Supplementary Information for
"Are carbodiphosphoranes better ligands than N-heterocyclic carbenes for Grubb's catalysts?" by R. Tonner, G. Frenking

Computational Methods in detail

Geometry optimizations without symmetry constraints have been carried out using the Gaussian03 optimizer[i] together with TurboMole5[ii] energies and gradients at the BP86[iii]/def-SVP[iv] level of theory. Stationary points were characterized as minima by calculating the Hessian matrix analytically at this level of theory.[v] Thermodynamic corrections have been taken from these calculations. The standard state for all thermodynamic data is 298.15 K and 1 atm. Single-point energies at the BP86/def-SVP optimized geometries have been calculated with the MP2 method[vi] applying the frozen core approximation for non-valence shell electrons. For the BP86 and the MP2 calculations the resolution-of-identity method has been applied.[vii] Transition state search have been done using the intrinsic reaction coordinate method as implemented in Gaussian03.[viii]

[i] Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.

[ii] R. Ahlrichs, M. Baer, M. Haeser, H. Horn, C. Koelmel, *Chem. Phys. Lett.* **1989** , *162* , 165.

[iii] a) A. D. Becke, *Phys. Rev. A* **1988**, *38* , 3098; b) J. P. Perdew, *Phys. Rev. B* **1986**, *33* , 8822.

[iv] A. Schaefer, H. Horn, R. Ahlrichs, *J. Chem. Phys* **1992**, *97* , 2571.

[v] P. Deglmann, F. Furche, R. Ahlrichs, *Chem. Phys. Lett.* **2002**, *362* , 511.

[vi] a) C. Møller, M.S. Plesset *Phys. Rev.* **1934**, *46* , 618; b) J.S. Binkley, J.A. Pople *Intern. J. Quantum Chem.* **1975**, *9S* , 229.

[vii] a) K. Eichkorn, O. Treutler, H. Ohm, M. Häser, R. Ahlrichs, *Chem. Phys. Lett.* **1995**, *242* , 652; b) F. Weigend, *PCCP* **2006**, *8* , 1057.

[viii] K. Fukui, *Acc. Chem. Res* . **1981**. *14* , 363.

Optimized structures are given for the molecules investigated.
For Nomenclature please refer to the article.
SCF energies refer to BP86/def-SVP energies.

Table S1 Geometries and SCF energies of investigated molecules

Reaction I

Aa-1Me

46			
E(SCF)	-2475.505812		
C	0.106603	0.243130	-0.275484
Ru	-0.242504	0.018303	1.835319
P	0.434347	-0.263613	4.063512
C	0.100749	-1.890717	4.867219
C	-1.993770	0.126941	2.324159
Cl	0.277987	2.363511	2.220582
Cl	-0.539322	-2.401662	1.556228
C	2.272386	-0.080877	4.177356
C	-0.185172	0.961929	5.294342
H	-2.679916	-0.753143	2.317985
H	-2.441555	1.107904	2.616933
H	0.613534	-1.971940	5.847050
H	-0.992622	-1.996384	5.008381
H	0.422878	-2.696303	4.180161
H	2.630553	-0.208231	5.219374
H	2.761491	-0.836147	3.531189
H	2.531903	0.930828	3.808660
H	0.321947	0.848457	6.273786
H	-0.010922	1.970521	4.871716
H	-1.275612	0.814345	5.420143
P	1.153729	-0.906892	-1.015696
P	-1.058091	1.142968	-1.159622
C	2.194020	-0.214196	-2.383081
H	2.977465	-0.948084	-2.660110
H	2.671203	0.721052	-2.032394
H	1.588411	0.003203	-3.281661
C	2.414760	-1.485876	0.182514
H	3.153813	-2.135794	-0.326589
H	1.878818	-2.054579	0.968993
H	2.923089	-0.604255	0.618593
C	0.486532	-2.471752	-1.752817
H	1.293411	-3.109062	-2.169843
H	-0.236017	-2.224225	-2.555725
H	-0.043057	-2.993667	-0.930679
C	-0.807500	1.264580	-2.992653

H	0.148017	1.776433	-3.213363
H	-1.636033	1.857369	-3.428205
H	-0.809759	0.262458	-3.463855
C	-1.235467	2.894619	-0.655205
H	-0.329969	3.448052	-0.969705
H	-1.275525	2.943053	0.452014
H	-2.137280	3.338813	-1.121991
C	-2.780875	0.475532	-1.074276
H	-2.783078	-0.559534	-1.467696
H	-3.492920	1.101889	-1.648254
H	-3.084307	0.438094	-0.010915

Ab-1Me

46

E(SCF) -2475.460397

C	0.051718	0.214074	-0.320135
Ru	-0.015488	0.071208	1.913226
C	-0.043171	1.890657	2.061212
H	-0.155505	2.489819	2.996007
H	0.098255	2.498235	1.138849
Cl	2.258062	-0.618997	2.245614
Cl	-2.225755	-0.828516	1.839824
P	-0.186982	-0.141828	4.233770
C	-0.151029	-1.897664	4.815905
C	1.133777	0.655979	5.257859
C	-1.739478	0.516237	4.998457
H	-1.774735	0.328318	6.090721
H	-1.802198	1.607133	4.814542
H	-2.599864	0.032069	4.497887
H	-0.234919	-1.977424	5.919094
H	-0.990172	-2.438658	4.336505
H	0.801354	-2.351861	4.479170
H	0.989315	0.464393	6.340508
H	2.111804	0.258798	4.925141
H	1.126659	1.749131	5.077178
P	1.429388	-0.391075	-1.150101
P	-1.383602	0.637832	-1.166557
C	1.410976	-0.441583	-3.007598
H	2.344322	-0.930769	-3.350694
H	1.372971	0.578033	-3.433253
H	0.550645	-1.031031	-3.379897
C	2.979917	0.549293	-0.827718
H	3.836510	0.106287	-1.374647
H	3.172040	0.520042	0.262066
H	2.823840	1.596711	-1.151136
C	1.851561	-2.146431	-0.765354

