

Supporting Information

Rational design of model Pd(II)-catalysts for C-H activations involving ligands with charge-shift bonding characters

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Cartesian coordinates and electronic energies of the complexes and the transition states.

Methane

E = -40.51766309 a.u.

C	0.000000	0.000000	0.000000
H	0.631397	0.631397	0.631397
H	-0.631397	-0.631397	0.631397
H	-0.631397	0.631397	-0.631397
H	0.631397	-0.631397	-0.631397

HOTFA4-OTFA

E = -2633.484697 a.u.

C	0.387504	4.527111	-0.513503
F	-0.438834	4.604487	0.547188
C	0.720604	3.065006	-0.889226
O	0.899893	2.349227	0.206420
F	-0.185114	5.164329	-1.541671
F	1.523782	5.187349	-0.194615
O	0.823589	2.716767	-2.040972
O	1.356338	-0.259361	-0.100736
C	0.431555	-1.075692	0.137273
C	0.857288	-2.568573	0.185328
F	2.043801	-2.711414	0.808475
O	-0.785463	-0.827787	0.312767
F	-0.039893	-3.326393	0.841415
F	0.985765	-3.051491	-1.062630
O	-2.047684	1.495757	-0.162264
C	-2.496373	2.154417	0.893036
C	-3.330103	3.377668	0.446915
F	-4.608378	2.992656	0.226330
O	-2.364071	1.878114	2.060776
F	-2.871029	3.935108	-0.685963
F	-3.342886	4.314765	1.404256
O	-2.873258	-2.478848	0.560043
C	-2.987176	-3.324731	-0.446971
C	-4.283482	-4.152270	-0.290864
F	-4.396804	-5.051188	-1.277668
O	-2.238825	-3.482994	-1.382550
F	-4.294942	-4.815614	0.882705
F	-5.369559	-3.354036	-0.324385
O	3.936088	-0.784308	-0.572193
C	4.704905	-0.862653	0.498341
C	6.163930	-1.144700	0.070920
F	6.977131	-1.160444	1.135678
O	4.394493	-0.746384	1.659856
F	6.259018	-2.340553	-0.545337
F	6.611807	-0.203792	-0.783821
H	1.076489	1.382677	-0.013508
H	-1.529304	0.681556	0.115020
H	-2.029008	-1.940838	0.465423
H	2.976352	-0.632284	-0.313226

HOTFA4

E = -2107.167475 a.u.

C	3.893274	-0.529590	-0.165411
O	3.622195	-1.029119	1.011674
O	3.309845	0.358182	-0.763964
C	5.123422	-1.224763	-0.792642
H	2.806408	-0.608344	1.421462
O	1.471198	0.061002	2.185908
C	0.369082	-0.380456	1.907198
O	0.180541	-1.409674	1.124056
C	-0.896348	0.293922	2.497814
F	6.185569	-1.105567	0.019698
F	5.418248	-0.676958	-1.972434
F	-0.575859	1.146004	3.463756
F	-1.543994	0.971063	1.520068
F	-1.734445	-0.635061	2.982417

F	4.866043	-2.530625	-0.972207
H	2.065867	1.460796	-0.612027
O	1.418569	2.228589	-0.616813
C	0.200935	1.826579	-0.855417
O	-0.159607	0.673594	-1.042227
C	-0.791225	3.011352	-0.857728
F	-0.780839	3.620162	0.336143
F	-2.030527	2.568341	-1.105159
F	-0.452936	3.900439	-1.800637
H	-1.738649	0.076345	-1.240517
O	-2.640621	-0.310237	-1.439103
C	-2.951358	-1.309010	-0.655280
O	-2.288956	-1.806194	0.241246
C	-4.365542	-1.844988	-0.975090
F	-4.600693	-2.971114	-0.300998
F	-4.488003	-2.088820	-2.287772
F	-5.280298	-0.926579	-0.621344
H	-0.772756	-1.557796	0.850413

HOTFA

E = -526.7759289 a.u.

C	0.600885	-0.000723	0.000063
C	-0.934212	0.159937	0.000195
O	-1.497900	1.222281	0.000068
O	-1.520766	-1.045970	0.000121
H	-2.485768	-0.895031	0.000184
F	1.188232	1.196097	-0.000673
F	0.997128	-0.679273	1.090297
F	0.996313	-0.680239	-1.089985

Br₂

E = -5142.796232 a.u.

Br	0.000000	0.000000	1.167257
Br	0.000000	0.000000	-1.167257

Me-OTFA

E = -566.0840522 a.u.

C	0.994905	-0.089970	-0.000220
C	-0.468462	0.403957	-0.001145
O	-0.778970	1.568101	-0.000556
O	-1.293887	-0.643843	-0.001066
F	1.832143	0.948796	-0.013592
F	1.239053	-0.827567	1.097722
F	1.234262	-0.851874	-1.082264
C	-2.700226	-0.322066	0.000363
H	-3.215247	-1.281797	-0.004382
H	-2.954198	0.251509	0.895014
H	-2.954115	0.260513	-0.888427

H₂S₂O₈

E = -1399.090546 a.u.

S	0.055730	1.909059	-0.071437
O	-1.247530	2.263275	-0.583629
O	1.247530	2.708539	-0.178073
O	0.565910	0.466475	-0.779552
O	-0.565910	-0.466475	-0.779552
S	-0.055730	-1.909059	-0.071437
O	-1.247530	-2.708539	-0.178073
O	0.086852	-1.461707	1.479429
H	1.002634	-1.156327	1.637578
O	-0.086852	1.461707	1.479429
H	-1.002634	1.156327	1.637578
O	1.247530	-2.263275	-0.583629

HSO₄-HOTFA3

E = -2280.124612 a.u.

C	-6.614259	0.481794	0.487743	H	-2.839539	2.283606	-2.077439
F	-6.368298	0.658870	1.800835	B	-1.225890	3.120566	0.676719
C	-5.472333	-0.299944	-0.205478	B	1.224866	3.121358	0.676102
O	-5.697887	-1.297270	-0.850742	Pd	0.000113	0.557568	-0.384805
O	-4.324102	0.302437	0.021384	O	-1.387904	-0.949757	-0.478266
F	-6.765285	1.702033	-0.070354	O	2.654823	-0.004164	1.150731
F	-7.780132	-0.171118	0.369822	C	-2.380131	-0.882586	0.334930
O	-2.264767	-0.847968	-1.160268	O	-2.652648	-0.005947	1.152687
S	-0.872870	-0.789385	-0.669130	C	-3.398388	-2.035650	0.137086
O	0.127978	-1.135844	-1.726747	F	-4.352997	-1.604390	-0.725811
O	-0.798955	-1.979567	0.429738	F	-2.850709	-3.145351	-0.372303
O	-0.531560	0.472756	0.047054	F	-4.000548	-2.352441	1.291174
O	2.616367	-1.448981	-1.135430	C	2.381259	-0.881669	0.334268
C	2.774231	-1.917663	0.072627	O	1.388611	-0.949199	-0.478406
C	4.268463	-2.061778	0.432214	C	3.398491	-2.035857	0.137601
F	4.440254	-2.108914	1.757505	F	2.849516	-3.145976	-0.369496
O	1.922938	-2.287520	0.863880	F	4.001062	-2.351177	1.291906
F	5.014227	-1.066152	-0.063741	F	4.352871	-1.606934	-0.726589
F	4.732514	-3.224462	-0.088781	C	-0.000434	3.545840	1.526961
O	1.455641	2.098277	-0.423280	H	-0.000695	4.607418	1.792621
C	2.572092	1.819988	0.210992	H	-0.000042	2.963322	2.459948
C	3.608184	2.942676	-0.032272				
F	4.782167	2.642996	0.538690				
O	2.834456	0.866049	0.909541				
F	3.819901	3.136971	-1.348524				
F	3.176334	4.110009	0.491555				
H	0.156072	-2.103805	0.670999				
H	1.619985	-1.338912	-1.363189				
H	-3.553040	-0.175809	-0.426890				
H	0.738629	1.397193	-0.253912				

HOTFA3

E = -1580.371851 a.u.

O	-2.534751	0.661642	-0.700050
C	-2.697762	-0.429404	-0.184379
O	-1.799197	-1.303851	0.191331
C	-4.121187	-0.960447	0.108543
F	-5.037516	-0.073554	-0.281725
F	-4.326563	-2.114847	-0.543747
F	-4.262782	-1.180423	1.425818
H	-1.430923	1.917771	-0.745256
O	-0.764364	2.666229	-0.725669
C	0.271402	2.284896	-0.027449
O	0.394794	1.211916	0.543363
C	1.364497	3.373135	0.047848
F	1.549894	3.957173	-1.140905
F	2.518712	2.823433	0.447064
F	1.000292	4.308380	0.938750
H	1.785673	0.232355	0.768258
O	2.468586	-0.489897	0.708674
C	1.955608	-1.526765	0.081323
O	0.820855	-1.656893	-0.335002
C	3.015100	-2.635191	-0.110038
F	2.454566	-3.731733	-0.621793
F	3.586305	-2.945395	1.063948
F	3.971875	-2.204302	-0.950323
H	-0.861115	-1.049224	-0.013039

A1

E = -1498.994830 a.u.

C	2.402584	3.082991	-0.085162
C	1.510752	1.943001	-0.312199
C	-1.511370	1.942141	-0.311529
C	-2.403970	3.081433	-0.083980
C	2.858934	2.069409	-1.011226
H	2.837967	2.285287	-2.078701
H	3.633646	1.377107	-0.687716
C	-2.859935	2.067593	-1.009982
H	-3.633976	1.374616	-0.686297

A2

E = -1013.065026 a.u.

