

Supporting Information

Mechanism of the Pd-catalysed C(sp³)-H arylation of thioethers with Ag(I) additives

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Experimental section

All chemicals and solvents were purchased from commercial suppliers and were used without purification. Dong group's original procedure of catalytic experiment was consulted for the design of the mass spectrometry experiment.^[1] [An oven-dried 4.0 mL vial was charged with the thioether substrate **1a** (0.2 mmol, 1.0 equiv.), Pd(OAc)₂ (22.0 mg, 0.1 mmol, 0.5 equiv.), NaTFA (15.1 mg, 0.1 mmol, 0.5 equiv.) and 3-nitrobenzoic acid (8.4 mg, 0.05 mmol, 0.25 equiv.). The vial was partially capped and transferred in a nitrogen-filled glovebox. In the glovebox, AgTFA (22.1 mg, 0.1 mmol, 0.5 equiv) was added to the vial. Then HFIP (1.8 mL) and acetic acid (0.2 mL) were added to the vial. The vial was tightly sealed, transferred out of glovebox and stirred on a pie-block preheated to 90 °C for 8 hrs. Upon completion of the reaction, the mixture was filtered through a thin pad of celite. The filter cake was washed with ethyl acetate, and the combined filtrate was concentrated. The mixtures were analyzed by mass spectrometry.] All lab manipulations were performed in fume hoods. MALDI-TOF mass spectra were obtained on a Bruker Autoflex III TOF/TOF 200 mass spectrometer.

[1] L. Jin, J. Wang and G. Dong, *Angew. Chem., Int. Ed.*, 2018, **57**, 12352.

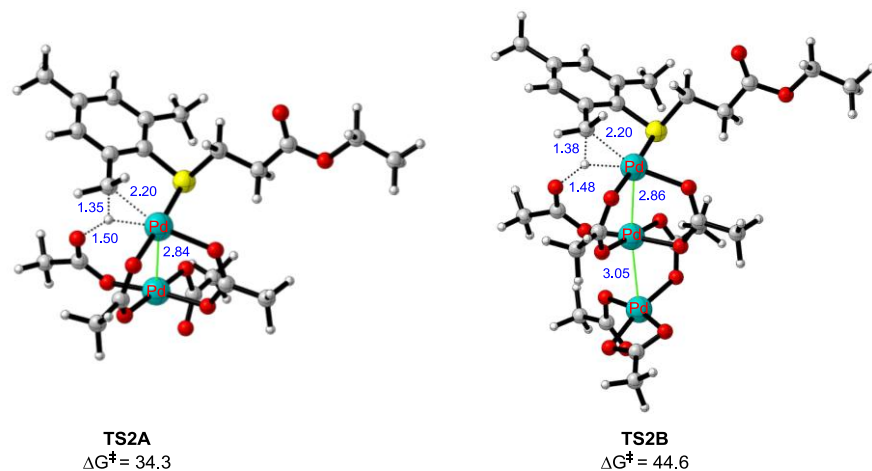


Fig. S1 C(sp³)–H activation pathways via dimeric Pd₂(OAc)₄ (**TS2A**) and trimeric Pd₃(OAc)₆ mechanism (**TS2B**). Energies are relative to Pd₃(OAc)₆ + **1a** and are mass-balanced.

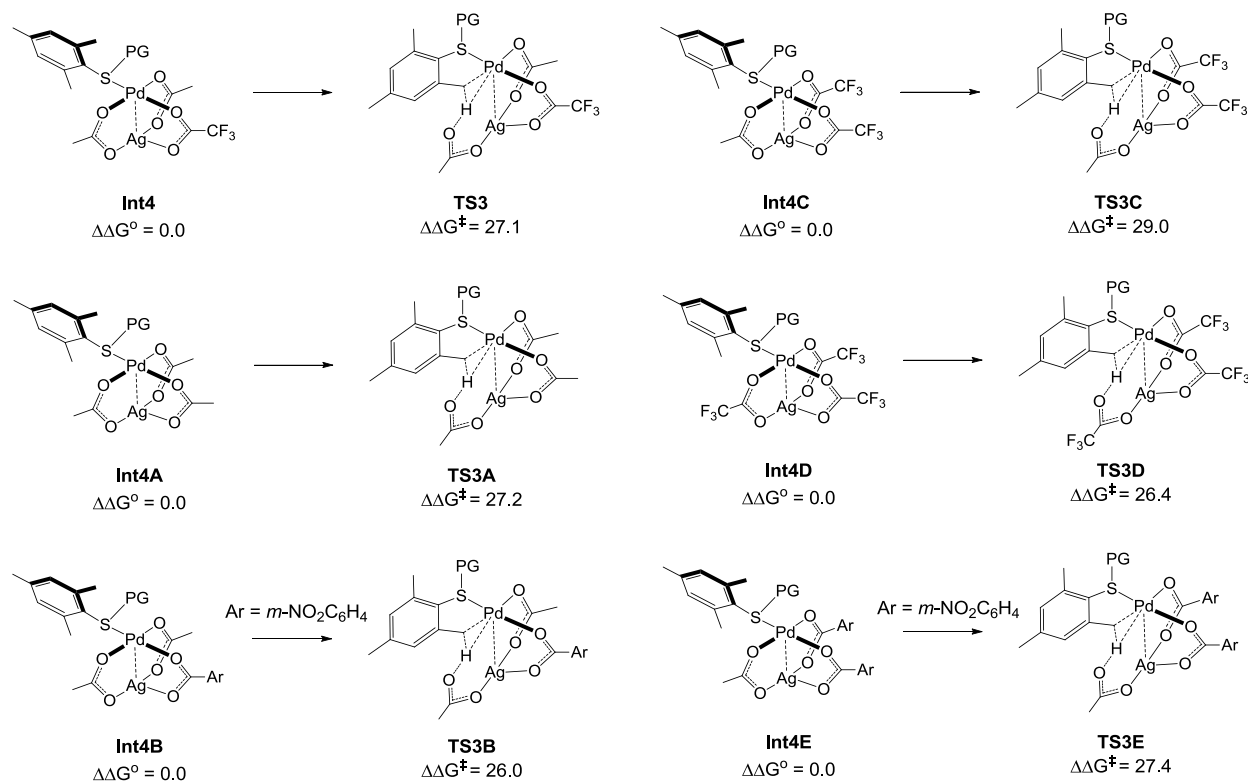


Fig. S2 C(sp³)–H activation pathways involving **Int4** and **Int4A–Int4E** via heterodimeric mechanism

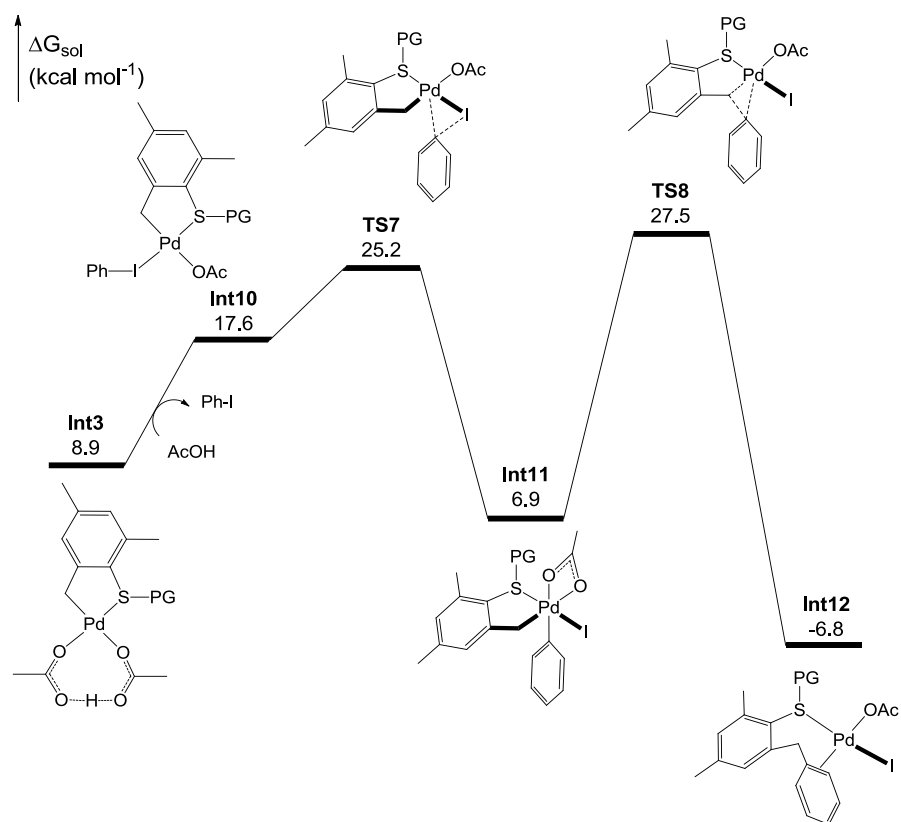


Fig. S3 Free energy profile for the Pd(II)-catalyzed oxidative addition and reductive elimination.

Energies and Cartesian Coordinates (Å) for the Optimized Structures

Pd₃(OAc)₆

SCF energy in solvent: -1754.972114 a.u.

Free energy in solvent: -1754.737223 a.u.

No imaginary frequency

Pd	-1.576568	0.910220	-0.007787
C	0.037084	2.601998	1.890640
O	-1.068151	2.431599	1.269820
O	1.159518	2.029524	1.663660
C	2.308851	-1.263694	-1.858271
O	1.584588	-2.133505	-1.263350
O	2.362537	-0.003231	-1.637443
C	3.242391	-1.793558	-2.933672
C	0.003399	3.587928	3.046276
Pd	0.000758	-1.816177	0.000172
C	2.223497	-1.338735	1.897681
O	2.636417	-0.296817	1.280111
O	1.167337	-2.023125	1.661872
C	-0.039532	2.600538	-1.892099
O	-1.161568	2.027464	-1.664622
O	1.065833	2.431450	-1.271157
C	-0.006576	3.585586	-3.048503
C	3.079064	-1.803599	3.063991
Pd	1.575821	0.911603	0.007609
C	-2.222645	-1.341496	-1.896944
O	-2.636346	-0.299905	-1.279373
O	-1.165716	-2.024812	-1.661392
C	-3.078127	-1.807400	-3.062898
C	-2.307281	-1.264917	1.858999
O	-2.361674	-0.004474	1.638133
O	-1.582976	-2.134391	1.263654
C	-3.240031	-1.795144	2.934898
H	-1.024780	3.876805	-3.339997
H	0.497457	3.110283	-3.906838
H	0.582339	4.471029	-2.765117
H	-0.586929	4.472311	2.762536
H	-0.499434	3.112577	3.905291
H	1.021364	3.880786	3.336965
H	-3.509524	-0.992656	3.635799

H	-2.771730	-2.637086	3.464577
H	-4.162835	-2.160573	2.452591
H	4.143267	-1.647269	2.833684
H	2.881901	-2.859952	3.292647
H	2.832515	-1.192226	3.948735
H	2.774585	-2.635521	-3.463760
H	3.512152	-0.990923	-3.634299
H	4.164948	-2.158903	-2.450834
H	-2.831846	-1.196480	-3.948031
H	-4.142372	-1.651354	-2.832612
H	-2.880547	-2.863808	-3.290947

Pd(OAc)₂

SCF energy in solvent: -584.955053 a.u.

Free energy in solvent: -584.893608 a.u.

No imaginary frequency

C	2.446647	-0.000031	-0.004163
O	1.762660	1.096589	-0.011734
O	1.762618	-1.096635	-0.011652
C	3.944415	-0.000052	0.042663
C	-2.446643	0.000182	-0.004025
O	-1.762726	-1.096502	-0.011609
O	-1.762539	1.096725	-0.011496
C	-3.944415	0.000168	0.042542
Pd	-0.000002	0.000001	-0.011018
H	4.338211	0.904969	-0.442996
H	4.274912	-0.000753	1.095845
H	4.338206	-0.904487	-0.444103
H	-4.338614	-0.891415	-0.467288
H	-4.337598	0.917369	-0.420010
H	-4.275173	-0.028743	1.095236

1a

SCF energy in solvent: -1094.149449 a.u.

Free energy in solvent: -1093.901783 a.u.

No imaginary frequency

C	-2.551121	-1.233685	-0.265356
C	-1.923366	-2.566090	-0.615187

H	-1.741472	-2.655395	-1.699307
H	-2.573769	-3.397955	-0.299593
C	-1.927357	0.000120	-0.589617
H	-0.942963	-2.696554	-0.124464
C	-2.550920	1.233969	-0.264636
C	-3.792472	-1.205703	0.397983
C	-4.427881	0.000026	0.743127
C	-3.792180	1.205926	0.398626
H	-4.276906	-2.157583	0.648933
H	-4.276396	2.157808	0.650037
S	-0.360960	0.000226	-1.487333
C	-1.922795	2.566375	-0.613805
H	-0.942132	2.696121	-0.123422
H	-1.741329	2.656360	-1.697944
H	-2.572752	3.398272	-0.297376
C	-5.746390	0.000252	1.486834
H	-5.586387	0.014570	2.581055
H	-6.352951	0.886345	1.236005
H	-6.341299	-0.899274	1.257148
C	0.845843	-0.000158	-0.081391
C	2.265126	0.000007	-0.654581
H	0.681968	-0.890275	0.546996
H	0.681916	0.889618	0.547481
H	2.434489	-0.880516	-1.301376
H	2.434830	0.881177	-1.300374
C	3.319905	-0.000937	0.445094
O	3.094771	-0.002993	1.648091
O	4.570567	0.000720	-0.096787
C	5.662018	-0.000273	0.870613
H	5.562337	0.887879	1.518674
H	5.563185	-0.890532	1.515908
C	6.964840	0.001571	0.085278
H	7.040879	0.896085	-0.554016
H	7.820161	0.000912	0.781413
H	7.041742	-0.890896	-0.556766

AcOH

SCF energy in solvent: -229.085158 a.u.

Free energy in solvent: -229.052699 a.u.

No imaginary frequency

C	-0.092409	0.125082	-0.000111
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O	-0.644066	1.202455	0.000024
O	-0.779434	-1.045643	0.000002
H	-1.720518	-0.802681	0.000146
C	1.396816	-0.110601	-0.000002
H	1.682976	-0.691605	0.881725
H	1.682913	-0.693761	-0.880305
H	1.916185	0.846660	-0.001099

Int1

SCF energy in solvent: -2773.306315 a.u.

