530	4.009449	0.643932
H	-2.525617	3.375113	2.209700
H	-1.095623	4.454989	2.103720
O	0.493823	2.568720	1.635844
C	2.814754	-1.170394	1.512804
H	2.938909	-0.143220	1.881386
H	3.279686	-1.844478	2.248070
H	3.383438	-1.253284	0.578942
C	0.494939	-0.281961	3.428282
H	1.063925	0.627809	3.199885
H	-0.476106	0.036940	3.823958
H	1.018356	-0.831460	4.224844
C	-2.222572	-1.605691	2.430085
H	-3.037327	-1.942463	1.777558
H	-2.271143	-2.197212	3.356115
H	-2.425592	-0.558263	2.688590
C	-1.547278	-3.316061	-0.203553
H	-1.356307	-3.239847	-1.281298
H	-1.445981	-4.375706	0.074768
H	-2.591099	-3.022445	-0.042009
C	1.521920	-3.023299	-0.797952
H	2.487544	-2.556073	-1.024699
H	1.720402	-4.062841	-0.494987
H	0.942364	-3.063284	-1.730128
C	0.801797	0.992270	-0.891267
C	2.255672	0.834935	-1.045874
C	3.122187	1.625059	-0.278059
C	2.781708	-0.044984	-1.997085
C	4.496481	1.510997	-0.451659
H	2.691918	2.297606	0.465390
C	4.158457	-0.138683	-2.174971
H	2.099932	-0.643293	-2.604083
C	5.018975	0.633614	-1.399040
H	5.165372	2.117794	0.156961
H	4.559719	-0.818885	-2.925099
H	6.096044	0.554496	-1.535963
C	0.291402	2.196785	-1.594129

H	-0.749180	2.449161	-1.377568
H	0.946969	3.060323	-1.401466
H	0.370084	1.989631	-2.676676

TS_{D-E}

E = -1322.5088509au

N	1.953242	0.203539	-0.977547
C	1.615573	2.190839	0.143101
C	2.070726	3.427812	0.602641
C	1.284057	4.162992	1.476818
H	1.637576	5.130240	1.830820
C	0.052717	3.667626	1.900191
H	-0.570434	4.245206	2.580676
C	-0.384040	2.428340	1.440086
H	-1.354948	2.068240	1.776594
C	0.380497	1.657270	0.561902
C	0.217597	-2.651046	0.173255
C	1.387090	-2.212740	0.893655
C	0.971863	-1.435183	2.001553
C	-0.472144	-1.388482	1.981422
C	-0.931993	-2.170133	0.872038
Rh	0.291996	-0.390369	0.092405
C	-2.338535	-2.538783	0.540746
H	-2.593082	-2.312880	-0.504541
H	-2.492994	-3.617501	0.689410
H	-3.064662	-2.013169	1.170021
C	0.223213	-3.550809	-1.013560
H	0.546245	-4.566477	-0.737526
H	-0.777161	-3.628250	-1.456458
H	0.904593	-3.163829	-1.781239
C	2.783962	-2.540020	0.497172
H	3.071954	-3.525672	0.892052
H	2.878735	-2.565267	-0.595400
H	3.497707	-1.801939	0.881510
C	1.840423	-0.763047	3.010144
H	1.922655	-1.350189	3.937506
H	2.854878	-0.613425	2.620194
H	1.449410	0.227724	3.277339
C	-1.296164	-0.797185	3.075979
H	-1.121552	-1.338383	4.017787
H	-1.042506	0.255463	3.263172
H	-2.371117	-0.855168	2.864340
C	-0.802482	0.732051	-1.077640
C	-2.266546	0.702010	-0.977790
C	-3.045890	0.706518	-2.152543
C	-2.948060	0.584690	0.243614
C	-4.426419	0.573800	-2.101170
H	-2.561485	0.775872	-3.123918
C	-4.331779	0.503356	0.298437
H	-2.371206	0.556731	1.162645
C	-5.079728	0.486865	-0.874857
H	-4.997841	0.550183	-3.027545
H	-4.827196	0.433915	1.266630
H	-6.164299	0.404118	-0.834503
O	2.417664	1.531596	-0.716120
C	2.448714	-0.294990	-2.133063
O	2.085273	-1.398186	-2.553850
C	3.481976	0.525797	-2.871589
H	3.048195	1.468074	-3.231324
H	4.325821	0.793783	-2.225658
H	3.833353	-0.063722	-3.722495
C	-0.284873	1.473020	-2.274264
H	-0.176927	0.737849	-3.090111
H	-0.965399	2.267196	-2.609547
H	0.705610	1.904854	-2.129966
H	3.041521	3.787530	0.266217

E

E = -1322.6068475au

N	0.244964	-1.687334	0.683701
C	2.483622	-1.354089	0.147221
C	3.608614	-2.172049	0.177225
H	3.665537	-2.933535	0.953595
C	4.623072	-2.003120	-0.753915
H	5.505107	-2.640531	-0.727270
C	4.483825	-1.017162	-1.721406
H	5.261072	-0.863055	-2.468390
C	3.352141	-0.209190	-1.734876
H	3.295044	0.567090	-2.494025
C	2.312757	-0.332828	-0.800247
C	-2.489509	0.330780	-1.472801
C	-2.951144	-0.751690	-0.592098
C	-2.855659	-0.307427	0.728623
C	-2.282272	1.034094	0.686480
C	-2.203612	1.466480	-0.683022
Rh	-0.765577	-0.190703	-0.176826
C	-1.964186	2.868063	-1.120191
H	-2.836170	3.488692	-0.865284

H	-1.091025	3.313883	-0.625717
H	-1.817540	2.947224	-2.203852
C	-2.517889	0.239252	-2.956663
H	-3.553691	0.280241	-3.326443
H	-1.960558	1.053461	-3.432631
H	-2.086496	-0.709609	-3.301861
C	-3.428074	-2.060134	-1.107090
H	-4.222255	-1.907506	-1.853214
H	-2.611506	-2.613184	-1.590184
H	-3.810581	-2.700239	-0.308951
C	-3.186802	-1.034606	1.982884
H	-4.091261	-0.617515	2.450392
H	-3.330680	-2.102870	1.802438
H	-2.368844	-0.945536	2.710882
C	-2.035572	1.895329	1.871164
H	-2.959882	2.421015	2.158971
H	-1.708474	1.302282	2.733855
H	-1.265780	2.650326	1.669387
C	1.144075	0.641969	-0.817394
O	1.576075	-1.570744	1.153486
C	-0.280683	-2.919104	0.997043
O	-1.449417	-3.183789	0.732426
C	0.629102	-3.936585	1.641893
H	1.465311	-4.181662	0.974908
H	1.062494	-3.562283	2.575849
H	0.041461	-4.838251	1.834647
C	0.884926	1.111862	-2.245299
H	-0.012576	1.733580	-2.315570
H	1.709249	1.719545	-2.657126
H	0.753145	0.249560	-2.912569
C	1.369215	1.774033	0.153785
C	1.631365	1.529209	1.516228
C	1.333594	3.116898	-0.252230
C	1.814214	2.568069	2.416625
H	1.673181	0.500077	1.869419
C	1.515788	4.161353	0.653713
H	1.172189	3.365408	-1.299662
C	1.751712	3.896476	1.995680
H	2.010698	2.337568	3.463408
H	1.483043	5.190232	0.295867
H	1.897006	4.709532	2.705129

TS_{E-F}

E = -1322.5697499au

N	1.381195	1.481294	-0.873195
C	-0.658341	2.369892	0.633467
C	-0.909878	3.659595	1.132589
H	-0.184840	4.098031	1.816859
C	-2.072314	4.322336	0.775929
H	-2.272438	5.314697	1.178207
C	-2.982936	3.724588	-0.097655
H	-3.890453	4.250722	-0.388662
C	-2.718660	2.458050	-0.608372
H	-3.432036	1.989050	-1.288524
C	-1.545556	1.778124	-0.278585
C	1.638448	-2.005318	-0.687637
C	2.630139	-1.410318	0.195136
C	2.035602	-1.273165	1.457838
C	0.689306	-1.838216	1.396579
C	0.502996	-2.392424	0.100501
Rh	0.701518	-0.139029	-0.040659
C	-0.605866	-3.262954	-0.364837
H	-0.281221	-4.314118	-0.351286
H	-1.499045	-3.175918	0.262522
H	-0.910831	-3.026014	-1.392128
C	1.889260	-2.338738	-2.117317
H	2.537393	-3.224132	-2.207884
H	0.956536	-2.554286	-2.651852
H	2.386726	-1.506887	-2.634091
C	4.009089	-1.041634	-0.226997
H	4.558846	-1.937639	-0.550399
H	4.015079	-0.337060	-1.071582
H	4.577451	-0.587274	0.592996
C	2.612645	-0.646313	2.678479
H	2.717172	-1.381854	3.489584
H	3.603732	-0.217781	2.488367
H	1.965647	0.160413	3.050125
C	-0.194100	-1.978992	2.587548
H	0.192263	-2.747327	3.274267
H	-0.253066	-1.036400	3.149470
H	-1.215127	-2.258444	2.306711
C	-1.241921	0.414358	-0.875163
O	0.412097	1.704005	1.046527
C	2.685621	1.812876	-0.950956
O	3.232303	1.654311	-2.047372
C	3.347250	2.441079	0.243359
H	3.119016	1.894643	1.165580
H	4.427494	2.480883	0.065100

H	2.962688	3.460043	0.375032
C	-1.022138	0.482947	-2.381441
H	-0.656324	-0.472105	-2.787224
H	-1.963730	0.725247	-2.904582
H	-0.290036	1.255332	-2.629203
C	-2.318992	-0.547064	-0.476693
C	-2.764240	-0.586127	0.857358
C	-2.966545	-1.389577	-1.391387
C	-3.778347	-1.441880	1.260532
H	-2.296460	0.077936	1.585831
C	-3.993966	-2.241656	-0.992503
H	-2.674284	-1.379684	-2.439986
C	-4.401579	-2.279683	0.334776
H	-4.095785	-1.446807	2.302957
H	-4.479945	-2.877672	-1.731430
H	-5.206150	-2.943619	0.646707

F

E = -1322.5868863au

N	1.317169	1.578287	-0.790687
C	-1.175690	1.963637	1.017803
C	-1.693170	3.037687	1.754429
H	-1.310182	3.213992	2.758243
C	-2.642823	3.871778	1.178746
H	-3.022396	4.719845	1.748007
C	-3.098230	3.647009	-0.119541
H	-3.839788	4.306904	-0.565854
C	-2.603434	2.561892	-0.838696
H	-2.978656	2.360788	-1.843075
C	-1.656646	1.710653	-0.274322
C	1.420525	-2.017004	-0.416390
C	2.576022	-1.244552	-0.012540
C	2.394405	-0.871329	1.348988
C	1.155672	-1.460430	1.799668
C	0.584506	-2.205749	0.734698
Rh	0.723918	0.056889	0.101331
C	-0.576169	-3.127249	0.846784
H	-0.248702	-4.097153	1.250488
H	-1.350913	-2.730816	1.512680
H	-1.051738	-3.313757	-0.121570
C	1.247722	-2.671265	-1.743085
H	1.776073	-3.635741	-1.779441
H	0.190497	-2.867767	-1.960813
H	1.648764	-2.046665	-2.552544
C	3.798347	-1.003535	-0.825759
H	4.538443	-1.793919	-0.632587
H	3.585980	-1.015708	-1.902253
H	4.264104	-0.041282	-0.579629
C	3.295017	-0.006680	2.161272
H	4.113369	-0.589367	2.610472
H	3.725151	0.795100	1.545673
H	2.736145	0.472633	2.974196
C	0.571089	-1.271589	3.152269
H	-0.213588	-2.007986	3.358304
H	1.337633	-1.359911	3.932663
H	0.123425	-0.266295	3.221175
C	-1.213216	0.440990	-0.959880
O	-0.237689	1.171791	1.525699
C	2.595164	1.858221	-1.137710
O	3.478922	2.171334	-0.340224
C	2.816822	1.861150	-2.637902
H	2.183883	1.122965	-3.148454
H	2.576293	2.851104	-3.044213
H	3.875377	1.653169	-2.833390
C	-0.903032	0.636358	-2.433498
H	-0.255767	-0.157160	-2.834634
H	-1.828794	0.628243	-3.032449
H	-0.391593	1.592556	-2.583651
C	-2.140851	-0.701211	-0.693826
C	-2.892299	-0.767464	0.493445
C	-2.381736	-1.691127	-1.661686
C	-3.839942	-1.761774	0.693578
H	-2.747980	-0.005159	1.257857
C	-3.331902	-2.687831	-1.461105
H	-1.839127	-1.672318	-2.605622
C	-4.069057	-2.728826	-0.283020
H	-4.417127	-1.772003	1.617251
H	-3.504417	-3.428764	-2.240905
H	-4.823311	-3.499073	-0.131145

TS_{F-G}

E = -1322.58178au

N	-0.859357	-1.759848	-0.699163
C	1.658237	-1.547651	1.147824
C	2.401908	-2.398655	2.000361
H	2.186614	-2.367927	3.066926
C	3.272691	-3.323369	1.460896
H	3.787875	-4.018923	2.123153

C	3.480159	-3.409271	0.073943
H	4.168780	-4.146135	-0.333866
C	2.832857	-2.521578	-0.764652
H	3.040378	-2.542707	-1.834164
C	1.993853	-1.522284	-0.239424
C	-1.680941	1.858176	-0.383595
C	-2.705804	0.851663	-0.214806
C	-2.700961	0.447158	1.158428
C	-1.636060	1.155622	1.809096
C	-1.036824	2.062479	0.871146
Rh	-0.756243	-0.108565	0.196219
C	0.019009	3.056183	1.204972
H	-0.396721	3.891760	1.787508
H	0.820596	2.602826	1.803209
H	0.488940	3.473846	0.307129
C	-1.446500	2.603753	-1.649332
H	-2.229069	3.362046	-1.801901
H	-0.479473	3.118088	-1.646400
H	-1.471509	1.932202	-2.519588
C	-3.729011	0.448688	-1.219566
H	-4.642417	1.050283	-1.098754
H	-3.374778	0.593968	-2.248022
H	-4.008148	-0.606906	-1.101183
C	-3.624215	-0.549318	1.766186
H	-4.647505	-0.146489	1.809647
H	-3.640633	-1.475827	1.174031
H	-3.322278	-0.803898	2.788150
C	-1.236382	0.994506	3.232386
H	-1.871309	1.605810	3.890278
H	-1.318713	-0.051685	3.549245
H	-0.193706	1.293068	3.385890
C	1.549451	-0.418266	-1.067470
O	0.662759	-0.856300	1.594120
C	-2.023844	-2.247336	-1.191412
O	-2.939497	-2.718151	-0.510380
C	-2.098858	-2.253077	-2.710209
H	-1.782372	-1.286462	-3.127403
H	-1.436587	-3.024469	-3.122542
H	-3.129196	-2.470787	-3.013930
C	1.296042	-0.729810	-2.515691
H	0.517964	-0.082397	-2.937577
H	2.208099	-0.565423	-3.112908
H	0.961086	-1.764233	-2.631313
C	2.047000	0.941283	-0.780205
C	2.853188	1.213114	0.343406
C	1.891269	1.976388	-1.722222
C	3.446023	2.454110	0.520506
H	3.052690	0.422565	1.063424
C	2.489929	3.216317	-1.545643
H	1.296279	1.808844	-2.617597
C	3.270704	3.466314	-0.420427
H	4.072884	2.625063	1.394220
H	2.353893	3.989086	-2.301482
H	3.751163	4.433912	-0.286790

G

E = -1322.6034817au

N	-0.631672	-1.089241	1.044494
C	-3.334310	-0.948136	-1.134495
C	-3.760999	-0.420493	0.134141
C	-3.613978	1.027166	0.083153
C	-3.072804	1.370794	-1.181324
C	-2.857554	0.155477	-1.918769
Rh	-1.674565	-0.038960	-0.068158
C	3.002049	-0.134665	-0.444763
C	2.137343	-1.077467	-1.212258
H	1.230537	-1.347010	-0.650875
C	-3.986166	1.955217	1.187526
H	-3.691161	1.548677	2.163367
H	-3.499584	2.932171	1.077847
H	-5.072654	2.127973	1.216159
C	-2.678353	2.728254	-1.656000
H	-1.627748	2.748052	-1.976476
H	-3.290439	3.049733	-2.511528
H	-2.794178	3.481621	-0.867387
C	-2.248995	0.083089	-3.276328
H	-2.994531	0.267455	-4.064770
H	-1.453477	0.831280	-3.389456
H	-1.800997	-0.900419	-3.462372
C	-3.381360	-2.388248	-1.506630
H	-4.417481	-2.705006	-1.702234
H	-2.794036	-2.592564	-2.409313
H	-2.973467	-3.001248	-0.691619
C	-4.402316	-1.212419	1.218262
H	-5.433075	-1.487996	0.948501
H	-3.842985	-2.140823	1.403432
H	-4.446352	-0.645236	2.156596
C	1.092573	1.334649	0.153070

C	2.514337	0.952600	0.259457
C	0.602633	2.337642	1.070163
C	3.339220	1.676877	1.200627
C	1.435734	2.973314	1.931727
H	-0.461614	2.566756	1.008000
C	2.827601	2.642790	2.002428
H	4.383075	1.390174	1.303477
H	1.043400	3.744565	2.594448
H	3.461612	3.147723	2.727996
C	-1.045661	-1.987793	3.255377
H	-1.965293	-1.509658	3.622839
H	-0.972463	-2.978571	3.717852
H	-0.198808	-1.361390	3.554771
O	0.351703	0.841013	-0.724519
C	-1.150264	-2.130753	1.747374
O	-1.683399	-3.134099	1.258713
H	2.699451	-1.972080	-1.500615
C	4.447444	-0.432186	-0.468842
C	5.375167	0.548276	-0.847004
C	4.914696	-1.719708	-0.170207
C	6.729971	0.250114	-0.920609
H	5.018747	1.543197	-1.111457
C	6.271934	-2.006892	-0.215333
H	4.205902	-2.491065	0.129188
C	7.182904	-1.025194	-0.596888
H	7.434869	1.017813	-1.234860
H	6.620404	-3.005175	0.043075
H	8.245425	-1.256528	-0.646495
H	1.772540	-0.593696	-2.129139

TS_{G-H}

E = -1322.5955045au

N	-0.062414	-1.266883	0.098646
C	3.260575	-1.305684	-0.232858
C	2.939439	-0.452218	-1.340452
C	3.006139	0.912989	-0.869193
C	3.441373	0.909121	0.493725
C	3.562879	-0.447807	0.902592
Rh	1.487011	-0.197148	0.222157
C	-2.549476	0.494587	0.942283
C	-1.795630	-0.190317	1.940287
H	-1.034584	-0.791876	1.197014
C	2.686614	2.125046	-1.670040
H	1.830414	1.949058	-2.333431
H	2.428900	2.969219	-1.019627
H	3.540766	2.427283	-2.294359
C	3.561248	2.122726	1.351415
H	3.923524	1.873384	2.355113
H	4.262302	2.850872	0.920231
H	2.583859	2.614144	1.462876
C	3.932887	-0.929576	2.261298
H	5.021548	-1.059871	2.352831
H	3.612294	-0.226380	3.038769
H	3.464549	-1.896747	2.479087
C	3.396758	-2.784856	-0.304123
H	4.317189	-3.063752	-0.838968
H	3.443619	-3.238308	0.693206
H	2.543046	-3.220603	-0.841147
C	2.618554	-0.910022	-2.718893
H	1.896551	-1.737241	-2.681446
H	2.185096	-0.100479	-3.317874
H	3.530293	-1.254405	-3.230734
C	-0.748342	2.172722	0.416243
C	-2.117519	1.687235	0.308538
C	-0.492078	3.481639	-0.104489
C	-3.073718	2.486210	-0.387180
C	-1.456356	4.218892	-0.739156
H	0.521623	3.862241	0.017215
C	-2.768927	3.719931	-0.895488
H	-4.095159	2.116324	-0.459130
H	-1.207660	5.205786	-1.130240
H	-3.530549	4.318001	-1.390685
C	-1.183726	-3.404431	0.242107
H	-1.158664	-4.403628	-0.204297
H	-0.976970	-3.472866	1.318092
H	-2.195615	-2.987172	0.134570
O	0.211383	1.499659	0.914971
C	-0.172848	-2.504206	-0.450421
O	0.422384	-2.899821	-1.459865
H	-2.350986	-0.949212	2.499768
C	-3.745775	-0.211575	0.445155
C	-4.706882	-0.727297	1.323036
C	-3.865251	-0.483733	-0.925399
C	-5.774923	-1.472914	0.841200
H	-4.620647	-0.520623	2.389324
C	-4.919064	-1.253617	-1.401330
H	-3.095845	-0.118172	-1.604285
C	-5.879438	-1.743329	-0.520775

H	-6.524812	-1.852988	1.532843
H	-4.986300	-1.477348	-2.464436
H	-6.708063	-2.342202	-0.894988
H	-1.107530	0.411642	2.537747