C	-4.171749	-0.399596	-0.360286
C	-2.766048	-0.568504	-0.015105
C	-0.631405	1.461627	0.498942
C	-0.863070	2.898556	0.658242
C	-3.835313	-1.600569	0.368613
H	-4.100913	-1.665222	1.423183
H	-3.830822	-2.551051	-0.163743
C	0.118684	2.314816	1.538593
H	1.170525	2.505481	1.338413
H	-0.148843	2.153258	2.581935
B	-1.635954	2.327263	-0.359766
B	-3.350128	0.644174	-0.826881
Pd	-0.702996	-0.522776	0.197130
O	1.293128	-0.665576	0.325243
C	2.020263	0.242244	-0.254779
O	1.647108	1.297774	-0.743802
C	3.530373	-0.136564	-0.223796
F	3.974467	-0.025797	1.039681
F	3.706411	-1.399052	-0.636484
F	4.231756	0.680137	-1.004553
C	-2.760372	1.971769	-1.363589
H	-3.512826	2.761612	-1.460252
H	-2.329345	1.803196	-2.361653
C	-0.457108	-3.123679	-0.078562
H	-1.182003	-3.926788	-0.229462
H	-0.579373	-2.421432	-0.927677
H	-0.632012	-2.701969	0.925412
H	0.572690	-3.482371	-0.109846

TS_{A1}

E = -1013.038346 a.u.

C	1.449168	3.104868	-0.194674
C	1.045508	1.699168	-0.146705
C	2.557506	-0.946423	-0.253204
C	3.974764	-1.191396	-0.521159
C	0.068386	2.820693	-0.511794
H	-0.703329	3.053502	0.219553
H	-0.252012	2.873604	-1.551479
C	3.076358	-2.264402	-0.857374
H	2.839831	-2.445239	-1.905337
H	3.057382	-3.148535	-0.221606
B	3.716968	0.067550	0.051524
B	2.473263	2.206525	0.174674
Pd	0.634631	-0.324305	0.161304
O	-1.320765	0.329505	0.456191

C	-2.197743	-0.441846	-0.038784
O	-1.990044	-1.599018	-0.474843
C	-3.636972	0.129189	-0.068328
F	-4.446573	-0.646379	-0.779539
F	-3.607261	1.356004	-0.611288
F	-4.090266	0.218490	1.187905
C	0.183427	-2.486578	0.750069
H	0.605926	-3.234851	0.079050
H	-0.789833	-1.899663	-0.013186
H	0.898802	-2.258604	1.548070
C	3.817817	1.530248	0.545148
H	3.943544	1.546723	1.638488
H	4.684800	2.051817	0.123610
H	-0.675259	-2.909164	1.288211

A3

E = -1013.073676 a.u.

C	-1.307947	3.216814	0.268276
C	-0.943269	1.797899	0.301757
C	-2.699015	-0.915055	0.149359
C	-4.155952	-1.015223	0.263342
C	0.025898	2.882622	0.729131
H	0.874172	3.082433	0.075006
H	0.246959	2.969016	1.792772
C	-3.409762	-2.185449	0.644860
H	-3.305620	-2.421817	1.703241
H	-3.409179	-3.049217	-0.018972
B	-3.714762	0.227979	-0.225958
B	-2.301623	2.298617	-0.166961
Pd	-0.749848	-0.423647	-0.102424
O	1.353087	0.018841	-0.397208
C	2.323379	-0.436213	0.198606
O	2.309637	-1.377973	1.110245
C	3.742154	0.089231	-0.128247
F	4.573972	-0.119369	0.887525
F	3.665345	1.397291	-0.385451
F	4.183446	-0.553562	-1.213934
C	-0.437707	-2.393217	-0.608754
H	-0.536266	-3.031771	0.274657
H	1.392896	-1.703935	1.237697
H	-1.166060	-2.689673	-1.366222
C	-3.642910	1.703984	-0.679514
H	-3.653275	1.749099	-1.779431
H	-4.512553	2.278240	-0.339405
H	0.567987	-2.446137	-1.033670

A4

E = -486.2674123 a.u.

C	3.152167	0.545063	0.064878
C	1.907460	-0.223983	0.042477
C	-1.354608	0.796599	0.046415
C	-1.887791	2.163534	0.097219
C	3.267567	-0.896204	0.158971
H	3.632292	-1.449264	-0.706018
H	3.528677	-1.338948	1.119616
C	-2.855837	1.102554	0.194506
H	-3.307544	0.890614	1.163046
H	-3.491750	0.892084	-0.664724
B	-0.486055	2.105163	-0.044719
B	1.946972	1.293675	-0.051002
Pd	-0.238224	-0.878704	-0.031722
C	-1.972772	-1.916989	-0.099217
H	-2.544104	-1.793197	0.822400
H	-2.561929	-1.670103	-0.983956
C	0.997978	2.517743	-0.179818
H	1.152976	3.001015	-1.156686
H	1.248998	3.286530	0.564143
H	-1.528904	-2.922450	-0.172595

A5

E = -5629.085566 a.u.

C	2.251237	2.991642	-0.164907
C	1.424090	1.782803	-0.202276
C	2.452965	-1.354286	-0.120510
C	3.847144	-1.804696	-0.051952
C	0.952169	3.110251	-0.788198
H	0.169190	3.654145	-0.259310
H	0.893699	3.181969	-1.873891
C	2.912523	-2.717878	-0.656944
H	2.919759	-2.839666	-1.739574
H	2.605954	-3.602903	-0.100546
B	3.622613	-0.532417	0.511149
B	2.806352	1.829528	0.438208
Pd	0.642988	-0.387338	-0.083332
C	-0.177146	-2.269029	-0.028687
H	-0.023797	-2.715070	-1.013625
H	0.287742	-2.859647	0.761973
C	3.827478	0.876683	1.114377
H	3.616280	0.838846	2.194122
H	4.860389	1.225804	1.007005
H	-1.236038	-2.103819	0.176508
Br	-1.628797	0.860163	-0.039066
Br	-3.535723	-0.492752	0.191307

TS_{A2}

E = -5629.065738 a.u.

C	-1.407787	3.134771	0.640775
C	-0.792032	1.840565	0.329295
C	-2.115274	-1.127043	0.014101
C	-3.496455	-1.484852	0.338951
C	0.017058	3.004996	0.868378
H	0.704807	3.499100	0.183129
H	0.381093	2.926420	1.892239
C	-2.526265	-2.543502	0.441199
H	-2.201406	-2.866988	1.429930
H	-2.516267	-3.321734	-0.321421
B	-3.315445	-0.138517	-0.055281
B	-2.270432	2.123870	0.134069
Pd	-0.217504	-0.296259	-0.402622
C	0.232906	-2.133712	-1.275946
H	0.116670	-2.898548	-0.510952
H	-0.484548	-2.227634	-2.093637
C	-3.552835	1.367092	-0.311202
H	-3.713554	1.535171	-1.387215
H	-4.452304	1.731752	0.197694
H	1.257573	-2.057341	-1.632260
Br	2.052727	0.557039	-0.983525
Br	1.681176	-0.699009	1.386264

A6

E = -5629.093155 a.u.

C	2.162978	2.831186	-0.040301
C	1.214479	1.750418	0.228270
C	1.616736	-1.388579	0.237927
C	2.808765	-2.196818	-0.020961
C	1.006899	3.169034	0.758052
H	1.140867	3.323351	1.828541
H	0.199356	3.741654	0.304243
C	1.775378	-2.808189	0.782680
H	1.141415	-3.571851	0.334968
H	1.940756	-2.912099	1.854628
B	2.831616	-0.903732	-0.593630
B	2.516051	1.581486	-0.599912
Pd	-0.019498	-0.001429	0.120956
C	-0.447514	-0.005354	2.199032
H	-1.027265	-0.913586	2.329033
H	0.548848	-0.018318	2.633121
C	3.258227	0.411492	-1.297321
H	4.346237	0.548872	-1.284661

H	2.965832	0.371007	-2.358015
H	-1.009310	0.912115	2.338906
Br	-1.890597	1.499291	-0.354839
Br	-1.436942	-1.938814	-0.349769

A

E = -5589.485928 a.u.

C	-2.482415	2.505688	0.110407
C	-1.380099	1.549306	0.304445
C	-1.384763	-1.546430	0.304070
C	-2.490192	-2.499184	0.108717
C	-1.339267	2.945576	0.888562
H	-0.614305	3.624066	0.443230
H	-1.439190	3.029436	1.970404
C	-1.347422	-2.943770	0.885154
H	-1.446664	-3.030102	1.966865
H	-0.624781	-3.623218	0.437483
B	-2.669341	-1.236642	-0.497505
B	-2.665530	1.245402	-0.498835
Pd	0.006498	-0.000497	0.158100
C	-3.264445	0.004929	-1.218814
H	-2.922429	0.003438	-2.264564
H	-4.359462	0.006559	-1.238680
Br	1.714817	1.763049	-0.170619
Br	1.711294	-1.766700	-0.169406

B1

E = -1656.268762 a.u.

C	2.293002	-3.108308	-0.896456
C	1.466660	-1.958425	-0.516433
C	-1.466669	-1.889582	0.262010
C	-2.349245	-3.043442	0.452332
C	2.986963	-2.001120	-0.253230
C	-2.563618	-1.912840	1.345951
B	-1.424746	-3.169928	-0.603822
B	0.932464	-3.210528	-1.254755
Pd	0.029491	-0.529017	-0.137265
O	-1.285677	1.014622	0.170796
O	1.898755	0.947941	1.701308
C	-2.226313	1.097350	-0.709026
O	-2.524057	0.309315	-1.598205
C	-3.070009	2.384404	-0.498895
F	-3.681303	2.345210	0.710804
F	-2.301464	3.485273	-0.535400
F	-4.021972	2.504496	-1.432222
C	1.964829	1.389923	0.561418
O	1.418279	0.936964	-0.517813
C	2.885367	2.609313	0.286408
F	2.488050	3.345324	-0.760607
F	4.142250	2.158147	0.018004
F	2.963858	3.407229	1.358034
C	-0.465502	-3.728699	-1.687251
H	-0.513866	-4.815650	-1.803186
H	-0.725176	-3.274388	-2.654669
C	-3.807162	-1.057201	1.153114
H	-3.629171	-0.045887	1.528405
H	-4.093987	-0.992523	0.102176
H	-4.633657	-1.495094	1.724592
C	-2.072963	-1.999075	2.786120
H	-2.871095	-2.389147	3.427589
H	-1.198449	-2.647835	2.882996
H	-1.806203	-0.997884	3.139801
C	3.889303	-1.125558	-1.113358
H	3.470736	-0.968417	-2.110288
H	4.042482	-0.151981	-0.644550
H	4.865542	-1.613975	-1.215645
C	3.412837	-2.125007	1.203968
H	2.805406	-2.857399	1.742695
H	4.462767	-2.433314	1.258673

H	3.301436	-1.151688	1.692245
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B2

E = -1170.346000 a.u.