Free energy in solvent: -2772.695395 a.u.

No imaginary frequency

Pd	-0.000048	0.000023	-0.000014
S	1.174941	1.930242	0.716547
O	1.816431	-0.939436	-0.151986
C	2.110862	-1.454905	-1.334215
O	1.391073	-1.386946	-2.345295
C	3.443438	-2.206755	-1.340112
H	4.196494	-1.714511	-0.705255
H	3.276086	-3.220455	-0.937175
H	3.813366	-2.295193	-2.371822
O	-1.391168	1.386927	2.345256
C	-2.110940	1.454946	1.334172
O	-1.816515	0.939492	0.151928
C	-3.443431	2.206939	1.340078
H	-3.275685	3.221003	0.938214
H	-4.196248	1.715426	0.704382
H	-3.813859	2.294508	2.371686
C	2.794230	1.993382	-0.196901
C	3.873714	1.328074	0.663150
H	3.021648	3.056285	-0.370519
H	2.692611	1.484274	-1.164960
H	3.941326	1.817779	1.653324
H	3.626934	0.269684	0.844133
C	5.238118	1.438954	-0.004605
O	5.544057	2.259285	-0.860655
O	6.094152	0.504216	0.495830
C	7.452786	0.566644	-0.034264
H	7.410810	0.438781	-1.129710
H	7.863149	1.572111	0.164121
C	8.256660	-0.530561	0.646226

H	7.825796	-1.523532	0.439103
H	9.293975	-0.519425	0.272007
H	8.281869	-0.384416	1.738272
C	0.001595	-3.602046	1.253466
C	-0.299691	-2.585570	2.329924
H	-0.090451	-1.552163	1.991289
H	0.308170	-2.782943	3.227016
C	-0.336309	-3.419065	-0.114340
H	-1.359606	-2.617595	2.638966
C	-0.007363	-4.390862	-1.099190
C	0.654180	-4.797429	1.611772
C	0.977501	-5.791506	0.672740
C	0.643976	-5.563674	-0.673936
H	0.922167	-4.946944	2.664788
H	0.898818	-6.320361	-1.425901
S	-1.174989	-1.930287	-0.716462
C	-0.308435	-4.200164	-2.570582
H	-1.384583	-4.038654	-2.753168
H	0.227660	-3.317566	-2.961808
H	0.005505	-5.087668	-3.142941
C	1.645683	-7.079574	1.102406
H	0.894503	-7.842766	1.378390
H	2.260975	-7.506293	0.293184
H	2.291642	-6.926448	1.982735
C	-2.794261	-1.993375	0.197001
C	-3.873735	-1.328153	-0.663123
H	-2.692676	-1.484200	1.165029
H	-3.021653	-3.056270	0.370715
H	-3.626930	-0.269779	-0.844198
H	-3.941353	-1.817916	-1.653265
C	-5.238138	-1.438882	0.004649
O	-5.543855	-2.258522	0.861442
O	-6.094451	-0.504898	-0.496712
C	-7.453066	-0.567222	0.033426
H	-7.863319	-1.572835	-0.164465
H	-7.411100	-0.438822	1.128807
C	-8.257082	0.529540	-0.647612
H	-8.282268	0.382853	-1.739586
H	-9.294398	0.518454	-0.273393
H	-7.826346	1.522669	-0.440978
C	0.336359	3.419123	0.114551

C	0.007490	4.390878	1.099472
C	-0.001509	3.602241	-1.253246
C	-0.643721	5.563785	0.674296
C	-0.653956	4.797725	-1.611475
C	-0.977192	5.791759	-0.672373
H	-0.898505	6.320441	1.426313
H	-0.921904	4.947353	-2.664484
C	0.308545	4.200037	2.570851
H	-0.227608	3.317445	2.962007
H	1.384683	4.038444	2.753420
H	-0.005336	5.087516	3.143282
C	-1.645223	7.079939	-1.101936
H	-2.260731	7.506489	-0.292786
H	-0.893946	7.843177	-1.377528
H	-2.290941	6.927032	-1.982479
C	0.299692	2.585815	-2.329778
H	0.090360	1.552406	-1.991216
H	-0.308155	2.783310	-3.226854
H	1.359608	2.617785	-2.638823

TS1

SCF energy in solvent: -2773.281872 a.u.

Free energy in solvent: -2772.675487 a.u.

imaginary frequency: -61.663000

Pd	-0.345350	-0.202079	-1.043635
S	2.288331	0.940585	-0.705918
O	-0.921028	1.536611	-1.850730
C	-1.075288	2.615825	-1.133514
O	-0.909430	2.687226	0.088234
C	-1.532379	3.816631	-1.949865
H	-1.139809	3.779093	-2.967775
H	-2.626323	3.803066	-2.006786
H	-1.224111	4.738104	-1.452683
O	0.925684	-1.479839	-2.655191
C	0.886330	-2.354321	-1.764683
O	0.258254	-2.116846	-0.646696
C	1.573484	-3.687493	-1.908124
H	2.581874	-3.607709	-1.488160
H	1.032538	-4.463957	-1.362470
H	1.657297	-3.950502	-2.964035
C	2.588010	1.729805	0.939552

C	2.215315	3.209822	0.890957
H	3.647640	1.601529	1.169379
H	2.005327	1.225321	1.709564
H	2.790642	3.747005	0.129426
H	1.155286	3.329865	0.635001
C	2.446011	3.872003	2.233983
O	2.740953	3.298452	3.262717
O	2.271388	5.208392	2.148353
C	2.432964	5.946008	3.380717
H	1.723304	5.560718	4.119926
H	3.440430	5.768797	3.771010
C	2.191930	7.411138	3.069597
H	1.182142	7.566358	2.678981
H	2.305355	8.008349	3.979885
H	2.907487	7.776190	2.327104
C	-4.174147	0.016623	-1.506675
C	-3.544844	-1.059968	-2.356552
H	-2.462728	-0.917464	-2.452724
H	-3.976782	-1.049030	-3.360083
C	-3.654459	0.442904	-0.263594
H	-3.711542	-2.059933	-1.941508
C	-4.265780	1.488092	0.468757
C	-5.335946	0.639780	-1.977450
C	-5.979146	1.658540	-1.271759
C	-5.423359	2.069863	-0.057613
H	-5.742419	0.318271	-2.933353
H	-5.899996	2.871134	0.501931
S	-2.163107	-0.260251	0.470807
C	-3.711660	2.012326	1.774170
H	-3.629009	1.225129	2.530332
H	-2.712824	2.434863	1.626199
H	-4.364165	2.793967	2.171697
C	-7.249246	2.284648	-1.794885
H	-7.317080	2.203002	-2.883456
H	-8.133171	1.789155	-1.374019
H	-7.313383	3.343515	-1.526769
C	-2.592004	-2.044886	0.694961
C	-1.745259	-2.626016	1.825117
H	-2.412299	-2.592666	-0.227663
H	-3.657106	-2.082855	0.932874
H	-0.680723	-2.556983	1.578716

H	-1.892849	-2.082774	2.765146
C	-2.079193	-4.088797	2.052272
O	-2.870963	-4.734957	1.397969
O	-1.372747	-4.586998	3.085797
C	-1.599643	-5.983694	3.393130
H	-2.662351	-6.127741	3.612038
H	-1.362500	-6.582192	2.507911
C	-0.718790	-6.338794	4.575561
H	-0.967701	-5.726735	5.447161
H	-0.861777	-7.390810	4.841286
H	0.337405	-6.184551	4.336956
C	3.604878	-0.281617	-0.837799
C	4.369687	-0.269645	-2.028518
C	3.839774	-1.260024	0.153533
C	5.388824	-1.214023	-2.179453
C	4.883141	-2.174807	-0.046831
C	5.674281	-2.166758	-1.196970
H	5.976982	-1.200919	-3.094336
H	5.070681	-2.921937	0.721531
C	4.104479	0.710908	-3.146533
H	3.110659	0.555224	-3.580145
H	4.138756	1.745908	-2.792720
H	4.843676	0.591039	-3.943129
C	6.811945	-3.144809	-1.370607
H	6.909354	-3.465587	-2.412591
H	7.769223	-2.693250	-1.080968
H	6.672347	-4.036275	-0.752047
C	3.007123	-1.380955	1.408638
H	1.947411	-1.221254	1.193846
H	3.120618	-2.378149	1.842932
H	3.307646	-0.658248	2.174846

Int2

SCF energy in solvent: -1679.126939 a.u.

Free energy in solvent: -1678.791727 a.u.

No imaginary frequency

C	1.456206	1.925493	-1.226470
C	1.070041	0.984520	-2.344655
H	1.269900	-0.069062	-2.063485
H	1.638601	1.216832	-3.258773
Pd	1.211505	-1.569514	0.011840

C	1.079979	1.718487	0.128324
H	-0.002932	1.044809	-2.597079
C	1.529347	2.583783	1.162742
C	2.252797	3.048276	-1.520962
C	2.691085	3.943089	-0.529817
C	2.325514	3.685472	0.803403
H	2.549228	3.216622	-2.563362
H	2.672754	4.360014	1.595307
S	0.059194	0.314699	0.655433
C	1.192458	2.357957	2.623024
H	0.103493	2.344887	2.799907
H	1.584893	1.392649	2.986338
H	1.629097	3.156161	3.243865
C	3.521173	5.156458	-0.886890
H	2.882854	6.050831	-1.011183
H	4.256078	5.389663	-0.098581
H	4.066510	5.009328	-1.833292
O	-0.367259	-2.444378	-0.881368
C	-1.408237	-2.713895	-0.110159
O	-1.534585	-2.348114	1.072483
C	-2.507159	-3.475826	-0.847059
H	-3.243157	-2.741112	-1.218025
H	-2.111236	-4.039920	-1.703710
H	-3.016636	-4.151181	-0.143660
O	2.716691	-3.071677	-0.217283
C	3.559328	-2.278453	0.343911
O	3.134696	-1.111141	0.713504
C	4.994168	-2.678250	0.549331
H	5.512812	-2.693905	-0.424305
H	5.499720	-1.965917	1.216816
H	5.041689	-3.695457	0.968741
C	-1.511781	0.575070	-0.317535
C	-2.727279	0.480520	0.612975
H	-1.566314	-0.187852	-1.106723
H	-1.424207	1.572194	-0.775874
H	-2.659889	-0.463360	1.189309
H	-2.774882	1.318130	1.326558
C	-4.012682	0.409527	-0.199493
O	-4.123466	-0.123801	-1.298622
O	-5.044041	0.990070	0.469113
C	-6.340703	0.901876	-0.197192

H	-6.256435	1.366599	-1.194711
H	-6.587080	-0.163231	-0.349416
C	-7.354607	1.609393	0.688403
H	-7.086207	2.668913	0.830069
H	-8.352192	1.565763	0.220417
H	-7.416981	1.131399	1.679362

TS2

SCF energy in solvent: -1679.087697 a.u.

Free energy in solvent: -1678.75882 a.u.

imaginary frequency: -939.950700

C	-2.422726	-1.161666	-0.577580
C	-2.028259	0.080571	-1.331304
C	-2.078370	3.385835	-0.965508
O	-0.817699	3.105714	-0.987707
O	-2.993402	2.535335	-0.712885
H	-2.310195	1.286006	-0.752370
H	-2.834220	0.378626	-2.025844
Pd	-0.455476	1.215295	-0.210081
C	-1.575280	-1.724727	0.403921
H	-1.156838	-0.094789	-1.995320
C	-2.455595	4.830244	-1.231741
H	-2.475860	5.364203	-0.266269
H	-3.457988	4.887002	-1.679162
H	-1.709505	5.315566	-1.876587
C	-1.896656	-2.925851	1.078957
C	-3.631409	-1.823572	-0.863575
C	-3.994893	-3.015982	-0.211596
C	-3.112411	-3.552087	0.744795
H	-4.302283	-1.393889	-1.617357
H	-3.385137	-4.476951	1.267010
S	-0.099138	-0.787800	0.872674
C	-0.995821	-3.531152	2.133326
H	-0.106784	-4.013067	1.686282
H	-0.629589	-2.768144	2.841290
H	-1.530119	-4.304850	2.706739
C	-5.319158	-3.686553	-0.506099
H	-5.638603	-3.511234	-1.546496
H	-5.267864	-4.774994	-0.339915
H	-6.115613	-3.291246	0.150892
C	1.240850	-1.672937	-0.075423

H	1.207266	-2.729500	0.237380
H	1.014128	-1.620583	-1.150171
C	2.596202	-1.030166	0.231681
H	2.923600	-1.234769	1.265364
H	2.531618	0.072776	0.144789
C	3.656523	-1.526776	-0.743099
O	3.431101	-2.133022	-1.783635
O	4.898607	-1.184017	-0.311707
C	5.989159	-1.557838	-1.208198
C	7.281400	-1.052377	-0.586014
H	5.798036	-1.112782	-2.199849
H	5.983523	-2.654822	-1.331658
H	8.133908	-1.314921	-1.234379
H	7.261609	0.043099	-0.468388
H	7.449123	-1.505349	0.404607
O	1.258227	1.961539	0.617364
C	1.038022	2.551513	1.789112
O	-0.044942	2.576428	2.385832
C	2.292456	3.243753	2.329258
H	3.187679	2.616925	2.192118
H	2.456749	4.181202	1.771221
H	2.152124	3.480504	3.393409

Int3

SCF energy in solvent: -1679.131383 a.u.

Free energy in solvent: -1678.799963 a.u.

