Electronic Supplementary Information for:

Radical Pd(III) C–C Reductive Eliminations in Palladium Catalyzed Sequences

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Contents

1. General Remarks

Unless otherwise noted calculations were performed at the DFT level using the M06[1] functionals as implemented in Gaussian09.[2] Geometry optimization were carried out employing LACVP(d)[3] basis set. It consists of the standard 6-31G(d) basis set for lighter atoms (H, C, N, and O) and the LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double-ζ) basis set for Pd. Unless otherwise noted, for all of the intermediates and transition states presented in the article, full optimization, without any restriction, was carried out using the CPCM[4] approach as implemented in Gaussian09, employing MeOH as a solvent as experimentally adopted (energetic trends and geometries were comparable with those observed with gas-phase optimized structures and with single point solvent calculations on gas-phase optimized ones, see next Table to compare data). The basic system presented in the article, denoted with the letter "a", has been studied by carrying out *full optimizations* at the M06-L, M06-2X, mPW2PLYP[5] and MP2 level,[6] using the LACVP(d), the Def2-SVP and Def2-TZVP[7] basis sets. Also in all of these cases the geometry optimization included solvent effects. The two Pd/Ru adducts presented in Figure 3 were obtained by using optimized geometry of the corresponding open-shell species (Pd(III) IIIa, Pd(I) Va and Ru(III) Iox) as a starting point and re-optimizing the two binuclear adducts imposing a 12 Å distance between metal cores (at the M06/Def2-SVP level with methanol as implicit solvent). In both cases, converged structures and molecular orbitals matched those of the stand-alone redox products (Pd(IV) IV a, Pd(II) II a and Ru(II) Ired). Transition states were identified by having one imaginary frequency in the Hessian matrix (for CPCM optimized structures, as implemented in Gaussina09, the implicit solvent effect was taken into account during optimization and thus before the frequency calculation). *In all cases, no differences in energetic trend aroused and the C-C reductive elimination remain favored on radical Pd(III) over diamagnetic Pd(IV) (either cationic or neutral, penta- or hexacoordinated).* Reaction Figures from which relevant transition states have been presented in the article on form of table or within the text for sake of space, are presented herein with captions of the relevant species thereby involved (Section 2-4). XYZ coordinates of all optimized structures with a different functionals and basis sets could be found in the last section, below the corresponding M06/LACVP(d) one. Structures optimized in the gas phase are labeled with the appendix "GAS" in the XYZ coordinate section and in the final Table in atomic units.

COMPREHENSIVE COMPARISON OF CALCULATED BARRIERS

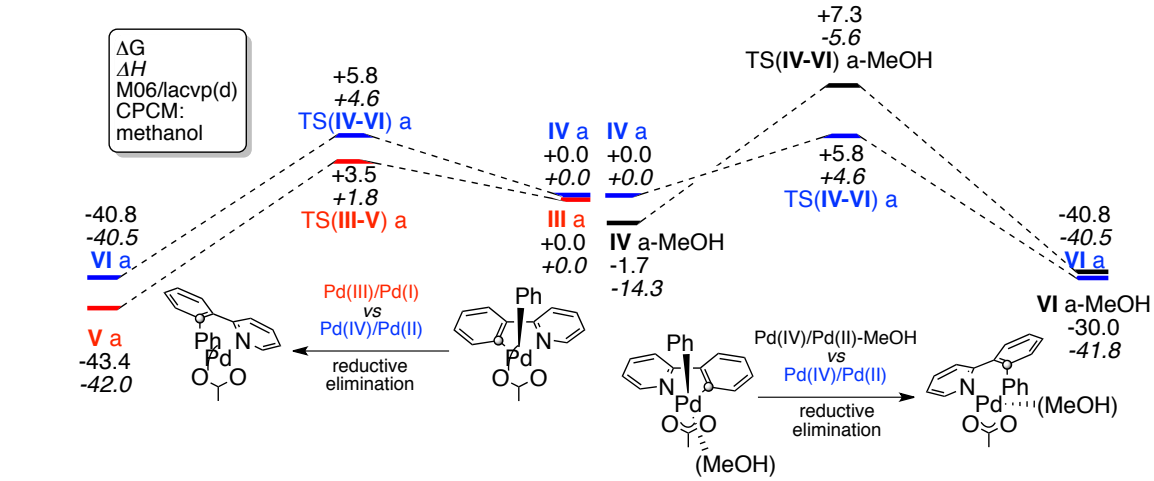
Level	Optimization/Solvent	Radical Pd (III) pathway ΔG TS(III)	Pd(IV) pathway ΔG TS(IV)	ΔG TS(IV)-MeOH	ΔG TS(IV)-BF4
M06/lacvp(d)	Full optimization including MeOH (CPCM)	3,5	5,8	9,0	11,5
M06-L/lacvp(d)		3,9	7,5	10,6	
M06-2X/lacvp(d)		2,7	6,0	8,3	
mPW2PLYP/lacvp(d)		4,7	8,7		
MP2/lacvp(d)		0,9	15,8		
M06/Def2-SVP		3,2	5,2		
M06/Def2-TZVP		2,7	5,1		
M06/lacvp(d)	Full optimization gas phase	1,9	2,2		11,9
M06/lacvp(d)	SP PCM on gas phase optimized geometries	4,5	5,3		
M06/lacvp(d)	*ON BINUCLEAR COMPLEX, vide infra* (full optimization including MeOH (CPCM))	3,8	5,5		

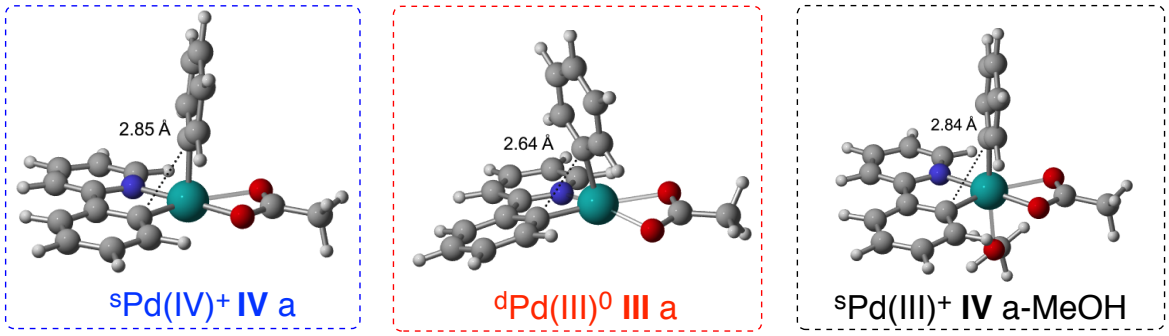
ΔG values in kcal/mol at 298.15 K.

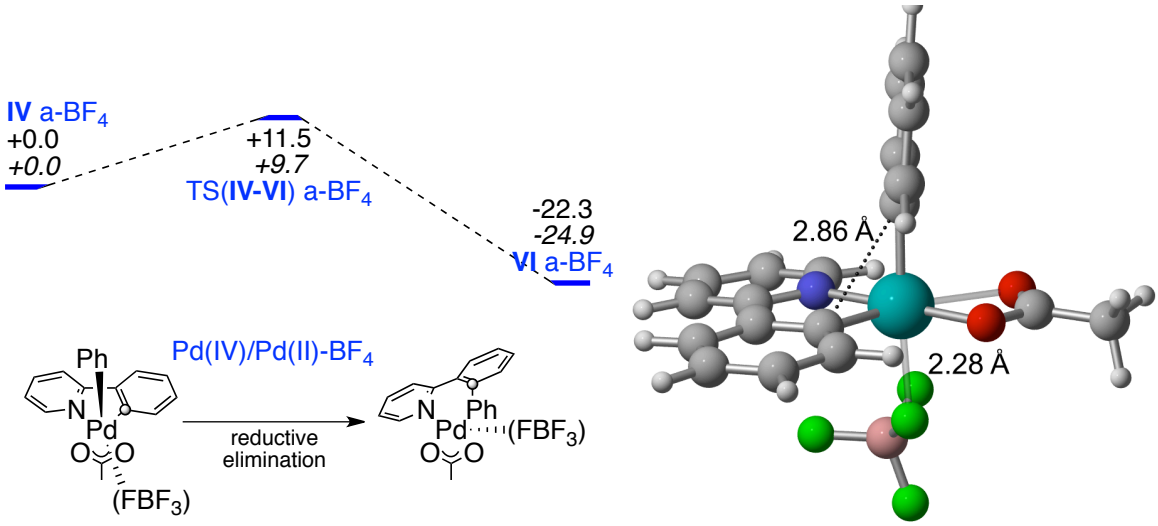
Level	Solvent	Radical Pd (III) ΔH TS(III)	Pd(IV) pathway ΔH TS(IV)	ΔH TS(IV)-MeOH	ΔH TS(IV)-BF4
	Full optimization including MeOH				
M06/lacvp(d)	(CPCM)	1,8	4,7	8,6	9,7
M06-L/lacvp(d)		4,1	6,4	13,1	
M06-2X/lacvp(d)		2,7	4,2	6,8	
mPW2PLYP/lacvp(d)		3,6	7,4		
MP2/lacvp(d)		1,9	15,4		
M06/Def2-SVP		1,9	4,2		
M06/Def2-TZVP		1,9	4,3		
M06/lacvp(d)	Full optimization gas phase	0,9	1,1		11,2
M06/lacvp(d)	SP PCM on gas phase optimized geometries	1,4	3,3		
M06/lacvp(d)	*ON BINUCLEAR COMPLEX, vide infra* (full optimization including MeOH (CPCM))	3,1	5,3		

ΔH values in kcal/mol at 298.15 K.

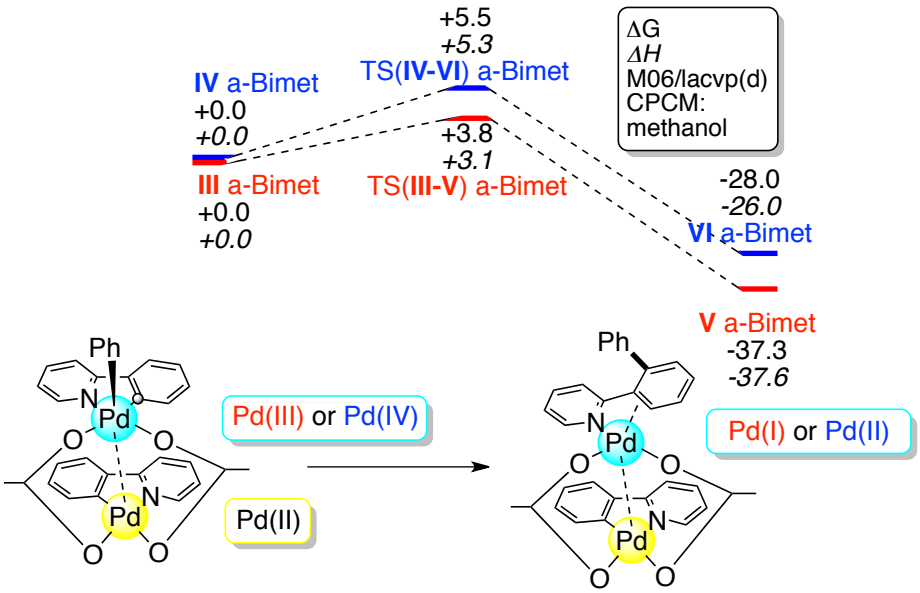
2. Reaction scheme comparing octahedric Pd(IV) (cationic a-MeOH & neutral a-BF_4)

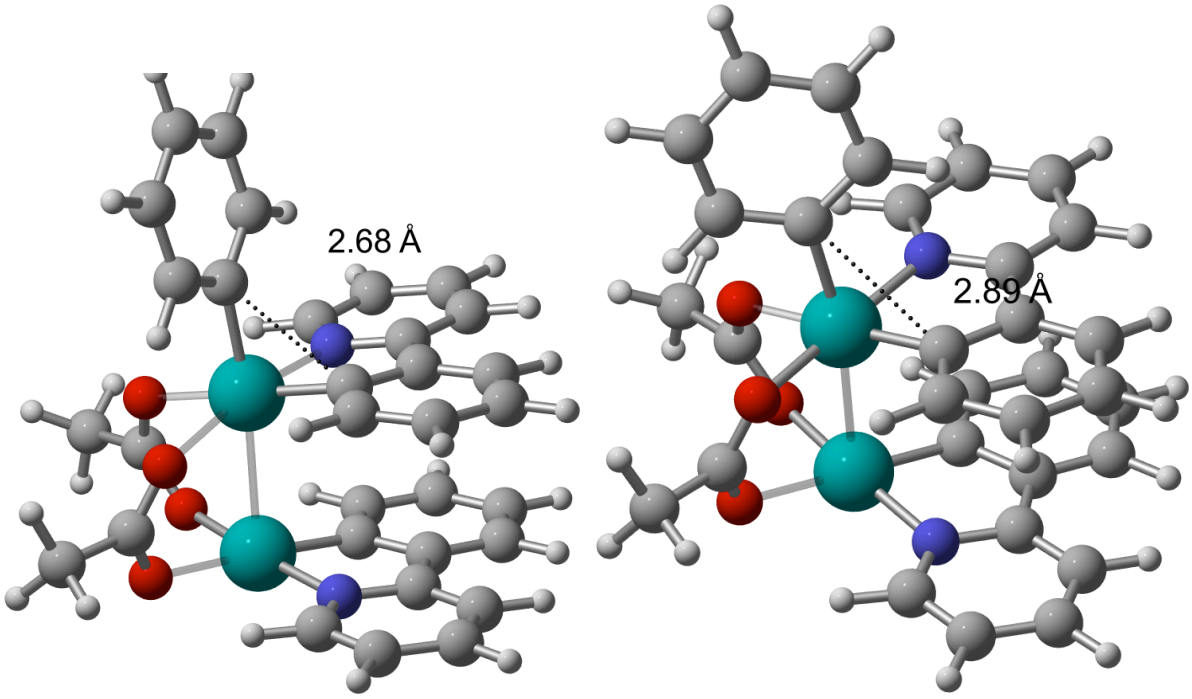






Reaction scheme comparing bimetallic complexes



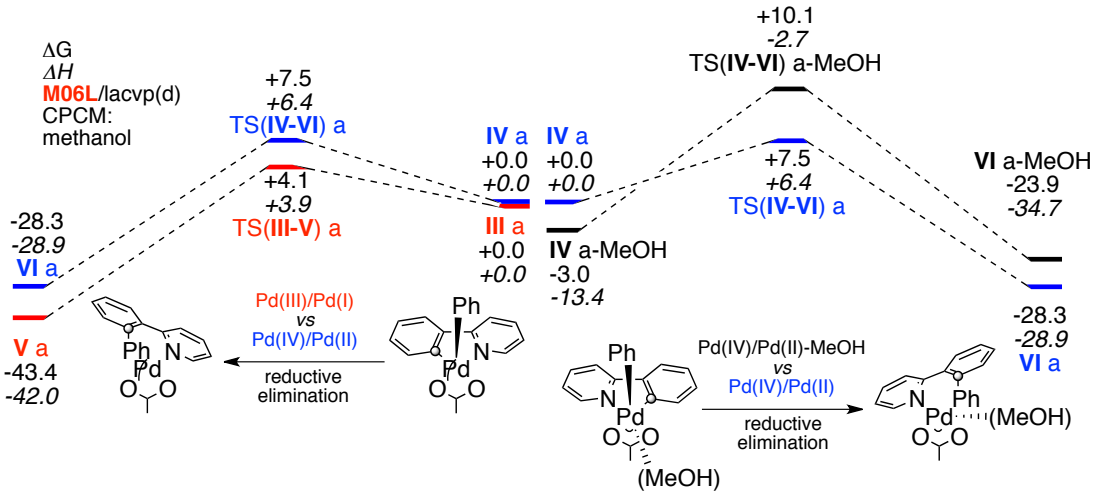


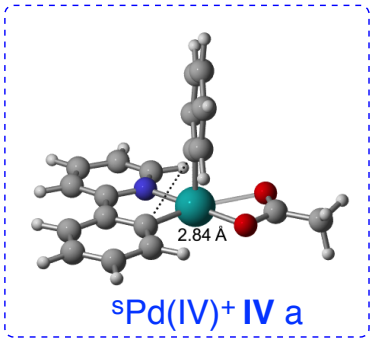
Pd(III) IIIa-Bimet

Pd(IV) IVa-Bimet

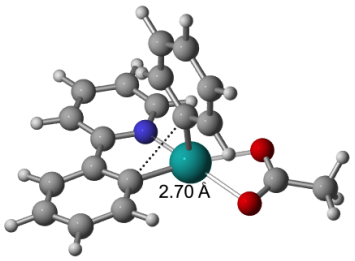
3. Reaction scheme (a) comparing different functional/basis set

M06-L (full optimization with CPCM: MeOH)

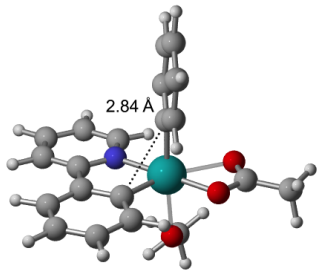




^{s}Pd(IV)$^{+}$ **IV** a

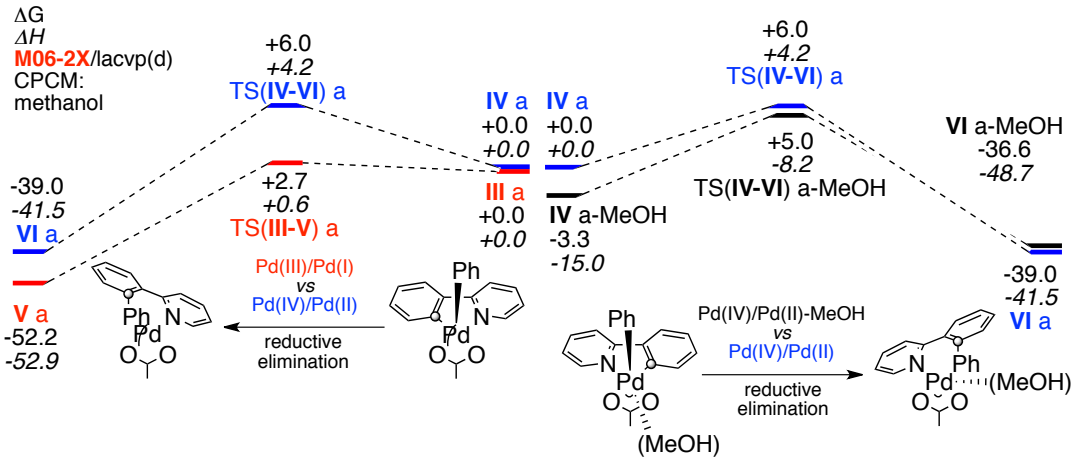


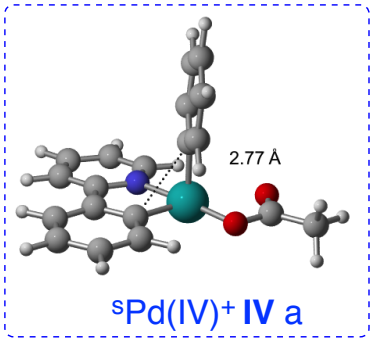
^{d}Pd(III)^{0} **III** a



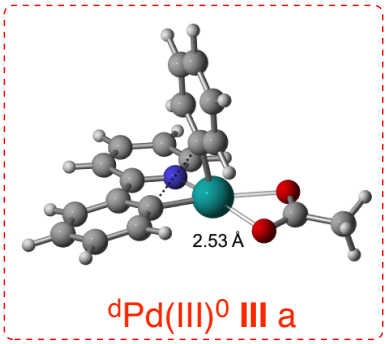
^{s}Pd(III)$^{+}$ **IV** a-MeOH

M06-2X (full optimization with CPCM: MeOH)

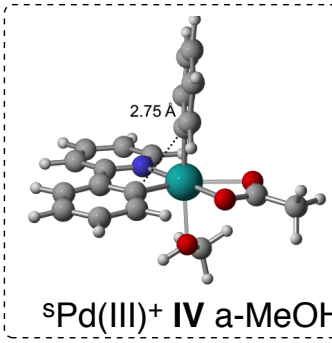




$^{s}Pd(IV)^{+}$ **IV** a

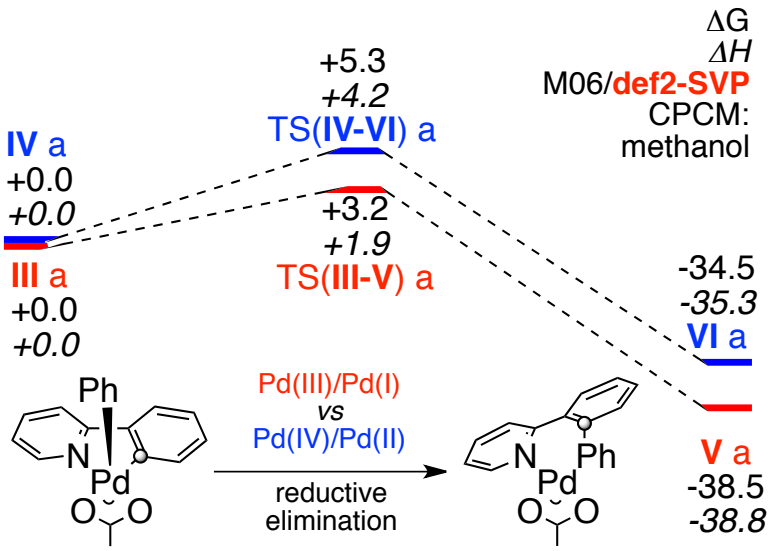


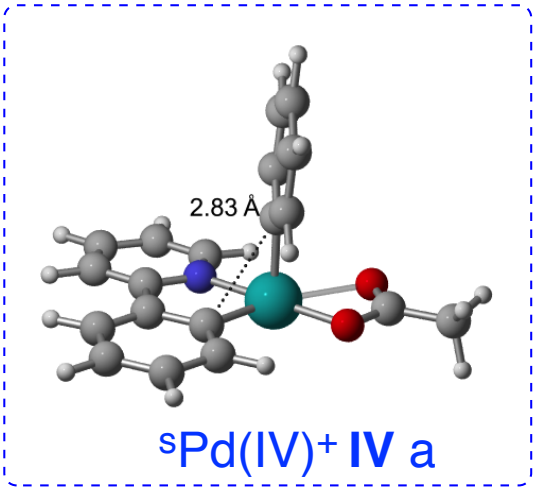
$^{d}Pd(III)^{0}$ **III** a

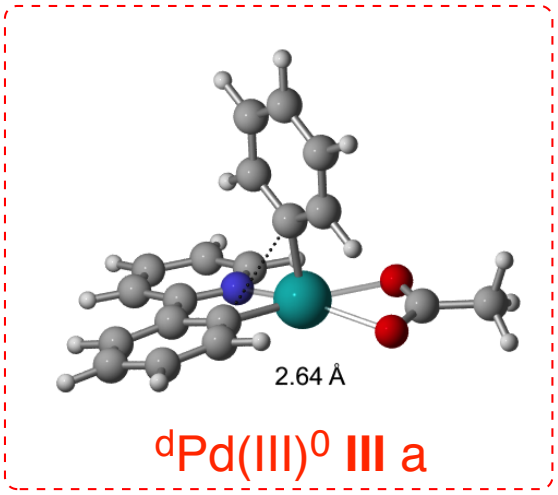


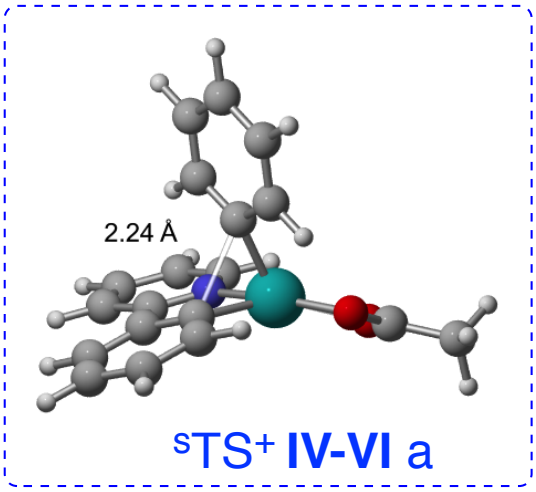
$^{s}Pd(III)^{+}$ **IV** a-MeOH

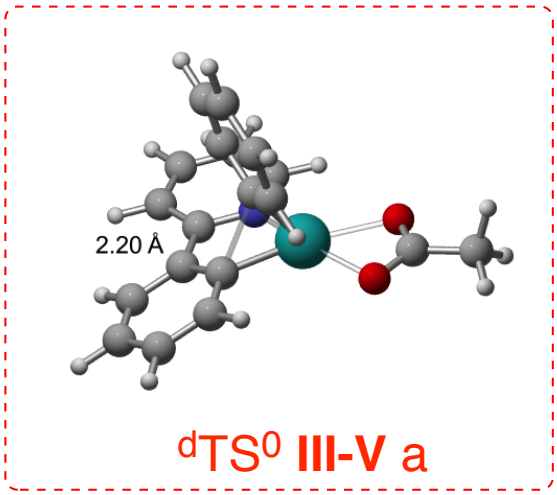
M06/def2-SVP (full optimization with CPCM: MeOH)



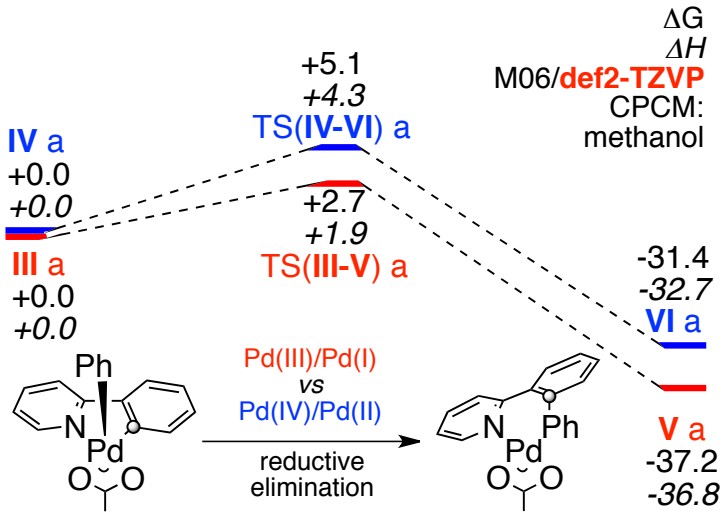


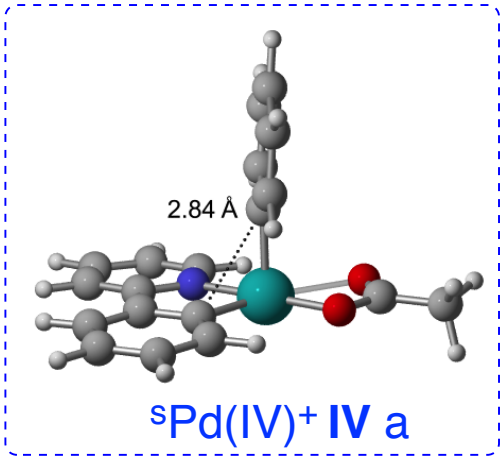


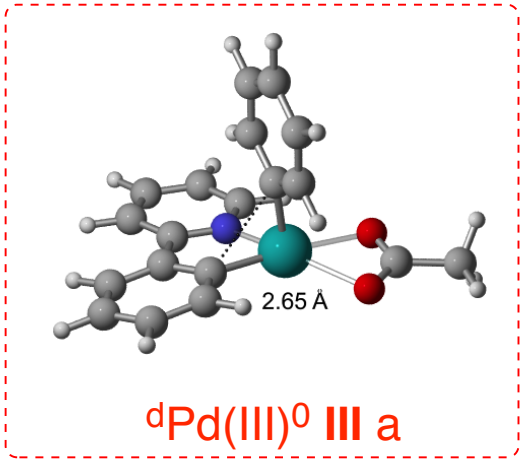


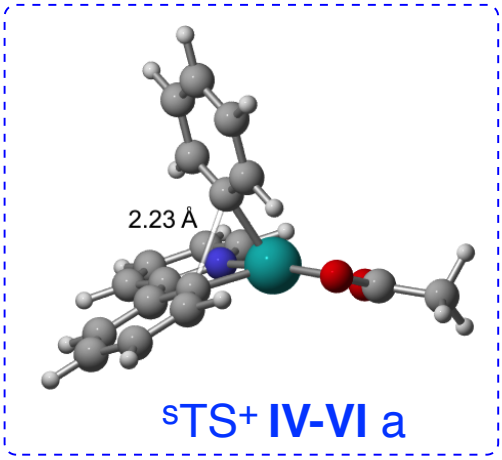


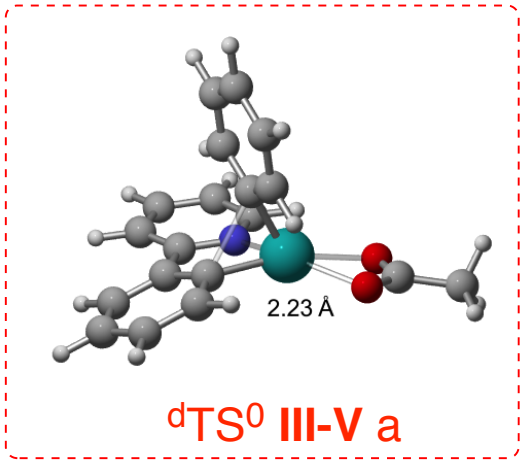
M06/def2-TZVP (full optimization with CPCM: MeOH)



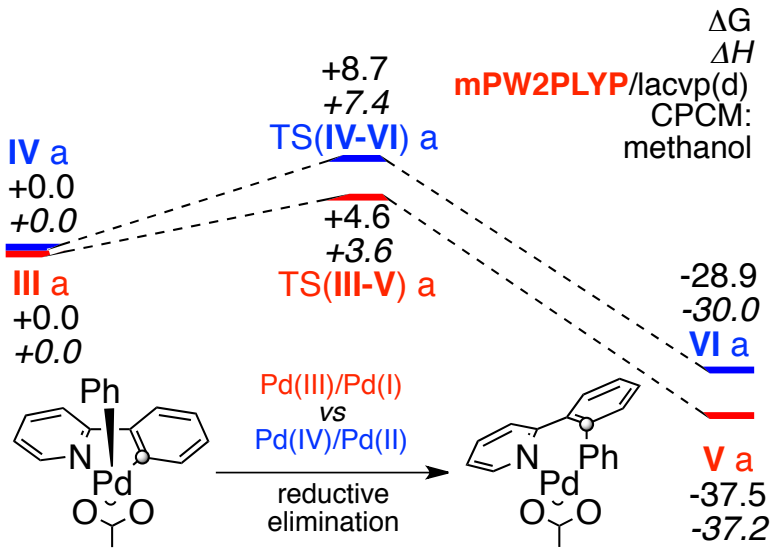


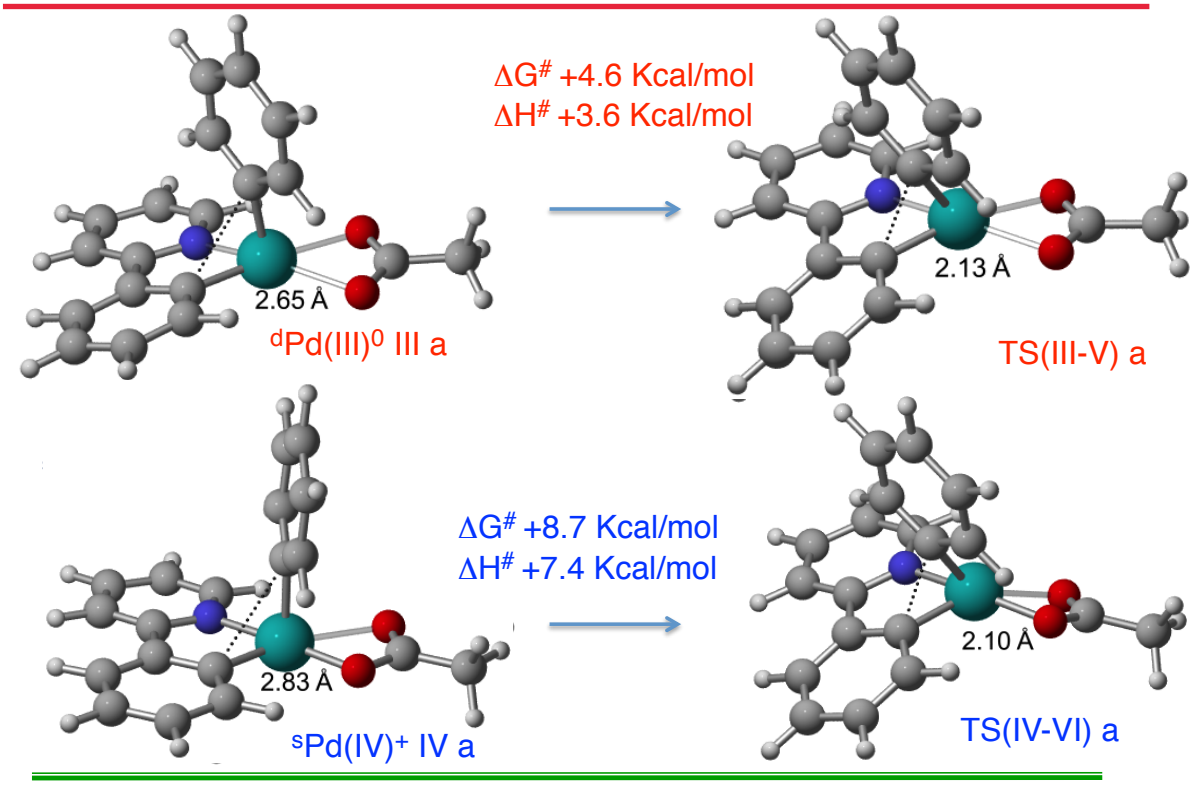




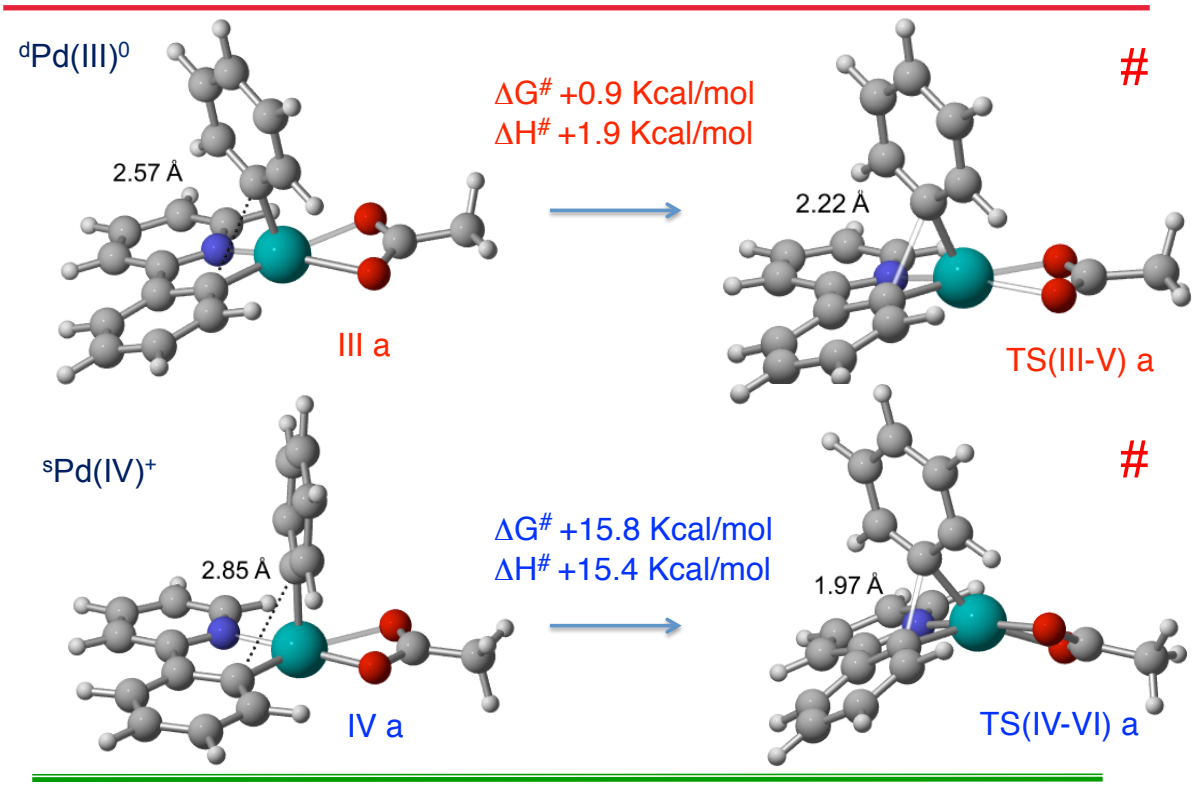


mPW2PLYP/LACVP(d) (full optimization with CPCM: MeOH)



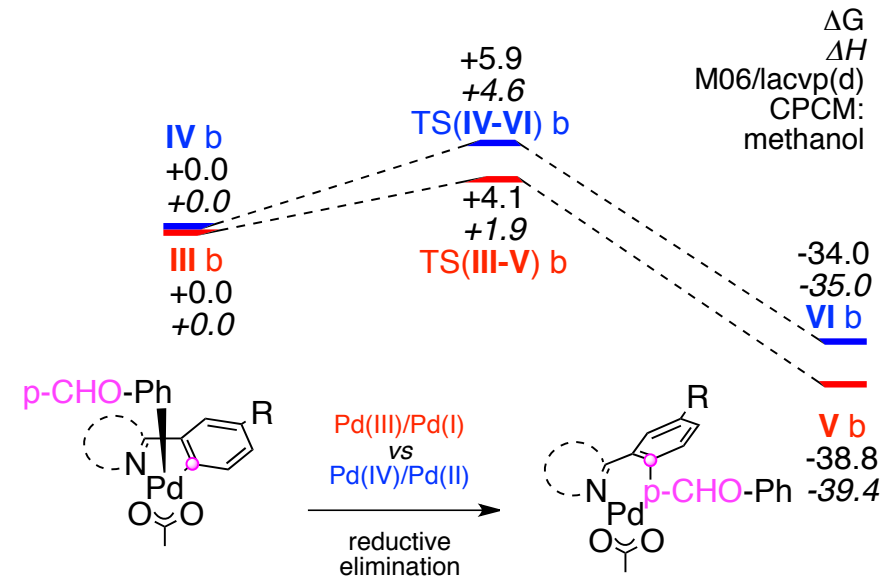


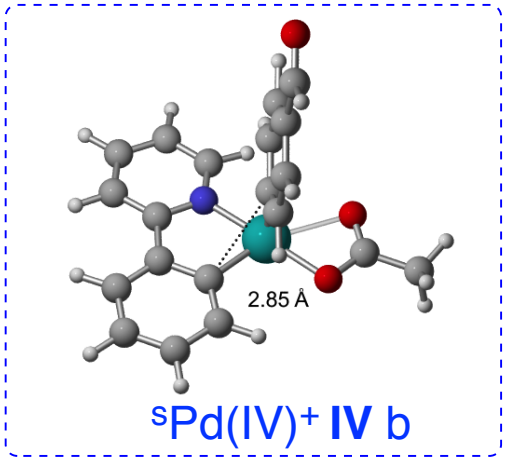
MP2/LACVP(d) (full optimization with CPCM: MeOH)

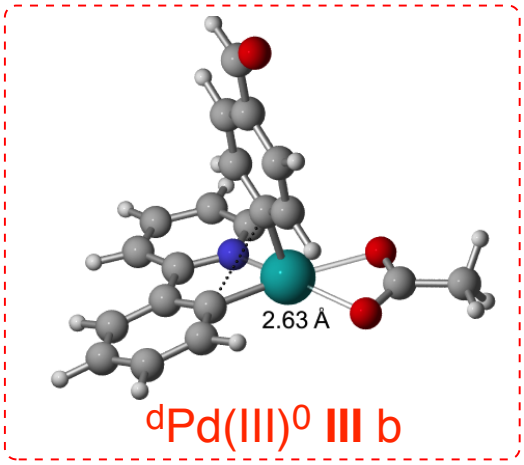


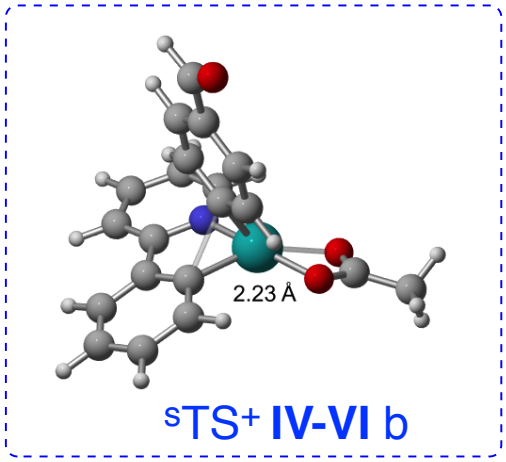
A particular case occurs modeling reactions barriers at the MP2 level. While geometries of intermediates remains unchanged, the cost of the Pd(III) barrier decreases to +0.9 kcal/mol in ΔG (ΔH +1.9 kcal/mol) while its Pd(IV) counterpart climbs to +15.8 kcal/mol. This steep increase arouses from a calculated transition state presenting a developed late character compared to DFT ones and thus more energy costly for an overall exoergonic, C-C forming reaction (distance between reacting atoms shrinks to 1.97 Å from 2.22 Å in **TS(IV-VI)a-MP2**).