C	3.873113	0.170401	0.791461
C	2.539868	-0.153868	0.298145
C	0.125180	1.590712	0.116833
C	0.064941	3.019732	0.403283
C	3.834568	-0.804613	-0.281581
C	-0.752276	2.587983	-0.716333
B	0.875996	2.292073	1.294558
B	2.831422	0.846788	1.459695
Pd	0.509994	-0.370493	-0.107741
O	-1.427340	-0.710853	-0.530426
C	-2.247632	-0.516305	0.467334
O	-1.999998	-0.003796	1.544268
C	-3.672956	-1.024073	0.112225
F	-4.134258	-0.364654	-0.969210
F	-3.632410	-2.335739	-0.174566
F	-4.511189	-0.825694	1.125173
C	1.977797	1.842934	2.285883
H	2.559883	2.672052	2.700273
H	1.509733	1.310537	3.127286
C	-2.263470	2.566486	-0.544823
H	-2.706489	1.802181	-1.189407
H	-2.556290	2.375613	0.488936
H	-2.663987	3.539225	-0.850587
C	-0.270472	2.866559	-2.134139
H	-0.646518	3.841158	-2.462936
H	0.820186	2.874255	-2.208241
H	-0.669772	2.105340	-2.812149
C	4.115765	-2.264013	0.049591
H	3.747757	-2.541074	1.040671
H	3.657751	-2.916526	-0.700349
H	5.197000	-2.437729	0.023679
C	4.248511	-0.373574	-1.682959
H	4.030447	0.680683	-1.870803
H	5.324549	-0.532458	-1.811622
H	3.728209	-0.982058	-2.430204
C	0.512533	-3.000920	-0.275347
H	0.853634	-2.295581	-1.062745
H	0.461870	-2.583997	0.742144
H	-0.482554	-3.344357	-0.559920
H	1.244355	-3.811583	-0.259958

TS_{B1}

E = -1170.318722 a.u.

C	3.840030	-0.050490	0.798404
C	2.479561	-0.309395	0.330714
C	0.271200	1.771251	0.172354
C	0.239896	3.161447	0.622439
C	3.746025	-0.997236	-0.289677
C	-0.593224	2.856235	-0.529570
B	1.051410	2.301545	1.395405
B	2.846498	0.647637	1.511309
Pd	0.462473	-0.293330	-0.136139
O	-1.592158	-0.240892	-0.510141
C	-2.231331	-1.153335	0.091004
O	-1.720886	-2.153340	0.654668
C	-3.764069	-0.957072	0.158502
F	-4.012738	-0.009822	1.082523
F	-4.226077	-0.536184	-1.023688
F	-4.382058	-2.080339	0.503167
C	2.103487	1.702515	2.366496
H	2.773370	2.452650	2.798900
H	1.582669	1.208278	3.199790
C	-2.104147	2.809846	-0.345696
H	-2.555025	2.182153	-1.118221
H	-2.389901	2.414921	0.631699

H	-2.506310	3.824021	-0.444928	C	3.317063	0.101764	0.337625
C	-0.132126	3.305569	-1.910087	B	1.501041	1.784432	-0.381564
H	-0.522572	4.307316	-2.118621	B	-1.031680	1.943333	-0.384804
H	0.957480	3.335552	-1.992162	Pd	-0.041894	-0.844209	-0.260814
H	-0.528295	2.624486	-2.670337	C	0.279001	2.651089	-0.804555
C	4.014658	-2.466248	0.010411	H	0.334322	3.669471	-0.402071
H	3.639936	-2.761158	0.993805	H	0.292044	2.757282	-1.900740
H	3.563043	-3.105215	-0.753508	C	4.179318	-0.652009	-0.667641
H	5.096521	-2.638728	-0.008929	H	4.075156	-1.731945	-0.515180
C	4.138014	-0.548858	-1.692286	H	3.911602	-0.411958	-1.699644
H	3.942807	0.514072	-1.854652	H	5.232472	-0.392956	-0.514832
H	5.206425	-0.732477	-1.849342	C	3.637254	-0.198764	1.796646
H	3.586488	-1.128763	-2.439817	H	4.674320	0.082063	2.009391
C	0.602540	-2.518184	-0.569775	H	2.983734	0.348222	2.480622
H	1.192965	-2.157645	-1.418704	H	3.533663	-1.271952	1.989920
H	-0.494222	-2.169510	0.194844	C	-4.095081	-0.036607	-0.523780
H	-0.122467	-3.200376	-1.033373	H	-3.847063	0.158056	-1.570315
H	1.242930	-3.067645	0.118749	H	-4.241796	-1.111604	-0.384296

B3

E = -1170.352947 a.u.

C	3.987088	0.028690	0.549585
C	2.590245	-0.303642	0.255072
C	0.225763	1.890453	0.147952
C	0.276835	3.321753	0.468005
C	3.813341	-1.074882	-0.362429
C	-0.739156	2.898329	-0.489037
B	1.205205	2.481720	1.143456
B	3.047420	0.829025	1.229221
Pd	0.579611	-0.352839	-0.074519
O	-1.562485	-0.527237	-0.418606
C	-2.363182	-1.056140	0.344457
O	-2.082613	-1.625950	1.491895
C	-3.872090	-1.049296	0.001995
F	-4.339491	0.185264	0.250336
F	-4.025494	-1.324682	-1.292120
F	-4.540532	-1.931600	0.735711
C	2.404310	2.000277	2.009115
H	3.121369	2.797905	2.229856
H	2.022711	1.636137	2.974545
C	-2.194733	2.878884	-0.039933
H	-2.754552	2.129188	-0.606418
H	-2.289746	2.660943	1.027244
H	-2.650162	3.856392	-0.231257
C	-0.540377	3.213945	-1.966229
H	-0.961360	4.199193	-2.193538
H	0.516366	3.216487	-2.244960
H	-1.065419	2.472281	-2.577702
C	4.122125	-2.479892	0.138559
H	3.844995	-2.611962	1.187582
H	3.603108	-3.228539	-0.466289
H	5.198311	-2.662974	0.043710
C	4.071138	-0.853339	-1.847578
H	3.843600	0.170249	-2.155334
H	5.124613	-1.055522	-2.070153
H	3.464852	-1.543946	-2.442773
C	0.748991	-2.377248	-0.380144
H	1.344879	-2.511554	-1.285036
H	-1.112982	-1.580642	1.649398
H	-0.263913	-2.749693	-0.550691
H	1.216724	-2.879752	0.468292

B4

E = -643.5470772 a.u.

C	-2.341790	1.712901	0.086524
C	-1.538461	0.495504	-0.069348
C	1.843426	0.347075	-0.029768
C	2.830399	1.429190	-0.014728
C	-3.022594	0.481892	0.425963

C	3.317063	0.101764	0.337625
B	1.501041	1.784432	-0.381564
B	-1.031680	1.943333	-0.384804
Pd	-0.041894	-0.844209	-0.260814
C	0.279001	2.651089	-0.804555
H	0.334322	3.669471	-0.402071
H	0.292044	2.757282	-1.900740
C	4.179318	-0.652009	-0.667641
H	4.075156	-1.731945	-0.515180
H	3.911602	-0.411958	-1.699644
H	5.232472	-0.392956	-0.514832
C	3.637254	-0.198764	1.796646
H	4.674320	0.082063	2.009391
H	2.983734	0.348222	2.480622
H	3.533663	-1.271952	1.989920
C	-4.095081	-0.036607	-0.523780
H	-3.847063	0.158056	-1.570315
H	-4.241796	-1.111604	-0.384296
H	-5.044997	0.460522	-0.298159
C	-3.251043	0.151844	1.895713
H	-2.451551	0.538254	2.532568
H	-4.199117	0.591012	2.224841
H	-3.320120	-0.932153	2.032561
C	-1.429698	-2.294062	-0.512940
H	-2.008397	-2.456346	0.397535
H	-0.721425	-3.119523	-0.692485
H	-2.069280	-2.120533	-1.378686

B5

E = -5786.363935 a.u.

C	-3.914173	-0.724792	-0.394522
C	-2.460065	-0.750847	-0.216371
C	-0.678999	1.996741	-0.168882
C	-1.238402	3.338200	-0.367410
C	-3.420137	-1.752326	0.497615
C	-0.110817	3.241842	0.544360
B	-1.843865	2.283305	-1.105710
B	-3.213411	0.238457	-1.151315
Pd	-0.451982	-0.305832	-0.123691
C	-2.879425	1.510254	-1.968419
H	-3.766271	2.106327	-2.205618
H	-2.409952	1.220587	-2.919745
C	1.237867	3.787390	0.089327
H	2.049742	3.307708	0.646693
H	1.401573	3.640505	-0.981399
H	1.284778	4.861627	0.298512
C	-0.362626	3.357563	2.042841
H	-0.307365	4.408945	2.344997
H	-1.344203	2.968140	2.323616
H	0.406672	2.807317	2.595223
C	-3.457990	-3.200059	0.024651
H	-3.270919	-3.288124	-1.048590
H	-2.722212	-3.801005	0.566854
H	-4.449051	-3.617403	0.234402
C	-3.592343	-1.570261	2.000511
H	-3.580355	-0.516601	2.289990
H	-4.546486	-2.005847	2.316249
H	-2.791433	-2.092147	2.534647
C	-0.143772	-2.333634	-0.029992
H	-0.458126	-2.662723	0.962520
H	0.932521	-2.452203	-0.166022
H	-0.697506	-2.841449	-0.819065
Br	2.059567	0.309623	-0.081517
Br	3.553902	-1.509184	-0.041929

TS_{B2}

E = -5786.344159 a.u.