No imaginary frequency

C	-2.650032	-0.944066	-0.479293
C	-2.131493	0.323646	-1.118668
C	-1.204738	3.906512	-0.867764
O	-0.843913	2.799367	-1.420710
O	-1.196402	4.167876	0.376461
H	-0.281505	3.614177	1.218103
H	-2.907762	1.108186	-1.150805
Pd	-0.479417	1.119279	-0.253549
C	-1.845993	-1.666486	0.422093
H	-1.799870	0.133185	-2.159374
C	-1.702112	4.991291	-1.814260
H	-1.153064	5.927435	-1.624853
H	-2.765987	5.190445	-1.601489
H	-1.589424	4.690203	-2.864672

C	-2.270802	-2.870624	1.033622
C	-3.931042	-1.452928	-0.773724
C	-4.392704	-2.652636	-0.204661
C	-3.550611	-3.342166	0.692792
H	-4.576756	-0.896050	-1.463836
H	-3.909632	-4.267158	1.160833
S	-0.287018	-0.863006	0.873856
C	-1.413505	-3.630966	2.021094
H	-0.659115	-4.257794	1.510223
H	-0.868532	-2.949280	2.696539
H	-2.030324	-4.304783	2.636696
C	-5.759740	-3.203678	-0.550416
H	-6.410734	-2.427066	-0.983032
H	-5.682830	-4.020979	-1.291030
H	-6.265002	-3.619334	0.337822
C	0.959391	-1.884886	-0.063787
H	0.855230	-2.925565	0.281762
H	0.707405	-1.842574	-1.133048
C	2.364916	-1.344508	0.204509
H	2.633950	-1.435796	1.272757
H	2.426219	-0.265534	-0.028084
C	3.401332	-2.094459	-0.621915
O	3.159927	-3.010333	-1.398180
O	4.647155	-1.603529	-0.381498
C	5.719587	-2.242178	-1.138181
C	7.013020	-1.523431	-0.786632
H	5.480589	-2.175365	-2.213472
H	5.750004	-3.313451	-0.872679
H	7.853285	-1.977444	-1.337908
H	6.958640	-0.456661	-1.057731
H	7.227873	-1.597513	0.291806
O	1.403643	1.833561	0.646090
C	1.472213	2.661400	1.598835
O	0.530298	3.482350	1.959444
C	2.740225	2.749548	2.426351
H	2.495410	2.599227	3.490626
H	3.472919	2.000165	2.099308
H	3.171352	3.759944	2.334285

Int4

SCF energy in solvent: -2352.439029 a.u.

Free energy in solvent: -2352.091131 a.u.

No imaginary frequency

C	-1.909559	2.907076	-1.457322
C	-1.541870	1.976196	-2.587996
C	3.533228	-0.508720	-0.570926
O	2.627804	0.320246	-0.915805
O	3.515809	-1.417313	0.268862
H	-0.667396	1.362886	-2.355481
H	-1.318681	2.550244	-3.490239
Pd	0.690506	0.427100	-0.224028
C	-1.937062	2.523559	-0.097670
H	-2.362588	1.292925	-2.833325
C	4.829732	-0.326125	-1.404705
C	-2.264584	3.447319	0.920925
C	-2.245027	4.229603	-1.766997
C	-2.589820	5.166267	-0.789601
C	-2.587460	4.754734	0.545175
H	-2.222921	4.535453	-2.810146
H	-2.838882	5.471267	1.323074
S	-1.517140	0.856371	0.466458
C	-2.267858	3.088931	2.390441
H	-2.959027	2.269763	2.613049
H	-1.276413	2.771769	2.727852
H	-2.566170	3.953392	2.988349
C	-2.969679	6.576680	-1.169294
H	-4.037270	6.642217	-1.413665
H	-2.777925	7.277262	-0.351794
H	-2.414171	6.916574	-2.048224
O	0.151210	-0.964791	-1.621308
C	0.108639	-2.217128	-1.305501
O	0.293352	-2.700991	-0.162734
C	-0.267612	-3.140778	-2.448152
H	-1.360254	-3.182800	-2.515670
H	0.119232	-2.759329	-3.394675
H	0.112590	-4.144662	-2.254135
Ag	1.496380	-1.663643	1.494508
O	1.582142	0.190681	2.802938
C	1.595628	1.369408	2.380054
O	1.258456	1.778385	1.202513
C	2.076659	2.467355	3.312707
H	3.170660	2.498273	3.268109

H	1.692768	3.442951	3.011573
H	1.788840	2.235492	4.339830
C	-2.698775	-0.243853	-0.427407
C	-2.934181	-1.510978	0.396823
H	-2.299075	-0.492936	-1.407951
H	-3.618343	0.334277	-0.545829
H	-1.976847	-1.978655	0.661111
H	-3.459654	-1.301746	1.332149
C	-3.707882	-2.543402	-0.405195
O	-3.731922	-2.602155	-1.619004
O	-4.339122	-3.409815	0.402689
C	-5.048730	-4.493014	-0.252746
H	-5.811913	-4.062945	-0.908521
H	-4.342249	-5.042384	-0.882192
C	-5.649084	-5.365396	0.832076
H	-6.346454	-4.795769	1.452909
H	-6.195016	-6.197032	0.376091
H	-4.869414	-5.778759	1.477955
F	5.126568	0.972440	-1.584424
F	5.880164	-0.914517	-0.816682
F	4.660779	-0.888526	-2.620392

TS3

SCF energy in solvent: -2352.38952 a.u.

Free energy in solvent: -2352.047944 a.u.

imaginary frequency: -593.139300

C	-0.359985	2.746156	1.130061
C	-0.827426	1.419432	1.667324
C	-2.177196	-2.358308	0.994165
O	-1.346344	-1.556469	1.594398
O	-2.436922	-2.491900	-0.207738
H	-1.577955	0.901789	0.682799
H	-1.765101	1.495153	2.241960
Pd	-0.176122	-0.300583	0.476939
C	0.617478	2.804081	0.113457
H	-0.092284	0.963201	2.361743
C	-2.919720	-3.245282	2.044758
C	1.081910	4.032714	-0.415336
C	-0.882575	3.953230	1.625724
C	-0.440240	5.197023	1.140347
C	0.537718	5.211782	0.126982

H	-1.654766	3.915647	2.402658
H	0.877130	6.174221	-0.274350
S	1.219372	1.235894	-0.572553
C	2.110990	4.113498	-1.521674
H	3.138184	3.964283	-1.140533
H	1.936619	3.350283	-2.299124
H	2.086270	5.103991	-2.002124
C	-1.033983	6.488134	1.659936
H	-1.870637	6.822298	1.019355
H	-1.430621	6.368233	2.680921
H	-0.288479	7.300190	1.672242
O	0.905972	-1.928750	-0.236103
C	0.763695	-2.457560	-1.413198
O	-0.012474	-2.079472	-2.335905
C	1.625083	-3.687780	-1.665257
Ag	-1.648647	-0.720974	-1.973733
O	-3.162241	0.739600	-2.041507
C	-3.550847	1.318257	-0.962905
O	-2.986487	1.288754	0.178570
C	-4.861152	2.096494	-1.068908
H	-5.695252	1.411083	-0.838733
H	-4.885692	2.921037	-0.341824
H	-5.005256	2.474445	-2.091585
C	2.863566	1.092304	0.298960
C	3.633266	-0.129307	-0.203918
H	2.679012	1.042001	1.382226
H	3.409331	2.024840	0.085640
H	3.077034	-1.060732	0.001309
H	3.777681	-0.089529	-1.299390
C	5.003247	-0.197924	0.461687
O	5.448911	0.639857	1.236333
O	5.666199	-1.316813	0.073664
C	6.999602	-1.478958	0.651139
H	7.610938	-0.602761	0.373986
H	6.906955	-1.484248	1.750700
C	7.573163	-2.779480	0.111382
H	7.648944	-2.754190	-0.987738
H	8.583639	-2.938223	0.523198
H	6.945601	-3.638754	0.397886
F	-3.644304	-2.469062	2.895033
F	-3.762231	-4.112753	1.445728

F	-2.030348	-3.962592	2.783831
H	2.534718	-3.679842	-1.048126
H	1.033507	-4.579702	-1.396327
H	1.878028	-3.756295	-2.733028

Int5

SCF energy in solvent: -2352.436883 a.u.

Free energy in solvent: -2352.090251 a.u.

No imaginary frequency

C	-0.669999	2.484699	1.111723
C	-0.774725	1.061995	1.608758
C	-2.043419	-2.237762	1.211859
O	-0.850652	-1.859327	1.455017
O	-2.900428	-1.769524	0.413723
H	-3.407789	-0.343081	0.140698
H	-1.824078	0.780639	1.799341
Pd	0.112222	-0.330643	0.415840
C	0.285121	2.824949	0.134441
H	-0.213264	0.938259	2.557840
C	-2.468104	-3.470524	2.067541
C	0.462332	4.146928	-0.337775
C	-1.488361	3.513535	1.621234
C	-1.342305	4.846002	1.193012
C	-0.365820	5.138789	0.217957
H	-2.245517	3.264262	2.374722
H	-0.258167	6.170622	-0.138276
S	1.165787	1.422124	-0.600092
C	1.479100	4.503498	-1.399298
H	2.496837	4.589699	-0.975651
H	1.520734	3.740696	-2.195837
H	1.238284	5.473085	-1.863098
C	-2.199743	5.949185	1.776469
H	-2.469837	6.699340	1.014303
H	-3.129600	5.551298	2.213988
H	-1.661812	6.484230	2.580572
O	1.294500	-1.837224	-0.629144
C	0.907664	-2.609886	-1.571988
O	-0.187696	-2.532218	-2.232294
C	1.829482	-3.769940	-1.929791
Ag	-1.575818	-0.962900	-1.853615
O	-3.006892	0.664763	-2.047117

C	-3.731175	1.119870	-1.128354
O	-3.916502	0.552709	0.046065
C	-4.460135	2.430232	-1.303023
H	-5.475976	2.366028	-0.884948
H	-3.914793	3.209628	-0.743143
H	-4.490965	2.706255	-2.365053
C	2.846065	1.552784	0.200073
C	3.732816	0.395578	-0.265506
H	2.716116	1.541841	1.291536
H	3.265424	2.528635	-0.094174
H	3.218196	-0.575484	-0.130564
H	3.966581	0.465917	-1.342368
C	5.033420	0.369877	0.527906
O	5.275183	1.062500	1.509001
O	5.893361	-0.544087	0.006294
C	7.158327	-0.680298	0.723694
H	7.669337	0.298185	0.724923
H	6.941033	-0.941154	1.773810
C	7.968490	-1.755305	0.016334
H	8.169616	-1.476609	-1.030782
H	8.935263	-1.890104	0.529435
H	7.436897	-2.720557	0.023460
F	-2.719502	-3.067118	3.344785
F	-3.586741	-4.053179	1.583524
F	-1.486962	-4.405320	2.106344
H	2.880981	-3.500812	-1.752425
H	1.584070	-4.625710	-1.277365
H	1.678738	-4.078667	-2.974024

AcOHAgTFA

SCF energy in solvent: -902.363555 a.u.

Free energy in solvent: -902.323077 a.u.

No imaginary frequency

C	1.898927	0.201551	-0.019255
O	1.518799	1.390040	-0.043994
O	1.140108	-0.848477	0.011282
C	3.416524	-0.130023	-0.004884
Ag	-0.746180	0.152475	0.010540
O	-2.824658	0.750247	0.018520
C	-3.724646	-0.116232	-0.001993
O	-3.477169	-1.428582	-0.027420

C	-5.185333	0.232217	-0.008799
H	-5.310889	1.315885	0.103799
H	-5.635236	-0.101353	-0.958884
H	-5.702005	-0.303492	0.803416
H	-2.487204	-1.543485	-0.028053
F	4.172840	0.981121	-0.137600
F	3.751198	-0.731046	1.169522
F	3.733331	-0.979493	-1.017830

Ph-I

SCF energy in solvent: -243.034153 a.u.

Free energy in solvent: -242.978642 a.u.

No imaginary frequency

C	-1.270867	1.224462	0.000000
C	-2.676594	1.213943	-0.000001
C	-3.380829	-0.000012	0.000000
C	-2.676556	-1.213958	0.000000
C	-1.270848	-1.224457	-0.000002
C	-0.589288	0.000020	0.000001
H	-0.722858	2.170027	0.000004
H	-3.217023	2.166368	-0.000004
H	-4.475273	-0.000044	0.000007
H	-3.216998	-2.166379	0.000000
H	-0.722784	-2.169988	0.000003
I	1.576318	0.000001	0.000000

Int6

SCF energy in solvent: -2366.383712 a.u.

Free energy in solvent: -2366.016749 a.u.

No imaginary frequency

C	0.309278	2.283327	1.635439
C	0.274965	0.815058	1.994940
C	-0.834559	-2.466343	1.596291
O	0.360983	-2.040255	1.731333
O	-1.724476	-2.142875	0.764542
H	-0.757687	0.477532	2.194480
Pd	1.107146	-0.435420	0.620141
C	1.112499	2.738725	0.573614
H	0.876007	0.618615	2.906169
C	-1.248055	-3.508770	2.676437
C	1.197308	4.103073	0.204879

C	-0.439705	3.239007	2.351386
C	-0.379094	4.607202	2.033575
C	0.441433	5.015629	0.961109
H	-1.081792	2.900850	3.173893
H	0.479539	6.078062	0.690690
S	1.921751	1.439900	-0.396991
C	2.047443	4.584571	-0.950143
H	3.111278	4.678070	-0.662909
H	2.000820	3.891739	-1.807963
H	1.716603	5.578061	-1.292179
C	-1.166650	5.626898	2.828496
H	-1.601436	6.401650	2.174509
H	-1.986600	5.153829	3.392306
H	-0.519304	6.145791	3.559161
O	2.166104	-1.765894	-0.725108
C	1.717255	-2.188575	-1.852599
O	0.571761	-1.952251	-2.360293
C	2.646686	-3.101298	-2.649374
Ag	-1.021837	-1.015669	-1.132994
C	3.692082	1.571338	0.178323
C	4.548363	0.524684	-0.538027
H	3.715367	1.431174	1.268311
H	4.026761	2.595925	-0.050953
H	4.095038	-0.482041	-0.451774
H	4.623556	0.730249	-1.620497
C	5.949209	0.480337	0.058496
O	6.311435	1.089043	1.057949
O	6.750058	-0.345677	-0.665833
C	8.108925	-0.494480	-0.152603
H	8.596089	0.496258	-0.153597
H	8.054722	-0.835078	0.895696
C	8.826242	-1.491971	-1.048787
H	8.862543	-1.135340	-2.090961
H	9.861493	-1.631962	-0.695541
H	8.321319	-2.471362	-1.033725
F	-0.200613	-4.249552	3.104001
F	-1.766049	-2.847973	3.753501
F	-2.199183	-4.353258	2.210716
H	3.700607	-2.917273	-2.395257
H	2.410559	-4.149382	-2.396109
H	2.479526	-2.970054	-3.728583

I	-3.117655	0.551621	-2.220741
C	-4.729851	0.377692	-0.759701
C	-5.862488	1.178812	-0.946721
C	-4.599902	-0.521206	0.303126
C	-6.913503	1.067656	-0.019090
H	-5.935865	1.873582	-1.787811
C	-5.666916	-0.612269	1.217079
H	-3.705521	-1.138260	0.436741
C	-6.817749	0.174858	1.059609
H	-7.807377	1.686415	-0.149802
H	-5.584116	-1.311890	2.055081
H	-7.640451	0.092891	1.776782

TS4

SCF energy in solvent: -2366.369212 a.u.