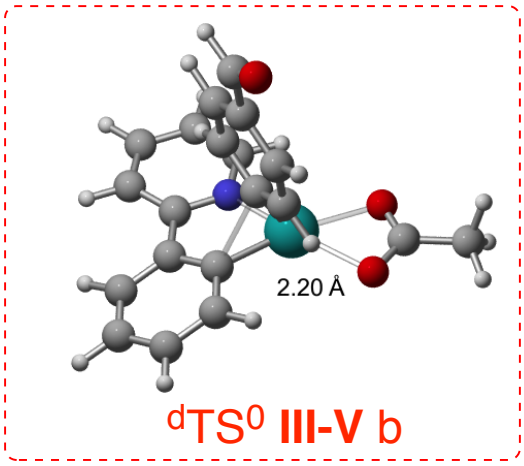
9. Reaction scheme (b-g) varying organic fragments on reactants (full optimization with CPCM: MeOH)

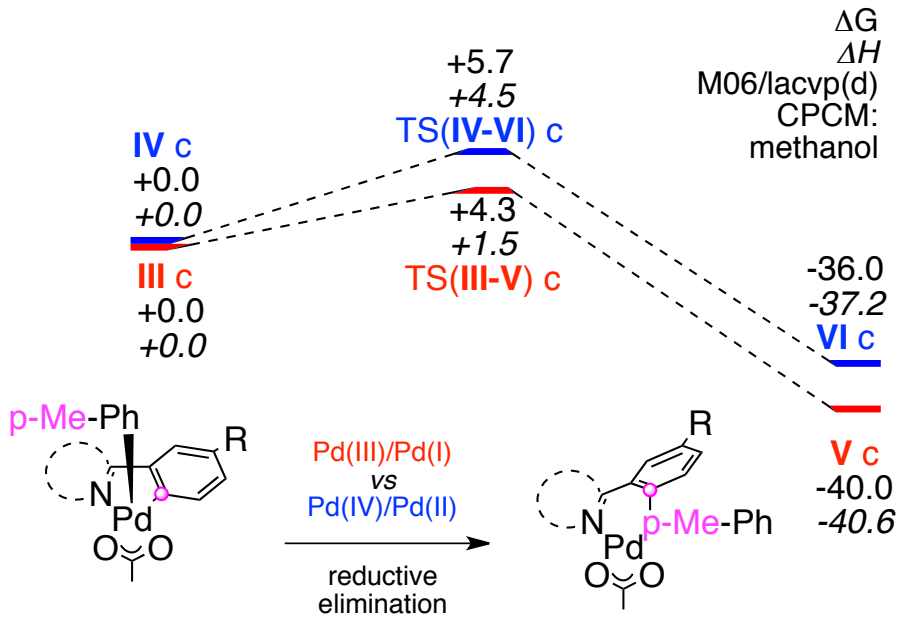


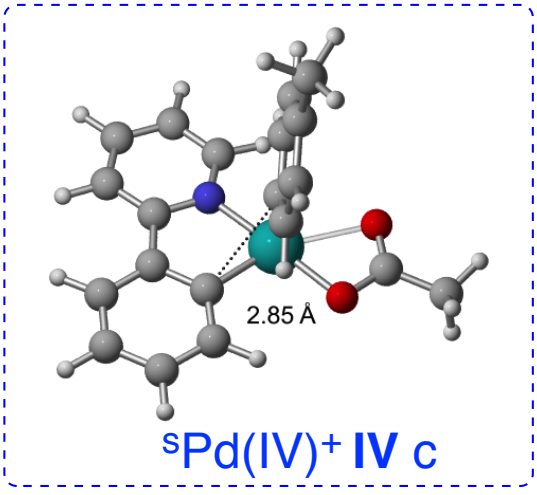


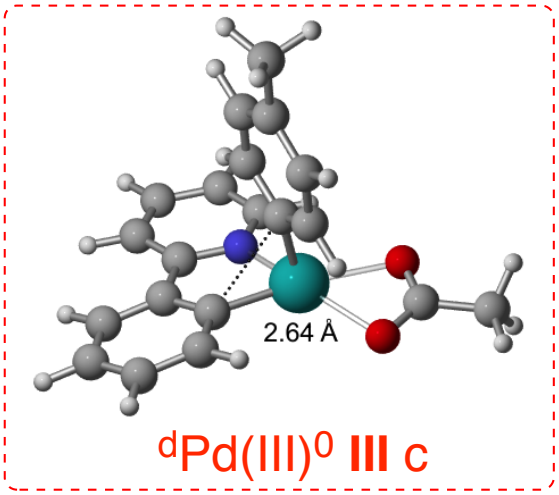


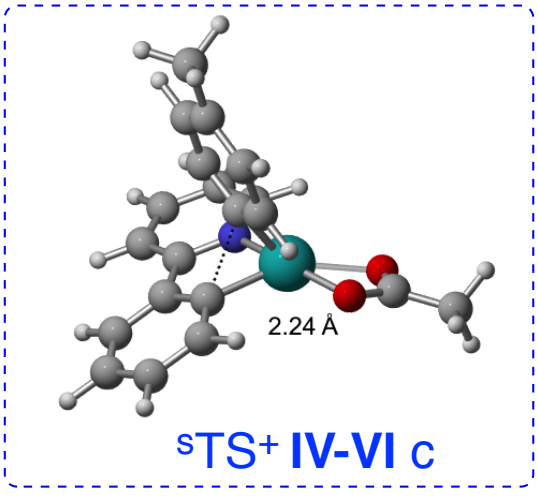


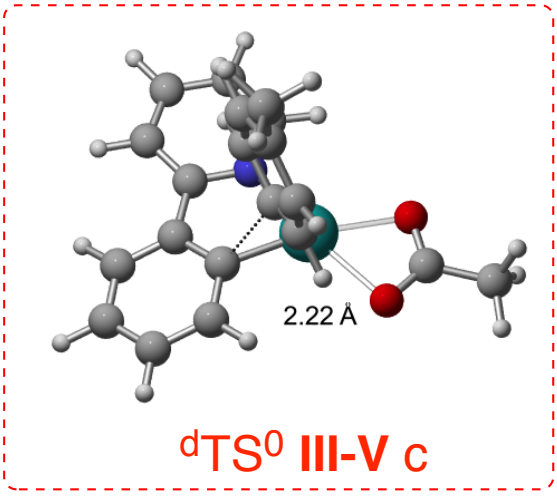


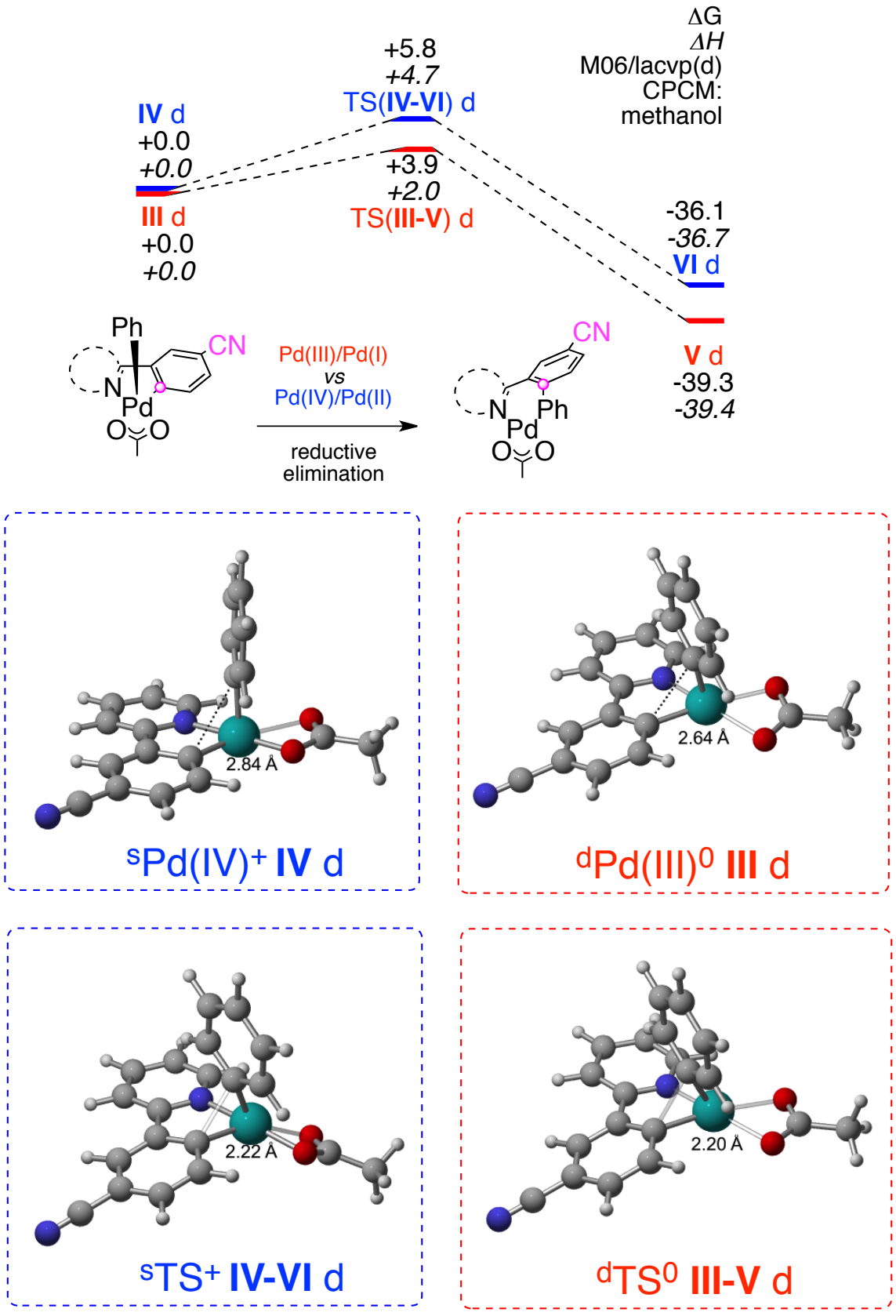

ΔG
ΔH
M06/lacvp(d)
CPCM:
methanol
IV c
+0.0
+0.0
III c
+0.0
+0.0
+5.7
+4.5
TS(IV-VI) c
+4.3
+1.5
TS(III-V) c
-36.0
-37.2
VI c
V c
-40.0
-40.6
p-Me-Ph
R
N
Pd
O
O
Pd(III)/Pd(I)
vs
Pd(IV)/Pd(II)
reductive
elimination

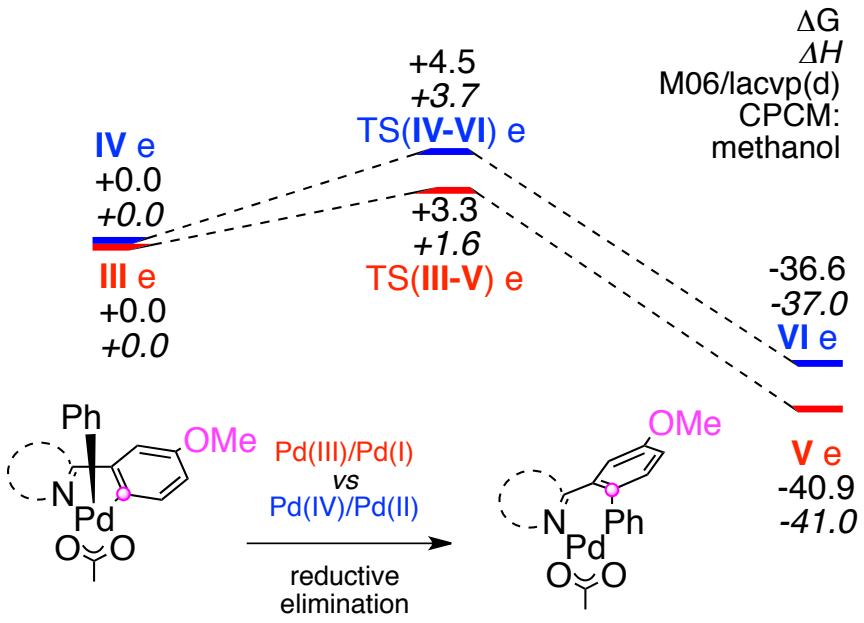

2.85 Å
sPd(IV)+ IV c

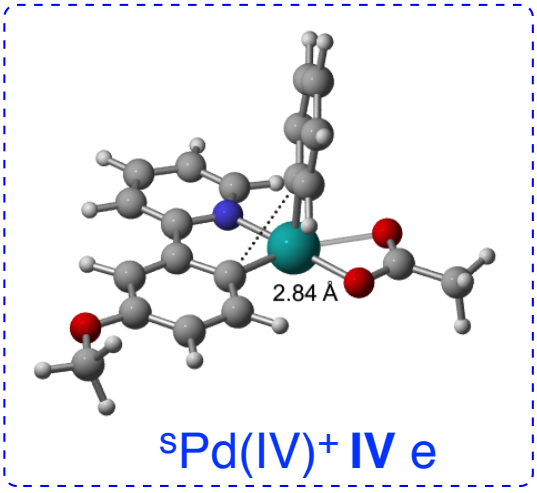

2.64 Å
dPd(III)0 III c

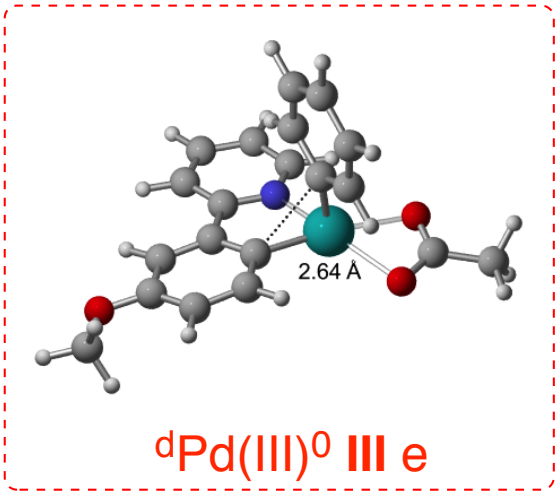

2.24 Å
sTS+ IV-VI c

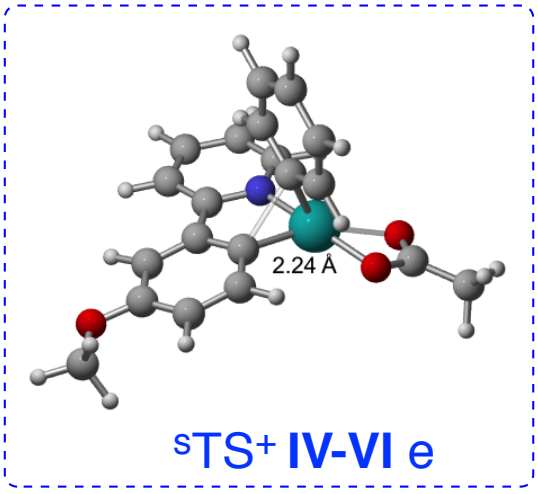

2.22 Å
dTS0 III-V c

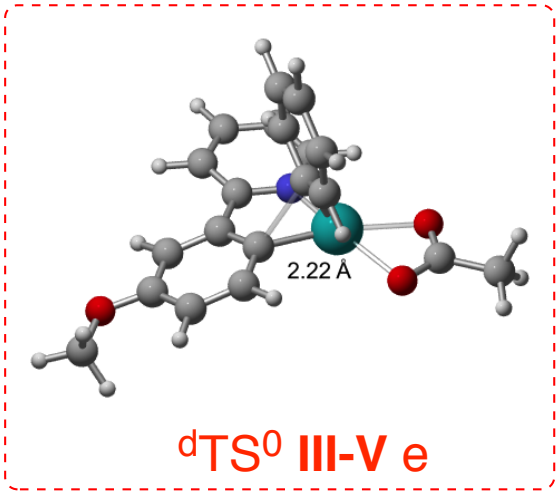

ΔG
ΔH
M06/lacvp(d)
CPCM:
methanol
IV d
+0.0
+0.0
III d
+0.0
+0.0
+5.8
+4.7
TS(IV-VI) d
+3.9
+2.0
TS(III-V) d
-36.1
-36.7
VI d
V d
-39.3
-39.4
Ph
CN
N
Pd
O
O
Pd(III)/Pd(I)
vs
Pd(IV)/Pd(II)
reductive
elimination
CN
N
Ph
Pd
O
O
2.84 Å
sPd(IV)+ IV d
2.64 Å
dPd(III)0 III d
2.22 Å
sTS+ IV-VI d
2.20 Å
dTS0 III-V d

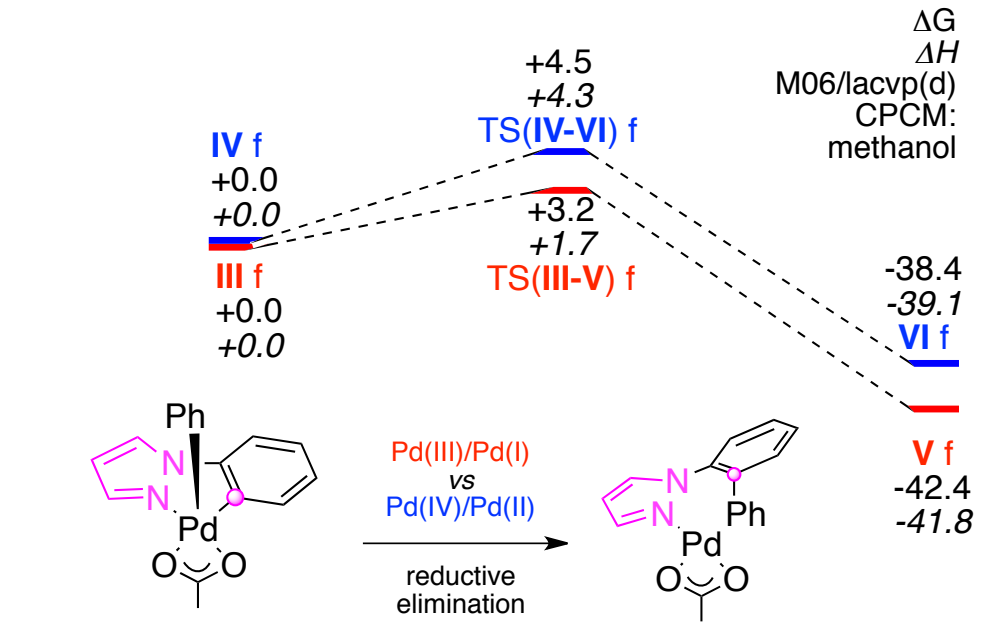

ΔG
ΔH
M06/lacvp(d)
CPCM:
methanol
IV e
+0.0
+0.0
III e
+0.0
+0.0
+4.5
+3.7
TS(IV-VI) e
+3.3
+1.6
TS(III-V) e
-36.6
-37.0
VI e
V e
-40.9
-41.0
Ph
OMe
N
Pd
O
O
Pd(III)/Pd(I)
vs
Pd(IV)/Pd(II)
reductive
elimination
OMe
N
Ph
Pd
O
O

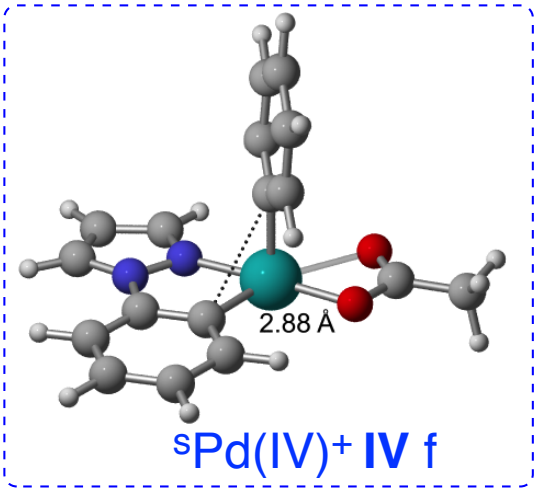

2.84 Å
sPd(IV)+ IV e

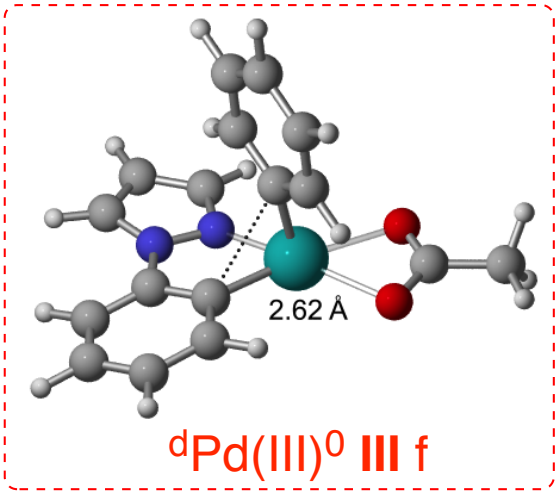

2.64 Å
dPd(III)0 III e

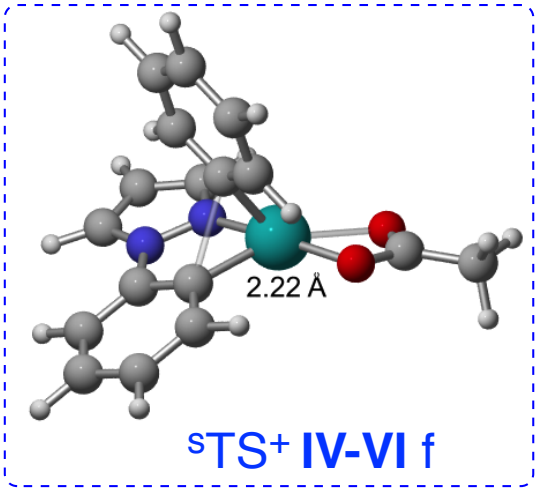

2.24 Å
sTS+ IV-VI e

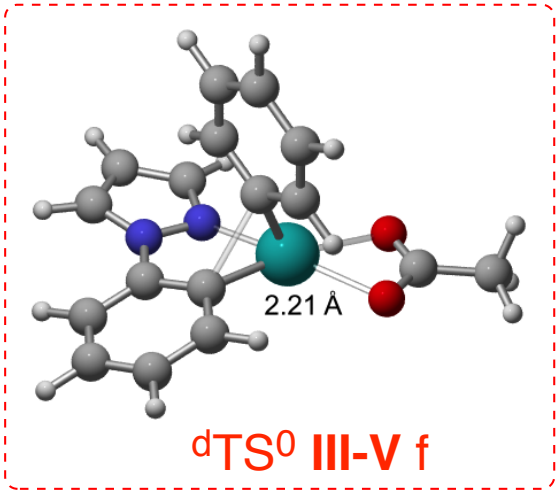

2.22 Å
dTS0 III-V e

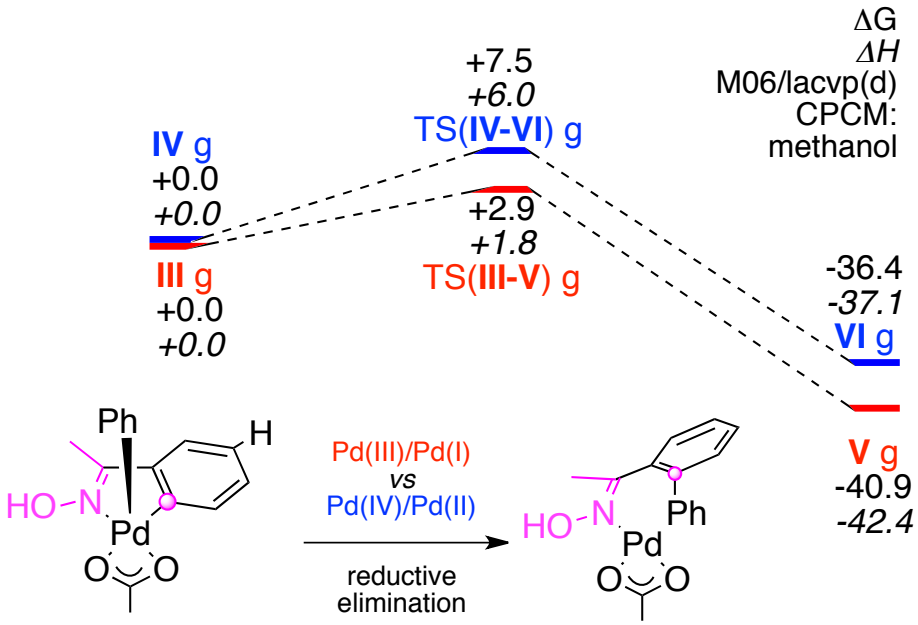


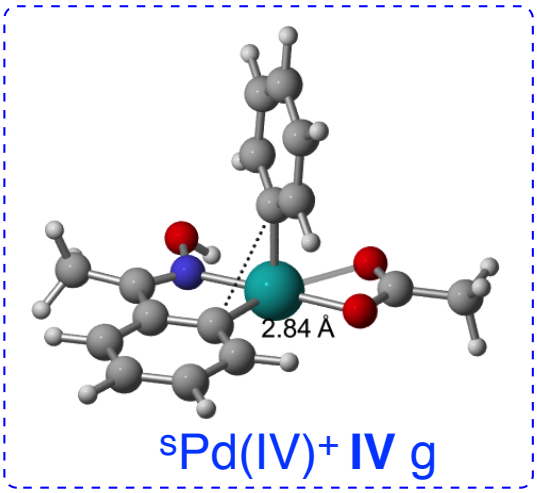


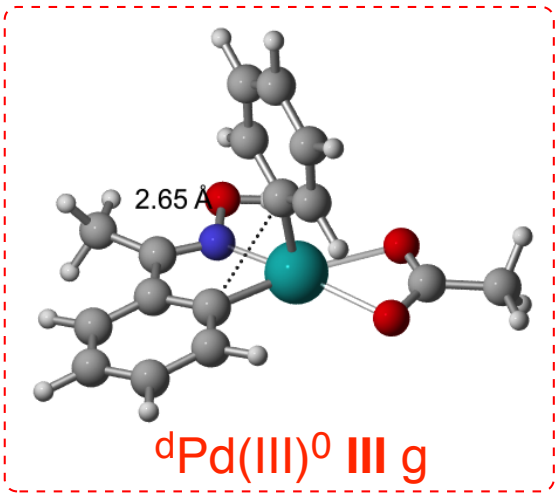


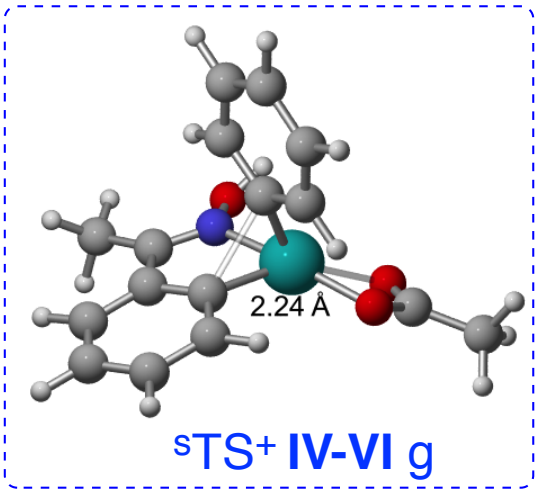


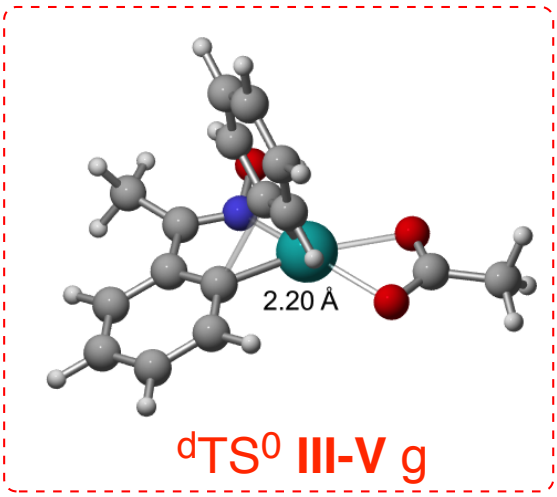












5. XYZ coordinates

Unless otherwise noted, coordinates refers to M06/LACVP(d) ones, optimized using MeOH as an implicit solvent.