C	-3.410792	1.335550	0.032142
C	-2.220211	0.518385	-0.194363

C	0.741332	1.808726	-0.013558
C	1.081080	3.231245	0.113387
C	-3.482601	-0.011673	0.556366
C	2.003617	2.285024	0.725923
B	-0.108167	2.918525	-0.600952
B	-2.378446	1.977601	-0.693724
Pd	-0.278925	-0.234243	-0.538306
C	-1.484859	3.080085	-1.309940
H	-1.909781	4.082231	-1.194374
H	-1.358696	2.900054	-2.387582
C	3.358901	2.059188	0.068724
H	3.743196	1.069064	0.331703
H	3.305549	2.139965	-1.019665
H	4.068950	2.807130	0.437730
C	2.010474	2.148107	2.243744
H	2.720370	2.862685	2.673782
H	1.024817	2.337407	2.676351
H	2.331090	1.139530	2.523243
C	-4.390867	-1.012814	-0.145835
H	-4.402823	-0.871009	-1.229446
H	-4.080378	-2.037813	0.077866
H	-5.413587	-0.888879	0.226939
C	-3.333177	-0.228310	2.056850
H	-2.685462	0.521769	2.517329
H	-4.317863	-0.176074	2.533867
H	-2.917590	-1.222285	2.251976
C	-1.210959	-1.960767	-1.236530
H	-1.793883	-2.374772	-0.417217
H	-0.409865	-2.626365	-1.550575
H	-1.827749	-1.632154	-2.074292
Br	1.957769	-1.202488	-1.111753
Br	0.934107	-1.690439	1.325364

B6

E = -5786.371671 a.u.

C	-2.428272	2.521595	0.001252
C	-1.570149	1.337271	-0.097104
C	1.576197	1.333191	-0.099529
C	2.439777	2.514251	-0.006485
C	-2.975674	1.333630	0.614341
C	2.984776	1.325019	0.606049
B	1.228866	2.693502	-0.719143
B	-1.219530	2.697083	-0.716207
Pd	-0.000692	-0.179403	-0.138941
C	0.004725	3.359244	-1.396992
H	0.006521	4.449937	-1.302722
H	0.002845	3.127953	-2.472241
C	4.148739	0.635551	-0.090554
H	4.187423	-0.416956	0.196375
H	4.074885	0.703185	-1.178804
H	5.081471	1.116915	0.223984
C	2.970050	1.189736	2.121721
H	3.907369	1.579831	2.532379
H	2.139616	1.735125	2.578158
H	2.894748	0.131422	2.390098
C	-4.145502	0.649677	-0.077811
H	-4.080449	0.724381	-1.166198
H	-4.182847	-0.404625	0.202777
H	-5.075394	1.129724	0.246919
C	-2.954497	1.195287	2.129675
H	-2.119947	1.736703	2.583315
H	-3.888460	1.587841	2.545581
H	-2.881675	0.136128	2.395481
C	-0.026471	-0.501993	-2.245311
H	-0.992037	-0.095265	-2.528834
H	0.068689	-1.573220	-2.382914
H	0.839523	0.072279	-2.560239
Br	1.692365	-1.940997	0.037577
Br	-1.696345	-1.938903	0.034120

B

E = -5746.758704 a.u.

C	-2.368541	2.396210	-0.475385
C	-1.543546	1.206357	-0.208673
C	1.543588	1.206448	-0.208594
C	2.368339	2.396474	-0.475107
C	-2.841468	1.478484	0.557939
C	2.841611	1.478263	0.557723
B	1.213802	2.265716	-1.278768
B	-1.214165	2.265185	-1.279291
Pd	-0.000039	-0.221248	-0.121071
C	-0.000045	2.599683	-2.188992
H	-0.000170	3.629577	-2.558303
H	0.000425	1.923864	-3.055431
C	4.067422	0.624457	0.268473
H	4.021734	-0.296806	0.853555
H	4.130307	0.351205	-0.786727
H	4.967909	1.184601	0.547646
C	2.684421	1.867514	2.022984
H	3.577674	2.401496	2.366143
H	1.812523	2.507078	2.184529
H	2.571990	0.961512	2.627603
C	-4.067246	0.624385	0.269440
H	-4.130477	0.350776	-0.785643
H	-4.021231	-0.296684	0.854806
H	-4.967710	1.184489	0.548780
C	-2.683818	1.868379	2.022970
H	-1.811787	2.507893	2.183990
H	-3.576897	2.402661	2.366132
H	-2.571373	0.962650	2.627991
Br	1.740282	-1.981864	-0.063745
Br	-1.740386	-1.981888	-0.064032

C1

E = -1649.434841 a.u.

C	-3.297352	-2.461518	-0.063698
C	-2.258928	-1.437441	-0.244362
C	-2.259834	1.436714	-0.245468
C	-3.298613	2.460399	-0.064880
C	-2.013820	-2.858498	0.423513
C	-2.015206	2.857744	0.422467
B	-3.734775	1.215812	-0.588020
B	-3.734037	-1.216997	-0.586526
Pd	-0.821158	0.000031	-0.355706
O	0.698094	1.369429	-0.603510
O	0.816370	-2.449458	1.403519
C	1.236741	2.101750	0.298440
O	0.815303	2.449807	1.403907
C	2.642189	2.595256	-0.147775
F	3.487082	1.554060	-0.242831
F	2.571071	3.193567	-1.353156
F	3.150454	3.474610	0.723539
C	1.237595	-2.101110	0.298079
O	0.698759	-1.368615	-0.603630
C	2.642978	-2.594519	-0.148497
F	2.571711	-3.192356	-1.354153
F	3.151182	-3.474286	0.722409
F	3.487947	-1.553392	-0.243163
C	-4.567770	-0.001163	-1.082278
H	-5.607652	-0.001248	-0.740732
H	-4.588244	-0.002029	-2.182344
H	-1.407496	-3.530251	-0.185151
H	-1.409139	3.529809	-0.186114
O	-1.786100	2.856313	1.754289
H	-0.798623	2.743739	1.851173
O	-1.784586	-2.857082	1.755327
H	-0.797168	-2.744161	1.852115

C2

E = -1163.493805 a.u.

C	4.063406	-0.160950	0.675144
C	2.649927	-0.280939	0.259449
C	0.472274	1.692392	0.082222
C	0.304135	3.133429	0.306785
C	3.513367	-1.492538	0.669923
C	-0.952983	2.476397	0.228361
B	1.632794	2.681951	0.066464
B	3.472465	1.042077	0.218877
Pd	0.611714	-0.280461	-0.193108
O	-1.372121	-0.264992	-0.590164
C	-2.065496	-0.797782	0.383573
O	-1.640564	-1.366717	1.370937
C	-3.579398	-0.547184	0.160345
F	-3.771756	0.814457	0.091374
F	-4.001567	-1.073805	-0.990228
F	-4.308487	-1.010318	1.162298
C	3.172004	2.538931	-0.044374
H	3.478446	2.793700	-1.071570
H	3.732383	3.209685	0.616745
H	3.263640	-1.961981	1.621252
H	-1.479562	2.219860	1.146811
O	-1.687279	2.624173	-0.890072
H	-2.450612	2.016361	-0.845697
O	3.850302	-2.337262	-0.359849
H	4.130188	-3.197756	-0.005452
C	0.575087	-2.793034	-0.894084
H	1.395773	-3.508539	-0.840262
H	0.359625	-2.449722	0.137805
H	0.872052	-2.020625	-1.624503
H	-0.347450	-3.246907	-1.260763

TS_{C1}

E = -1163.465466 a.u.

C	4.034887	-0.517256	0.623542
C	2.606574	-0.483491	0.237132
C	0.686491	1.816353	0.153701
C	0.758278	3.274777	0.331895
C	3.383652	-1.788129	0.625394
C	-0.568745	2.738842	0.373125
B	1.983521	2.618868	0.039880
B	3.575214	0.730700	0.135931
Pd	0.584163	-0.242720	-0.138993
O	-1.463495	0.094705	-0.393012
C	-2.215650	-0.792230	0.105871
O	-1.840804	-1.908590	0.538220
C	-3.725039	-0.453634	0.133324
F	-3.884432	0.886490	0.171925
F	-4.294063	-0.922298	-0.979926
F	-4.311045	-0.986624	1.199105
C	3.474352	2.246413	-0.158988
H	3.746352	2.425494	-1.211541
H	4.165123	2.847699	0.442650
H	3.096700	-2.243368	1.571852
O	3.670039	-2.640273	-0.409308
H	3.493291	-3.558828	-0.148926
C	0.458278	-2.464564	-0.636836
H	1.223617	-2.195140	-1.370490
H	-0.626084	-2.022274	0.095828
H	-0.305131	-2.986395	-1.228413
H	0.901039	-3.148347	0.090597
H	-1.056341	2.616854	1.340771
O	-1.379643	2.961516	-0.696524
H	-2.145128	2.362107	-0.631629

C3

E = -1163.497423 a.u.

C	-4.077757	-0.669531	-0.558848
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C	-2.625147	-0.674720	-0.254665
C	-0.597441	1.835282	-0.107224
C	-0.844776	3.286911	-0.293428
C	-3.618252	-1.758627	0.247262
C	0.264917	2.872819	0.556176
B	-1.776506	2.378945	-0.884248
B	-3.362685	0.461371	-1.017856
Pd	-0.635912	-0.446514	0.043338
O	1.540159	-0.310186	0.333298
C	2.451269	-0.641348	-0.404444
O	2.269903	-1.247030	-1.558566
C	3.911769	-0.324205	0.008149
F	4.056530	0.996525	0.126437
F	4.199814	-0.915261	1.161134
F	4.754649	-0.774440	-0.947378
C	-3.004072	1.824279	-1.656715
H	-3.851384	2.518253	-1.673819
H	-2.715105	1.657678	-2.706332
H	-3.520837	-2.747289	-0.199064
H	1.282807	2.998597	0.187423
C	-0.547049	-2.471535	0.317795
H	-1.140982	-2.713100	1.201559
H	0.507063	-2.693273	0.495737
H	-0.910808	-2.994993	-0.569361
H	3.126096	-1.433540	-1.994233
O	0.112371	2.969812	1.923629
H	0.869932	3.441331	2.304935
O	-3.899685	-1.726259	1.592260
H	-3.860570	-2.623653	1.959083

C4

E = -636.6912396 a.u.