Free energy in solvent: -2365.998205 a.u.

imaginary frequency: -101.004400

C	0.111244	2.330812	1.808399
C	0.016824	0.867769	2.174971
C	-1.099702	-2.632097	1.551082
O	-0.062322	-1.980202	1.912350
O	-1.848248	-2.495568	0.549440
H	-1.018764	0.576561	2.423302
Pd	0.740290	-0.427390	0.781819
C	0.900548	2.741957	0.717967
H	0.651279	0.642265	3.056667
C	-1.512734	-3.732357	2.575055
C	1.044347	4.100323	0.342992
C	-0.562455	3.326678	2.546865
C	-0.443023	4.689208	2.221446
C	0.361459	5.051788	1.120305
H	-1.184444	3.024343	3.398437
H	0.447035	6.110276	0.845523
S	1.615151	1.400913	-0.271414
C	1.884046	4.536655	-0.837240
H	2.956530	4.593156	-0.573735
H	1.791136	3.837561	-1.685766
H	1.582868	5.538215	-1.182812
C	-1.158335	5.751794	3.028408
H	-1.750086	6.420140	2.378942
H	-1.839526	5.305794	3.770332

H	-0.439051	6.388045	3.574789
O	1.739887	-1.844999	-0.508415
C	1.220535	-2.368003	-1.558417
O	0.060779	-2.128364	-2.031295
C	2.061533	-3.403364	-2.296641
Ag	-1.475533	-0.905369	-1.051850
C	3.406924	1.452374	0.248574
C	4.189515	0.363159	-0.488304
H	3.458451	1.317056	1.338350
H	3.780922	2.459085	0.001836
H	3.695415	-0.621557	-0.377207
H	4.235948	0.558282	-1.574359
C	5.607261	0.260587	0.059598
O	6.033138	0.867321	1.034878
O	6.340342	-0.614744	-0.677606
C	7.708924	-0.821559	-0.211484
H	8.243577	0.143524	-0.250758
H	7.677188	-1.139382	0.844822
C	8.341895	-1.870064	-1.112884
H	8.355975	-1.535293	-2.162795
H	9.381733	-2.054551	-0.795422
H	7.790717	-2.822762	-1.058839
F	-0.433073	-4.333605	3.129221
F	-2.237414	-3.156910	3.576819
F	-2.277714	-4.687498	2.000140
H	3.130431	-3.280683	-2.071005
H	1.749086	-4.409030	-1.966342
H	1.883788	-3.336903	-3.380220
C	-3.264942	0.239395	-0.616334
C	-4.398344	-0.590454	-0.655269
C	-3.107191	1.254544	0.341163
C	-5.363114	-0.444470	0.356999
H	-4.523700	-1.341963	-1.439033
C	-4.089646	1.382116	1.338412
H	-2.242262	1.922260	0.323686
C	-5.213068	0.538385	1.348850
H	-6.238836	-1.101832	0.354660
H	-3.970579	2.158434	2.101713
H	-5.978808	0.655950	2.121899
I	-2.369840	0.883287	-2.921100

Int7

SCF energy in solvent: -2366.370276 a.u.

Free energy in solvent: -2366.001114 a.u.

No imaginary frequency

C	-0.086297	2.533596	-1.709306
C	0.122227	1.109607	-2.168690
C	1.353832	-2.470399	-1.652960
O	0.403581	-1.748192	-2.084978
O	1.961223	-2.460044	-0.541751
H	1.184464	0.900518	-2.382968
Pd	-0.575930	-0.325133	-0.907803
C	-0.956591	2.815006	-0.639899
H	-0.462068	0.900716	-3.088416
C	1.899009	-3.500146	-2.688591
C	-1.207011	4.130183	-0.179471
C	0.557467	3.617455	-2.340878
C	0.325829	4.943617	-1.934257
C	-0.553434	5.175238	-0.855474
H	1.246778	3.415184	-3.169721
H	-0.720633	6.203857	-0.513442
S	-1.621925	1.365465	0.219665
C	-2.120055	4.425335	0.989746
H	-3.184365	4.413039	0.689734
H	-1.997924	3.685505	1.799393
H	-1.912741	5.424279	1.404588
C	0.994927	6.103598	-2.640017
H	1.334334	6.871092	-1.924087
H	1.865873	5.771870	-3.227640
H	0.294818	6.598771	-3.337588
O	-1.563613	-1.892609	0.227236
C	-1.099285	-2.482544	1.263032
O	0.030972	-2.264625	1.821159
C	-1.956769	-3.567273	1.901487
Ag	1.548403	-0.967130	1.021019
C	-3.393429	1.335568	-0.367803
C	-4.129738	0.172476	0.300314
H	-3.403976	1.245125	-1.463354
H	-3.833664	2.307214	-0.091718
H	-3.580137	-0.776771	0.149413
H	-4.203201	0.311377	1.393374
C	-5.530748	0.019437	-0.277808

O	-5.965183	0.628547	-1.247633
O	-6.236127	-0.904274	0.426480
C	-7.587068	-1.160741	-0.066303
H	-8.156941	-0.215777	-0.038918
H	-7.522952	-1.478043	-1.121400
C	-8.198761	-2.231134	0.824015
H	-8.247034	-1.895411	1.872587
H	-9.224170	-2.454934	0.485726
H	-7.611452	-3.162711	0.783747
F	0.934540	-3.901406	-3.546287
F	2.893597	-2.912117	-3.408224
F	2.406441	-4.593617	-2.077135
H	-2.960477	-3.591623	1.455417
H	-1.467837	-4.544337	1.751433
H	-2.023332	-3.397995	2.987522
C	3.201228	0.094812	0.393008
C	4.385468	-0.647968	0.356605
C	3.113259	1.403653	-0.088870
C	5.521488	-0.060284	-0.236108
H	4.438063	-1.667206	0.750284
C	4.259885	1.969308	-0.682374
H	2.191968	1.985450	-0.009115
C	5.457915	1.242071	-0.754560
H	6.452698	-0.634761	-0.285571
H	4.205046	2.991949	-1.070982
H	6.346733	1.694200	-1.206509
I	1.683447	0.559136	3.201439

TS5

SCF energy in solvent: -2366.356263 a.u.

Free energy in solvent: -2365.985556 a.u.

imaginary frequency: -112.489000

C	0.047872	3.166105	-1.121436
C	0.485252	1.924672	-1.837232
C	2.147316	-1.665549	-2.094098
O	1.220883	-0.811011	-2.322221
O	2.643121	-2.050955	-1.009234
H	1.534542	1.960044	-2.163801
Pd	0.119646	0.172430	-0.826434
C	-0.959962	3.104294	-0.136774
H	-0.164731	1.692987	-2.706645

C	2.782755	-2.223862	-3.403945
C	-1.457509	4.256999	0.513367
C	0.590015	4.423791	-1.445913
C	0.111772	5.600922	-0.840855
C	-0.906560	5.493866	0.127447
H	1.391570	4.481017	-2.191583
H	-1.267067	6.402344	0.624802
S	-1.454037	1.444772	0.390618
C	-2.519832	4.194273	1.587898
H	-3.531021	4.076860	1.156413
H	-2.358111	3.344849	2.273816
H	-2.528444	5.119937	2.184301
C	0.670003	6.952957	-1.227808
H	0.660051	7.653662	-0.376919
H	1.705432	6.872406	-1.596061
H	0.068957	7.410521	-2.035039
O	-1.059096	-1.636097	-0.458867
C	-0.805122	-2.895882	-0.223922
O	0.265263	-3.354053	0.251914
C	-1.949037	-3.855044	-0.535835
Ag	1.579181	-1.524421	0.900679
C	-3.093820	1.238884	-0.467442
C	-3.781398	-0.038151	0.018484
H	-2.928597	1.220703	-1.555286
H	-3.677941	2.141491	-0.224959
H	-3.115364	-0.907927	-0.144790
H	-3.995460	-0.003843	1.100821
C	-5.077334	-0.259112	-0.749283
O	-5.428594	0.382323	-1.732981
O	-5.787772	-1.278606	-0.203352
C	-7.039619	-1.600141	-0.885658
H	-7.676412	-0.698669	-0.894761
H	-6.812368	-1.855563	-1.935029
C	-7.681954	-2.755174	-0.133675
H	-7.892178	-2.479479	0.912343
H	-8.634644	-3.028434	-0.616952
H	-7.027916	-3.641967	-0.134465
F	1.839440	-2.475379	-4.341256
F	3.641214	-1.288089	-3.900591
F	3.473437	-3.357062	-3.177427
H	-2.741630	-3.729915	0.221723

H	-2.384578	-3.625098	-1.520993
H	-1.594204	-4.894436	-0.508563
C	1.907237	0.777654	0.471233
C	3.136136	0.927599	-0.200492
C	1.600013	1.593715	1.578335
C	4.057503	1.895671	0.245657
H	3.398971	0.305136	-1.056657
C	2.531052	2.555414	2.008083
H	0.680387	1.448170	2.148673
C	3.758011	2.713496	1.344271
H	5.010974	1.998780	-0.283912
H	2.292469	3.161828	2.888423
H	4.479053	3.461984	1.687921
I	0.828559	-1.441135	3.494534

Int8

SCF energy in solvent: -2366.392334 a.u.

Free energy in solvent: -2366.017285 a.u.

No imaginary frequency

C	2.327274	2.408278	-1.053094
C	2.056319	1.081492	-1.676131
C	1.378229	-2.953549	-0.883084
O	1.665994	-1.790774	-1.389003
O	0.635863	-3.240053	0.067074
H	2.953638	0.496575	-1.920887
Pd	0.842393	-0.132120	-0.488446
C	1.387973	2.987441	-0.173595
H	1.347522	1.112332	-2.520797
C	2.089678	-4.093956	-1.673684
C	1.558367	4.281508	0.365107
C	3.486402	3.136452	-1.379834
C	3.684941	4.439986	-0.885759
C	2.714077	4.987566	-0.024881
H	4.235527	2.682103	-2.038513
H	2.875025	5.989824	0.389549
S	0.060558	1.902859	0.413789
C	0.572028	4.899718	1.330071
H	-0.325086	5.279538	0.807361
H	0.225940	4.170397	2.082607
H	1.024446	5.751857	1.860615
C	4.911533	5.234969	-1.275753

H	5.173915	5.977235	-0.504809
H	5.783229	4.579648	-1.435146
H	4.739813	5.786138	-2.218538
O	-0.574904	-0.026423	-2.158342
C	-1.421620	-0.967129	-2.406222
O	-1.771315	-1.882192	-1.594476
C	-2.067553	-0.937324	-3.782698
Ag	-1.257774	-1.731914	0.531813
C	-1.379430	2.459993	-0.622316
C	-2.678557	1.825730	-0.121188
H	-1.180434	2.172312	-1.664804
H	-1.393622	3.558986	-0.535875
H	-2.541575	0.739671	0.059298
H	-3.011057	2.243014	0.842661
C	-3.780941	1.965900	-1.165438
O	-3.599671	2.190749	-2.357850
O	-4.996383	1.770347	-0.600228
C	-6.128347	1.794535	-1.525519
H	-6.161828	2.785562	-2.010425
H	-5.952297	1.043434	-2.314499
C	-7.381285	1.500867	-0.716189
H	-7.532030	2.257081	0.071006
H	-8.261981	1.512160	-1.379769
H	-7.320084	0.509522	-0.239300
F	1.527345	-4.214387	-2.906654
F	3.412478	-3.824305	-1.838817
F	1.975371	-5.274838	-1.036424
H	-2.688015	-0.028380	-3.858456
H	-1.291100	-0.876940	-4.561505
H	-2.691845	-1.827665	-3.937449
C	2.295152	-0.238323	0.944983
C	3.590209	-0.656148	0.590986
C	1.980964	0.053789	2.283408
C	4.578642	-0.770971	1.586068
H	3.833995	-0.923814	-0.440990
C	2.978964	-0.071960	3.269240
H	0.964146	0.322585	2.586201
C	4.277409	-0.474815	2.924255
H	5.584004	-1.103360	1.304667
H	2.720494	0.137569	4.312845
H	5.047817	-0.570537	3.696326

I -1.812418 -0.838884 2.965067

TS6

SCF energy in solvent: -2366.369745 a.u.

Free energy in solvent: -2365.994638 a.u.

imaginary frequency: -334.179500

C	1.489268	3.141281	-0.991581
C	2.102375	1.840928	-1.378784
C	2.186880	-2.540268	-0.875660
O	2.046888	-1.424287	-1.529861
O	1.703804	-2.904745	0.203674
H	3.182475	1.906370	-1.537990
Pd	0.853286	0.061601	-0.736710
C	0.185196	3.230894	-0.447952
H	1.652851	1.410825	-2.298304
C	3.141182	-3.498602	-1.654770
C	-0.381610	4.481541	-0.090150
C	2.221568	4.329375	-1.191951
C	1.670531	5.588796	-0.905942
C	0.376159	5.637339	-0.351767
H	3.239830	4.261893	-1.592326
H	-0.049876	6.609864	-0.077316
S	-0.629900	1.691934	0.052430
C	-1.730153	4.611203	0.584516
H	-2.561410	4.601523	-0.144102
H	-1.910904	3.791374	1.301415
H	-1.795679	5.563443	1.133675
C	2.443817	6.859240	-1.180847
H	2.139691	7.303265	-2.146341
H	2.262335	7.618861	-0.402581
H	3.527967	6.670238	-1.232060
O	-0.629831	-0.647488	-2.092949
C	-1.157949	-1.831257	-2.047201
O	-1.115033	-2.631682	-1.071371
C	-1.919404	-2.231530	-3.304885
Ag	-0.453763	-1.908534	0.927970
C	-2.154186	1.621144	-1.009180
C	-3.225264	0.798940	-0.284786
H	-1.883215	1.156872	-1.969149
H	-2.468020	2.662994	-1.172785
H	-2.796426	-0.147938	0.101415

H	-3.630403	1.319688	0.597643
C	-4.356507	0.426849	-1.236887
O	-4.265759	0.389085	-2.460000
O	-5.476509	0.111300	-0.543640
C	-6.606610	-0.344364	-1.352500
H	-6.882291	0.462581	-2.053269
H	-6.280469	-1.210315	-1.953582
C	-7.735300	-0.694694	-0.396219
H	-8.038904	0.182077	0.198296
H	-8.610746	-1.043985	-0.968575
H	-7.432264	-1.496498	0.295991
F	2.622061	-3.800183	-2.873338
F	4.352478	-2.899137	-1.851404
F	3.346969	-4.647314	-0.983728
H	-1.274604	-2.105526	-4.188635
H	-2.260540	-3.272381	-3.226952
H	-2.785175	-1.558268	-3.422055
C	2.510143	0.782953	0.353290
C	2.248299	1.460417	1.566973
C	3.747837	0.105464	0.201381
C	3.167035	1.400634	2.624709
H	1.317805	2.011624	1.723336
C	4.666000	0.065538	1.257169
H	3.981019	-0.402199	-0.737742
C	4.377838	0.705639	2.475521
H	2.923825	1.893681	3.571053
H	5.610423	-0.472712	1.125780
H	5.093793	0.664747	3.302424
I	-1.070225	-0.854493	3.289856

Int9

SCF energy in solvent: -2366.440857 a.u.