H

E = -1322.6662246au

N	1.580420	1.585553	-0.328938
C	2.322601	-1.724581	-0.809361
C	2.765415	-1.566504	0.531565
C	1.655765	-1.930730	1.410901
C	0.559237	-2.359299	0.611286
C	0.941744	-2.167154	-0.758432
Rh	1.072856	-0.258089	0.206812
C	-2.243867	0.896752	-1.150462
C	-1.832933	1.031120	-2.421558
C	1.646697	-1.857506	2.895063
H	2.380337	-1.133688	3.267879
H	0.659065	-1.548810	3.258868
H	1.882981	-2.836278	3.338377
C	-0.786699	-2.738511	1.126120
H	-1.417808	-3.169630	0.340415
H	-0.701870	-3.477234	1.933993
H	-1.311209	-1.853748	1.519494
C	0.078818	-2.399621	-1.943193
H	0.249054	-3.406055	-2.354402
H	-0.983143	-2.308445	-1.684457
H	0.296826	-1.672269	-2.734560
C	3.136630	-1.516786	-2.035962
H	3.716990	-2.421142	-2.272786
H	2.503424	-1.292890	-2.902958
H	3.821601	-0.672632	-1.901173
C	4.119906	-1.124035	0.947748
H	4.417837	-0.249217	0.355461
H	4.149772	-0.851955	2.008834
H	4.854686	-1.926057	0.784258
C	-1.063395	1.719564	0.921889
C	-1.905054	1.978369	-0.188993
C	-0.727432	2.790533	1.769586
C	-2.378385	3.273825	-0.402939
C	-1.215373	4.070896	1.539890
H	-0.058948	2.578548	2.604059
C	-2.044244	4.322186	0.449109
H	-3.027409	3.451204	-1.261357
H	-0.939382	4.881245	2.214274
H	-2.428867	5.323401	0.263915
C	2.784581	3.554828	-1.101347
H	3.817502	3.914292	-1.077387
H	2.387558	3.726336	-2.110781
H	2.172386	4.137594	-0.401455
O	-0.586541	0.505668	1.141271
C	2.759930	2.067859	-0.797047
O	3.759863	1.377998	-0.998439
H	-2.084901	0.324180	-3.210860
C	-3.067449	-0.246607	-0.686824
C	-3.334512	-1.352541	-1.507422
C	-3.633534	-0.241545	0.594370
C	-4.115749	-2.411933	-1.063525
H	-2.926686	-1.389934	-2.517124
C	-4.417936	-1.298967	1.041353
H	-3.455638	0.610636	1.247345
C	-4.660488	-2.393207	0.218303
H	-4.305883	-3.254890	-1.726850
H	-4.844566	-1.262836	2.042762
H	-5.274201	-3.222123	0.567279
H	-1.220318	1.883020	-2.712199
H	0.877103	2.306744	-0.166199

H1

E = -1551.6497857au

N	-0.143214	-0.303948	1.630431
C	-2.460352	-1.824473	-0.039464
C	-3.244486	-0.663402	-0.301798
C	-2.832153	-0.126227	-1.592216
C	-1.779520	-0.933671	-2.096421
C	-1.480602	-1.946890	-1.096720
Rh	-1.162016	-0.080198	-0.192658
C	3.091389	0.301220	0.728912
C	3.497915	0.508646	1.993714
H	3.424580	1.493637	2.451996
C	-3.398936	1.105947	-2.203157
H	-2.870834	1.378688	-3.123521
H	-4.462703	0.971693	-2.444637
H	-3.312299	1.950936	-1.506901
C	-0.979329	-0.729395	-3.331459
H	-0.990162	-1.631263	-3.958991
H	-1.357317	0.106621	-3.930467
H	0.063557	-0.509216	-3.056130

C	-0.390963	-2.953913	-1.202508
H	-0.666510	-3.784382	-1.869320
H	0.527413	-2.489831	-1.588550
H	-0.142673	-3.373942	-0.219433
C	-2.622332	-2.736005	1.121627
H	-3.422894	-3.460922	0.913862
H	-1.706343	-3.305999	1.320067
H	-2.883065	-2.180315	2.029228
C	-4.306801	-0.114735	0.583306
H	-5.253376	-0.662282	0.462954
H	-3.991434	-0.178756	1.632993
H	-4.497126	0.941309	0.357754
C	1.447546	1.341305	-0.879568
C	2.628537	1.442957	-0.093520
C	1.025114	2.480715	-1.595441
C	3.319680	2.657754	-0.056497
C	1.724253	3.676594	-1.533334
H	0.113111	2.388294	-2.188797
C	2.878913	3.775056	-0.755814
H	4.235915	2.712656	0.532500
H	1.373697	4.538419	-2.102450
H	3.441558	4.706011	-0.713468
C	0.071824	-1.473139	3.758349
H	0.244429	-2.479594	3.348643
H	1.056206	-1.010910	3.914039
H	-0.446529	-1.563042	4.717233
O	0.787279	0.205914	-0.949606
C	-0.767217	-0.664972	2.786302
O	-1.926335	-0.351645	3.049604
H	0.777265	-0.721506	1.493869
H	3.930828	-0.286753	2.599045
C	3.131177	-1.061046	0.142549
C	3.400604	-1.252040	-1.218241
C	2.916380	-2.195112	0.935280
C	3.472554	-2.528440	-1.759602
H	3.557662	-0.379723	-1.851886
C	2.984508	-3.475545	0.395222
H	2.683815	-2.070718	1.994374
C	3.265477	-3.648723	-0.956041
H	3.694811	-2.651852	-2.818941
H	2.814843	-4.341062	1.034829
H	3.322226	-4.648893	-1.383159
C	-0.809443	2.812404	1.020403
O	-1.470384	2.110771	0.244698
O	0.040712	2.345189	1.885645
H	0.055058	1.323297	1.810894
C	-0.908143	4.302481	1.005754
H	-1.006744	4.690289	2.024930
H	0.029515	4.693507	0.587950
H	-1.746980	4.626228	0.385648

$TS_{H1\text{-}I}$

E = -1551.6477376au

N	-0.109207	-0.235726	1.691256
C	-2.516038	-1.773655	-0.093575
C	-3.243990	-0.588334	-0.405663
C	-2.731093	-0.066875	-1.662703
C	-1.679964	-0.926501	-2.103728
C	-1.486208	-1.945945	-1.093750
Rh	-1.154254	-0.050322	-0.199073
C	3.096962	0.330003	0.779417
C	3.471096	0.508965	2.058259
H	3.370457	1.480257	2.539261
C	-3.209006	1.184774	-2.308596
H	-4.271196	1.108199	-2.579592
H	-3.090015	2.032360	-1.619663
H	-2.641334	1.413863	-3.217373
C	-0.802103	-0.763946	-3.290454
H	-0.829872	-1.663179	-3.921180
H	-1.096984	0.094647	-3.903751
H	0.233971	-0.601083	-2.955276
C	-0.439537	-3.002618	-1.139054
H	-0.715856	-3.822735	-1.818318
H	0.520428	-2.586912	-1.477005
H	-0.268127	-3.433875	-0.144383
C	-2.786550	-2.668602	1.061035
H	-3.642815	-3.318291	0.828078
H	-1.931520	-3.319547	1.281705
H	-3.025506	-2.102321	1.969414
C	-4.333680	0.003908	0.416218
H	-5.287585	-0.521490	0.260789
H	-4.077986	-0.048958	1.482358
H	-4.484676	1.060046	0.165595
C	1.451022	1.388737	-0.809488
C	2.628103	1.485221	-0.020768
C	1.014554	2.531325	-1.507624
C	3.307691	2.705037	0.038741
C	1.701139	3.732558	-1.421885

H	0.097240	2.439667	-2.092934
C	2.854929	3.827884	-0.643246
H	4.221456	2.759215	0.631700
H	1.338679	4.603503	-1.968511
H	3.404797	4.765350	-0.581150
C	-0.068180	-1.990693	3.404284
H	0.838390	-1.629086	3.909677
H	-0.723912	-2.467264	4.138567
H	0.254469	-2.728117	2.654127
O	0.802880	0.243679	-0.894317
C	-0.784331	-0.838610	2.740135
O	-1.886614	-0.458177	3.099179
H	0.805715	-0.642899	1.491517
H	3.903743	-0.295142	2.652523
C	3.161370	-1.015148	0.155767
C	3.423366	-1.163331	-1.211899
C	2.961742	-2.175246	0.914120
C	3.495175	-2.421685	-1.793664
H	3.571553	-0.271197	-1.819462
C	3.029590	-3.438156	0.334007
H	2.741035	-2.084855	1.979059
C	3.296923	-3.567851	-1.024817
H	3.709571	-2.510748	-2.858025
H	2.868845	-4.323868	0.948149
H	3.351746	-4.553973	-1.483659
C	-0.829263	2.724628	1.112088
O	-1.456400	2.063280	0.239106
O	-0.036423	2.233420	1.967172
H	-0.027775	0.986016	1.854406
C	-1.057248	4.209559	1.165956
H	-1.802965	4.428210	1.940853
H	-0.127840	4.717154	1.442136
H	-1.426632	4.581585	0.206053

I

E = -1342.5431552au

C	-3.439983	-0.470541	0.942088
C	-3.301425	0.876684	0.475021
C	-3.035807	0.820872	-0.932702
C	-3.117164	-0.572555	-1.348708
C	-3.383759	-1.365903	-0.204206
Rh	-1.507749	-0.307395	0.077854
C	2.635976	0.340713	1.106346
C	2.177756	-0.287426	2.202456
H	1.284802	0.049819	2.718515
C	-2.816905	1.953804	-1.872954
H	-1.873508	1.835391	-2.423399
H	-3.631460	2.010125	-2.609586
H	-2.768318	2.915512	-1.351480
C	-2.880876	-1.033238	-2.742535
H	-3.689784	-0.700604	-3.408665
H	-1.936955	-0.625536	-3.127713
H	-2.817074	-2.124890	-2.805172
C	-3.499543	-2.846333	-0.121947
H	-4.508931	-3.143423	0.195763
H	-3.295088	-3.320791	-1.087959
H	-2.781973	-3.253264	0.602590
C	-3.650092	-0.894150	2.351686
H	-4.718859	-1.041613	2.567707
H	-3.132418	-1.839864	2.556155
H	-3.259963	-0.145548	3.051030
C	-3.291167	2.075425	1.356737
H	-4.151190	2.064900	2.038649
H	-2.368430	2.092263	1.955758
H	-3.332082	3.005606	0.778908
C	0.570262	1.733868	0.579967
C	1.979655	1.532568	0.529000
C	0.052004	2.908594	-0.003580
C	2.772759	2.518741	-0.074065
C	0.860378	3.863303	-0.596569
H	-1.025868	3.057351	0.053735
C	2.239602	3.671727	-0.632206
H	3.852317	2.370056	-0.097552
H	0.417064	4.763749	-1.022332
H	2.894625	4.414082	-1.084862
O	-0.243622	0.887846	1.194825
C	0.458215	-1.885061	-0.267453
O	-0.320694	-2.031983	0.722329
O	0.235089	-0.951792	-1.099003
C	1.622037	-2.808557	-0.441686
H	1.959587	-2.821477	-1.482586
H	2.455003	-2.456181	0.181351
H	1.352354	-3.816758	-0.110422
H	2.670863	-1.184450	2.577525
C	3.844003	-0.187200	0.421128
C	3.889431	-0.285745	-0.976566
C	4.938000	-0.662900	1.152831
C	4.979459	-0.863438	-1.614818

H	3.038947	0.071489	-1.556885
C	6.031991	-1.237403	0.514291
H	4.927038	-0.563433	2.238053
C	6.056222	-1.343122	-0.872423
H	4.987750	-0.942736	-2.701267
H	6.875111	-1.594404	1.104511
H	6.912786	-1.791510	-1.373796

I1

E = -1571.5142467au

C	-3.265925	-0.567877	0.661631
C	-3.174375	0.824618	0.379665
C	-2.786812	0.974073	-1.007998
C	-2.777327	-0.346501	-1.609794
C	-3.037744	-1.292621	-0.579072
Rh	-1.268316	-0.132954	-0.053696
C	2.632788	0.527796	1.353664
C	2.589015	0.216887	2.657020
H	2.097143	0.878953	3.367165
C	-2.520308	2.232902	-1.754244
H	-1.556215	2.165007	-2.276887
H	-3.305359	2.421223	-2.500911
H	-2.467469	3.099717	-1.086117
C	-2.515431	-0.606520	-3.050713
H	-3.340156	-0.207246	-3.658601
H	-1.590129	-0.123137	-3.393845
H	-2.429332	-1.677257	-3.265534
C	-3.069271	-2.775166	-0.695710
H	-4.073093	-3.159852	-0.466291
H	-2.799149	-3.112001	-1.702076
H	-2.364585	-3.236665	0.009146
C	-3.604275	-1.172049	1.980112
H	-4.693133	-1.217200	2.131201
H	-3.219829	-2.196523	2.061059
H	-3.173463	-0.591078	2.805265
C	-3.316639	1.905423	1.391206
H	-4.207934	1.740879	2.010277
H	-2.433326	1.924890	2.047268
H	-3.406906	2.891184	0.921137
C	0.616288	2.020717	0.970803
C	2.011117	1.811134	0.924685
C	0.114235	3.278220	0.597220
C	2.836865	2.861061	0.514455
C	0.949959	4.305650	0.192538
H	-0.965187	3.424321	0.653234
C	2.326743	4.099617	0.147809
H	3.913389	2.686702	0.485275
H	0.528679	5.271087	-0.085824
H	2.997519	4.897214	-0.166103
O	-0.254416	1.084788	1.376486
C	0.669372	-0.422816	-2.340835
O	0.285343	0.316535	-1.334317
O	1.029036	0.067033	-3.404272
C	0.721684	-1.922685	-2.126011
H	0.932719	-2.424900	-3.075460
H	1.527010	-2.145340	-1.412596
H	-0.201163	-2.317033	-1.682651
C	0.051219	-1.922765	2.111954
O	-0.159359	-1.857692	0.895485
O	-0.065687	-0.920915	2.934947
H	-0.088217	-0.047502	2.386026
C	0.489873	-3.200375	2.752262
H	1.580600	-3.167184	2.872174
H	0.051943	-3.302103	3.750335
H	0.235378	-4.056368	2.122653
H	3.026269	-0.687827	3.077279
C	3.320882	-0.306093	0.337327
C	3.332077	0.075245	-1.010158
C	3.983747	-1.494683	0.681991
C	3.972674	-0.697708	-1.973833
H	2.803746	0.974753	-1.317060
C	4.626009	-2.265204	-0.276454
H	4.019510	-1.819470	1.721224
C	4.624588	-1.870431	-1.613315
H	3.927484	-0.384065	-3.015280
H	5.136808	-3.179803	0.023031
H	5.125188	-2.477526	-2.366065

$TS_{I1\text{-}A}$

E = -1571.5169503au

C	2.867887	-0.499539	-1.433047
C	2.813793	0.909550	-1.243776
C	3.000935	1.182227	0.166554
C	3.264596	-0.074205	0.826195
C	3.150464	-1.113970	-0.146488
Rh	1.277989	-0.064066	-0.032527
C	-3.284484	0.805393	-0.944856
C	-4.066210	0.963750	-2.022543

H	-4.048683	1.891716	-2.591257
C	3.065457	2.504044	0.847945
H	2.320389	2.565463	1.653325
H	4.057950	2.658621	1.295200
H	2.881506	3.332205	0.154689
C	3.574381	-0.191593	2.275214
H	4.554955	0.257942	2.488813
H	2.824473	0.339900	2.875643
H	3.604010	-1.233168	2.611893
C	3.262035	-2.580745	0.072611
H	4.075407	-3.002867	-0.533864
H	3.460495	-2.821856	1.122237
H	2.325848	-3.081226	-0.214112
C	2.693175	-1.224591	-2.721162
H	3.644975	-1.301461	-3.267341
H	2.328810	-2.244923	-2.549132
H	1.971588	-0.715820	-3.372238
C	2.488996	1.897478	-2.307626
H	3.073364	1.696991	-3.214619
H	1.421016	1.840027	-2.564883
H	2.697508	2.924190	-1.987288
C	-1.067545	1.984142	-0.521706
C	-2.474321	1.962339	-0.479500
C	-0.393133	3.125639	-0.074805
C	-3.145778	3.094037	-0.005395
C	-1.078185	4.229222	0.407633
H	0.694049	3.123185	-0.122373
C	-2.469137	4.221048	0.442151
H	-4.234991	3.062714	0.017724
H	-0.523331	5.100655	0.753140
H	-3.021495	5.080051	0.817992
O	-0.341682	0.977967	-1.051562
C	-0.062210	-0.419064	2.701193
O	0.244788	0.360166	1.697448
O	-0.701036	-0.005200	3.658060
C	0.389138	-1.865174	2.639199
H	0.074246	-2.383646	3.550116
H	-0.041616	-2.358333	1.759295
H	1.482107	-1.934799	2.549339
C	-0.617186	-1.980719	-1.503647
O	0.118646	-1.880331	-0.491224
O	-1.023358	-1.001224	-2.213627
H	-0.807123	0.003760	-1.680986
C	-0.996017	-3.356816	-1.967271
H	-1.081144	-4.033063	-1.111872
H	-1.932150	-3.331087	-2.531670
H	-0.204550	-3.736862	-2.627927
H	-4.754224	0.192274	-2.364644
C	-3.282679	-0.436120	-0.140396
C	-2.877517	-0.417251	1.198153
C	-3.715027	-1.654085	-0.686211
C	-2.928381	-1.572422	1.974596
H	-2.507456	0.505558	1.644091
C	-3.763258	-2.805498	0.085374
H	-3.983879	-1.698970	-1.741755
C	-3.372022	-2.769154	1.423793
H	-2.599234	-1.518337	3.011547
H	-4.099638	-3.741315	-0.361786
H	-3.408120	-3.673109	2.030581

2a

E = -615.4451672au

C	2.232347	0.591901	-0.440922
C	3.378973	-0.202628	-0.488666
C	1.106237	0.166432	0.288619
C	3.421365	-1.411027	0.188317
C	1.168880	-1.071994	0.939792
C	2.312518	-1.854958	0.908170
H	4.325918	-2.016043	0.149290
H	0.290224	-1.407755	1.491031
H	2.340033	-2.805427	1.436952
O	2.264670	1.750145	-1.139675
H	1.391078	2.173802	-1.067763
H	4.225368	0.157145	-1.070201
C	-0.123975	0.990238	0.361438
C	-0.071179	2.303489	0.653341
H	0.862811	2.788044	0.936552
H	-0.966765	2.922476	0.655393
C	-1.420414	0.325311	0.094191
C	-1.522465	-0.675972	-0.879262
C	-2.573245	0.692970	0.797562
C	-2.746397	-1.269818	-1.160458
H	-0.629775	-0.979367	-1.425439
C	-3.795830	0.093075	0.522533
H	-2.497748	1.440097	1.587151
C	-3.887467	-0.887296	-0.461089
H	-2.809873	-2.037622	-1.929854
H	-4.679774	0.384678	1.087668

H	-4.844948	-1.359529	-0.674767

TS_{G-J}

E = -1322.5781049au

N	-0.680485	-0.988579	1.231449
C	-3.316428	-1.041107	-1.048323
C	-3.731734	-0.286871	0.106053
C	-3.469538	1.118994	-0.168782
C	-2.878607	1.213131	-1.455057
C	-2.749389	-0.115279	-1.985489
Rh	-1.620855	-0.094338	-0.079904
C	2.909288	-0.395309	-0.116803
C	1.978670	-1.272035	-0.704800
H	1.196043	-0.343973	-1.163519
C	-3.783848	2.237833	0.762900
H	-3.585133	1.953021	1.803985
H	-3.178629	3.126296	0.546618
H	-4.842509	2.530682	0.695354
C	-2.352265	2.437550	-2.122470
H	-1.296802	2.304878	-2.398957
H	-2.911848	2.671928	-3.039850
H	-2.413324	3.314449	-1.466346
C	-2.135790	-0.449249	-3.300583
H	-2.854899	-0.317832	-4.123417
H	-1.273387	0.196399	-3.511241
H	-1.784304	-1.487602	-3.327426
C	-3.454290	-2.517248	-1.185287
H	-4.509667	-2.800344	-1.318223
H	-2.896467	-2.896538	-2.049442
H	-3.069013	-3.017131	-0.286344
C	-4.459601	-0.851483	1.274862
H	-5.494319	-1.109369	1.002669
H	-3.970501	-1.768558	1.637100
H	-4.505423	-0.135795	2.105029
C	1.200084	1.364539	0.005784
C	2.417790	0.794991	0.518648
C	0.852027	2.668687	0.419871
C	3.162466	1.522015	1.474070
C	1.585232	3.325760	1.382921
H	-0.058655	3.096175	0.001346
C	2.747639	2.752904	1.927836
H	4.065289	1.066226	1.879747
H	1.252424	4.302634	1.732470
H	3.310776	3.276931	2.696703
C	-1.273607	-1.351970	3.547803
H	-0.313729	-0.884854	3.793911
H	-2.053237	-0.588820	3.688457
H	-1.479753	-2.190392	4.221757
O	0.454111	0.738779	-0.867179
C	-1.314050	-1.820483	2.105795
O	-1.903154	-2.861652	1.798350
H	1.125620	-1.566075	-0.071385
C	4.348893	-0.599022	-0.323680
C	5.231746	0.470989	-0.534710
C	4.860436	-1.905671	-0.341082
C	6.581322	0.237750	-0.761335
H	4.843173	1.487703	-0.551918
C	6.212597	-2.135522	-0.549615
H	4.186163	-2.740235	-0.155403
C	7.075335	-1.064011	-0.765548
H	7.251352	1.076106	-0.942692
H	6.596078	-3.154085	-0.542738
H	8.135059	-1.244094	-0.938636
H	2.357539	-2.048779	-1.369341

J

E = -707.1498705au

Rh	0.102976	0.002836	-0.632701
C	-0.619786	0.700437	1.269718
C	-1.568099	1.149533	0.270153
C	-2.187354	0.009260	-0.317743
C	-0.625928	-0.730561	1.252664
C	-1.581231	-1.149376	0.245548
N	1.834249	0.008152	-1.066798
C	2.991637	0.004107	-0.320502
C	4.264363	0.010230	-1.128598
H	4.295413	-0.866331	-1.787737
H	4.294286	0.895465	-1.776105
H	5.133948	0.006400	-0.464317
O	2.995677	-0.004296	0.909452
C	-1.886900	-2.563872	-0.101761
H	-2.610794	-2.996180	0.605030
H	-2.314022	-2.648392	-1.107789
H	-0.984210	-3.186019	-0.073432
C	0.190485	-1.598769	2.144012
H	-0.179264	-1.553304	3.179608
H	0.161105	-2.647340	1.825896
H	1.239577	-1.271429	2.139276