C	-2.272953	1.788550	-0.321179
C	-1.475438	0.544462	-0.178671
C	1.867363	0.285051	-0.259053
C	2.925552	1.320016	-0.212005
C	-2.981522	0.549623	-0.510249
C	3.322025	-0.056626	-0.474457
B	1.595961	1.733052	0.108668
B	-0.938924	1.979868	0.119176
Pd	-0.044739	-0.867062	-0.033014
C	0.403239	2.663070	0.468234
H	0.429366	2.841477	1.555898
H	0.491927	3.653259	0.005068
H	-3.253492	0.244742	-1.519829
O	-3.811807	0.123012	0.499910
H	-4.598400	-0.305191	0.124630
C	-1.509795	-2.243053	0.211827
H	-0.889215	-3.029158	0.669601
H	-1.867242	-2.524656	-0.782639
H	-2.318929	-1.929549	0.868618
H	3.631646	-0.325737	-1.484129
O	3.903829	-0.778783	0.544779
H	4.740151	-1.165328	0.237993

C5

E = -5779.513146 a.u.

C	-3.959111	-1.191572	-0.241278
C	-2.495098	-0.971713	-0.148401
C	-1.175806	1.927447	-0.329058
C	-1.720190	3.293316	-0.130041
C	-3.127846	-2.246402	-0.750838
C	-0.430878	3.145653	-0.785315
B	-2.470347	2.207450	0.418700
B	-3.562231	-0.028297	0.465277
Pd	-0.576836	-0.247228	-0.053348
C	-3.607872	1.388771	1.085527
H	-3.383221	1.315199	2.161472
H	-4.589480	1.866630	0.999753

H	-3.022902	-2.366457	-1.828006	C	2.542858	2.461747	-0.271930
O	-3.019995	-3.395893	-0.001832	C	1.498036	1.421068	-0.141427
H	-2.847783	-4.153704	-0.583844	C	-1.497484	1.421709	-0.141840
C	0.068601	-2.162490	0.322936	C	-2.542103	2.462544	-0.271675
H	0.680447	-2.059959	1.222574	C	3.014484	1.117179	-0.393232
H	0.667694	-2.420621	-0.554780	C	-3.014228	1.118115	-0.392880
H	-0.751148	-2.857915	0.481264	B	-1.235796	2.915402	0.045767
H	-0.353698	3.334787	-1.855599	B	1.236908	2.914815	0.046826
O	0.720219	3.401563	-0.052263	Pd	-0.000053	-0.039571	-0.056914
H	1.264913	4.063875	-0.510160	C	0.000663	3.818210	0.303467
Br	3.429051	-1.108634	0.064491	H	0.001250	4.734110	-0.298291
Br	1.888661	0.668961	0.072453	H	0.000066	4.141289	1.355473

TS_{C2}

E = -5779.489059 a.u.

C	3.693871	-0.389124	0.539470
C	2.267732	-0.469329	0.149283
C	0.064573	1.933301	0.150203
C	0.171976	3.346619	0.590089
C	3.339720	-1.400749	-0.424811
C	-0.843247	3.009630	-0.395009
B	1.136995	2.423702	1.095877
B	2.849492	0.611307	1.091427
Pd	0.200858	-0.344726	-0.302817
C	2.345046	1.841408	1.877881
H	3.135768	2.577357	2.059750
H	1.993969	1.509512	2.867928
H	3.315164	-2.442974	-0.107143
O	3.620937	-1.180655	-1.754005
H	4.069163	-1.955109	-2.131881
C	0.349138	-2.332262	-0.889590
H	-0.658669	-2.665839	-1.125475
H	0.784896	-2.896154	-0.065940
H	0.992182	-2.280625	-1.769988
Br	-2.226015	-0.344838	-0.915474
Br	-1.542597	-1.042028	1.588363
H	-1.887128	2.989590	-0.084070
O	-0.613648	3.353322	-1.708897
H	-1.406980	3.768619	-2.083134

C6

E = -5779.524902 a.u.

C	-2.576191	2.456343	-0.249815
C	-1.526539	1.418949	-0.215664
C	1.535111	1.411763	-0.216156
C	2.590877	2.444093	-0.251091
C	-3.049551	1.143031	0.051506
C	3.052994	1.127782	0.055811
B	1.250845	2.894109	-0.442103
B	-1.235199	2.900074	-0.442885
Pd	0.000280	-0.090378	-0.166520
C	0.010265	3.784103	-0.710479
H	0.012159	4.698245	-0.103456
H	0.011845	4.124997	-1.757188
H	-3.556127	0.567697	-0.720260
O	-3.380407	0.855806	1.344856
H	-3.683157	-0.069020	1.385026
C	0.005775	-0.245006	1.969742
H	-0.006490	-1.311580	2.166859
H	-0.911247	0.279116	2.223921
H	0.936101	0.257615	2.218677
Br	1.718606	-1.843633	-0.263489
Br	-1.729641	-1.833376	-0.256561
H	3.560296	0.545755	-0.710267
O	3.375884	0.845435	1.353092
H	3.711479	-0.067321	1.396571

C

E = -5739.924041 a.u.

C	2.542858	2.461747	-0.271930
C	1.498036	1.421068	-0.141427
C	-1.497484	1.421709	-0.141840
C	-2.542103	2.462544	-0.271675
C	3.014484	1.117179	-0.393232
C	-3.014228	1.118115	-0.392880
B	-1.235796	2.915402	0.045767
B	1.236908	2.914815	0.046826
Pd	-0.000053	-0.039571	-0.056914
C	0.000663	3.818210	0.303467
H	0.001250	4.734110	-0.298291
H	0.000066	4.141289	1.355473
H	-3.221234	0.714349	-1.384554
O	-3.730713	0.586309	0.638517
H	-3.501917	-0.372908	0.644370
Br	-1.725358	-1.845259	0.003075
Br	1.724681	-1.845692	0.003327
H	3.221079	0.713084	-1.384842
O	3.731368	0.585319	0.637996
H	3.502705	-0.373888	0.643869

D1

E = -1728.037515 a.u.

C	-2.474716	-2.793685	0.700059
C	-1.498732	-1.738213	0.374490
C	1.498851	-1.738157	0.374378
C	2.474910	-2.793594	0.699738
C	-2.911320	-1.826776	-0.264849
C	2.911379	-1.826700	-0.265242
B	1.227714	-2.904131	1.350765
B	-1.227356	-2.904225	1.350776
Pd	0.000049	-0.373966	0.062734
O	1.403442	1.074960	-0.324118
O	-2.530723	0.596527	1.587887
C	2.336691	1.221532	0.550142
O	2.530910	0.596561	1.588010
C	3.402779	2.260498	0.114099
F	4.394346	1.588535	-0.538598
F	2.930620	3.196335	-0.718031
F	3.952975	2.869462	1.170129
C	-2.336638	1.221492	0.549973
O	-1.403559	1.074795	-0.324447
C	-3.402699	2.260565	0.114115
F	-2.930595	3.196396	-0.718045
F	-3.952704	2.869559	1.170212
F	-4.394371	1.588679	-0.538456
C	0.000210	-3.379618	2.172223
H	0.000243	-4.450815	2.396184
H	0.000169	-2.842551	3.133291
H	-3.607970	-1.047397	0.044384
H	3.607997	-1.047255	0.043912
O	2.994107	-2.214352	-1.575294
O	-2.994143	-2.214368	-1.574957
C	3.212225	-1.124578	-2.486712
H	4.054858	-0.503716	-2.161044
H	3.437839	-1.582726	-3.450137
H	2.316818	-0.498930	-2.565428
C	-3.213402	-1.124566	-2.486041
H	-3.436928	-1.582655	-3.449984
H	-4.057778	-0.505669	-2.161077
H	-2.319232	-0.496980	-2.563380

D2

E = -1242.109024 a.u.

C	-3.918137	0.377895	-0.895601
C	-2.532262	-0.009642	-0.569793
C	-0.022214	1.560202	-0.227050
C	0.241224	3.012718	-0.213216

C	-3.738349	-0.847151	-0.137978	H	-0.233339	-3.135975	0.790646
C	1.100899	2.259788	0.648554	H	-1.477077	-2.883172	-0.475336
B	-0.868012	2.601136	-0.988067				
B	-2.929864	1.307036	-1.299643				
Pd	-0.511950	-0.381523	-0.227348				
O	1.392343	-0.902903	0.145932				
C	2.326289	-0.430784	-0.631440				
O	2.218946	0.404521	-1.512421				
C	3.717578	-0.996846	-0.231354				
F	4.097290	-0.385643	0.916119				
F	3.669754	-2.316051	-0.013269				
F	4.622494	-0.739408	-1.169771				
C	-2.156714	2.532403	-1.844961				
H	-2.746409	3.455144	-1.833191				
H	-1.881648	2.342831	-2.894458				
H	-3.898766	-1.799713	-0.648681				
H	2.121214	2.064467	0.323526				
O	0.867153	2.281665	1.983541				
O	-3.966233	-0.850697	1.208661				
C	1.960354	1.805340	2.801691				
H	2.788403	2.521143	2.778005				
H	1.559652	1.739053	3.812328				
H	2.298620	0.821421	2.463864				
C	-5.097725	-1.638758	1.626720				
H	-5.080570	-1.625299	2.715861				
H	-6.031513	-1.196418	1.263591				
H	-5.007454	-2.671345	1.268076				
C	-0.845889	-2.983817	-0.149118				
H	-1.061317	-2.378043	0.747824				
H	-0.717531	-2.419429	-1.093252				
H	0.079849	-3.531600	0.030838				
H	-1.697282	-3.651901	-0.299928				

TS_{D1}

E = -1242.082485 a.u.