Free energy in solvent: -2366.064817 a.u.

No imaginary frequency

C	2.024108	1.434898	1.980511
C	1.344612	0.355840	2.802754
C	-3.360113	-1.521523	0.417839
O	-2.255034	-1.753145	1.057063
O	-3.616975	-0.718421	-0.491125
H	1.542066	0.574426	3.867703
Pd	-0.526398	-0.796716	0.508188

C	2.133714	1.381799	0.567313
H	1.792598	-0.638415	2.625030
C	-4.499343	-2.448895	0.950436
C	2.706690	2.446732	-0.178455
C	2.535028	2.565933	2.640683
C	3.137623	3.629191	1.943118
C	3.206674	3.548262	0.541666
H	2.450594	2.620140	3.732700
H	3.652479	4.376525	-0.021266
S	1.483671	-0.018802	-0.366108
C	2.756176	2.459029	-1.690647
H	3.203166	1.541932	-2.109137
H	1.734886	2.548755	-2.106144
H	3.344439	3.318784	-2.047293
C	3.707217	4.819856	2.681157
H	4.772105	4.656834	2.930103
H	3.650422	5.736006	2.071415
H	3.173966	5.002342	3.628252
O	-0.166742	-2.433663	-0.746596
C	-0.733515	-2.523881	-1.919549
O	-1.411671	-1.646605	-2.507724
C	-0.542383	-3.880307	-2.592226
Ag	-1.836569	0.435271	-1.778589
C	2.690475	-1.368614	0.052263
C	4.063125	-1.126868	-0.581874
H	2.201039	-2.276837	-0.333295
H	2.792365	-1.463238	1.143135
H	4.041880	-1.221919	-1.679412
H	4.418449	-0.103777	-0.351681
C	5.090637	-2.094899	0.005634
O	5.004881	-2.618583	1.109452
O	6.127028	-2.271533	-0.850586
C	7.198775	-3.137437	-0.356761
H	7.611379	-2.692043	0.565029
H	6.762134	-4.113925	-0.086634
C	8.237214	-3.249627	-1.461312
H	8.652402	-2.261895	-1.718784
H	9.065807	-3.895069	-1.125707
H	7.802059	-3.692837	-2.371466
F	-4.167333	-3.755687	0.778713
F	-4.705518	-2.239784	2.281711

F	-5.661933	-2.220199	0.308287
H	-1.439396	-4.490931	-2.393027
H	-0.457477	-3.744529	-3.680136
H	0.333466	-4.412362	-2.195178
C	-0.180512	0.253480	2.651152
C	-0.936800	1.091377	1.761472
C	-0.891663	-0.489581	3.640365
C	-2.350699	1.232011	1.939533
H	-0.435321	1.827910	1.123561
C	-2.267164	-0.345730	3.786239
H	-0.331271	-1.143346	4.318153
C	-3.000954	0.535130	2.948072
H	-2.888825	1.908664	1.268979
H	-2.789020	-0.910112	4.565363
H	-4.079104	0.649756	3.092928
I	-1.411987	3.073033	-1.749001

2a

SCF energy in solvent: -1325.187374 a.u.

Free energy in solvent: -1324.866458 a.u.

No imaginary frequency

C	-1.587650	0.506970	0.159809
C	-1.336836	-0.995897	0.134882
H	-0.629698	-1.214047	-0.671850
C	-0.718300	1.428378	-0.464426
H	-0.836068	-1.286672	1.067982
C	-0.989908	2.816383	-0.407154
C	-2.702439	0.996068	0.853381
C	-2.983757	2.359371	0.935478
C	-2.119422	3.250847	0.290615
H	-3.372550	0.284466	1.328227
H	-2.328859	4.317539	0.332992
S	0.717983	0.867268	-1.398267
C	-0.102545	3.840394	-1.077626
H	0.929251	3.778151	-0.717488
H	-0.061562	3.694060	-2.161610
H	-0.471937	4.851297	-0.884399
C	-4.176259	2.864437	1.712538
H	-3.877636	3.222864	2.705727
H	-4.662295	3.701697	1.201282
H	-4.920875	2.076945	1.858727

C	1.900852	0.467296	-0.039731
C	3.223919	0.013241	-0.650616
H	1.485692	-0.320818	0.592055
H	2.047177	1.353074	0.582565
H	3.079289	-0.853432	-1.307411
H	3.662674	0.795282	-1.280901
C	4.237129	-0.369383	0.412872
O	4.030932	-0.379953	1.607909
O	5.415946	-0.707387	-0.149839
C	6.464036	-1.103856	0.766324
H	6.656360	-0.279533	1.460355
H	6.112551	-1.955231	1.357707
C	7.686407	-1.449741	-0.062475
H	8.018683	-0.588027	-0.648477
H	8.506055	-1.755725	0.595079
H	7.472249	-2.272164	-0.750994
C	-2.578018	-1.850381	-0.039461
C	-3.320894	-1.790553	-1.228620
C	-2.999020	-2.730503	0.964318
C	-4.449013	-2.589026	-1.407542
H	-3.008960	-1.109866	-2.016713
C	-4.130187	-3.532532	0.789454
H	-2.433106	-2.792522	1.890980
C	-4.858691	-3.464406	-0.397576
H	-5.009260	-2.530484	-2.336749
H	-4.438780	-4.209678	1.581231
H	-5.737555	-4.087392	-0.537259

TS2A

SCF energy in solvent: -2264.085112 a.u.

Free energy in solvent: -2263.67191 a.u.

imaginary frequency: -721.479800

C	0.629387	3.005299	-0.792757
C	0.901410	1.907853	-1.783722
C	2.141331	-1.794341	-2.503133
O	1.134201	-1.007726	-2.706717
O	2.604059	-2.186892	-1.386836
H	1.650276	1.004723	-1.106830
H	1.794306	2.097300	-2.401178
Pd	0.161509	-0.061112	-1.152718
C	-0.248103	2.786680	0.290708

H	0.062097	1.767822	-2.495642
C	2.856140	-2.267343	-3.757868
H	2.151969	-2.348029	-4.598606
H	3.349396	-3.231226	-3.569300
H	3.628434	-1.525825	-4.025195
C	-0.526036	3.793820	1.246637
C	1.238125	4.266677	-0.919130
C	0.970558	5.303741	-0.007944
C	0.093683	5.043820	1.063435
H	1.938455	4.434884	-1.745503
H	-0.097761	5.832356	1.801023
S	-0.926870	1.118205	0.509788
C	-1.428654	3.561955	2.438585
H	-2.498223	3.608032	2.161514
H	-1.251932	2.573727	2.896831
H	-1.261613	4.331851	3.208013
C	1.603749	6.667568	-0.176789
H	1.758584	7.165009	0.794607
H	2.577572	6.600530	-0.688362
H	0.959120	7.329464	-0.784042
O	-1.181422	-1.690052	-0.970682
C	-0.840684	-2.828022	-0.468570
O	0.259796	-3.127470	0.094053
C	-1.888590	-3.927564	-0.551666
H	-2.699915	-3.707740	0.162984
H	-2.327858	-3.957503	-1.560596
H	-1.442488	-4.898175	-0.296567
O	3.344911	-0.605643	0.974492
C	3.701163	0.454699	0.337048
O	3.106263	1.032292	-0.625538
C	5.010237	1.073072	0.821945
H	5.695553	1.187931	-0.033341
H	4.807908	2.081059	1.220419
H	5.479297	0.453900	1.598381
C	-2.675265	1.378419	-0.089596
C	-3.529392	0.152509	0.237107
H	-2.651560	1.582151	-1.170090
H	-3.047336	2.280084	0.422091
H	-3.119945	-0.744465	-0.262280
H	-3.528734	-0.065434	1.320155
C	-4.965291	0.368539	-0.222892

O	-5.365867	1.346219	-0.843050
O	-5.747413	-0.678439	0.147963
C	-7.149174	-0.577553	-0.251930
H	-7.564525	0.360018	0.156160
H	-7.197014	-0.509276	-1.352573
C	-7.863420	-1.808914	0.282719
H	-7.797461	-1.859836	1.381589
H	-8.929236	-1.771133	0.002465
H	-7.429836	-2.731950	-0.134869
Pd	1.758345	-1.765892	0.466756
O	0.935080	-1.363014	2.261326
C	1.377283	-2.189339	3.205311
O	2.159748	-3.129538	3.029053
C	0.825690	-1.825752	4.587713
H	-0.227710	-1.508950	4.531939
H	0.928653	-2.689170	5.260621
H	1.408457	-0.984061	5.000071

TS2B

SCF energy in solvent: -2849.062781 a.u.

Free energy in solvent: -2848.568009 a.u.

imaginary frequency: -974.117000

C	2.904976	2.888958	0.710004
C	2.370843	2.099014	1.870532
C	-0.652045	-0.075197	3.289381
O	0.626806	-0.121080	3.137838
O	-1.542197	-0.017006	2.377126
H	1.039970	1.909297	1.567100
H	2.025003	2.732922	2.702776
Pd	1.540525	0.138584	1.300686
C	3.116837	2.262522	-0.537399
H	3.133810	1.418426	2.302476
C	-1.146656	-0.060576	4.724903
H	-0.460295	-0.624359	5.373136
H	-2.163810	-0.472292	4.781542
H	-1.172500	0.985237	5.076008
C	3.615991	2.966489	-1.659438
C	3.196580	4.260109	0.826963
C	3.710549	4.995010	-0.256574
C	3.908411	4.331834	-1.483702
H	3.011016	4.760454	1.784508

H	4.278803	4.900111	-2.345279
S	2.624016	0.524177	-0.704270
C	3.818426	2.314641	-3.009949
H	4.736145	1.698181	-3.036771
H	2.974817	1.654497	-3.274222
H	3.918109	3.076969	-3.798296
C	4.050198	6.461937	-0.107620
H	3.896691	7.010502	-1.051386
H	3.437975	6.941387	0.673211
H	5.109923	6.594597	0.178287
O	1.482803	-1.970229	0.958410
C	0.393726	-2.612452	0.728639
O	-0.767970	-2.125061	0.519428
C	0.498847	-4.129136	0.687410
H	1.028708	-4.428956	-0.232629
H	1.086987	-4.488129	1.546010
H	-0.501950	-4.581194	0.687853
O	-1.655238	1.831577	0.123196
C	-1.146912	2.809055	0.787885
O	-0.145142	2.789148	1.573681
C	-1.871105	4.136706	0.599419
H	-2.301591	4.445029	1.566784
H	-1.148172	4.910517	0.295412
H	-2.672827	4.042851	-0.144630
C	4.290260	-0.304654	-0.560261
C	4.174764	-1.803132	-0.844900
H	4.692019	-0.116788	0.446026
H	4.943993	0.199212	-1.290618
H	3.433744	-2.269561	-0.168892
H	3.827298	-1.999732	-1.874205
C	5.521017	-2.485142	-0.630948
O	6.501119	-1.959428	-0.117351
O	5.482977	-3.767110	-1.077136
C	6.718402	-4.525706	-0.889241
H	7.541203	-3.985724	-1.388584
H	6.949956	-4.557945	0.189430
C	6.494375	-5.910961	-1.474659
H	6.259954	-5.854194	-2.549938
H	7.407090	-6.517403	-1.352112
H	5.665893	-6.428453	-0.964592
Pd	-1.144612	-0.113759	0.360398

O	-0.712960	-0.215932	-1.634218
C	-1.507614	-0.764564	-2.491353
O	-2.689881	-1.193181	-2.312603
C	-0.951165	-0.890652	-3.902081
H	0.147494	-0.926167	-3.892750
H	-1.366234	-1.785943	-4.387336
H	-1.272291	-0.009468	-4.483245
Pd	-3.923063	-0.765456	-0.717428
O	-4.238163	1.024383	-1.590607
C	-5.346073	1.003246	-2.317925
O	-6.068114	0.012592	-2.500925
O	-3.957538	-2.483876	0.535583
C	-4.867146	-1.910036	1.243624
O	-5.218394	-0.711486	0.910749
C	-5.533220	-2.614560	2.394170
H	-5.845004	-1.885711	3.157282
H	-6.434738	-3.135243	2.027349
H	-4.852165	-3.362026	2.827451
C	-5.684606	2.378619	-2.900228
H	-4.775586	2.941064	-3.164053
H	-6.327574	2.253080	-3.783742
H	-6.238047	2.962427	-2.144522

Int4A

SCF energy in solvent: -2054.742862 a.u.

Free energy in solvent: -2054.367142 a.u.