$Ru(II)(bpy)_3^{2+}$ **Ired**

61

scf done: -1578.767660

C	2.993941	-0.602824	-0.422835
N	2.490696	0.414407	0.322322
C	3.324785	1.339923	0.818575
C	4.692597	1.303369	0.598752
C	5.218049	0.265617	-0.161807
C	4.359783	-0.695585	-0.676402
Ru	0.419095	0.380723	0.629119
H	4.755156	-1.514000	-1.270852
C	2.001247	-1.560057	-0.930132
N	0.719005	-1.320961	-0.553676
N	0.792574	-0.499141	2.495146
H	5.327101	2.077498	1.019928
H	6.285792	0.203098	-0.354440
H	2.866981	2.134663	1.404345
C	2.317773	-2.647429	-1.740016
C	1.308416	-3.497397	-2.169161
H	3.345412	-2.831299	-2.039236
H	1.545162	-4.349051	-2.801511
C	-0.001134	-3.243024	-1.779316
C	-0.252883	-2.144896	-0.972099
H	-0.822603	-3.881140	-2.091410
H	-1.260812	-1.907017	-0.637622
N	-0.132989	1.391376	-1.119031
C	-1.467567	1.498193	-1.342906
C	-1.952756	2.156339	-2.469727
C	-1.059770	2.709006	-3.376640
C	0.304746	2.590753	-3.140018
C	0.726133	1.923245	-2.000875
C	-2.327681	0.891662	-0.318135
H	-3.022115	2.240621	-2.639801
H	-1.427992	3.226741	-4.258429
H	1.038621	3.007347	-3.823588
H	1.783349	1.809607	-1.769069
C	-3.718885	0.907890	-0.367095
C	-4.446053	0.304244	0.648776
C	-3.766571	-0.305156	1.696875
C	-2.380720	-0.287583	1.689605
N	-1.673260	0.292302	0.709338
H	-4.235179	1.388963	-1.192620
H	-5.532362	0.310621	0.619883
H	-4.294501	-0.790907	2.512215
H	-1.804151	-0.755174	2.485148
C	0.792223	0.348118	3.556330
C	1.014852	-0.122896	4.847439
C	1.242894	-1.476028	5.051775
C	1.245787	-2.334143	3.958393
C	1.017985	-1.805657	2.697525
C	0.531127	1.758030	3.236113
H	1.007744	0.559767	5.692139
H	1.414948	-1.855850	6.055429
H	1.419502	-3.400103	4.072258
H	1.004901	-2.436909	1.811157
C	0.505235	2.776597	4.185263
C	0.255301	4.080674	3.782471
C	0.034293	4.341898	2.435519
C	0.075050	3.286407	1.538581
N	0.319776	2.024532	1.922016
H	0.682198	2.557406	5.234112
H	0.233660	4.883074	4.515178
H	-0.164974	5.346991	2.075824
H	-0.084295	3.442819	0.473522

$Ru(III)(bpy)_3^{3+}$ **Iox**

61

scf done: -1578.555887

C	3.001359	-0.630266	-0.404426
N	2.506736	0.379389	0.357642
C	3.336093	1.280308	0.903434
C	4.706380	1.224706	0.706415
C	5.226968	0.197507	-0.070575
C	4.367647	-0.739587	-0.629766
Ru	0.423044	0.388860	0.621558
H	4.762867	-1.548562	-1.236347
C	2.001407	-1.557327	-0.944202
N	0.715754	-1.287816	-0.599982
N	0.853814	-0.481705	2.480699
H	5.345212	1.976722	1.158331
H	6.297165	0.122106	-0.242069
H	2.881189	2.067935	1.499517
C	2.300535	-2.645051	-1.754913
C	1.270612	-3.458649	-2.209610
H	3.327937	-2.859103	-2.032609
H	1.494711	-4.313295	-2.842025
C	-0.039958	-3.169103	-1.850335
C	-0.279992	-2.068285	-1.044399
H	-0.871857	-3.781082	-2.184292
H	-1.287724	-1.800848	-0.735327
N	-0.126115	1.348885	-1.160490
C	-1.461360	1.492787	-1.363433
C	-1.934722	2.133215	-2.501495
C	-1.028995	2.627322	-3.431591
C	0.333561	2.466750	-3.212787
C	0.748806	1.814940	-2.062968
C	-2.321962	0.934690	-0.314724
H	-3.001660	2.249839	-2.664290
H	-1.389575	3.133104	-4.323065
H	1.071281	2.838633	-3.916721
H	1.803551	1.665282	-1.844608
C	-3.709958	0.987481	-0.337723
C	-4.430339	0.428967	0.710161
C	-3.752029	-0.173028	1.762477
C	-2.367048	-0.192077	1.735501
N	-1.672270	0.344009	0.721891
H	-4.229157	1.462080	-1.164632
H	-5.516063	0.465892	0.701854
H	-4.278474	-0.624117	2.597592
H	-1.790731	-0.655745	2.532559
C	0.825937	0.355909	3.549685
C	1.095369	-0.120477	4.826361
C	1.395458	-1.464849	5.002352
C	1.426616	-2.308642	3.898987
C	1.155173	-1.777903	2.648411
C	0.492685	1.751097	3.247151
H	1.071306	0.548326	5.681051
H	1.604122	-1.848935	5.997056
H	1.657763	-3.364747	3.995043
H	1.163107	-2.398154	1.755529
C	0.416802	2.759071	4.200331
C	0.081951	4.047147	3.803661
C	-0.174883	4.304946	2.463008

C	-0.085190	3.261025	1.556861
N	0.247259	2.019430	1.938870
H	0.617426	2.546533	5.245843
H	0.019003	4.842214	4.541593
H	-0.441641	5.297535	2.114212
H	-0.270265	3.415006	0.496390

MeOH

6

scf done: -115.646183

C	0.334954	0.619616	3.628860
O	0.816267	-0.316886	2.694140
H	0.431401	-1.175684	2.913126
H	0.629318	0.376859	4.661981
H	0.773854	1.589774	3.371942
H	-0.760903	0.724258	3.598250

Phenyldiazonium

13

scf done: -340.662853

C	-0.002838	-2.558683	4.475422
C	-0.397534	-1.761601	3.418425
C	0.620744	-1.129550	2.687721
C	1.991925	-1.256997	2.960614
C	2.343202	-2.062976	4.026041
C	1.354125	-2.706295	4.774378
H	2.728641	-0.738853	2.354177
H	3.391863	-2.192401	4.276810
H	1.647148	-3.335786	5.610986
H	-0.754003	-3.068910	5.070983
H	-1.440763	-1.618927	3.152729
N	0.251239	-0.332197	1.634250
N	-0.048406	0.314471	0.779866

Phenyldiazoyl

13

scf done: -340.828034

C	0.003493	-2.513360	4.419122
C	-0.313560	-1.696251	3.343702
C	0.722136	-1.083773	2.639550
C	2.054439	-1.271464	2.986150
C	2.361613	-2.092682	4.065900
C	1.337881	-2.711450	4.778869
H	2.828607	-0.772120	2.406751
H	3.399700	-2.250330	4.350117
H	1.579401	-3.353052	5.624018
H	-0.790691	-3.000879	4.980979
H	-1.344523	-1.523211	3.039523
N	0.462260	-0.217371	1.503264
N	-0.615412	0.037238	1.084457

N_2

2

scf done: -109.455402

N	0.348257	-0.186478	1.453755
N	-0.700740	-0.016431	1.151201

Phenyl

11

scf done: -231.367337

C	-0.292954	-1.672289	3.312954
C	0.773529	-1.099138	2.661313

C	2.098392	-1.270226	2.986503
C	2.375035	-2.101380	4.078162
C	1.332979	-2.709519	4.776714
C	0.006811	-2.499569	4.401435
H	2.902975	-0.788139	2.432693
H	3.408095	-2.271833	4.379641
H	1.557855	-3.353801	5.624881
H	-0.800160	-2.980168	4.953702
H	-1.324730	-1.499728	3.009454

Pd(II) Complex II

28

scf done: -833.521090

C	4.196628	-0.507725	-0.777806
C	2.847485	-0.538794	-0.434738
N	2.281799	0.525879	0.191555
C	3.007348	1.610609	0.482702
C	4.353610	1.698002	0.164634
C	4.951975	0.616902	-0.475695
C	1.911073	-1.629637	-0.672220
C	2.223525	-2.839161	-1.298373
C	1.238746	-3.806715	-1.462764
C	-0.056990	-3.573492	-1.004721
C	-0.382948	-2.368085	-0.378322
C	0.598494	-1.400979	-0.215250
Pd	0.275965	0.336928	0.647721
O	-0.751035	2.098518	1.724086
C	-1.793806	1.396575	1.674105
C	-3.100931	1.910194	2.195848
O	-1.766473	0.229740	1.145726
H	4.651522	-1.359536	-1.277109
H	4.914093	2.593259	0.416882
H	6.006538	0.649257	-0.739540
H	2.479254	2.419558	0.984986
H	3.233739	-3.030280	-1.659980
H	1.482403	-4.748138	-1.951007
H	-0.823556	-4.336122	-1.135842
H	-1.396322	-2.188525	-0.020735
H	-3.718091	1.089801	2.574615
H	-2.936992	2.655504	2.979597
H	-3.649446	2.392273	1.376619

Pd(III) Complex III a

39

scf done: -1064.919129

Pd	0.124460	0.322269	0.411977
C	0.699321	-1.341193	-0.543635
C	2.084631	-1.534359	-0.695834
C	2.978640	-0.450028	-0.273904
N	2.368464	0.570626	0.366913
O	-0.853849	2.026855	1.528645
C	-1.947047	1.398676	1.675350
O	-2.103055	0.220483	1.247713
C	-0.387147	0.872980	-1.485829
C	-1.726885	0.802909	-1.851745
C	0.564477	1.429911	-2.332069
C	0.157283	1.953168	-3.560767
C	-1.182110	1.903632	-3.937181
C	-2.120293	1.329313	-3.083619
C	4.354952	-0.407861	-0.499870

C	5.083761	0.688342	-0.059256
C	4.434562	1.731966	0.593791
C	3.063452	1.630074	0.781783
C	-0.201129	-2.326590	-0.921785
C	0.270905	-3.535550	-1.434532
C	1.640783	-3.743801	-1.582573
C	2.541444	-2.750896	-1.216737
C	-3.078735	2.092373	2.384888
H	-2.461356	0.363392	-1.177953
H	4.851389	-1.219865	-1.025352
H	4.973484	2.605950	0.948276
H	6.156910	0.730671	-0.231696
H	2.493943	2.412916	1.282417
H	3.610216	-2.933934	-1.324703
H	2.010131	-4.685713	-1.983263
H	-0.434280	-4.312532	-1.725864
H	-1.273612	-2.154681	-0.820198
H	-3.170107	1.287941	-3.372184
H	-1.494993	2.310237	-4.897423
H	0.897815	2.395535	-4.226239
H	1.616557	1.467419	-2.050688
H	-3.985460	1.481123	2.384017
H	-2.787943	2.306019	3.420502
H	-3.283718	3.055522	1.903137

TS (III-V) a

39

scf done: -1064.915796

C	-0.018446	-0.045881	0.173342
C	-0.077015	0.120916	2.376661
Pd	1.686572	-0.035316	1.287767
N	1.660809	2.077927	0.516257
C	0.563222	2.318822	-0.233048
C	-0.223112	1.129646	-0.577499
O	2.330371	-2.192434	1.930214
C	3.357865	-1.702059	2.480293
O	3.603611	-0.458091	2.446762
C	-1.122706	1.104575	-1.648480
C	-1.798762	-0.063852	-1.977016
C	-1.573805	-1.226704	-1.242755
C	-0.691371	-1.215222	-0.164751
C	2.436066	3.084143	0.924030
C	2.166924	4.405200	0.594654
C	1.041147	4.672038	-0.179027
C	0.230292	3.624792	-0.594889
C	-0.552435	1.366271	2.781042
C	-1.420868	1.447264	3.869682
C	-1.817901	0.296158	4.543400
C	-1.340569	-0.944681	4.127834
C	-0.474385	-1.038844	3.040308
C	4.306423	-2.606061	3.219493
H	-0.089143	-2.009070	2.729664
H	-0.668430	3.821131	-1.174461
H	2.821966	5.199833	0.940385
H	0.788561	5.695266	-0.448194
H	3.298695	2.810384	1.531243
H	-1.270468	1.998146	-2.254311
H	-2.491091	-0.070877	-2.816205
H	-2.094998	-2.146478	-1.503181

H	-0.539938	-2.120918	0.422339
H	-1.639429	-1.850844	4.653353
H	-2.498017	0.364872	5.390465
H	-1.787421	2.422239	4.188338
H	-0.254436	2.278266	2.264780
H	4.112963	-3.658177	2.991513
H	5.343203	-2.354109	2.971476
H	4.183199	-2.452251	4.298969

V a

39

scf done: -1064.985473

C	-1.109783	0.107415	0.369606
C	-1.063590	0.233858	1.846356
Pd	1.576525	-0.089165	2.007913
N	1.334982	1.819159	0.967155
C	0.422631	2.099610	0.013405
C	-0.453234	1.015323	-0.485772
O	2.445712	-1.887867	2.997953
C	3.636019	-1.534656	2.734140
O	3.890708	-0.471584	2.101890
C	-0.593895	0.873212	-1.869852
C	-1.351694	-0.155837	-2.416003
C	-1.984724	-1.062651	-1.573262
C	-1.864008	-0.924459	-0.194844
C	2.164411	2.786103	1.384500
C	2.128681	4.080107	0.887792
C	1.187205	4.382529	-0.088617
C	0.330312	3.383685	-0.528450
C	-1.440698	1.430182	2.483079
C	-1.466202	1.517530	3.865599
C	-1.114616	0.415277	4.651111
C	-0.752561	-0.776574	4.042017
C	-0.732169	-0.877175	2.644043
C	4.777813	-2.394017	3.206652
H	-0.522010	-1.837123	2.170244
H	-0.425906	3.588485	-1.282761
H	2.823645	4.825761	1.263533
H	1.116693	5.386117	-0.502122
H	2.889948	2.492940	2.142689
H	-0.068542	1.564633	-2.527851
H	-1.437716	-0.252454	-3.496219
H	-2.580953	-1.874019	-1.986111
H	-2.385355	-1.614168	0.468379
H	-0.485569	-1.645328	4.641013
H	-1.135952	0.490431	5.736487
H	-1.770465	2.448476	4.340729
H	-1.728303	2.288741	1.876080
H	4.425077	-3.364845	3.566700
H	5.503369	-2.538110	2.398473
H	5.301356	-1.883522	4.024771

IV a

39

scf done: -1064.754227

C	2.277450	-2.891610	-1.203223
C	1.978393	-1.629043	-0.684241
C	0.669286	-1.402847	-0.248286
C	-0.328412	-2.350121	-0.284587
C	0.001310	-3.607749	-0.801487

C	1.289007	-3.867864	-1.263537
Pd	0.338608	0.415127	0.510405
C	-0.162712	1.097260	-1.333351
C	-1.168197	0.473937	-2.046349
C	-1.545703	1.064173	-3.254500
C	-0.934821	2.233467	-3.695199
C	0.062639	2.831681	-2.933407
C	0.469354	2.262193	-1.724003
C	2.918452	-0.534626	-0.491681
N	2.367367	0.549766	0.108480
C	3.102888	1.620531	0.427635
C	4.455569	1.674537	0.135942
C	5.038713	0.585091	-0.504740
C	4.270314	-0.528690	-0.816076
O	-0.907455	2.217177	1.459329
C	-1.854458	1.407333	1.415061
C	-3.215522	1.707189	1.948191
O	-1.665023	0.228805	0.906858
H	-1.665497	-0.423127	-1.692352
H	4.718150	-1.390378	-1.303515
H	5.031318	2.554995	0.403381
H	6.095791	0.600124	-0.757815
H	2.579798	2.438784	0.921699
H	3.283852	-3.115644	-1.553056
H	1.527847	-4.846713	-1.672358
H	-0.762633	-4.381076	-0.846447
H	-1.334474	-2.132485	0.070897
H	-2.334406	0.596478	-3.840544
H	-1.243367	2.685221	-4.635366
H	0.538615	3.752148	-3.265419
H	1.238391	2.745213	-1.127817
H	-3.984985	1.326069	1.269560
H	-3.342661	1.199861	2.912388
H	-3.337261	2.783159	2.096868

TS (IV-VI) a

39

scf done: -1064.746516

C	-0.348081	-0.058804	0.184860
C	-0.187993	-0.032134	2.405105
Pd	1.471969	0.034896	1.213778
N	1.428894	-1.974307	1.614604
C	0.508981	-2.368945	2.528627
C	-0.312805	-1.279416	3.039067
O	1.792837	2.048354	0.896704
C	3.051140	1.901139	0.664116
O	3.531577	0.734870	0.716579
C	-0.829862	1.103012	2.862414
C	-1.650700	0.988070	3.985506
C	-1.816765	-0.241383	4.617633
C	-1.147789	-1.368395	4.154735
C	-0.834003	-1.271632	-0.282988
C	-1.775348	-1.241920	-1.312519
C	-2.215138	-0.032745	-1.838700
C	-1.710179	1.165209	-1.342290
C	-0.768255	1.165452	-0.315219
C	2.282023	-2.833173	1.049731
C	2.248676	-4.180604	1.372509
C	1.307652	-4.618231	2.299851

C	0.432713	-3.710753	2.884032
C	3.883770	3.088398	0.342950
H	-0.368652	2.103556	0.060734
H	-0.306137	-4.042257	3.608520
H	2.944480	-4.866145	0.899326
H	1.254199	-5.669953	2.569049
H	2.986092	-2.418381	0.330786
H	-1.253095	-2.314936	4.681887
H	-2.463696	-0.320011	5.487772
H	-2.166578	1.870105	4.358342
H	-0.714761	2.062455	2.362861
H	-2.046305	2.117156	-1.748410
H	-2.952998	-0.023075	-2.637769
H	-2.161600	-2.184468	-1.695427
H	-0.509581	-2.229304	0.111963
H	3.278748	3.998622	0.325789
H	4.680007	3.188407	1.089213
H	4.362903	2.943294	-0.631948

VI a

39

scf done: -1064.813990

C	-0.980237	0.110371	0.912662
C	-1.217167	-0.206442	2.344622
Pd	1.306945	-0.115111	0.552785
N	1.353620	-1.824757	1.649436
C	0.425221	-2.189598	2.560642
C	-0.574819	-1.231730	3.082873
O	1.789808	1.561126	-0.602873
C	3.024456	1.450644	-0.296296
O	3.350043	0.482235	0.465277
C	-2.191850	0.561346	2.997007
C	-2.507621	0.380734	4.335695
C	-1.838038	-0.587167	5.070874
C	-0.892618	-1.381329	4.440455
C	-0.766279	-0.895598	-0.079763
C	-0.830453	-0.582075	-1.456485
C	-1.080570	0.709984	-1.859382
C	-1.254752	1.722890	-0.896074
C	-1.201054	1.439130	0.448633
C	2.313940	-2.674556	1.246538
C	2.395468	-3.968013	1.725209
C	1.424230	-4.393094	2.624010
C	0.443589	-3.505861	3.036862
C	4.030437	2.425483	-0.783601
H	-1.319888	2.239243	1.175289
H	-0.335782	-3.833870	3.718062
H	3.190097	-4.622589	1.381346
H	1.424981	-5.413571	2.998503
H	3.025951	-2.284667	0.521495
H	-0.356820	-2.123108	5.028190
H	-2.048332	-0.731247	6.127892
H	-3.273573	0.999669	4.797010
H	-2.746204	1.303974	2.428884
H	-1.429961	2.746537	-1.218710
H	-1.140179	0.953082	-2.917427
H	-0.704821	-1.380658	-2.183228
H	-0.752287	-1.944768	0.209818
H	3.688080	2.898286	-1.708498

H	4.168509	3.205894	-0.024987
H	4.994268	1.931213	-0.938979

IV a-MeOH

45

scf done: -1180.425908

C	4.294312	-0.555880	-0.884366
C	2.942978	-0.565313	-0.554947
N	2.394069	0.516913	0.050107
C	3.126365	1.591612	0.363241
C	4.477316	1.649102	0.064744
C	5.060944	0.559418	-0.576037
C	2.002708	-1.658650	-0.750568
C	2.298255	-2.920059	-1.276261
C	1.308256	-3.894158	-1.337121
C	0.022619	-3.634083	-0.868365
C	-0.303375	-2.378674	-0.343833
C	0.694944	-1.432435	-0.311905
Pd	0.374372	0.368989	0.484278
O	-1.627055	0.187822	0.913209
C	-1.771234	1.336974	1.490304
C	-3.100472	1.641059	2.096459
C	-0.137108	1.082355	-1.340408
C	-1.150243	0.476366	-2.065606
C	-1.538318	1.067760	-3.268469
C	-0.928575	2.237573	-3.710868
C	0.075078	2.829487	-2.951783
C	0.485626	2.250804	-1.748990
O	-0.803535	2.126021	1.541263
H	-1.647222	-0.423881	-1.715596
H	4.741945	-1.416484	-1.373973
H	5.051867	2.531586	0.328085
H	6.117250	0.576534	-0.832113
H	2.602715	2.408890	0.860155
H	3.303241	-3.144057	-1.630198
H	1.544250	-4.872457	-1.748860
H	-0.742163	-4.406736	-0.912044
H	-1.306062	-2.161387	0.021567
H	-2.331102	0.603914	-3.852632
H	-1.241391	2.692669	-4.648348
H	0.550835	3.749853	-3.285349
H	1.263681	2.731190	-1.160326
H	-3.908826	1.274991	1.456133
H	-3.179344	1.125489	3.061503
H	-3.204329	2.716313	2.263917
O	0.794816	-0.400818	2.616008
H	1.222540	-1.272117	2.600992
C	1.523741	0.463480	3.489656
H	1.495849	0.075662	4.513614
H	2.566340	0.576455	3.165760
H	1.022280	1.434166	3.454027

TS (IV-VI) a-MeOH

45

scf done: -1180.412053

C	-0.186456	-0.104712	0.361797
C	-0.219047	-0.183316	2.444480
H	4.772494	0.060653	2.567955
N	2.070942	-1.365123	1.779124
O	0.869858	2.511999	1.300743

C	1.784846	2.967027	0.496313
O	2.663934	2.215370	0.048048
O	3.144877	1.353815	2.844915
C	4.509442	1.123728	2.492279
C	3.186127	-1.851813	1.226693
C	3.581170	-3.159716	1.457855
C	2.784817	-3.958028	2.274824
C	1.622986	-3.440798	2.832891
C	1.271702	-2.120362	2.569604
C	-1.222863	0.635397	2.936609
C	-1.987919	0.185325	4.010836
C	-1.742758	-1.061224	4.583229
C	-0.703797	-1.854474	4.113104
C	0.086991	-1.419822	3.047126
C	-0.130978	-1.361774	-0.247011
C	-0.923176	-1.614764	-1.363879
C	-1.760215	-0.630772	-1.877518
C	-1.801436	0.622087	-1.270991
C	-1.017066	0.893038	-0.156097
Pd	1.450166	0.567701	1.488328
C	1.682624	4.415903	0.139579
H	-1.051591	1.879290	0.297163
H	0.984445	-4.059467	3.457624
H	4.486609	-3.541064	0.996407
H	3.063049	-4.990714	2.469476
H	3.746265	-1.174481	0.583125
H	-0.480811	-2.799983	4.604688
H	-2.349819	-1.405371	5.416860
H	-2.784534	0.817915	4.396404
H	-1.420850	1.604684	2.485433
H	-2.447658	1.403557	-1.665891
H	-2.376660	-0.838485	-2.749412
H	-0.876502	-2.597135	-1.829527
H	0.503443	-2.160071	0.124898
H	0.899990	4.544327	-0.618548
H	1.399697	5.013059	1.012308
H	2.631541	4.771315	-0.271321
H	2.990826	1.029581	3.746658
H	5.168623	1.710559	3.141563
H	4.616579	1.460282	1.458431

VI a-MeOH

45

scf done: -1180.472066

C	-0.781002	-0.287655	0.983787
C	-0.696710	-0.700258	2.410589
H	2.462796	0.529434	3.963994
N	2.127611	-1.356591	1.295462
O	1.127024	2.086320	-0.651678
C	2.366765	2.373082	-0.529948
O	3.116107	1.512869	0.032571
O	1.412417	1.809042	2.678675
C	2.554221	1.502854	3.456474
C	3.249387	-1.819403	0.720038
C	3.827572	-3.015489	1.100999
C	3.194889	-3.759309	2.090426
C	2.041582	-3.267224	2.680150
C	1.514824	-2.029983	2.291890
C	-1.755120	-0.294326	3.236456

C	-1.785926	-0.566907	4.597065
C	-0.739037	-1.267593	5.177950
C	0.299310	-1.716531	4.375762
C	0.341899	-1.466771	2.996551
C	-0.392969	-1.128603	-0.103942
C	-0.753712	-0.810308	-1.432564
C	-1.473332	0.331937	-1.700486
C	-1.825728	1.198075	-0.647259
C	-1.486280	0.905754	0.652653
Pd	1.381467	0.289401	0.373975
C	2.898630	3.675361	-1.003822
H	-1.746485	1.604478	1.444451
H	1.524472	-3.848024	3.438193
H	4.738682	-3.354439	0.618088
H	3.593688	-4.721799	2.401009
H	3.677960	-1.195885	-0.062162
H	1.127785	-2.246324	4.840987
H	-0.726489	-1.471329	6.245837
H	-2.629063	-0.228832	5.195014
H	-2.598940	0.228723	2.793488
H	-2.369037	2.114944	-0.864008
H	-1.763610	0.571479	-2.720608
H	-0.478032	-1.497754	-2.228348
H	0.012887	-2.118582	0.094619
H	2.227947	4.116342	-1.746750
H	2.975989	4.361152	-0.151070
H	3.901020	3.545325	-1.423615
H	0.636487	1.774874	3.257186
H	2.754762	2.275052	4.212779
H	3.403198	1.456559	2.766313

BF4-

5

scf done: -424.465828

F	0.754420	-0.355913	2.611814
B	2.141186	-0.392406	2.784199
F	2.438687	-0.862084	4.067313
F	2.707378	-1.245331	1.832400
F	2.665390	0.892889	2.625811

IV a-BF4

44

scf done: -1489.254186

C	4.286946	-0.641431	-0.871420
C	2.924634	-0.611630	-0.599297
N	2.375882	0.495738	-0.046015
C	3.118147	1.552617	0.291589
C	4.480809	1.575167	0.044625
C	5.065772	0.462147	-0.550697
C	1.973385	-1.694934	-0.793910
C	2.257802	-2.964053	-1.307308
C	1.256947	-3.926621	-1.370198
C	-0.029802	-3.646619	-0.915879
C	-0.343057	-2.384403	-0.401072
C	0.665781	-1.449581	-0.368976
Pd	0.370291	0.349048	0.429439
O	-1.618242	0.153496	0.901086
C	-1.774308	1.313655	1.455444
C	-3.103390	1.602201	2.072382
C	-0.154297	1.099694	-1.369284

C	-1.129524	0.483416	-2.135158
C	-1.524040	1.111203	-3.317987
C	-0.957026	2.322597	-3.700392
C	0.008786	2.922737	-2.899114
C	0.423371	2.310837	-1.714965
O	-0.825438	2.122433	1.473699
H	-1.590229	-0.453201	-1.834554
H	4.734536	-1.525434	-1.317575
H	5.065222	2.447453	0.320400
H	6.132914	0.449380	-0.758305
H	2.600636	2.374794	0.782045
H	3.263374	-3.203004	-1.649900
H	1.484445	-4.911020	-1.772355
H	-0.804231	-4.409646	-0.961327
H	-1.344404	-2.152806	-0.041143
H	-2.287450	0.640947	-3.935200
H	-1.273142	2.803964	-4.623516
H	0.450792	3.875449	-3.184854
H	1.167951	2.796958	-1.088941
H	-3.911913	1.262701	1.417183
H	-3.187943	1.051072	3.016826
H	-3.203994	2.671393	2.276257
F	0.822075	-0.478850	2.507598
B	2.062592	-0.049868	3.139039
F	1.998840	-0.408503	4.465402
F	3.103290	-0.681768	2.480506
F	2.139795	1.327774	2.984697

TS IV a-BF4

44

scf done: -1489.238354

C	-0.375380	-0.019392	0.279251
C	-0.369701	-0.073793	2.341058
Pd	1.434651	-0.010481	1.362427
N	1.272524	-2.030476	1.626265
O	3.332699	0.885495	0.215034
O	1.693195	2.003422	1.161166
F	2.962101	0.190420	3.157732
C	-0.532253	-1.329064	2.962367
C	0.296392	-2.424329	2.475840
C	2.139249	-2.890869	1.091785
C	2.059499	-4.244536	1.380029
C	1.064671	-4.682135	2.248076
C	0.173620	-3.770299	2.799838
C	-0.984463	1.063681	2.846636
C	-1.833860	0.940560	3.943047
C	-2.054900	-0.303436	4.531265
C	-1.398365	-1.430068	4.052469
C	-0.841709	-1.197004	-0.308535
C	-1.683575	-1.116508	-1.414971
C	-2.052693	0.117719	-1.938353
C	-1.571481	1.284816	-1.351262
C	-0.730824	1.225003	-0.245525
C	2.831761	1.979147	0.539238
C	3.485041	3.294054	0.272607
B	3.739874	-0.981546	3.479937
F	4.290523	-1.451864	2.293769
F	4.720129	-0.612220	4.377622
F	2.880706	-1.924922	4.026391

H	-0.349730	2.143906	0.190580
H	-0.611505	-4.100331	3.474811
H	2.762610	-4.935369	0.925262
H	0.977464	-5.738152	2.491398
H	2.888424	-2.477942	0.421481
H	-1.530837	-2.387493	4.553429
H	-2.726105	-0.391351	5.382068
H	-2.329197	1.826388	4.334658
H	-0.823666	2.035184	2.384785
H	-1.846033	2.257715	-1.754473
H	-2.709468	0.170041	-2.804002
H	-2.049195	-2.037621	-1.864722
H	-0.578892	-2.177822	0.075327
H	2.753895	4.014587	-0.108670
H	3.886119	3.694997	1.211430
H	4.303943	3.173513	-0.441677

VI a-BF4

44

scf done: -1489.296253

C	-1.405508	1.039861	0.807632
C	-0.722132	-0.187148	1.066984
C	-0.376130	-0.987547	-0.067310
C	-0.765014	-0.606479	-1.367463
C	-1.466727	0.562902	-1.562691
C	-1.769643	1.396488	-0.468090
C	-0.719441	-0.715276	2.455735
C	-1.851368	-0.413205	3.227161
C	-1.989691	-0.837870	4.539765
C	-0.973040	-1.579100	5.126586
C	0.142304	-1.910280	4.374888
C	0.287718	-1.517725	3.037051
Pd	1.416192	0.407033	0.490319
O	3.178746	1.461016	-0.296432
C	2.387969	2.299175	-0.817866
C	2.879919	3.490886	-1.557004
C	1.522291	-1.977073	2.368717
N	2.146157	-1.233887	1.432745
C	3.324584	-1.608012	0.908823
C	3.947265	-2.787967	1.265276
C	3.297583	-3.614627	2.175139
C	2.090877	-3.209048	2.719114
O	1.129835	2.105887	-0.665507
F	1.547484	1.706646	2.790198
B	2.663678	1.364408	3.597786
F	2.366330	0.212044	4.322052
H	-1.635844	1.695659	1.644536
H	1.562604	-3.857750	3.410789
H	4.901869	-3.052607	0.821449
H	3.725041	-4.573516	2.457790
H	3.759245	-0.922909	0.182833
H	0.954187	-2.449546	4.856626
H	-1.040719	-1.896755	6.164463
H	-2.886805	-0.581692	5.099092
H	-2.665432	0.144890	2.770543
H	-2.294124	2.334600	-0.634402
H	-1.781699	0.850172	-2.563315
H	-0.524894	-1.260405	-2.202155
H	0.032538	-1.985513	0.084853

H	2.119997	3.855232	-2.254334
H	3.102388	4.289415	-0.838435
H	3.804147	3.249776	-2.091000
F	2.924603	2.423259	4.460657
F	3.763801	1.131699	2.773387

III a-Bimet

67

scf done: -1898.494378

C	1.382324	-0.619056	2.916180
C	0.207925	-0.609489	2.169115
C	-0.977403	-1.104235	2.705903
C	-0.989496	-1.583221	4.017097
C	0.176115	-1.582022	4.779034
C	1.359607	-1.100119	4.227185
Pd	0.132139	0.310937	0.329576
O	-2.211770	0.117938	0.170212
C	-2.909312	0.909403	-0.512383
C	-4.402536	0.915121	-0.261303
O	-2.497500	1.673869	-1.434891
Pd	-0.428721	1.574554	-2.165701
O	0.030451	3.328230	-1.131021
C	-0.011669	3.410104	0.139519
C	0.165134	4.796725	0.712253
N	-0.719883	-0.153889	-3.249291
C	0.398042	-0.662967	-3.827988
C	0.332879	-1.879496	-4.505017
C	-0.878084	-2.549699	-4.595972
C	-2.015589	-1.999131	-4.012248
C	-1.890085	-0.795016	-3.338617
C	1.579024	0.177172	-3.667975
C	1.392886	1.367612	-2.932882
C	2.460332	2.235156	-2.740156
C	3.715974	1.916287	-3.260498
C	3.907560	0.733543	-3.973934
C	2.841544	-0.132378	-4.184336
C	0.634463	-1.512181	-0.314038
C	1.980219	-1.659548	-0.705635
C	2.357554	-2.823449	-1.388283
C	1.426918	-3.817709	-1.661045
C	0.103605	-3.665485	-1.250739
C	-0.292083	-2.513450	-0.570250
C	2.923591	-0.572103	-0.413669
N	2.370266	0.547035	0.094091
C	3.120201	1.593892	0.430832
C	4.497702	1.596121	0.269074
C	5.091271	0.457644	-0.269163
C	4.305168	-0.632523	-0.613339
O	-0.145348	2.465918	0.953543
H	4.764885	-1.530141	-1.020060
H	5.084161	2.465677	0.553028
H	6.168509	0.416147	-0.416214
H	2.585834	2.452031	0.841004
H	3.384226	-2.944467	-1.733951
H	1.732941	-4.712108	-2.200587
H	-0.628649	-4.442987	-1.466306
H	-1.329404	-2.382997	-0.262824
H	-4.634165	0.579611	0.753854
H	-4.825728	1.909343	-0.436421

H	-4.880637	0.222084	-0.966964
H	0.022351	5.570813	-0.046405
H	-0.531574	4.951050	1.542612
H	1.181268	4.885543	1.118737
H	2.999654	-1.056152	-4.741307
H	4.891849	0.486697	-4.367583
H	4.555283	2.590950	-3.092366
H	2.319273	3.149488	-2.164110
H	1.228601	-2.296259	-4.959427
H	-0.935117	-3.499043	-5.124008
H	-2.982852	-2.489528	-4.071321
H	-2.735532	-0.304258	-2.860897
H	-1.888880	-1.097189	2.109432
H	-1.919663	-1.961956	4.440892
H	0.162728	-1.958821	5.800603
H	2.277519	-1.099141	4.814785
H	2.317979	-0.250336	2.496179

TS III a-Bimet

67

scf done: -1898.489552

C	-0.070241	-0.116948	0.036193
C	0.022341	-0.045861	2.222618
Pd	1.735974	-0.061207	1.113799
N	1.546748	2.135965	1.534129
O	3.733785	0.331007	0.055920
O	2.178432	-2.336876	0.890775
Pd	3.687146	-0.559262	3.196197
N	2.432298	-1.361343	4.613705
C	3.301924	1.086622	4.234069
O	5.013499	0.427002	1.918248
O	4.114754	-2.381847	2.047922
C	3.283521	-2.846067	1.214290
C	3.676628	-4.132798	0.518967
C	-0.427804	-1.366614	-0.470427
C	-1.303749	-1.451864	-1.550770
C	-1.839747	-0.297589	-2.116964
C	-1.489663	0.946088	-1.599684
C	-0.609921	1.042179	-0.521471
C	-0.583668	-1.193954	2.726218
C	-1.404471	-1.117801	3.848059
C	-1.635288	0.109606	4.468428
C	-1.032960	1.256724	3.971165
C	-0.200336	1.199676	2.847227
C	2.241981	3.130246	0.984889
C	1.931677	4.462391	1.220657
C	0.850362	4.745333	2.051165
C	0.124046	3.704914	2.613883
C	0.496845	2.386972	2.340273
C	2.113454	-2.658049	4.683984
C	1.250535	-3.147410	5.651567
C	0.707441	-2.247951	6.565154
C	1.036818	-0.902931	6.484486
C	1.911053	-0.465592	5.490587
C	3.809359	2.355544	3.979599
C	3.404606	3.436679	4.764235
C	2.481368	3.259417	5.794639
C	1.967030	1.995162	6.055237
C	2.376849	0.902224	5.285304

C	4.790113	0.593143	0.675450
C	5.924780	1.232647	-0.091416
H	-0.738260	3.913587	3.242561
H	2.517942	5.252946	0.760397
H	0.566923	5.776267	2.252525
H	3.070043	2.830139	0.341225
H	-1.185288	2.207821	4.481073
H	-2.272553	0.167509	5.348758
H	-1.860301	-2.024930	4.243193
H	-0.415011	-2.154793	2.240381
H	4.216459	-3.883618	-0.403973
H	4.341274	-4.734994	1.146043
H	2.791660	-4.713330	0.240548
H	6.893730	0.868085	0.263537
H	5.822384	1.054165	-1.165384
H	5.895744	2.316926	0.082823
H	1.243494	1.863650	6.860412
H	2.164429	4.109142	6.396491
H	3.802786	4.430217	4.558487
H	4.510813	2.507265	3.159468
H	0.618504	-0.189307	7.190557
H	0.027078	-2.595136	7.339755
H	1.016053	-4.207324	5.685126
H	2.583340	-3.301630	3.942610
H	-0.002880	-2.270834	-0.037692
H	-1.568934	-2.430796	-1.949050
H	-2.529624	-0.367571	-2.956221
H	-1.903385	1.856263	-2.032712
H	-0.356293	2.026430	-0.129943

V a-Bimet

67

scf done: -1898.557182

C	-0.730784	-1.253290	0.642583
C	-1.111383	0.020580	1.094376
C	-1.604449	0.947599	0.164675
C	-1.705310	0.614596	-1.178877
C	-1.312471	-0.649801	-1.623132
C	-0.827301	-1.580472	-0.713255
C	-1.048973	0.344230	2.538688
C	-0.390194	1.488182	3.033140
C	-0.444711	1.762253	4.403883
C	-1.118516	0.924286	5.283223
C	-1.744093	-0.219441	4.799901
C	-1.708175	-0.498949	3.438573
C	0.387351	2.417298	2.180549
N	1.236634	1.932321	1.250057
C	1.952476	2.793774	0.510546
C	1.871843	4.170215	0.656451
C	1.000602	4.680675	1.611047
C	0.251777	3.795745	2.371179
Pd	1.678250	-0.191059	0.885072
O	2.234155	-2.268999	0.503214
C	3.282087	-2.772681	0.992419
C	3.721760	-4.114647	0.447320
Pd	3.539691	-0.484146	3.104511
O	3.991084	-2.294708	1.920238
O	3.814602	0.401455	0.016976
C	4.761781	0.801019	0.725606

C	5.858771	1.597997	0.054498
N	2.328084	-1.452004	4.473105
C	2.002833	-0.715225	5.567513
C	1.242784	-1.286799	6.587367
C	0.803131	-2.596207	6.463177
C	1.125098	-3.324236	5.320984
C	1.900487	-2.712913	4.348306
C	2.473235	0.664218	5.508499
C	3.186658	1.017921	4.343069
C	3.556410	2.343293	4.137968
C	3.246621	3.308499	5.098038
C	2.581645	2.953013	6.271874
C	2.192695	1.634524	6.476322
O	4.888284	0.657645	1.985861
H	-0.456958	4.161565	3.110532
H	2.478312	4.817938	0.029117
H	0.896739	5.753870	1.755383
H	2.628289	2.339693	-0.212301
H	0.089645	2.629297	4.791587
H	-1.133271	1.155890	6.347344
H	-2.263497	-0.892735	5.479781
H	-2.224511	-1.375869	3.048677
H	3.147065	-4.399574	-0.438369
H	4.789736	-4.089657	0.203392
H	3.586472	-4.880118	1.222267
H	6.781352	1.599176	0.641775
H	6.051239	1.213569	-0.952070
H	5.513778	2.636476	-0.047745
H	1.650349	1.369200	7.384492
H	2.357677	3.707651	7.023474
H	3.532169	4.346621	4.929647
H	4.090513	2.619885	3.229491
H	0.986610	-0.701217	7.467298
H	0.206114	-3.046668	7.253025
H	0.792131	-4.349051	5.185293
H	2.208196	-3.230598	3.442190
H	-0.386059	-1.997826	1.362094
H	-0.521024	-2.570094	-1.047118
H	-1.393546	-0.907392	-2.677531
H	-2.102204	1.340587	-1.886549
H	-1.922524	1.931835	0.509373

IV a-Bimet

67

scf done: -1898.340956

C	1.195991	-1.353790	2.625102
C	0.235342	-0.456777	2.192642
C	-0.707477	0.120775	3.024576
C	-0.674007	-0.226290	4.376894
C	0.275174	-1.124628	4.853351
C	1.203342	-1.684676	3.982481
Pd	0.115530	0.236742	0.268456
O	-1.927183	-0.078462	0.346126
C	-2.733338	0.608598	-0.377959
C	-4.190296	0.362219	-0.094133
O	-2.424072	1.399364	-1.294088
Pd	-0.381227	1.530176	-2.192466
O	0.002947	3.274855	-1.131594
C	-0.043510	3.333471	0.135501