H	2.767441	-2.467699	-1.301444
H	0.996241	-2.783994	-1.062916
H	2.011336	-2.225435	0.326776
C	-1.193478	1.543361	-2.781105
H	-0.477885	2.378383	-2.651932
H	-2.178378	1.953740	-3.081384
H	-0.836980	0.877859	-3.587245
C	-2.550146	-0.727037	-1.637541
H	-2.010855	-1.461499	-2.267992
H	-3.437470	-0.349322	-2.186190
H	-2.860131	-1.220557	-0.696054
C	-2.459648	1.818257	-0.256175
H	-1.928405	2.780387	-0.133860
H	-2.704388	1.393539	0.734183
H	-3.388196	1.978093	-0.839469

B-1Me

33

E(SCF)	-2014.518990		
C	-0.109448	-0.203256	-0.044077
Ru	0.044038	-0.778309	1.926825
C	-1.151683	0.422156	2.555233
Cl	2.167883	-0.060259	2.637275
Cl	-1.018008	-2.863528	1.782486
H	-1.606778	1.216563	1.919066
H	-1.463013	0.418600	3.629664
P	1.211227	0.736075	-0.661623
P	-1.398157	-0.861436	-1.007077
C	1.508576	2.292749	0.270138
H	2.345143	2.858951	-0.185762
H	1.761388	2.026125	1.314452
H	0.582792	2.899054	0.250775
C	2.844456	-0.118658	-0.689175
H	3.636272	0.551311	-1.080987
H	2.762237	-1.019861	-1.327584
H	3.087480	-0.417870	0.349216
C	1.086657	1.341390	-2.407971
H	2.001084	1.928826	-2.621553
H	0.206346	1.994836	-2.546643
H	1.042731	0.497353	-3.121531
C	-1.184029	-2.586483	-1.636122
H	-0.275156	-2.627582	-2.268076
H	-2.064149	-2.919792	-2.223021
H	-1.044930	-3.238284	-0.751434
C	-1.848279	0.064708	-2.547434
H	-1.070743	-0.021464	-3.326732

H	-2.025295	1.131631	-2.314091
H	-2.784872	-0.375145	-2.943014
C	-3.007307	-0.896086	-0.123680
H	-2.899081	-1.521487	0.781953
H	-3.781000	-1.325618	-0.790816
H	-3.283700	0.136062	0.162281

Ca-1Me

39

E(SCF) -2093.043848

C	0.008897	0.181937	0.133690
Ru	0.009024	-0.200946	-1.993470
Cl	-2.350521	0.139210	-2.284959
C	0.622945	1.501256	-2.309182
Cl	1.960187	-1.553365	-1.743751
H	0.953963	1.917727	-3.282740
H	0.635941	2.213812	-1.457865
C	0.142065	-0.243634	-4.284493
C	-0.242018	-1.502844	-3.833924
H	-0.607412	0.471668	-4.657094
H	-1.306541	-1.787159	-3.828711
H	0.493191	-2.316918	-3.746794
H	1.191805	-0.048935	-4.556488
P	1.508939	0.339751	0.990700
P	-1.481200	0.042205	1.006817
C	2.282823	-1.200902	1.669783
H	3.221868	-0.981877	2.217981
H	2.482504	-1.864657	0.806953
H	1.565944	-1.699515	2.351307
C	2.854312	1.119185	0.012309
H	3.788290	1.070800	0.606645
H	2.602886	2.177237	-0.188101
H	2.982703	0.564163	-0.934716
C	1.506914	1.455457	2.478206
H	2.555976	1.677125	2.759156
H	1.011459	0.987825	3.347134
H	0.993336	2.404038	2.228121
C	-1.385518	-0.063304	2.857584
H	-0.674024	-0.849021	3.177109
H	-2.392423	-0.329611	3.235491
H	-1.094518	0.905759	3.301910
C	-2.424719	-1.495304	0.632948
H	-1.796351	-2.363604	0.911617
H	-2.635085	-1.514918	-0.452878
H	-3.377367	-1.519525	1.199247
C	-2.674342	1.427248	0.779788