No imaginary frequency

C	2.876345	1.761316	-1.320690
C	2.033341	1.335179	-2.499538
C	-0.365781	-3.865482	-1.185742
O	0.426103	-2.869329	-1.468569
O	-1.250893	-3.923234	-0.295480
H	1.633636	0.312681	-2.361178
H	2.627943	1.351901	-3.426222
Pd	0.470799	-1.041742	-0.528797
C	2.437813	1.663417	0.026938
H	1.162684	1.996249	-2.649872
C	-0.166506	-5.071012	-2.106029
H	-0.928378	-5.033410	-2.903354
H	-0.320113	-5.998479	-1.534780
H	0.828808	-5.063597	-2.572093

C	3.281708	2.029384	1.110773
C	4.169451	2.266212	-1.552685
C	5.026435	2.657286	-0.509249
C	4.564148	2.523644	0.811309
H	4.517471	2.344054	-2.589730
H	5.220968	2.808638	1.641875
S	0.799096	1.032376	0.486384
C	2.862415	1.902687	2.561705
H	1.961467	2.498583	2.787207
H	2.626465	0.858630	2.827759
H	3.672327	2.247656	3.223743
C	6.398592	3.223537	-0.800432
H	6.352363	4.319370	-0.941224
H	7.100286	3.029877	0.027271
H	6.825755	2.795061	-1.721967
O	-0.928917	-0.370058	-1.881885
C	-2.196325	-0.406169	-1.584757
O	-2.718109	-0.762854	-0.485721
C	-3.108009	0.106788	-2.692050
H	-3.225731	1.197741	-2.570011
H	-2.669691	-0.085396	-3.682087
H	-4.097294	-0.365670	-2.608781
Ag	-1.564943	-2.009360	1.027654
O	0.203082	-2.219459	2.420491
C	1.392058	-2.206897	1.990588
O	1.822915	-1.782879	0.836956
C	2.486422	-2.772231	2.890841
H	2.457881	-3.873181	2.821551
H	3.483307	-2.427400	2.582275
H	2.286265	-2.498834	3.937744
C	-0.363383	2.287704	-0.231603
C	-1.652555	2.296979	0.599253
H	-0.580692	2.036407	-1.278820
H	0.163799	3.253955	-0.184105
H	-2.060147	1.268878	0.672579
H	-1.482216	2.653532	1.627851
C	-2.727346	3.142028	-0.072742
O	-2.805485	3.356579	-1.278205
O	-3.616084	3.606834	0.841139
C	-4.737444	4.364049	0.287940
H	-4.335656	5.219001	-0.282527

H	-5.280635	3.717124	-0.422274
C	-5.608752	4.802006	1.454505
H	-5.044971	5.441642	2.152701
H	-6.470507	5.377844	1.078017
H	-5.992047	3.931829	2.011386

TS3A

SCF energy in solvent: -2054.692715 a.u.

Free energy in solvent: -2054.323855 a.u.

imaginary frequency: -720.809900

C	-1.301745	2.363264	0.927960
C	-1.259857	1.090371	1.732148
C	-1.334324	-2.989911	1.827451
O	-0.762707	-1.862934	2.197348
O	-1.589304	-3.356828	0.664046
H	-1.881594	0.176066	0.953539
H	-2.122063	0.985459	2.410525
Pd	-0.145690	-0.534147	0.775265
C	-0.461569	2.531828	-0.194067
H	-0.364077	1.037062	2.385617
C	-1.723686	-3.866676	3.018773
H	-1.130670	-3.631241	3.914130
H	-1.604876	-4.925455	2.744803
H	-2.789102	-3.692285	3.247036
C	-0.478930	3.711379	-0.977371
C	-2.180679	3.407113	1.266864
C	-2.219709	4.602818	0.527236
C	-1.367124	4.730431	-0.586390
H	-2.853494	3.273538	2.121699
H	-1.409086	5.645345	-1.189662
S	0.590294	1.135709	-0.676158
C	0.398389	3.898426	-2.195685
H	1.419330	4.221045	-1.918878
H	0.496182	2.966039	-2.776859
H	-0.015918	4.674702	-2.858054
C	-3.150392	5.729327	0.920394
H	-3.502836	6.288532	0.038032
H	-4.031769	5.354101	1.465082
H	-2.638334	6.452339	1.581815
O	1.362259	-1.858153	0.201330
C	1.337406	-2.573631	-0.881484

O	0.434716	-2.599302	-1.764590
C	2.537911	-3.495663	-1.059686
H	3.425732	-3.111437	-0.537444
H	2.281814	-4.478554	-0.628223
H	2.746553	-3.638425	-2.129792
Ag	-1.556363	-1.827380	-1.355109
O	-3.462963	-0.906839	-1.501966
C	-3.956950	-0.315546	-0.477417
O	-3.352619	0.007962	0.598640
C	-5.450824	-0.000447	-0.551448
H	-6.013537	-0.871869	-0.173806
H	-5.700421	0.867543	0.075792
H	-5.756719	0.172370	-1.593756
C	2.236480	1.710222	-0.008675
C	3.330917	0.695571	-0.341382
H	2.140903	1.862489	1.076565
H	2.438552	2.687225	-0.475873
H	3.088067	-0.297842	0.077221
H	3.430906	0.553212	-1.432950
C	4.671092	1.161138	0.214833
O	4.852037	2.202228	0.834502
O	5.645038	0.257999	-0.069297
C	6.974438	0.603509	0.429332
H	7.277486	1.567103	-0.015882
H	6.913342	0.748155	1.521651
C	7.912191	-0.530566	0.046508
H	7.952105	-0.660920	-1.047055
H	8.930838	-0.306872	0.404683
H	7.588940	-1.481914	0.499038

Int4B

SCF energy in solvent: -2450.969943 a.u.

Free energy in solvent: -2450.548662 a.u.

No imaginary frequency

C	2.895161	-2.649735	-1.556104
C	2.152781	-1.884633	-2.627246
C	-2.903128	-0.092266	-0.064689
O	-1.923581	-0.810727	-0.532681
O	-2.846297	0.850953	0.764758
H	1.182352	-1.505436	-2.258109
H	1.962399	-2.530370	-3.498747

Pd	0.078176	-0.578659	-0.098251
C	3.036959	-2.186699	-0.220127
H	2.724541	-1.010216	-2.984430
C	3.703554	-2.961647	0.767913
C	3.468677	-3.892994	-1.881120
C	4.153987	-4.679223	-0.938364
C	4.251696	-4.197051	0.378097
H	3.361917	-4.260335	-2.908921
H	4.767588	-4.801147	1.133842
S	2.358580	-0.605000	0.355403
C	3.836836	-2.520352	2.211544
H	4.365677	-1.556425	2.304705
H	2.850596	-2.390130	2.687883
H	4.396657	-3.272130	2.789854
C	4.780397	-5.997652	-1.335056
H	5.790469	-5.843904	-1.757789
H	4.886220	-6.672188	-0.470031
H	4.182095	-6.513903	-2.103891
O	0.190758	0.829632	-1.591242
C	0.097149	2.098230	-1.307696
O	-0.008394	2.621638	-0.157654
C	0.194718	3.014506	-2.519204
Ag	-0.704277	1.401757	1.620836
O	-0.435332	-0.333945	3.028875
C	-0.337104	-1.530196	2.631022
O	-0.103108	-1.955326	1.421308
C	-0.533975	-2.645393	3.652071
C	3.242064	0.655148	-0.679882
C	3.329317	1.966222	0.111529
H	2.702664	0.805199	-1.625202
H	4.238258	0.232211	-0.886578
H	2.319910	2.265596	0.457429
H	3.965419	1.870014	1.005982
C	3.838875	3.101746	-0.768034
O	3.706413	3.164237	-1.986150
O	4.435701	4.059120	-0.015900
C	4.889210	5.239082	-0.751096
H	5.619323	4.916978	-1.513388
H	4.025177	5.675126	-1.281130
C	5.492561	6.198798	0.262219
H	6.348164	5.739720	0.783434

H	5.848740	7.106441	-0.252713
H	4.746454	6.499587	1.015196
C	-4.258461	-0.480704	-0.621284
C	-5.390562	0.241516	-0.204850
C	-4.402877	-1.537144	-1.544686
C	-6.640190	-0.111297	-0.724544
H	-5.292021	1.061901	0.508334
C	-5.669522	-1.872864	-2.049224
H	-3.510086	-2.085013	-1.856937
C	-6.804930	-1.159076	-1.642763
H	-5.773336	-2.694467	-2.764799
H	-7.805737	-1.388857	-2.014435
N	-7.837106	0.650458	-0.292613
O	-8.935064	0.314762	-0.774060
O	-7.669811	1.574976	0.521078
H	-1.617499	-2.783731	3.808778
H	-0.107573	-3.595547	3.300871
H	-0.091868	-2.351512	4.615749
H	-0.181546	2.513715	-3.422775
H	-0.364400	3.941964	-2.329484
H	1.257367	3.268898	-2.677782

TS3B

SCF energy in solvent: -2450.919841 a.u.

Free energy in solvent: -2450.50715 a.u.

imaginary frequency: -650.331400

C	2.009920	-2.355919	-1.386187
C	0.748942	-1.595166	-1.700373
C	-2.577268	0.404016	-0.390745
O	-1.512868	0.345423	-1.159490
O	-2.622689	0.249921	0.846142
H	-0.026112	-1.762352	-0.614026
H	0.003840	-2.204971	-2.236865
Pd	0.323634	0.043577	-0.306492
C	2.932791	-1.853444	-0.444237
H	0.941009	-0.718311	-2.352684
C	4.123572	-2.544074	-0.113744
C	2.293823	-3.581923	-2.012566
C	3.474784	-4.292310	-1.730837
C	4.367332	-3.758955	-0.780740
H	1.569517	-3.990823	-2.726334

H	5.276450	-4.317736	-0.528318
S	2.508242	-0.314848	0.418418
C	5.102395	-2.038007	0.923650
H	5.686822	-1.174941	0.555408
H	4.588674	-1.713005	1.844626
H	5.823187	-2.825685	1.192764
C	3.782361	-5.595483	-2.435244
H	4.378567	-5.418573	-3.349378
H	4.365390	-6.275129	-1.792434
H	2.860629	-6.116189	-2.741110
O	0.226562	1.919371	0.587994
C	-0.006806	2.124751	1.849307
O	-0.201504	1.255533	2.744522
C	-0.072734	3.592962	2.249656
Ag	-0.719581	-0.787521	2.238600
O	-0.935494	-2.891918	2.177775
C	-1.026227	-3.487075	1.044438
O	-0.793015	-2.997358	-0.109576
C	-1.505287	-4.937051	1.097538
H	-1.212353	-5.405667	2.048381
H	-2.607637	-4.945348	1.040479
H	-1.113759	-5.510068	0.244620
C	3.544008	0.905251	-0.544008
C	3.431542	2.304170	0.063237
H	3.213327	0.891684	-1.592865
H	4.579250	0.530763	-0.505794
H	2.380957	2.646419	0.072536
H	3.771047	2.318015	1.114823
C	4.270447	3.294059	-0.737041
O	4.930185	3.012540	-1.730104
O	4.182549	4.537398	-0.199381
C	4.942666	5.571229	-0.899964
H	6.009292	5.287235	-0.893532
H	4.612622	5.596892	-1.952605
C	4.689774	6.886745	-0.180749
H	5.019929	6.835329	0.869354
H	5.249628	7.695483	-0.679138
H	3.619368	7.148032	-0.197180
C	-3.852636	0.691342	-1.157628
C	-5.059724	0.751861	-0.439239
C	-3.858186	0.897168	-2.552960

C	-6.242995	1.015796	-1.136082
H	-5.066466	0.595107	0.641149
C	-5.060472	1.160600	-3.229172
H	-2.910260	0.847891	-3.094910
C	-6.269600	1.222010	-2.523588
H	-5.056438	1.318970	-4.312139
H	-7.224604	1.423414	-3.013444
N	-7.519225	1.081379	-0.382771
O	-8.556530	1.312453	-1.031318
O	-7.473017	0.902693	0.846139
H	0.540894	4.221749	1.588712
H	-1.121798	3.924305	2.163163
H	0.236912	3.710605	3.297933

Int4C

SCF energy in solvent: -2650.135488 a.u.

Free energy in solvent: -2649.813109 a.u.

No imaginary frequency

C	3.084773	-1.797474	1.560202
C	1.980539	-1.578466	2.566650
C	-0.620046	3.423678	0.618311
O	0.137249	2.497558	1.060742
O	-1.308033	3.478497	-0.409092
H	1.370385	-0.701546	2.328905
H	2.402767	-1.429043	3.562850
Pd	0.553463	0.669209	0.213189
C	2.896568	-1.750689	0.160728
H	1.306516	-2.439713	2.625283
C	-0.608830	4.662573	1.553671
C	3.973052	-1.942806	-0.735015
C	4.373476	-2.065291	2.033906
C	5.459304	-2.274935	1.180059
C	5.236822	-2.203579	-0.197133
H	4.529863	-2.101429	3.109137
H	6.070280	-2.352788	-0.878879
S	1.296028	-1.409265	-0.606038
C	3.819822	-1.876874	-2.238674
H	3.110629	-2.622737	-2.611962
H	3.456181	-0.898711	-2.567971
H	4.782143	-2.057653	-2.723214
C	6.828286	-2.589447	1.731350

H	6.941787	-3.667090	1.903054
H	7.618488	-2.283782	1.039968
H	6.998418	-2.088641	2.688842
O	-1.092731	-0.136965	1.153518
C	-2.219239	-0.163614	0.553188
O	-2.527806	0.214435	-0.587614
C	-3.320006	-0.826935	1.421968
Ag	-1.166903	1.624407	-1.849678
O	0.946426	1.856684	-2.661131
C	1.991283	1.904239	-1.974425
O	2.144216	1.474590	-0.764116
C	3.231973	2.545092	-2.568837
H	3.197040	3.618905	-2.355327
H	4.140695	2.138653	-2.122616
H	3.236153	2.413809	-3.652071
C	0.188154	-2.752948	0.006244
C	-0.925535	-2.997436	-1.015120
H	-0.228621	-2.464900	0.969867
H	0.809444	-3.640899	0.131615
H	-1.468678	-2.081205	-1.257462
H	-0.509198	-3.382505	-1.953843
C	-1.902893	-4.027100	-0.467540
O	-1.590396	-4.936593	0.272092
O	-3.147038	-3.790377	-0.908137
C	-4.192466	-4.656304	-0.394490
H	-4.089871	-5.640570	-0.863317
H	-4.040629	-4.778487	0.680922
C	-5.519639	-3.997258	-0.715984
H	-5.648730	-3.875286	-1.795253
H	-6.340816	-4.614313	-0.338165
H	-5.577535	-3.012472	-0.245614
F	0.599136	5.259508	1.497322
F	-1.534427	5.560237	1.195489
F	-0.841155	4.305407	2.828927
F	-2.981612	-2.114634	1.676361
F	-4.509219	-0.826878	0.807898
F	-3.448887	-0.193558	2.596844

TS3C

SCF energy in solvent: -2650.082739 a.u.