C	-3.965462	0.237609	-0.815966
C	-2.537947	0.006075	-0.484717
C	-0.135640	1.873334	-0.265581
C	0.148165	3.310059	-0.492573
C	-3.648922	-1.026599	-0.204137
C	1.177260	2.571573	0.193378
B	-1.143606	2.851717	-0.865632
B	-3.111467	1.341696	-1.045552
Pd	-0.508744	-0.172590	-0.067171
O	1.546219	-0.300833	0.269401
C	2.114017	-1.281270	-0.295092
O	1.531761	-2.254730	-0.831529
C	3.657703	-1.203809	-0.333562
F	3.998890	-0.209159	-1.172935
F	4.123317	-0.909289	0.889307
F	4.197113	-2.340362	-0.751434
C	-2.575941	2.736778	-1.444561
H	-3.237071	3.539186	-1.093048
H	-2.549156	2.832566	-2.540556
H	-3.657880	-1.927512	-0.820260
H	2.078592	2.283698	-0.346262
O	1.307083	2.747327	1.535639
O	-3.909474	-1.214336	1.126148
C	2.611429	2.452885	2.076076
H	3.351171	3.168038	1.700206
H	2.510836	2.565907	3.155023
H	2.909564	1.429055	1.832102
C	-4.854907	-2.262414	1.414707
H	-4.874312	-2.351777	2.500296
H	-5.851031	-1.995455	1.046199
H	-4.531832	-3.211701	0.970707
C	-0.862768	-2.393366	0.282577
H	-1.506453	-2.008311	1.079710
H	0.305073	-2.147746	-0.418655

D3

E = -1242.115342 a.u.

C	-4.065629	0.412828	-0.730630
C	-2.668182	0.005941	-0.424133
C	0.066220	1.821292	-0.352040
C	0.326005	3.266211	-0.575457
C	-3.886064	-0.871186	-0.099744
C	1.352337	2.460834	0.083617
B	-0.960548	2.757281	-0.939129
B	-3.079257	1.385637	-1.017921
Pd	-0.685101	-0.330719	-0.112313
O	1.438291	-0.784594	0.235904
C	2.280532	-1.340135	-0.444383
O	2.009787	-1.998643	-1.551459
C	3.769002	-1.238204	-0.024038
F	4.157020	0.040040	-0.125100
F	3.931787	-1.657785	1.222413
F	4.525867	-1.987155	-0.854325
C	-2.408350	2.695510	-1.494960
H	-2.999073	3.574264	-1.207339
H	-2.378231	2.707656	-2.595519
H	-4.016429	-1.775855	-0.697819
H	2.259613	2.212246	-0.471420
O	1.523890	2.577141	1.440151
O	-4.146137	-1.013694	1.239169
C	2.815208	3.058089	1.835915
H	2.977352	4.084751	1.487691
H	2.821687	3.036008	2.925646
H	3.609020	2.404569	1.451564
C	-5.280551	-1.843686	1.537282
H	-5.299760	-1.943688	2.622259
H	-6.208297	-1.373376	1.192261
H	-5.172570	-2.834349	1.077845
C	-1.162884	-2.291152	0.217377
H	-1.911282	-2.332370	1.009033
H	-0.227632	-2.755346	0.536629
H	-1.526328	-2.733597	-0.713609
H	2.821018	-2.388065	-1.935405

D4

E = -715.3097878 a.u.

C	-2.394718	1.721235	-0.304565
C	-1.527163	0.522592	-0.182452
C	1.841796	0.454573	-0.282980
C	2.836844	1.548977	-0.246124
C	-3.026550	0.429847	-0.481608
C	3.307844	0.189725	-0.507341
B	1.484898	1.884432	0.074185
B	-1.063299	1.986306	0.104286
Pd	-0.005987	-0.800107	-0.076767
C	0.242002	2.744916	0.436869
H	0.265505	2.933732	1.522718
H	0.269612	3.734539	-0.035220
H	-3.307230	0.115102	-1.488867
H	3.631369	-0.060695	-1.520481
O	3.932472	-0.508414	0.492998
O	-3.791811	-0.080573	0.532862
C	5.340659	-0.708909	0.285867
H	5.878206	0.245162	0.322729
H	5.673576	-1.351567	1.100513
H	5.527799	-1.205198	-0.674642
C	-5.183695	-0.252510	0.207312
H	-5.630318	-0.748468	1.068477
H	-5.665557	0.718001	0.047138
H	-5.301580	-0.881099	-0.683751
C	-1.380835	-2.272685	0.125668

H	-2.242193	-2.017656	0.739258
H	-0.726103	-3.009870	0.615813
H	-1.668081	-2.575424	-0.885530

D5

E = -5858.131797 a.u.

C	4.004986	0.792424	0.175065
C	2.609530	0.293023	0.078672
C	0.059435	2.228230	0.286966
C	-0.121583	3.686786	0.090827
C	3.758575	-0.554299	0.638917
C	-1.189081	2.927196	0.728959
B	1.069861	3.099078	-0.438178
B	3.096402	1.647358	-0.499457
Pd	0.568903	0.033249	0.008634
C	2.468515	2.933111	-1.089657
H	2.323450	2.796589	-2.173011
H	3.105639	3.815530	-0.966952
H	3.739348	-0.751065	1.712271
H	-1.366690	3.055698	1.798524
O	-2.308268	2.588629	-0.006765
O	4.154695	-1.606734	-0.145048
C	-3.530454	3.212732	0.428839
H	-3.488512	4.293065	0.255775
H	-4.322850	2.772481	-0.175889
H	-3.716193	3.008688	1.490070
C	5.076976	-2.514488	0.483077
H	5.217829	-3.330785	-0.224765
H	6.035918	-2.020688	0.674026
H	4.663641	-2.905877	1.420651
C	0.887852	-1.964869	-0.348732
H	1.938994	-2.208381	-0.474785
H	0.317803	-2.161332	-1.260327
H	0.450644	-2.456354	0.524739
Br	-2.045071	-0.324807	-0.088121
Br	-2.549780	-2.625577	-0.081377

TS_{D2}

E = -5858.107761 a.u.

C	-3.128899	2.038241	0.072155
C	-2.087386	1.010549	-0.147263
C	1.100256	1.653854	-0.226190
C	1.779070	2.944093	0.046390
C	-3.513588	0.871671	-0.690614
C	2.465769	1.956722	-0.784305
B	0.539704	2.695707	0.713890
B	-1.904429	2.246379	0.764372
Pd	-0.346880	-0.185474	-0.376944
C	-0.759572	2.948509	1.525599
H	-0.644014	2.459621	2.506080
H	-0.957070	4.008204	1.715312
H	-3.639062	0.961452	-1.771369
H	2.541503	2.142685	-1.858121
O	3.499702	1.240917	-0.243493
O	-4.279395	-0.087910	-0.084552
C	4.785120	1.523828	-0.817842
H	5.096499	2.549421	-0.589484
H	5.478512	0.818650	-0.360127
H	4.770491	1.372828	-1.904639
C	-5.534310	-0.364768	-0.733495
H	-5.967214	-1.206547	-0.194028
H	-6.202174	0.500626	-0.667025
H	-5.378721	-0.639276	-1.783846
C	-1.621467	-1.795296	-0.715506
H	-2.474535	-1.689796	-0.051099
H	-1.047419	-2.700998	-0.537905
H	-1.878004	-1.663662	-1.769875
Br	1.601198	-1.693311	-0.758196
Br	0.639056	-1.422126	1.748624

D6

E = -5858.142358 a.u.

C	-2.565342	2.392827	-0.575593
C	-1.546946	1.330987	-0.403824
C	1.547216	1.330650	-0.403580
C	2.565805	2.392245	-0.575715
C	-2.995679	1.202275	0.114649
C	2.996088	1.201658	0.114492
B	1.242412	2.704520	-1.003060
B	-1.242032	2.704670	-1.003583
Pd	-0.000046	-0.158277	-0.310039
C	0.000351	3.430329	-1.581413
H	0.000294	4.506509	-1.373068
H	0.000737	3.333358	-2.678594
H	-3.627295	0.481376	-0.401662
H	3.627418	0.480537	-0.401849
O	3.116762	1.246502	1.475189
O	-3.116142	1.246955	1.475368
C	4.179845	0.434596	2.022304
H	5.152983	0.792464	1.671768
H	4.113127	0.556661	3.102879
H	4.036576	-0.616429	1.751694
C	-4.179057	0.434889	2.022557
H	-4.111789	0.556320	3.103171
H	-5.152322	0.793094	1.672703
H	-4.036066	-0.616008	1.751298
C	-0.000599	-0.265891	1.822535
H	-0.923515	0.257395	2.057128
H	0.922380	0.257214	2.057335
H	-0.000712	-1.328265	2.041971
Br	1.726801	-1.892667	-0.414288
Br	-1.727278	-1.892318	-0.414360

D

E = -5818.528265 a.u.

C	-2.520366	2.339925	-0.575014
C	-1.520025	1.271664	-0.331705
C	1.520584	1.271118	-0.331942
C	2.520615	2.339880	-0.574421
C	-2.934646	1.254874	0.274466
C	2.934601	1.255023	0.275442
B	1.234024	2.547425	-1.132448
B	-1.233135	2.548306	-1.131325
Pd	0.000162	-0.154395	-0.273127
C	0.000335	3.149757	-1.860564
H	0.000909	4.243910	-1.899268
H	-0.000652	2.792264	-2.901777
H	-3.593709	0.479072	-0.115162
H	3.594525	0.479570	-0.113400
O	3.042412	1.508374	1.618268
O	-3.044124	1.508172	1.617095
C	3.434705	0.367066	2.397597
H	4.430723	0.017767	2.096910
H	3.466307	0.713106	3.431467
H	2.714806	-0.449712	2.288157
C	-3.436141	0.366551	2.396162
H	-3.470600	0.713118	3.429757
H	-4.430870	0.015340	2.093446
H	-2.714640	-0.449040	2.288604
Br	1.766178	-1.896594	-0.323364
Br	-1.765977	-1.896532	-0.322894

E1

E = -1963.939996 a.u.