H	-2.189699	2.364278	1.117005
H	-3.602974	1.251692	1.359602
H	-2.904659	1.492949	-0.300957

Cb-1Me

39

E(SCF) -2093.062655

C	0.005072	-0.115372	-0.073719
Ru	-0.045617	0.398328	2.063692
Cl	1.063616	2.394194	1.318403
C	1.184055	-0.861364	2.483490
Cl	-2.040081	-0.961411	2.240977
C	-0.592692	0.557394	4.275819
C	0.424778	1.468037	4.018580
H	1.718702	-0.893753	3.464223
H	1.401826	-1.706276	1.793961
H	1.474743	1.240753	4.266970
H	-0.395137	-0.420135	4.741840
H	0.207946	2.533823	3.856664
H	-1.645201	0.878778	4.302594
P	1.478991	-0.063364	-0.967342
P	-1.486307	-0.131651	-0.945692
C	-1.423697	0.350128	-2.738792
H	-1.126255	1.411461	-2.835146
H	-2.435163	0.223613	-3.173594
H	-0.720883	-0.279984	-3.315383
C	-2.732112	1.069717	-0.319767
H	-2.276460	2.078866	-0.335584
H	-2.995328	0.793099	0.718082
H	-3.637959	1.051162	-0.957994
C	-2.367458	-1.753813	-1.030368
H	-1.716842	-2.480422	-1.555946
H	-3.337750	-1.666266	-1.560702
H	-2.522673	-2.090160	0.012062
C	1.842993	1.427178	-2.018711
H	2.839705	1.349347	-2.498812
H	1.809988	2.298898	-1.336905
H	1.074691	1.550869	-2.803790
C	1.724408	-1.474069	-2.150753
H	2.701420	-1.393008	-2.669827
H	0.922857	-1.499469	-2.913357
H	1.686480	-2.420207	-1.576760
C	3.003188	-0.164714	0.049478
H	3.872407	-0.019331	-0.621563
H	3.081712	-1.150697	0.540329
H	2.971832	0.638600	0.808925

Cc-1Me

39

E(SCF) -2093.072770

C	-0.124109	0.118454	-0.055335
Ru	0.076128	0.447342	2.012210
Cl	1.788872	2.104962	1.393459
C	1.356494	-0.633693	2.716827
Cl	-1.450882	-1.478287	2.275988
C	-1.060237	0.997166	3.829364
C	-0.132794	2.016855	3.560098
H	1.146171	-1.686283	3.005676
H	2.393798	-0.248189	2.833210
H	-0.441871	2.938421	3.040328
H	-0.881382	0.243110	4.609082
H	0.813083	2.097862	4.115125
H	-2.114099	1.103963	3.524734
P	1.236498	0.008927	-1.125003
P	-1.734833	-0.025547	-0.670187
C	1.753251	1.540406	-2.019421
H	2.649314	1.361026	-2.647752
H	1.968506	2.290546	-1.233548
H	0.921792	1.901872	-2.654719
C	2.755919	-0.593178	-0.308687
H	3.545790	-0.743750	-1.070772
H	2.529863	-1.545077	0.207458
H	3.061912	0.172013	0.430086
C	1.018281	-1.233688	-2.483116
H	1.927122	-1.263533	-3.116951
H	0.154288	-0.989031	-3.129396
H	0.856043	-2.231884	-2.032535
C	-1.976284	0.884150	-2.265947
H	-1.740413	1.954219	-2.108854
H	-3.029416	0.785516	-2.597848
H	-1.322991	0.488724	-3.066342
C	-2.994657	0.763684	0.403808
H	-2.682752	1.801968	0.629206
H	-3.057132	0.169472	1.336083
H	-3.971573	0.771772	-0.119541
C	-2.426107	-1.704715	-1.023982
H	-1.802330	-2.212023	-1.784860
H	-3.473918	-1.646446	-1.382788
H	-2.369274	-2.262765	-0.069149

TSCD-1Me

39

E(SCF)	-2093.060953		
C	0.059699	-0.478788	-0.010678
Ru	-0.015280	-0.085780	-2.097982
Cl	1.937318	-1.464659	-2.395970
Cl	-2.088024	1.191531	-1.734651
C	0.712779	1.524125	-2.576601
C	-1.043702	-0.706591	-3.915292
C	0.081940	-0.087830	-4.474297
H	1.786902	1.583126	-2.874016
H	0.128253	2.471952	-2.593261
H	-0.021838	0.898267	-4.953988
H	-2.043096	-0.247507	-3.974964
H	-1.003597	-1.799897	-3.748289
H	1.011034	-0.647283	-4.658660
P	-1.402247	-1.059357	0.698068
P	1.305438	0.276155	0.900911
C	-2.604782	0.101893	1.498377
H	-2.110912	0.629721	2.338204
H	-3.498804	-0.433497	1.878901
H	-2.886852	0.836021	0.717734
C	-1.124531	-2.340370	2.004817
H	-0.442759	-3.115757	1.606044
H	-2.093145	-2.803869	2.280784
H	-0.679032	-1.899834	2.915288
C	-2.408534	-1.960322	-0.539664
H	-1.777289	-2.724862	-1.032474
H	-2.763970	-1.217138	-1.280587
H	-3.268161	-2.448322	-0.039078
C	1.268752	-0.006240	2.728725
H	2.098170	0.563560	3.191796
H	1.410177	-1.080381	2.951615
H	0.315095	0.343826	3.168799
C	1.309759	2.122123	0.802777
H	2.130851	2.562723	1.402726
H	0.331282	2.501292	1.155597
H	1.424982	2.415115	-0.258091
C	3.014848	-0.195380	0.441511
H	3.189049	-1.244295	0.748333
H	3.743497	0.477061	0.936997
H	3.107521	-0.163693	-0.662421