Free energy in solvent: -2649.766936 a.u.

imaginary frequency: -486.333300

C	-1.395862	2.795515	0.947905
C	-1.454572	1.439542	1.602837
C	-1.563726	-2.616645	1.261666
O	-1.041555	-1.547435	1.787106
O	-1.728636	-2.926104	0.074297
H	-1.968082	0.643078	0.671348
H	-2.390581	1.270060	2.160193
Pd	-0.278545	-0.091778	0.565330
C	-0.452621	3.060529	-0.067794
H	-0.640390	1.285851	2.340349
C	-2.063102	-3.586116	2.380535
C	-0.374491	4.316769	-0.714858
C	-2.280548	3.819604	1.324277
C	-2.224782	5.091641	0.724322
C	-1.273027	5.313499	-0.289245
H	-3.032086	3.612850	2.094697
H	-1.240845	6.289945	-0.787002
S	0.629975	1.704529	-0.596696
C	0.606330	4.601967	-1.830812
H	1.634950	4.744496	-1.451214
H	0.641171	3.777420	-2.563236
H	0.328708	5.523622	-2.365354
C	-3.164253	6.193275	1.162957
H	-4.157121	5.794379	1.428022
H	-2.772207	6.711969	2.056980
H	-3.296431	6.951267	0.374319
O	1.262880	-1.365030	-0.038507
C	1.275814	-1.989660	-1.161651
O	0.441863	-2.005056	-2.095898
C	2.566752	-2.843998	-1.338420
Ag	-1.564284	-1.195413	-1.801324
O	-3.415953	-0.216350	-2.041333
C	-3.967363	0.342747	-1.023524
O	-3.439844	0.567259	0.112821
C	-5.430474	0.740928	-1.207586
H	-5.629197	1.004219	-2.256878
H	-6.064911	-0.124886	-0.950255
H	-5.696667	1.573166	-0.540378
C	2.187094	2.137693	0.340403
C	3.354222	1.239371	-0.072013

H	1.980435	2.057885	1.417434
H	2.389008	3.196046	0.108831
H	3.100911	0.170034	0.041554
H	3.629550	1.382239	-1.131316
C	4.564979	1.537370	0.808802
O	4.544387	2.254202	1.802585
O	5.661974	0.888019	0.350592
C	6.869259	1.062911	1.157890
H	7.118783	2.137717	1.186285
H	6.647487	0.745874	2.191231
C	7.967527	0.228942	0.518058
H	8.166971	0.558941	-0.514248
H	8.898301	0.333882	1.099940
H	7.692536	-0.837747	0.495796
F	-3.163769	-3.058599	2.983385
F	-2.396721	-4.788730	1.869149
F	-1.112307	-3.777202	3.330653
F	2.659618	-3.765114	-0.349673
F	3.666096	-2.037904	-1.271786
F	2.586045	-3.481330	-2.523806

Int4D

SCF energy in solvent: -2947.82798 a.u.

Free energy in solvent: -2947.53067 a.u.

No imaginary frequency

C	-0.713275	3.186018	1.979812
C	-0.068656	2.151911	2.873437
C	-1.562363	-3.066500	0.799424
O	-1.431370	-1.903950	1.341341
O	-1.201473	-3.495173	-0.316089
H	-0.372946	1.125983	2.590697
H	-0.359935	2.313216	3.922692
Pd	-0.594212	-0.232439	0.474031
C	-0.682693	3.125039	0.559814
H	1.033340	2.185941	2.826915
C	-2.301105	-4.048817	1.764292
C	-1.341777	4.093985	-0.245274
C	-1.399874	4.261746	2.570090
C	-2.048311	5.252575	1.810742
C	-2.008714	5.144968	0.410600
H	-1.434065	4.317056	3.664558

H	-2.518396	5.899405	-0.199984
S	0.172244	1.807929	-0.347411
C	-1.376728	4.035071	-1.759088
H	-0.372569	3.927028	-2.201060
H	-1.983767	3.183713	-2.110581
H	-1.829033	4.953926	-2.163680
C	-2.752969	6.407871	2.485478
H	-2.033915	7.201438	2.760369
H	-3.508841	6.862189	1.825133
H	-3.253170	6.087555	3.414324
O	1.222274	-0.740240	1.304893
C	2.032909	-1.485380	0.634418
O	1.931989	-1.979790	-0.514103
C	3.360051	-1.729761	1.414849
Ag	-0.050706	-1.936873	-1.647848
O	-1.824362	-0.756320	-2.439617
C	-2.569119	-0.128679	-1.649463
O	-2.395389	0.216059	-0.418536
C	-3.951930	0.350262	-2.188893
C	1.954372	2.035291	0.119853
C	2.848978	1.522370	-1.013317
H	2.158323	1.497444	1.055981
H	2.095428	3.114881	0.279716
H	2.707919	0.445065	-1.199991
H	2.617190	2.037765	-1.964056
C	4.315857	1.787451	-0.678389
O	4.704287	2.597211	0.153580
O	5.125092	1.020438	-1.448009
C	6.558447	1.212170	-1.227080
H	6.804826	2.270289	-1.421714
H	6.775730	1.009089	-0.164727
C	7.291776	0.263094	-2.161189
H	7.052627	0.478741	-3.215100
H	8.380090	0.376099	-2.024262
H	7.024382	-0.784784	-1.950243
F	-4.043558	1.708451	-2.092551
F	-4.957362	-0.191208	-1.461693
F	-4.123299	0.009770	-3.480881
F	-1.580766	-4.213881	2.903940
F	-3.519677	-3.552619	2.096971
F	-2.476750	-5.258681	1.194781

F	4.173934	-2.579752	0.761148
F	4.016319	-0.538848	1.560166
F	3.113399	-2.226971	2.647972

TS3D

SCF energy in solvent: -2947.777072 a.u.

Free energy in solvent: -2947.48863 a.u.

imaginary frequency: -737.662900

C	-1.477797	2.408710	1.433737
C	-1.445084	0.965371	1.862425
C	-1.139268	-2.958588	1.307150
O	-0.665998	-1.882605	1.857448
O	-1.353198	-3.226277	0.115126
H	-1.777526	0.273565	0.687870
H	-2.416021	0.606315	2.241332
Pd	-0.068590	-0.263690	0.739571
C	-0.536663	2.906575	0.508828
H	-0.714326	0.783536	2.675466
C	-1.455437	-4.034597	2.395270
C	-0.533928	4.261265	0.094319
C	-2.437186	3.291144	1.958868
C	-2.456767	4.649265	1.594725
C	-1.499902	5.107730	0.668264
H	-3.184369	2.905097	2.661651
H	-1.518859	6.159097	0.357517
S	0.600491	1.720982	-0.262325
C	0.442097	4.808853	-0.923712
H	1.413224	5.071531	-0.465000
H	0.644621	4.082494	-1.729528
H	0.044990	5.726172	-1.385543
C	-3.511803	5.584028	2.143416
H	-3.859297	5.262267	3.138308
H	-3.134386	6.616230	2.225986
H	-4.395085	5.608977	1.479407
O	1.715723	-1.230407	0.221443
C	1.892976	-1.999259	-0.792560
O	1.128897	-2.286137	-1.742517
C	3.317409	-2.632517	-0.806752
Ag	-0.964876	-1.604403	-1.687373
O	-2.721729	-0.497635	-2.228049
C	-3.363737	0.125114	-1.328510

O	-3.093045	0.325398	-0.107652
C	-4.682027	0.803339	-1.817652
C	2.226581	2.158803	0.542759
C	3.402556	1.662345	-0.299648
H	2.235414	1.731958	1.556603
H	2.244078	3.255736	0.631125
H	3.481804	0.564082	-0.293511
H	3.287931	1.965365	-1.357658
C	4.702588	2.271507	0.223292
O	4.765263	3.194958	1.026700
O	5.773412	1.662055	-0.336872
C	7.076364	2.184289	0.075820
H	7.119722	3.257821	-0.176718
H	7.154780	2.097052	1.172982
C	8.138534	1.373075	-0.648557
H	8.037891	1.472423	-1.741371
H	9.140097	1.732793	-0.359910
H	8.066653	0.304944	-0.388069
F	-2.321985	-3.537774	3.316991
F	-2.004839	-5.136550	1.847766
F	-0.314836	-4.398810	3.037785
F	3.586526	-3.233418	0.376005
F	4.248812	-1.651323	-1.004170
F	3.451097	-3.539911	-1.790881
F	-5.633407	0.788417	-0.853536
F	-5.186486	0.206253	-2.919501
F	-4.416722	2.106446	-2.126166

Int4E

SCF energy in solvent: -2847.19827 a.u.

Free energy in solvent: -2846.732836 a.u.

No imaginary frequency

C	-2.542037	-3.239247	1.946087
C	-1.845145	-2.204196	2.797932
C	3.005304	-0.542587	-0.028465
O	2.077665	-1.180014	0.626188
O	2.897209	0.076411	-1.118461
H	-0.873860	-1.907975	2.354921
H	-1.657447	-2.598141	3.808938
Pd	0.084009	-1.289271	0.104931
C	-2.731240	-3.095446	0.545654

H	-2.443591	-1.282940	2.905172
C	-3.355186	-4.109911	-0.229480
C	-3.019478	-4.415381	2.552904
C	-3.657802	-5.434787	1.824527
C	-3.808198	-5.262548	0.437760
H	-2.876969	-4.537429	3.633326
H	-4.293105	-6.050218	-0.151006
S	-2.171684	-1.635861	-0.374935
C	-3.552551	-3.999446	-1.728113
H	-4.187608	-3.138069	-1.998185
H	-2.595811	-3.867489	-2.260578
H	-4.035739	-4.909417	-2.117166
C	-4.185382	-6.671235	2.517849
H	-5.202702	-6.497203	2.914622
H	-4.245489	-7.528156	1.827419
H	-3.549194	-6.959507	3.370964
O	-0.197209	0.545175	0.999834
C	-0.211242	1.613864	0.256376
O	-0.133385	1.672180	-1.006436
Ag	0.818440	-0.025782	-2.216518
O	0.747729	-2.168766	-2.898089
C	0.704345	-3.132851	-2.081721
O	0.438011	-3.091738	-0.805982
C	1.020988	-4.531173	-2.599522
C	-3.197435	-0.259581	0.337900
C	-3.467358	0.785483	-0.749657
H	-2.664420	0.181755	1.190930
H	-4.130696	-0.721710	0.693761
H	-2.529798	1.206541	-1.152662
H	-4.001132	0.338390	-1.608331
C	-4.320410	1.922841	-0.194201
O	-4.862654	1.918059	0.904660
O	-4.396928	2.935820	-1.091722
C	-5.201787	4.087453	-0.681792
H	-6.265389	3.790442	-0.711492
H	-4.953728	4.333161	0.364127
C	-4.893143	5.225966	-1.641113
H	-5.123595	4.942944	-2.681116
H	-5.507008	6.104313	-1.380116
H	-3.832373	5.518695	-1.583524
C	4.361316	-0.581234	0.645453

C	5.437918	0.084694	0.033412
C	4.561161	-1.263571	1.863839
C	6.688748	0.051823	0.657917
H	5.297533	0.616821	-0.909187
C	5.827805	-1.281838	2.469246
H	3.711861	-1.776406	2.322587
C	6.908095	-0.620677	1.869280
H	5.975132	-1.814186	3.414063
H	7.907337	-0.611836	2.309814
N	7.827946	0.754091	0.017378
O	8.928360	0.707418	0.597131
O	7.611950	1.343403	-1.055119
H	2.117878	-4.643160	-2.645514
H	0.618171	-5.308638	-1.935472
H	0.628993	-4.647991	-3.620757
C	-0.375375	2.904943	1.019624
C	-0.661465	4.082267	0.305434
C	-0.248340	2.949127	2.424433
C	-0.822388	5.274501	1.017967
H	-0.757068	4.064629	-0.781508
C	-0.395618	4.163692	3.112635
H	-0.024767	2.023892	2.961842
C	-0.687533	5.342417	2.412663
H	-0.285854	4.192687	4.200889
H	-0.815212	6.303987	2.914394
N	-1.155676	6.512870	0.273562
O	-1.226456	7.571189	0.921803
O	-1.348517	6.414030	-0.952339

TS3E

SCF energy in solvent: -2847.146807 a.u.

Free energy in solvent: -2846.688619 a.u.

imaginary frequency: -561.501900

C	-2.070758	-3.489105	0.580597
C	-0.818699	-2.928145	1.202026
C	2.541106	-0.625510	0.773016
O	1.481193	-0.968568	1.472571
O	2.565917	-0.274904	-0.423687
H	-0.010651	-2.674185	0.175160
H	-0.093450	-3.708575	1.485551
Pd	-0.346964	-0.882761	0.559034

C	-2.966144	-2.646009	-0.111273
H	-1.025782	-2.364349	2.135160
C	-4.146020	-3.137721	-0.720132
C	-2.370828	-4.859664	0.664395
C	-3.541902	-5.389091	0.092216
C	-4.406666	-4.514953	-0.594681
H	-1.667734	-5.524835	1.178564
H	-5.306420	-4.919669	-1.073321
S	-2.516825	-0.898344	-0.289246
C	-5.097223	-2.252375	-1.495226
H	-5.724206	-1.635073	-0.825727
H	-4.558216	-1.561374	-2.165654
H	-5.780985	-2.860434	-2.107615
C	-3.868700	-6.861151	0.214511
H	-2.957956	-7.468108	0.341788
H	-4.515115	-7.049656	1.091388
H	-4.408100	-7.230447	-0.673056
O	-0.197587	1.194719	0.437600
C	0.014178	1.833730	-0.672215
O	0.136160	1.339702	-1.829807
Ag	0.681241	-0.742928	-2.127398
O	0.921253	-2.720456	-2.839211
C	1.032324	-3.680690	-1.993043
O	0.805022	-3.635941	-0.740343
C	1.530076	-5.006462	-2.565830
H	2.633804	-5.002641	-2.552480
H	1.181290	-5.852354	-1.956219
H	1.206664	-5.120527	-3.610901
C	-3.573716	-0.137283	1.048296
C	-3.458646	1.387456	1.022519
H	-3.263601	-0.548320	2.020078
H	-4.605125	-0.469069	0.847985
H	-2.404016	1.701127	1.131302
H	-3.810849	1.809603	0.065029
C	-4.267607	1.993800	2.164719
O	-4.789661	1.353370	3.069267
O	-4.320955	3.344087	2.047520
C	-5.055405	4.031399	3.109187
H	-6.083763	3.632141	3.138598
H	-4.579489	3.792946	4.076038
C	-5.019091	5.518782	2.796416

H	-5.493789	5.732023	1.825136
H	-5.564486	6.075166	3.576678
H	-3.983101	5.892884	2.766400
C	3.829044	-0.686782	1.567212
C	5.027584	-0.353128	0.911972
C	3.855695	-1.065007	2.925810
C	6.223837	-0.406819	1.633786
H	5.018212	-0.058791	-0.139292
C	5.070984	-1.110959	3.627848
H	2.914660	-1.321313	3.419317
C	6.271665	-0.780728	2.985005
H	5.083836	-1.406061	4.681698
H	7.236102	-0.804862	3.496747
N	7.491891	-0.055969	0.947636
O	8.539967	-0.113957	1.616720
O	7.427315	0.273166	-0.248666
C	0.106771	3.332287	-0.531425
C	0.196328	3.941134	0.738488
C	0.121099	4.127422	-1.691842
C	0.303407	5.336162	0.850720
H	0.195755	3.306349	1.628526
C	0.213720	5.514958	-1.549938
H	0.063950	3.672251	-2.682218
C	0.309105	6.139489	-0.297735
H	0.385780	5.800782	1.838009
H	0.387778	7.227745	-0.250822
N	0.212016	6.360903	-2.770129
O	0.112905	5.786446	-3.867039
O	0.305936	7.591209	-2.612011

Int10

SCF energy in solvent: -1693.068648 a.u.