C	0.068659	4.704413	0.747510
N	-0.628235	-0.156572	-3.347819
C	0.505758	-0.617215	-3.936443
C	0.475799	-1.810036	-4.655353
C	-0.719669	-2.503565	-4.779467
C	-1.875237	-1.997819	-4.191257
C	-1.785343	-0.815874	-3.473983
C	1.664591	0.243918	-3.730887
C	1.446906	1.402819	-2.955971
C	2.481103	2.294051	-2.712944
C	3.749123	2.029103	-3.237458
C	3.978062	0.881375	-3.993845
C	2.940141	-0.009364	-4.243667
C	0.517709	-1.588304	-0.454163
C	1.865356	-1.723843	-0.828614
C	2.244748	-2.877586	-1.519873
C	1.301206	-3.859574	-1.800374
C	-0.020811	-3.709558	-1.388348
C	-0.428763	-2.558839	-0.705321
C	2.765790	-0.643600	-0.444335
N	2.154338	0.375873	0.209073
C	2.836191	1.420393	0.690409
C	4.208008	1.510256	0.522127
C	4.860898	0.493462	-0.169374
C	4.140345	-0.589926	-0.652975
O	-0.138071	2.358047	0.926589
H	4.640463	-1.394305	-1.186097
H	4.745064	2.363848	0.923910
H	5.935524	0.541613	-0.327131
H	2.253337	2.177240	1.211666
H	3.275636	-3.007635	-1.847004
H	1.601283	-4.753281	-2.342839
H	-0.751326	-4.487092	-1.604508
H	-1.464680	-2.424328	-0.400444
H	-4.356080	0.135236	0.962559
H	-4.788102	1.225003	-0.400107
H	-4.515585	-0.506766	-0.681299
H	-0.071315	5.489561	0.000504
H	-0.663563	4.815277	1.553723
H	1.065617	4.811195	1.194189
H	3.129817	-0.903575	-4.837007
H	4.970293	0.680675	-4.392612
H	4.564883	2.724935	-3.045344
H	2.309083	3.180555	-2.103525
H	1.385007	-2.191971	-5.113131
H	-0.749328	-3.436335	-5.337914
H	-2.830090	-2.507780	-4.277187
H	-2.646833	-0.368406	-2.982136
H	-1.449417	0.820017	2.651047
H	-1.403969	0.216592	5.052339
H	0.291148	-1.389417	5.908509
H	1.948460	-2.389348	4.347672
H	1.927152	-1.800979	1.957641

TS IV a-Bimet

67

scf done: -1898.332032

C	-0.043637	-0.030406	-0.039979
C	-0.010459	-0.041214	2.184170

Pd	1.724278	-0.030609	1.116857
N	1.570204	1.980764	1.448797
O	3.765105	0.166420	0.418380
O	1.913784	-2.077468	0.952942
Pd	3.258074	-0.323655	3.661435
N	1.903564	-0.926459	5.089132
C	3.050482	1.388679	4.625053
O	4.781235	0.431970	2.417393
O	3.493982	-2.268473	2.567514
C	2.781578	-2.720980	1.650263
C	2.873955	-4.184436	1.307877
C	-0.376954	-1.262826	-0.582636
C	-1.246616	-1.292725	-1.671686
C	-1.776226	-0.114509	-2.188147
C	-1.434149	1.105126	-1.615023
C	-0.564271	1.162273	-0.525691
C	-0.682861	-1.179109	2.595448
C	-1.571324	-1.080280	3.665928
C	-1.777815	0.141900	4.302481
C	-1.086658	1.275080	3.890008
C	-0.187259	1.200448	2.824070
C	2.390487	2.887670	0.909039
C	2.318400	4.220850	1.279476
C	1.377901	4.594932	2.234870
C	0.528749	3.642304	2.781376
C	0.633495	2.317498	2.369436
C	1.443018	-2.176140	5.208068
C	0.544076	-2.530528	6.201675
C	0.117636	-1.545854	7.088714
C	0.591145	-0.248382	6.955514
C	1.497476	0.051045	5.940075
C	3.688180	2.577553	4.301416
C	3.383117	3.737457	5.019133
C	2.440423	3.711837	6.044549
C	1.800174	2.521824	6.371658
C	2.102724	1.350959	5.671482
C	4.762195	0.417773	1.156141
C	6.040273	0.772715	0.442386
H	-0.213070	3.925035	3.523282
H	2.988617	4.943469	0.824343
H	1.302661	5.631915	2.552918
H	3.100651	2.518131	0.172556
H	-1.232392	2.217146	4.417087
H	-2.472918	0.210091	5.136342
H	-2.102957	-1.968499	4.002001
H	-0.524498	-2.133682	2.098151
H	2.753494	-4.347706	0.233192
H	3.825636	-4.596299	1.653948
H	2.059439	-4.712178	1.820842
H	6.887052	0.795633	1.132303
H	6.229142	0.055351	-0.362736
H	5.926906	1.761080	-0.020789
H	1.064571	2.508722	7.175697
H	2.203722	4.621599	6.592428
H	3.883899	4.671241	4.765218
H	4.419511	2.606995	3.495473
H	0.264082	0.530384	7.639930
H	-0.585737	-1.787771	7.882113

H	0.191710	-3.555191	6.274061
H	1.820150	-2.893967	4.481131
H	0.040478	-2.184637	-0.188212
H	-1.506232	-2.253952	-2.111549
H	-2.457118	-0.146789	-3.035953
H	-1.842227	2.034454	-2.008286
H	-0.321342	2.128220	-0.093728

VI a-Bimet

67

scf done: -1898.384729

C	-0.902818	-0.870849	-0.521340
C	-1.097878	0.143921	0.426497
C	-1.816346	1.285438	0.054068
C	-2.310936	1.418171	-1.238790
C	-2.099955	0.412233	-2.177377
C	-1.397758	-0.733813	-1.812349
C	-0.614710	-0.019145	1.832839
C	-0.233150	1.095268	2.658043
C	-0.233037	0.983616	4.046787
C	-0.553414	-0.222988	4.653572
C	-0.826452	-1.350549	3.874544
C	-0.875907	-1.244709	2.497684
Pd	1.644944	-0.043313	1.163846
O	1.815264	-2.081056	1.082218
C	2.741689	-2.730776	1.680076
C	2.755590	-4.210421	1.400407
C	0.362238	2.295060	2.036273
N	1.332404	1.973122	1.158854
C	2.029390	2.916220	0.517605
C	1.767706	4.260097	0.742845
C	0.782912	4.612213	1.662149
C	0.069072	3.619187	2.325283
Pd	3.465361	-0.264364	3.455533
O	3.585930	-2.267195	2.476414
O	3.434134	0.136786	0.101003
C	4.506336	0.478438	0.697118
C	5.665767	0.827838	-0.197278
N	2.606731	-0.991266	5.178572
C	2.349705	-0.060638	6.134945
C	1.814401	-0.454666	7.359561
C	1.534350	-1.795759	7.583244
C	1.794501	-2.730504	6.584836
C	2.341469	-2.285316	5.391556
C	2.662300	1.300706	5.719111
C	3.227860	1.431622	4.433100
C	3.489194	2.691681	3.910672
C	3.187751	3.826511	4.667614
C	2.636455	3.704456	5.941691
C	2.376124	2.444930	6.469897
O	4.674668	0.593512	1.934749
H	-0.709888	3.856143	3.046191
H	2.331233	5.014293	0.201900
H	0.568878	5.659922	1.858630
H	2.788148	2.571324	-0.181082
H	0.073037	1.840861	4.646646
H	-0.554983	-0.297654	5.739757
H	-1.046138	-2.302625	4.352466
H	-1.177059	-2.103511	1.900671

H	2.271398	-4.444905	0.448958
H	3.783976	-4.583281	1.407634
H	2.207710	-4.721676	2.202857
H	6.602586	0.483831	0.250606
H	5.540424	0.401952	-1.195657
H	5.717936	1.920485	-0.287438
H	1.934010	2.357760	7.462117
H	2.403311	4.593495	6.523830
H	3.379602	4.814604	4.250382
H	3.916181	2.799933	2.913636
H	1.619771	0.285968	8.131146
H	1.114667	-2.111935	8.535417
H	1.587643	-3.787249	6.725354
H	2.588988	-2.961267	4.575280
H	-0.336358	-1.762026	-0.250845
H	-1.229651	-1.526298	-2.539070
H	-2.488608	0.517680	-3.188317
H	-2.874962	2.309025	-1.508508
H	-2.011852	2.066629	0.788021

III b

41

scf done: -1178.191214

C	2.512955	-2.761655	-1.222774
C	2.064574	-1.542482	-0.701346
C	0.683137	-1.356637	-0.515613
C	-0.224137	-2.348137	-0.856713
C	0.240653	-3.560179	-1.369321
C	1.606943	-3.762279	-1.553562
Pd	0.120479	0.311182	0.441799
C	-0.377350	0.864393	-1.453153
C	-1.702195	0.723200	-1.870758
C	-2.084813	1.250292	-3.096518
C	-1.148788	1.906905	-3.904306
C	0.174880	2.029673	-3.475634
C	0.569660	1.502033	-2.250060
C	2.961122	-0.451043	-0.305799
N	2.362963	0.556625	0.366338
C	3.060162	1.621936	0.763039
C	4.421382	1.742538	0.522193
C	5.057895	0.712718	-0.164598
C	4.326630	-0.389774	-0.585103
O	-0.855893	2.021468	1.545575
C	-1.954789	1.398804	1.671086
C	-3.093134	2.090152	2.370012
O	-2.107967	0.224639	1.229093
H	-2.429499	0.226239	-1.230704
H	4.811700	-1.190945	-1.137107
H	4.962782	2.620860	0.861770
H	6.122515	0.770959	-0.379787
H	2.500456	2.394661	1.289649
H	3.579322	-2.941449	-1.356444
H	1.969939	-4.706663	-1.954050
H	-0.467986	-4.344689	-1.630028
H	-1.293853	-2.181916	-0.722573
H	-3.113149	1.163719	-3.445408
C	-1.541146	2.467368	-5.201183
H	0.900675	2.539344	-4.111190
H	1.605169	1.598636	-1.926266

H	-3.999393	1.478480	2.359655
H	-2.811811	2.303205	3.408281
H	-3.293754	3.053493	1.886825
O	-2.659391	2.412729	-5.676664
H	-0.711622	2.972111	-5.750668

III c

42

scf done: -1104.203130

C	2.542205	-2.758289	-1.202274
C	2.085501	-1.540639	-0.683872
C	0.700443	-1.348078	-0.528578
C	-0.199989	-2.335664	-0.901355
C	0.271850	-3.545729	-1.411626
C	1.641557	-3.753194	-1.562688
Pd	0.126436	0.316106	0.425371
C	-0.379378	0.867660	-1.473703
C	-1.718202	0.805403	-1.845486
C	-2.104699	1.329553	-3.078337
C	-1.174624	1.904163	-3.948911
C	0.164118	1.935044	-3.555266
C	0.571070	1.414765	-2.325746
C	2.979501	-0.453872	-0.268132
N	2.371020	0.565401	0.376443
C	3.065938	1.627346	0.784870
C	4.435265	1.733362	0.586382
C	5.082751	0.691118	-0.070577
C	4.353967	-0.407750	-0.504586
O	-0.854315	2.020103	1.544620
C	-1.947370	1.391050	1.687430
C	-3.081291	2.082946	2.395458
O	-2.102185	0.213627	1.257171
H	-2.458563	0.369495	-1.175690
H	4.848794	-1.218506	-1.033520
H	4.974176	2.609431	0.935729
H	6.154376	0.736698	-0.251515
H	2.497809	2.409109	1.288787
H	3.610895	-2.940731	-1.312233
H	2.010739	-4.696036	-1.961366
H	-0.433335	-4.324387	-1.698497
H	-1.272350	-2.164518	-0.797146
H	-3.155842	1.289409	-3.369704
C	-1.610329	2.485057	-5.262108
H	0.908858	2.367738	-4.225271
H	1.625496	1.445356	-2.051942
H	-3.986166	1.468942	2.396222
H	-2.791096	2.300596	3.430392
H	-3.289517	3.044054	1.910966
H	-2.379919	1.866198	-5.740849
H	-2.042127	3.487659	-5.132767
H	-0.768874	2.580464	-5.958991

III d

40

scf done: -1157.108910

C	2.523040	-2.755291	-1.223539
C	2.068555	-1.546318	-0.699473
C	0.685211	-1.360573	-0.510027
C	-0.221172	-2.356303	-0.854244
C	0.232936	-3.562949	-1.371597

C	1.608368	-3.758872	-1.557146
Pd	0.118041	0.300094	0.451966
C	-0.361205	0.870587	-1.446292
C	-1.671316	0.716480	-1.882992
C	-2.036962	1.256000	-3.117696
C	-1.100525	1.927904	-3.899127
C	0.209531	2.062161	-3.448773
C	0.591286	1.524958	-2.217737
C	2.967612	-0.453275	-0.302894
N	2.371158	0.543304	0.384273
C	3.068535	1.607230	0.782692
C	4.426804	1.735604	0.526232
C	5.059991	0.716081	-0.177358
C	4.327967	-0.386271	-0.599209
O	-0.860444	2.006932	1.538636
C	-1.964059	1.389853	1.657252
C	-3.105348	2.090701	2.340825
O	-2.117074	0.214294	1.220023
H	-2.406259	0.204575	-1.263515
H	4.810975	-1.178805	-1.165220
H	4.968359	2.613263	0.867216
H	6.121432	0.781060	-0.405193
H	2.512165	2.373241	1.322260
H	3.586229	-2.943498	-1.364199
C	2.082801	-4.997984	-2.088564
H	-0.466287	-4.353144	-1.637120
H	-1.290184	-2.193600	-0.715737
H	-3.063680	1.147676	-3.465346
H	-1.392201	2.345049	-4.861369
H	0.948284	2.583833	-4.055904
H	1.620494	1.631707	-1.876216
H	-4.012234	1.479964	2.331779
H	-2.830234	2.316134	3.378104
H	-3.301892	3.048292	1.844629
N	2.466932	-6.007655	-2.521816

III e

43

scf done: -1179.380953

C	2.476960	-2.752019	-1.208543
C	2.034693	-1.535832	-0.691662
C	0.651650	-1.316742	-0.536661
C	-0.251279	-2.292731	-0.922729
C	0.192170	-3.513785	-1.436282
C	1.562736	-3.741639	-1.578920
Pd	0.103641	0.357397	0.415265
C	-0.412317	0.905614	-1.480485
C	-1.755440	0.853300	-1.837290
C	-2.150058	1.380267	-3.068561
C	-1.209934	1.937432	-3.931239
C	0.132676	1.969171	-3.564359
C	0.540896	1.444940	-2.336460
C	2.948720	-0.465614	-0.272409
N	2.355158	0.568798	0.361168
C	3.069208	1.615777	0.774537
C	4.442877	1.690368	0.590683
C	5.074330	0.632427	-0.056157
C	4.325642	-0.451579	-0.494601
O	-0.846627	2.075675	1.540083

C	-1.946107	1.460452	1.693273
C	-3.065494	2.167084	2.409894
O	-2.119174	0.284150	1.266687
H	-2.491464	0.426625	-1.156948
H	4.807369	-1.275983	-1.014444
H	4.997298	2.555407	0.943244
H	6.148618	0.653409	-0.225189
H	2.513436	2.411432	1.270422
H	3.537028	-2.975559	-1.322876
O	2.103184	-4.886484	-2.062570
H	-0.535717	-4.267459	-1.726000
H	-1.323127	-2.112413	-0.829236
H	-3.202368	1.352456	-3.349655
H	-1.523718	2.344324	-4.891078
H	0.874783	2.397878	-4.237018
H	1.595420	1.467778	-2.062779
H	-3.979805	1.567236	2.412329
H	-2.766909	2.374812	3.444511
H	-3.260770	3.133811	1.931257
C	1.221618	-5.924676	-2.435074
H	1.847703	-6.757038	-2.764424
H	0.604168	-6.250025	-1.585772
H	0.564683	-5.617093	-3.261125

III f

37

scf done: -1042.856106

C	2.490820	-2.724751	-1.185632
C	2.002661	-1.528645	-0.666101
C	0.636207	-1.344171	-0.439929
C	-0.249792	-2.362836	-0.761635
C	0.226761	-3.564524	-1.287461
C	1.592160	-3.739358	-1.500107
Pd	0.078142	0.328096	0.523232
C	-0.339868	0.895029	-1.382093
C	-1.630560	0.736413	-1.871148 424242
C	-1.948092	1.276308	-3.118912
C	-0.982869	1.950773	-3.862204
C	0.307751	2.088209	-3.359896
C	0.641862	1.551299	-2.114888
N	2.866126	-0.459713	-0.322530
C	4.136680	-0.184800	-0.704240
C	4.484601	1.022542	-0.135138
N	2.375876	0.522502	0.470076
C	3.347781	1.424280	0.582601
O	-0.967709	2.020923	1.603031
C	-2.056538	1.375458	1.668832
C	-3.243795	2.030634	2.318309
O	-2.161754	0.203055	1.204021
H	-2.386639	0.218455	-1.283275
H	4.689164	-0.852943	-1.352480
H	5.430570	1.538903	-0.226809
H	3.187701	2.317096	1.175043
H	3.559902	-2.873784	-1.329579
H	1.966950	-4.676411	-1.906501
H	-0.470865	-4.363119	-1.533361
H	-1.319318	-2.216727	-0.603502
H	-2.959341	1.164226	-3.508317
H	-1.236337	2.367441	-4.835437

H	1.069008	2.612224	-3.936490
H	1.655033	1.662404	-1.728851
H	-4.121412	1.378730	2.301215
H	-3.000344	2.287441	3.355995
H	-3.475119	2.968619	1.799850

III g

37

scf done: -1025.820126

C	2.489306	-2.760339	-1.180925
C	2.041118	-1.537215	-0.669923
C	0.662694	-1.350229	-0.461927
C	-0.243408	-2.354955	-0.758621
C	0.219726	-3.576328	-1.254664
C	1.581361	-3.774492	-1.468185
Pd	0.112848	0.336820	0.470623
C	-0.343606	0.902566	-1.428469
C	-1.628274	0.689365	-1.913206
C	-1.982001	1.235143	-3.148215
C	-1.057533	1.973637	-3.883018
C	0.226652	2.170572	-3.383757
C	0.596362	1.627512	-2.151185
C	2.952406	-0.437970	-0.337978
C	4.374752	-0.437945	-0.776522
N	2.398978	0.513035	0.341293
O	3.184555	1.620609	0.563827
O	-0.919899	2.038800	1.563697
C	-2.005026	1.389354	1.650211
C	-3.183875	2.046407	2.314550
O	-2.115618	0.213715	1.196048
H	-2.353653	0.126404	-1.327731
H	2.646078	2.167421	1.159470
H	3.552937	-2.925717	-1.349430
H	1.939978	-4.723243	-1.862291
H	-0.489971	-4.370330	-1.482126
H	-1.311242	-2.192736	-0.605733
H	-2.988935	1.079631	-3.534047
H	-1.338947	2.395586	-4.846296
H	0.954146	2.747663	-3.953381
H	1.601978	1.788970	-1.763539
H	-4.064122	1.397877	2.303525
H	-2.929398	2.296816	3.351259
H	-3.416629	2.988134	1.803658
H	4.884183	0.484033	-0.491824
H	4.907920	-1.284595	-0.324776
H	4.436043	-0.560840	-1.865197

IV b

41

scf done: -1178.021833

C	4.279241	-0.538656	-0.805968
C	2.925709	-0.541252	-0.489559
N	2.374171	0.544812	0.107433
C	3.110251	1.613861	0.431680
C	4.464633	1.664054	0.147558
C	5.048556	0.573300	-0.490065
C	1.984522	-1.633842	-0.685775
C	2.282757	-2.898372	-1.200390
C	1.292559	-3.872839	-1.261786
C	0.003740	-3.609967	-0.804797

C	-0.326205	-2.350605	-0.291647
C	0.673994	-1.406721	-0.255957
Pd	0.344757	0.413370	0.505926
O	-1.661018	0.233225	0.890673
C	-1.851679	1.414219	1.394591
C	-3.214129	1.717399	1.920673
C	-0.154509	1.096320	-1.328257
C	-1.158303	0.471095	-2.045041
C	-1.542590	1.067039	-3.244513
C	-0.937909	2.246402	-3.676969
C	0.064498	2.846437	-2.912520
C	0.473258	2.270954	-1.714972
O	-0.903019	2.221852	1.438591
H	-1.647965	-0.431559	-1.695642
H	4.727768	-1.401653	-1.290385
H	5.040967	2.543078	0.418316
H	6.107053	0.585733	-0.737116
H	2.586975	2.433164	0.923704
H	3.290221	-3.125390	-1.545036
H	1.531253	-4.853097	-1.667171
H	-0.761265	-4.382138	-0.850011
H	-1.332620	-2.131487	0.061911
H	-2.331151	0.608191	-3.841058
C	-1.372200	2.867528	-4.941642
H	0.517304	3.772570	-3.262354
H	1.240286	2.751181	-1.114236
H	-3.981004	1.335222	1.239727
H	-3.346068	1.213241	2.885835
H	-3.334495	2.794053	2.065145
O	-0.903814	3.891095	-5.394302
H	-2.185504	2.320713	-5.470248

IV c

42

scf done: -1104.038934

C	4.283619	-0.545082	-0.797983
C	2.930405	-0.548287	-0.479200
N	2.376914	0.540714	0.110348
C	3.111433	1.613687	0.424173
C	4.465248	1.665526	0.137240
C	5.050921	0.571038	-0.492373
C	1.990959	-1.643924	-0.668205
C	2.292769	-2.910532	-1.175546
C	1.304213	-3.886731	-1.235090
C	0.013385	-3.622093	-0.784474
C	-0.318784	-2.360605	-0.278763
C	0.679365	-1.413696	-0.241662
Pd	0.347837	0.405932	0.510216
O	-1.656182	0.219249	0.904417
C	-1.847928	1.399147	1.408354
C	-3.212668	1.701836	1.930737
C	-0.152271	1.087982	-1.333130
C	-1.159751	0.471578	-2.048715
C	-1.550534	1.077263	-3.242991
C	-0.962429	2.261183	-3.692583
C	0.040564	2.842281	-2.914979
C	0.465203	2.262023	-1.719043
O	-0.901019	2.208778	1.457037
H	-1.654655	-0.430440	-1.703618

H	4.733295	-1.410714	-1.276691
H	5.040000	2.547943	0.400350
H	6.109064	0.583920	-0.741103
H	2.586856	2.435277	0.911037
H	3.301461	-3.137997	-1.516472
H	1.545457	-4.869002	-1.634200
H	-0.750825	-4.395188	-0.829157
H	-1.326918	-2.139645	0.068653
H	-2.346404	0.613582	-3.825844
C	-1.391450	2.888915	-4.984351
H	0.504770	3.774218	-3.237173
H	1.234338	2.748218	-1.125221
H	-3.977308	1.322963	1.245349
H	-3.349373	1.194323	2.893485
H	-3.333156	2.778056	2.078675
H	-1.277697	3.978990	-4.957496
H	-0.784956	2.519497	-5.822568
H	-2.438262	2.657891	-5.213860

IV d

40

scf done: -1156.938199

C	4.266106	-0.519658	-0.815923
C	2.916702	-0.528954	-0.488246
N	2.362686	0.547163	0.122799
C	3.096032	1.616726	0.448949
C	4.448644	1.675214	0.154315
C	5.033351	0.593738	-0.496322
C	1.975879	-1.624582	-0.685627
C	2.278566	-2.872810	-1.222995
C	1.282661	-3.852502	-1.284244
C	-0.008855	-3.605952	-0.802728
C	-0.325885	-2.357195	-0.271538
C	0.668751	-1.403671	-0.237044
Pd	0.333670	0.408225	0.524228
O	-1.668701	0.224024	0.915306
C	-1.848600	1.408823	1.413221
C	-3.203255	1.729996	1.945287
C	-0.167214	1.081433	-1.329112
C	-1.173163	0.453990	-2.036141
C	-1.543618	1.035079	-3.251253
C	-0.925956	2.197349	-3.700255
C	0.071063	2.799068	-2.940722
C	0.471923	2.240126	-1.724310
O	-0.889437	2.206844	1.445790
H	-1.678003	-0.436325	-1.675964
H	4.716117	-1.375569	-1.311289
H	5.022633	2.554935	0.427791
H	6.089749	0.612996	-0.751258
H	2.572874	2.430855	0.949286
H	3.277777	-3.098961	-1.589686
C	1.592174	-5.132244	-1.846282
H	-0.764245	-4.386551	-0.852102
H	-1.328148	-2.147454	0.098457
H	-2.332645	0.565136	-3.834881
H	-1.229334	2.641542	-4.645594
H	0.551898	3.714530	-3.279229
H	1.239581	2.726319	-1.129328
H	-3.977894	1.354016	1.269683

H	-3.335832	1.230863	2.912984
H	-3.310253	2.808526	2.086125
N	1.842797	-6.170819	-2.305031

IV e

43

scf done: -1179.216846

C	4.235967	-0.554851	-0.793153
C	2.886209	-0.541576	-0.462423
N	2.348650	0.555153	0.126934
C	3.096404	1.622380	0.428033
C	4.448330	1.658459	0.128478
C	5.017573	0.554860	-0.499994
C	1.931264	-1.627056	-0.640382
C	2.216385	-2.882891	-1.159805
C	1.213694	-3.859388	-1.224814
C	-0.072868	-3.585327	-0.748896
C	-0.372138	-2.321552	-0.230956
C	0.627226	-1.377865	-0.192052
Pd	0.319513	0.450803	0.536378
O	-1.682998	0.294496	0.953041
C	-1.852210	1.486626	1.435025
C	-3.203995	1.820261	1.971677
C	-0.178498	1.104110	-1.318720
C	-1.209689	0.494927	-2.007559
C	-1.580364	1.065543	-3.227150
C	-0.936834	2.202678	-3.703864
C	0.086696	2.787889	-2.967062
C	0.487212	2.237009	-1.746937
O	-0.893651	2.284291	1.452622
H	-1.730911	-0.377504	-1.627577
H	4.671318	-1.428312	-1.271000
H	5.034145	2.536525	0.381542
H	6.073582	0.555795	-0.757886
H	2.583691	2.452633	0.912763
H	3.209486	-3.142339	-1.522200
O	1.588494	-5.035030	-1.761387
H	-0.853520	-4.340740	-0.782472
H	-1.376362	-2.099857	0.127621
H	-2.388346	0.607385	-3.794203
H	-1.239671	2.639200	-4.653065
H	0.588759	3.683491	-3.327458
H	1.278299	2.710117	-1.172292
H	-3.984730	1.444297	1.303086
H	-3.335531	1.329849	2.943967
H	-3.303993	2.900537	2.104517
C	0.611937	-6.052062	-1.891308
H	1.111064	-6.891422	-2.379329
H	0.236971	-6.372783	-0.909968
H	-0.229266	-5.717992	-2.513570

IV f

37

scf done: -1042.684365

C	0.445839	2.306114	-1.695258
C	-0.179639	1.128424	-1.336112
C	-1.165888	0.497515	-2.066021
C	-1.533008	1.100914	-3.271510
C	-0.930909	2.284140	-3.686304
C	0.047990	2.885775	-2.902864

Pd	0.324719	0.437616	0.506038
O	-1.667289	0.224290	0.885347
C	-1.878732	1.396700	1.404398
C	-3.244252	1.666996	1.937897
C	0.654687	-1.391585	-0.227352
C	1.960822	-1.638378	-0.643898
C	2.301295	-2.890615	-1.140243
C	1.314680	-3.870868	-1.202044
C	0.016379	-3.614495	-0.769975
C	-0.330157	-2.353668	-0.275068
N	2.857372	-0.568045	-0.490242
C	4.170869	-0.395686	-0.752993
C	4.518687	0.865801	-0.312396
N	2.352054	0.537170	0.110065
C	3.346916	1.415698	0.219508
O	-0.943238	2.217911	1.455342
H	-1.655798	-0.410356	-1.729695
H	4.758038	-1.172379	-1.225341
H	5.493340	1.329507	-0.370191
H	3.174775	2.386751	0.667836
H	3.316787	-3.103287	-1.467572
H	1.570204	-4.853093	-1.591838
H	-0.740985	-4.393354	-0.820016
H	-1.343662	-2.137912	0.059967
H	-2.307113	0.631893	-3.875533
H	-1.231838	2.744829	-4.624524
H	0.516922	3.816230	-3.216393
H	1.200022	2.784431	-1.076754
H	-4.006217	1.280751	1.253763
H	-3.363667	1.147173	2.896352
H	-3.383024	2.739305	2.097590

IV g

37

scf done: -1025.651932

C	0.544796	2.176614	-1.750414
C	-0.174280	1.076128	-1.329918
C	-1.225158	0.501798	-2.016982
C	-1.571239	1.091188	-3.235329
C	-0.882556	2.204366	-3.706188
C	0.165826	2.745235	-2.970010
Pd	0.289149	0.410897	0.531793
O	-1.718391	0.227473	0.920544
C	-1.902318	1.407858	1.425217
C	-3.259686	1.719081	1.959647
C	0.638276	-1.407452	-0.224582
C	1.959984	-1.615046	-0.635933
C	2.298977	-2.867839	-1.150410
C	1.328181	-3.863174	-1.229239
C	0.027756	-3.622214	-0.798894
C	-0.340814	-2.367771	-0.291627
C	2.878344	-0.499147	-0.464748
C	4.285574	-0.509484	-0.920333
N	2.314693	0.512376	0.124943
O	3.028616	1.669272	0.226370
O	-0.949509	2.211994	1.466245
H	-1.777494	-0.352364	-1.638759
H	2.796573	2.043255	1.097582
H	3.314077	-3.064032	-1.491074

H	1.591691	-4.837862	-1.632193
H	-0.721218	-4.409160	-0.858661
H	-1.359828	-2.170625	0.037706
H	-2.395701	0.667801	-3.805559
H	-1.167387	2.655880	-4.653954
H	0.707409	3.616926	-3.331803
H	1.367249	2.595664	-1.175247
H	-4.033229	1.342412	1.283221
H	-3.388735	1.215050	2.925322
H	-3.372524	2.796343	2.106064
H	4.850319	0.318892	-0.489725
H	4.763717	-1.458614	-0.655062
H	4.312913	-0.422281	-2.015004

V b

41

scf done: -1178.256152

C	-0.725402	-0.899976	2.623816
C	-1.055543	0.225504	1.838375
C	-1.430374	1.420363	2.483342
C	-1.451212	1.493987	3.862952
C	-1.094852	0.381779	4.639175
C	-0.734588	-0.811593	4.016298
C	-1.111676	0.108342	0.362420
C	-0.460404	1.021462	-0.491389
C	-0.611983	0.885036	-1.874538
C	-1.377971	-0.139023	-2.418855
C	-2.006360	-1.049274	-1.576614
C	-1.871839	-0.920749	-0.198674
C	0.422493	2.099554	0.008161
N	1.326838	1.814316	0.968120
C	2.163165	2.774569	1.387035
C	2.141926	4.066954	0.885199
C	1.207700	4.374901	-0.096256
C	0.343545	3.382809	-0.537402
Pd	1.558108	-0.091047	2.021131
O	3.869344	-0.451836	2.119197
C	3.624358	-1.515533	2.754701
C	4.771570	-2.365454	3.228418
O	2.435857	-1.875582	3.019382
H	-0.522630	-1.855082	2.138304
H	-0.407701	3.593137	-1.295031
H	2.841960	4.807431	1.261649
H	1.148024	5.377889	-0.512745
H	2.881729	2.477514	2.150293
H	-0.089080	1.576510	-2.534138
H	-1.472894	-0.229830	-3.498740
H	-2.607974	-1.856707	-1.988885
H	-2.387741	-1.613985	0.464914
H	-0.470267	-1.672792	4.627454
C	-1.119216	0.480172	6.104174
H	-1.752307	2.417382	4.358549
H	-1.718073	2.282689	1.883077
H	4.424777	-3.336664	3.593020
H	5.496141	-2.508666	2.419226
H	5.293593	-1.848447	4.043345
O	-0.814469	-0.417682	6.864923
H	-1.451010	1.471351	6.492342

V c

42

scf done: -1104.270170

C	-0.743712	-0.884975	2.639440
C	-1.037860	0.232323	1.837981
C	-1.399925	1.431474	2.483450
C	-1.443408	1.508073	3.862803
C	-1.127864	0.400007	4.667339
C	-0.784617	-0.789275	4.036874
C	-1.091792	0.110049	0.361074
C	-0.446311	1.022735	-0.498400
C	-0.599022	0.884749	-1.881595
C	-1.357491	-0.145308	-2.424852
C	-1.979358	-1.057050	-1.579128
C	-1.847756	-0.922086	-0.201423
C	0.433310	2.106106	-0.004476
N	1.349831	1.822786	0.944190
C	2.184472	2.786286	1.358224
C	2.150370	4.080736	0.862336
C	1.204573	4.386545	-0.108911
C	0.342046	3.390837	-0.545038
Pd	1.567591	-0.085859	1.991254
O	3.875282	-0.480430	2.094417
C	3.617619	-1.542602	2.727800
C	4.758294	-2.402578	3.202464
O	2.426964	-1.893423	2.990195
H	-0.543448	-1.848693	2.169138
H	-0.417422	3.598822	-1.295208
H	2.849458	4.824175	1.234839
H	1.135094	5.390641	-0.521385
H	2.912464	2.489776	2.112795
H	-0.081822	1.580088	-2.541955
H	-1.452556	-0.238793	-3.504589
H	-2.576437	-1.869367	-1.988976
H	-2.362459	-1.614844	0.463772
H	-0.543911	-1.668232	4.635137
C	-1.169290	0.511991	6.160946
H	-1.737483	2.443293	4.340709
H	-1.665316	2.301085	1.881762
H	4.404043	-3.371731	3.565558
H	5.483149	-2.550548	2.394325
H	5.283338	-1.890564	4.018659
H	-1.003493	-0.459110	6.641694
H	-0.399436	1.203667	6.529918
H	-2.136149	0.901702	6.506466

V d

40

scf done: -1157.174019

C	-0.734684	-0.878738	2.645992
C	-1.051497	0.234639	1.845377
C	-1.423607	1.437080	2.473876
C	-1.458150	1.526930	3.855606
C	-1.118053	0.423950	4.645192
C	-0.760312	-0.772582	4.042802
C	-1.095466	0.103609	0.370313
C	-0.447884	1.019260	-0.486445
C	-0.584824	0.877822	-1.865296
C	-1.338497	-0.167737	-2.406087
C	-1.963286	-1.089173	-1.560622

C	-1.837944	-0.941398	-0.188777
C	0.421218	2.111376	0.011676
N	1.339090	1.827148	0.957642
C	2.165650	2.795316	1.375519
C	2.117954	4.092660	0.886476
C	1.169221	4.396693	-0.081394
C	0.314955	3.395309	-0.523392
Pd	1.574342	-0.086934	1.994142
O	3.880224	-0.482551	2.088763
C	3.620440	-1.545012	2.720542
C	4.756997	-2.410071	3.193450
O	2.427549	-1.891204	2.982562
H	-0.526179	-1.841098	2.176834
H	-0.446716	3.600786	-1.272079
H	2.810725	4.840047	1.262626
H	1.090693	5.402303	-0.487988
H	2.897509	2.501831	2.127240
H	-0.072858	1.568369	-2.533330
C	-1.457859	-0.297469	-3.824683
H	-2.548512	-1.904270	-1.979409
H	-2.349206	-1.636123	0.475288
H	-0.501378	-1.640589	4.645977
H	-1.144973	0.502447	5.730097
H	-1.759283	2.460674	4.326690
H	-1.700886	2.296169	1.863205
H	4.398631	-3.378613	3.554037
H	5.481567	-2.558624	2.385237
H	5.283268	-1.901819	4.011167
N	-1.557065	-0.403638	-4.979166

V e

43

scf done: -1179.448338

C	-0.729263	-0.870167	2.709753
C	-1.059924	0.231892	1.898758
C	-1.418698	1.440144	2.525410
C	-1.426997	1.547065	3.906549
C	-1.079001	0.451791	4.703680
C	-0.735828	-0.751435	4.106591
C	-1.125151	0.086274	0.425402
C	-0.481027	0.981269	-0.457208
C	-0.637480	0.825784	-1.830679
C	-1.408352	-0.211974	-2.362585
C	-2.030531	-1.112472	-1.499342
C	-1.882571	-0.946191	-0.125289
C	0.402913	2.073353	0.012856
N	1.325929	1.804580	0.959264
C	2.159560	2.777209	1.354433
C	2.116450	4.065102	0.842398
C	1.163460	4.354906	-0.126512
C	0.302688	3.349848	-0.544235
Pd	1.574912	-0.089400	2.029195
O	3.888502	-0.481544	2.096130
C	3.638446	-1.534187	2.747382
C	4.782868	-2.393411	3.213949
O	2.450896	-1.876699	3.036203
H	-0.529165	-1.837675	2.247139
H	-0.462073	3.544037	-1.292635
H	2.814531	4.816043	1.201472

H	1.087050	5.353320	-0.551318
H	2.894171	2.494628	2.107819
H	-0.127598	1.491743	-2.525558
O	-1.479312	-0.260079	-3.711282
H	-2.635267	-1.932711	-1.877025
H	-2.397692	-1.632464	0.546430
H	-0.470951	-1.615003	4.714056
H	-1.088101	0.541666	5.788147
H	-1.716517	2.487586	4.372110
H	-1.706389	2.293061	1.910428
H	4.431777	-3.364733	3.574379
H	5.505924	-2.535877	2.403363
H	5.308252	-1.884105	4.031696
C	-2.223730	-1.311019	-4.293557
H	-2.156354	-1.172536	-5.374751
H	-1.806153	-2.291912	-4.026502
H	-3.278602	-1.272112	-3.987803