D-1Me

39			
E(SCF)	-2093.098956		
C	0.064700	0.034229	-1.417556
Ru	-0.188159	0.216108	0.581620

C	-0.664749	1.660029	1.849972
C	-0.470917	0.420386	2.820945
C	-0.071915	-0.967811	2.164372
Cl	2.180457	0.641196	0.956875
Cl	-2.585328	-0.189483	0.430132
H	0.107070	2.440283	1.998498
H	-1.704922	2.038005	1.840009
H	-1.443154	0.265108	3.326549
H	-0.874089	-1.726093	2.254133
H	0.929608	-1.318244	2.479159
H	0.350251	0.684987	3.514337
P	-0.872617	-1.169160	-2.264018
P	1.210715	1.086474	-2.206804
C	0.006709	-1.898220	-3.721154
H	0.116100	-1.171358	-4.546384
H	-0.578198	-2.760611	-4.097835
H	1.007831	-2.252828	-3.408736
C	-1.184981	-2.657832	-1.244343
H	-0.217017	-3.038311	-0.866377
H	-1.689004	-3.430044	-1.859451
H	-1.828645	-2.349167	-0.396886
C	-2.515206	-0.680218	-2.942717
H	-2.383266	0.149583	-3.663931
H	-3.111493	-0.330312	-2.076598
H	-3.015212	-1.534542	-3.442673
C	0.735856	1.525995	-3.941647
H	1.415779	2.320361	-4.308352
H	-0.302815	1.908993	-3.954729
H	0.816977	0.662202	-4.626082
C	1.298063	2.739404	-1.423545
H	1.957189	3.399358	-2.022455
H	1.704625	2.600472	-0.402158
H	0.276382	3.161316	-1.370933
C	2.957574	0.518629	-2.361583
H	3.585466	1.279936	-2.867464
H	2.987102	-0.429503	-2.932796
H	3.314042	0.341962	-1.327305

Reaction II

Aa-2Me

36

E(SCF) -1821.409214

C	-0.366094	0.518562	-2.403622
N	-0.850244	0.761524	-1.035404
C	-0.140576	0.068408	-0.111947
N	0.860344	-0.589540	-0.756772

C	0.983315	-0.179258	-2.160030
Ru	-0.255790	0.009736	1.927002
P	0.453088	-0.445255	4.158038
C	-0.728592	-1.392914	5.205057
C	1.902905	-1.337188	-0.085297
C	-2.063679	1.516827	-0.830047
C	-1.845718	0.709936	2.446341
Cl	0.880415	2.144005	1.963580
Cl	-1.062744	-2.286189	1.882032
C	1.936887	-1.544069	4.086750
C	0.973732	0.983472	5.196517
H	1.845482	0.515259	-2.291426
H	1.146250	-1.055791	-2.820505
H	-1.086321	-0.127983	-2.956862
H	-0.266415	1.471209	-2.963278
H	2.264910	-2.150300	-0.746903
H	2.769063	-0.698797	0.201132
H	1.464119	-1.814323	0.815585
H	-1.940896	2.564881	-1.177491
H	-2.914245	1.058645	-1.382619
H	-2.300892	1.524146	0.247845
H	-2.740972	0.062294	2.603123
H	-1.964166	1.800722	2.651588
H	-0.253678	-1.756254	6.138461
H	-1.586722	-0.738236	5.453231
H	-1.096699	-2.238405	4.590293
H	2.313690	-1.782622	5.102035
H	1.633968	-2.476483	3.570732
H	2.740724	-1.050175	3.506279
H	1.512589	0.655839	6.108171
H	1.602668	1.646950	4.570915
H	0.070648	1.556550	5.484583

Ab-2Me

36

E(SCF) -1821.371882

C	-0.001433	0.123514	-0.159963
Ru	-0.013523	0.173135	1.923834
N	0.978681	-0.352501	-0.983739
N	-1.037362	0.510717	-0.964893
C	0.573076	-0.402720	-2.395516
C	2.147970	-1.118856	-0.600665
C	-0.723473	0.415342	-2.397183
C	-2.365218	0.951999	-0.586291
H	1.361404	0.024076	-3.049767
H	0.412878	-1.460911	-2.709608

H	-1.550793	-0.078235	-2.949089
H	-0.587902	1.431069	-2.835445
H	1.980964	-2.207584	-0.771886
H	3.022055	-0.804752	-1.208955
H	2.385323	-0.931795	0.461036
H	-2.517260	2.037527	-0.780801
H	-3.118404	0.391975	-1.181724
H	-2.539559	0.734670	0.480817
C	-0.756301	1.844140	1.939463
H	-1.118977	2.359321	2.859417
H	-0.839935	2.462954	1.018119
Cl	2.304808	0.635443	2.217012
Cl	-1.691506	-1.499904	1.873144
P	-0.102781	0.029661	4.319294
C	0.680503	-1.526839	4.936436
C	0.761146	1.349659	5.283197
C	-1.790755	-0.018302	5.072384
H	-1.756892	-0.189785	6.167310
H	-2.308103	0.940513	4.869952
H	-2.359405	-0.826869	4.573263
H	0.638538	-1.610343	6.041501
H	0.153710	-2.386125	4.476862
H	1.735914	-1.538598	4.600359
H	0.741540	1.150229	6.373671
H	1.805420	1.404357	4.919311
H	0.277042	2.326187	5.083159