Free energy in solvent: -1692.712008 a.u.

No imaginary frequency

C	-2.152186	3.477842	0.100976
C	-1.175509	2.485231	-0.120706
C	0.094646	2.899646	-0.561328
C	0.424619	4.259423	-0.780872
C	-0.580036	5.208916	-0.527061
C	-1.869649	4.841473	-0.088512
H	-3.152484	3.171727	0.431194

H	-0.355186	6.268487	-0.700775
C	1.783247	4.698580	-1.280864
H	2.167787	4.022053	-2.063763
H	2.532767	4.716210	-0.467930
H	1.736005	5.716470	-1.699371
C	-2.918816	5.899927	0.178428
H	-2.899868	6.690718	-0.590602
H	-2.747570	6.392577	1.153262
H	-3.932060	5.467570	0.200816
C	-1.464937	1.021772	0.129548
H	-2.479847	0.763195	-0.220547
H	-1.429274	0.807873	1.217871
S	1.224531	1.560750	-1.011180
C	2.456164	1.576834	0.389579
C	3.538054	0.525697	0.128912
H	2.876102	2.594912	0.434088
H	1.923130	1.372978	1.328835
H	4.208413	0.820609	-0.696314
H	3.074960	-0.432532	-0.184582
C	4.360924	0.274507	1.384220
O	4.053115	0.623218	2.517772
O	5.490741	-0.421268	1.082099
C	6.326289	-0.768677	2.226951
C	7.487544	-1.600976	1.705401
H	6.664347	0.163377	2.712868
H	5.711312	-1.318174	2.960347
H	8.149152	-1.883087	2.541398
H	8.082728	-1.035456	0.970097
H	7.127188	-2.524296	1.223734
Pd	-0.094055	-0.285323	-0.648520
O	0.358578	-3.433667	-1.697553
C	1.398275	-2.730615	-1.761953
O	1.519836	-1.491743	-1.381930
C	2.671389	-3.338145	-2.356487
H	2.902477	-2.838260	-3.312326
H	2.539772	-4.414777	-2.531773
H	3.526663	-3.166992	-1.682958
I	-1.688281	-2.432544	-0.328411
C	-3.383265	-1.660086	0.827986
C	-4.577664	-1.331693	0.167949
C	-3.277260	-1.542153	2.222540

C	-5.679907	-0.882804	0.917409
H	-4.652992	-1.424762	-0.920211
C	-4.383674	-1.090403	2.963262
H	-2.342978	-1.801347	2.730687
C	-5.583822	-0.761472	2.312826
H	-6.613951	-0.628413	0.404989
H	-4.304072	-0.999118	4.051857
H	-6.444253	-0.413127	2.893364

TS7

SCF energy in solvent: -1693.057798 a.u.

Free energy in solvent: -1692.699992 a.u.

imaginary frequency: -115.656600

C	1.162703	2.123758	-0.981299
C	0.968231	0.765776	-1.593260
H	1.857283	0.441677	-2.159696
Pd	0.351387	-0.659219	-0.234870
C	0.366601	2.503362	0.120393
H	0.100038	0.759541	-2.284081
C	0.426436	3.789328	0.699067
C	2.078693	3.064218	-1.490330
C	2.178499	4.358309	-0.944157
C	1.346638	4.698864	0.140253
H	2.716712	2.781473	-2.336992
H	1.431555	5.697278	0.586267
S	-0.650727	1.178737	0.824742
C	-0.428729	4.192904	1.879991
H	-1.473706	4.389001	1.576962
H	-0.458429	3.401889	2.648809
H	-0.045487	5.114799	2.345209
C	3.143613	5.370800	-1.523844
H	2.668461	5.949896	-2.337151
H	3.479111	6.093952	-0.762326
H	4.034627	4.881821	-1.950959
C	-2.289595	1.573251	0.031416
C	-3.348122	0.544937	0.427954
H	-2.144221	1.597588	-1.058837
H	-2.561273	2.587104	0.367738
H	-3.080417	-0.455706	0.034389
H	-3.429725	0.445185	1.526097
C	-4.706783	0.944796	-0.126731

O	-4.932926	1.946192	-0.796538
O	-5.650824	0.027153	0.215449
C	-6.988854	0.295125	-0.298527
H	-7.348770	1.248030	0.128266
H	-6.927452	0.426343	-1.392517
C	-7.869138	-0.881396	0.094829
H	-7.910061	-0.997752	1.190066
H	-8.895760	-0.719439	-0.274118
H	-7.489228	-1.820063	-0.339775
C	2.647447	-1.219942	0.654795
C	3.595941	-0.207797	0.437174
C	2.364633	-1.723764	1.933347
C	4.237711	0.354220	1.553866
H	3.820616	0.148738	-0.570763
C	3.021841	-1.142691	3.032075
H	1.609295	-2.501223	2.069023
C	3.956414	-0.110136	2.849337
H	4.966618	1.156737	1.398237
H	2.793081	-1.510561	4.038094
H	4.468902	0.326633	3.712185
O	-0.498070	-2.157542	1.074702
C	-1.539856	-2.616562	0.436945
O	-1.954055	-2.134990	-0.650447
C	-2.233034	-3.814215	1.081519
H	-3.259202	-3.913970	0.698780
H	-1.675782	-4.732873	0.827556
H	-2.239897	-3.723166	2.179124
I	2.093966	-2.532717	-1.160106

Int11

SCF energy in solvent: -1693.0894 a.u.

Free energy in solvent: -1692.729075 a.u.

No imaginary frequency

C	1.426539	1.975770	-1.047961
C	1.503235	0.537075	-1.469572
H	2.528041	0.222714	-1.716028
Pd	0.604224	-0.770533	-0.144631
C	0.424035	2.431340	-0.166047
H	0.843646	0.321794	-2.331196
C	0.290106	3.795903	0.186110
C	2.328895	2.920499	-1.576142

C	2.218730	4.289283	-1.272739
C	1.196514	4.701729	-0.395093
H	3.124314	2.574970	-2.247239
H	1.116772	5.762480	-0.128435
S	-0.572498	1.165623	0.651130
C	-0.760258	4.286065	1.157721
H	-1.769389	4.287751	0.706623
H	-0.808106	3.647740	2.057099
H	-0.544709	5.317189	1.478461
C	3.167943	5.298603	-1.880955
H	2.737410	5.742390	-2.797496
H	3.376668	6.127909	-1.185100
H	4.126896	4.833810	-2.161379
C	-2.198181	1.271485	-0.242478
C	-3.293424	0.651067	0.629034
H	-2.092908	0.738369	-1.199031
H	-2.402775	2.335747	-0.434422
H	-3.124095	-0.424817	0.796017
H	-3.306414	1.120122	1.631639
C	-4.665984	0.872871	0.000414
O	-4.926182	1.740103	-0.824011
O	-5.570535	-0.005852	0.503503
C	-6.935921	0.157691	0.007609
H	-7.269605	1.186393	0.228135
H	-6.926274	0.041288	-1.089772
C	-7.796456	-0.891116	0.694261
H	-7.787736	-0.757817	1.788128
H	-8.838421	-0.803822	0.344102
H	-7.440018	-1.908352	0.465218
C	1.944874	-0.446369	1.359560
C	3.178162	0.212345	1.258012
C	1.501913	-0.954817	2.592555
C	3.966484	0.380583	2.412853
H	3.546364	0.586799	0.299843
C	2.299396	-0.780234	3.739234
H	0.551166	-1.494573	2.661781
C	3.530018	-0.110742	3.652388
H	4.931967	0.892282	2.330192
H	1.951594	-1.179309	4.698604
H	4.150046	0.020071	4.545408
O	-0.918609	-2.216635	0.713030

C	-1.501616	-2.266464	-0.431715
O	-1.118041	-1.499583	-1.391567
C	-2.614160	-3.265914	-0.665732
H	-3.329908	-2.887817	-1.410861
H	-2.167333	-4.193683	-1.063035
H	-3.124751	-3.508793	0.277798
I	2.156888	-2.761330	-1.010673

TS8

SCF energy in solvent: -1693.056965 a.u.

Free energy in solvent: -1692.69637 a.u.

imaginary frequency: -237.852000

C	1.395372	3.426679	-1.444880
C	0.898865	2.238743	-0.874119
C	-0.298797	2.295619	-0.125744
C	-1.013581	3.507909	0.046480
C	-0.490675	4.659082	-0.570963
C	0.704679	4.643627	-1.316736
H	2.334226	3.390431	-2.009714
H	-1.027449	5.606717	-0.442486
C	-2.280083	3.596058	0.869133
H	-2.167025	3.073801	1.835945
H	-3.145760	3.138003	0.356405
H	-2.536710	4.647018	1.074758
C	1.222585	5.904629	-1.973029
H	2.310393	5.855588	-2.141683
H	1.008400	6.795895	-1.360300
H	0.743460	6.062774	-2.956704
C	1.604982	0.943690	-1.106143
H	2.587506	1.062866	-1.572873
H	1.010123	0.275304	-1.771523
Pd	0.941293	-0.734861	0.155323
C	2.563006	0.553927	0.666285
C	3.915951	0.257180	0.388670
C	2.255473	1.333833	1.801981
C	4.926068	0.673144	1.266741
H	4.177099	-0.317917	-0.502949
C	3.275001	1.735858	2.683632
H	1.229394	1.635025	2.029479
C	4.611990	1.406496	2.422792
H	5.966410	0.419073	1.037611

H	3.009567	2.317374	3.572914
H	5.403954	1.730194	3.105690
S	-0.821652	0.799752	0.743100
C	-2.351975	0.320442	-0.210427
C	-3.462648	-0.182080	0.721364
H	-2.679125	1.233815	-0.729763
H	-2.047213	-0.449132	-0.938403
H	-3.398263	0.308182	1.712225
H	-3.398106	-1.266296	0.897010
C	-4.833315	0.185318	0.154675
O	-5.075535	1.214620	-0.467206
O	-5.757364	-0.755286	0.463934
C	-7.118268	-0.463686	0.013731
C	-7.989882	-1.643539	0.413303
H	-7.097552	-0.304345	-1.077734
H	-7.447279	0.480561	0.481280
H	-9.028715	-1.463325	0.090431
H	-7.637801	-2.573924	-0.060521
H	-7.988142	-1.786854	1.505937
I	2.544250	-2.700487	-0.765979
O	-0.315700	-2.260867	0.765277
C	-1.036701	-2.806782	-0.201153
O	-1.173214	-2.343352	-1.346126
C	-1.686745	-4.120955	0.228993
H	-1.936514	-4.123500	1.300843
H	-2.580040	-4.316242	-0.381947
H	-0.956453	-4.929772	0.053924

Int12

SCF energy in solvent: -1693.113988 a.u.

Free energy in solvent: -1692.75096 a.u.

No imaginary frequency

C	0.125082	2.849681	-0.760321
C	0.994146	1.910172	-1.571194
H	1.384400	2.467221	-2.441110
Pd	1.125587	-0.588625	0.121419
C	-0.739036	2.399424	0.269066
H	0.396619	1.078054	-1.987869
C	-1.477585	3.326117	1.055789
C	0.209988	4.231819	-1.012768
C	-0.530235	5.172082	-0.276038

C	-1.358212	4.695748	0.755975	O	-5.696657	-1.040728	-0.142487
H	0.880098	4.580056	-1.808161	C	-6.670773	-1.837405	-0.885301
H	-1.929819	5.413220	1.357127	H	-6.610612	-1.561232	-1.952153
S	-0.869001	0.639939	0.708203	H	-6.389902	-2.901613	-0.803800
C	-2.380862	2.896226	2.193101	C	-8.040108	-1.552338	-0.288665
H	-3.275766	2.363874	1.825746	H	-8.297217	-0.484281	-0.377159
H	-1.870184	2.208582	2.887220	H	-8.807275	-2.137093	-0.823014
H	-2.728472	3.772935	2.762112	H	-8.074136	-1.831099	0.776938
C	-0.450993	6.649241	-0.592372	H	-0.841314	-4.647885	-0.250128
H	-1.226868	6.938537	-1.325069	H	-1.982392	-4.440207	1.136614
H	-0.608596	7.264579	0.308561	H	-2.353077	-3.726867	-0.469689
H	0.525275	6.918762	-1.027191	C	2.208950	1.339566	-0.812706
O	-0.018124	-2.241920	-0.277727	C	2.325324	1.342258	0.619065
C	-0.852444	-2.664934	0.652501	C	3.381755	1.052576	-1.573161
O	-1.115324	-2.074191	1.715993	C	3.590744	1.094581	1.234453
C	-1.547077	-3.965459	0.245706	H	1.553695	1.822737	1.228600
C	-2.227824	0.066975	-0.441031	C	4.604407	0.826482	-0.951859
C	-3.464446	-0.388198	0.344679	H	3.312634	1.044790	-2.666316
H	-1.817453	-0.772988	-1.021380	C	4.715488	0.847475	0.460578
H	-2.446199	0.904950	-1.120699	H	3.659028	1.122445	2.326151
H	-3.136516	-1.061693	1.160652	H	5.491274	0.628725	-1.562141
H	-4.010496	0.451876	0.801933	H	5.683974	0.664835	0.935029
C	-4.407053	-1.187701	-0.546591	I	3.107765	-2.374372	-0.037537
O	-4.059972	-1.896676	-1.484694				