C	0.202799	1.541325	2.181348
H	1.250919	1.211295	2.163612
H	0.175017	2.598259	1.892053
H	-0.163758	1.468353	3.216514
C	-1.866662	2.572655	-0.046874
H	-2.287008	2.681804	-1.053426
H	-2.595246	2.989913	0.664348
H	-0.963138	3.192179	0.003098
C	-3.215143	0.032198	-1.397093
H	-4.227656	0.162409	-0.987567
H	-3.040650	0.850146	-2.107195
H	-3.212697	-0.900536	-1.973582
C	0.682212	-3.242584	-0.065803
H	0.684483	-3.796354	-1.011600
H	1.658794	-2.743821	0.043189
H	0.572129	-3.972622	0.745636
C	3.134724	0.339690	-0.011298
O	2.102156	-0.447993	0.016038
O	3.126381	1.566890	-0.056438
H	1.349662	2.110230	-0.031198
C	4.444143	-0.424892	0.016388
H	5.290400	0.267558	0.010760
H	4.489346	-1.058779	0.910187
H	4.505897	-1.090211	-0.853441

K

E = -936.1744781au

Rh	0.050819	-0.061752	-0.010811
C	-1.951600	-0.581037	-0.671730
C	-0.985522	-1.560386	-1.152458
C	-0.410279	-2.230388	-0.031338
C	-1.908363	-0.601239	0.748375
C	-0.914287	-1.593471	1.141376
N	0.351517	1.866496	-0.009328
C	-0.538749	2.893564	0.017526
C	0.077562	4.276699	-0.027390
H	0.566072	4.438810	-0.997049
H	-0.699766	5.032884	0.113125
H	0.849547	4.390486	0.743777
O	-1.761057	2.747974	0.062830
C	-0.482750	-1.906321	2.528500
H	-1.059038	-2.748601	2.939503
H	0.579538	-2.179407	2.548451
H	-0.619202	-1.048224	3.196096
C	-2.753377	0.219425	1.653722
H	-3.795086	-0.133374	1.628451
H	-2.408248	0.165276	2.692402
H	-2.731801	1.269047	1.332018
C	-2.855416	0.255209	-1.504256
H	-3.891694	-0.105336	-1.423833
H	-2.820285	1.298198	-1.163073
H	-2.573962	0.224726	-2.563021
C	-0.657928	-1.822196	-2.578039
H	-1.354364	-2.554645	-3.012629
H	-0.722074	-0.904948	-3.174930
H	0.360117	-2.214934	-2.681938

$TS_{F\text{-}L}$

E = -1322.5542311au

N	2.278155	0.279020	-1.583670
C	2.364570	-1.550142	0.670912
C	1.742114	-0.810846	1.726749
C	0.358660	-1.235666	1.825306
C	0.126809	-2.185084	0.788407
C	1.340554	-2.304133	0.017375
Rh	0.704732	-0.160069	-0.082588
C	-1.394386	0.516754	-0.828029
C	-0.469322	0.383922	-1.966183
H	-0.438319	1.298859	-2.575069
C	-0.600317	-0.769068	2.864974
H	-0.629527	0.328949	2.907993
H	-1.616735	-1.122223	2.655289
H	-0.316110	-1.132907	3.862771
C	-1.086476	-3.012891	0.571375
H	-0.888206	-4.044917	0.896697
H	-1.950667	-2.643748	1.133108
H	-1.376967	-3.056336	-0.486126
C	1.537202	-3.142196	-1.196204
H	2.060102	-4.081332	-0.963295
H	0.578138	-3.400427	-1.662997
H	2.135084	-2.593197	-1.935557
C	3.811204	-1.585176	0.348567
H	4.282127	-2.429014	0.876459
H	3.975818	-1.725823	-0.726044
H	4.306351	-0.658554	0.653385
C	2.417829	0.167348	2.618275
H	3.132720	-0.344531	3.278931
H	2.955571	0.903968	2.005515

H	1.694045	0.701236	3.243160
C	-0.408403	2.509229	0.241287
C	-1.566698	1.857967	-0.257347
C	-0.498894	3.877001	0.593790
C	-2.791609	2.549697	-0.296321
C	-1.708972	4.534207	0.522159
H	0.405268	4.368593	0.947774
C	-2.869712	3.875942	0.083988
H	-3.677420	2.039915	-0.676444
H	-1.764303	5.582180	0.816602
H	-3.816401	4.408876	0.022777
C	4.277989	1.244019	-2.262712
H	5.223235	0.782640	-1.947939
H	3.964408	0.820265	-3.221381
H	4.445704	2.321971	-2.373009
O	0.696315	1.853567	0.432857
C	3.262362	1.047153	-1.119013
O	3.535188	1.513899	-0.009922
H	0.772256	0.472561	-1.825178
H	-0.581218	-0.512510	-2.580391
C	-2.524929	-0.422390	-0.681301
C	-3.284611	-0.402427	0.502426
C	-2.919315	-1.313487	-1.690016
C	-4.375743	-1.240346	0.674495
H	-2.999698	0.291164	1.292728
C	-4.016209	-2.152613	-1.520066
H	-2.389297	-1.333540	-2.640267
C	-4.746963	-2.124655	-0.337639
H	-4.944318	-1.201893	1.602411
H	-4.307085	-2.823647	-2.326680
H	-5.607001	-2.779062	-0.208110

L

E = -1322.6751961au

N	1.906087	1.484030	-0.414982
C	2.569941	-1.395495	0.436031
C	1.894820	-1.155622	1.679689
C	0.590907	-1.789497	1.610116
C	0.455037	-2.357699	0.317700
C	1.661801	-2.069437	-0.435485
Rh	0.764059	-0.127142	0.162573
C	-1.350217	0.533937	-0.912409
C	-0.321547	0.348382	-1.812257
H	0.276194	1.185674	-2.155561
C	-0.394176	-1.798792	2.725063
H	-1.365726	-2.194410	2.406514
H	-0.034532	-2.416188	3.560975
H	-0.553285	-0.779806	3.104338
C	-0.677204	-3.189286	-0.164618
H	-0.448795	-4.254224	-0.010191
H	-1.608312	-2.962882	0.366553
H	-0.868272	-3.049718	-1.234934
C	1.980536	-2.495916	-1.826909
H	2.751132	-3.280500	-1.830789
H	1.098954	-2.898870	-2.339422
H	2.355092	-1.635705	-2.398911
C	3.962423	-1.004674	0.099182
H	4.649578	-1.829992	0.336794
H	4.047753	-0.765103	-0.965164
H	4.281606	-0.124547	0.669860
C	2.433649	-0.451008	2.872974
H	2.736723	-1.164914	3.652979
H	3.307653	0.157682	2.614384
H	1.677011	0.219243	3.299927
C	-0.848133	2.171103	0.918169
C	-1.572983	1.851033	-0.249017
C	-1.071037	3.425969	1.518322
C	-2.538093	2.729807	-0.740206
C	-2.015650	4.297820	0.999967
H	-0.495714	3.675316	2.409180
C	-2.760110	3.958872	-0.131159
H	-3.110495	2.443392	-1.624583
H	-2.176370	5.260394	1.485528
H	-3.498047	4.648320	-0.536403
C	3.545835	2.813151	-1.618969
H	3.493617	3.165233	-2.655083
H	3.246190	3.625193	-0.946161
H	4.594557	2.559108	-1.416153
O	-0.019016	1.301678	1.459623
C	2.706034	1.553072	-1.484436
O	2.818602	0.659822	-2.336151
H	1.864621	2.283390	0.210280
H	-0.253827	-0.560971	-2.411484
C	-2.441794	-0.455983	-0.751225
C	-3.108706	-0.564663	0.477181
C	-2.869177	-1.255924	-1.816744
C	-4.141261	-1.477476	0.645007
H	-2.796010	0.074003	1.303633

C	-3.916470	-2.157601	-1.654425
H	-2.394416	-1.148611	-2.791857
C	-4.548908	-2.278226	-0.421594
H	-4.640114	-1.558113	1.609837
H	-4.244248	-2.761800	-2.498957
H	-5.367547	-2.984514	-0.293507

TS_{E-M}

E = -1322.5338625au

N	0.550322	-1.885321	0.239260
C	2.597140	-1.374531	-0.684442
C	3.881922	-1.903436	-0.776164
H	3.984294	-2.985533	-0.836081
C	4.989955	-1.066687	-0.758352
H	5.989981	-1.491649	-0.826775
C	4.810595	0.305037	-0.618421
H	5.668682	0.973283	-0.578125
C	3.524456	0.826505	-0.547398
H	3.389835	1.905350	-0.478524
C	2.385286	0.014085	-0.608230
C	-2.926435	-1.231598	-0.552818
C	-2.526353	-1.173609	0.815183
C	-2.301653	0.209921	1.182353
C	-2.527745	0.993156	0.018611
C	-2.870556	0.106363	-1.064448
Rh	-0.810143	-0.493104	-0.471493
C	-3.256023	0.526588	-2.442766
H	-4.334154	0.736019	-2.504535
H	-2.733402	1.440937	-2.750579
H	-3.028867	-0.251950	-3.182409
C	-3.346439	-2.462691	-1.280300
H	-4.422331	-2.657578	-1.150894
H	-3.151807	-2.384228	-2.357051
H	-2.804866	-3.342577	-0.911256
C	-2.465390	-2.363817	1.708631
H	-3.470202	-2.788542	1.849918
H	-1.826852	-3.138905	1.264011
H	-2.031126	-2.121358	2.680274
C	-1.980124	0.719270	2.544247
H	-2.893153	0.870130	3.139364
H	-1.317974	0.024929	3.077120
H	-1.456786	1.682214	2.486843
C	-2.480253	2.476721	-0.085658
H	-3.490808	2.903034	0.002694
H	-1.857888	2.924643	0.698841
H	-2.072184	2.803523	-1.052111
O	1.565617	-2.281612	-0.669801
C	0.928234	-1.976083	1.546773
O	0.290518	-1.400844	2.429691
C	2.078599	-2.885868	1.906959
H	2.211841	-3.697558	1.185667
H	3.015422	-2.316539	1.957124
H	1.879474	-3.289039	2.904839
C	0.883580	1.983068	-0.119018
C	0.963361	2.056993	1.280424
C	0.727062	3.167274	-0.845067
C	0.856386	3.280006	1.926900
H	1.086044	1.132558	1.850386
C	0.626866	4.395835	-0.194034
H	0.710952	3.128999	-1.934939
C	0.685470	4.455781	1.192426
H	0.909521	3.319532	3.014191
H	0.510953	5.308278	-0.777443
H	0.609575	5.414399	1.703086
C	1.051826	0.671020	-0.793189
C	0.413697	0.384164	-2.050142
H	-0.394821	-1.019732	-1.939967
H	-0.254059	1.131278	-2.485885
H	0.989017	-0.168132	-2.796894

M

E = -1322.5953236au

N	0.563823	-1.662579	0.621952
C	2.562815	-1.482527	-0.504334
C	3.819303	-2.078582	-0.628539
H	3.897823	-3.140954	-0.402427
C	4.922253	-1.329432	-1.004306
H	5.896863	-1.806835	-1.091910
C	4.778773	0.034977	-1.242200
H	5.637207	0.642881	-1.521162
C	3.525147	0.617149	-1.123334
H	3.406146	1.683217	-1.321808
C	2.384278	-0.117586	-0.771261
C	-2.933512	-1.171151	-0.690097
C	-2.629012	-1.038087	0.698157
C	-2.424095	0.369739	0.996948
C	-2.500511	1.071906	-0.215913
C	-2.759505	0.119351	-1.284289

Rh	-0.790115	-0.544034	-0.504770
C	-3.063990	0.471332	-2.701681
H	-4.142065	0.641128	-2.842175
H	-2.551241	1.388824	-3.015790
H	-2.761218	-0.327084	-3.390588
C	-3.376985	-2.414089	-1.385256
H	-4.468251	-2.532782	-1.310478
H	-3.117052	-2.396977	-2.450299
H	-2.916153	-3.307946	-0.949309
C	-2.697744	-2.119628	1.719304
H	-3.701255	-2.154091	2.170575
H	-2.498530	-3.102977	1.276253
H	-1.959530	-1.948380	2.511991
C	-2.265604	0.933273	2.364878
H	-3.224868	0.906183	2.904387
H	-1.531915	0.350097	2.931227
H	-1.928438	1.976209	2.338288
C	-2.386015	2.543655	-0.402213
H	-3.381778	2.999576	-0.508838
H	-1.880874	3.022719	0.444376
H	-1.816007	2.802881	-1.304199
O	1.558948	-2.325658	-0.124111
C	0.791455	-1.696088	1.954271
O	0.074012	-1.075454	2.748057
C	1.951483	-2.531763	2.451256
H	1.941808	-3.541286	2.025893
H	2.908632	-2.071392	2.172413
H	1.883695	-2.579160	3.541473
C	1.005376	1.882827	-0.043294
C	1.034921	1.857506	1.357174
C	0.965819	3.123346	-0.690139
C	0.993425	3.042224	2.080968
H	1.038609	0.902021	1.883316
C	0.939897	4.310116	0.037677
H	0.978159	3.157775	-1.780402
C	0.947534	4.273291	1.426855
H	0.996163	3.001528	3.169313
H	0.917168	5.264811	-0.486101
H	0.924834	5.198277	2.000952
H	-0.430201	-1.666307	-1.533779
C	1.080959	0.627701	-0.847892
C	0.341236	0.502869	-2.036448
H	0.695904	-0.157464	-2.825760
H	-0.315077	1.310016	-2.363770

$TS_{M\text{-}N}$

E = -1322.573965au

N	0.191455	-2.156518	-0.133729
C	2.425523	-1.752377	-0.497376
C	3.549736	-2.535487	-0.268878
H	3.468108	-3.608290	-0.435584
C	4.740527	-1.950389	0.142931
H	5.621670	-2.565303	0.316028
C	4.781218	-0.576096	0.336285
H	5.701251	-0.091866	0.658995
C	3.650160	0.196794	0.100732
H	3.723047	1.274638	0.225946
C	2.434635	-0.355913	-0.333139
C	-2.829864	0.391907	-1.003904
C	-2.991605	-0.599592	0.004539
C	-2.561107	-0.030981	1.278828
C	-2.086298	1.259649	1.044853
C	-2.146896	1.496018	-0.390040
Rh	-0.801040	-0.271693	-0.380887
C	-1.904285	2.816623	-1.037637
H	-2.801564	3.448979	-0.953352
H	-1.071998	3.359451	-0.574084
H	-1.679814	2.716741	-2.107555
C	-3.292886	0.324764	-2.420463
H	-4.274702	0.807592	-2.542940
H	-2.595311	0.828682	-3.101499
H	-3.389820	-0.711664	-2.765904
C	-3.732699	-1.887120	-0.131803
H	-4.772124	-1.769138	0.212233
H	-3.768573	-2.222403	-1.175985
H	-3.259189	-2.676241	0.460843
C	-2.715393	-0.711101	2.594170
H	-3.779695	-0.778871	2.868269
H	-2.312712	-1.729133	2.553823
H	-2.202645	-0.166028	3.395384
C	-1.674911	2.262908	2.063798
H	-2.546663	2.832686	2.421573
H	-1.207864	1.795474	2.940408
H	-0.958271	2.987383	1.660521
O	1.309045	-2.417837	-0.956033
C	-0.208060	-3.226217	0.622645
O	-1.246221	-3.177302	1.272508
C	0.687017	-4.440865	0.636794

H	0.866527	-4.823118	-0.374319
H	1.664225	-4.198820	1.073017
H	0.199747	-5.205835	1.247017
C	1.396625	1.922512	-0.170293
C	1.495352	2.150115	1.209266
C	1.506256	3.024005	-1.025308
C	1.679207	3.429967	1.714153
H	1.421938	1.297236	1.886329
C	1.678796	4.311166	-0.521904
H	1.475766	2.868195	-2.103339
C	1.764423	4.520856	0.849755
H	1.746699	3.579383	2.791197
H	1.761299	5.151353	-1.210025
H	1.906901	5.524873	1.245863
H	-0.791712	-1.664621	-1.174062
C	1.294670	0.535165	-0.708273
C	0.572785	0.295427	-1.907681
H	0.847122	-0.546870	-2.540737
H	0.134824	1.138015	-2.446136

N

E = -1322.6019967au

N	-0.568953	-2.129323	-0.320710
C	1.680791	-2.450766	0.178004
C	2.527694	-3.528874	0.438549
H	2.097350	-4.416827	0.897861
C	3.870927	-3.456639	0.113252
H	4.527688	-4.298857	0.322378
C	4.357859	-2.305603	-0.501797
H	5.406198	-2.232721	-0.785305
C	3.500913	-1.245844	-0.750250
H	3.891806	-0.339825	-1.213339
C	2.136403	-1.264031	-0.408555
C	-2.607189	1.274744	-0.867287
C	-2.980288	0.477982	0.237136
C	-2.199211	0.885064	1.400028
C	-1.326139	1.903589	0.991998
C	-1.508257	2.098146	-0.436589
Rh	-0.771079	0.039618	-0.305684
C	-0.923876	3.213052	-1.235759
H	-1.556208	4.111696	-1.166898
H	0.079798	3.488040	-0.889932
H	-0.851231	2.952187	-2.300538
C	-3.221429	1.255824	-2.225752
H	-4.007131	2.020893	-2.334345
H	-2.473553	1.443140	-3.007799
H	-3.677576	0.280847	-2.441612
C	-4.151205	-0.446817	0.260594
H	-5.088792	0.129093	0.269643
H	-4.180348	-1.110687	-0.613060
H	-4.160566	-1.081815	1.155925
C	-2.390197	0.403529	2.799544
H	-3.090381	1.042401	3.360335
H	-2.801258	-0.613762	2.835203
H	-1.443360	0.392552	3.355447
C	-0.424123	2.702905	1.864350
H	-0.931775	3.612045	2.222662
H	-0.103257	2.134676	2.747751
H	0.484684	3.019929	1.338991
O	0.379426	-2.673410	0.588169
C	-1.859754	-2.719116	-0.072443
O	-2.606612	-2.873208	-1.007128
C	-2.134776	-3.087680	1.347989
H	-1.602448	-4.017703	1.584767
H	-1.764453	-2.323967	2.040283
H	-3.209498	-3.248463	1.468340
C	2.047173	1.197369	-0.196196
C	2.480386	1.237185	1.138309
C	2.362280	2.289368	-1.012722
C	3.181236	2.324603	1.639032
H	2.244522	0.390362	1.785403
C	3.055059	3.389025	-0.509885
H	2.074811	2.272722	-2.063861
C	3.468790	3.413896	0.817334
H	3.500303	2.326967	2.680699
H	3.287514	4.224294	-1.169765
H	4.017367	4.269480	1.207668
C	1.344528	-0.015631	-0.703224
C	0.560362	0.020265	-1.910345
H	0.543911	-0.869504	-2.549927
H	0.480215	0.945861	-2.485845
H	-0.283349	-2.400924	-1.270589

TS_{N-O}

E = -1322.5832337au

N	2.000422	1.807613	0.283338
C	2.168771	-2.017539	-0.001040
C	1.572033	-1.843155	1.325691

C	0.234597	-2.240713	1.273783
C	-0.059215	-2.543046	-0.124811
C	1.190971	-2.524290	-0.869946
Rh	0.463745	-0.491973	-0.255402
C	-1.286447	0.695096	-0.698475
C	-0.601071	0.238588	-1.879940
H	-0.016848	0.945367	-2.471081
H	1.803642	2.411807	1.083555
C	-0.723160	-2.389670	2.402524
H	-1.745345	-2.122846	2.104740
H	-0.754588	-3.430478	2.761723
H	-0.450418	-1.756798	3.257143
C	-1.333174	-3.150255	-0.602552
H	-1.336795	-4.233545	-0.403844
H	-2.207672	-2.715621	-0.101229
H	-1.470595	-3.013089	-1.682680
C	1.379060	-2.946122	-2.286247
H	1.536208	-4.033185	-2.368635
H	0.506394	-2.695324	-2.902920
H	2.248529	-2.450876	-2.736208
C	3.606174	-1.805188	-0.337037
H	4.143940	-2.764106	-0.394991
H	3.731926	-1.291257	-1.298464
H	4.117359	-1.199647	0.421988
C	2.323962	-1.403458	2.534772
H	2.968217	-2.206879	2.924322
H	2.982543	-0.551121	2.318801
H	1.647474	-1.099920	3.343214
C	0.055504	2.840316	-0.388060
C	-1.150101	2.122746	-0.294651
C	0.161016	4.190739	-0.074231
C	-2.257507	2.871847	0.142841
C	-0.953790	4.894555	0.361831
H	1.130430	4.673318	-0.199780
C	-2.165279	4.218728	0.468098
H	-3.225330	2.380082	0.213378
H	-0.879559	5.953271	0.601610
H	-3.058833	4.749233	0.793776
C	4.240694	1.658233	1.172397
H	3.702010	1.615661	2.126860
H	4.950785	0.826002	1.119771
H	4.825213	2.586459	1.141480
O	1.211367	2.204318	-0.826140
C	3.340865	1.614096	-0.038974
O	3.730028	1.393452	-1.162030
H	-1.047613	-0.567870	-2.467350
C	-2.559603	0.038415	-0.284878
C	-3.474490	-0.448892	-1.224221
C	-2.897559	-0.076366	1.071850
C	-4.663122	-1.057279	-0.826403
H	-3.255064	-0.338656	-2.285916
C	-4.086335	-0.671034	1.472858
H	-2.195437	0.305522	1.815726
C	-4.975134	-1.174038	0.523132
H	-5.354864	-1.431339	-1.580372
H	-4.318635	-0.749652	2.534757
H	-5.905660	-1.645050	0.835840