B-2Me

23

E(SCF)	-1360.429372		
C	0.813482	0.282777	-1.973819
C	-0.651585	-0.162823	-2.044280
N	-1.092320	-0.008207	-0.654821
C	-0.032915	0.087495	0.214902
N	1.111103	0.167412	-0.542914
C	-2.513710	-0.005685	-0.368477
Ru	-0.142302	0.146396	2.143824
C	-1.342015	-1.206352	2.278739
C	2.435458	0.552800	-0.094078
Cl	-1.266522	2.176040	2.146804
Cl	1.825528	-0.809110	2.940049
H	0.953057	1.336943	-2.312854
H	1.493392	-0.357033	-2.572730
H	-0.756886	-1.222812	-2.374515
H	-1.264764	0.464191	-2.723609
H	3.199649	-0.023132	-0.655472

H	2.619279	1.638070	-0.269201
H	2.550644	0.322663	0.980145
H	-3.024789	0.676220	-1.081128
H	-2.966905	-1.016068	-0.479687
H	-2.687633	0.371142	0.653804
H	-1.653571	-1.896915	1.465907
H	-1.777710	-1.409118	3.287228

Ca-2Me

29

E(SCF) -1438.954862

C	-0.579451	-0.178936	2.268562
N	-1.006166	-0.123252	0.863938
C	0.025946	0.156736	0.014843
N	1.125081	0.423542	0.781471
C	0.814966	0.456897	2.217496
Ru	-0.053061	0.042055	-2.009511
Cl	-2.130955	1.200988	-2.146581
C	2.506732	0.579974	0.367721
C	-2.274072	-0.743262	0.524539
C	1.031770	1.516440	-2.135953
Cl	1.266795	-1.911028	-1.800281
H	0.819209	1.505544	2.593534
H	1.573734	-0.110564	2.795081
H	-0.554323	-1.237511	2.618693
H	-1.288497	0.374194	2.917995
H	2.856978	1.632451	0.454500
H	2.627446	0.226459	-0.670664
H	3.150797	-0.048134	1.019620
H	-2.231822	-1.845950	0.678485
H	-2.535771	-0.509578	-0.522293
H	-3.074547	-0.331032	1.172504
H	1.523205	1.836282	-3.078797
H	1.198298	2.194755	-1.271945
C	0.428640	-0.133874	-4.352325
C	-0.744400	-0.803035	-4.092676
H	0.406273	0.888988	-4.759591
H	-1.721578	-0.333294	-4.276968
H	-0.733072	-1.883581	-3.871976
H	1.397876	-0.654774	-4.343871

Cb-2Me

29

E(SCF) -1438.972521

N	1.026733	0.036868	-0.766446
C	0.683024	0.043621	-2.198902

C	-0.826224	-0.206607	-2.182062
N	-1.163614	0.037922	-0.774797
C	-0.079312	0.082947	0.028022
C	-2.559368	0.161288	-0.405736
Ru	-0.127211	0.225280	2.083650
Cl	0.210248	2.497510	1.574054
C	2.370066	0.475857	-0.427538
C	1.412605	-0.716605	2.253661
Cl	-1.633051	-1.599283	2.047696
C	-0.687491	0.048665	4.312318
C	0.272302	1.028476	4.218658
H	0.943307	1.024189	-2.633670
H	1.243022	-0.729807	-2.741308
H	-1.085456	-1.242209	-2.457632
H	-1.386304	0.472911	-2.839293
H	2.625063	1.363368	-1.029524
H	2.420269	0.753926	0.627044
H	3.107908	-0.311855	-0.641416
H	-3.043696	0.860695	-1.104298
H	-3.078129	-0.807145	-0.442066
H	-2.647553	0.555722	0.608535
H	1.960710	-0.756401	3.209667
H	1.832008	-1.341214	1.451975
H	1.317483	0.820320	4.448604
H	-0.445398	-0.970504	4.607775
H	0.006973	2.082393	4.166741
H	-1.748876	0.297512	4.333451

Cc-2Me

29

E(SCF) -1438.969823

N	0.812309	-0.037021	-0.881201
C	0.288342	0.220103	-2.236131
C	-1.230761	0.135274	-2.020601
N	-1.334880	0.349363	-0.569790
C	-0.149741	0.136957	0.047058
C	-2.616568	0.338805	0.114359
Ru	-0.090120	0.180647	2.103896
Cl	0.835231	2.384072	1.606357
C	2.242449	0.003422	-0.641162
C	1.569154	-0.420237	2.506583
Cl	-0.896464	-2.104741	1.836141
C	-1.215989	-0.041605	3.993800
C	-0.688129	1.258981	3.942542
H	0.606576	1.232517	-2.575663
H	0.670069	-0.526658	-2.960363

H	-1.637079	-0.866892	-2.290223
H	-1.795987	0.904791	-2.583638
H	2.594418	1.046536	-0.489878
H	2.476990	-0.578576	0.268692
H	2.767003	-0.455395	-1.501249
H	-3.376534	0.825093	-0.527702
H	-2.931531	-0.693352	0.377332
H	-2.547571	0.934444	1.048141
H	1.742590	-1.502623	2.698108
H	2.422779	0.286738	2.604572
H	-1.308506	2.110931	3.620188
H	-0.741114	-0.837357	4.586860
H	0.222336	1.534895	4.495017
H	-2.263126	-0.239043	3.711900