V f

37

scf done: -1042.924858

C	-0.679978	-0.823725	2.659846
C	-1.059576	0.263039	1.854756
C	-1.419282	1.470752	2.471445
C	-1.395029	1.589280	3.853312
C	-1.005620	0.509182	4.648907
C	-0.651873	-0.693739	4.053724
C	-1.095140	0.117588	0.381536
C	-0.399445	0.991885	-0.466743
C	-0.466486	0.868742	-1.850958
C	-1.235224	-0.141168	-2.417721
C	-1.911197	-1.036651	-1.595045
C	-1.835542	-0.907627	-0.212324
N	0.413393	2.026030	0.078831
C	0.374546	3.346453	-0.231107
C	1.334412	3.979439	0.525931
Pd	1.726536	-0.099454	2.021352
O	4.048666	-0.652928	2.099383
C	3.689617	-1.682056	2.729288
C	4.725908	-2.649572	3.232620
N	1.369522	1.776095	1.006276
C	1.924925	2.954448	1.279947
O	2.464571	-1.918173	2.983067
H	-0.455622	-1.785685	2.196514
H	-0.340583	3.721538	-0.953265
H	1.574954	5.033589	0.534462
H	2.728647	3.008300	2.005306
H	0.106287	1.552469	-2.475204
H	-1.289268	-0.236841	-3.499693
H	-2.505603	-1.837049	-2.030547
H	-2.384181	-1.594882	0.430622
H	-0.352161	-1.544948	4.662223
H	-0.985868	0.609287	5.732283
H	-1.685478	2.529779	4.318000
H	-1.722895	2.317677	1.856017
H	4.298327	-3.646415	3.377382
H	5.573933	-2.700037	2.542287
H	5.105533	-2.297545	4.200454

V g

37

scf done: -1025.890763

C	-0.885770	-1.186728	2.391503
C	-1.029948	0.072525	1.765111
C	-1.205749	1.213219	2.583244
C	-1.245268	1.096131	3.959916
C	-1.105133	-0.157571	4.572840
C	-0.924930	-1.287637	3.795226
C	-1.250370	0.163583	0.297107
C	-0.545988	1.042005	-0.554023
C	-0.920196	1.132214	-1.900099
C	-1.947353	0.355301	-2.419404
C	-2.628325	-0.525805	-1.587411
C	-2.282202	-0.609322	-0.243762
C	0.642090	1.814656	-0.136859
C	0.900585	3.188235	-0.665532
Pd	1.364951	-0.481104	1.991292
O	3.607589	-0.337962	2.167941
C	3.665141	-1.181399	3.127950
C	5.011346	-1.431116	3.749835
N	1.485029	1.229405	0.641178
O	2.602925	1.971632	0.934653
O	2.644738	-1.773800	3.551140
H	-0.863447	-2.090199	1.780196
H	3.154088	1.338384	1.450237
H	-0.369257	1.798538	-2.562317
H	-2.208713	0.435699	-3.472360
H	-3.438319	-1.138857	-1.977277
H	-2.841589	-1.268739	0.418833
H	-0.821668	-2.267170	4.258364
H	-1.146627	-0.241430	5.656774
H	-1.402996	1.983236	4.570352
H	-1.348631	2.184918	2.110817
H	4.986781	-2.299097	4.414552
H	5.768650	-1.577651	2.971925
H	5.309839	-0.548850	4.329978
H	1.156898	3.858465	0.163670
H	1.761938	3.188369	-1.346651
H	0.028982	3.588279	-1.189406

VI b

41

scf done: -1178.080289

C	0.434731	-3.508573	3.035996
C	0.418429	-2.194188	2.554875
N	1.346886	-1.836430	1.640511
C	2.307207	-2.688543	1.242817
C	2.387399	-3.979604	1.728418
C	1.414346	-4.399230	2.627428
Pd	1.299068	-0.137675	0.527659
C	-0.764653	-0.884932	-0.065174
C	-1.012666	0.115017	0.924442
C	-1.233196	1.448236	0.468958
C	-1.257905	1.744743	-0.870031
C	-1.043745	0.739691	-1.838971
C	-0.799752	-0.557223	-1.440807
C	-1.233945	-0.208435	2.354098
C	-0.578643	-1.233830	3.082577
C	-0.880196	-1.381792	4.443705

C	-1.823738	-0.592784	5.084278
C	-2.507664	0.371196	4.357808
C	-2.204766	0.555878	3.017060
O	1.760891	1.525471	-0.641313
C	2.996633	1.443229	-0.324759
C	3.987227	2.427594	-0.820941
O	3.331141	0.491757	0.453879
H	-1.369607	2.240957	1.199993
H	-0.344948	-3.832777	3.718606
H	3.181958	-4.636430	1.388818
H	1.412987	-5.417967	3.006517
H	3.019830	-2.302920	0.515888
H	-0.333962	-2.119253	5.026993
H	-2.020982	-0.738359	6.143545
H	-3.272599	0.984798	4.827476
H	-2.768157	1.297104	2.456242
H	-1.430994	2.763321	-1.211131
C	-1.069691	1.075706	-3.275929
H	-0.652004	-1.344331	-2.179211
H	-0.765480	-1.936916	0.213488
H	3.636950	2.887378	-1.749395
H	4.115504	3.215622	-0.068554
H	4.957554	1.945087	-0.973136
O	-1.276668	2.191085	-3.703276
H	-0.880014	0.216510	-3.956984

VI c

42

scf done: -1104.100922

C	0.444933	-3.511284	3.046420
C	0.423940	-2.192101	2.578722
N	1.351167	-1.817159	1.670589
C	2.311848	-2.663040	1.260326
C	2.395345	-3.960226	1.728536
C	1.426489	-4.393808	2.625994
Pd	1.299248	-0.099457	0.582990
C	-0.786136	-0.903813	-0.068721
C	-0.966945	0.101861	0.930417
C	-1.190648	1.431735	0.460781
C	-1.251343	1.711189	-0.880213
C	-1.090489	0.704050	-1.863675
C	-0.858309	-0.590682	-1.440228
C	-1.213358	-0.211606	2.362003
C	-0.578058	-1.239005	3.102494
C	-0.903028	-1.392401	4.457755
C	-1.847203	-0.594765	5.085529
C	-2.507475	0.378991	4.349270
C	-2.186435	0.560307	3.011744
O	1.784329	1.575966	-0.583367
C	3.022774	1.443497	-0.304208
C	4.033587	2.402639	-0.813943
O	3.350161	0.470338	0.450075
H	-1.299964	2.235524	1.185216
H	-0.333279	-3.844732	3.726402
H	3.190249	-4.611125	1.378321
H	1.429781	-5.417040	2.992927
H	3.023195	-2.267171	0.538049
H	-0.373134	-2.138632	5.045375
H	-2.063173	-0.739602	6.141318

H	-3.271109	1.001931	4.809151
H	-2.734592	1.307214	2.443120
H	-1.419602	2.737415	-1.204938
C	-1.147596	1.062975	-3.311257
H	-0.747157	-1.392777	-2.167732
H	-0.764849	-1.953048	0.220374
H	3.685956	2.867018	-1.741251
H	4.185160	3.191856	-0.067095
H	4.991474	1.898222	-0.972822
H	-2.040641	1.659596	-3.537164
H	-0.278353	1.676413	-3.586962
H	-1.150222	0.173928	-3.950635

VI d

40

scf done: -1156.999048

C	0.442572	-3.511920	3.032651
C	0.430911	-2.195846	2.561647
N	1.360093	-1.824492	1.654900
C	2.319353	-2.673278	1.250548
C	2.396204	-3.970416	1.723031
C	1.423188	-4.399463	2.616474
Pd	1.310877	-0.107550	0.568133
C	-0.770923	-0.899991	-0.076172
C	-0.973659	0.108098	0.916013
C	-1.197023	1.437614	0.456588
C	-1.254638	1.722664	-0.887965
C	-1.087511	0.709251	-1.850865
C	-0.839443	-0.585094	-1.450396
C	-1.214232	-0.211346	2.347803
C	-0.567799	-1.234712	3.085599
C	-0.877661	-1.384493	4.440140
C	-1.831028	-0.585165	5.067528
C	-2.511272	0.384186	4.330972
C	-2.193913	0.555059	2.995920
O	1.784874	1.568942	-0.581849
C	3.022913	1.453678	-0.289167
C	4.027433	2.425706	-0.782010
O	3.349997	0.479507	0.465133
H	-1.310584	2.237717	1.184203
H	-0.338371	-3.842596	3.711049
H	3.190133	-4.624593	1.376910
H	1.421450	-5.421754	2.985539
H	3.033613	-2.281976	0.528667
H	-0.344151	-2.121045	5.035566
C	-2.109904	-0.769031	6.458356
H	-3.277541	0.996830	4.798375
H	-2.751721	1.293105	2.426792
H	-1.428760	2.746699	-1.209322
H	-1.151497	0.952385	-2.908592
H	-0.720336	-1.382973	-2.178783
H	-0.751783	-1.948964	0.213439
H	3.680128	2.899123	-1.704762
H	4.171190	3.205838	-0.024163
H	4.989159	1.929233	-0.943096
N	-2.339550	-0.917080	7.588715

VI e

43

scf done: -1179.278089

C	0.407025	-3.474915	3.051383
C	0.397071	-2.164596	2.560153
N	1.341871	-1.808180	1.662586
C	2.313682	-2.659935	1.293506
C	2.389640	-3.946936	1.790815
C	1.399025	-4.364456	2.671469
Pd	1.314871	-0.119251	0.525679
C	-0.743376	-0.880009	-0.107344
C	-0.984401	0.133480	0.872471
C	-1.199245	1.457122	0.390325
C	-1.231305	1.727173	-0.957342
C	-1.034453	0.706546	-1.909502
C	-0.786378	-0.579294	-1.489734
C	-1.230988	-0.167983	2.300365
C	-0.609855	-1.197818	3.057385
C	-0.943572	-1.341340	4.402649
C	-1.896460	-0.535161	5.028856
C	-2.544577	0.445392	4.281890
C	-2.197993	0.609363	2.949352
O	1.808399	1.531149	-0.659698
C	3.039454	1.436729	-0.332160
C	4.044778	2.407293	-0.830653
O	3.361529	0.490966	0.457534
H	-1.330830	2.264890	1.106162
H	-0.385884	-3.795544	3.720340
H	3.194897	-4.602281	1.474140
H	1.393999	-5.380220	3.058541
H	3.039534	-2.276721	0.578529
H	-0.437695	-2.077597	5.022846
O	-2.112737	-0.785319	6.331424
H	-3.311187	1.080558	4.716488
H	-2.740205	1.359326	2.379090
H	-1.404024	2.747256	-1.292723
H	-1.075509	0.940489	-2.970451
H	-0.643754	-1.384544	-2.205999
H	-0.742440	-1.927032	0.190576
H	3.702285	2.869984	-1.760547
H	4.183963	3.195154	-0.080026
H	5.008709	1.911542	-0.981174
C	-3.078763	0.001867	7.005594
H	-3.095780	-0.354509	8.037184
H	-2.804288	1.065115	6.992011
H	-4.074513	-0.125819	6.560152

VI f

37

scf done: -1042.749177

C	-1.185382	1.460849	0.480802
C	-0.931065	0.134856	0.930091
C	-0.677144	-0.855657	-0.070896
C	-0.754451	-0.529834	-1.444597
C	-1.040903	0.758273	-1.834805
C	-1.243893	1.756193	-0.861822
C	-1.186419	-0.209699	2.352004
C	-0.561929	-1.243006	3.079310
C	-0.883787	-1.482629	4.413565
C	-1.865181	-0.736844	5.049353
C	-2.516574	0.269135	4.347746
C	-2.170771	0.525526	3.029100

Pd	1.382075	-0.035378	0.532572
O	3.406590	0.592419	0.388752
C	3.049279	1.513775	-0.414380
C	4.019812	2.488210	-0.965752
N	0.416966	-2.108117	2.510214
C	0.592393	-3.425550	2.783612
C	1.738404	-3.849595	2.146469
N	1.436132	-1.670771	1.729538
C	2.225604	-2.719196	1.487825
O	1.804655	1.575788	-0.703427
H	-1.330686	2.249969	1.214524
H	-0.116217	-3.959029	3.403936
H	2.161834	-4.843915	2.154030
H	3.092954	-2.598840	0.849063
H	-0.342215	-2.249806	4.961837
H	-2.108544	-0.940604	6.089053
H	-3.297031	0.858386	4.822710
H	-2.713492	1.297937	2.490511
H	-1.447529	2.777793	-1.173936
H	-1.106889	1.010188	-2.890280
H	-0.602660	-1.316750	-2.178925
H	-0.629733	-1.907035	0.208423
H	3.644871	2.914698	-1.900518
H	4.158209	3.301243	-0.242307
H	4.990317	2.008184	-1.124484

VI g

37

scf done: -1025.714003

C	-1.154808	1.526514	0.575765
C	-0.961952	0.165060	0.959798
C	-0.790733	-0.791239	-0.091264
C	-0.871669	-0.400835	-1.442851
C	-1.090216	0.921494	-1.766625
C	-1.215054	1.887621	-0.749716
C	-1.262462	-0.235767	2.359118
C	-0.647014	-1.293169	3.077449
C	-1.089486	-1.576843	4.378734
C	-2.103103	-0.851511	4.983677
C	-2.722805	0.168191	4.274511
C	-2.305554	0.459393	2.983126
Pd	1.291380	0.001348	0.574518
O	3.360616	0.436920	0.362801
C	3.073508	1.345792	-0.487682
C	4.130450	2.173270	-1.116435
C	0.493897	-2.098788	2.618219
C	0.712700	-3.487863	3.126117
N	1.365214	-1.587999	1.808584
O	2.393610	-2.418353	1.447082
O	1.839433	1.525935	-0.753638
H	-1.251307	2.282940	1.351431
H	3.115712	-1.818131	1.174352
H	-0.602172	-2.364084	4.947697
H	-2.407253	-1.089904	5.999757
H	-3.538477	0.734980	4.717163
H	-2.832793	1.231149	2.427691
H	-1.362382	2.931922	-1.014030
H	-1.161739	1.223282	-2.808728
H	-0.777205	-1.158631	-2.216201

H	-0.765042	-1.853077	0.148033
H	3.777072	2.587581	-2.064904
H	4.381321	3.004058	-0.445351
H	5.035648	1.578323	-1.271203
H	1.058142	-4.129190	2.309766
H	1.496882	-3.495038	3.894549
H	-0.203638	-3.907872	3.543686

TS (III-V) b

41

scf done: -1178.187986

C	-0.469235	-1.063318	3.014673
C	-0.055904	0.107636	2.367607
C	-0.519487	1.354117	2.790787
C	-1.389697	1.425857	3.872521
C	-1.805015	0.264441	4.527033
C	-1.335440	-0.981135	4.092494
Pd	1.697642	-0.032502	1.276844
O	3.599426	-0.444164	2.457786
C	3.354615	-1.688123	2.492491
C	4.294282	-2.591361	3.241952
C	-0.014692	-0.045193	0.168711
C	-0.232507	1.134891	-0.570822
C	-1.144426	1.111015	-1.630976
C	-1.817855	-0.059438	-1.958556
C	-1.577810	-1.226218	-1.236033
C	-0.682723	-1.217025	-0.168310
C	0.555555	2.323837	-0.230217
N	1.656114	2.081961	0.514391
C	2.437258	3.086399	0.915547
C	2.169886	4.407187	0.583794
C	1.040348	4.675352	-0.183848
C	0.223957	3.629652	-0.592841
O	2.331423	-2.177845	1.932030
H	-0.088814	-2.030047	2.689207
H	-0.676807	3.827351	-1.168630
H	2.829169	5.200820	0.923559
H	0.789328	5.698595	-0.454198
H	3.301956	2.811463	1.519114
H	-1.304951	2.007111	-2.229555
H	-2.520447	-0.064526	-2.789090
H	-2.096018	-2.147322	-1.497063
H	-0.516884	-2.126879	0.408130
H	-1.660043	-1.878478	4.617561
C	-2.727880	0.362137	5.661163
H	-1.754227	2.395360	4.215378
H	-0.206336	2.270186	2.292523
H	4.099888	-3.643653	3.015921
H	5.333438	-2.342493	3.001076
H	4.162622	-2.433059	4.319736
O	-3.157630	-0.583731	6.294403
H	-3.026208	1.405525	5.919710

TS (III-V) c

42

scf done: -1104.199973

C	0.231747	3.623711	-0.608190
C	0.567722	2.318755	-0.245345
N	1.664995	2.081225	0.505523
C	2.436679	3.089814	0.914116

C	2.164419	4.410019	0.583861
C	1.039085	4.673379	-0.191678
C	-0.214890	1.127295	-0.590348
C	-0.006841	-0.047251	0.160971
C	-0.677193	-1.218406	-0.176125
C	-1.560074	-1.232576	-1.253720
C	-1.788114	-0.070710	-1.988745
C	-1.114828	1.099530	-1.661047
Pd	1.694853	-0.032396	1.277851
O	2.339814	-2.189235	1.921226
C	3.364829	-1.698527	2.475661
C	4.309927	-2.602726	3.219385
C	-0.065880	0.122931	2.369790
C	-0.467257	-1.034398	3.035155
C	-1.338325	-0.938548	4.116275
C	-1.831443	0.297034	4.545954
C	-1.425689	1.440149	3.855953
C	-0.551792	1.363672	2.772101
C	-2.751496	0.387511	5.727037
O	3.611052	-0.454769	2.443244
H	-0.084041	-2.006741	2.728280
H	-0.666629	3.817291	-1.189243
H	2.816793	5.206621	0.930129
H	0.784174	5.695785	-0.461810
H	3.299283	2.818667	1.522562
H	-1.265261	1.992515	-2.267125
H	-2.480677	-0.079967	-2.827735
H	-2.079253	-2.153736	-1.513397
H	-0.523113	-2.123182	0.411749
H	-1.641308	-1.846718	4.639979
H	-1.801407	2.415426	4.169094
H	-0.261814	2.278501	2.255919
H	4.116345	-3.654959	2.992005
H	5.347849	-2.352102	2.974774
H	4.183064	-2.447439	4.298237
H	-3.447365	-0.460228	5.760976
H	-2.189796	0.378071	6.671982
H	-3.341186	1.312093	5.709544

TS (III-V) d

40

scf done: -1157.105439

C	-0.453539	-1.034403	3.029020
C	-0.057543	0.127011	2.368275
C	-0.532355	1.372735	2.770882
C	-1.404113	1.451922	3.856938
C	-1.802260	0.299831	4.527880
C	-1.322965	-0.940693	4.113769
Pd	1.705806	-0.024832	1.268891
O	3.602104	-0.457268	2.454750
C	3.345665	-1.698526	2.474442
C	4.258607	-2.624620	3.228194
C	-0.003960	-0.041464	0.174894
C	-0.226541	1.134970	-0.574286
C	-1.131457	1.109196	-1.632384
C	-1.800181	-0.075235	-1.954604
C	-1.555056	-1.247830	-1.226189
C	-0.664048	-1.221278	-0.164047
C	0.557133	2.330076	-0.236322

N	1.662425	2.087713	0.499401
C	2.440371	3.093897	0.901029
C	2.163203	4.415192	0.577263
C	1.028640	4.682079	-0.182164
C	0.214628	3.633768	-0.591631
O	2.321288	-2.171926	1.899785
H	-0.065239	-2.003879	2.720697
H	-0.691064	3.831390	-1.159647
H	2.820180	5.210511	0.917452
H	0.770908	5.705230	-0.445903
H	3.310002	2.820851	1.498056
H	-1.303461	1.995953	-2.240347
C	-2.723502	-0.091819	-3.044608
H	-2.070860	-2.167771	-1.493058
H	-0.490054	-2.127875	0.413877
H	-1.622504	-1.847095	4.638118
H	-2.485131	0.367585	5.372664
H	-1.771776	2.426373	4.175282
H	-0.232749	2.285788	2.258022
H	4.195939	-3.643897	2.835375
H	5.292231	-2.267076	3.188178
H	3.953085	-2.647286	4.282184
N	-3.477049	-0.105270	-3.931750

TS (III-V) e

43

scf done: -1179.378012

C	-0.440520	-1.055549	3.084256
C	-0.053290	0.101056	2.409241
C	-0.541849	1.345811	2.799410
C	-1.411772	1.429883	3.886716
C	-1.798345	0.282179	4.572394
C	-1.308822	-0.958269	4.169973
Pd	1.704309	-0.049426	1.317676
O	3.618189	-0.427827	2.492549
C	3.395950	-1.675892	2.542250
C	4.357574	-2.549297	3.301610
C	0.008051	-0.086810	0.193839
C	-0.210393	1.078761	-0.572210
C	-1.111058	1.044063	-1.632926
C	-1.795968	-0.132137	-1.948458
C	-1.567626	-1.289370	-1.200291
C	-0.673555	-1.251470	-0.130701
C	0.567679	2.279761	-0.243698
N	1.663464	2.057014	0.512966
C	2.430614	3.074486	0.907132
C	2.152916	4.388813	0.557232
C	1.027711	4.636398	-0.223201
C	0.225888	3.576977	-0.626059
O	2.382622	-2.194641	1.992906
H	-0.045720	-2.025223	2.783734
H	-0.672028	3.757533	-1.211915
H	2.800942	5.193381	0.893108
H	0.768558	5.653651	-0.508176
H	3.293306	2.816083	1.520923
H	-1.280496	1.914438	-2.265576
O	-2.644983	-0.052267	-2.999364
H	-2.083001	-2.217876	-1.432758
H	-0.524252	-2.153570	0.462665

H	-1.599633	-1.861752	4.704663
H	-2.480058	0.353227	5.418003
H	-1.788204	2.404595	4.194614
H	-0.253038	2.254636	2.272265
H	4.185785	-3.608597	3.090108
H	5.390793	-2.281693	3.055008
H	4.225415	-2.379946	4.377713
C	-3.362618	-1.215097	-3.357439
H	-3.982905	-0.941310	-4.213849
H	-2.686147	-2.031452	-3.647391
H	-4.008558	-1.555977	-2.536049

TS (III-V) f

37

scf done: -1042.853043

C	-0.440279	-1.031710	3.040809
C	-0.011081	0.116617	2.379206
C	-0.464062	1.375984	2.763167
C	-1.344437	1.481980	3.840365
C	-1.773529	0.343884	4.516460
C	-1.318054	-0.910163	4.116226
Pd	1.746825	-0.065468	1.300184
O	3.630244	-0.544402	2.494437
C	3.347471	-1.779731	2.507411
C	4.249081	-2.725047	3.251208
C	0.044887	-0.071424	0.177169
C	-0.173378	1.096554	-0.565741
C	-1.067354	1.120302	-1.632013
C	-1.759778	-0.039288	-1.961872
C	-1.537730	-1.214937	-1.247989
C	-0.641423	-1.227839	-0.181725
N	0.578626	2.243798	-0.219138
C	0.328399	3.561274	-0.422424
C	1.352494	4.268072	0.170900
N	1.724867	2.069793	0.480144
C	2.193601	3.290140	0.725356
O	2.314708	-2.228424	1.928545
H	-0.071753	-2.011066	2.739586
H	-0.554885	3.890904	-0.954892
H	1.474600	5.342298	0.199526
H	3.116026	3.411596	1.280471
H	-1.202573	2.028732	-2.216711
H	-2.461449	-0.025826	-2.792870
H	-2.070568	-2.125149	-1.516500
H	-0.488602	-2.143334	0.389682
H	-1.643819	-1.805764	4.643643
H	-2.463648	0.433232	5.353358
H	-1.694967	2.466520	4.147007
H	-0.138584	2.275647	2.242350
H	4.024908	-3.766782	3.004630
H	5.298132	-2.504352	3.026471
H	4.109367	-2.581271	4.330021

TS (III-V) g

37

scf done: -1025.816476

C	-0.528533	-1.030873	2.999588
C	-0.060389	0.124023	2.375535
C	-0.468243	1.381691	2.814862
C	-1.343514	1.477512	3.897447

C	-1.812934	0.330813	4.529932
C	-1.399850	-0.921513	4.081106
Pd	1.717542	-0.044843	1.308862
O	3.631300	-0.482159	2.473342
C	3.367825	-1.721817	2.500217
C	4.299432	-2.646973	3.232681
C	0.021243	-0.059345	0.180208
C	-0.189560	1.120738	-0.563799
C	-1.104420	1.106524	-1.622080
C	-1.769366	-0.065671	-1.962108
C	-1.520126	-1.237444	-1.251317
C	-0.633257	-1.232342	-0.175893
C	0.586447	2.314353	-0.218163
C	0.150124	3.681613	-0.611777
N	1.643868	2.059724	0.482112
O	2.316309	3.158807	0.962533
O	2.331517	-2.190719	1.945367
H	-0.203227	-2.013159	2.660930
H	3.133331	2.784333	1.332289
H	-1.284874	2.013915	-2.196915
H	-2.476569	-0.066458	-2.788727
H	-2.031285	-2.159714	-1.522405
H	-0.469347	-2.145844	0.395287
H	-1.756190	-1.825533	4.573196
H	-2.498128	0.411725	5.371742
H	-1.656154	2.461732	4.243752
H	-0.103454	2.291535	2.340238
H	4.088227	-3.693880	2.996857
H	5.340267	-2.410310	2.986863
H	4.177750	-2.498647	4.313052
H	0.854216	4.441954	-0.269730
H	0.058656	3.755292	-1.702596
H	-0.840917	3.893970	-0.189192

TS (IV-VI) b

41

scf done: -1178.014307

C	0.428948	-3.713690	2.880799
C	0.505948	-2.371795	2.526626
N	1.428394	-1.976455	1.615305
C	2.284834	-2.833982	1.053167
C	2.250821	-4.181526	1.375482
C	1.306538	-4.620232	2.298912
Pd	1.475053	0.034362	1.217405
O	3.530219	0.729957	0.709875
C	3.053071	1.897599	0.659542
C	3.885437	3.083758	0.337490
C	-0.316502	-1.282496	3.036340
C	-0.184199	-0.032249	2.410531
C	-0.823429	1.104756	2.865469
C	-1.652945	0.987940	3.982205
C	-1.827290	-0.243516	4.607773
C	-1.159436	-1.371835	4.145730
C	-0.336100	-0.051063	0.188055
C	-0.820492	-1.263026	-0.286697
C	-1.764552	-1.228019	-1.309527
C	-2.209333	-0.013127	-1.826513
C	-1.701954	1.187885	-1.323634
C	-0.760414	1.179788	-0.305264

O	1.794910	2.045037	0.896837
H	-0.356141	2.113939	0.075072
H	-0.311734	-4.046037	3.602985
H	2.948624	-4.866432	0.904376
H	1.252665	-5.672129	2.567186
H	2.990839	-2.418643	0.336481
H	-1.272337	-2.319605	4.668885
H	-2.480692	-0.323276	5.472895
H	-2.168080	1.870344	4.354897
H	-0.699865	2.066217	2.371938
H	-2.055105	2.130348	-1.738430
C	-3.215690	-0.003367	-2.902855
H	-2.158151	-2.164724	-1.704498
H	-0.490883	-2.221836	0.100014
H	3.280270	3.993828	0.318668
H	4.680826	3.184648	1.084556
H	4.365462	2.936953	-0.636691
O	-3.664453	1.004101	-3.408827
H	-3.550279	-1.013202	-3.232463

TS (IV-VI) c

42

scf done: -1104.031548

C	0.436863	-3.711539	2.884407
C	0.516176	-2.368796	2.533155
N	1.434732	-1.973991	1.617802
C	2.283314	-2.833782	1.047445
C	2.246717	-4.182140	1.365741
C	1.307086	-4.619831	2.294550
Pd	1.480387	0.035572	1.220343
O	3.545175	0.743904	0.729068
C	3.059228	1.907441	0.678870
C	3.887560	3.100240	0.365439
C	-0.301932	-1.278759	3.048182
C	-0.174501	-0.030467	2.417482
C	-0.815729	1.104580	2.875110
C	-1.637425	0.988617	3.997620
C	-1.805283	-0.241613	4.627885
C	-1.137826	-1.368731	4.163261
C	-0.331407	-0.058440	0.186484
C	-0.824410	-1.269451	-0.280451
C	-1.772077	-1.237696	-1.300416
C	-2.230707	-0.034335	-1.840109
C	-1.712265	1.157437	-1.329724
C	-0.762394	1.161942	-0.311379
O	1.799205	2.049511	0.906793
H	-0.367764	2.103554	0.061438
H	-0.301090	-4.043118	3.609781
H	2.939015	-4.868262	0.888281
H	1.251003	-5.672297	2.560313
H	2.986623	-2.418587	0.327969
H	-1.245469	-2.316437	4.687903
H	-2.452911	-0.320803	5.497467
H	-2.152760	1.870603	4.371423
H	-0.699298	2.064311	2.376423
H	-2.056515	2.110939	-1.729859
C	-3.236700	-0.028882	-2.949810
H	-2.163133	-2.182219	-1.678944
H	-0.500863	-2.229212	0.110537

H	3.278643	4.007884	0.349304
H	4.680393	3.201084	1.115229
H	4.371270	2.961068	-0.608053
H	-3.736950	0.942425	-3.035144
H	-2.755989	-0.236683	-3.915719
H	-4.002578	-0.799679	-2.800405

TS (IV-VI) d

40

scf done: -1156.930172

C	-0.189937	-0.036685	2.447770
C	-0.371945	-0.055098	0.237584
Pd	1.460698	0.035499	1.251105
N	1.423176	-1.977300	1.645245
C	0.508912	-2.376997	2.561893
C	-0.306887	-1.285367	3.083488
C	-1.123268	-1.382251	4.206156
C	0.429113	-3.718594	2.911025
O	1.770071	2.047351	0.936054
C	3.024871	1.901855	0.681023
O	3.502589	0.733694	0.726619
C	-0.796270	1.171599	-0.252040
C	-1.755252	1.173123	-1.263087
C	-2.269303	-0.023992	-1.752222
C	-1.822548	-1.234821	-1.235912
C	-0.864212	-1.268073	-0.222284
C	2.269952	-2.834524	1.069836
C	2.234064	-4.184423	1.385663
C	1.298440	-4.625569	2.315452
C	-1.786606	-0.247003	4.679206
C	-1.629367	0.992508	4.047806
C	-0.824334	1.099387	2.919283
C	3.851955	3.087096	0.344860
C	-2.622739	-0.350809	5.835732
N	-3.302505	-0.434079	6.775395
H	-0.388317	2.108646	0.117262
H	-0.306070	-4.053658	3.637536
H	2.925055	-4.868824	0.903938
H	1.243496	-5.678596	2.578599
H	2.970740	-2.418064	0.348842
H	-1.228090	-2.324986	4.738922
H	-2.140493	1.869320	4.437426
H	-0.711710	2.060955	2.424161
H	-2.096842	2.125848	-1.662423
H	-3.020636	-0.012240	-2.538479
H	-2.215963	-2.176225	-1.613920
H	-0.534114	-2.226785	0.164890
H	3.245202	3.996162	0.328611
H	4.655009	3.192257	1.083078
H	4.321827	2.936482	-0.633686

TS (IV-VI) e

43

scf done: -1179.210073

C	0.399435	-3.691251	2.915498
C	0.503526	-2.352611	2.557752
N	1.434099	-1.975114	1.647479
C	2.271502	-2.851605	1.086842
C	2.210216	-4.198251	1.410678
C	1.258435	-4.616833	2.335308

Pd	1.519505	0.033348	1.238507
O	3.536498	0.697251	0.469659
C	3.079971	1.869547	0.511526
C	3.882848	3.064481	0.141268
C	-0.301066	-1.244248	3.059572
C	-0.124653	0.001550	2.426473
C	-0.758161	1.141201	2.884486
C	-1.613426	1.053997	3.981313
C	-1.825846	-0.180303	4.605248
C	-1.159205	-1.324678	4.145879
C	-0.301907	-0.026494	0.191738
C	-0.793125	-1.233353	-0.283373
C	-1.726473	-1.191121	-1.320382
C	-2.152850	0.023586	-1.844537
C	-1.641663	1.214842	-1.338841
C	-0.707326	1.203417	-0.304461
O	1.862553	2.038606	0.905877
H	-0.301097	2.135772	0.077965
H	-0.347385	-4.006515	3.639048
H	2.893699	-4.897628	0.939740
H	1.183624	-5.666992	2.605485
H	2.986193	-2.453063	0.368999
H	-1.317125	-2.257715	4.683501
O	-2.639118	-0.369278	5.656435
H	-2.111766	1.953356	4.331610
H	-0.611990	2.103799	2.398517
H	-1.966592	2.171490	-1.743215
H	-2.884485	0.042790	-2.649154
H	-2.116834	-2.129276	-1.710053
H	-0.478946	-2.195086	0.109890
H	3.289931	3.734512	-0.489976
H	4.151005	3.616976	1.049909
H	4.797010	2.764419	-0.377646
C	-3.328910	0.751384	6.183834
H	-3.916976	0.376899	7.023599
H	-2.626561	1.515394	6.542575
H	-4.001705	1.190616	5.435405

TS (IV-VI) f

37

scf done: -1042.676645

C	-0.730402	1.184949	-0.268978
C	-0.292802	-0.038101	0.214505
C	-0.758061	-1.257267	-0.255459
C	-1.704487	-1.232698	-1.280784
C	-2.164480	-0.026330	-1.795567
C	-1.676226	1.175834	-1.292673
Pd	1.544820	0.042662	1.240695
O	3.543898	0.784909	0.540535
C	3.043677	1.938374	0.576520
C	3.803855	3.167936	0.240617
C	-0.116280	-0.023525	2.423562
C	-0.291218	-1.273927	3.026785
C	-1.137606	-1.417557	4.117595
C	-1.792112	-0.291173	4.605804
C	-1.588344	0.960019	4.028355
C	-0.744350	1.102682	2.928072
N	0.479340	-2.323820	2.498956
C	0.472650	-3.667412	2.659419

C	1.495880	-4.179608	1.888000
N	1.472623	-1.962986	1.652520
C	2.096314	-3.074338	1.270482
O	1.806700	2.047612	0.938107
H	-0.343789	2.125064	0.114303
H	-0.249084	-4.151210	3.304786
H	1.772442	-5.218984	1.780751
H	2.926460	-3.025595	0.577439
H	-1.264055	-2.386526	4.595802
H	-2.457130	-0.392127	5.459659
H	-2.091771	1.836093	4.429986
H	-0.596683	2.078444	2.470160
H	-2.028991	2.125542	-1.689740
H	-2.905963	-0.022055	-2.591208
H	-2.078153	-2.178232	-1.668537
H	-0.415515	-2.211646	0.131697
H	3.193041	3.830722	-0.380949
H	4.046088	3.707528	1.164193
H	4.732261	2.910409	-0.275986

TS (IV-VI) g

37

scf done: -1025.642223

C	-0.747929	1.194650	-0.345771
C	-0.345158	-0.040202	0.140113
C	-0.832599	-1.243548	-0.345459
C	-1.760728	-1.193722	-1.386627
C	-2.183953	0.025580	-1.902615
C	-1.676415	1.213555	-1.384929
Pd	1.465429	0.011804	1.194654
O	3.548649	0.718398	0.732367
C	3.066870	1.881150	0.686216
C	3.881318	3.085106	0.380204
C	-0.205514	-0.040310	2.371599
C	-0.328441	-1.289060	3.008507
C	-1.187312	-1.395268	4.104564
C	-1.881179	-0.276190	4.552153
C	-1.708879	0.955267	3.927697
C	-0.860112	1.085989	2.824407
C	0.537504	-2.368563	2.557162
C	0.519442	-3.735544	3.125717
N	1.355563	-1.989838	1.623020
O	2.335534	-2.844426	1.236336
O	1.802749	2.023792	0.902803
H	-0.345313	2.124622	0.046442
H	2.482833	-2.662394	0.288484
H	-1.287337	-2.344826	4.626985
H	-2.550722	-0.363171	5.403928
H	-2.247852	1.829651	4.285617
H	-0.746313	2.049010	2.331657
H	-1.999639	2.172886	-1.783990
H	-2.910807	0.051364	-2.711327
H	-2.148909	-2.128513	-1.786169
H	-0.515639	-2.204909	0.044659
H	3.720856	3.849860	1.148056
H	4.941595	2.826236	0.324161
H	3.556371	3.508451	-0.577533
H	1.091958	-4.429421	2.507679
H	0.960655	-3.720919	4.131453

H -0.512069 -4.092128 3.220645

III a (mPW2PLYP)

39

FINAL HEAT OF FORMATION = 0.000000

Pd 0.123418 0.302007 0.414093

C 0.686238 -1.360798 -0.551460

C 2.073626 -1.553850 -0.705557

C 2.970811 -0.466410 -0.279003

N 2.357363 0.557698 0.360615

O -0.800557 2.013883 1.549953

C -1.913631 1.407825 1.697725

O -2.090661 0.227682 1.266484

C -0.387898 0.884289 -1.462282

C -1.718670 0.766355 -1.863403

C 0.546852 1.510424 -2.285670

C 0.139058 2.042560 -3.513082

C -1.190969 1.936581 -3.919519

C -2.117218 1.299544 -3.093117

C 4.352107 -0.427609 -0.495797

C 5.085886 0.662598 -0.040630

C 4.435083 1.705090 0.618380

C 3.059934 1.611841 0.793729

C -0.207072 -2.355611 -0.938915

C 0.269731 -3.561265 -1.460503

C 1.643115 -3.763811 -1.607712

C 2.540440 -2.767746 -1.231744

C -3.059494 2.135406 2.360012

H -2.443311 0.286694 -1.216779

H 4.847380 -1.233477 -1.019952

H 4.973972 2.568104 0.985683

H 6.155943 0.699873 -0.203570

H 2.494345 2.389571 1.292508

H 3.603819 -2.947829 -1.339292

H 2.015558 -4.697394 -2.012296

H -0.429054 -4.335530 -1.757062

H -1.275282 -2.194942 -0.840915

H -3.153848 1.214496 -3.401155

H -1.503160 2.347000 -4.872943

H 0.866548 2.534220 -4.149975

H 1.583957 1.594066 -1.984027

H -3.712330 1.433123 2.877185

H -2.688690 2.887496 3.055179

H -3.647479 2.641144 1.589322

TS (III-V) a (mPW2PLYP)