O

E = -1322.6034672au

N	2.577935	1.020427	0.647338
C	1.367844	-2.619981	-0.193553
C	0.954531	-2.219581	1.152522
C	-0.446787	-2.206450	1.211510
C	-0.920924	-2.465990	-0.138478
C	0.216797	-2.846486	-0.961905
Rh	0.175840	-0.652353	-0.373297
C	-1.137866	1.003244	-0.715078
C	-0.748802	0.357904	-1.940702
H	-0.037096	0.863082	-2.598916
H	2.223503	0.391776	1.366209
C	-1.314698	-1.987537	2.400836
H	-2.190067	-1.368210	2.157438
H	-1.694749	-2.941484	2.799274
H	-0.773082	-1.485747	3.213717
C	-2.350584	-2.680653	-0.499336
H	-2.655198	-3.715125	-0.275891
H	-3.014179	-2.009168	0.060206
H	-2.531777	-2.509671	-1.568100
C	0.132342	-3.341390	-2.364771
H	-0.142973	-4.406965	-2.398801
H	-0.623147	-2.792896	-2.941625
H	1.086916	-3.228749	-2.892666
C	2.786921	-2.784271	-0.618508
H	3.261706	-3.652906	-0.135999
H	2.871190	-2.917019	-1.703131
H	3.390981	-1.902061	-0.362149
C	1.900538	-2.027508	2.291493

H	2.115227	-2.978498	2.802937
H	2.873104	-1.640941	1.952496
H	1.501703	-1.338469	3.049288
C	0.945010	2.360851	-0.303832
C	-0.443326	2.289858	-0.409835
C	1.642704	3.549204	-0.161079
C	-1.135328	3.504925	-0.313772
C	0.925733	4.735870	-0.073531
H	2.729366	3.533250	-0.120306
C	-0.465230	4.709135	-0.141107
H	-2.222313	3.490648	-0.385372
H	1.454536	5.679535	0.045933
H	-1.032312	5.635883	-0.071057
C	4.808296	0.457698	1.352472
H	4.322255	0.392099	2.333388
H	5.165582	-0.540542	1.068357
H	5.683477	1.110222	1.425600
O	1.639955	1.138955	-0.372300
C	3.906509	0.981885	0.261505
O	4.298636	1.373909	-0.813509
H	-1.461589	-0.281722	-2.468230
C	-2.499532	0.847357	-0.145704
C	-3.607713	0.533921	-0.940667
C	-2.710971	1.021318	1.230944
C	-4.870952	0.365015	-0.379849
H	-3.476863	0.429842	-2.017423
C	-3.970349	0.860161	1.792143
H	-1.855136	1.270843	1.861694
C	-5.059054	0.521447	0.989018
H	-5.715992	0.118009	-1.021524
H	-4.104056	0.993987	2.865244
H	-6.046756	0.391294	1.428424

$TS_{O\text{-}L}$

E = -1322.5623833au

N	2.279376	1.138138	-0.770848
C	1.908767	-2.192239	0.054581
C	1.422351	-1.867008	1.388739
C	0.037485	-2.135695	1.448006
C	-0.379201	-2.489173	0.109426
C	0.803888	-2.600983	-0.724566
Rh	0.422206	-0.496309	-0.150070
C	-1.243657	0.824662	-0.710499
C	-0.477590	0.360926	-1.831535
H	0.161944	1.064849	-2.370461
C	-0.858161	-2.036731	2.633390
H	-1.854383	-1.668223	2.353539
H	-1.000120	-3.015024	3.118117
H	-0.453085	-1.352258	3.389110
C	-1.739870	-2.959089	-0.270223
H	-1.833374	-4.041385	-0.091727
H	-2.523001	-2.457740	0.310903
H	-1.957241	-2.781449	-1.331157
C	0.850275	-3.094032	-2.129414
H	1.012364	-4.182440	-2.166911
H	-0.084642	-2.887058	-2.665302
H	1.665016	-2.619254	-2.691108
C	3.316141	-2.103527	-0.425635
H	3.714532	-3.095798	-0.684694
H	3.380802	-1.477969	-1.331471
H	3.974089	-1.648773	0.323344
C	2.286838	-1.382389	2.499936
H	2.931486	-2.192002	2.874627
H	2.938837	-0.562307	2.165272
H	1.687483	-1.018518	3.342789
C	0.348355	2.507539	0.306939
C	-0.942480	2.168426	-0.165361
C	0.685886	3.835997	0.623874
C	-1.909101	3.186636	-0.154676
C	-0.280289	4.821162	0.579082
H	1.701736	4.035688	0.962902
C	-1.586483	4.487549	0.199492
H	-2.922492	2.949032	-0.476545
H	-0.033104	5.845285	0.853018
H	-2.353281	5.259605	0.159535
C	4.565542	1.638378	-1.383029
H	5.201783	0.782526	-1.638969
H	4.110227	2.020345	-2.303763
H	5.212780	2.410208	-0.949843
O	1.236997	1.551043	0.584269
C	3.573948	1.189754	-0.324272
O	3.944365	0.812506	0.774621
H	2.020978	1.863863	-1.441966
H	-0.909055	-0.406884	-2.478540
C	-2.609104	0.306822	-0.445606
C	-3.121659	0.313648	0.861524
C	-3.430661	-0.183328	-1.467039
C	-4.390474	-0.176461	1.138697

H	-2.496065	0.700998	1.667801
C	-4.702922	-0.677249	-1.191416
H	-3.071416	-0.161611	-2.495543
C	-5.187979	-0.680839	0.111390
H	-4.760841	-0.166394	2.163183
H	-5.323169	-1.050069	-2.005632
H	-6.183636	-1.065219	0.326620

P

E = -1322.5930417au

N	3.184864	1.776738	-0.770635
C	1.270580	-2.761369	0.012944
C	0.723289	-2.452193	1.335618
C	-0.664819	-2.335601	1.233641
C	-0.989986	-2.423187	-0.184551
C	0.210114	-2.828989	-0.905221
Rh	0.302577	-0.714393	-0.181483
C	-0.829374	1.085955	-0.661672
C	-0.341249	0.396554	-1.826771
H	0.458058	0.819506	-2.429178
H	3.896244	2.014473	-1.452975
C	-1.650373	-2.188808	2.339226
H	-2.521514	-1.599740	2.028062
H	-2.028704	-3.169152	2.670048
H	-1.212300	-1.693625	3.215749
C	-2.378206	-2.490409	-0.724064
H	-2.801166	-3.497774	-0.584065
H	-3.043669	-1.775418	-0.222551
H	-2.410389	-2.267432	-1.798014
C	0.272065	-3.223461	-2.341032
H	0.009154	-4.283769	-2.481620
H	-0.421683	-2.634155	-2.954161
H	1.276656	-3.075781	-2.757649
C	2.713585	-3.028738	-0.244612
H	2.985182	-4.071405	-0.014925
H	2.982209	-2.841261	-1.293134
H	3.344180	-2.385558	0.384142
C	1.561151	-2.329397	2.561328
H	2.076387	-3.273976	2.794419
H	2.331737	-1.555680	2.428868
H	0.960886	-2.053895	3.436521
C	1.117190	2.767398	-0.462358
C	-0.204717	2.361366	-0.192290
C	1.655033	3.964598	-0.012450
C	-0.952734	3.300256	0.546527
C	0.888862	4.839709	0.743716
H	2.688105	4.199144	-0.262571
C	-0.430182	4.498333	1.012628
H	-1.993995	3.077548	0.762584
H	1.313551	5.775971	1.100697
H	-1.067381	5.168913	1.587099
C	4.790445	0.403673	0.397758
H	4.892938	0.212207	1.470553
H	5.060102	-0.518626	-0.132674
H	5.488158	1.196469	0.105087
O	1.915012	1.945933	-1.272219
C	3.356779	0.737940	0.099388
O	2.414653	0.164167	0.625539
C	-2.280191	0.922114	-0.332039
C	-3.247209	0.929310	-1.343148
C	-2.727609	0.778464	0.989417
C	-4.600252	0.767457	-1.055186
H	-2.929697	1.071982	-2.375824
C	-4.077181	0.630762	1.284143
H	-1.984756	0.770241	1.789462
C	-5.023794	0.616284	0.259755
H	-5.327596	0.770656	-1.866390
H	-4.392222	0.515395	2.321308
H	-6.081127	0.492363	0.488913
H	-1.061974	-0.186035	-2.407297

$TS_{P\text{-}Q}$

E = -1322.551575au

N	0.739752	3.286324	-0.970190
C	2.900971	-1.137973	0.226893
C	2.287553	-1.015994	1.537813
C	1.106625	-1.777488	1.534449
C	0.952275	-2.347937	0.203096
C	2.113898	-2.013739	-0.570101
Rh	0.927094	-0.157188	-0.105226
C	-1.335312	0.287867	-0.644528
C	-0.342944	0.374262	-1.673932
H	-0.079719	1.360210	-2.056112
H	0.713650	4.305120	-0.891507
C	0.201200	-2.019871	2.691286
H	-0.823695	-2.236035	2.366603
H	0.540720	-2.885061	3.281461
H	0.163207	-1.155794	3.366663

C	-0.015364	-3.409180	-0.186879
H	0.439370	-4.401224	-0.037229
H	-0.939864	-3.372806	0.398258
H	-0.295638	-3.332764	-1.244987
C	2.419436	-2.523086	-1.935384
H	2.877044	-3.524490	-1.900252
H	1.509422	-2.606363	-2.544601
H	3.112390	-1.862098	-2.469788
C	4.208433	-0.532659	-0.140056
H	4.260209	0.514768	0.179328
H	5.035837	-1.075966	0.341165
H	4.373785	-0.553280	-1.224002
C	2.843793	-0.196169	2.650079
H	3.197007	0.775184	2.279453
H	2.089684	0.002465	3.420963
H	3.696911	-0.693173	3.137530
C	-1.385603	2.658222	0.398480
C	-2.015385	1.459303	-0.064403
C	-2.166161	3.782293	0.780929
C	-3.431656	1.457608	-0.002597
C	-3.536387	3.734286	0.811064
H	-1.614129	4.667012	1.096676
C	-4.170804	2.549274	0.405307
H	-3.968957	0.576092	-0.344263
H	-4.120042	4.594716	1.134035
H	-5.258166	2.491211	0.385122
C	3.167600	3.676401	-1.081006
H	4.030844	3.059148	-1.350160
H	2.980804	4.405395	-1.878318
H	3.414692	4.232251	-0.165732
O	-0.098479	2.760029	0.561764
C	1.974479	2.788110	-0.821613
O	2.172782	1.611841	-0.461929
H	-0.327486	-0.419456	-2.425274
C	-2.131373	-0.970530	-0.534511
C	-2.633354	-1.382662	0.710056
C	-2.497742	-1.719715	-1.657746
C	-3.443231	-2.502965	0.830975
H	-2.384945	-0.788156	1.590518
C	-3.309311	-2.846137	-1.542106
H	-2.167134	-1.398390	-2.644988
C	-3.782978	-3.247708	-0.298737
H	-3.814401	-2.797806	1.812193
H	-3.584007	-3.404194	-2.436587
H	-4.421269	-4.125152	-0.209336

Q

E = -1322.6481529au

N	1.518984	2.555012	-2.215871
C	2.600663	-1.673891	0.499614
C	1.889848	-1.273069	1.667633
C	0.523623	-1.717611	1.533201
C	0.411752	-2.439586	0.291684
C	1.679408	-2.370910	-0.376079
Rh	0.947188	-0.358674	-0.109504
C	-1.542074	0.548059	-0.754838
C	-0.551467	0.190563	-1.668224
H	0.058857	0.979043	-2.123426
C	-0.528080	-1.512134	2.566859
H	-1.523718	-1.778603	2.193560
H	-0.329142	-2.123045	3.459993
H	-0.557668	-0.459578	2.881605
C	-0.789970	-3.171742	-0.189500
H	-0.749968	-4.219160	0.143871
H	-1.722738	-2.736348	0.189322
H	-0.850309	-3.179457	-1.284734
C	2.047756	-2.958237	-1.693357
H	2.610918	-3.895799	-1.573058
H	1.160429	-3.179481	-2.298221
H	2.670177	-2.259253	-2.266534
C	4.005386	-1.356374	0.143176
H	4.544127	-2.257903	-0.177968
H	3.995798	-0.633053	-0.688878
H	4.549368	-0.906982	0.981695
C	2.384924	-0.416013	2.776202
H	2.144641	-0.852702	3.755151
H	3.469375	-0.269845	2.723253
H	1.907637	0.575796	2.719777
C	-0.282120	2.288472	0.534661
C	-1.491514	1.833146	-0.071053
C	-0.218100	3.637160	0.961211
C	-2.620161	2.675443	-0.067502
C	-1.328491	4.450733	0.904389
H	0.727349	3.984418	1.376653
C	-2.548898	3.971131	0.403284
H	-3.549526	2.304040	-0.500739
H	-1.259153	5.477452	1.263484
H	-3.421719	4.619364	0.362116

C	3.376039	2.484310	-0.566570
H	4.368270	2.070786	-0.792666
H	3.425119	3.578531	-0.633619
H	3.121744	2.203162	0.466229
O	0.703407	1.488150	0.816014
C	2.334568	1.880749	-1.482041
O	2.311626	0.565974	-1.462907
H	1.687025	3.554349	-2.089314
H	-0.682370	-0.724888	-2.250327
C	-2.724575	-0.310407	-0.542180
C	-3.342533	-0.364688	0.716266
C	-3.253249	-1.092432	-1.578169
C	-4.424865	-1.205138	0.942177
H	-2.945943	0.252746	1.521864
C	-4.346113	-1.921171	-1.357489
H	-2.813204	-1.026902	-2.572251
C	-4.928227	-1.988481	-0.094343
H	-4.881480	-1.246847	1.929771
H	-4.750556	-2.512648	-2.177101
H	-5.781112	-2.642218	0.080342

TS_{E-N}

E = -1322.5628293au

N	-1.128979	-1.792902	-0.322834
C	0.970907	-2.677510	0.240271
C	1.518614	-3.912101	0.593306
H	0.854159	-4.651579	1.037702
C	2.860042	-4.177617	0.377069
H	3.273693	-5.146289	0.651874
C	3.660856	-3.201837	-0.210950
H	4.713629	-3.394528	-0.409183
C	3.108061	-1.975636	-0.545989
H	3.742247	-1.212097	-0.995874
C	1.757521	-1.657917	-0.320026
C	-2.703073	1.536643	-0.140084
C	-2.398786	0.895106	1.113198
C	-1.193146	1.457694	1.657634
C	-0.691766	2.369783	0.681621
C	-1.617656	2.402779	-0.429463
Rh	-0.766155	0.305764	-0.210297
C	-1.450076	3.246764	-1.646269
H	-1.839160	4.264042	-1.489484
H	-0.390763	3.342013	-1.919405
H	-1.975706	2.818467	-2.508536
C	-3.919787	1.291389	-0.962821
H	-4.816634	1.707316	-0.479357
H	-3.833341	1.758900	-1.950995
H	-4.080153	0.217441	-1.122060
C	-3.249651	-0.130649	1.781488
H	-3.900857	0.330328	2.538610
H	-3.891456	-0.647333	1.056979
H	-2.633056	-0.885441	2.289504
C	-0.603540	1.163032	2.994273
H	-0.988365	1.842963	3.770031
H	-0.831659	0.137548	3.312167
H	0.489317	1.264618	2.979683
C	0.458592	3.295584	0.851658
H	0.105790	4.269301	1.224253
H	1.193923	2.911077	1.567419
H	0.990447	3.474391	-0.091104
O	-0.350604	-2.548450	0.580740
C	-2.347638	-2.380658	-0.594074
O	-3.147652	-1.817771	-1.327814
C	-2.623810	-3.718006	0.040588
H	-1.837193	-4.444333	-0.194249
H	-2.654564	-3.625904	1.133655
H	-3.588796	-4.074884	-0.328549
C	2.230599	0.799084	-0.408568
C	2.829656	0.847355	0.862199
C	2.613672	1.771245	-1.340891
C	3.766059	1.819266	1.182432
H	2.553179	0.092166	1.599292
C	3.549069	2.752038	-1.018195
H	2.199331	1.744590	-2.348371
C	4.132325	2.783000	0.243127
H	4.216594	1.825337	2.174336
H	3.834270	3.487043	-1.770079
H	4.871394	3.542748	0.490984
C	1.279784	-0.293871	-0.732408
C	0.464428	-0.251456	-1.937801
H	0.466271	-1.158195	-2.559606
H	0.428829	0.644944	-2.559140
H	-0.713013	-1.034958	-1.388646

TS_{M-J}

E = -1322.5117916au

N	0.679278	-1.698163	0.635093
C	2.595207	-1.213317	-0.639013

C	3.818435	-1.860256	-0.632388
H	3.845077	-2.944089	-0.727963
C	4.978372	-1.106311	-0.493204
H	5.949826	-1.596028	-0.489739
C	4.877885	0.272593	-0.341911
H	5.777195	0.873879	-0.221283
C	3.635027	0.897943	-0.358817
H	3.572542	1.980830	-0.260040
C	2.448925	0.175380	-0.528956
C	-2.713118	-0.760259	-1.160875
C	-2.601605	-1.321350	0.134025
C	-2.524168	-0.222889	1.108723
C	-2.546973	0.984457	0.410199
C	-2.541921	0.662131	-1.002763
Rh	-0.665912	-0.356540	-0.360731
C	-2.694054	1.679523	-2.082085
H	-3.737191	2.026758	-2.136734
H	-2.072470	2.566339	-1.895024
H	-2.432079	1.278125	-3.069296
C	-2.964748	-1.472821	-2.446506
H	-4.029580	-1.439297	-2.725537
H	-2.395433	-1.026582	-3.272701
H	-2.675050	-2.528959	-2.385305
C	-2.758499	-2.757723	0.501976
H	-3.813263	-2.999492	0.705013
H	-2.417070	-3.419238	-0.305854
H	-2.179753	-3.001063	1.400953
C	-2.460274	-0.426704	2.582205
H	-3.414337	-0.818771	2.966937
H	-1.675489	-1.151215	2.838539
H	-2.247212	0.511617	3.108604
C	-2.505245	2.368125	0.953570
H	-3.454573	2.896642	0.775637
H	-2.318736	2.374169	2.033661
H	-1.709310	2.963528	0.482214
O	1.450592	-2.036325	-0.676024
C	0.539888	-2.816411	1.397235
O	-0.126892	-2.735401	2.427560
C	1.235474	-4.093880	0.994700
H	0.847752	-4.470394	0.039834
H	2.315149	-3.944351	0.873235
H	1.056037	-4.831640	1.781305
C	0.967219	2.159072	-0.002777
C	1.136478	2.207605	1.389876
C	0.664820	3.347972	-0.674641
C	1.004824	3.402315	2.082085
H	1.357015	1.279702	1.920458
C	0.527927	4.548000	0.022304
H	0.564685	3.338845	-1.760338
C	0.699735	4.581181	1.400704
H	1.136672	3.415950	3.163113
H	0.297729	5.462962	-0.522238
H	0.598179	5.519160	1.944030
H	0.536288	-1.518063	-1.217800
C	1.142365	0.869555	-0.715861
C	0.465586	0.569782	-1.933030
H	0.969663	-0.049767	-2.679090
H	-0.196124	1.313442	-2.378287

$TS_{D\text{-}E1}$

E = -1322.5592514au

Rh	0.274762	0.385385	-0.022298
C	-1.187585	1.912017	1.025729
C	0.150132	2.075777	1.560543
C	1.015152	2.477353	0.519245
C	-1.128368	2.164123	-0.360304
C	0.245811	2.454042	-0.705451
C	4.186358	-0.331376	-1.891541
C	4.547391	-1.524602	-1.275202
C	3.664901	-2.144358	-0.395888
C	2.439531	-1.538701	-0.142440
C	2.051907	-0.323249	-0.710980
C	2.950725	0.255122	-1.607804
H	4.862747	0.145100	-2.600214
H	5.512171	-1.984581	-1.483002
H	3.906790	-3.091515	0.084359
H	2.681264	1.180012	-2.119623
O	1.556222	-2.251977	0.636770
N	0.366187	-1.540380	0.902973
C	-0.039559	-1.768256	2.208616
C	0.760206	-2.755804	3.019020
H	0.847978	-3.720643	2.508181
H	1.779977	-2.386086	3.176320
H	0.258423	-2.879926	3.982205
O	-1.004683	-1.187102	2.687799
C	-2.253205	2.180475	-1.335585
H	-3.141018	1.661834	-0.955902
H	-2.544004	3.214639	-1.575678

H	-1.970470	1.693634	-2.278939
C	-2.392228	1.657981	1.864778
H	-3.257270	1.358749	1.260690
H	-2.204423	0.861285	2.595975
H	-2.673039	2.565452	2.421509
C	0.489425	1.879504	2.996654
H	1.572447	1.822852	3.157273
H	0.101347	2.706624	3.610070
H	0.038011	0.952973	3.374763
C	2.449567	2.862753	0.637586
H	2.856248	2.587887	1.617979
H	3.072457	2.366896	-0.119047
H	2.577951	3.948794	0.517666
C	0.690991	2.983113	-2.028147
H	0.399923	2.326144	-2.858521
H	0.247268	3.972269	-2.220526
H	1.779801	3.107729	-2.065089
C	-0.597929	-1.208194	-0.873190
C	-2.069925	-1.236156	-0.866708
C	-2.881445	-1.179291	0.272663
C	-2.697112	-1.237440	-2.129710
C	-4.265629	-1.146203	0.152156
H	-2.418455	-1.167226	1.255782
C	-4.079143	-1.156000	-2.240872
H	-2.090559	-1.262224	-3.034832
C	-4.873962	-1.122166	-1.099448
H	-4.874170	-1.127755	1.055693
H	-4.535699	-1.131683	-3.229253
H	-5.958290	-1.079153	-1.185894
C	0.027240	-2.246731	-1.748044
H	0.740686	-1.807532	-2.457017
H	0.604046	-2.953911	-1.139345
H	-0.731526	-2.830085	-2.283598