TSCD-2Me

29

E(SCF)	-1438.963899		
C	0.610673	-0.194522	2.099284
C	-0.842714	-0.668888	1.945229
N	-0.940412	-0.856284	0.490788
C	0.042338	-0.189107	-0.163188
N	0.928329	0.285580	0.742786
C	-2.176785	-1.286674	-0.141343
Ru	-0.007169	-0.037137	-2.181328
Cl	1.522917	-1.898639	-2.253129
C	2.244426	0.816653	0.455830
Cl	-1.648368	1.724368	-1.824573
C	1.226186	1.199968	-2.701361
C	-1.184724	-0.393041	-4.013786
C	0.085366	-0.211912	-4.562801
H	0.729355	0.615412	2.846827
H	1.296542	-1.027851	2.378015
H	-1.054360	-1.611533	2.488947
H	-1.572178	0.102555	2.284647
H	2.214934	1.355031	-0.508583
H	3.008703	0.011736	0.386025
H	2.536264	1.529784	1.252279
H	-2.681395	-2.025347	0.511369
H	-1.947104	-1.796452	-1.099468
H	-2.850547	-0.429190	-0.352799
H	2.266693	0.898074	-2.965008
H	0.953052	2.272933	-2.826625
H	0.327106	0.723757	-5.091789
H	-1.974069	0.369349	-4.100580
H	-1.508016	-1.423272	-3.770532

H	0.791869	-1.049907	-4.664744

D-2Me

29

E(SCF) -1438.987570

C	0.000193	-0.000094	-1.301516
N	0.542185	0.963223	-2.080131
C	0.522410	0.565660	-3.496254
C	-0.522491	-0.565578	-3.496207
N	-0.541923	-0.963349	-2.080133
C	1.418939	2.011652	-1.592417
C	-1.418803	-2.011652	-1.592348
Ru	0.000292	-0.000183	0.685945
C	0.642308	1.182687	2.132296
C	0.000057	-0.000079	2.963756
C	-0.642628	-1.182590	2.132277
Cl	2.124124	-1.117490	0.657266
Cl	-2.123663	1.117137	0.656565
H	0.241622	1.417984	-4.147235
H	1.529553	0.204573	-3.808946
H	-0.241867	-1.417804	-4.147384
H	-1.529711	-0.204437	-3.808591
H	1.118076	2.286114	-0.563616
H	2.482637	1.688088	-1.576338
H	1.317253	2.910175	-2.233226
H	-1.317621	-2.910028	-2.233439
H	-1.117646	-2.286474	-0.563730
H	-2.482393	-1.687761	-1.575778
H	1.740502	1.249706	2.244521
H	0.091531	2.136309	2.236251
H	-0.814635	0.441650	3.568172
H	-1.740872	-1.249089	2.244292
H	-0.092310	-2.136462	2.236398
H	0.814882	-0.441887	3.567925

Reaction III

Aa-1Ph

127

E(SCF) -4210.783341

C	0.113033	0.206490	0.084909
Ru	0.189750	0.481588	2.337572
C	-1.624135	0.589579	2.452421
P	0.445163	0.708853	4.707975
C	2.233110	0.881892	5.324809
C	2.942175	2.201135	4.955245
C	4.309874	2.292992	5.659617

C	5.206470	1.084708	5.348933
C	4.487154	-0.244322	5.628017
C	3.118484	-0.318158	4.925250
C	-0.120447	-0.816378	5.707413
C	0.363659	-0.960885	7.168579
C	-0.014952	-2.336331	7.752033
C	-1.525669	-2.595113	7.665890
C	-2.020817	-2.442864	6.221353
C	-1.639860	-1.077793	5.617751
C	-0.322632	2.294769	5.428340
C	-1.748737	2.622831	4.938596
C	-2.178186	4.035390	5.377096
C	-2.063725	4.231643	6.896191
C	-0.649751	3.890959	7.389371
C	-0.226528	2.473101	6.959003
Cl	0.801067	2.782804	2.070013
Cl	0.699391	-1.850993	2.530701
H	-2.245106	0.943783	1.598863
H	-2.237238	0.329266	3.341695
H	0.365403	-1.617296	5.103002
H	-2.196686	-0.274420	6.151013
H	-1.963449	-1.053142	4.559901
H	-3.122021	-2.581699	6.168211
H	-1.573457	-3.245648	5.593529
H	-2.060079	-1.867200	8.318427
H	-1.771880	-3.604707	8.059373
H	0.334728	-2.405233	8.804693
H	0.525545	-3.131312	7.190273
H	-0.089257	-0.168772	7.802110
H	1.461875	-0.830953	7.242182
H	2.135262	0.870529	6.434012
H	3.064447	2.257935	3.853175
H	2.328483	3.079896	5.238200
H	4.820079	3.236989	5.370409
H	4.146302	2.355602	6.760125
H	5.492914	1.116506	4.275987
H	6.152665	1.144213	5.929010
H	5.120675	-1.100106	5.310743
H	4.338603	-0.359278	6.726537
H	3.257181	-0.316792	3.822890
H	2.624420	-1.281953	5.162372
H	0.335531	3.053061	4.945636
H	-0.895321	1.736932	7.456822
H	0.799305	2.263237	7.325991
H	-0.587970	3.983968	8.495101
H	0.072902	4.628682	6.972803