39

FINAL HEAT OF FORMATION = 0.000000

C -0.067713 -0.034873 0.268582

C -0.151202 0.143653 2.391449

Pd 1.662011 -0.013439 1.366293

N 1.641031 2.089588 0.602853

C 0.565959 2.321475 -0.186629

C -0.225958 1.126269 -0.521403

O 2.315842 -2.167754 1.981492

C 3.409881 -1.699018 2.425438

O 3.683472 -0.457102 2.351459

C -1.070271 1.085890 -1.639931

C -1.742029 -0.084602 -1.980173

C -1.564392 -1.235702 -1.210392

C	-0.736580	-1.207325	-0.088170
C	2.436141	3.100794	0.975304
C	2.208407	4.410627	0.569947
C	1.101420	4.668412	-0.237728
C	0.269433	3.619425	-0.615031
C	-0.665363	1.380850	2.788729
C	-1.534902	1.455008	3.879651
C	-1.899675	0.302116	4.574022
C	-1.385158	-0.932108	4.174224
C	-0.519126	-1.016006	3.083102
C	4.392659	-2.629867	3.096884
H	-0.113439	-1.976391	2.789513
H	-0.607602	3.808127	-1.219394
H	2.876876	5.201209	0.883568
H	0.882199	5.677810	-0.563279
H	3.274262	2.839445	1.609761
H	-1.174517	1.961112	-2.270880
H	-2.387992	-0.102629	-2.849625
H	-2.075995	-2.153565	-1.476860
H	-0.630233	-2.096535	0.521568
H	-1.654810	-1.835228	4.710704
H	-2.577193	0.364017	5.417573
H	-1.927501	2.419982	4.180976
H	-0.402296	2.288170	2.260859
H	4.330602	-3.628743	2.666347
H	5.408017	-2.244985	3.010821
H	4.142881	-2.702087	4.158822

V a (mPW2PLYP)

39

FINAL HEAT OF FORMATION = 0.000000

C	-1.035911	0.090948	0.444173
C	-1.088503	0.301552	1.915852
Pd	1.751340	0.002696	1.946703
N	1.347127	1.939071	1.044224
C	0.425356	2.138757	0.073617
C	-0.353059	0.974548	-0.421137
O	2.495738	-1.889536	2.761961
C	3.725356	-1.684024	2.471653
O	4.113621	-0.632032	1.894620
C	-0.385775	0.746564	-1.803286
C	-1.064501	-0.346472	-2.336570
C	-1.726983	-1.227613	-1.484202
C	-1.712746	-1.003730	-0.109296
C	2.075918	2.984965	1.474851
C	1.929363	4.269989	0.968126
C	0.986234	4.483597	-0.033379
C	0.228445	3.407094	-0.481669
C	-1.506523	1.528412	2.459404
C	-1.588144	1.701962	3.837228
C	-1.254103	0.655703	4.702223
C	-0.851152	-0.569779	4.178330
C	-0.773396	-0.751654	2.792854
C	4.728145	-2.743804	2.875723
H	-0.497111	-1.720038	2.391178
H	-0.523777	3.539171	-1.248293
H	2.541885	5.074572	1.352466
H	0.838153	5.470372	-0.454314
H	2.802343	2.767940	2.247493

H 0.151709 1.419529 -2.461588

H -1.069257 -0.509501 -3.407544

H -2.261330 -2.080380 -1.885945

H -2.253735 -1.672092 0.550819

H -0.601700 -1.391737 4.839101

H -1.318284 0.795113 5.774875

H -1.920549 2.652186 4.238985

H -1.780152 2.341031 1.796322

H 4.332253 -3.738663 2.669302

H 5.673275 -2.602750 2.353822

H 4.907578 -2.675943 3.951762

IV a (mPW2PLYP)

39

FINAL HEAT OF FORMATION = 0.000000

C 2.289248 -2.876622 -1.200896

C 1.981319 -1.614588 -0.678925

C 0.668281 -1.384267 -0.250375

C -0.327523 -2.339757 -0.302536

C 0.005835 -3.597457 -0.821633

C 1.300470 -3.855982 -1.274681

Pd 0.347525 0.428786 0.512980

C -0.160530 1.096099 -1.328078

C -1.230743 0.516773 -1.992477

C -1.626663 1.088795 -3.205625

C -0.965871 2.206648 -3.712452

C 0.100008 2.764590 -3.009935

C 0.522631 2.207719 -1.796993

C 2.924274 -0.518603 -0.480041

N 2.369065 0.568369 0.118037

C 3.109690 1.638575 0.449430

C 4.466274 1.688176 0.164872

C 5.052978 0.598775 -0.479295

C 4.281175 -0.513646 -0.797982

O -0.902621 2.214791 1.483802

C -1.847823 1.396185 1.439407

C -3.224878 1.688853 1.950544

O -1.641311 0.214423 0.923893

H -1.759575 -0.334793 -1.592712

H 4.726133 -1.371647 -1.282888

H 5.040301 2.562443 0.438284

H 6.106964 0.612445 -0.725324

H 2.590224 2.451804 0.940759

H 3.293437 -3.098110 -1.542051

H 1.543608 -4.828958 -1.682765

H -0.753815 -4.368014 -0.874607

H -1.331580 -2.127613 0.044138

H -2.460977 0.652499 -3.742045

H -1.283689 2.644477 -4.650735

H 0.616500 3.636911 -3.392364

H 1.346491 2.654892 -1.260774

H -3.946510 1.571522 1.140489

H -3.482765 0.972779 2.732731

H -3.270036 2.701071 2.346161

TS (IV-VI) a (mPW2PLYP)

39

FINAL HEAT OF FORMATION = 0.000000

C -0.404350 -0.069824 0.249257

C -0.200544 -0.034550 2.336814

Pd	1.486957	0.015613	1.173836
N	1.429330	-1.987774	1.553081
C	0.515485	-2.375419	2.480375
C	-0.297163	-1.275897	2.998535
O	1.796855	2.025722	0.895682
C	3.067767	1.894807	0.675306
O	3.556289	0.726911	0.710608
C	-0.816217	1.107520	2.835086
C	-1.590193	1.002694	3.991761
C	-1.738504	-0.227777	4.635026
C	-1.087050	-1.359097	4.150037
C	-0.938376	-1.273332	-0.209130
C	-1.861514	-1.238947	-1.256241
C	-2.242433	-0.027743	-1.830395
C	-1.694573	1.164064	-1.356750
C	-0.771781	1.153757	-0.310526
C	2.277739	-2.858456	0.988332
C	2.243743	-4.204923	1.325008
C	1.308875	-4.635014	2.265843
C	0.438849	-3.717513	2.848214
C	3.885225	3.111289	0.396094
H	-0.345962	2.082751	0.041305
H	-0.290307	-4.038806	3.579057
H	2.930462	-4.892847	0.851996
H	1.255314	-5.679631	2.543929
H	2.972926	-2.456687	0.263061
H	-1.167941	-2.296355	4.686820
H	-2.348517	-0.302578	5.526259
H	-2.082541	1.884738	4.382450
H	-0.719079	2.057983	2.327636
H	-1.978755	2.112534	-1.796679
H	-2.961131	-0.012151	-2.640441
H	-2.279676	-2.171918	-1.614838
H	-0.670640	-2.225416	0.222465
H	3.451548	3.656600	-0.443467
H	3.864672	3.767896	1.268009
H	4.911549	2.829803	0.170353

VI a (mPW2PLYP)

39

FINAL HEAT OF FORMATION = 0.000000

C	-0.982779	0.113943	0.913820
C	-1.236406	-0.217801	2.344777
Pd	1.311284	-0.099272	0.571068
N	1.363200	-1.803690	1.661863
C	0.428977	-2.185328	2.564056
C	-0.583342	-1.234675	3.086997
O	1.789726	1.554746	-0.604039
C	3.032937	1.424587	-0.316595
O	3.350497	0.452988	0.455973
C	-2.233371	0.534024	2.988561
C	-2.553956	0.348417	4.328538
C	-1.868842	-0.607331	5.071017
C	-0.903754	-1.388235	4.447115
C	-0.787175	-0.882264	-0.091302
C	-0.853433	-0.549984	-1.464142
C	-1.089408	0.754379	-1.851750
C	-1.250969	1.757617	-0.875431
C	-1.194631	1.453462	0.469119

C	2.344217	-2.643832	1.273369
C	2.435598	-3.938728	1.753774
C	1.455759	-4.381356	2.638669
C	0.455270	-3.505178	3.037953
C	4.057403	2.376585	-0.830505
H	-1.305239	2.240795	1.202705
H	-0.323814	-3.840830	3.706875
H	3.241398	-4.578857	1.422739
H	1.465887	-5.397522	3.011468
H	3.056941	-2.243727	0.564572
H	-0.362359	-2.117282	5.035533
H	-2.081430	-0.751033	6.122926
H	-3.330544	0.950983	4.783108
H	-2.791285	1.263822	2.417590
H	-1.417651	2.782591	-1.182486
H	-1.151464	1.008574	-2.902427
H	-0.742266	-1.337688	-2.198423
H	-0.774086	-1.928765	0.185678
H	3.685098	2.886693	-1.717163
H	4.270030	3.118583	-0.057125
H	4.980320	1.842619	-1.054707

III a (MP2)

39

scf done: -1061.924210

Pd	0.128644	0.277857	0.451697
C	0.657590	-1.350152	-0.495570
C	2.038290	-1.551654	-0.705728
C	2.933247	-0.455764	-0.305119
N	2.321945	0.525892	0.412997
O	-0.794377	2.009149	1.520442
C	-1.919975	1.401409	1.659599
O	-2.092854	0.205891	1.254043
C	-0.337285	0.840078	-1.414977
C	-1.645134	0.666214	-1.869476
C	0.610510	1.516922	-2.183721
C	0.233149	2.046464	-3.426396
C	-1.075390	1.884226	-3.893876
C	-2.013337	1.198962	-3.113409
C	4.294878	-0.352718	-0.619078
C	5.020232	0.754996	-0.179743
C	4.372978	1.751638	0.554761
C	3.013188	1.604209	0.825281
C	-0.248511	-2.350529	-0.852775
C	0.206966	-3.556678	-1.398547
C	1.577104	-3.756863	-1.602639
C	2.493343	-2.762614	-1.253341
C	-3.049606	2.148349	2.329438
H	-2.376112	0.148470	-1.254632
H	4.781763	-1.123901	-1.208134
H	4.905966	2.627344	0.910178
H	6.077173	0.842897	-0.416796
H	2.451654	2.346550	1.386630
H	3.556838	-2.942943	-1.401504
H	1.933381	-4.692387	-2.027063
H	-0.504387	-4.333003	-1.673093
H	-1.316455	-2.192614	-0.705120
H	-3.033234	1.071022	-3.470576

H	-1.363319	2.292657	-4.859266
H	0.968030	2.577605	-4.027928
H	1.629079	1.646431	-1.828192
H	-3.962680	1.552574	2.327990
H	-2.766329	2.383078	3.359219
H	-3.221105	3.094236	1.808937

TS (III-V) a (MP2)

39

scf done: -1061.920210

C	-0.002141	-0.050150	0.188020
C	-0.042554	0.138510	2.352769
Pd	1.665095	-0.026728	1.259482
N	1.673501	2.051950	0.496544
C	0.551438	2.313735	-0.226465
C	-0.231291	1.118965	-0.570599
O	2.316721	-2.191509	1.872063
C	3.337035	-1.689553	2.454006
O	3.575850	-0.429933	2.439741
C	-1.138903	1.087529	-1.641902
C	-1.809611	-0.095360	-1.957528
C	-1.564545	-1.259626	-1.219547
C	-0.667921	-1.232764	-0.146213
C	2.460952	3.061136	0.911677
C	2.177664	4.391446	0.603308
C	1.030134	4.677698	-0.140512
C	0.203651	3.631135	-0.551633
C	-0.526021	1.390344	2.746649
C	-1.403878	1.480549	3.835713
C	-1.801710	0.329670	4.523989
C	-1.307384	-0.918128	4.126793
C	-0.431989	-1.018487	3.037753
C	4.265184	-2.605244	3.219651
H	-0.034017	-1.986464	2.744876
H	-0.709256	3.836976	-1.102766
H	2.840278	5.180641	0.943809
H	0.772879	5.704880	-0.385047
H	3.335001	2.777786	1.492151
H	-1.300783	1.975937	-2.249950
H	-2.509656	-0.113514	-2.788991
H	-2.078643	-2.184692	-1.471651
H	-0.500345	-2.133026	0.441711
H	-1.602639	-1.819664	4.659871
H	-2.485977	0.404740	5.365349
H	-1.779137	2.455980	4.138102
H	-0.232303	2.295565	2.223777
H	4.381243	-3.552198	2.689006
H	5.237341	-2.133572	3.367934
H	3.823885	-2.818538	4.198506

IV a (MP2)

39

scf done: -1061.793980

C	2.242168	-2.862860	-1.265214
C	1.955275	-1.610810	-0.699080
C	0.663738	-1.400091	-0.198306
C	-0.336945	-2.357364	-0.216397
C	-0.024654	-3.603629	-0.779370
C	1.249227	-3.844020	-1.309791
Pd	0.351162	0.404444	0.578668

C	-0.117796	1.071464	-1.250750
C	-1.131714	0.447516	-1.972062
C	-1.504112	1.006656	-3.201945
C	-0.878972	2.162029	-3.678106
C	0.125456	2.771163	-2.922038
C	0.521965	2.226273	-1.692491
C	2.893380	-0.512048	-0.513940
N	2.347831	0.548659	0.146177
C	3.082583	1.627638	0.481898
C	4.428854	1.703454	0.137585
C	5.007218	0.647113	-0.570616
C	4.238753	-0.470653	-0.889992
O	-0.879785	2.208362	1.492514
C	-1.846060	1.404116	1.427057
C	-3.234090	1.732967	1.883441
O	-1.650611	0.200031	0.936544
H	-1.637849	-0.435163	-1.599040
H	4.677500	-1.306196	-1.426528
H	5.003162	2.581262	0.414634
H	6.052384	0.689196	-0.863176
H	2.569430	2.416868	1.024442
H	3.230590	-3.074647	-1.667097
H	1.473422	-4.810143	-1.753872
H	-0.784870	-4.380377	-0.811180
H	-1.326130	-2.151892	0.185463
H	-2.294476	0.530869	-3.778139
H	-1.178343	2.590500	-4.631100
H	0.612646	3.676078	-3.277873
H	1.294351	2.718773	-1.111446
H	-3.930125	1.599371	1.051780
H	-3.525113	1.043811	2.680335
H	-3.273931	2.759624	2.246350

TS (IV-VI) a (MP2)

39

scf done: -1061.768830

C	-0.427151	-0.136049	0.269645
C	-0.247991	0.005093	2.229586
Pd	1.446777	0.049693	1.121881
N	1.426230	-1.902296	1.527287
C	0.517747	-2.300149	2.462165
C	-0.311802	-1.207326	2.954451
O	1.769608	2.060116	0.826351
C	3.057698	1.884768	0.789844
O	3.497565	0.690616	0.931360
C	-0.875344	1.161627	2.702140
C	-1.628935	1.088587	3.874916
C	-1.752320	-0.122574	4.570925
C	-1.082387	-1.261505	4.125013
C	-0.965876	-1.363259	-0.142767
C	-1.879858	-1.383275	-1.200090
C	-2.253260	-0.203842	-1.849703
C	-1.698431	1.011344	-1.438265
C	-0.787720	1.054269	-0.380198
C	2.284926	-2.760162	0.945762
C	2.263922	-4.109630	1.286795
C	1.342616	-4.554718	2.239305
C	0.462813	-3.648240	2.829051
C	3.964628	3.056427	0.624386

H	-0.362026	2.005617	-0.077592
H	-0.261334	-3.981174	3.566100
H	2.954413	-4.793684	0.804910
H	1.305528	-5.604311	2.516042
H	2.968054	-2.342603	0.212145
H	-1.133416	-2.180629	4.704300
H	-2.353334	-0.170038	5.474908
H	-2.129715	1.981060	4.241836
H	-0.802699	2.095910	2.153524
H	-1.970201	1.937929	-1.938201
H	-2.967754	-0.231606	-2.668189
H	-2.299195	-2.336924	-1.511763
H	-0.713564	-2.298194	0.343478
H	4.095395	3.539690	1.597327
H	4.935821	2.724430	0.256868
H	3.516905	3.777037	-0.061766

$Ru(II)(bpy)_3^{2+}$ Ired (Def2-SVP)

61

scf done: -1578.693140

C	2.983735	-0.593589	-0.421946
N	2.480831	0.421986	0.324354
C	3.311841	1.350399	0.817044
C	4.681626	1.320839	0.591082
C	5.209846	0.284985	-0.173990
C	4.350881	-0.681248	-0.684459
Ru	0.418545	0.378803	0.631397
H	4.747726	-1.503100	-1.286048
C	1.990945	-1.556175	-0.922563
N	0.710672	-1.321122	-0.539687
N	0.783960	-0.502915	2.487686
H	5.317967	2.103451	1.013016
H	6.284105	0.227192	-0.373729
H	2.855258	2.151036	1.410560
C	2.308261	-2.645984	-1.733424
C	1.297906	-3.501337	-2.157112
H	3.341953	-2.826953	-2.039126
H	1.534939	-4.358606	-2.794619
C	-0.011582	-3.248654	-1.758555
C	-0.260926	-2.147737	-0.949642
H	-0.839386	-3.893460	-2.066146
H	-1.276868	-1.915947	-0.609035
N	-0.121628	1.391288	-1.108699
C	-1.455041	1.498004	-1.334806
C	-1.939723	2.162250	-2.461494
C	-1.043671	2.720613	-3.365669
C	0.322014	2.600292	-3.124532
C	0.739814	1.926160	-1.984580
C	-2.317253	0.885162	-0.313485
H	-3.015859	2.246596	-2.633537
H	-1.412396	3.246650	-4.251541
H	1.063948	3.022570	-3.807763
H	1.805689	1.814365	-1.753465
C	-3.710980	0.899907	-0.365486
C	-4.440501	0.288176	0.647114
C	-3.758899	-0.326792	1.693442
C	-2.370362	-0.305253	1.686949
N	-1.664296	0.281836	0.711595

H	-4.229214	1.387821	-1.195059
H	-5.534165	0.292572	0.616538
H	-4.289359	-0.822324	2.511237
H	-1.794205	-0.781786	2.488516
C	0.788950	0.345164	3.547180
C	1.011022	-0.125864	4.841199
C	1.231835	-1.482386	5.047445
C	1.228182	-2.341237	3.951905
C	1.001945	-1.809484	2.689036
C	0.533837	1.757065	3.224769
H	1.008724	0.563651	5.689479
H	1.403799	-1.864944	6.058195
H	1.396489	-3.415682	4.064959
H	0.985057	-2.450143	1.799492
C	0.510605	2.778546	4.174616
C	0.265454	4.085267	3.769251
C	0.046446	4.343400	2.419175
C	0.084681	3.282836	1.523906
N	0.324657	2.022327	1.910826
H	0.685751	2.557906	5.230728
H	0.246024	4.894611	4.505364
H	-0.150168	5.354852	2.053287
H	-0.074800	3.444443	0.451481

$Ru(III)(bpy)_3^{3+}$ Iox (Def2-SVP)

61

scf done: -1578.479904

C	2.993915	-0.624367	-0.401763
N	2.498319	0.385124	0.358362
C	3.323774	1.291796	0.897117
C	4.696572	1.243799	0.696082
C	5.221167	0.215489	-0.080163
C	4.362104	-0.729160	-0.633099
Ru	0.420789	0.385855	0.623522
H	4.760118	-1.543712	-1.243079
C	1.994220	-1.556740	-0.937524
N	0.709339	-1.291425	-0.590178
N	0.849958	-0.487795	2.476272
H	5.336284	2.006501	1.146789
H	6.298366	0.144467	-0.256821
H	2.868084	2.086399	1.498294
C	2.296764	-2.646005	-1.749247
C	1.267136	-3.465298	-2.201583
H	3.331345	-2.856404	-2.030910
H	1.493550	-4.325095	-2.839060
C	-0.044606	-3.178384	-1.837141
C	-0.284308	-2.075296	-1.029379
H	-0.882102	-3.796900	-2.169424
H	-1.301425	-1.813938	-0.716845
N	-0.118829	1.346829	-1.155683
C	-1.452735	1.491818	-1.361149
C	-1.925086	2.135736	-2.500728
C	-1.015879	2.632425	-3.429718
C	0.347581	2.469566	-3.206267
C	0.758165	1.813949	-2.053568
C	-2.316825	0.933318	-0.313048
H	-2.998826	2.253236	-2.665355
H	-1.376624	3.144489	-4.326665
H	1.093980	2.844254	-3.911091

H	1.821527	1.665926	-1.835021
C	-3.707215	0.988330	-0.339705
C	-4.432080	0.429100	0.707779
C	-3.754012	-0.175125	1.761520
C	-2.366314	-0.195071	1.734446
N	-1.670263	0.341409	0.723599
H	-4.226556	1.466878	-1.173535
H	-5.525164	0.466958	0.697237
H	-4.284380	-0.630094	2.601787
H	-1.791664	-0.666027	2.539607
C	0.827696	0.350285	3.543939
C	1.100314	-0.125312	4.822934
C	1.396118	-1.472865	5.000481
C	1.419462	-2.317815	3.895351
C	1.145469	-1.783961	2.643549
C	0.495389	1.747415	3.241436
H	1.081163	0.550770	5.681100
H	1.608127	-1.859242	6.001792
H	1.646974	-3.382448	3.990169
H	1.149602	-2.413614	1.747206
C	0.420468	2.756122	4.197605
C	0.085731	4.046999	3.801690
C	-0.170555	4.304399	2.458860
C	-0.080457	3.257226	1.552361
N	0.249554	2.016287	1.934221
H	0.621972	2.540407	5.249641
H	0.023177	4.847215	4.545022
H	-0.437886	5.303592	2.105998
H	-0.265843	3.418020	0.484604

III a (Def2-SVP)

39

scf done: -1065.381679

Pd	0.142099	0.298465	0.428805
C	0.700991	-1.352276	-0.548223
C	2.088591	-1.547489	-0.704727
C	2.979247	-0.465624	-0.264447
N	2.364887	0.549149	0.378660
O	-0.800465	2.000111	1.536524
C	-1.903363	1.397011	1.685348
O	-2.069250	0.219325	1.273817
C	-0.389723	0.871244	-1.453819
C	-1.733215	0.796985	-1.818568
C	0.551303	1.447061	-2.304977
C	0.134304	1.977509	-3.529743
C	-1.208464	1.920311	-3.901924
C	-2.138394	1.330122	-3.046056
C	4.360578	-0.421966	-0.475918
C	5.084588	0.674922	-0.021299
C	4.425242	1.714602	0.632927
C	3.049984	1.606158	0.808554
C	-0.199389	-2.334809	-0.944677
C	0.272347	-3.536841	-1.479377
C	1.644422	-3.744179	-1.632700
C	2.546496	-2.755576	-1.249443
C	-3.050341	2.127759	2.325548
H	-2.468937	0.341674	-1.144170
H	4.866553	-1.237039	-1.002224
H	4.962345	2.593145	1.001844

H	6.166834	0.720082	-0.182842
H	2.471836	2.389856	1.315680
H	3.622099	-2.936268	-1.364404
H	2.015756	-4.685337	-2.053208
H	-0.438331	-4.313483	-1.785814
H	-1.279701	-2.165080	-0.840452
H	-3.196565	1.282077	-3.331531
H	-1.531511	2.334745	-4.864049
H	0.873086	2.435065	-4.199169
H	1.613377	1.493606	-2.031670
H	-3.754112	1.424778	2.800719
H	-2.688682	2.864740	3.061632
H	-3.600658	2.678763	1.539881

TS (III-V) a (Def2-SVP)

39

scf done: -1065.377838

C	-0.016975	-0.046506	0.175266
C	-0.067125	0.113827	2.364054
Pd	1.689457	-0.030843	1.273431
N	1.661392	2.069149	0.520200
C	0.569711	2.315917	-0.233045
C	-0.228938	1.132183	-0.574405
O	2.333595	-2.173677	1.923447
C	3.352833	-1.679744	2.474729
O	3.588638	-0.437882	2.429947
C	-1.147210	1.113580	-1.632535
C	-1.829762	-0.054666	-1.958752
C	-1.593277	-1.223054	-1.232024
C	-0.696253	-1.215621	-0.163689
C	2.447044	3.063740	0.928558
C	2.194759	4.390190	0.595599
C	1.075103	4.668158	-0.187201
C	0.254322	3.626395	-0.605718
C	-0.557884	1.355243	2.774207
C	-1.434109	1.428456	3.859764
C	-1.824794	0.272013	4.532877
C	-1.331094	-0.965338	4.117587
C	-0.457060	-1.049480	3.032962
C	4.299596	-2.569928	3.230346
H	-0.060830	-2.024182	2.723396
H	-0.641443	3.832166	-1.199701
H	2.862131	5.183337	0.945005
H	0.834697	5.700251	-0.464184
H	3.311631	2.782286	1.544176
H	-1.307619	2.016078	-2.234629
H	-2.538643	-0.057256	-2.793789
H	-2.120523	-2.148466	-1.491702
H	-0.537633	-2.131379	0.419876
H	-1.624317	-1.880917	4.645589
H	-2.514202	0.334130	5.382591
H	-1.813029	2.406887	4.179146
H	-0.267329	2.280685	2.260983
H	4.119486	-3.633458	3.005008
H	5.345597	-2.305632	2.997914
H	4.157202	-2.410625	4.315164

V a (Def2-SVP)

39

scf done: -1065.445112

C	-1.104117	0.102497	0.362207
C	-1.040029	0.222201	1.840488
Pd	1.566198	-0.090534	1.977048
N	1.338479	1.810433	0.950934
C	0.426953	2.095766	0.000176
C	-0.456760	1.015908	-0.498669
O	2.429869	-1.877286	2.976515
C	3.618715	-1.512123	2.745368
O	3.872421	-0.448412	2.123535
C	-0.619143	0.882337	-1.883642
C	-1.387248	-0.143782	-2.426975
C	-2.011208	-1.055703	-1.579488
C	-1.870152	-0.925489	-0.199723
C	2.170683	2.768307	1.376651
C	2.139407	4.068905	0.889307
C	1.199634	4.380602	-0.089000
C	0.340016	3.384791	-0.538166
C	-1.404890	1.421810	2.486163
C	-1.431654	1.502734	3.871069
C	-1.094726	0.389552	4.652151
C	-0.745711	-0.804504	4.035260
C	-0.722452	-0.897349	2.634945
C	4.759591	-2.356461	3.245410
H	-0.517145	-1.863907	2.156185
H	-0.417657	3.599238	-1.298748
H	2.840596	4.815305	1.273759
H	1.132453	5.393969	-0.499107
H	2.901468	2.466865	2.138355
H	-0.100445	1.581561	-2.550436
H	-1.488726	-0.233944	-3.513887
H	-2.619924	-1.868449	-1.991031
H	-2.387693	-1.623577	0.469391
H	-0.487310	-1.684766	4.634619
H	-1.116339	0.458897	5.745368
H	-1.726204	2.441359	4.354210
H	-1.686287	2.292635	1.880377
H	4.410018	-3.335746	3.610768
H	5.507733	-2.498856	2.446187
H	5.268731	-1.828762	4.072872

IV a (Def2-SVP)

39

scf done: -1065.212221

C	2.279179	-2.883760	-1.235600
C	1.974886	-1.629476	-0.694875
C	0.666065	-1.411037	-0.244654
C	-0.324496	-2.370304	-0.285898
C	0.008577	-3.620793	-0.822449
C	1.295324	-3.867741	-1.301481
Pd	0.332533	0.399501	0.525175
C	-0.165860	1.078064	-1.316643
C	-1.171306	0.453182	-2.035286
C	-1.547274	1.036768	-3.249286
C	-0.935258	2.205891	-3.696226
C	0.060030	2.809926	-2.931878
C	0.463100	2.245802	-1.716798
C	2.908353	-0.529486	-0.490634
N	2.352278	0.544110	0.123988
C	3.081664	1.613886	0.455090

C	4.436427	1.681000	0.164084
C	5.027379	0.601765	-0.491049
C	4.262405	-0.513320	-0.816782
O	-0.871891	2.199690	1.443772
C	-1.839129	1.417443	1.413847
C	-3.188736	1.761588	1.943602
O	-1.670662	0.233973	0.923182
H	-1.676341	-0.447822	-1.678187
H	4.716516	-1.372847	-1.317847
H	5.010302	2.567977	0.444660
H	6.091855	0.625311	-0.744674
H	2.553032	2.432080	0.960673
H	3.290759	-3.096721	-1.599695
H	1.538184	-4.846030	-1.728764
H	-0.755725	-4.404175	-0.870060
H	-1.337290	-2.166491	0.081819
H	-2.339131	0.562095	-3.839580
H	-1.243205	2.655394	-4.646349
H	0.538233	3.736410	-3.268919
H	1.231304	2.743494	-1.117459
H	-3.974990	1.394083	1.263479
H	-3.331516	1.259598	2.917802
H	-3.280054	2.849317	2.087240

TS (IV-VI) a (Def2-SVP)

39

scf done: -1065.205287

C	-0.323654	-0.059245	0.186364
C	-0.171885	-0.026300	2.417804
Pd	1.476593	0.037467	1.226453
N	1.436535	-1.966176	1.622672
C	0.514886	-2.364354	2.532696
C	-0.309821	-1.276742	3.047257
O	1.796668	2.046452	0.901508
C	3.047320	1.898007	0.655029
O	3.518094	0.731972	0.701587
C	-0.822973	1.108276	2.870586
C	-1.662192	0.990868	3.982297
C	-1.839537	-0.242413	4.609209
C	-1.164348	-1.370406	4.150367
C	-0.814871	-1.272808	-0.283839
C	-1.770972	-1.244659	-1.302744
C	-2.223028	-0.034273	-1.821641
C	-1.714385	1.165481	-1.326704
C	-0.758401	1.164832	-0.309958
C	2.287001	-2.822302	1.052941
C	2.251609	-4.174848	1.364965
C	1.308595	-4.618239	2.290800
C	0.435749	-3.710002	2.882746
C	3.885370	3.079079	0.329678
H	-0.357697	2.111010	0.066743
H	-0.307775	-4.045024	3.611537
H	2.951524	-4.862445	0.883451
H	1.251846	-5.679041	2.554123
H	2.999598	-2.403622	0.332241
H	-1.282823	-2.325968	4.673286
H	-2.504806	-0.324052	5.474574
H	-2.186685	1.878322	4.352385
H	-0.700723	2.076343	2.372662

H	-2.060584	2.124035	-1.729265
H	-2.975517	-0.025202	-2.617255
H	-2.160785	-2.194310	-1.686177
H	-0.483096	-2.240428	0.102581
H	3.279344	3.997490	0.289991
H	4.675419	3.188413	1.093282
H	4.386745	2.916837	-0.640464

VI a (Def2-SVP)

39

scf done: -1065.271280

C	-0.969348	0.115185	0.913134
C	-1.214858	-0.203123	2.345939
Pd	1.298413	-0.121830	0.553061
N	1.351545	-1.822934	1.646189
C	0.426808	-2.189970	2.559585
C	-0.575154	-1.232790	3.085052
O	1.784468	1.547524	-0.606651
C	3.014332	1.439202	-0.298823
O	3.335127	0.475456	0.463483
C	-2.190105	0.567267	2.999237
C	-2.512383	0.383900	4.338537
C	-1.848207	-0.590453	5.074039
C	-0.901285	-1.386189	4.442977
C	-0.762870	-0.892184	-0.079700
C	-0.834703	-0.580538	-1.459216
C	-1.079848	0.713428	-1.864304
C	-1.246212	1.729707	-0.900233
C	-1.189754	1.446273	0.446235
C	2.316418	-2.666097	1.245590
C	2.406866	-3.961874	1.723745
C	1.436737	-4.393083	2.623709
C	0.451985	-3.507655	3.038874
C	4.021468	2.414258	-0.781722
H	-1.307062	2.254518	1.174878
H	-0.326897	-3.843380	3.728246
H	3.210644	-4.616342	1.377005
H	1.442170	-5.420560	3.001011
H	3.032545	-2.273589	0.513953
H	-0.368854	-2.135500	5.037179
H	-2.063283	-0.737923	6.137287
H	-3.282735	1.008967	4.801874
H	-2.743025	1.321099	2.431055
H	-1.417544	2.761212	-1.225001
H	-1.142803	0.955864	-2.930002
H	-0.717617	-1.386513	-2.190420
H	-0.760174	-1.949972	0.207524
H	3.678283	2.898943	-1.709713
H	4.160496	3.194736	-0.011399
H	4.992756	1.916991	-0.938448

III a (M06-L)

39

scf done: -1065.548845

Pd	0.091301	0.302264	0.431365
C	0.691418	-1.372454	-0.491291
C	2.079973	-1.547925	-0.667805
C	2.972830	-0.453789	-0.280717
N	2.376882	0.562968	0.388737
O	-0.915571	2.014678	1.531527

C	-2.005194	1.372520	1.666023
O	-2.143419	0.190259	1.225725
C	-0.386616	0.904866	-1.450859
C	-1.726804	0.904387	-1.831292
C	0.595294	1.406288	-2.301551
C	0.224395	1.942983	-3.537120
C	-1.114183	1.962854	-3.922221
C	-2.085872	1.443198	-3.069917
C	4.339688	-0.392892	-0.571700
C	5.077922	0.712030	-0.170085
C	4.445549	1.749141	0.512300
C	3.085177	1.630325	0.765935
C	-0.196954	-2.376789	-0.857857
C	0.283777	-3.581307	-1.375564
C	1.655675	-3.771989	-1.541190
C	2.545503	-2.763880	-1.191267
C	-3.154497	2.041370	2.368634
H	-2.488076	0.501999	-1.165150
H	4.818940	-1.198818	-1.121155
H	4.989392	2.630293	0.840117
H	6.140401	0.767310	-0.395937
H	2.531366	2.407688	1.290553
H	3.615122	-2.931345	-1.312694
H	2.032871	-4.709548	-1.943674
H	-0.415550	-4.367609	-1.656151
H	-1.270467	-2.224530	-0.742575
H	-3.134739	1.452293	-3.364155
H	-1.399169	2.378994	-4.886854
H	0.992176	2.341030	-4.199664
H	1.646492	1.389038	-2.016900
H	-4.049263	1.414746	2.363945
H	-2.879430	2.262835	3.405691
H	-3.380481	2.999815	1.889301

TS (III-V) a (M06-L)

39

scf done: -1065.542289

C	-0.031294	-0.046977	0.214944
C	-0.114101	0.116650	2.341099
Pd	1.693165	-0.041955	1.309843
N	1.663074	2.080953	0.537737
C	0.556634	2.320524	-0.207921
C	-0.230210	1.133226	-0.541038
O	2.333718	-2.182813	1.966355
C	3.381180	-1.695388	2.494217
O	3.633370	-0.449922	2.444801
C	-1.122133	1.108665	-1.621780
C	-1.792426	-0.058632	-1.965559
C	-1.570289	-1.226349	-1.234380
C	-0.702194	-1.216213	-0.145332
C	2.446551	3.094550	0.919113
C	2.184475	4.412149	0.566843
C	1.052198	4.676382	-0.201212
C	0.230558	3.626319	-0.587940
C	-0.576686	1.361542	2.772523
C	-1.428666	1.439976	3.875006
C	-1.827898	0.285878	4.544547
C	-1.371784	-0.955603	4.103586
C	-0.524962	-1.045503	3.000142

C	4.336406	-2.603374	3.216857
H	-0.166273	-2.018416	2.669173
H	-0.672020	3.817087	-1.163050
H	2.851337	5.206651	0.889072
H	0.804874	5.695951	-0.487463
H	3.312647	2.825566	1.521697
H	-1.261347	2.004962	-2.225323
H	-2.475556	-0.062924	-2.811908
H	-2.084583	-2.147161	-1.504631
H	-0.560963	-2.122569	0.442660
H	-1.672551	-1.865666	4.621143
H	-2.492443	0.352061	5.403674
H	-1.778832	2.416048	4.208189
H	-0.279546	2.277783	2.265468
H	4.138129	-3.654853	2.995044
H	5.370790	-2.359275	2.956205
H	4.234798	-2.453307	4.298047

V a (M06-L)

39

scf done: -1065.601895

C	-1.012829	0.080352	0.420790
C	-1.024478	0.260705	1.891540
Pd	1.625326	-0.031883	1.970835
N	1.329782	1.913134	1.019002
C	0.419251	2.139346	0.040796
C	-0.389041	1.003816	-0.449475
O	2.384931	-1.934342	2.842165
C	3.597616	-1.644500	2.578476
O	3.909343	-0.563335	1.996353
C	-0.499032	0.822521	-1.833138
C	-1.184577	-0.262984	-2.367729
C	-1.776398	-1.188211	-1.512631
C	-1.692949	-1.009623	-0.135625
C	2.089543	2.935877	1.444557
C	1.989211	4.222118	0.933439
C	1.060438	4.462741	-0.074032
C	0.273366	3.410622	-0.522192
C	-1.381271	1.491957	2.474193
C	-1.455748	1.630232	3.853012
C	-1.176412	0.545076	4.688634
C	-0.833256	-0.681907	4.133331
C	-0.762736	-0.830427	2.744922
C	4.682453	-2.596547	2.999051
H	-0.532082	-1.803886	2.313366
H	-0.473535	3.563011	-1.297618
H	2.629218	5.009903	1.320294
H	0.946513	5.456048	-0.501649
H	2.810353	2.692734	2.223008
H	-0.003355	1.529199	-2.497587
H	-1.245950	-0.388625	-3.446356
H	-2.314786	-2.043639	-1.915643
H	-2.189640	-1.711854	0.532793
H	-0.616381	-1.535440	4.772643
H	-1.235469	0.658926	5.769076
H	-1.742814	2.588322	4.282269
H	-1.614213	2.338845	1.829488
H	4.293422	-3.608870	3.136402
H	5.496972	-2.607866	2.269038