E1

E = -1322.5790856au

Rh	0.410345	0.413101	-0.042044
C	-0.749218	2.195025	0.930067
C	0.616161	2.215350	1.390113
C	1.458879	2.389823	0.268434
C	-0.743700	2.345778	-0.481669
C	0.626676	2.414565	-0.916049
C	4.401154	-1.054588	-1.218979
C	4.401623	-2.295756	-0.591479
C	3.255426	-2.736970	0.064695
C	2.149294	-1.899567	0.083466
C	2.109042	-0.629811	-0.492851
C	3.267697	-0.240626	-1.167319
H	5.286777	-0.714530	-1.754871
H	5.285710	-2.930438	-0.618653
H	3.207181	-3.714976	0.541222
H	3.295800	0.723650	-1.676460
O	0.995030	-2.428181	0.643387
N	-0.074629	-1.473957	0.630870
C	-0.755287	-1.858982	1.902935
C	-1.395663	-3.206683	1.859859
H	-2.266102	-3.164653	1.190919
H	-0.698909	-3.945597	1.449922
H	-1.719849	-3.495302	2.862965
O	-0.713695	-1.112144	2.837534
C	-1.932478	2.430240	-1.375803
H	-2.807951	1.933579	-0.939401
H	-2.206239	3.477117	-1.576059
H	-1.739821	1.950974	-2.344939
C	-1.922701	2.186257	1.851320
H	-2.869368	2.043074	1.317861
H	-1.835299	1.396868	2.612950
H	-1.992165	3.143036	2.391683
C	1.040855	2.126067	2.815156
H	2.120798	1.955099	2.897983
H	0.805753	3.052750	3.362025
H	0.533842	1.299946	3.329665
C	2.933914	2.610482	0.330932
H	3.461960	1.778274	0.815144
H	3.370001	2.739397	-0.666138
H	3.156206	3.524991	0.899771
C	1.085569	2.709603	-2.304044
H	0.390544	2.304699	-3.050036
H	1.169983	3.793072	-2.482588
H	2.068655	2.267444	-2.510368
C	-0.709464	-1.280341	-0.684344
C	-2.173047	-1.002101	-0.710169
C	-2.918987	-0.559917	0.396850
C	-2.882315	-1.148910	-1.917852
C	-4.282575	-0.308100	0.311921
H	-2.435385	-0.369664	1.349896
C	-4.241694	-0.875677	-2.008483
H	-2.366187	-1.478955	-2.814921

C	-4.959917	-0.461030	-0.893204
H	-4.814035	0.024613	1.203407
H	-4.742592	-0.998945	-2.967825
H	-6.026721	-0.257255	-0.962066
C	-0.248699	-2.218056	-1.775971
H	-0.339617	-1.718508	-2.747092
H	0.795430	-2.512798	-1.685788
H	-0.865472	-3.132674	-1.804899

C1’

E = -1322.60738au

N	-0.907437	1.741707	-0.418233
C	-2.862974	0.698291	-0.918265
C	-4.195643	0.683356	-1.327654
H	-4.763323	1.612546	-1.326833
C	-4.763909	-0.517674	-1.737625
H	-5.804277	-0.535418	-2.058560
C	-4.004540	-1.684146	-1.759756
H	-4.443688	-2.620568	-2.101133
C	-2.670625	-1.649214	-1.347529
H	-2.076297	-2.566001	-1.372216
C	-2.094487	-0.467527	-0.893578
C	0.901223	-0.072887	2.022695
C	-0.527711	0.031338	2.196193
C	-1.131137	-1.211700	1.815495
C	-0.096442	-2.040450	1.276598
C	1.159377	-1.339305	1.448179
Rh	-0.269801	-0.212416	0.002259
C	0.398885	-0.879417	-2.028232
C	1.224701	0.195120	-1.731201
C	2.493159	-1.933678	1.171723
H	2.805067	-2.557643	2.023262
H	2.478544	-2.580715	0.285900
H	3.264257	-1.172819	1.007328
C	1.889254	0.959436	2.442498
H	1.861094	1.102069	3.532850
H	2.911355	0.669976	2.172857
H	1.675778	1.921434	1.956403
C	-1.239950	1.195159	2.794778
H	-1.498993	0.995097	3.845158
H	-0.612832	2.094491	2.767962
H	-2.170646	1.418180	2.256083
C	-2.563210	-1.565701	2.016798
H	-2.717751	-1.945618	3.037655
H	-3.218153	-0.695508	1.881901
H	-2.902928	-2.335269	1.314770
C	-0.230932	-3.455919	0.829308
H	0.055285	-4.156314	1.628502
H	-1.261986	-3.691634	0.539620
H	0.412598	-3.670398	-0.034324
H	0.874480	1.192991	-1.996578
H	0.762857	-1.906410	-1.939211
H	-0.463862	-0.746701	-2.674606
C	2.656563	0.096170	-1.407733
C	3.308705	1.165266	-0.776198
C	3.414239	-1.013088	-1.805604
C	4.671784	1.101583	-0.518079
H	2.714063	2.028952	-0.474057
C	4.780164	-1.070198	-1.553177
H	2.932243	-1.828494	-2.345140
C	5.412476	-0.016330	-0.900727
H	5.163538	1.935647	-0.019021
H	5.354507	-1.937261	-1.876439
H	6.482811	-0.058047	-0.704310
O	-2.328816	1.868296	-0.499955
C	-0.324872	2.901672	-0.047568
O	0.886656	2.957530	0.203302
C	-1.194636	4.135421	0.025328
H	-0.549966	4.992888	0.235850
H	-1.747457	4.296817	-0.906676
H	-1.942681	4.030422	0.822218

$TS_{C1'\text{-}D'}$

E = -1322.5846389au

N	-1.322858	1.462290	-0.818306
C	-2.689964	-0.343217	-1.155519
C	-3.944169	-0.934668	-1.287742
H	-4.811176	-0.296361	-1.448770
C	-4.065430	-2.316797	-1.195997
H	-5.046888	-2.775336	-1.305107
C	-2.942822	-3.109858	-0.964148
H	-3.036756	-4.192164	-0.894512
C	-1.692997	-2.508981	-0.841984
H	-0.805724	-3.129679	-0.695461
C	-1.536563	-1.122924	-0.930533
C	0.890822	0.974822	1.934105
C	-0.540913	0.955317	2.148926
C	-0.978980	-0.401002	2.231813

C	0.174843	-1.227807	2.009137
C	1.326518	-0.380493	1.878552
Rh	-0.153082	0.054588	0.182966
C	0.030424	-0.692197	-2.013158
C	1.056044	0.222475	-1.584194
C	2.735439	-0.847249	1.824320
H	3.145233	-0.918464	2.843206
H	2.825109	-1.837370	1.362503
H	3.374696	-0.161575	1.255833
C	1.736166	2.200259	1.872642
H	1.810289	2.682457	2.859143
H	2.755645	1.962243	1.544356
H	1.312999	2.920176	1.159144
C	-1.380846	2.174665	2.303836
H	-1.427710	2.469982	3.362398
H	-0.959375	3.010700	1.732731
H	-2.407574	2.009439	1.953872
C	-2.377494	-0.871908	2.438289
H	-2.578449	-1.105490	3.494093
H	-3.102291	-0.110339	2.122888
H	-2.589517	-1.774504	1.849081
C	0.216468	-2.716034	2.058633
H	0.532543	-3.063196	3.053884
H	-0.764119	-3.159033	1.849380
H	0.932249	-3.122693	1.330930
C	-2.250535	3.582843	-1.619936
H	-1.895492	4.606740	-1.764042
H	-2.572796	3.157912	-2.577501
H	-3.129958	3.588417	-0.962759
H	0.929719	1.266631	-1.873572
H	0.327486	-1.723382	-2.204077
H	-0.636908	-0.300490	-2.780759
C	2.456890	-0.169458	-1.395226
C	3.410343	0.851458	-1.254309
C	2.910298	-1.496676	-1.384486
C	4.762332	0.560666	-1.126396
H	3.063352	1.886799	-1.249081
C	4.264267	-1.787299	-1.264592
H	2.195829	-2.317791	-1.472498
C	5.198684	-0.762782	-1.136660
H	5.482153	1.371831	-1.025299
H	4.592932	-2.825970	-1.272413
H	6.258755	-0.993829	-1.047885
O	-2.618473	1.002383	-1.219975
C	-1.129575	2.780853	-0.999533
O	-0.064160	3.309841	-0.652535

D’

E = -1322.6103484au

Rh	-0.091484	0.528228	-0.022382
C	0.536129	2.199636	-1.451596
C	0.233229	0.913438	-2.072162
C	-1.179106	0.645023	-1.934321
C	-0.624652	2.624876	-0.804798
C	-1.683251	1.632403	-1.054784
C	3.537576	-2.958880	-1.333499
C	4.341801	-2.151008	-0.535286
C	3.762931	-1.434840	0.504084
C	2.395961	-1.526269	0.754616
C	1.562745	-2.321503	-0.042676
C	2.173305	-3.032051	-1.082553
H	3.971521	-3.529739	-2.152817
H	5.412585	-2.079689	-0.718346
H	4.361661	-0.796119	1.151408
H	1.544353	-3.664241	-1.712882
O	1.894062	-0.805672	1.823248
N	1.386470	0.443263	1.356532
C	1.932610	1.519027	1.998564
C	2.957089	1.266396	3.078966
H	2.595624	0.540001	3.814886
H	3.884514	0.857794	2.659449
H	3.174252	2.221165	3.565607
O	1.567296	2.659452	1.712921
C	-0.675274	-1.338768	0.809695
C	-2.151917	-1.459000	0.857570
C	-2.853180	-0.684830	1.801498
C	-2.912606	-2.304542	0.036748
C	-4.234438	-0.727574	1.901924
H	-2.276807	-0.031302	2.460605
C	-4.302841	-2.347120	0.132183
H	-2.417661	-2.951845	-0.687156
C	-4.974148	-1.557613	1.058400
H	-4.741275	-0.114267	2.646325
H	-4.863746	-3.016267	-0.519908
H	-6.059385	-1.597702	1.134694
C	0.072060	-2.480463	0.146098
C	-3.085245	1.779561	-0.582933
H	-3.622225	2.515508	-1.201250

H	-3.634941	0.832376	-0.627719
H	-3.121442	2.134314	0.455555
C	-0.794193	3.813276	0.070504
H	-1.757920	4.307376	-0.113246
H	-0.742721	3.521938	1.128933
H	0.006179	4.543437	-0.086316
C	1.882958	2.832458	-1.433713
H	2.100009	3.336738	-2.387015
H	1.971302	3.550453	-0.613176
H	2.664788	2.077061	-1.274185
C	1.206098	0.113144	-2.861103
H	1.311213	0.523322	-3.877500
H	2.198563	0.121332	-2.392337
H	0.894142	-0.934291	-2.948008
C	-1.942745	-0.444156	-2.598757
H	-2.355766	-0.099063	-3.558067
H	-1.310416	-1.316346	-2.810683
H	-2.777396	-0.789572	-1.976908
H	-0.349411	-2.665481	-0.856172
H	-0.115560	-3.417499	0.707812
H	-0.308781	-1.206443	1.834510

$TS_{D'-D1'}$

E = -1322.5466393au

N	1.512257	-0.888948	-0.824384
C	-0.845954	-2.614144	1.115700
C	-1.669731	-1.599527	1.713525
C	-2.434540	-0.972488	0.674128
C	-2.062910	-1.560990	-0.576052
C	-1.083414	-2.569174	-0.299502
Rh	-0.178429	-0.638482	0.344855
C	0.840374	1.280515	0.793678
H	0.476824	1.773291	1.700075
C	0.008598	1.411012	-0.360073
H	0.490230	1.322765	-1.333772
H	0.835388	-0.237549	1.537763
C	3.185528	0.325228	0.244891
C	2.331362	1.337506	0.713525
C	4.571637	0.489877	0.283250
C	2.932397	2.503264	1.206618
C	5.133688	1.657050	0.773876
H	5.185405	-0.328915	-0.088912
C	4.307685	2.678708	1.235542
H	2.280866	3.294194	1.581293
H	6.216138	1.771292	0.789158
H	4.731001	3.603874	1.621447
C	-3.520646	0.021604	0.878847
H	-3.603054	0.724348	0.041102
H	-4.488323	-0.493139	0.978067
H	-3.369572	0.613735	1.789351
C	-2.606622	-1.236573	-1.924333
H	-3.292441	-2.020864	-2.278674
H	-3.161919	-0.290291	-1.914707
H	-1.786272	-1.136443	-2.647074
C	-1.793866	-1.305565	3.170675
H	-1.959422	-0.235378	3.350576
H	-2.640307	-1.848833	3.616370
H	-0.888618	-1.592732	3.718686
C	0.061061	-3.573939	1.809060
H	0.323557	-3.225983	2.815309
H	-0.400194	-4.567912	1.910245
H	1.001492	-3.696475	1.256603
C	-0.460496	-3.467743	-1.308736
H	0.536984	-3.794212	-0.991730
H	-1.079570	-4.367027	-1.446039
H	-0.358087	-2.964635	-2.276595
C	2.928703	-0.820674	-2.828950
H	3.513025	-1.694837	-2.519170
H	2.785984	-0.829970	-3.912836
H	3.508322	0.068692	-2.547624
O	2.773713	-0.898699	-0.204346
C	1.563375	-0.803413	-2.177067
O	0.528945	-0.723129	-2.846399
C	-1.248226	2.167480	-0.390401
C	-1.888228	2.325202	-1.629894
C	-1.828723	2.773948	0.731675
C	-3.060487	3.060844	-1.743183
H	-1.444157	1.851130	-2.507030
C	-2.996287	3.518590	0.616559
H	-1.365268	2.663024	1.713059
C	-3.619795	3.666258	-0.619232
H	-3.535856	3.171000	-2.716916
H	-3.423580	3.987786	1.502029
H	-4.533254	4.251875	-0.706635

D1’

E = -1322.5988705au

N	-1.489695	-0.838930	0.935054

C	0.774837	-2.632090	-1.066736
C	1.541132	-1.629167	-1.768916
C	2.352240	-0.954168	-0.804841
C	2.092388	-1.515924	0.490335
C	1.130331	-2.552488	0.322660
Rh	0.083714	-0.664715	-0.379019
C	-0.832889	1.287232	-0.749467
H	-0.458522	1.680030	-1.698576
C	0.005628	1.435403	0.371610
H	-0.438469	1.327259	1.360045
C	-3.182389	0.362912	-0.122246
C	-2.320698	1.318763	-0.690387
C	-4.568560	0.531990	-0.170068
C	-2.927813	2.423123	-1.309098
C	-5.130080	1.639965	-0.780662
H	-5.183235	-0.241677	0.287281
C	-4.301569	2.598890	-1.358664
H	-2.275223	3.169736	-1.764263
H	-6.212257	1.755661	-0.803098
H	-4.722305	3.476695	-1.845065
C	3.401634	0.049016	-1.122157
H	3.594427	0.732543	-0.287609
H	4.347323	-0.464896	-1.353064
H	3.139446	0.657199	-1.996447
C	2.737801	-1.147289	1.780593
H	3.463322	-1.912029	2.096069
H	3.273386	-0.193394	1.703912
H	1.976137	-1.044608	2.564851
C	1.595367	-1.420594	-3.245169
H	1.759489	-0.364255	-3.494354
H	2.415335	-1.996763	-3.700011
H	0.662627	-1.727493	-3.732228
C	-0.118756	-3.664009	-1.669063
H	-0.475509	-3.358921	-2.659643
H	0.403732	-4.625891	-1.780905
H	-1.004428	-3.836073	-1.045100
C	0.590509	-3.417633	1.405823
H	-0.426330	-3.756239	1.174719
H	1.221147	-4.309644	1.536203
H	0.550961	-2.872982	2.355541
C	-2.719142	-0.664197	3.049636
H	-3.348630	-1.532342	2.823672
H	-2.482803	-0.638430	4.116680
H	-3.298891	0.229788	2.783319
O	-2.797018	-0.824031	0.435482
C	-1.415653	-0.707472	2.283318
O	-0.325417	-0.630362	2.859816
C	1.281730	2.160704	0.382490
C	1.987266	2.230397	1.593810
C	1.799099	2.845588	-0.724965
C	3.174027	2.944798	1.690399
H	1.586028	1.700108	2.459381
C	2.982930	3.566727	-0.626174
H	1.265665	2.825990	-1.675671
C	3.678619	3.617371	0.578702
H	3.704566	2.984415	2.640742
H	3.362889	4.098690	-1.497418
H	4.604054	4.185813	0.653796
H	-1.011654	-0.775539	-1.519260

$TS_{D1'\text{-}E'}$

E = -1322.5762887au

N	1.643287	-0.435192	-1.241953
C	-1.234961	-2.579078	0.026890
C	-0.146420	-2.610905	1.000132
C	-0.438731	-1.675397	2.032515
C	-1.611004	-0.959360	1.616969
C	-2.148913	-1.599350	0.423618
Rh	-0.005259	-0.519662	0.174313
C	0.363106	1.573257	0.562957
H	-0.151644	1.862127	1.485699
C	-0.414107	1.477449	-0.619561
H	0.121558	1.477962	-1.568505
H	1.597465	-0.633415	0.250472
C	0.312726	-1.455463	3.302671
H	0.394589	-0.387132	3.545217
H	-0.181567	-1.949193	4.153470
H	1.333580	-1.850585	3.238016
C	-2.344998	0.039677	2.444493
H	-3.052874	-0.467349	3.118026
H	-1.663856	0.628525	3.073031
H	-2.923273	0.737464	1.825329
C	-3.442921	-1.239059	-0.214156
H	-4.287494	-1.712666	0.309642
H	-3.618158	-0.155003	-0.198282
H	-3.482425	-1.556316	-1.263508
C	-1.321107	-3.489236	-1.148844
H	-1.527623	-4.522002	-0.827989

H	-2.122640	-3.189450	-1.834417
H	-0.374264	-3.494991	-1.703252
C	0.931402	-3.641354	1.015440
H	0.540665	-4.600118	1.390350
H	1.336891	-3.797580	0.010735
H	1.762035	-3.345744	1.668554
C	2.684959	1.498938	-0.440570
C	1.803931	1.877011	0.589946
C	4.032977	1.820647	-0.401575
C	2.356539	2.555235	1.680422
C	4.548813	2.528155	0.681622
H	4.661776	1.514871	-1.236127
C	3.707638	2.882809	1.729882
H	1.696710	2.847495	2.498579
H	5.605128	2.788574	0.707647
H	4.100851	3.423299	2.589104
C	3.292043	-1.133569	-2.927306
H	4.166495	-0.745767	-2.390082
H	3.563488	-2.052968	-3.452495
H	2.990376	-0.364845	-3.646943
C	-1.823699	1.871294	-0.752823
C	-2.502507	1.524534	-1.931336
C	-2.512254	2.634480	0.199074
C	-3.818456	1.908742	-2.145923
H	-1.973874	0.930452	-2.678899
C	-3.835132	3.013449	-0.010336
H	-1.998062	2.959093	1.103723
C	-4.495350	2.652496	-1.180990
H	-4.321014	1.625162	-3.069583
H	-4.347952	3.610926	0.742280
H	-5.527220	2.957533	-1.346039
O	2.212780	0.832758	-1.551778
C	2.177685	-1.463731	-1.965061
O	1.748270	-2.604918	-1.829855

E’

E = -1322.6209908au

N	1.686156	-0.570890	-1.324056
C	-1.012040	-2.593125	0.254231
C	0.187195	-2.566584	1.092339
C	0.004324	-1.624606	2.124116
C	-1.246077	-0.950722	1.849169
C	-1.906983	-1.629211	0.748938
Rh	0.010419	-0.501876	0.138088
C	0.496945	1.532559	0.484891
H	0.077926	1.859357	1.442502
C	-0.405831	1.445801	-0.626198
H	0.035160	1.523469	-1.623115
H	2.451934	-1.095004	-0.882694
C	0.924610	-1.297813	3.251711
H	1.093441	-0.214557	3.337995
H	0.525210	-1.645529	4.217257
H	1.907587	-1.766439	3.118164
C	-1.898663	0.026085	2.766074
H	-2.448153	-0.497997	3.563546
H	-1.162073	0.676907	3.256708
H	-2.614843	0.665259	2.235843
C	-3.283486	-1.325185	0.270886
H	-4.043026	-1.791398	0.917303
H	-3.478868	-0.244247	0.265004
H	-3.447528	-1.688705	-0.751571
C	-1.236896	-3.565869	-0.850505
H	-1.376051	-4.585334	-0.457585
H	-2.131770	-3.312289	-1.432257
H	-0.385620	-3.602340	-1.545098
C	1.349853	-3.479170	0.894405
H	1.139010	-4.488235	1.279999
H	1.590016	-3.584896	-0.172313
H	2.247022	-3.112609	1.410940
C	2.752785	1.371148	-0.671531
C	1.936711	1.780512	0.398592
C	4.119437	1.605781	-0.704807
C	2.597777	2.428320	1.454080
C	4.734008	2.284608	0.342047
H	4.681936	1.254071	-1.568258
C	3.962996	2.682604	1.430170
H	2.002298	2.755784	2.307396
H	5.802545	2.486590	0.311740
H	4.427597	3.202451	2.266576
C	0.594239	-0.555162	-3.563134
H	1.371511	0.013482	-4.089414
H	0.128890	-1.263692	-4.252660
H	-0.145456	0.164085	-3.198129
C	-1.811517	1.881513	-0.580979
C	-2.654965	1.568858	-1.658965
C	-2.364766	2.611985	0.479327
C	-3.987742	1.954532	-1.675372
H	-2.246278	0.990400	-2.490495

C	-3.703835	2.991547	0.471316
H	-1.731508	2.907189	1.315693
C	-4.524594	2.666469	-0.603975
H	-4.614021	1.694694	-2.528058
H	-4.103806	3.561873	1.309083
H	-5.569869	2.970349	-0.611872
O	2.221964	0.686041	-1.758936
C	1.213132	-1.327907	-2.445196
O	1.368678	-2.530271	-2.427014