C	-2.459012	-1.662456	2.256789
C	-1.497876	-0.927813	1.414409
C	1.498059	-0.927885	1.414352
C	2.459217	-1.662587	2.256672

C	-2.879636	-1.405967	0.902565	F	3.654315	2.281946	-1.993061
C	2.879699	-1.406215	0.902383	F	4.812725	2.385305	-0.156437
B	1.223741	-1.371674	2.870426	C	-0.991157	0.294357	3.681425
B	-1.223448	-1.371684	2.870437	H	-1.366193	-0.241617	4.558998
Pd	0.000083	0.172932	0.548787	H	-0.611920	1.267182	4.030414
O	1.385766	1.370072	-0.387529	H	-3.774016	1.731289	0.007332
O	-2.667530	1.609713	1.473813	H	2.675497	-1.253913	0.943696
C	2.374832	1.820379	0.301199	O	1.139098	-2.604484	0.459788
O	2.667755	1.609549	1.473715	O	-3.734098	-0.341122	-0.290692
C	3.347450	2.655219	-0.574067	C	1.966226	-3.262702	-0.590134
F	4.131729	1.793369	-1.281676	C	-4.967051	-0.353465	-1.123888
F	2.714203	3.442842	-1.452485	C	3.252849	-3.806477	0.037757
F	4.154767	3.416244	0.172848	H	3.797593	-4.400375	-0.703044
C	-2.374731	1.820302	0.301220	H	3.929129	-3.010288	0.368526
O	-1.385700	1.369923	-0.387496	H	3.025610	-4.452857	0.891364
C	-3.347444	2.654998	-0.574062	C	1.057651	-4.400038	-1.054915
F	-2.714344	3.442356	-1.452820	H	1.552876	-4.972652	-1.844993
F	-4.154552	3.416266	0.172835	H	0.829717	-5.077715	-0.226674
F	-4.131925	1.792998	-1.281277	H	0.116758	-4.005830	-1.451454
C	0.000147	-1.286166	3.821098	C	2.241492	-2.272268	-1.723187
H	0.000143	-2.033190	4.620555	H	1.304226	-1.864318	-2.115522
H	0.000172	-0.292305	4.294174	H	2.880241	-1.440642	-1.412497
H	-3.600517	-0.611364	0.731521	H	2.757002	-2.786832	-2.540723
H	3.600652	-0.611711	0.731185	C	-4.828399	0.657521	-2.265970
O	2.907920	-2.476280	0.052166	H	-4.816135	1.695678	-1.913819
O	-2.908120	-2.476001	0.052320	H	-3.917715	0.467462	-2.843355
C	3.480930	-2.314265	-1.296487	H	-5.683328	0.565260	-2.943371
C	-3.481198	-2.313941	-1.296305	C	-4.994306	-1.784749	-1.657114
C	4.899376	-1.732813	-1.223491	H	-5.038147	-2.502750	-0.832876
H	5.379993	-1.831997	-2.202647	H	-5.874057	-1.930810	-2.291259
H	4.905885	-0.667004	-0.975765	C	-6.179180	-0.064249	-0.234884
H	5.505400	-2.277741	-0.491636	H	-6.159401	0.952469	0.174516
C	3.514331	-3.755391	-1.810150	H	-7.098912	-0.160364	-0.820629
H	3.889270	-3.781246	-2.838298	H	-6.229803	-0.774504	0.596543
H	4.166336	-4.373922	-1.184884	C	-0.936781	2.714933	-1.567202
H	2.509567	-4.189378	-1.795534	H	-1.057790	1.630097	-1.740301
C	2.555793	-1.441507	-2.149388	H	-0.638445	3.005581	-0.543864
H	1.544584	-1.861934	-2.171195	H	-0.159697	3.068506	-2.246339
H	2.495402	-0.416151	-1.774271	H	-1.903440	3.182941	-1.766388
H	2.930612	-1.398334	-3.178287	H	-4.100314	-1.992788	-2.253178
C	-2.556094	-1.441235	-2.149297	TS_{E1}			
H	-2.495676	-0.415854	-1.774259	E = -1477.988767 a.u.			
H	-1.544883	-1.861666	-2.171123	C	3.405695	0.574180	1.756072
H	-2.930958	-1.398138	-3.178181	C	2.140657	0.075712	1.172485
C	-3.514655	-3.755064	-1.809965	C	-0.662373	1.239975	1.233907
H	-4.166718	-4.373556	-1.184719	C	-1.341779	2.353496	1.935662
H	-3.889552	-3.780905	-2.838129	C	3.525957	-0.265430	0.583737
H	-2.509912	-4.189094	-1.795304	C	-1.983557	1.861436	0.730029
C	-4.899633	-1.732477	-1.223301	B	-0.066948	1.976250	2.435440
H	-4.906126	-0.666582	-0.975950	B	2.230853	1.064381	2.370973
H	-5.380371	-1.831994	-2.202365	Pd	0.269547	-0.468566	0.482877
H	-5.505559	-2.277171	-0.491190	O	-1.662970	-1.004767	-0.112397
E2				C	-1.941646	-2.224915	0.064613
E = -1478.016445 a.u.				O	-1.122549	-3.127607	0.369962
C	-3.270902	0.680144	1.859615	C	-3.418255	-2.619453	-0.173529
C	-2.037315	0.764163	1.056284	F	-4.226151	-1.617801	0.213473
C	0.654107	-0.398870	1.464198	F	-3.593927	-2.833616	-1.484405
C	1.143893	-1.339885	2.490005	F	-3.735770	-3.719122	0.502360
C	-3.436415	0.780846	0.418295	C	1.232418	1.832260	3.270206
C	1.659174	-1.569678	1.162858	H	1.630321	2.791542	3.620047
B	0.139163	-0.447376	2.922968	H	1.018238	1.239502	4.172879
B	-2.069875	0.533632	2.594405	H	3.873148	-1.288620	0.721846
Pd	-0.157383	0.918507	0.193618	H	-2.862980	1.229861	0.825747
O	1.611403	1.192936	-0.732281	O	-1.865826	2.602441	-0.402081
C	2.663273	1.384870	0.007074	O	3.752380	0.301946	-0.634537
O	2.755129	1.297879	1.221425	C	-3.060095	2.780597	-1.270111
C	3.934571	1.658621	-0.843829	C	5.034060	0.004208	-1.331419
F	4.498652	0.461533	-1.132572	C	-4.188996	3.417579	-0.454118

H	-5.032122	3.651725	-1.111849
H	-4.566102	2.749025	0.328197
H	-3.852222	4.348463	0.013126
C	-2.547996	3.738339	-2.344735
H	-3.344044	3.952420	-3.064503
H	-2.221295	4.682285	-1.898128
H	-1.703777	3.297239	-2.883599
C	-3.464907	1.434087	-1.876273
H	-2.626985	0.992406	-2.424601
H	-3.802180	0.713296	-1.124707
H	-4.292391	1.584561	-2.577393
C	5.099222	-1.481880	-1.696086
H	5.181948	-2.131440	-0.817278
H	4.220188	-1.781298	-2.275708
H	5.986622	-1.666944	-2.309794
C	4.941855	0.874563	-2.583541
H	4.849160	1.930787	-2.313625
H	5.842548	0.749881	-3.192272
C	6.200996	0.430618	-0.437438
H	6.264116	-0.174501	0.474211
H	7.145187	0.305693	-0.977041
H	6.108446	1.483776	-0.153438
C	1.262074	-2.296082	-0.431843
H	1.745784	-1.536638	-1.054632
H	0.040031	-2.586056	0.157935
H	0.903331	-3.038651	-1.157447
H	1.996372	-2.757203	0.230017
H	4.074351	0.592755	-3.188521

E3

E = -1478.020472 a.u.

C	3.489501	0.698551	1.682586
C	2.264494	0.112058	1.087811
C	-0.785165	1.229507	1.187369
C	-1.398156	2.418626	1.830998
C	3.686518	-0.208700	0.576113
C	-2.117194	1.785197	0.727890
B	-0.091458	2.034016	2.260392
B	2.272319	1.191610	2.209112
Pd	0.450320	-0.508224	0.399424
O	-1.454515	-1.288822	-0.314153
C	-2.060788	-2.222171	0.197292
O	-1.624585	-3.004613	1.155932
C	-3.516319	-2.520451	-0.227633
F	-4.312482	-1.708067	0.493576
F	-3.668870	-2.245262	-1.520914
F	-3.845743	-3.784918	0.009802
C	1.248460	1.994422	3.045904
H	1.621232	2.994131	3.297857
H	1.085204	1.482200	4.006910
H	4.060226	-1.209649	0.789189
H	-3.003483	1.198193	0.962603
O	-2.096105	2.391148	-0.495482
O	3.948223	0.290006	-0.667183
C	-3.376492	2.613244	-1.201801
C	5.277849	0.023315	-1.273056
C	-4.288113	3.492597	-0.340478
H	-5.199295	3.740637	-0.894442
H	-4.594613	2.988177	0.582970
H	-3.784016	4.427045	-0.074558
C	-2.937334	3.346990	-2.469018
H	-3.808500	3.586332	-3.086644
H	-2.425335	4.279981	-2.214986
H	-2.255118	2.725788	-3.057785
C	-4.025642	1.268392	-1.547216
H	-3.322845	0.627071	-2.088136
H	-4.380020	0.728745	-0.662402
H	-4.898090	1.436903	-2.187052
C	5.446863	-1.477068	-1.532789

H	5.511154	-2.062498	-0.608690
H	4.621403	-1.863419	-2.139352
H	6.378119	-1.649334	-2.081834
C	5.209586	0.802016	-2.586140
H	5.042202	1.866222	-2.395094
H	6.149160	0.691454	-3.136189
C	6.370630	0.574764	-0.353288
H	6.418295	0.034744	0.599282
H	7.348053	0.473104	-0.835654
H	6.202669	1.636236	-0.144710
C	1.422166	-2.095987	-0.461984
H	2.123104	-1.666368	-1.179300
H	0.656970	-2.680468	-0.978826
H	1.947327	-2.700352	0.282592
H	4.394739	0.429739	-3.214904
H	-0.713064	-2.733761	1.407703

E4

E = -951.2154145 a.u.