H	5.106361	-2.265526	3.954652

IV a (M06-L)

39

scf done: -1065.393274

C	2.306956	-2.874734	-1.223560
C	1.993412	-1.623823	-0.677290
C	0.673868	-1.408398	-0.259085
C	-0.319738	-2.358779	-0.356066
C	0.021893	-3.602296	-0.901443
C	1.322931	-3.850851	-1.335894
Pd	0.324364	0.400320	0.527973
C	-0.177821	1.092552	-1.306888
C	-1.223328	0.484188	-1.978104
C	-1.616174	1.043214	-3.196707
C	-0.975518	2.173641	-3.695103
C	0.065752	2.759014	-2.981555
C	0.486997	2.216619	-1.762125
C	2.927899	-0.533675	-0.462181
N	2.368459	0.553426	0.133186
C	3.101815	1.626338	0.455772
C	4.459272	1.680084	0.178332
C	5.053168	0.588871	-0.452433
C	4.286909	-0.524103	-0.770493
O	-0.880483	2.203614	1.456513
C	-1.858082	1.419815	1.426691
C	-3.204469	1.773361	1.959029
O	-1.702796	0.227995	0.930943
H	-1.737335	-0.382866	-1.576849
H	4.735498	-1.388641	-1.251710
H	5.029045	2.562427	0.450303
H	6.112962	0.603700	-0.692254
H	2.572433	2.444181	0.939986
H	3.321958	-3.083877	-1.557118
H	1.572763	-4.817233	-1.766522
H	-0.742336	-4.371352	-0.989886
H	-1.335883	-2.154973	-0.022599
H	-2.435974	0.582208	-3.743642
H	-1.292522	2.604078	-4.642130
H	0.568116	3.647545	-3.358557
H	1.294322	2.685513	-1.207526
H	-3.991801	1.411337	1.292362
H	-3.349665	1.286738	2.929927
H	-3.291344	2.853168	2.094040

TS (IV-VI) a (M06-L)

39

scf done: -1065.382374

C	-0.382730	-0.059185	0.231911
C	-0.209134	-0.031124	2.355699
Pd	1.477238	0.047420	1.194911
N	1.439223	-1.975795	1.593933
C	0.505682	-2.368155	2.500777
C	-0.321985	-1.281211	2.998702
O	1.809615	2.077875	0.873824
C	3.073593	1.919714	0.664930
O	3.544424	0.743322	0.732579
C	-0.848327	1.100869	2.836804
C	-1.657084	0.984001	3.967102
C	-1.819557	-0.250409	4.595624

C	-1.151045	-1.373124	4.121790
C	-0.881071	-1.270528	-0.237507
C	-1.810694	-1.245249	-1.277708
C	-2.231551	-0.037420	-1.825451
C	-1.720278	1.161633	-1.334054
C	-0.791243	1.162245	-0.295217
C	2.302897	-2.839147	1.049494
C	2.271160	-4.185596	1.383714
C	1.320843	-4.621608	2.303492
C	0.435020	-3.711264	2.866632
C	3.922605	3.095476	0.352752
H	-0.391289	2.100947	0.076718
H	-0.310422	-4.036407	3.586753
H	2.975674	-4.869707	0.922334
H	1.268797	-5.670629	2.581856
H	3.012410	-2.428179	0.336107
H	-1.244813	-2.321535	4.647264
H	-2.459093	-0.334033	5.470274
H	-2.167456	1.865548	4.348126
H	-0.739079	2.060408	2.337418
H	-2.040377	2.113089	-1.753413
H	-2.957851	-0.029365	-2.634779
H	-2.201765	-2.188725	-1.652207
H	-0.573535	-2.224983	0.176615
H	3.332459	4.013758	0.330209
H	4.714847	3.188709	1.102340
H	4.410227	2.950387	-0.616579

IV a-MeOH (M06-L)

45

scf done: -1181.113671

C	4.333266	-0.552809	-0.797109
C	2.967339	-0.553944	-0.518107
N	2.403540	0.538822	0.061572
C	3.133900	1.611907	0.391316
C	4.496715	1.657194	0.140994
C	5.098215	0.557575	-0.468471
C	2.030416	-1.638129	-0.750706
C	2.345998	-2.892429	-1.289293
C	1.357577	-3.861304	-1.419920
C	0.049819	-3.602539	-1.011524
C	-0.293319	-2.357038	-0.471834
C	0.704309	-1.412958	-0.359012
Pd	0.363361	0.376088	0.467934
O	-1.651568	0.193602	0.936853
C	-1.755248	1.336495	1.541052
C	-3.056641	1.665126	2.188668
C	-0.160185	1.093009	-1.354082
C	-1.264239	0.536124	-1.982735
C	-1.678925	1.080733	-3.199249
C	-0.997509	2.159549	-3.756146
C	0.102682	2.702404	-3.099243
C	0.539925	2.166831	-1.882840
O	-0.761545	2.103576	1.580891
H	-1.807826	-0.293646	-1.541001
H	4.787526	-1.422529	-1.263461
H	5.065305	2.538758	0.417996
H	6.163431	0.564692	-0.683599
H	2.597797	2.435044	0.860402

H	3.366189	-3.109519	-1.601225
H	1.609275	-4.831067	-1.841721
H	-0.717750	-4.366673	-1.113067
H	-1.312377	-2.147679	-0.150997
H	-2.543323	0.652238	-3.703166
H	-1.326427	2.580538	-4.703674
H	0.638678	3.548833	-3.524477
H	1.399410	2.602525	-1.379638
H	-3.894735	1.282739	1.600520
H	-3.098501	1.187038	3.173956
H	-3.152510	2.744124	2.326582
O	0.750425	-0.397634	2.611624
H	1.176244	-1.270498	2.612658
C	1.481048	0.463729	3.493734
H	1.422748	0.083729	4.518331
H	2.531112	0.554355	3.191744
H	0.995219	1.439271	3.435528

TS (IV-VI) a-MeOH (M06-L)

45

scf done: -1181.096420

C	-0.211408	-0.119301	0.385009
C	-0.221732	-0.187092	2.402891
H	4.767809	0.063353	2.599270
N	2.077343	-1.377081	1.755963
O	0.861604	2.530934	1.291414
C	1.796886	3.000976	0.513581
O	2.690253	2.253042	0.074175
O	3.152461	1.391247	2.811733
C	4.517336	1.123109	2.470646
C	3.201570	-1.872215	1.227100
C	3.596533	-3.177847	1.479816
C	2.792015	-3.970081	2.296561
C	1.622202	-3.446661	2.831320
C	1.266275	-2.128077	2.547667
C	-1.217564	0.637019	2.914778
C	-1.980835	0.192924	3.991218
C	-1.746156	-1.061104	4.557865
C	-0.714122	-1.859041	4.080473
C	0.080739	-1.426728	3.012701
C	-0.153479	-1.377278	-0.229736
C	-0.940207	-1.635382	-1.348996
C	-1.776099	-0.652410	-1.870780
C	-1.821779	0.601991	-1.264562
C	-1.043224	0.876355	-0.145907
Pd	1.452111	0.570096	1.465745
C	1.699688	4.454713	0.180189
H	-1.084836	1.861801	0.307015
H	0.977355	-4.055344	3.458622
H	4.508607	-3.560028	1.032985
H	3.070953	-4.999015	2.507461
H	3.768378	-1.201478	0.585085
H	-0.491457	-2.807299	4.566714
H	-2.352613	-1.404396	5.391833
H	-2.767682	0.832927	4.384173
H	-1.412031	1.608812	2.468477
H	-2.466760	1.382631	-1.662908
H	-2.387004	-0.861102	-2.745935
H	-0.889596	-2.618800	-1.811508

H	0.481135	-2.170494	0.150429
H	0.916404	4.603239	-0.571866
H	1.420404	5.041531	1.059716
H	2.646171	4.817341	-0.226238
H	2.996961	1.076835	3.717518
H	5.181508	1.732394	3.092045
H	4.625788	1.408125	1.423427

VI a-MeOH (M06-L)

45

scf done: -1181.149008

C	-0.810273	-0.267109	0.978951
C	-0.728605	-0.671448	2.402344
H	2.608442	0.244316	3.808323
N	2.123174	-1.318553	1.305186
O	1.082759	2.099960	-0.722314
C	2.319460	2.412347	-0.589508
O	3.080075	1.575455	0.001514
O	1.496659	1.715025	2.802395
C	2.677292	1.286833	3.459917
C	3.272811	-1.769978	0.772186
C	3.860829	-2.951793	1.185832
C	3.209998	-3.700340	2.161288
C	2.033137	-3.219015	2.711863
C	1.495301	-1.991445	2.298131
C	-1.791090	-0.268632	3.228828
C	-1.827651	-0.548090	4.587989
C	-0.778874	-1.249177	5.170404
C	0.264403	-1.691025	4.370564
C	0.314216	-1.436542	2.989310
C	-0.387036	-1.106009	-0.103762
C	-0.735293	-0.794768	-1.438459
C	-1.461132	0.343259	-1.719750
C	-1.846247	1.203867	-0.672889
C	-1.529132	0.914496	0.635793
Pd	1.358764	0.302858	0.339008
C	2.832501	3.714511	-1.081819
H	-1.813591	1.606527	1.424373
H	1.503052	-3.799408	3.460351
H	4.793796	-3.275514	0.735963
H	3.613790	-4.654008	2.490782
H	3.710213	-1.143777	-0.001584
H	1.094912	-2.216506	4.835726
H	-0.768412	-1.456603	6.237352
H	-2.673880	-0.215664	5.184138
H	-2.631810	0.254335	2.781673
H	-2.396626	2.113775	-0.899892
H	-1.733272	0.580473	-2.744992
H	-0.437542	-1.478086	-2.229447
H	0.025010	-2.090589	0.108710
H	2.152410	4.146409	-1.819520
H	2.917267	4.410910	-0.239860
H	3.830172	3.595521	-1.512894
H	0.759848	1.607525	3.422516
H	2.926394	1.926445	4.318132
H	3.483686	1.352373	2.724317

III a (M06-2X)

39

scf done: -1065.088519

C	2.471385	-2.723594	-1.197539
C	2.035411	-1.491272	-0.695168
C	0.658110	-1.279631	-0.519517
C	-0.258840	-2.268548	-0.851938
C	0.189073	-3.493405	-1.349048
C	1.554060	-3.717197	-1.523164
Pd	0.113718	0.360997	0.461454
C	-0.318254	0.866811	-1.437835
C	-1.636807	0.738623	-1.865031
C	-2.003605	1.256823	-3.108440
C	-1.059088	1.888278	-3.915628
C	0.258085	2.003919	-3.477840
C	0.636845	1.487924	-2.236131
C	2.969104	-0.409125	-0.310738
N	2.416081	0.603448	0.386240
C	3.160796	1.639359	0.775438
C	4.519745	1.724472	0.497214
C	5.105494	0.688673	-0.225205
C	4.326696	-0.386006	-0.637332
O	-0.947875	2.046833	1.602377
C	-2.024982	1.384025	1.671232
C	-3.219778	2.003527	2.364785
O	-2.124692	0.213587	1.204329
H	-2.373065	0.258925	-1.226752
H	4.767538	-1.187704	-1.217683
H	5.093681	2.580311	0.831623
H	6.161134	0.719446	-0.474053
H	2.643820	2.420640	1.324614
H	3.532068	-2.921489	-1.319174
H	1.906478	-4.668642	-1.907488
H	-0.527594	-4.268548	-1.603151
H	-1.323304	-2.084291	-0.727758
H	-3.032705	1.165153	-3.443649
H	-1.349156	2.287421	-4.882513
H	1.000600	2.492170	-4.102294
H	1.668043	1.577588	-1.906908
H	-4.149355	1.610843	1.950595
H	-3.181960	1.744839	3.427911
H	-3.192440	3.090534	2.276907

TS (III-V) a (M06-2X)

39

scf done: -1065.087004

C	-0.003011	-0.028657	0.183939
C	-0.029409	0.116855	2.387123
Pd	1.697907	-0.031130	1.285637
N	1.652086	2.154664	0.528170
C	0.552211	2.362648	-0.221050
C	-0.218776	1.145968	-0.559877
O	2.310039	-2.213999	1.897237
C	3.322977	-1.754576	2.497219
O	3.599915	-0.518364	2.502056
C	-1.112861	1.114058	-1.636109
C	-1.775102	-0.061540	-1.972899
C	-1.541887	-1.224711	-1.241070
C	-0.660865	-1.205363	-0.160661
C	2.419058	3.182424	0.894833
C	2.134450	4.491847	0.525502
C	0.996021	4.723791	-0.240885

C	0.192430	3.653030	-0.615799
C	-0.512508	1.356153	2.801601
C	-1.387825	1.423934	3.887095
C	-1.780629	0.264758	4.551121
C	-1.290004	-0.970262	4.129963
C	-0.416471	-1.049823	3.045955
C	4.226481	-2.698516	3.262541
H	-0.019354	-2.010281	2.731035
H	-0.711922	3.820603	-1.189011
H	2.783879	5.300908	0.837509
H	0.729075	5.732569	-0.538080
H	3.286245	2.939035	1.501254
H	-1.268991	2.004559	-2.237814
H	-2.460446	-0.072421	-2.813772
H	-2.049910	-2.146972	-1.505395
H	-0.498323	-2.106638	0.424406
H	-1.583208	-1.879155	4.647036
H	-2.462835	0.322658	5.393214
H	-1.761918	2.391160	4.209236
H	-0.220400	2.269904	2.293853
H	4.003167	-3.737781	3.021107
H	5.272121	-2.475684	3.039398
H	4.075736	-2.539633	4.334825

V a (M06-2X)

39

scf done: -1065.174902

C	-1.054692	0.098165	0.416999
C	-1.084650	0.289153	1.894458
Pd	1.727186	-0.026575	1.971652
N	1.329616	1.953357	1.003936
C	0.401729	2.154408	0.049193
C	-0.384219	0.989266	-0.445002
O	2.478903	-1.926636	2.850159
C	3.697317	-1.701697	2.563531
O	4.071750	-0.660558	1.968393
C	-0.430266	0.775307	-1.826171
C	-1.110106	-0.313456	-2.362714
C	-1.759958	-1.203556	-1.512902
C	-1.731761	-0.992591	-0.137763
C	2.058803	2.992522	1.430802
C	1.904891	4.281040	0.935224
C	0.951264	4.496487	-0.053597
C	0.193417	3.421377	-0.501176
C	-1.425338	1.526255	2.462703
C	-1.457426	1.685041	3.842324
C	-1.146047	0.613976	4.683324
C	-0.819349	-0.621056	4.134665
C	-0.797101	-0.787925	2.746898
C	4.722477	-2.732604	2.995510
H	-0.561795	-1.760895	2.322045
H	-0.568566	3.552324	-1.261400
H	2.520652	5.085896	1.318495
H	0.796302	5.486731	-0.468892
H	2.796867	2.772584	2.196304
H	0.099616	1.459139	-2.483328
H	-1.125187	-0.466558	-3.436660
H	-2.295555	-2.056254	-1.917710
H	-2.264141	-1.669728	0.524195

H	-0.581692	-1.462727	4.777470
H	-1.166767	0.744084	5.760489
H	-1.729714	2.646687	4.265982
H	-1.673836	2.362147	1.814341
H	4.344599	-3.740269	2.810132
H	5.669182	-2.582852	2.475884
H	4.890740	-2.633985	4.072652

IV a (M06-2X)

39

scf done: -1064.914625

C	2.263319	-2.841480	-1.196188
C	1.979374	-1.576721	-0.676655
C	0.674660	-1.328703	-0.244073
C	-0.337605	-2.263218	-0.284589
C	-0.026452	-3.524114	-0.805302
C	1.259340	-3.804158	-1.263033
Pd	0.378914	0.458988	0.521861
C	-0.140706	1.102484	-1.296329
C	-1.235769	0.532757	-1.921765
C	-1.640274	1.088973	-3.136164
C	-0.964380	2.180516	-3.675446
C	0.124480	2.728786	-3.005136
C	0.559399	2.187967	-1.790599
C	2.946985	-0.492146	-0.486376
N	2.414299	0.600767	0.105927
C	3.172781	1.655583	0.423953
C	4.528930	1.680623	0.133693
C	5.091797	0.576825	-0.502368
C	4.298617	-0.522477	-0.811730
O	-0.987375	2.235515	1.496367
C	-1.873212	1.368851	1.426799
C	-3.286688	1.591324	1.880465
O	-1.594768	0.198040	0.933657
H	-1.775293	-0.298234	-1.486846
H	4.723536	-1.395185	-1.292984
H	5.120190	2.547557	0.399695
H	6.147206	0.568369	-0.751392
H	2.669722	2.484358	0.912509
H	3.264748	-3.078047	-1.541220
H	1.484382	-4.783162	-1.671556
H	-0.800073	-4.283254	-0.854442
H	-1.336030	-2.029552	0.072538
H	-2.495121	0.660838	-3.649354
H	-1.290612	2.607423	-4.617822
H	0.651534	3.584001	-3.415231
H	1.403328	2.628246	-1.274582
H	-3.955946	1.501388	1.020634
H	-3.564674	0.819465	2.602147
H	-3.387039	2.579149	2.328274

TS (IV-VI) a (M06-2X)

39

scf done: -1064.907502

C	-0.324555	-0.086003	0.195643
C	-0.131371	-0.041369	2.360981
Pd	1.510152	-0.018537	1.173580
N	1.426642	-2.041828	1.558277
C	0.513769	-2.402902	2.489040
C	-0.269929	-1.276420	3.010819

O	1.768101	1.993725	0.924041
C	3.038916	1.936270	0.690826
O	3.602379	0.817245	0.699463
C	-0.716841	1.120112	2.831333
C	-1.512358	1.037768	3.975250
C	-1.701766	-0.183775	4.619681
C	-1.077579	-1.334745	4.148227
C	-0.841594	-1.295333	-0.252040
C	-1.797219	-1.262809	-1.268777
C	-2.217714	-0.052824	-1.811451
C	-1.678831	1.142154	-1.340662
C	-0.722779	1.138260	-0.326192
C	2.234862	-2.936896	0.985059
C	2.158652	-4.283110	1.315976
C	1.222125	-4.681817	2.265003
C	0.391785	-3.736825	2.860485
C	3.767797	3.215881	0.423495
H	-0.301161	2.070234	0.030596
H	-0.343744	-4.032494	3.598991
H	2.818011	-4.993495	0.833451
H	1.135323	-5.726759	2.541663
H	2.937517	-2.555935	0.251632
H	-1.195032	-2.271993	4.682428
H	-2.325394	-0.236582	5.504992
H	-1.985108	1.936079	4.357491
H	-0.570880	2.067033	2.322731
H	-1.998218	2.091724	-1.757331
H	-2.963650	-0.040000	-2.599050
H	-2.208681	-2.200157	-1.628220
H	-0.537246	-2.249758	0.156209
H	3.275769	3.748400	-0.393802
H	3.718905	3.848704	1.313675
H	4.807282	3.010803	0.170258

VI a (M06-2X)

39

scf done: -1064.982882

C	-1.064356	0.088116	0.902468
C	-1.278662	-0.228407	2.346705
Pd	1.320892	-0.057903	0.590633
N	1.359661	-1.782835	1.661907
C	0.420817	-2.174870	2.546061
C	-0.597019	-1.226876	3.080363
O	1.819250	1.605027	-0.568812
C	3.054600	1.439350	-0.300750
O	3.364117	0.458650	0.452469
C	-2.260551	0.523353	3.006277
C	-2.544473	0.348995	4.354853
C	-1.835841	-0.595543	5.086893
C	-0.882119	-1.374146	4.445769
C	-0.876790	-0.913507	-0.085367
C	-0.882394	-0.586968	-1.454256
C	-1.068021	0.724981	-1.853344
C	-1.239645	1.731665	-0.890468
C	-1.233858	1.426317	0.457001
C	2.341224	-2.612303	1.270658
C	2.429777	-3.913923	1.731547
C	1.444141	-4.366426	2.602038
C	0.441438	-3.496392	3.006443

C	4.095911	2.374071	-0.819983
H	-1.346351	2.217014	1.190628
H	-0.343054	-3.835774	3.671255
H	3.239596	-4.550225	1.397784
H	1.452490	-5.388880	2.963319
H	3.061263	-2.199661	0.571291
H	-0.320297	-2.099164	5.024754
H	-2.022684	-0.733494	6.146143
H	-3.314162	0.951784	4.824815
H	-2.836730	1.246198	2.439369
H	-1.366817	2.762138	-1.203990
H	-1.077760	0.976793	-2.908243
H	-0.759440	-1.378308	-2.185197
H	-0.838832	-1.958344	0.208067
H	3.750222	2.845229	-1.740404
H	4.270796	3.150450	-0.068875
H	5.030002	1.835850	-0.986054

IV a-MeOH (M06-2X)

45

scf done: -1180.600260

C	4.315502	-0.543333	-0.850044
C	2.958042	-0.529009	-0.545543
N	2.410739	0.551704	0.054139
C	3.152504	1.611676	0.394739
C	4.512098	1.651553	0.124444
C	5.093832	0.558384	-0.514530
C	1.998476	-1.613995	-0.767061
C	2.293743	-2.871105	-1.299823
C	1.293360	-3.834893	-1.392620
C	0.000772	-3.563742	-0.947614
C	-0.320662	-2.311281	-0.412849
C	0.687763	-1.374426	-0.348400
Pd	0.386841	0.386871	0.473799
O	-1.592402	0.163366	0.916984
C	-1.762329	1.288392	1.537361
C	-3.116603	1.550915	2.127498
C	-0.128360	1.066805	-1.328688
C	-1.246339	0.534095	-1.955043
C	-1.651179	1.086975	-3.169591
C	-0.951145	2.154427	-3.727064
C	0.157708	2.677679	-3.069608
C	0.585846	2.132534	-1.855332
O	-0.812732	2.091546	1.624513
H	-1.805332	-0.280959	-1.512146
H	4.754959	-1.406282	-1.335813
H	5.092203	2.520854	0.406894
H	6.153104	0.561470	-0.746618
H	2.631555	2.430175	0.883756
H	3.300769	-3.100251	-1.633703
H	1.526406	-4.808716	-1.808905
H	-0.769624	-4.324647	-1.016142
H	-1.323244	-2.087317	-0.060623
H	-2.521598	0.677681	-3.672423
H	-1.273165	2.580344	-4.671623
H	0.703997	3.514124	-3.493649
H	1.449825	2.555086	-1.356316
H	-3.878788	1.441111	1.352589
H	-3.318693	0.807860	2.903559

H	-3.153384	2.552310	2.554610
O	0.833406	-0.361535	2.595687
H	1.263140	-1.231214	2.626663
C	1.510746	0.534122	3.485157
H	1.445414	0.161783	4.509686
H	2.559917	0.655460	3.199082
H	0.991754	1.489660	3.406669

TS (IV-VI) a-MeOH (M06-2X)

45

scf done: -1180.588884

C	-0.176701	-0.122427	0.350268
C	-0.227453	-0.183500	2.426465
H	4.866417	0.092809	2.488136
N	2.064871	-1.393334	1.782855
O	0.839801	2.465457	1.333939
C	1.746452	2.988169	0.557759
O	2.639777	2.291574	0.062221
O	3.193491	1.327836	2.732183
C	4.554754	1.129880	2.332894
C	3.183827	-1.894875	1.254074
C	3.572274	-3.202047	1.512825
C	2.764033	-3.983579	2.335103
C	1.596837	-3.450106	2.872284
C	1.259553	-2.132542	2.578636
C	-1.226234	0.652525	2.897883
C	-2.005565	0.219105	3.970002
C	-1.773765	-1.023579	4.558727
C	-0.734549	-1.830168	4.106967
C	0.066598	-1.412188	3.041801
C	-0.122032	-1.388431	-0.235233
C	-0.891853	-1.648717	-1.367954
C	-1.705143	-0.661748	-1.915197
C	-1.747111	0.599451	-1.324911
C	-0.985999	0.877543	-0.193354
Pd	1.442233	0.543338	1.485057
C	1.619580	4.468297	0.316755
H	-1.022632	1.865003	0.249171
H	0.949773	-4.051410	3.499434
H	4.479663	-3.592932	1.070030
H	3.035418	-5.011195	2.550447
H	3.753250	-1.234312	0.607445
H	-0.522170	-2.770059	4.606626
H	-2.388323	-1.354016	5.388533
H	-2.798033	0.860065	4.341374
H	-1.404178	1.617322	2.436114
H	-2.374492	1.380183	-1.742543
H	-2.302283	-0.873774	-2.795720
H	-0.847088	-2.635747	-1.816323
H	0.490364	-2.184538	0.166245
H	0.645746	4.680965	-0.132136
H	1.669319	4.998326	1.271384
H	2.416697	4.811087	-0.342027
H	3.092081	1.077714	3.664291
H	5.206672	1.798015	2.900250
H	4.596034	1.383699	1.274400

VI a-MeOH (M06-2X)

45

scf done: -1180.655424

C	-0.878243	-0.322276	0.956346
C	-0.767533	-0.691179	2.400361
H	2.748347	0.208979	3.747679
N	2.130776	-1.301454	1.299102
O	1.111046	2.128032	-0.629879
C	2.343442	2.453497	-0.513351
O	3.126580	1.620761	0.036501
O	1.497554	1.567284	2.761768
C	2.729836	1.248097	3.394953
C	3.255093	-1.786230	0.748989
C	3.813592	-2.986149	1.154403
C	3.157545	-3.710466	2.143629
C	1.999617	-3.194930	2.708873
C	1.498117	-1.956852	2.292800
C	-1.833559	-0.304130	3.224519
C	-1.828715	-0.521919	4.597344
C	-0.733839	-1.139180	5.188215
C	0.315712	-1.568606	4.386082
C	0.317852	-1.377854	2.996189
C	-0.457721	-1.172112	-0.098484
C	-0.735851	-0.847513	-1.440350
C	-1.424975	0.312487	-1.747299
C	-1.833468	1.171875	-0.717332
C	-1.560901	0.869717	0.603625
Pd	1.407172	0.349711	0.373832
C	2.824025	3.789423	-0.979192
H	-1.858844	1.561066	1.384331
H	1.466338	-3.751312	3.469413
H	4.725412	-3.340818	0.690557
H	3.540740	-4.669692	2.473758
H	3.700625	-1.181791	-0.034938
H	1.173031	-2.042943	4.852168
H	-0.693391	-1.295814	6.260409
H	-2.676486	-0.205222	5.195033
H	-2.701882	0.162205	2.773122
H	-2.359011	2.090097	-0.956222
H	-1.646860	0.557634	-2.780223
H	-0.421939	-1.531362	-2.221401
H	-0.022800	-2.141424	0.126227
H	2.138552	4.199050	-1.721330
H	2.860486	4.463603	-0.117867
H	3.830869	3.699803	-1.389514
H	0.775990	1.385603	3.383160
H	2.929559	1.914955	4.240198
H	3.508017	1.380489	2.640967

III a (def2-TZVP)

39

scf done: -1066.471561

C	2.514047	-2.772716	-1.237650
C	2.048985	-1.568151	-0.714431
C	0.669817	-1.387861	-0.547823
C	-0.214546	-2.385042	-0.908427
C	0.263650	-3.583310	-1.421363
C	1.627158	-3.773515	-1.588329
Pd	0.099843	0.265119	0.404868
C	-0.382017	0.853116	-1.482479
C	-1.658395	0.631025	-1.967807
C	-2.025571	1.177559	-3.190986

C	-1.120652	1.929223	-3.923152
C	0.157565	2.134011	-3.431699
C	0.535697	1.589605	-2.210353
C	2.925869	-0.476823	-0.293329
N	2.307673	0.512224	0.373261
C	2.979889	1.576406	0.793271
C	4.337018	1.713635	0.582945
C	4.996900	0.701858	-0.094871
C	4.291085	-0.398506	-0.538562
O	-0.779943	1.979675	1.511344
C	-1.908347	1.429662	1.673807
C	-2.971021	2.198274	2.401002
O	-2.144767	0.271033	1.260626
H	-2.374391	0.049048	-1.398586
H	4.793532	-1.188076	-1.082009
H	4.858577	2.590281	0.942503
H	6.061155	0.773723	-0.283271
H	2.404115	2.335249	1.314191
H	3.579281	-2.938671	-1.357069
H	2.000511	-4.707944	-1.989601
H	-0.432302	-4.368062	-1.695776
H	-1.283696	-2.236246	-0.788110
H	-3.027793	1.010186	-3.570363
H	-1.410992	2.352569	-4.877585
H	0.873371	2.718889	-3.999020
H	1.541377	1.757619	-1.839835
H	-3.947646	1.732183	2.284773
H	-2.721570	2.230543	3.463721
H	-3.003238	3.227845	2.044135

TS (III-V) a (def2-TZVP)

39

scf done: -1066.467628

C	-0.061433	-0.055332	0.220261
C	-0.171858	0.115111	2.445403
Pd	1.584286	-0.062510	1.387829
N	1.652002	2.018938	0.585190
C	0.593806	2.277713	-0.199974
C	-0.217105	1.110192	-0.544192
O	2.341357	-2.227950	2.087096
C	3.412625	-1.672039	2.417762
O	3.599319	-0.429635	2.250271
C	-1.082977	1.091289	-1.634565
C	-1.770991	-0.059590	-1.969431
C	-1.593600	-1.212516	-1.220061
C	-0.748323	-1.206005	-0.121204
C	2.447730	2.999776	0.992630
C	2.238691	4.314113	0.625228
C	1.154846	4.600929	-0.187864
C	0.324480	3.579245	-0.603699
C	-0.633878	1.359877	2.841453
C	-1.534725	1.452484	3.893832
C	-1.979919	0.311266	4.539079
C	-1.520650	-0.930422	4.129110
C	-0.623903	-1.033684	3.076436
C	4.508900	-2.470381	3.056083
H	-0.267477	-2.009204	2.764362
H	-0.539599	3.789965	-1.220403
H	2.909217	5.089372	0.970734

H	0.951741	5.621137	-0.489873
H	3.278423	2.713712	1.630371
H	-1.193774	1.977983	-2.249227
H	-2.435172	-0.062040	-2.825020
H	-2.121850	-2.121134	-1.485493
H	-0.632290	-2.105289	0.474773
H	-1.860739	-1.830463	4.629330
H	-2.684991	0.388403	5.358253
H	-1.889076	2.428696	4.205836
H	-0.297926	2.266344	2.349456
H	4.365823	-3.537877	2.898803
H	5.480293	-2.160359	2.671324
H	4.505862	-2.274096	4.130544

V a (def2-TZVP)

39

scf done: -1066.532531

C	-1.072412	0.102165	0.381538
C	-1.040769	0.254579	1.852524
Pd	1.696742	-0.008174	1.888555
N	1.336628	1.878907	0.961776
C	0.408425	2.119387	0.020998
C	-0.423375	1.003154	-0.475982
O	2.420010	-1.830788	2.777513
C	3.659090	-1.587955	2.656546
O	4.081198	-0.538581	2.128614
C	-0.536951	0.833543	-1.852527
C	-1.259803	-0.216000	-2.389191
C	-1.886441	-1.114709	-1.544563
C	-1.792706	-0.949757	-0.174205
C	2.102818	2.884784	1.392127
C	1.985289	4.174649	0.920887
C	1.033501	4.433744	-0.047860
C	0.243707	3.396937	-0.500663
C	-1.438375	1.447239	2.463653
C	-1.435860	1.569870	3.838037
C	-1.037577	0.504952	4.637680
C	-0.657546	-0.686132	4.051964
C	-0.663988	-0.818104	2.666045
C	4.637282	-2.594860	3.187644
H	-0.408399	-1.770470	2.213001
H	-0.520039	3.566748	-1.249009
H	2.630202	4.951791	1.308194
H	0.904313	5.433239	-0.444661
H	2.844772	2.630919	2.141842
H	-0.020926	1.523287	-2.511335
H	-1.324795	-0.334105	-3.463888
H	-2.456404	-1.941861	-1.950539
H	-2.306856	-1.636817	0.489056
H	-0.350306	-1.525695	4.664311
H	-1.033796	0.607146	5.716213
H	-1.753513	2.500260	4.294025
H	-1.762541	2.279264	1.847227
H	4.151316	-3.537863	3.431845
H	5.433037	-2.763418	2.461759
H	5.102195	-2.195253	4.091298

IV a (def2-TZVP)

39

scf done: -1066.306726

C	2.273172	-2.880132	-1.208258
C	1.962717	-1.628614	-0.687670
C	0.658941	-1.408649	-0.253745
C	-0.321913	-2.364239	-0.297306
C	0.015917	-3.611528	-0.814464
C	1.299320	-3.860194	-1.273462
Pd	0.320484	0.397619	0.502839
C	-0.165998	1.081686	-1.334116
C	-1.152164	0.461028	-2.062906
C	-1.517123	1.049152	-3.268087
C	-0.909863	2.216145	-3.696868
C	0.069179	2.813759	-2.923953
C	0.459127	2.245124	-1.717056
C	2.889643	-0.531157	-0.490518
N	2.330394	0.539282	0.112148
C	3.057074	1.608117	0.432985
C	4.401840	1.673461	0.143924
C	4.991552	0.598344	-0.499623
C	4.234817	-0.512453	-0.814504
O	-0.866894	2.195682	1.444599
C	-1.827465	1.410126	1.416973
C	-3.166643	1.744045	1.967274
O	-1.665526	0.235958	0.911654
H	-1.648646	-0.436263	-1.723189
H	4.683098	-1.366156	-1.305012
H	4.967152	2.553759	0.415630
H	6.044052	0.624061	-0.751833
H	2.534598	2.420776	0.926924
H	3.278425	-3.090085	-1.555410
H	1.545251	-4.832159	-1.682263
H	-0.738585	-4.387598	-0.860398
H	-1.327437	-2.163416	0.054636
H	-2.292596	0.581417	-3.862946
H	-1.206935	2.666742	-4.635860
H	0.542365	3.733922	-3.245284
H	1.212236	2.731553	-1.112184
H	-3.953188	1.373059	1.311432
H	-3.281517	1.248260	2.933404
H	-3.263339	2.817911	2.109831

TS (IV-VI) a (def2-TZVP)

39

scf done: -1066.299535

C	-0.351986	-0.055137	0.173660
C	-0.191305	-0.022195	2.401832
Pd	1.446008	0.047356	1.206763
N	1.423269	-1.939096	1.615727
C	0.513755	-2.340739	2.527190
C	-0.316797	-1.262418	3.032182
O	1.794534	2.039145	0.889282
C	3.047645	1.861488	0.703660
O	3.493298	0.687832	0.787710
C	-0.839018	1.102867	2.851686
C	-1.663683	0.987349	3.963017
C	-1.830406	-0.236335	4.591090
C	-1.155951	-1.354186	4.136230
C	-0.813185	-1.264343	-0.307389
C	-1.752194	-1.247346	-1.330025
C	-2.218484	-0.049973	-1.840077

C	-1.743987	1.146708	-1.330646
C	-0.806443	1.155454	-0.309164
C	2.279095	-2.789829	1.056994
C	2.261643	-4.128615	1.383846
C	1.334084	-4.571168	2.311698
C	0.455823	-3.674921	2.889451
C	3.913041	3.013956	0.373289
H	-0.443330	2.097204	0.080165
H	-0.273477	-4.005429	3.616862
H	2.962898	-4.803947	0.914443
H	1.295231	-5.617606	2.586040
H	2.979681	-2.377986	0.339775
H	-1.260617	-2.298189	4.658280
H	-2.481395	-0.316554	5.452273
H	-2.182430	1.864303	4.330572
H	-0.719149	2.058410	2.355848
H	-2.101884	2.091411	-1.722233
H	-2.953443	-0.048356	-2.635477
H	-2.114357	-2.190552	-1.721403
H	-0.469001	-2.216243	0.070988
H	3.478332	3.941828	0.740234
H	4.910978	2.867065	0.782851
H	3.999540	3.080811	-0.713456

VI a (def2-TZVP)

39

scf done: -1066.361721

C	-0.965024	0.109544	0.910414
C	-1.204000	-0.204799	2.340147
Pd	1.302000	-0.118902	0.555559
N	1.347323	-1.812597	1.640417
C	0.433826	-2.177646	2.555972
C	-0.567821	-1.225414	3.076356
O	1.774395	1.541996	-0.581611
C	3.001520	1.426557	-0.277044
O	3.320123	0.457189	0.474711
C	-2.176356	0.559220	2.986462
C	-2.496749	0.379172	4.316581
C	-1.834494	-0.585186	5.049950
C	-0.891374	-1.374173	4.426141
C	-0.756688	-0.888972	-0.077676
C	-0.834871	-0.577900	-1.448563
C	-1.088333	0.705011	-1.849437
C	-1.250284	1.714558	-0.889871
C	-1.185471	1.433046	0.446088
C	2.302434	-2.658348	1.236575
C	2.391135	-3.943544	1.713284
C	1.435540	-4.367170	2.618217
C	0.463099	-3.485451	3.035820
C	4.009516	2.394056	-0.757395
H	-1.299898	2.230928	1.168514
H	-0.302248	-3.810965	3.726116
H	3.181297	-4.593360	1.364280
H	1.443024	-5.382163	2.994867
H	3.006543	-2.273949	0.507723
H	-0.363278	-2.114692	5.013112
H	-2.048778	-0.728828	6.101494
H	-3.261233	0.995129	4.773514
H	-2.721768	1.302147	2.419463