$TS_{E'-F'}$

E = -1322.5919802au

N	2.402140	-0.525127	-1.671954
C	-1.065419	-2.555263	0.346644
C	0.155434	-2.496044	1.156727
C	-0.021387	-1.572013	2.204508
C	-1.276521	-0.900640	1.931959
C	-1.960380	-1.608722	0.844866
Rh	-0.073179	-0.426991	0.253128
C	0.393545	1.632882	0.406909
H	-0.059717	2.053972	1.310939
C	-0.475036	1.397345	-0.706773
H	-0.008768	1.253339	-1.687013
H	3.391636	-0.771552	-1.680439
C	0.921997	-1.266558	3.316923
H	0.904614	-0.199276	3.576994
H	0.683089	-1.830651	4.232301
H	1.956783	-1.508922	3.042025
C	-1.933024	0.116092	2.799197
H	-2.618605	-0.365656	3.513640
H	-1.199878	0.690448	3.379935
H	-2.524256	0.823905	2.201937
C	-3.341096	-1.309671	0.381139
H	-4.094607	-1.754458	1.049774
H	-3.527318	-0.227697	0.354277
H	-3.518660	-1.688878	-0.632709
C	-1.271764	-3.436066	-0.842588
H	-2.337261	-3.648817	-0.994982
H	-0.905369	-2.964995	-1.768570
H	-0.762537	-4.403409	-0.728115
C	1.344333	-3.373547	0.956146
H	1.294349	-4.275872	1.584728
H	1.420624	-3.713974	-0.084544
H	2.277372	-2.850104	1.205723
C	2.708806	1.521168	-0.688739
C	1.838708	1.874225	0.358201
C	4.065906	1.813793	-0.661801
C	2.447365	2.510251	1.456617
C	4.630028	2.454585	0.434699
H	4.666926	1.541519	-1.530058
C	3.804599	2.791477	1.504052
H	1.810434	2.798892	2.293913
H	5.691970	2.690315	0.450648
H	4.218738	3.291997	2.378085
C	2.094598	-2.715913	-2.613247
H	2.902558	-2.975306	-1.918514
H	1.278515	-3.437929	-2.505500
H	2.475341	-2.798533	-3.639210
C	-1.889625	1.782519	-0.774669
C	-2.657232	1.298652	-1.847243
C	-2.527206	2.597624	0.170748
C	-4.004637	1.607149	-1.964053
H	-2.166879	0.655134	-2.580890
C	-3.881721	2.900209	0.057817
H	-1.949274	3.023651	0.991292
C	-4.628567	2.408925	-1.008114
H	-4.575893	1.219460	-2.806952
H	-4.351944	3.541495	0.802861
H	-5.685654	2.653526	-1.098838
O	2.241233	0.856334	-1.826899
C	1.547521	-1.324399	-2.410615
O	0.468320	-0.958771	-2.830062

F'

E = -1322.607538au

N	-2.914194	-0.728839	-2.235922
C	1.170545	2.647836	-0.229032
C	0.063563	2.744776	0.722923
C	0.352417	1.944050	1.841963
C	1.572872	1.220816	1.526185
C	2.125967	1.764977	0.291613
Rh	0.168235	0.572818	0.054419
C	-0.324220	-1.391914	0.694306
H	0.212576	-1.580366	1.630679
C	0.460441	-1.450002	-0.503749
H	-0.069581	-1.562220	-1.451712
H	-3.420376	-1.127876	-3.018762
C	-0.449859	1.795551	3.089022

H	-0.397389	0.770820	3.480743
H	-0.098162	2.466776	3.888523
H	-1.511385	2.014492	2.915114
C	2.332373	0.365101	2.481883
H	2.973547	0.981423	3.131310
H	1.663604	-0.209239	3.137047
H	2.980553	-0.348622	1.957448
C	3.445611	1.386254	-0.281997
H	4.271470	1.906921	0.227500
H	3.631009	0.307610	-0.185726
H	3.508314	1.627142	-1.351024
C	1.224605	3.402706	-1.512705
H	1.293396	4.488653	-1.343107
H	2.089680	3.106112	-2.117903
H	0.323797	3.226957	-2.117798
C	-1.121392	3.627196	0.527444
H	-0.873054	4.684436	0.710115
H	-1.505021	3.558549	-0.499389
H	-1.942350	3.358422	1.203425
C	-2.733519	-1.687490	-0.142017
C	-1.767297	-1.585187	0.870001
C	-4.089005	-1.822927	0.119410
C	-2.271294	-1.649288	2.184946
C	-4.548417	-1.858372	1.429181
H	-4.779671	-1.899620	-0.719219
C	-3.621901	-1.774217	2.466660
H	-1.554697	-1.580432	3.005263
H	-5.611709	-1.963179	1.635106
H	-3.954811	-1.809231	3.502840
C	-2.868528	1.370790	-3.420371
H	-3.082193	2.349093	-2.977052
H	-2.119754	1.521560	-4.206966
H	-3.786490	0.977240	-3.871087
C	1.855807	-1.911921	-0.552783
C	2.586401	-1.732683	-1.739564
C	2.511259	-2.532686	0.520101
C	3.908883	-2.138026	-1.846039
H	2.092536	-1.244405	-2.582302
C	3.841198	-2.930275	0.419490
H	1.964088	-2.727356	1.442562
C	4.550138	-2.735985	-0.761966
H	4.446720	-1.983811	-2.781158
H	4.322258	-3.412954	1.269948
H	5.588351	-3.054187	-0.841352
O	-2.294491	-1.696928	-1.474092
C	-2.289461	0.479491	-2.356549
O	-1.371705	0.845792	-1.638484

$TS_{F'-G'}$

E = -1322.570443au

N	-1.850325	-0.013156	-2.686450
C	1.578071	2.344244	0.566484
C	0.283230	2.616982	1.172379
C	0.021522	1.617922	2.133709
C	1.122041	0.671189	2.072117
C	2.127125	1.187961	1.170726
Rh	0.177929	0.612302	0.125413
C	-0.708478	-1.372680	0.396602
H	-0.280523	-1.795995	1.310999
C	0.187264	-1.329221	-0.713427
H	-0.252365	-1.230040	-1.706672
H	-2.608360	0.028009	-3.368946
C	-1.183315	1.499894	3.003484
H	-1.421552	0.450204	3.220169
H	-1.045655	2.011064	3.968794
H	-2.069257	1.930369	2.519469
C	1.340979	-0.465593	3.011080
H	1.930234	-0.140307	3.881863
H	0.395250	-0.871797	3.392992
H	1.894265	-1.284266	2.530916
C	3.449485	0.556086	0.916046
H	4.169256	0.788246	1.716003
H	3.361437	-0.538480	0.858035
H	3.883009	0.893563	-0.033456
C	2.187275	3.187084	-0.497672
H	1.458262	3.392240	-1.292822
H	2.527477	4.155595	-0.100761
H	3.048354	2.691356	-0.961428
C	-0.579723	3.776449	0.811490
H	-1.593487	3.665497	1.214022
H	-0.168288	4.720679	1.200308
H	-0.666950	3.881377	-0.277991
C	-3.059624	-0.740071	-0.444684
C	-2.157074	-1.428206	0.425292
C	-4.438382	-1.068829	-0.431173
C	-2.748317	-2.238096	1.420643
C	-4.966016	-1.906517	0.523887
H	-5.071586	-0.554390	-1.152592

C	-4.106331	-2.480294	1.474569
H	-2.088702	-2.724881	2.141210
H	-6.035469	-2.106907	0.555102
H	-4.505703	-3.141324	2.242392
C	-0.926843	1.756949	-4.117293
H	-1.649070	2.585112	-4.102948
H	0.073500	2.180353	-4.248547
H	-1.164253	1.115521	-4.974051
C	1.520486	-1.955926	-0.710411
C	2.407394	-1.636999	-1.752516
C	1.963993	-2.858118	0.265937
C	3.680101	-2.184301	-1.811750
H	2.074635	-0.927000	-2.512734
C	3.245050	-3.402856	0.211943
H	1.285785	-3.164979	1.062090
C	4.110615	-3.070921	-0.824477
H	4.344401	-1.918506	-2.633382
H	3.560934	-4.107181	0.980983
H	5.108569	-3.503724	-0.869598
O	-2.711745	0.302622	-1.155486
C	-0.991855	1.016490	-2.803755
O	-0.250844	1.385299	-1.871170

G’

E = -1322.6532933au

N	-0.268541	-0.477503	3.475584
C	-0.310614	2.693464	-0.583629
C	0.938514	2.339823	-1.158215
C	0.719850	1.229278	-2.055490
C	-0.701498	0.965135	-2.088722
C	-1.331029	1.818419	-1.131996
Rh	0.108676	0.552388	-0.084883
C	0.416229	-1.673533	-0.535158
H	0.059262	-1.933608	-1.539060
C	-0.529798	-1.543247	0.481183
H	-0.186183	-1.509372	1.522166
C	1.779621	0.593803	-2.886918
H	1.458387	-0.376137	-3.284008
H	2.051708	1.231618	-3.740864
H	2.687852	0.414559	-2.296090
C	-1.407630	0.029535	-3.002977
H	-1.819501	0.586335	-3.857103
H	-0.737835	-0.739211	-3.406805
H	-2.243910	-0.475817	-2.503070
C	-2.771768	1.873216	-0.765257
H	-3.249151	2.783226	-1.157854
H	-3.323706	1.007996	-1.151283
H	-2.882525	1.872329	0.327609
C	-0.572444	3.706263	0.466686
H	-1.350125	4.412409	0.144781
H	-0.924226	3.186702	1.372623
H	0.328912	4.274157	0.723071
C	2.277082	2.861942	-0.781355
H	2.900026	3.042123	-1.666962
H	2.205012	3.796725	-0.214710
H	2.787294	2.117324	-0.147049
C	2.516613	-0.939147	0.539878
C	1.852532	-1.867607	-0.293682
C	3.845244	-1.209453	0.914893
C	2.545576	-2.951119	-0.835298
C	4.505010	-2.312866	0.395377
H	4.346853	-0.508208	1.580039
C	3.871822	-3.184431	-0.495123
H	2.019748	-3.633997	-1.505771
H	5.544301	-2.488607	0.672722
H	4.404842	-4.038776	-0.907149
C	0.853174	1.739624	3.423909
H	0.309279	2.684069	3.560239
H	1.337439	1.471732	4.370876
H	1.630138	1.901814	2.663677
C	-1.977232	-1.734386	0.317409
C	-2.822394	-1.332483	1.363809
C	-2.547309	-2.338777	-0.812091
C	-4.198325	-1.485923	1.252681
H	-2.366378	-0.896542	2.252766
C	-3.925354	-2.490494	-0.918763
H	-1.905605	-2.720233	-1.607043
C	-4.756848	-2.052777	0.109187
H	-4.841842	-1.165742	2.070959
H	-4.350402	-2.968503	-1.800522
H	-5.836044	-2.174103	0.027423
O	1.924021	0.185257	0.885261
C	-0.081595	0.667404	2.915071
O	-0.734627	0.997620	1.821086
H	0.295990	-0.542216	4.323786

G1’

E = -1551.6411484au

C	-2.290376	0.398717	-1.766309
C	-0.934628	0.750944	-2.129820
C	-0.210722	-0.454022	-2.333514
C	-1.135543	-1.570549	-2.191503
C	-2.418557	-1.041106	-1.865781
Rh	-1.011976	-0.520412	-0.330482
C	1.243290	-0.585727	-2.618261
H	1.669749	-1.442884	-2.082796
H	1.422846	-0.732535	-3.693351
H	1.796193	0.303772	-2.291727
C	-0.753417	-3.000789	-2.329960
H	-0.481462	-3.234883	-3.369365
H	0.109580	-3.231092	-1.691533
H	-1.573748	-3.664376	-2.036235
C	-3.670258	-1.799846	-1.607260
H	-4.297511	-1.820527	-2.510670
H	-3.458007	-2.834208	-1.313634
H	-4.233586	-1.328764	-0.791380
C	-3.393303	1.350186	-1.475492
H	-4.059291	1.443549	-2.346645
H	-3.965126	0.991520	-0.607413
H	-3.003165	2.345771	-1.229336
C	-0.434666	2.139818	-2.276880
H	-0.843487	2.579800	-3.198339
H	-0.744043	2.776678	-1.439292
H	0.658142	2.177399	-2.340034
C	-0.407279	2.029174	1.117368
C	-1.626698	2.689707	1.353911
C	0.727365	2.798457	0.732594
C	-1.734542	4.067712	1.245540
C	0.577520	4.192112	0.622948
C	-0.623618	4.831778	0.881108
H	-2.690932	4.551674	1.442849
H	1.447841	4.778390	0.321464
H	-0.699300	5.914198	0.793215
O	-0.360295	0.706910	1.231369
C	0.951079	-2.134859	1.609764
O	0.673568	-1.953184	0.424668
O	0.660611	-1.308472	2.582404
H	0.166534	-0.510914	2.214674
C	1.705076	-3.353476	2.044625
H	1.924178	-3.332563	3.115117
H	1.112478	-4.243735	1.805771
H	2.637404	-3.416676	1.470910
N	-3.787679	-0.206669	1.339411
C	-3.284793	-1.881712	3.103749
H	-2.436571	-1.736820	3.784792
H	-4.204326	-1.552142	3.601124
H	-3.354021	-2.958402	2.904951
C	-3.021624	-1.137065	1.810822
O	-1.939604	-1.557414	1.230876
H	-4.569832	-0.063747	1.977829
H	-2.481376	2.061243	1.609969
C	2.013607	2.221924	0.366996
H	2.651799	2.887715	-0.226175
C	2.493271	1.008708	0.700062
H	1.902726	0.396830	1.374459
C	3.767287	0.432571	0.289660
C	4.265134	-0.667638	1.003898
C	4.515707	0.900836	-0.800493
C	5.468828	-1.267378	0.658448
H	3.693412	-1.030831	1.860724
C	5.720192	0.303767	-1.146228
H	4.137314	1.736332	-1.390635
C	6.204163	-0.782854	-0.419864
H	5.837144	-2.115120	1.235169
H	6.284990	0.683096	-1.996911
H	7.146906	-1.251584	-0.697048

$TS_{G1'-H'}$

E = -1551.6310835au

C	-2.735389	0.087525	-1.368798
C	-1.510420	0.379563	-2.091209
C	-0.831035	-0.843217	-2.330451
C	-1.635874	-1.918802	-1.773110
C	-2.830789	-1.337318	-1.223800
Rh	-1.083669	-0.652564	-0.184658
C	0.504775	-1.034002	-2.955537
H	1.176094	-1.555830	-2.259495
H	0.428842	-1.633781	-3.873537
H	0.966907	-0.073905	-3.213744
C	-1.265613	-3.358517	-1.802282
H	-1.374055	-3.774039	-2.814823
H	-0.224011	-3.495658	-1.485234
H	-1.897235	-3.944528	-1.125638
C	-3.937470	-2.069302	-0.555369
H	-4.704544	-2.354783	-1.289932
H	-3.568293	-2.980222	-0.070328

H	-4.391363	-1.445643	0.222635
C	-3.760235	1.074194	-0.939460
H	-4.643478	1.028082	-1.593579
H	-4.056787	0.856107	0.096268
H	-3.365584	2.097014	-0.968176
C	-1.090473	1.740422	-2.512508
H	-1.692692	2.065067	-3.373708
H	-1.234546	2.475938	-1.711373
H	-0.035504	1.774425	-2.808962
C	-0.324044	2.203823	0.809894
C	-1.489058	2.914636	1.120144
C	0.711094	2.824313	0.080400
C	-1.638114	4.235691	0.724130
C	0.525204	4.156334	-0.317621
C	-0.623765	4.865139	0.001303
H	-2.549641	4.776737	0.975037
H	1.318888	4.634953	-0.893169
H	-0.732263	5.900798	-0.316135
O	-0.322203	0.893829	1.156707
C	1.529117	-1.483337	1.234394
O	0.826588	-1.637125	0.190364
O	1.417497	-0.537680	2.059239
H	0.528019	0.360700	1.593903
C	2.607928	-2.508681	1.464837
H	3.139250	-2.311118	2.400248
H	2.167828	-3.512164	1.485478
H	3.320357	-2.474106	0.630518
N	-3.327194	-0.114375	2.081246
C	-2.287571	-1.528526	3.838997
H	-1.301064	-1.234259	4.219456
H	-3.061859	-1.156680	4.520355
H	-2.312992	-2.624681	3.829950
C	-2.444755	-0.993507	2.431400
O	-1.573722	-1.529791	1.627410
H	-3.885172	0.135739	2.897348
H	-2.269525	2.367059	1.650609
C	1.918449	2.101693	-0.342109
H	2.159931	2.150848	-1.410038
C	2.730071	1.436740	0.491558
H	2.524563	1.488853	1.561842
C	3.879531	0.610840	0.128778
C	4.794658	0.246949	1.125284
C	4.077601	0.113095	-1.166807
C	5.887065	-0.560485	0.834777
H	4.629803	0.602221	2.142988
C	5.167053	-0.696356	-1.458464
H	3.351601	0.343671	-1.946588
C	6.078834	-1.034509	-0.459512
H	6.587214	-0.828512	1.624566
H	5.301342	-1.078448	-2.469547
H	6.929482	-1.674091	-0.689232

H’

E = -936.1612294au

C	-1.318979	-0.972527	1.207293
C	-1.947586	0.308511	0.932621
C	-2.175648	0.389121	-0.470390
C	-1.672551	-0.829253	-1.081448
C	-1.187928	-1.680864	-0.029673
Rh	-0.068441	0.168822	-0.114955
C	-2.727074	1.545506	-1.225081
H	-2.093563	1.785050	-2.088367
H	-3.738708	1.325718	-1.594599
H	-2.778750	2.445161	-0.602414
C	-1.702475	-1.153248	-2.532898
H	-2.603994	-1.725838	-2.796026
H	-1.692514	-0.242713	-3.143495
H	-0.827370	-1.748602	-2.820047
C	-0.607363	-3.039287	-0.191624
H	-1.386426	-3.805421	-0.065113
H	-0.164848	-3.165736	-1.186756
H	0.188647	-3.198678	0.543989
C	-0.858612	-1.462241	2.532221
H	-1.391553	-2.381157	2.815319
H	0.219340	-1.680032	2.470743
H	-1.023053	-0.715015	3.316371
C	-2.226273	1.351456	1.956896
H	-3.091824	1.078666	2.577176
H	-1.361116	1.482797	2.618771
H	-2.434697	2.322719	1.494419
C	1.320601	2.288225	0.040483
O	0.648928	2.047732	-1.007138
O	1.199119	1.533935	1.049495
C	2.282975	3.435548	0.067900
H	1.947023	4.236551	-0.597646
H	2.410050	3.809499	1.088302
H	3.258173	3.083066	-0.290618
N	2.093705	-1.742939	1.094433

C	3.845648	-1.501745	-0.649930
H	4.350290	-0.536246	-0.778091
H	4.473420	-2.152696	-0.030452
H	3.747279	-1.943577	-1.648988
C	2.473638	-1.277814	-0.049578
O	1.722546	-0.558948	-0.833609
H	2.863118	-2.260012	1.518703

2b

E = -615.4472406au

C	0.337026	-0.569798	-0.093038
H	0.020614	-1.583335	-0.358062
C	-0.621250	0.341315	0.172149
H	-0.330961	1.319636	0.566873
C	2.429046	0.831330	-0.298896
C	1.783698	-0.387085	-0.006312
C	3.812631	0.945177	-0.175093
C	2.585869	-1.479953	0.354134
C	4.572110	-0.143281	0.226679
H	4.268459	1.904146	-0.413292
C	3.960817	-1.369495	0.485021
H	2.093820	-2.432565	0.554726
H	5.651462	-0.037986	0.323065
H	4.553937	-2.231602	0.782795
O	1.761558	1.928897	-0.731789
C	-2.062319	0.116421	0.084559
C	-2.929121	1.005407	0.733842
C	-2.623898	-0.952408	-0.628615
C	-4.305262	0.821419	0.697494
H	-2.506322	1.847330	1.283386
C	-3.998415	-1.137549	-0.664827
H	-1.975688	-1.634523	-1.178275
C	-4.846307	-0.253960	0.000098
H	-4.958372	1.522197	1.215049
H	-4.414435	-1.972844	-1.226085
H	-5.924593	-0.398949	-0.034785
H	0.861875	1.662090	-0.984251

I’

E = -1322.6118509au

N	2.908141	-0.544081	-0.994635
C	-0.451753	-2.624462	0.085308
C	0.482860	-2.389894	1.185424
C	-0.154001	-1.626580	2.183246
C	-1.437090	-1.236499	1.638694
C	-1.646788	-1.956098	0.385239
Rh	-0.029284	-0.342808	0.306861
C	-0.014797	1.753445	0.596496
H	-0.576016	2.113437	1.464385
C	-0.733293	1.429140	-0.608144
H	-0.177881	1.534444	-1.548565
C	0.374686	-1.242139	3.522879
H	0.105336	-0.209181	3.781101
H	-0.019871	-1.891680	4.320054
H	1.469222	-1.308461	3.560690
C	-2.494677	-0.515523	2.401305
H	-3.072533	-1.217578	3.022395
H	-2.059930	0.236138	3.074038
H	-3.200937	-0.001829	1.737601
C	-2.909676	-1.951401	-0.401062
H	-3.612841	-2.713163	-0.030618
H	-3.417928	-0.980145	-0.344836
H	-2.726900	-2.155994	-1.464135
C	-0.180019	-3.500583	-1.091846
H	-0.326221	-4.563099	-0.841548
H	-0.852263	-3.268947	-1.928160
H	0.850229	-3.404485	-1.461873
C	1.846834	-2.991265	1.262200
H	1.809968	-4.003758	1.692202
H	2.310902	-3.094684	0.270713
H	2.517394	-2.398465	1.900025
C	2.343950	1.603380	-0.219778
C	1.361090	2.282288	0.511253
C	3.636413	2.066451	-0.377828
C	1.759834	3.468828	1.131568
C	3.992660	3.261688	0.245397
H	4.353865	1.488640	-0.955002
C	3.057828	3.955371	1.005484
H	1.022891	4.018918	1.717139
H	5.007514	3.639874	0.139374
H	3.337784	4.882874	1.501765
C	1.765092	-0.821292	-3.146429
H	0.733451	-0.747797	-2.767859
H	2.074458	0.192074	-3.427582
H	1.794777	-1.487826	-4.011783
C	-2.185066	1.548636	-0.794792
C	-2.747339	1.116635	-2.006604
C	-3.052950	2.074483	0.171914