C	-2.464728	-1.839761	0.308193
C	-1.556552	-0.672684	0.186953
C	1.796019	-0.756493	0.292649
C	2.733506	-1.902011	0.263851
C	-3.049852	-0.533123	0.539096
C	3.277322	-0.578665	0.562066
B	1.382033	-2.153317	-0.125541
B	-1.161520	-2.139636	-0.163004
Pd	0.017591	0.584160	0.084825
C	0.106567	-2.935685	-0.550927
H	0.127359	-3.039037	-1.648154
H	0.088984	-3.957729	-0.154731
H	-3.266911	-0.239382	1.564985
H	3.567455	-0.363003	1.589213
O	3.962281	0.082989	-0.417175
O	-3.820399	0.024657	-0.438143
C	5.348965	0.523568	-0.136123
C	-5.235087	0.359188	-0.121654
C	6.198978	-0.685433	0.265627
H	7.244224	-0.381718	0.382164
H	5.876679	-1.119074	1.218959
H	6.152778	-1.463076	-0.503258
C	5.799757	1.094002	-1.480566
H	6.827918	1.461652	-1.407102
H	5.761057	0.324726	-2.257603
H	5.156407	1.926240	-1.783317
C	5.337400	1.609978	0.944658
H	4.677223	2.434743	0.656676
H	5.019729	1.229744	1.922282
H	6.347133	2.013027	1.073300
C	-5.285506	1.465161	0.937010
H	-4.920552	1.133234	1.915646
H	-4.702047	2.335123	0.619176
H	-6.322088	1.787150	1.078987
C	-5.769133	0.857642	-1.463421
H	-5.679331	0.079792	-2.227463
H	-6.824794	1.129424	-1.367815
C	-5.962226	-0.909971	0.330528
H	-5.573869	-1.293232	1.281153
H	-7.025532	-0.694812	0.476856
H	-5.875146	-1.697098	-0.425155
C	-1.296726	2.111616	-0.111280
H	-2.159177	1.892405	-0.736814
H	-0.613049	2.833568	-0.584520
H	-1.588244	2.415317	0.898262
H	-5.215256	1.740290	-1.798349

E5

E = -6094.037386 a.u.

C	3.125891	-2.403434	0.136521
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C	2.113993	-1.318789	0.135946	H	6.591789	2.242986	-1.086399
C	-1.006623	-1.932150	-0.084835	H	4.991010	2.972925	-1.226849
C	-1.806207	-3.152416	0.171858	H	5.668030	2.622621	0.379171
C	3.518923	-1.146651	-0.468916	C	5.818971	-0.121890	0.161175
C	-2.410880	-2.069704	-0.600053	H	6.827662	-0.209844	-0.254138
B	-0.514356	-3.080572	0.778673	H	5.898291	0.233570	1.192878
B	1.937089	-2.675163	0.860979	H	5.360406	-1.115517	0.171332
Pd	0.404398	-0.178080	0.126927	C	4.811874	0.323815	-2.107949
C	0.787582	-3.467055	1.532547	H	4.315434	-0.651937	-2.100385
H	0.684741	-3.133329	2.576860	H	4.233577	1.006498	-2.740965
H	0.965210	-4.547160	1.559155	H	5.792138	0.204528	-2.580371
H	3.556483	-1.084662	-1.554829	C	-5.377455	-0.226689	-2.063877
H	-2.544844	-2.208021	-1.671755	H	-4.876704	0.516824	-2.694609
O	-3.311936	-1.229432	0.015423	H	-4.817027	-1.165912	-2.111726
O	4.357674	-0.318547	0.219416	H	-6.364757	-0.400227	-2.503558
C	-4.715414	-1.214366	-0.480112	C	-6.254981	-0.819214	0.226356
C	5.616257	0.120370	-0.436388	H	-6.320213	-0.502731	1.271556
C	-5.286973	-2.632981	-0.405363	H	-7.269722	-0.974451	-0.152699
H	-6.345082	-2.617391	-0.685754	C	-6.240673	1.596169	-0.514734
H	-4.777016	-3.320270	-1.089170	H	-5.723677	2.370118	-1.093423
H	-5.208990	-3.030471	0.611386	H	-7.258040	1.517708	-0.910956
C	-5.416039	-0.283142	0.508110	H	-6.304981	1.924327	0.527479
H	-6.477621	-0.201431	0.255747	C	-1.745019	-1.627307	-0.679979
H	-5.331174	-0.668428	1.528584	H	-2.592657	-1.484593	-0.015677
H	-4.978481	0.719604	0.476788	H	-1.281523	-2.606030	-0.582298
C	-4.756111	-0.646064	-1.901822	H	-1.971631	-1.374132	-1.718836
H	-4.265987	0.331923	-1.943154	H	-5.722300	-1.774524	0.184148
H	-4.281796	-1.307867	-2.634920	Br	1.479317	-1.889898	-0.715554
H	-5.797074	-0.518384	-2.215458	Br	0.551742	-1.772773	1.798046
C	5.295767	0.978459	-1.664708	E6			
H	4.820899	0.405490	-2.469422	E = -6094.049752 a.u.			
H	4.642197	1.814505	-1.396019	C	2.538456	1.078477	2.122500
H	6.223494	1.390794	-2.074216	C	1.549682	0.342213	1.305552
C	6.291018	0.951559	0.653903	C	-1.549615	0.342273	1.305538
H	6.468189	0.344957	1.546988	C	-2.538392	1.078514	2.122508
H	7.253205	1.329542	0.294801	C	2.948044	0.688236	0.782624
C	6.451802	-1.112225	-0.792969	C	-2.948005	0.688223	0.782652
H	5.967183	-1.732189	-1.555773	C	-1.240228	0.928047	2.687190
H	7.421144	-0.799587	-1.194273	B	1.240289	0.928049	2.687180
H	6.631476	-1.727733	0.094080	Pd	0.000020	-0.819334	0.393123
C	1.580234	1.481362	0.421973	C	0.000035	1.000055	3.616960
H	2.626773	1.231682	0.571928	H	0.000033	1.883981	4.264098
H	1.148575	1.957208	1.306111	H	0.000040	0.125244	4.286121
H	1.425091	2.077947	-0.481643	H	3.632117	-0.149695	0.671298
H	5.667556	1.806805	0.933209	H	-3.632080	-0.149714	0.671391
Br	-1.787486	1.280711	0.155832	O	-2.945739	1.626984	-0.206351
Br	-1.237524	3.574260	0.213911	O	2.945715	1.627020	-0.206354
TS_{E2}				C	-4.209928	1.860862	-0.965653
E = -6094.013334 a.u.				C	4.209875	1.860911	-0.965693
C	-2.804279	2.249490	0.497094	C	-5.296968	2.305458	0.015612
C	-1.895014	1.133919	0.160369	H	-6.208137	2.562173	-0.534063
C	1.321157	1.428133	0.134903	H	-5.557951	1.513295	0.726353
C	2.106927	2.626339	0.519990	H	-4.977324	3.188901	0.577378
C	-3.315622	1.251248	-0.420591	C	-3.822123	2.990703	-1.917535
C	2.703984	1.687773	-0.427834	H	-4.686526	3.281760	-2.521989
B	0.878954	2.392142	1.211487	H	-3.479647	3.867217	-1.359354
B	-1.588678	2.203687	1.232298	H	-3.023468	2.673555	-2.596048
Pd	-0.300664	-0.212947	-0.191002	C	-4.601120	0.596630	-1.735161
C	-0.380531	2.655411	2.082101	H	-3.772776	0.243649	-2.357257
H	-0.316817	2.008893	2.971299	H	-4.914984	-0.221347	-1.078244
H	-0.463567	3.688135	2.434155	H	-5.448099	0.821023	-2.391427
H	-3.375737	1.501807	-1.478496	C	4.601013	0.596676	-1.735221
H	2.756382	1.978957	-1.475587	H	4.914886	-0.221315	-1.078324
O	3.684050	0.852415	0.021434	H	3.772637	0.243714	-2.357286
O	-4.208500	0.331453	0.043788	H	5.447970	0.821065	-2.391516
C	4.988386	0.848347	-0.678550	C	3.822048	2.990769	-1.917547
C	-5.540393	0.238213	-0.613297	H	3.479609	3.867277	-1.359332
C	5.588049	2.257738	-0.649658	H	4.686432	3.281827	-2.522028

C	5.296952	2.305475	0.015545
H	5.557905	1.513316	0.726302
H	6.208127	2.562129	-0.534147
H	4.977356	3.188948	0.577290
C	0.000068	0.276503	-1.433931
H	0.922621	0.842722	-1.336390
H	-0.922407	0.842846	-1.336374
H	0.000010	-0.486076	-2.205897
H	3.023362	2.673650	-2.596037
Br	-1.738357	-2.320032	-0.457024
Br	1.738332	-2.320116	-0.457001

E

E = -6054.42809 a.u.

C	-2.528324	0.364271	-2.374491
C	-1.532666	0.033333	-1.330133
C	1.532302	0.033186	-1.330080
C	2.528059	0.363808	-2.374441
C	-2.929211	0.572446	-0.999987
C	2.929094	0.571862	-1.000007
B	1.238058	0.001922	-2.838224
B	-1.238461	0.001772	-2.838234
Pd	-0.000242	-0.860548	-0.245943
C	-0.000177	-0.320716	-3.723252
H	-0.000243	0.199017	-4.687158
H	-0.000020	-1.399781	-3.941187
H	-3.590214	-0.148282	-0.525059
H	3.589834	-0.149104	-0.525080
O	3.028359	1.875546	-0.589192
O	-3.028081	1.876176	-0.589225
C	3.580626	2.165283	0.743773
C	-3.579560	2.166140	0.744016
C	5.000457	1.596965	0.872563
H	5.461446	1.970973	1.792905
H	5.011307	0.503630	0.932424
H	5.620764	1.912160	0.026671
C	3.612294	3.695196	0.761974
H	3.982930	4.054072	1.727638
H	4.266629	4.078756	-0.027673
H	2.607361	4.098846	0.603421
C	2.646878	1.615112	1.825421
H	1.644666	2.044436	1.720214
H	2.558334	0.524915	1.775114
H	3.029933	1.879102	2.817822
C	-2.645119	1.616185	1.825185
H	-2.556838	0.525955	1.775152
H	-1.642921	2.045329	1.719116
H	-3.027433	1.880548	2.817769
C	-3.611258	3.696057	0.761935
H	-4.266171	4.079445	-0.027316
H	-3.981203	4.055120	1.727795
C	-4.999280	1.597793	0.873830
H	-5.010046	0.504479	0.934097
H	-5.459722	1.972108	1.794323
H	-5.620121	1.912676	0.028214
H	-2.606451	4.099707	0.602575
Br	1.785058	-2.138577	0.920113
Br	-1.785789	-2.138356	0.919984