H	-1.423774	2.734349	-1.210460
H	-1.157880	0.945159	-2.902842
H	-0.716571	-1.374403	-2.171970
H	-0.745340	-1.933384	0.208691
H	3.670329	2.878290	-1.671137
H	4.150998	3.160007	0.008229
H	4.965471	1.897517	-0.916925

GEOMETRIES OPTIMIZED IN THE GAS PHASE FOLLOW (NAMES HIGHLIGHTED IN ORANGE)

Ru(II) I red

61

scf done: -1578.585946

C	2.999987	-0.607968	-0.424450
N	2.496079	0.409875	0.320612
C	3.333369	1.334216	0.816033
C	4.701522	1.298891	0.596328
C	5.227081	0.261758	-0.166095
C	4.366487	-0.698422	-0.679831
Ru	0.419194	0.379363	0.626314
H	4.762479	-1.515311	-1.276965
C	2.007622	-1.567498	-0.930972
N	0.723168	-1.324930	-0.561616
N	0.795142	-0.502918	2.497228
H	5.338394	2.072052	1.017202
H	6.295124	0.199970	-0.360010
H	2.874666	2.128699	1.402733
C	2.326539	-2.660631	-1.733480
C	1.319870	-3.512516	-2.166520
H	3.356201	-2.849772	-2.024481
H	1.559251	-4.368214	-2.793202
C	0.007723	-3.252957	-1.787056
C	-0.245961	-2.150640	-0.985683
H	-0.811952	-3.892106	-2.103646
H	-1.256229	-1.908008	-0.659737
N	-0.134890	1.393771	-1.125260
C	-1.470133	1.504678	-1.348022
C	-1.953924	2.160193	-2.478051
C	-1.062080	2.707541	-3.390010
C	0.302841	2.586060	-3.154267
C	0.722564	1.920801	-2.012836
C	-2.331977	0.904197	-0.319484
H	-3.023473	2.246039	-2.649805
H	-1.429973	3.222152	-4.274349
H	1.035921	2.998326	-3.842220
H	1.780364	1.802185	-1.783201
C	-3.724004	0.932944	-0.361762
C	-4.455132	0.336624	0.656246
C	-3.776825	-0.279279	1.702002
C	-2.390624	-0.273484	1.688552
N	-1.678505	0.298852	0.706055
H	-4.240745	1.420136	-1.184142
H	-5.541916	0.353743	0.632003
H	-4.308337	-0.759696	2.518929
H	-1.814147	-0.744803	2.482948
C	0.797662	0.344649	3.559136
C	1.031202	-0.126010	4.849320
C	1.265001	-1.478367	5.055584
C	1.262416	-2.337343	3.962193

C	1.025866	-1.808879	2.702572
C	0.527056	1.754353	3.241207
H	1.029795	0.556998	5.694580
H	1.446006	-1.856935	6.058653
H	1.440314	-3.403021	4.077830
H	1.011568	-2.440954	1.815974
C	0.488581	2.770835	4.193296
C	0.226673	4.074869	3.796437
C	0.006164	4.338179	2.449187
C	0.059028	3.284879	1.549793
N	0.315303	2.022633	1.926898
H	0.662978	2.550467	5.242864
H	0.193777	4.874718	4.532182
H	-0.203315	5.343588	2.094508
H	-0.102198	3.441723	0.484376

Ru(III) I ox

61

scf done: -1578.143849

C	3.005586	-0.624669	-0.413517
N	2.508588	0.383346	0.353741
C	3.343909	1.287313	0.893012
C	4.713499	1.243378	0.684720
C	5.235362	0.219661	-0.099599
C	4.373020	-0.721987	-0.650392
Ru	0.420509	0.381314	0.625036
H	4.772482	-1.526391	-1.262118
C	2.008596	-1.561990	-0.948260
N	0.717456	-1.301558	-0.605873
N	0.842639	-0.496298	2.495548
H	5.354790	1.998515	1.131299
H	6.305648	0.152032	-0.281758
H	2.889868	2.069348	1.499156
C	2.317806	-2.650129	-1.758014
C	1.298275	-3.475053	-2.220513
H	3.348041	-2.860624	-2.032367
H	1.532517	-4.329546	-2.851686
C	-0.017793	-3.192680	-1.868711
C	-0.267851	-2.092890	-1.062872
H	-0.842464	-3.812648	-2.210147
H	-1.281143	-1.833053	-0.761506
N	-0.136245	1.363245	-1.151644
C	-1.474564	1.495107	-1.359282
C	-1.950828	2.134130	-2.499491
C	-1.050658	2.643414	-3.429168
C	0.314886	2.498181	-3.205314
C	0.732623	1.845062	-2.056235
C	-2.335361	0.926018	-0.313817
H	-3.019161	2.239164	-2.669025
H	-1.414904	3.147059	-4.321947
H	1.048775	2.882811	-3.908589
H	1.789897	1.704471	-1.837916
C	-3.725500	0.966887	-0.341207
C	-4.450607	0.402368	0.702507
C	-3.770519	-0.191509	1.760985
C	-2.384542	-0.196722	1.739349
N	-1.683124	0.340026	0.726808
H	-4.248258	1.437617	-1.169510
H	-5.537891	0.428477	0.688057

H	-4.301168	-0.645936	2.593433
H	-1.807966	-0.650389	2.543618
C	0.816755	0.350212	3.561197
C	1.069278	-0.122627	4.844840
C	1.348114	-1.470976	5.038388
C	1.376135	-2.324171	3.939792
C	1.124390	-1.796917	2.682617
C	0.507664	1.751977	3.249439
H	1.049006	0.551440	5.697116
H	1.542508	-1.850746	6.039061
H	1.590213	-3.383950	4.049919
H	1.136034	-2.425781	1.794019
C	0.441650	2.766422	4.199383
C	0.133361	4.062488	3.800955
C	-0.108380	4.321897	2.455615
C	-0.032854	3.272153	1.553857
N	0.274425	2.021089	1.936461
H	0.629058	2.555008	5.248677
H	0.078928	4.861129	4.537525
H	-0.353286	5.321181	2.105759
H	-0.212587	3.425592	0.491211

Phenyldiazonium

13

scf done: -340.584264

C	-0.004095	-2.559078	4.475832
C	-0.398701	-1.761566	3.419302
C	0.620227	-1.127375	2.686353
C	1.993591	-1.256142	2.960938
C	2.344587	-2.062639	4.026069
C	1.354247	-2.706798	4.774572
H	2.734605	-0.739436	2.356088
H	3.393674	-2.193265	4.277701
H	1.647376	-3.337283	5.611364
H	-0.755337	-3.070108	5.071965
H	-1.444498	-1.621682	3.157094
N	0.250016	-0.330337	1.631092
N	-0.050347	0.317004	0.774033

Phenyldiazoyl

13

scf done: -340.823596

C	0.004697	-2.512843	4.418610
C	-0.310843	-1.695466	3.343147
C	0.723122	-1.082762	2.638596
C	2.053584	-1.272149	2.987225
C	2.360549	-2.093252	4.066626
C	1.337608	-2.711910	4.779370
H	2.824994	-0.771157	2.405363
H	3.398960	-2.251310	4.351112
H	1.578750	-3.353943	5.624760
H	-0.790324	-3.000307	4.980231
H	-1.340102	-1.518833	3.034523
N	0.463616	-0.215429	1.500951
N	-0.619267	0.030656	1.091888

N2

2

scf done: -109.455005

N	0.348370	-0.186496	1.453788
N	-0.700853	-0.016413	1.151168

Phenyl

11

scf done: -231.364726

C	-0.291485	-1.672562	3.313390
C	0.773562	-1.099230	2.661463
C	2.097250	-1.270898	2.987345
C	2.374002	-2.101346	4.078048
C	1.332900	-2.709259	4.776396
C	0.007723	-2.499227	4.401029
H	2.900849	-0.788235	2.432632
H	3.407121	-2.272169	4.379916
H	1.557783	-3.353609	5.624666
H	-0.799085	-2.980116	4.953729
H	-1.322794	-1.499140	3.008836

BF4-

39

scf done: -1066.361721

Palladacycle II a

28

scf done: -833.506824

C	4.178550	-0.494555	-0.768432
C	2.825974	-0.543028	-0.432618
N	2.250932	0.515740	0.194291
C	2.962337	1.605107	0.494720
C	4.309453	1.708516	0.184794
C	4.920363	0.635214	-0.457873
C	1.902481	-1.641307	-0.676260
C	2.229654	-2.845261	-1.306541
C	1.255819	-3.820384	-1.476127
C	-0.043142	-3.599479	-1.018636
C	-0.383013	-2.401939	-0.389047
C	0.587750	-1.425395	-0.220102
Pd	0.248811	0.307802	0.643405
O	-0.703507	2.068404	1.684181
C	-1.765939	1.394089	1.662360
C	-3.048256	1.952063	2.199335
O	-1.778880	0.220146	1.151153
H	4.642771	-1.341134	-1.269004
H	4.861136	2.607874	0.443712
H	5.976616	0.678934	-0.716688
H	2.415564	2.401665	0.998493
H	3.242864	-3.025724	-1.667515
H	1.508010	-4.758252	-1.967503
H	-0.801370	-4.370035	-1.154728
H	-1.396394	-2.225577	-0.029755
H	-3.676047	1.152828	2.605109
H	-2.844248	2.708247	2.963028
H	-3.600684	2.431249	1.381219

Pd(III) III a

39

scf done: -1064.900487

Pd	0.119138	0.347810	0.357449
C	0.690918	-1.318597	-0.585560
C	2.079984	-1.523902	-0.694126
C	2.962438	-0.448964	-0.234386
N	2.337688	0.551084	0.425775
O	-0.725665	1.995808	1.578425
C	-1.848969	1.415027	1.690000

O	-2.059216	0.277727	1.179694
C	-0.429391	0.864352	-1.555161
C	-1.773697	0.805216	-1.896421
C	0.521852	1.386244	-2.420369
C	0.107783	1.892463	-3.652618
C	-1.236556	1.855837	-4.009366
C	-2.172050	1.313833	-3.133461
C	4.342178	-0.385113	-0.441814
C	5.052239	0.707786	0.033119
C	4.384847	1.731202	0.700985
C	3.012900	1.610476	0.870013
C	-0.200045	-2.302671	-0.988154
C	0.283006	-3.511323	-1.486422
C	1.655469	-3.727993	-1.595733
C	2.548506	-2.741387	-1.201636
C	-2.946312	2.109579	2.446153
H	-2.503880	0.392962	-1.200932
H	4.850348	-1.178722	-0.984829
H	4.911211	2.602731	1.080856
H	6.127479	0.766448	-0.125992
H	2.417842	2.370728	1.376932
H	3.620147	-2.930994	-1.269825
H	2.030421	-4.672789	-1.984908
H	-0.416329	-4.286130	-1.797909
H	-1.272996	-2.123935	-0.911325
H	-3.226145	1.284737	-3.408359
H	-1.556012	2.248129	-4.973636
H	0.845620	2.310377	-4.337068
H	1.577197	1.408851	-2.147941
H	-3.855086	1.502038	2.470194
H	-2.612509	2.318453	3.469218
H	-3.158495	3.075924	1.973648

TS III a

39

scf done: -1064.898278

C	-0.030325	-0.045730	0.206563
C	-0.143235	0.113525	2.460034
Pd	1.618539	-0.044453	1.386171
N	1.691555	2.047577	0.541324
C	0.608599	2.299206	-0.224162
C	-0.197943	1.122915	-0.562933
O	2.283495	-2.179836	2.042156
C	3.371310	-1.667412	2.425860
O	3.604863	-0.424808	2.293935
C	-1.078478	1.101096	-1.650046
C	-1.774300	-0.055738	-1.972154
C	-1.589380	-1.210202	-1.213997
C	-0.725691	-1.202787	-0.122265
C	2.484803	3.038726	0.945056
C	2.252654	4.361238	0.593079
C	1.141665	4.642087	-0.197273
C	0.311012	3.609184	-0.607472
C	-0.674885	1.350117	2.808650
C	-1.578952	1.427747	3.867109
C	-1.955722	0.280255	4.556811
C	-1.424002	-0.952607	4.189124
C	-0.520312	-1.045164	3.132913
C	4.412453	-2.530569	3.080673

H	-0.084162	-2.005518	2.859332
H	-0.579057	3.816416	-1.197428
H	2.922654	5.146128	0.934031
H	0.915340	5.667751	-0.483178
H	3.331078	2.744100	1.566436
H	-1.190035	1.986975	-2.275791
H	-2.450174	-0.062451	-2.825043
H	-2.127741	-2.121695	-1.469737
H	-0.595987	-2.100238	0.482185
H	-1.708093	-1.854680	4.730013
H	-2.665500	0.346043	5.379767
H	-1.991648	2.396084	4.148302
H	-0.394973	2.256268	2.271479
H	4.231467	-3.588802	2.871054
H	5.412570	-2.238684	2.743547
H	4.373680	-2.376044	4.166321

Pd(I) V a

39

scf done: -1064.967869

C	-1.163943	0.125312	0.331676
C	-1.055745	0.187810	1.808873
Pd	1.565966	-0.148760	1.961658
N	1.361101	1.744006	0.870081
C	0.415406	2.085224	-0.027519
C	-0.522328	1.048840	-0.517279
O	2.436953	-1.877679	3.032144
C	3.610940	-1.415976	2.902320
O	3.836072	-0.323265	2.309873
C	-0.729044	0.962055	-1.897821
C	-1.538860	-0.022989	-2.447760
C	-2.157764	-0.944652	-1.612008
C	-1.970256	-0.862964	-0.237639
C	2.266435	2.655126	1.249795
C	2.267738	3.959399	0.776787
C	1.283483	4.330645	-0.130548
C	0.353744	3.385174	-0.537581
C	-1.422733	1.350835	2.508812
C	-1.408827	1.374806	3.893214
C	-1.020455	0.243033	4.616212
C	-0.658778	-0.913796	3.944975
C	-0.683758	-0.954147	2.543216
C	4.769933	-2.185978	3.474990
H	-0.474611	-1.890054	2.022701
H	-0.434940	3.641396	-1.242033
H	3.023504	4.661261	1.119543
H	1.238864	5.346570	-0.518792
H	3.020180	2.300039	1.952607
H	-0.206376	1.658149	-2.553416
H	-1.672806	-0.077318	-3.526338
H	-2.793787	-1.724445	-2.027045
H	-2.476761	-1.564281	0.424949
H	-0.339787	-1.798100	4.492689
H	-1.002542	0.271042	5.704011
H	-1.706087	2.280280	4.419958
H	-1.736675	2.231279	1.947640
H	4.439985	-3.140328	3.895454
H	5.519032	-2.361455	2.694290
H	5.254673	-1.590072	4.257757

Pd(IV) IV a

39

scf done: -1064.685649

C	2.329187	-2.946537	-1.174722
C	1.980140	-1.680103	-0.699878
C	0.647116	-1.465227	-0.326566
C	-0.325074	-2.439544	-0.389287
C	0.052172	-3.701015	-0.861989
C	1.364721	-3.944869	-1.258130
Pd	0.267825	0.345216	0.420536
C	-0.241544	1.085842	-1.418239
C	-1.164682	0.412137	-2.186918
C	-1.535283	1.031548	-3.383827
C	-0.998634	2.262478	-3.744469
C	-0.087029	2.902767	-2.913039
C	0.311184	2.314005	-1.709188
C	2.893036	-0.567274	-0.480518
N	2.298417	0.516431	0.079506
C	2.998925	1.604053	0.422699
C	4.363056	1.678664	0.199888
C	4.994250	0.590433	-0.398981
C	4.260525	-0.538459	-0.737045
O	-0.696616	2.108983	1.450674
C	-1.751690	1.429823	1.440203
C	-3.024455	1.892346	2.052268
O	-1.722119	0.254823	0.887995
H	-1.599156	-0.537552	-1.892455
H	4.746411	-1.397911	-1.191960
H	4.913574	2.568989	0.489095
H	6.063572	0.619554	-0.595841
H	2.437678	2.414463	0.889569
H	3.355906	-3.161513	-1.468436
H	1.642631	-4.928784	-1.628397
H	-0.691083	-4.493679	-0.920005
H	-1.349222	-2.240064	-0.074099
H	-2.259537	0.533789	-4.025706
H	-1.302064	2.732306	-4.677228
H	0.322564	3.874719	-3.180890
H	0.998232	2.828861	-1.043867
H	-3.877257	1.602724	1.430437
H	-3.149591	1.410294	3.029946
H	-3.000566	2.975627	2.196202

TS IV a

39

scf done: -1064.683530

C	-0.366710	-0.024521	0.134240
C	-0.170083	-0.027599	2.460981
Pd	1.423106	0.053841	1.200553
N	1.429254	-1.951143	1.617353
C	0.524567	-2.362781	2.540404
C	-0.304864	-1.287092	3.065859
O	1.789623	2.056028	0.869012
C	3.037979	1.847611	0.618142
O	3.448195	0.651308	0.662481
C	-0.824002	1.097273	2.917982
C	-1.659005	0.962701	4.030181
C	-1.829703	-0.275887	4.641921
C	-1.153554	-1.394804	4.170059

C	-0.859605	-1.237925	-0.314814
C	-1.816332	-1.201867	-1.330875
C	-2.262039	0.010738	-1.843032
C	-1.751352	1.206486	-1.349460
C	-0.792452	1.205376	-0.336284
C	2.297309	-2.793646	1.047560
C	2.294572	-4.141409	1.369211
C	1.366668	-4.597967	2.302190
C	0.478462	-3.708153	2.892769
C	3.929831	2.991529	0.314672
H	-0.381577	2.140623	0.035505
H	-0.248067	-4.053982	3.623831
H	3.004373	-4.813096	0.895600
H	1.336646	-5.651238	2.571933
H	2.993828	-2.360787	0.330446
H	-1.266627	-2.349797	4.681505
H	-2.487975	-0.368238	5.502292
H	-2.182481	1.837053	4.411108
H	-0.698783	2.063697	2.433695
H	-2.094195	2.159688	-1.747192
H	-3.012379	0.024776	-2.630151
H	-2.210523	-2.141295	-1.713738
H	-0.525750	-2.193703	0.078086
H	3.436636	3.686418	-0.372858
H	4.141019	3.539381	1.241596
H	4.872328	2.634430	-0.108994

Pd(II) VI a

39

scf done: -1064.753394

C	-0.986386	0.128069	0.924705
C	-1.233644	-0.212522	2.349134
Pd	1.297934	-0.109124	0.541474
N	1.365166	-1.802068	1.676736
C	0.420104	-2.190193	2.561516
C	-0.600439	-1.250988	3.076929
O	1.775970	1.531603	-0.646346
C	3.015051	1.401964	-0.363386
O	3.323126	0.428288	0.403121
C	-2.217333	0.542522	3.002333
C	-2.552711	0.337525	4.332567
C	-1.892906	-0.642843	5.059170
C	-0.938063	-1.423806	4.427527
C	-0.792563	-0.863071	-0.086197
C	-0.852980	-0.524306	-1.455891
C	-1.073991	0.781268	-1.834946
C	-1.229172	1.779559	-0.854761
C	-1.182558	1.468757	0.484878
C	2.367165	-2.623592	1.316613
C	2.466938	-3.915658	1.795809
C	1.468713	-4.372173	2.649396
C	0.451855	-3.511151	3.028290
C	4.035044	2.347020	-0.870971
H	-1.285224	2.256207	1.228240
H	-0.344793	-3.859356	3.679531
H	3.296615	-4.545364	1.488506
H	1.480272	-5.395470	3.017898
H	3.101088	-2.206852	0.628571
H	-0.404690	-2.169869	5.012487

H	-2.116936	-0.804726	6.110779
H	-3.325843	0.946691	4.794907
H	-2.765503	1.293464	2.438450
H	-1.379499	2.812751	-1.159001
H	-1.125305	1.044777	-2.888612
H	-0.744631	-1.310233	-2.199686
H	-0.790833	-1.916517	0.191057
H	3.692588	2.816797	-1.797591
H	4.197109	3.133502	-0.122945
H	4.987601	1.831149	-1.026526

Pd(IV) IV a-BF4

44

scf done: -1489.221966

C	4.267341	-0.675327	-0.825412
C	2.900575	-0.642279	-0.575536
N	2.337358	0.484988	-0.084550
C	3.065199	1.562410	0.205698
C	4.431139	1.584127	-0.022293
C	5.034025	0.445684	-0.544738
C	1.958056	-1.735934	-0.753839
C	2.253802	-3.015356	-1.232400
C	1.256723	-3.980647	-1.290312
C	-0.037973	-3.691107	-0.863894
C	-0.359415	-2.419777	-0.382004
C	0.644623	-1.479007	-0.359741
Pd	0.338093	0.321715	0.414156
O	-1.651724	0.174423	0.880709
C	-1.726103	1.332041	1.459037
C	-2.991681	1.664400	2.177205
C	-0.161431	1.118587	-1.366363
C	-0.942918	0.428089	-2.278279
C	-1.312223	1.074953	-3.458086
C	-0.911800	2.383761	-3.701833
C	-0.142344	3.060175	-2.761182
C	0.239737	2.428764	-1.578200
O	-0.745309	2.100529	1.426398
H	-1.271517	-0.590420	-2.088202
H	4.725811	-1.581139	-1.213750
H	5.005526	2.471593	0.225986
H	6.106764	0.427592	-0.725247
H	2.534420	2.402035	0.647227
H	3.266958	-3.262173	-1.548002
H	1.493274	-4.975608	-1.661315
H	-0.807691	-4.460160	-0.899101
H	-1.360313	-2.175719	-0.027143
H	-1.923973	0.542947	-4.185139
H	-1.207071	2.882044	-4.623383
H	0.161513	4.091077	-2.936155
H	0.811385	2.974941	-0.830602
H	-3.855441	1.223767	1.670013
H	-2.938705	1.241087	3.187781
H	-3.102090	2.748982	2.261317
F	0.760483	-0.600246	2.386595
B	2.008267	-0.091126	3.003078
F	1.955728	-0.358380	4.332082
F	3.050889	-0.724841	2.349553
F	2.014618	1.274031	2.718743

TS IV a-BF4

44

scf done: -1489.203178

C	-0.368304	0.007203	0.263866
C	-0.288386	-0.070507	2.288558
Pd	1.486262	0.020021	1.258239
N	1.365093	-1.990799	1.512537
O	1.816819	2.012345	0.961922
O	3.287655	0.689780	0.008980
F	3.064938	0.253585	2.888685
B	3.733022	-0.970030	3.347424
F	2.742736	-1.771660	3.909183
C	-0.879893	-1.161570	-0.306435
C	-1.761250	-1.077302	-1.379520
C	-2.133218	0.158476	-1.895993
C	-1.611798	1.319626	-1.333160
C	-0.730926	1.251581	-0.261029
C	-0.898799	1.050497	2.837153
C	-1.688153	0.910061	3.973264
C	-1.858537	-0.339037	4.566942
C	-1.205702	-1.449409	4.049645
C	-0.399673	-1.329142	2.917553
C	2.265741	-2.811810	0.978498
C	2.256698	-4.162143	1.295914
C	1.303273	-4.626644	2.193686
C	0.382021	-3.748573	2.749834
C	0.439960	-2.404233	2.405529
C	2.935683	1.843911	0.325684
C	3.762312	3.050628	0.041960
F	4.249865	-1.577268	2.205480
F	4.697440	-0.620013	4.240497
H	-0.308804	2.164983	0.150115
H	-0.363182	-4.097610	3.460164
H	2.992904	-4.825262	0.852002
H	1.277409	-5.679918	2.465176
H	2.984291	-2.365885	0.295869
H	-1.280907	-2.408365	4.560672
H	-2.478698	-0.440371	5.454692
H	-2.172985	1.786760	4.398501
H	-0.769995	2.027358	2.375609
H	-1.884016	2.294339	-1.734816
H	-2.821333	0.216782	-2.736996
H	-2.156791	-1.995226	-1.811416
H	-0.617035	-2.142982	0.078071
H	3.129214	3.911995	-0.194085
H	4.343218	3.293215	0.940328
H	4.457101	2.844328	-0.777045

Pd(II) VI a-BF4

44

scf done: -1489.262344

C	-1.335334	1.093919	0.889916
C	-0.660598	-0.138286	1.105439
C	-0.134981	-0.794310	-0.053266
C	-0.395043	-0.289394	-1.351248
C	-1.105807	0.875117	-1.512508
C	-1.551552	1.579276	-0.378928
C	-0.753947	-0.766114	2.452875
C	-1.943022	-0.512676	3.150784
C	-2.163327	-0.955402	4.446355

C	-1.169804	-1.668297	5.098637
C	-0.005266	-1.975738	4.414188
C	0.219041	-1.576571	3.089728
Pd	1.585539	0.436936	0.795138
O	3.043411	1.260934	-1.140051
C	2.268316	2.213054	-1.004829
C	2.398865	3.494252	-1.774560
C	1.490156	-2.051874	2.503357
N	2.173144	-1.314062	1.614609
C	3.383509	-1.674421	1.169061
C	3.981499	-2.855950	1.563131
C	3.271497	-3.685891	2.423178
C	2.027650	-3.289232	2.883182
O	1.275601	2.177782	-0.162464
F	1.422855	1.363669	3.302449
B	2.819477	1.257954	3.364856
F	3.180959	0.010800	3.842476
H	-1.649233	1.674549	1.754240
H	1.452924	-3.939698	3.536000
H	4.968561	-3.116299	1.192958
H	3.684561	-4.642784	2.735664
H	3.860833	-0.974829	0.481864
H	0.786711	-2.504075	4.939900
H	-1.293023	-1.985371	6.131748
H	-3.103201	-0.724686	4.943702
H	-2.734047	0.039533	2.648810
H	-2.064652	2.530579	-0.503925
H	-1.300495	1.267692	-2.508428
H	-0.026957	-0.845052	-2.211025
H	0.247168	-1.810742	0.037453
H	1.421680	3.824508	-2.144410
H	2.778149	4.275967	-1.105520
H	3.097987	3.363369	-2.605320
F	3.393600	2.286956	4.037249
F	3.267735	1.320018	1.954523

6. Comprehensive Tables

A: values obtained carrying out full optimization with MeOH as implicit solvent

	H (hartrees)	**ZPC** (hartrees)	**S** (cal/mol*K)	Imaginary freq.	Multipl.	Charge
M06/LACVP(d)						
$Ru(bpy)_3^{2+}$	-1578,284474	0,483186	189,204		s	2+
$Ru(bpy)_3^{3+}$ Iox	-1578,071709	0,484178	191,131		d	3+
Phenyldiazonium	-340,563860	0,098993	78,839		s	+
Phenyldiazoyl	-340,731037	0,096997	81,129		d	0
Phenyl	-231,280088	0,087249	70,287		d	0
N_2	-109,449780	0,005622	45,784		s	0
MeOH	-115,594791	0,051392	56,787		s	0
Palladacyle II	-833,309765	0,211325	127,149		s	0
Pd(III) III a	-1064,619707	0,299422	160,619		d	0
TS (III-V) a	-1064,616845	0,298951	154,923	-217.0132	d	0
Pd (I) V a	-1064,683814	0,301659	159,531		d	0
Pd(IV) IV a	-1064,452074	0,302154	149,468		s	+
TS (IV-VI) a	-1064,444643	0,301873	145,505	-192.9061	s	+
Pd(II) VI a	-1064,509177	0,304813	146,574		s	+
Pd(IV) IV a-MeOH	-1180,069595	0,356313	164,182		s	+
TS (IV-VI) a-MeOH	-1180,055818	0,356235	163,003	-296.5212	s	+
Pd(II) VI a-MeOH	-1180,113564	0,358502	166,513		s	+
BF4-	-424,451116	0,014711	69,026		s	-
Pd(IV)a-BF4	-1488,935867	0,318320	178,886		s	0
TS (IV) a	-1488,920465	0,317889	172,580	-298.1710	s	0
Pd(II)-BF4 VI a	-1488,975532	0,320722	170,179		s	0
Pd IIIa-Bimet	-1897,981057	0,513321	228,782		d	0
TS IIIa-Bimet	-1897,976146	0,513406	226,186	-231.5300	d	0
Va-Bimet	-1898,040924	0,516258	228,044		d	0
Pd IVa-Bimet	-1897,824521	0,516435	217,578		s	+
TS IVa-Bimet	-1897,816028	0,516003	216,871	-207.3267	s	+
VI a Bimet	-1897,865996	0,518734	224,188		s	+
M06-L/LACVP(d)						
MeOH	-115,644856	0,051511	56,817		s	0
Pd(III) III a	-1065,247985	0,300860	154,142		d	0
TS (III-V) a	-1065,241779	0,300510	153,404	-258.9158	d	0
Pd (I) V a	-1065,298658	0,303238	157,656		d	0
Pd(IV) IV a	-1065,089964	0,303310	149,995		s	+
TS (IV-VI) a	-1065,079758	0,302615	146,288	-260.6568	s	+
Pd(II) VI a	-1065,136031	0,305374	148,053		s	+
Pd(IV) IV a-	-1180,756136	0,357535	172,087		s	+

MeOH						
TS (IV-VI) a-MeOH	-1180,739208	0,357212	163,673	-313.2470	s	+
Pd(II) VI a-MeOH	-1180,790202	0,358808	170,540		s	+
M06-2X/LACVP(d)						
MeOH	-115,606463	0,052166	56,639		s	0
Pd(III) III a	-1064,784089	0,304430	160,197		d	0
TS (III-V) a	-1064,783041	0,303963	153,421	-176.4276	d	0
Pd (I) V a	-1064,868340	0,306562	158,040		d	0
Pd(IV) IV a	-1064,607786	0,306839	152,074		s	+
TS (IV-VI) a	-1064,601028	0,306474	146,017	-205.7218	s	+
Pd(II) VI a	-1064,673958	0,308924	143,757		s	+
Pd(IV) IV a-MeOH	-1180,238147	0,362113	169,378		s	+
TS (IV-VI) a-MeOH	-1180,227277	0,361607	164,542	-292.8430	s	+
Pd(II) VI a-MeOH	-1180,291906	0,363518	168,071		s	+
M06/Def2-SVP						
$Ru(bpy)_3^{2+}$	-1577,996807	0,483097	189,560		s	2+
$Ru(bpy)_3^{3+}$ lox	-1578,210918	0,482222	187,774		d	3+
Pd(III) III a	-1065,083055	0,298624	158,297		d	0
TS (III-V) a	-1065,080029	0,297809	153,935	-221.0342	d	0
Pd (I) V a	-1065,144454	0,300658	159,220		d	0
Pd(IV) IV a	-1064,911133	0,301088	148,270		s	+
TS (IV-VI) a	-1064,904369	0,300917	144,874	-178.0378	s	+
Pd(II) VI a	-1064,967395	0,303885	145,664		s	+
M06/Def2-TZVP						
Pd(III) III a	-1066,172826	0,298735	160,855		d	0
TS (III-V) a	-1066,169752	0,297876	158,113	-173.5296	d	0
Pd (I) V a	-1066,231427	0,301111	162,164		d	0
Pd(IV) IV a	-1066,005395	0,301330	150,815		s	+
TS (IV-VI) a	-1065,998550	0,300986	148,039	-161.5303	s	+
Pd(II) VI a	-1066,057502	0,304219	146,758		s	+
mPW2PLYP/LACVP(d)						
Pd(III) III a	-1064,043284	0,304560	159,700		d	0
TS (III-V) a	-1064,037472	0,303893	156,270	-227.6241	d	0
V a	-1064,102551	0,306345	160,908		d	0
Pd(IV) IV a	-1063,887608	0,306854	151,523		s	+
TS (IV-VI) a	-1063,875730	0,306226	147,388	-282.0649	s	+
VI a	-1063,935368	0,309100	148,067		s	+
MP2/LACVP(d)						
Pd(III) III a	-1061,620602	0,303610	153,774		d	0
TS (III-V) a	-1061,617581	0,302636	157,035	-216.9818	d	0
Pd(IV) IV a	-1061,488462	0,305518	150,684		s	+
TS (IV-VI) a	-1061,463941	0,304895	149,224	-360.2686	s	+
M06/LACVP(d)						

Pd(III) III b	-1177,882292	0,308922	171,131		d	0
TS (III-V) b	-1177,879288	0,308698	163,805	-217.0633	d	0
Pd (I) V b	-1177,945057	0,311094	169,335		d	0
Pd(IV) IV b	-1177,710183	0,311650	159,568		s	+
TS (IV-VI) b	-1177,702903	0,311404	155,191	-183.4848	s	+
Pd(II) VI b	-1177,766016	0,314273	156,291		s	+
Pd(III) III c	-1103,876346	0,326784	169,455		d	0
TS (III-V) c	-1103,873922	0,326048	160,186	-211.0327	d	0
Pd (I) V c	-1103,941017	0,329153	167,675		d	0
Pd(IV) IV c	-1103,709465	0,329469	158,291		s	+
TS (IV-VI) c	-1103,702345	0,329203	154,244	-185.9449	s	+
Pd(II) VI c	-1103,768715	0,332207	154,471		s	+
Pd(III) III d	-1156,810841	0,298069	169,633		d	0
TS (III-V) d	-1156,807635	0,297804	163,221	-220.3666	d	0
Pd (I) V d	-1156,873688	0,300331	169,249		d	0
Pd(IV) IV d	-1156,637187	0,301012	157,829		s	+
TS (IV-VI) d	-1156,629676	0,300496	154,242	-192.7329	s	+
Pd(II) VI d	-1156,695643	0,303404	156,000		s	+
Pd(III) III e	-1179,048725	0,332228	172,330		d	0
TS (III-V) e	-1179,046149	0,331863	166,762	-211.3585	d	0
Pd (I) V e	-1179,114154	0,334184	171,733		d	0
Pd(IV) IV e	-1178,881644	0,335202	160,404		s	+
TS (IV-VI) e	-1178,875653	0,334420	157,819	-208.1285	s	+
Pd(II) VI e	-1178,940672	0,337417	158,827		s	+
Pd(III) III f	-1042,574058	0,282048	154,522		d	0
TS (III-V) f	-1042,571337	0,281706	149,525	-210.0128	d	0
Pd (I) V f	-1042,640626	0,284232	156,517		d	0
Pd(IV) IV f	-1042,400168	0,284197	145,904		s	+
TS (IV-VI) f	-1042,393328	0,283317	145,253	-209.2556	s	+
Pd(II) VI f	-1042,462432	0,286745	143,757		s	+
Pd(III) III g	-1025,535674	0,284452	159,592		d	0
TS (III-V) g	-1025,532731	0,283745	155,939	-217.1434	d	0
Pd (I) V g	-1025,603269	0,287495	154,555		d	0
Pd(IV) IV g	-1025,365582	0,286351	151,751		s	+
TS (IV-VI) g	-1025,355975	0,286249	146,845	-184.7867	s	+
Pd(II) VI g	-1025,424750	0,289253	149,504		s	+

Values obtained carrying out SP calculations including CPCM on gas phase optimized geometries

Pd(III) III a	-1064,618593	0,299605	161,553		d	0
TS (III-V) a	-1064,616301	0,298853	151,257	-172.0693	d	0
Pd (I) V a	-1064,682800	0,301888	153,939		d	0
Pd(IV) IV a	-1064,450224	0,302242	149,311		s	+
TS (IV-VI) a	-1064,444903	0,301192	142,749	-101.3911	s	+
Pd(II) VI a	-1064,509036	0,304584	147,117		s	+

B: values obtained carrying out full optimization in the gas phase

	H (hartrees)	**ZPC** (hartrees)	**S** (cal/mol*K)	Imaginary freq.	Multipl.	Charge
M06/LACVP(d)						
$Ru(bpy)_3^{2+}$	-1578,102989	0,482956	189,304		s	2+
$Ru(bpy)_3^{3+}$ lox	-1577,660734	0,483116	190,217		d	3+
Phenyldiazonium	-340,485463	0,098801	78,845		s	+
Phenyldiazoyl	-340,726605	0,096991	81,167		d	0
Phenyl	-231,277461	0,087264	70,286		d	0
N_2	-109,449387	0,005618	45,785		s	0
Palladacyle II	-833,295140	0,211683	125,387		s	0
Pd(III) III a	-1064,600688	0,299799	159,314		d	0
TS (III-V) a	-1064,599238	0,299040	155,773	-163.7110	d	0
Pd (I) V a	-1064,665912	0,301957	158,983		d	0
Pd(IV) IV a	-1064,383702	0,301946	150,375		s	+
TS (IV-VI) a	-1064,381950	0,301579	146,525	-111.5000	s	+
Pd(II) VI a	-1064,448637	0,304757	147,824		s	+
BF4-	-424,357082	0,014855	69,060		s	-
Pd(IV)a-BF4	-1488,902787	0,319179	174,445		s	0
TS (IV) a	-1488,884838	0,318340	172,347	-297.5656	s	0
Pd(II)-BF4 VI a	-1488,941967	0,320378	176,508		s	0

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