C	-4.112939	1.192928	-2.240506
H	-2.082566	0.697400	-2.765627
C	-4.423685	2.144040	-0.056696
H	-2.647150	2.448551	1.112307
C	-4.963654	1.703567	-1.261722
H	-4.518366	0.847357	-3.190848
H	-5.075438	2.559402	0.711354
H	-6.035837	1.764529	-1.440036
O	1.898172	0.392053	-0.768981
C	2.643377	-1.388435	-2.074422
O	3.143340	-2.495660	-2.083942
H	3.102212	-1.053035	-0.129030

$TS_{I'-J'}$

E = -1322.5618786au

N	-1.591558	-0.305721	1.790682
C	0.532866	-2.602938	-0.196820
C	-0.383016	-2.411460	-1.313989
C	0.235377	-1.585058	-2.276305
C	1.490156	-1.147604	-1.707361
C	1.705291	-1.859678	-0.458502
Rh	0.014745	-0.399816	-0.326787
C	-0.020431	1.732177	-0.603871
H	0.580893	2.121772	-1.431473
C	0.650490	1.391717	0.617509
H	0.070850	1.481366	1.540404
C	-0.301936	-1.154957	-3.597866
H	-0.148109	-0.079924	-3.765273
H	0.186628	-1.686749	-4.429020
H	-1.379009	-1.344283	-3.674725
C	2.517641	-0.352636	-2.434244
H	3.142794	-1.011762	-3.056125
H	2.057208	0.386577	-3.103276
H	3.182973	0.181037	-1.745366
C	2.948336	-1.829256	0.357718
H	3.667301	-2.588138	0.012459
H	3.446491	-0.852709	0.305452
H	2.737119	-2.028971	1.416534
C	0.280062	-3.464186	0.991530
H	0.757578	-4.450368	0.881830
H	0.680400	-3.006248	1.907172
H	-0.792748	-3.622106	1.146607
C	-1.742834	-3.009745	-1.390016
H	-1.689413	-4.094142	-1.568409
H	-2.286660	-2.848327	-0.450004
H	-2.332687	-2.563830	-2.199273
C	-2.447615	1.377526	-0.055300
C	-1.414382	2.171967	-0.618701
C	-3.746223	1.895529	0.114766
C	-1.787730	3.402742	-1.179063
C	-4.063254	3.139063	-0.394940
H	-4.493864	1.255414	0.581377
C	-3.081767	3.884765	-1.063136
H	-1.021571	4.007819	-1.664819
H	-5.075222	3.528553	-0.300148
H	-3.330858	4.862131	-1.473412
C	-2.659049	-1.108859	3.808750
H	-1.922577	-0.478154	4.319761
H	-3.651137	-0.653932	3.932522
H	-2.680300	-2.096044	4.280015
C	2.091684	1.555122	0.857366
C	2.619520	1.129170	2.086741
C	2.977659	2.128175	-0.065343
C	3.970512	1.254467	2.377307
H	1.940855	0.675872	2.812655
C	4.333702	2.249138	0.221316
H	2.599377	2.500948	-1.017505
C	4.840191	1.812150	1.441918
H	4.350034	0.911335	3.339113
H	4.999162	2.701432	-0.513345
H	5.900769	1.912598	1.665963
O	-2.244258	0.082969	0.177450
C	-2.381300	-1.292444	2.326492
O	-2.791489	-2.261153	1.711155
H	-1.716596	0.606741	2.236363

J'

E = -1322.6754167au

N	0.396722	-1.244835	1.792109
C	0.640543	-2.335613	-1.141867
C	-0.706474	-2.139609	-1.567718
C	-0.801706	-0.834818	-2.175490
C	0.517267	-0.266518	-2.183294
C	1.407817	-1.168731	-1.510007
Rh	-0.180306	-0.549653	-0.091782
C	-0.891605	1.627276	0.015789
H	-0.695024	2.129416	-0.938830
C	0.195526	1.481092	0.872533

H	0.005713	1.192941	1.907794
C	-2.050022	-0.260501	-2.751510
H	-1.975781	0.825100	-2.884509
H	-2.278422	-0.704470	-3.731567
H	-2.905361	-0.446277	-2.088596
C	0.942158	0.999343	-2.839489
H	1.498559	0.766819	-3.759095
H	0.089432	1.627591	-3.122159
H	1.607576	1.591658	-2.197148
C	2.879659	-1.014648	-1.360849
H	3.408602	-1.655305	-2.082564
H	3.192247	0.021389	-1.537582
H	3.180230	-1.293728	-0.341743
C	1.185494	-3.549461	-0.479057
H	1.496297	-4.286515	-1.234186
H	2.053147	-3.292604	0.138276
H	0.436550	-4.022752	0.167665
C	-1.862894	-3.036489	-1.317274
H	-2.489055	-3.131368	-2.213995
H	-1.542136	-4.038768	-1.013795
H	-2.483846	-2.610060	-0.512062
C	-2.790814	0.304566	0.913592
C	-2.311264	1.525864	0.398038
C	-4.112855	0.253541	1.394422
C	-3.168417	2.619790	0.264854
C	-4.939011	1.361132	1.283990
H	-4.474075	-0.685876	1.810628
C	-4.482535	2.549580	0.708532
H	-2.782867	3.545424	-0.167739
H	-5.967656	1.293139	1.637629
H	-5.142519	3.409609	0.616572
C	1.458169	-2.449303	3.612843
H	2.263150	-2.078521	4.257138
H	0.497934	-2.330107	4.128176
H	1.640844	-3.520145	3.454111
C	1.524716	2.056485	0.573355
C	2.697817	1.450041	1.041816
C	1.632834	3.250000	-0.153635
C	3.938297	2.009593	0.761730
H	2.642258	0.497582	1.569946
C	2.876762	3.806090	-0.434569
H	0.729004	3.762702	-0.484093
C	4.035413	3.183815	0.018495
H	4.838943	1.513185	1.119942
H	2.937305	4.735872	-0.998523
H	5.010365	3.618235	-0.197366
O	-2.034116	-0.773917	0.883202
C	1.538804	-1.741965	2.268074
O	2.641857	-1.684131	1.698664
H	-0.438717	-1.404868	2.348344

$TS_{D'-K'}$

E = -1322.5672522au

Rh	0.053310	-0.484740	0.108660
C	-0.185948	-2.619027	0.949128
C	1.091463	-2.527181	0.379231
C	1.810165	-1.434601	1.038333
C	-0.285306	-1.569451	1.961901
C	0.984884	-0.937136	2.097341
C	-4.492632	2.862275	0.224847
C	-4.977157	1.558161	0.166188
C	-4.112553	0.508829	-0.101012
C	-2.735306	0.735533	-0.287752
C	-2.240280	2.056767	-0.256565
C	-3.137988	3.090634	0.006708
H	-5.163028	3.695108	0.428852
H	-6.035584	1.355505	0.326221
H	-4.464039	-0.520598	-0.155999
H	-2.754445	4.112137	0.031608
O	-1.993521	-0.354371	-0.464238
N	-0.394609	-0.286221	-1.809101
C	-0.424972	-1.420292	-2.547260
C	0.557957	-1.230348	-3.709133
H	1.308740	-0.451043	-3.534638
H	1.054374	-2.194457	-3.869048
H	-0.012348	-0.972793	-4.609051
O	-1.085842	-2.439779	-2.420689
C	0.220377	1.629740	0.277822
C	-0.804360	2.360251	-0.569812
C	1.370219	0.047181	3.142458
H	1.730982	-0.470785	4.042974
H	2.173916	0.709194	2.799818
H	0.522479	0.674793	3.447589
C	-1.501071	-1.295148	2.777097
H	-1.516325	-1.908761	3.690026
H	-1.550761	-0.240288	3.076246
H	-2.412073	-1.516128	2.207752
C	-1.304602	-3.525215	0.572437

H	-1.602130	-4.155134	1.423537
H	-2.179825	-2.944957	0.250793
H	-1.033840	-4.174260	-0.265789
C	1.632801	-3.358917	-0.729845
H	2.122371	-4.263997	-0.342328
H	0.836105	-3.668492	-1.417320
H	2.383497	-2.808125	-1.311806
C	3.227211	-1.057500	0.778059
H	3.919645	-1.712114	1.328523
H	3.472460	-1.134323	-0.288750
H	3.429005	-0.020563	1.075850
H	-0.608495	2.168950	-1.634028
H	-0.644494	3.443248	-0.423056
H	0.004836	1.809021	1.344625
C	1.626284	1.997222	-0.035884
C	2.447546	2.574357	0.944188
C	2.172449	1.824746	-1.317902
C	3.763851	2.934577	0.667869
H	2.030526	2.768447	1.933578
C	3.482274	2.187737	-1.597851
H	1.549940	1.376222	-2.092590
C	4.291388	2.736290	-0.603231
H	4.375384	3.384241	1.449338
H	3.880241	2.039098	-2.601106
H	5.320939	3.014019	-0.822576

K’

E = -1322.5933161au

Rh	0.074741	-0.576078	-0.073541
C	-1.967708	-1.506900	-0.329915
C	-1.523707	-1.147509	-1.653351
C	-0.342684	-1.881626	-1.934211
C	-1.083585	-2.526130	0.169702
C	-0.053872	-2.724886	-0.803983
C	4.812062	2.452794	0.245078
C	5.163770	1.198286	-0.250418
C	4.179269	0.290335	-0.601752
C	2.811507	0.610320	-0.485260
C	2.453193	1.878952	0.009287
C	3.466483	2.770812	0.365694
H	5.576198	3.173339	0.530871
H	6.212697	0.922853	-0.357272
H	4.431697	-0.696900	-0.987419
H	3.175751	3.751245	0.749680
O	1.941564	-0.309944	-0.886322
N	0.472769	-0.082786	1.676071
C	0.026889	-0.725785	2.780499
C	1.066297	-1.587812	3.461528
H	1.639514	-0.975244	4.167947
H	0.556824	-2.378222	4.024707
H	1.773958	-2.019382	2.742458
O	-1.102573	-0.549967	3.247253
C	-0.058365	1.542759	-0.528664
C	-1.420073	2.061760	-0.241732
C	-2.136687	2.704320	-1.261387
C	-1.995063	2.009753	1.036702
C	-3.387349	3.264437	-1.022375
H	-1.694102	2.774988	-2.256440
C	-3.243176	2.571518	1.276211
H	-1.482299	1.477478	1.839293
C	-3.947761	3.195528	0.249318
H	-3.920922	3.761116	-1.831714
H	-3.675106	2.505594	2.273689
H	-4.929220	3.627333	0.439184
C	1.025507	2.307769	0.194379
C	1.125518	-3.628503	-0.716558
H	1.047100	-4.459534	-1.432731
H	2.044361	-3.072196	-0.947315
H	1.235388	-4.059951	0.285122
C	-1.302717	-3.285791	1.429305
H	-2.127018	-4.002301	1.298185
H	-0.414543	-3.858433	1.722073
H	-1.577529	-2.622173	2.261868
C	-3.199640	-1.051445	0.370180
H	-3.986672	-1.818271	0.306197
H	-2.992159	-0.862731	1.433075
H	-3.595679	-0.122798	-0.056684
C	-2.236256	-0.266497	-2.616611
H	-2.838749	-0.876979	-3.305313
H	-2.911051	0.435910	-2.116386
H	-1.537902	0.320124	-3.227193
C	0.516565	-1.776153	-3.141870
H	0.793450	-2.769841	-3.518617
H	0.018683	-1.233312	-3.953368
H	1.446016	-1.242995	-2.882258
H	0.780287	2.346246	1.266284
H	0.937195	3.350382	-0.166384
H	0.138681	1.505124	-1.610911

$TS_{D1'-J}$

E = -1322.4792399au

N	-1.683607	-0.426693	1.105623
C	0.097493	-2.661021	-0.693083
C	0.374665	-1.919769	-1.871017
C	1.580856	-1.171028	-1.612467
C	2.141062	-1.623175	-0.353312
C	1.214751	-2.496048	0.235096
Rh	0.056897	-0.506028	-0.164068
C	-0.368368	1.574112	-0.582753
H	0.123010	1.899045	-1.506235
C	0.442190	1.472661	0.588986
H	-0.085314	1.516239	1.545432
C	-2.858974	1.251146	-0.193921
C	-1.767110	2.075660	-0.475242
C	-4.158447	1.711927	-0.071199
C	-2.053265	3.432078	-0.656240
C	-4.404472	3.069839	-0.239887
H	-4.957440	1.002988	0.137442
C	-3.348057	3.926108	-0.537933
H	-1.228644	4.109125	-0.880635
H	-5.417661	3.455000	-0.145338
H	-3.533022	4.990022	-0.675898
C	2.294264	-0.326668	-2.612940
H	2.959427	0.398135	-2.127170
H	2.913179	-0.945731	-3.280799
H	1.591946	0.232862	-3.245282
C	3.452266	-1.183333	0.192862
H	4.282842	-1.695363	-0.316550
H	3.606234	-0.103595	0.061817
H	3.536164	-1.393663	1.265834
C	-0.395749	-1.912479	-3.148749
H	-0.404948	-0.915091	-3.607145
H	0.041403	-2.606047	-3.883836
H	-1.439995	-2.213756	-2.996031
C	-1.040136	-3.596022	-0.454065
H	-1.919334	-3.333674	-1.058968
H	-0.765305	-4.631931	-0.704629
H	-1.336455	-3.586428	0.604206
C	1.305262	-3.189731	1.549812
H	0.418690	-2.979430	2.165800
H	1.374187	-4.280234	1.415941
H	2.188543	-2.868606	2.114090
C	-3.658889	-1.838252	1.670470
H	-3.812013	-2.334000	0.703639
H	-3.918528	-2.528763	2.477642
H	-4.322975	-0.966326	1.699714
O	-2.646370	-0.131675	-0.099758
C	-2.212633	-1.445173	1.849275
O	-1.492877	-1.977249	2.689420
C	1.859903	1.849008	0.677307
C	2.531348	1.659937	1.895433
C	2.577013	2.425450	-0.380377
C	3.861568	2.025060	2.049084
H	1.987142	1.205462	2.725036
C	3.912216	2.786566	-0.229610
H	2.078074	2.615558	-1.331049
C	4.562340	2.590432	0.985561
H	4.355936	1.869025	3.007092
H	4.443093	3.240895	-1.065549
H	5.604506	2.881408	1.105139
H	-1.670460	-0.327321	-0.763835

L'

E = -1551.5910204au

Rh	-0.148692	0.306182	-0.430032
C	0.941860	1.070733	-2.283501
C	0.964995	-0.384054	-2.159036
C	-0.382975	-0.860624	-2.309899
C	-0.391129	1.480707	-2.373421
C	-1.231123	0.280229	-2.309321
C	4.216027	-2.830945	0.504658
C	4.784867	-1.634965	0.929756
C	3.957993	-0.621640	1.396120
C	2.573015	-0.788826	1.441988
C	1.976705	-1.981948	1.011828
C	2.837132	-2.985821	0.551109
H	4.843229	-3.643375	0.141454
H	5.864207	-1.494224	0.910478
H	4.373806	0.311610	1.770925
H	2.393641	-3.927449	0.219217
O	1.838337	0.223732	2.026295
N	1.163257	1.065575	1.085532
C	1.700100	2.323126	0.979539
C	2.937482	2.687099	1.762832
H	2.974838	3.776933	1.846320
H	2.971721	2.223496	2.752656

H	3.826372	2.358391	1.206060
O	1.135507	3.157424	0.270392
C	-0.512104	-1.183495	1.086264
C	-1.930896	-1.616716	1.028414
C	-2.904490	-0.888613	1.735697
C	-2.381755	-2.742205	0.319918
C	-4.252188	-1.208622	1.672477
H	-2.574821	-0.066684	2.371855
C	-3.733008	-3.068551	0.252286
H	-1.664496	-3.390291	-0.179926
C	-4.681843	-2.293760	0.911048
H	-4.973914	-0.617489	2.236444
H	-4.043285	-3.948604	-0.310932
H	-5.738679	-2.549829	0.858820
C	0.502616	-2.309943	1.046967
C	-2.719469	0.278066	-2.344701
H	-3.098532	0.521608	-3.348399
H	-3.124363	-0.698826	-2.050456
H	-3.119618	1.017266	-1.639012
C	-0.876411	2.887210	-2.429098
H	-0.714017	3.321764	-3.426295
H	-1.948621	2.948143	-2.210935
H	-0.346727	3.504314	-1.691678
C	2.156677	1.927872	-2.297052
H	2.599179	1.952560	-3.304489
H	1.931242	2.950744	-1.979198
H	2.922660	1.533491	-1.614386
C	2.200017	-1.206934	-2.264930
H	2.532330	-1.247079	-3.314632
H	3.025749	-0.792403	-1.673861
H	2.040524	-2.236342	-1.926315
C	-0.787672	-2.271450	-2.542536
H	-0.727742	-2.502667	-3.616855
H	-0.131251	-2.982761	-2.024004
H	-1.817032	-2.461950	-2.219137
C	-1.918454	2.195262	1.514085
O	-1.836415	1.631860	0.426685
O	-1.003325	2.112646	2.448847
H	-0.210022	1.632735	2.052306
C	-3.132023	2.974351	1.906992
H	-2.900704	3.714115	2.677739
H	-3.567519	3.453181	1.025904
H	-3.874594	2.271054	2.308443
H	-0.364750	-0.599939	2.002241
H	0.309675	-2.955841	0.175348
H	0.323338	-2.971419	1.918365

$TS_{L'-M'}$

E = -1551.5443812au

Rh	0.156360	-0.522584	-0.367165
C	-0.400838	-1.483366	-2.403965
C	-0.244394	-0.035937	-2.455816
C	1.139585	0.264959	-2.227289
C	0.812503	-2.034799	-1.968274
C	1.770363	-0.941540	-1.804175
C	-3.712061	3.580274	-0.387407
C	-4.563465	2.627402	0.166325
C	-4.012200	1.557929	0.846764
C	-2.627060	1.423319	0.991062
C	-1.744219	2.356837	0.433970
C	-2.342407	3.432484	-0.242694
H	-4.112836	4.433847	-0.930918
H	-5.643398	2.716892	0.068214
H	-4.638362	0.788763	1.294983
H	-1.679490	4.182894	-0.677799
O	-2.281718	0.256524	1.628659
N	-1.689231	-0.914499	0.284610
C	-2.134829	-2.139201	0.704535
C	-3.120225	-2.277928	1.832153
H	-2.671198	-1.960020	2.779883
H	-4.011539	-1.663673	1.666382
H	-3.402282	-3.333649	1.886428
O	-1.738552	-3.112276	0.062645
C	0.609099	1.212757	0.860564
C	2.073948	1.506958	0.899277
C	2.962231	0.595241	1.501567
C	2.635593	2.697612	0.408313
C	4.324124	0.844233	1.580584
H	2.568846	-0.343505	1.885108
C	4.003845	2.948696	0.483671
H	2.001335	3.459857	-0.040497
C	4.860485	2.022536	1.064249
H	4.975839	0.108758	2.051230
H	4.396809	3.885515	0.089514
H	5.929466	2.219680	1.126207
C	-0.233236	2.416987	0.500913
C	3.203862	-1.130485	-1.452715
H	3.774895	-1.497544	-2.319150

H	3.666008	-0.197477	-1.108177
H	3.315635	-1.865891	-0.644955
C	1.104248	-3.453470	-1.631480
H	1.953989	-3.834761	-2.216063
H	1.357339	-3.544313	-0.565628
H	0.237251	-4.096345	-1.811479
C	-1.660925	-2.183203	-2.768512
H	-1.800479	-2.147782	-3.859910
H	-1.664512	-3.225163	-2.440399
H	-2.530461	-1.695096	-2.311548
C	-1.302559	0.905629	-2.916689
H	-1.446268	0.843054	-4.006356
H	-2.263810	0.677524	-2.437290
H	-1.059033	1.946083	-2.667712
C	1.800716	1.567481	-2.493335
H	2.073153	1.624890	-3.557744
H	1.140733	2.419227	-2.284239
H	2.714555	1.702001	-1.905134
C	0.415955	-1.594972	2.544852
O	0.836806	-1.662378	1.344880
O	-0.427573	-0.793356	3.010863
H	-1.416339	0.131270	2.154724
C	1.032401	-2.610395	3.481378
H	2.124393	-2.604025	3.381243
H	0.748367	-2.407097	4.517446
H	0.689975	-3.613712	3.199034
H	0.333083	0.809461	1.836721
H	0.086447	2.793988	-0.483895
H	0.025378	3.239801	1.198589

M’