H	-2.798439	3.569688	7.409266
H	-2.333995	5.272090	7.177230
H	-3.216722	4.234764	5.036055
H	-1.532013	4.780405	4.860677
H	-2.473822	1.879066	5.338074
H	-1.782651	2.553314	3.833102
P	1.584994	-0.081614	-0.755823
P	-1.362982	0.140736	-0.811529
C	3.084684	-0.129409	0.335269
C	5.572881	-0.026394	1.665379
C	3.826365	-1.308628	0.553212
C	3.589402	1.101814	0.811648
C	4.827471	1.148847	1.470635
C	5.062011	-1.255327	1.219310
H	3.454615	-2.274597	0.187411
H	3.013909	2.027073	0.663759
H	5.216143	2.117087	1.820962
H	5.633463	-2.183018	1.375581
H	6.553336	0.015384	2.164332
C	2.173708	1.238580	-1.944519
C	3.084100	3.347027	-3.587141
C	1.435991	2.432277	-2.045832
C	3.396128	1.122371	-2.645110
C	3.841170	2.167009	-3.470073
C	1.887507	3.481851	-2.865821
H	0.517761	2.542770	-1.449278
H	4.017954	0.221120	-2.530782
H	4.792419	2.065078	-4.015197
H	1.303308	4.412701	-2.929702
H	3.439198	4.168117	-4.228983
C	1.665246	-1.685014	-1.699429
C	1.712418	-4.213182	-2.960605
C	1.990346	-1.793698	-3.066531
C	1.339697	-2.854517	-0.972400
C	1.376163	-4.109830	-1.599151
C	2.008975	-3.052553	-3.692246
H	2.211778	-0.894912	-3.658603
H	1.063032	-2.770407	0.093516
H	1.135446	-5.013638	-1.018077
H	2.254087	-3.121592	-4.763303
H	1.734065	-5.197918	-3.452721
C	-1.283672	-0.501609	-2.553524
C	-1.168691	-1.471898	-5.206396
C	-0.903887	0.351260	-3.614142
C	-1.602967	-1.846812	-2.838738
C	-1.543958	-2.326636	-4.156677

C	-0.846360	-0.132743	-4.931038
H	-0.663421	1.405513	-3.417196
H	-1.906804	-2.523575	-2.027397
H	-1.798794	-3.377256	-4.362713
H	-0.553650	0.546419	-5.746492
H	-1.130442	-1.848814	-6.240118
C	-2.235585	1.774274	-1.047935
C	-3.515955	4.274288	-1.358597
C	-1.870346	2.867083	-0.234264
C	-3.236760	1.950328	-2.031778
C	-3.872604	3.193749	-2.183794
C	-2.513848	4.107647	-0.388972
H	-1.061264	2.756942	0.509116
H	-3.512364	1.119899	-2.699382
H	-4.646625	3.319259	-2.956892
H	-2.217281	4.949881	0.254950
H	-4.013979	5.248789	-1.480171
C	-2.656385	-0.962833	-0.048415
C	-4.522243	-2.812527	0.988020
C	-4.041559	-0.756692	-0.228513
C	-2.214452	-2.094332	0.668216
C	-3.145794	-3.013317	1.181189
C	-4.967220	-1.678472	0.286877
H	-4.408647	0.133628	-0.758120
H	-1.139491	-2.229191	0.864251
H	-2.785303	-3.885635	1.747788
H	-6.044818	-1.504382	0.142729
H	-5.250404	-3.532880	1.392112

B-1Ph

75

E(SCF)	-3164.135908		
C	-0.049894	0.013485	-0.027378
Ru	-0.077188	0.427933	2.000410
Cl	0.160973	2.767435	1.776158
Cl	0.848085	-1.668773	2.532680
C	-1.817378	0.279208	2.444551
H	-2.701851	0.039070	1.816262
H	-2.036958	0.459763	3.530634
P	1.509549	-0.037109	-0.799742
P	-1.507185	-0.297221	-0.916195
C	2.898476	0.083242	0.420205
C	5.042052	0.396116	2.228881
C	3.765480	-0.995962	0.690088
C	3.127658	1.328418	1.046439
C	4.187736	1.475591	1.955921