E = -1551.5661au

Rh	-0.142232	0.646801	-0.201166
C	-0.102310	2.531167	-1.510537
C	-0.287542	1.379062	-2.343615
C	-1.571947	0.794995	-2.030749
C	-1.180261	2.565929	-0.582534
C	-2.110934	1.493394	-0.920835
C	3.813660	-1.870599	-2.022721
C	4.544756	-2.127451	-0.867012
C	3.878599	-2.400071	0.322291
C	2.485236	-2.412855	0.374380
C	1.736050	-2.181436	-0.791207
C	2.424402	-1.910379	-1.974173
H	4.321548	-1.659682	-2.962537
H	5.633528	-2.117071	-0.890600
H	4.420516	-2.606680	1.244235
H	1.848055	-1.735304	-2.885637
O	1.866787	-2.722868	1.549043
N	1.682121	0.946811	0.029281
C	2.330061	1.562383	1.040926
C	3.640783	0.926926	1.415965
H	3.484681	0.375063	2.351841
H	3.992791	0.226406	0.649758
H	4.383613	1.715085	1.584001
O	1.913384	2.609756	1.551229
C	-0.551293	-1.460244	0.183230
C	-1.983906	-1.786808	0.338766
C	-2.667174	-1.375815	1.497441
C	-2.692691	-2.568523	-0.587974
C	-3.999691	-1.702077	1.703360
H	-2.130288	-0.775119	2.229958
C	-4.030784	-2.890861	-0.384726
H	-2.188445	-2.949579	-1.474966
C	-4.694018	-2.454170	0.757841
H	-4.500166	-1.372050	2.612744
H	-4.553638	-3.502451	-1.118981
H	-5.738783	-2.713936	0.920103
C	0.238133	-2.305114	-0.797688
C	-3.430824	1.300324	-0.262782
H	-4.089475	2.158373	-0.461789
H	-3.938191	0.394995	-0.613576
H	-3.318881	1.209424	0.826046
C	-1.322587	3.543792	0.526963
H	-1.444764	4.561721	0.129504
H	-2.186536	3.311211	1.157507
H	-0.422609	3.523946	1.159940
C	1.028523	3.494768	-1.570051
H	0.752029	4.363981	-2.185605
H	1.297283	3.848663	-0.568069
H	1.920436	3.037965	-2.012775
C	0.632815	0.964705	-3.435929
H	0.611680	1.686831	-4.265469
H	1.666984	0.904456	-3.070354
H	0.362922	-0.017661	-3.841715
C	-2.226125	-0.272039	-2.831101
H	-2.607363	0.148876	-3.773081
H	-1.522840	-1.072704	-3.097965

H	-3.066673	-0.733815	-2.302006
C	0.259928	0.490407	2.839602
O	-0.491285	0.882510	1.869073
O	1.133052	-0.384072	2.799173
C	0.001749	1.245497	4.123131
H	0.421467	0.707684	4.977978
H	0.494869	2.222695	4.034355
H	-1.069204	1.424682	4.268163
H	1.645352	-1.894293	2.034988
H	-0.070311	-1.429821	1.160320
H	-0.123826	-2.152023	-1.828370
H	-0.011309	-3.355635	-0.550184

$TS_{M'-K}$

E = -1551.5285197au

Rh	0.388103	-0.584952	-0.204242
C	1.284223	-2.340848	-1.398533
C	1.405256	-1.100326	-2.100803
C	2.309337	-0.244698	-1.363615
C	1.939238	-2.172500	-0.137670
C	2.639631	-0.900813	-0.147535
C	-4.386236	2.700005	-1.388164
C	-5.148266	2.367921	-0.269271
C	-4.596219	1.604561	0.743781
C	-3.271522	1.153610	0.681509
C	-2.478118	1.527457	-0.422348
C	-3.071327	2.269415	-1.452492
H	-4.809599	3.290618	-2.197700
H	-6.183652	2.696048	-0.192604
H	-5.175011	1.313472	1.618267
H	-2.461193	2.535579	-2.317355
O	-2.858923	0.414569	1.720402
N	-1.491648	-1.558400	-0.929317
C	-1.756587	-2.697967	-0.296156
C	-3.101207	-3.208264	-0.856385
H	-3.765294	-3.378037	-0.000859
H	-3.582658	-2.528367	-1.564603
H	-2.906795	-4.173539	-1.341329
O	-1.151095	-3.404325	0.514714
C	-0.025052	1.460213	0.456936
C	1.026442	2.475036	0.359313
C	1.992911	2.531093	1.378625
C	1.060712	3.442080	-0.653626
C	2.984029	3.500821	1.357471
H	1.952650	1.780445	2.171511
C	2.050064	4.420021	-0.665700
H	0.283645	3.456247	-1.418324
C	3.019409	4.446911	0.331346
H	3.730019	3.528417	2.150249
H	2.055146	5.172217	-1.452909
H	3.792024	5.213786	0.321408
C	-1.009887	1.217954	-0.589595
C	3.626373	-0.462928	0.872783
H	4.563995	-1.026903	0.757109
H	3.864014	0.603213	0.777401
H	3.236166	-0.633755	1.881598
C	2.009736	-3.195342	0.937662
H	2.743584	-3.972646	0.676584
H	2.301586	-2.745093	1.892544
H	1.023227	-3.661002	1.059793
C	0.668565	-3.579886	-1.933530
H	1.408230	-4.116932	-2.547383
H	0.330609	-4.237834	-1.128080
H	-0.194683	-3.351124	-2.570292
C	0.804046	-0.819719	-3.432618
H	1.326467	-1.373560	-4.226309
H	-0.250271	-1.126628	-3.445640
H	0.852498	0.246524	-3.684585
C	2.881712	1.027134	-1.874322
H	3.674676	0.807647	-2.604638
H	2.133779	1.646549	-2.384406
H	3.319485	1.632436	-1.073599
C	0.102166	-0.951624	2.770894
O	-0.560636	-0.899520	1.651973
O	1.281839	-0.645408	2.912492
C	-0.745712	-1.466220	3.909686
H	-1.055718	-2.492111	3.673459
H	-0.183265	-1.448075	4.847060
H	-1.660591	-0.869322	4.009032
H	-2.051373	-0.133900	1.558741
H	-0.371654	1.307863	1.478980
H	-0.677713	1.569019	-1.573669
H	-1.257198	-0.040707	-0.755828

$TS_{C1'-D2'}$

E = -1322.5767759au

N	1.490794	1.460565	-0.776300
C	-0.190895	2.384538	0.470386

C	-0.570403	3.370261	1.379048
H	-0.042689	4.322208	1.369038
C	-1.584674	3.106530	2.291158
H	-1.880320	3.877139	3.001393
C	-2.209912	1.859567	2.308789
H	-3.001150	1.650415	3.026636
C	-1.835968	0.889916	1.385225
H	-2.365356	-0.063600	1.370231
C	-0.827344	1.124827	0.443104
C	2.135589	-1.987748	-0.073291
C	2.522864	-1.001866	0.913444
C	1.525296	-0.943931	1.933084
C	0.489546	-1.862396	1.555465
C	0.879024	-2.525630	0.340445
Rh	0.667909	-0.342794	-0.095627
C	-1.238023	0.469813	-1.336930
C	-0.233100	-0.366001	-1.970585
C	0.156747	-3.651424	-0.318011
H	0.645071	-4.611358	-0.094634
H	-0.880759	-3.730111	0.030311
H	0.140858	-3.546646	-1.411143
C	2.949112	-2.405813	-1.249345
H	3.810714	-3.018115	-0.942428
H	2.350389	-3.002663	-1.949057
H	3.316978	-1.524953	-1.790903
C	3.785753	-0.218176	0.857145
H	4.609539	-0.796940	1.300669
H	4.043716	0.019316	-0.181732
H	3.702735	0.725793	1.408404
C	1.506286	-0.040215	3.119165
H	0.517990	0.421916	3.257763
H	1.759539	-0.571327	4.048567
H	2.227196	0.777739	2.998599
C	-0.729745	-2.172398	2.354464
H	-0.566153	-3.067803	2.972539
H	-0.988584	-1.348309	3.029254
H	-1.603408	-2.369758	1.717780
C	2.698576	3.101730	-2.142356
H	3.510949	3.090485	-2.873780
H	1.805020	3.557183	-2.586307
H	2.977555	3.724500	-1.284128
H	0.431318	0.097061	-2.698973
H	-1.220839	1.501297	-1.701577
O	0.808140	2.664662	-0.386585
C	2.430111	1.674986	-1.719197
O	3.068434	0.727452	-2.196624
H	-0.519955	-1.388070	-2.230284
C	-2.625614	-0.052245	-1.192108
C	-3.696379	0.843092	-1.242048
C	-2.897020	-1.407398	-0.992479
C	-5.005552	0.397535	-1.106410
H	-3.490410	1.906574	-1.373595
C	-4.204601	-1.855494	-0.844353
H	-2.074079	-2.120508	-0.944472
C	-5.264198	-0.954570	-0.902557
H	-5.826896	1.110569	-1.154926
H	-4.397524	-2.915808	-0.687042
H	-6.288355	-1.306317	-0.790724

D2’

E = -1322.6051014au

Rh	0.917811	0.303421	-0.300440
C	2.796990	0.211802	1.102488
C	2.410488	-1.081886	0.547537
C	2.551598	-1.052356	-0.867033
C	3.044187	1.069089	0.033083
C	2.824769	0.311717	-1.211141
C	-5.181660	0.242053	-0.139487
C	-5.036892	1.621430	-0.022254
C	-3.786482	2.188702	-0.211084
C	-2.676817	1.397294	-0.520208
C	-2.808325	0.015172	-0.692509
C	-4.080663	-0.530523	-0.475470
H	-6.151976	-0.228028	0.011268
H	-5.891170	2.251603	0.219282
H	-3.640617	3.264838	-0.139466
H	-4.199016	-1.608889	-0.598473
O	-1.502599	2.084689	-0.745669
N	-0.442141	1.720269	0.128709
C	-0.184020	2.709782	1.054138
C	-1.097945	3.907889	1.118193
H	-1.225815	4.379835	0.138102
H	-2.093478	3.608073	1.469282
H	-0.670918	4.618788	1.830897
O	0.761222	2.594965	1.828465
C	-0.439488	-0.346277	-1.725593
C	-1.740312	-0.943831	-1.185737
C	3.044965	0.846485	-2.581290

H	4.110353	0.805312	-2.855275
H	2.483325	0.274392	-3.329786
H	2.723477	1.892278	-2.656511
C	3.393998	2.512740	0.084478
H	4.476328	2.664732	-0.040232
H	2.890305	3.065567	-0.719658
H	3.075218	2.962324	1.030101
C	2.832083	0.507004	2.559619
H	3.565646	-0.134793	3.070214
H	3.088743	1.551569	2.755367
H	1.851251	0.334094	3.021825
C	2.092974	-2.270118	1.378822
H	3.024234	-2.724035	1.753045
H	1.490430	-1.992502	2.252487
H	1.541755	-3.037202	0.821835
C	2.409440	-2.212212	-1.790079
H	3.345098	-2.786950	-1.848416
H	1.617076	-2.894643	-1.453617
H	2.157266	-1.894561	-2.809283
H	-2.216895	-1.443585	-2.053460
H	-0.651096	0.512551	-2.378732
H	0.064219	-1.125913	-2.317685
C	-1.466709	-2.062405	-0.193535
C	-1.151559	-3.336682	-0.671575
C	-1.515849	-1.865522	1.188757
C	-0.895042	-4.390508	0.201766
H	-1.124382	-3.504663	-1.750744
C	-1.272599	-2.918462	2.065323
H	-1.766294	-0.877616	1.577266
C	-0.962272	-4.185142	1.577102
H	-0.664560	-5.378981	-0.194205
H	-1.332287	-2.748669	3.139948
H	-0.780842	-5.009388	2.265235

$TS_{C1'-D3'}$

E = -1322.5752818au

Rh	0.220467	0.149601	0.231456
C	0.891043	1.028461	2.130775
C	-0.269559	1.736692	1.654544
C	-1.401901	0.840939	1.758431
C	0.488789	-0.321132	2.367956
C	-0.944603	-0.422324	2.178710
C	3.466919	2.437325	-1.635255
C	4.345547	1.408347	-1.958169
C	3.987013	0.083175	-1.727335
C	2.751231	-0.185400	-1.147173
C	1.864244	0.826460	-0.767760
C	2.232349	2.138873	-1.051295
H	3.736833	3.473067	-1.837689
H	5.310547	1.630831	-2.410901
H	4.641906	-0.741844	-2.003928
H	1.547311	2.954752	-0.806900
O	2.406171	-1.502353	-0.982678
N	1.031410	-1.616475	-0.647368
C	0.681062	-2.906407	-0.344565
C	1.770970	-3.945448	-0.319961
H	2.235610	-4.048746	-1.307982
H	2.571267	-3.662716	0.374349
H	1.326685	-4.897538	-0.018181
O	-0.498523	-3.183300	-0.130202
C	-0.140773	-0.884755	-2.135909
C	-0.845578	0.275504	-1.766254
C	-2.805611	1.258180	1.514210
H	-3.195505	1.789514	2.395830
H	-2.882113	1.941682	0.659697
H	-3.465435	0.408748	1.307826
C	-1.754118	-1.647388	2.429494
H	-2.812649	-1.476098	2.201235
H	-1.416163	-2.485738	1.804277
H	-1.687834	-1.955598	3.483334
C	1.369411	-1.440160	2.804996
H	1.489957	-1.453054	3.898387
H	0.947065	-2.409579	2.509547
H	2.369932	-1.357309	2.359057
C	2.248343	1.595512	2.362792
H	2.322280	2.019364	3.375087
H	3.027995	0.829792	2.263954
H	2.488823	2.388961	1.645071
C	-0.371726	3.195208	1.362078
H	-0.850659	3.738534	2.191212
H	0.615938	3.644549	1.203491
H	-0.971176	3.382612	0.459709
H	0.754976	-0.793006	-2.747609
H	-0.450136	1.220449	-2.149677
H	-0.677628	-1.830634	-2.211569
C	-2.305865	0.235593	-1.578587
C	-3.062029	1.372616	-1.892468
C	-2.984893	-0.912150	-1.136912

C	-4.449084	1.366274	-1.788531
H	-2.545809	2.269180	-2.241948
C	-4.370274	-0.915046	-1.036154
H	-2.417552	-1.799864	-0.848626
C	-5.111994	0.220246	-1.361296
H	-5.014161	2.260621	-2.048631
H	-4.878180	-1.817150	-0.695961
H	-6.197699	0.209523	-1.281529

D3’

E = -1322.605818au

Rh	-0.255074	0.221087	0.203722
C	-0.927893	1.723124	1.771595
C	0.208174	0.922079	2.189752
C	1.354998	1.344069	1.414355
C	-0.515771	2.479530	0.658620
C	0.901484	2.236928	0.427665
C	-3.510050	-2.418577	1.546148
C	-4.224260	-2.585188	0.364065
C	-3.749259	-2.017628	-0.814183
C	-2.582055	-1.267461	-0.764250
C	-1.852852	-1.036342	0.403265
C	-2.336162	-1.662682	1.554400
H	-3.861327	-2.883513	2.466725
H	-5.139347	-3.174717	0.349231
H	-4.262239	-2.156755	-1.764821
H	-1.780656	-1.567004	2.489648
O	-2.139647	-0.749051	-1.977417
N	-0.793905	-0.338672	-1.878986
C	-0.540003	0.751140	-2.754993
C	-1.734508	1.585895	-3.100235
H	-2.365775	1.052493	-3.821247
H	-2.354419	1.782265	-2.218945
H	-1.382941	2.520134	-3.547632
O	0.586985	0.969541	-3.145109
C	0.157289	-1.497971	-1.851555
C	0.734037	-1.568138	-0.451542
C	2.752283	0.935895	1.707862
H	3.156212	1.550845	2.526804
H	2.810148	-0.112260	2.025774
H	3.415992	1.045707	0.843153
C	1.710877	2.908183	-0.628589
H	2.741665	2.534753	-0.639599
H	1.299093	2.735966	-1.634178
H	1.751918	3.996400	-0.470327
C	-1.330097	3.458525	-0.115179
H	-1.244215	4.469028	0.312806
H	-0.990123	3.526734	-1.156978
H	-2.396082	3.196232	-0.123536
C	-2.269424	1.732817	2.416853
H	-2.260515	2.339132	3.334915
H	-3.034072	2.149536	1.749791
H	-2.597954	0.721629	2.689984
C	0.291785	0.071314	3.411549
H	0.794734	0.602337	4.234663
H	-0.702584	-0.219901	3.771101
H	0.861993	-0.848187	3.215839
H	-0.437407	-2.376000	-2.133838
H	0.330374	-2.412538	0.118454
H	0.907806	-1.317823	-2.628940
C	2.207130	-1.530721	-0.350709
C	2.853275	-2.300354	0.628845
C	3.011656	-0.758989	-1.207493
C	4.238673	-2.311745	0.745817
H	2.244763	-2.911921	1.298614
C	4.396302	-0.776014	-1.094360
H	2.541405	-0.123290	-1.959993
C	5.020542	-1.550586	-0.117995
H	4.710853	-2.926879	1.511159
H	4.996618	-0.173683	-1.776020
H	6.106030	-1.563485	-0.035227

$TS_{C1'\text{-}D4'}$

E = -1322.5722567au

Rh	-0.716990	-0.375921	-0.161375
C	-2.426743	-1.455402	0.813266
C	-2.246766	-1.858846	-0.561198
C	-0.991659	-2.573426	-0.644914
C	-1.244081	-1.812670	1.515836
C	-0.369969	-2.544559	0.620849
C	-3.393993	2.966427	-1.137596
C	-2.762045	4.016417	-0.481208
C	-1.563836	3.794318	0.190776
C	-1.030902	2.509269	0.208196
C	-1.654144	1.420046	-0.408628
C	-2.832867	1.686764	-1.104078
H	-4.322892	3.138245	-1.680385
H	-3.190761	5.017224	-0.500311

H	-1.033817	4.601527	0.694736
H	-3.334749	0.879780	-1.642249
O	0.173742	2.352787	0.847255
N	0.669950	1.036612	0.686672
C	1.616745	0.752425	1.652774
C	2.023032	1.860817	2.587032
H	2.376951	2.735871	2.027809
H	1.172076	2.197211	3.190973
H	2.817847	1.482877	3.235409
O	2.123518	-0.361062	1.699819
C	1.378165	0.970888	-1.235093
C	0.393171	0.187032	-1.916081
C	-0.492176	-3.236690	-1.881843
H	-0.923353	-4.243690	-1.986588
H	-0.773122	-2.671539	-2.780143
H	0.599776	-3.346079	-1.883162
C	0.907790	-3.199685	1.021239
H	1.391561	-3.691673	0.167550
H	1.614197	-2.470733	1.437567
H	0.728553	-3.975172	1.781271
C	-0.943355	-1.557481	2.952199
H	-1.244802	-2.409600	3.580094
H	0.131673	-1.400855	3.099597
H	-1.467479	-0.668318	3.324326
C	-3.633634	-0.783041	1.369696
H	-4.447143	-1.504361	1.537282
H	-3.416856	-0.298692	2.329326
H	-4.008939	-0.003333	0.693565
C	-3.274618	-1.817707	-1.641342
H	-3.712888	-2.813004	-1.813170
H	-4.099127	-1.141217	-1.385316
H	-2.849622	-1.475520	-2.595587
H	1.233480	2.054425	-1.241625
H	-0.283402	0.753814	-2.559772
H	0.752018	-0.740426	-2.371071
C	2.765214	0.558029	-1.042920
C	3.731923	1.540549	-0.799211
C	3.155907	-0.785578	-1.067301
C	5.062979	1.194448	-0.611818
H	3.425520	2.587409	-0.763829
C	4.484250	-1.133159	-0.876296
H	2.401179	-1.559278	-1.202735
C	5.440504	-0.144915	-0.653528
H	5.807912	1.968265	-0.435540
H	4.776734	-2.181523	-0.888751
H	6.482973	-0.420916	-0.503533

D4’

E = -1322.5890282au

Rh	-0.776534	-0.307261	-0.195942
C	-2.747359	-1.264097	0.497743
C	-2.418286	-1.501937	-0.897019
C	-1.266050	-2.376926	-0.935323
C	-1.735129	-1.860880	1.271700
C	-0.818197	-2.562759	0.386841
C	-2.825754	3.491834	-1.036224
C	-2.061871	4.381919	-0.288806
C	-0.937394	3.922628	0.390182
C	-0.626675	2.571064	0.321568
C	-1.381261	1.631389	-0.386174
C	-2.477652	2.140605	-1.086380
H	-3.694018	3.847837	-1.589838
H	-2.325969	5.437177	-0.245230
H	-0.300278	4.594646	0.963658
H	-3.081383	1.468074	-1.698371
O	0.521147	2.179740	1.002127
N	0.907449	0.873188	0.637383
C	1.381202	0.164473	1.778948
C	0.960562	0.729607	3.104929
H	1.436397	1.700049	3.285328
H	-0.123395	0.894128	3.136761
H	1.262023	0.019812	3.880328
O	2.024185	-0.852442	1.651064
C	1.613827	0.889172	-0.741916
C	0.640507	0.162379	-1.647706
C	-0.688668	-2.957829	-2.179246
H	-1.227718	-3.869523	-2.477249
H	-0.754338	-2.250746	-3.016344
H	0.368761	-3.224977	-2.055059
C	0.325704	-3.397136	0.849770
H	0.900396	-3.794315	0.004244
H	1.021087	-2.825792	1.479349
H	-0.026640	-4.258104	1.438211
C	-1.602656	-1.862059	2.756248
H	-2.020213	-2.782469	3.191939
H	-0.546727	-1.820437	3.058985
H	-2.121187	-1.012889	3.218678
C	-3.926887	-0.491548	0.978523

H	-4.858361	-1.064774	0.859478
H	-3.832369	-0.231444	2.039635
H	-4.043873	0.451058	0.425462
C	-3.291791	-1.197651	-2.067127
H	-3.841783	-2.093444	-2.394647
H	-4.037328	-0.431001	-1.823975
H	-2.708930	-0.834943	-2.925232
H	1.603931	1.964843	-0.959428
H	0.257811	0.798560	-2.453747
H	1.034889	-0.770959	-2.066413
C	3.051885	0.452557	-0.694334
C	4.028386	1.412591	-0.425872
C	3.448995	-0.867770	-0.911971
C	5.376027	1.069457	-0.383549
H	3.723172	2.446035	-0.251308
C	4.792541	-1.214178	-0.875023
H	2.692215	-1.634936	-1.076345
C	5.760246	-0.246374	-0.613941
H	6.125536	1.832848	-0.180750
H	5.088333	-2.248457	-1.043431
H	6.813693	-0.520968	-0.589519