C	4.832065	-0.835676	1.587804
H	3.617003	-1.968025	0.202342
H	2.464854	2.182801	0.847070
H	4.341571	2.446994	2.449629
H	5.499459	-1.686924	1.791103
H	5.874789	0.514498	2.939130
C	1.937158	1.392097	-1.915324
C	2.584844	3.657380	-3.463118
C	1.027999	2.460910	-2.022939
C	3.193231	1.479801	-2.557761
C	3.508448	2.603642	-3.336929
C	1.351040	3.589397	-2.796929
H	0.080994	2.414544	-1.462922
H	3.938641	0.679030	-2.433869
H	4.486960	2.663912	-3.838002
H	0.636616	4.423845	-2.866837
H	2.838007	4.541226	-4.068776
C	-2.667406	1.137187	-1.178903
C	-4.426008	3.312279	-1.583322
C	-2.571601	2.288597	-0.369994
C	-3.642103	1.092387	-2.204690
C	-4.515816	2.174253	-2.402769
C	-3.451192	3.366292	-0.573852
H	-1.791859	2.361448	0.405735
H	-3.713413	0.216409	-2.867077
H	-5.266215	2.127930	-3.207202
H	-3.361915	4.257829	0.065629
H	-5.110498	4.160368	-1.739807
C	-2.564930	-1.613911	-0.141020
C	-4.058115	-3.744665	0.947891
C	-3.961332	-1.679716	-0.340712
C	-1.925078	-2.610848	0.623480
C	-2.672467	-3.670583	1.164333
C	-4.701380	-2.744917	0.198253
H	-4.482131	-0.893612	-0.905202
H	-0.848879	-2.526421	0.840899
H	-2.163555	-4.432100	1.774813
H	-5.789576	-2.787248	0.037051
H	-4.641748	-4.574731	1.375302
C	-1.243280	-0.905409	-2.644082
C	-0.876839	-1.809792	-5.292519
C	-0.951129	0.011479	-3.678662
C	-1.349106	-2.278998	-2.949196
C	-1.166041	-2.726153	-4.267325
C	-0.766619	-0.441437	-4.995026
H	-0.882900	1.087183	-3.462295

H	-1.582657	-3.001985	-2.154375
H	-1.254830	-3.799443	-4.493287
H	-0.543784	0.283544	-5.792785
H	-0.740915	-2.162756	-6.326420
C	1.841771	-1.588158	-1.757099
C	2.323579	-4.052986	-3.043297
C	2.229771	-1.618376	-3.111295
C	1.675834	-2.805299	-1.053825
C	1.927189	-4.028207	-1.694080
C	2.465269	-2.848453	-3.749953
H	2.334739	-0.683898	-3.680127
H	1.357680	-2.781060	0.002403
H	1.809831	-4.968704	-1.133988
H	2.759220	-2.860941	-4.810661
H	2.514943	-5.013799	-3.545660

Ca-1Ph

81

E(SCF)	-3242.687096		
C	-0.067230	0.257932	-0.120249
Ru	0.020966	0.757648	2.045653
Cl	0.619162	-1.502981	2.562225
C	-1.796943	0.687926	2.266315
C	-0.122988	1.125110	4.306681
C	1.181474	1.348717	3.887550
Cl	0.293895	3.074740	1.489087
H	-2.362533	1.007741	3.166281
H	-2.439273	0.287560	1.454189
H	1.546164	2.371468	3.707561
H	-0.805012	1.975706	4.463571
H	-0.416907	0.161393	4.750345
H	1.940905	0.554539	3.977285
P	1.501298	-0.022211	-0.783786
P	-1.481770	-0.052344	-1.061394
C	2.836331	0.083190	0.499250
C	4.947469	0.358515	2.352550
C	3.555051	-1.050481	0.933903
C	3.193291	1.359216	0.990813
C	4.240102	1.490421	1.919238
C	4.604333	-0.910168	1.854556
H	3.300744	-2.048985	0.555165
H	2.643424	2.253457	0.663284
H	4.501559	2.489523	2.299651
H	5.155473	-1.802920	2.187060
H	5.770947	0.463466	3.075725
C	1.766707	-1.673822	-1.594775

C	2.017902	-4.262569	-2.695234
C	2.313389	-1.850314	-2.883160
C	1.334740	-2.805993	-0.864340
C	1.468033	-4.091898	-1.412188
C	2.437035	-3.139956	-3.428162
H	2.626504	-0.980795	-3.477733
H	0.898781	-2.668826	0.140086
H	1.134167	-4.965705	-0.832024
H	2.860634	-3.264942	-4.436722
H	2.115070	-5.271289	-3.125615
C	2.132611	1.251028	-1.988014
C	3.114049	3.291688	-3.669461
C	1.321723	2.350353	-2.317847
C	3.457825	1.196004	-2.478416
C	3.940632	2.207394	-3.322736
C	1.808914	3.365730	-3.158860
H	0.315720	2.413580	-1.879079
H	4.126955	0.373739	-2.181130
H	4.973300	2.156517	-3.701057
H	1.166462	4.224844	-3.405309
H	3.497421	4.088384	-4.325510
C	-1.285454	-0.069904	-2.908064
C	-0.986146	-0.087655	-5.718743
C	-1.554574	1.091361	-3.665742
C	-0.872880	-1.243641	-3.576944
C	-0.723663	-1.248745	-4.973592
C	-1.403313	1.081739	-5.061077
H	-1.902177	2.006079	-3.163580
H	-0.679165	-2.164537	-3.008656
H	-0.402762	-2.171784	-5.479868
H	-1.621247	1.993533	-5.637793
H	-0.872639	-0.095652	-6.813706
C	-2.803527	1.230241	-0.806165
C	-4.731565	3.280902	-0.589748
C	-2.408631	2.546963	-0.489680
C	-4.173328	0.944939	-0.999165
C	-5.129653	1.967554	-0.893783
C	-3.372205	3.564463	-0.381650
H	-1.350940	2.766988	-0.268497
H	-4.504151	-0.080005	-1.217606
H	-6.194692	1.732374	-1.043583
H	-3.049878	4.582909	-0.116049
H	-5.484508	4.079620	-0.503276
C	-2.351787	-1.671936	-0.740583
C	-3.665983	-4.106632	-0.169123
C	-3.278620	-2.219644	-1.658882

C	-2.077664	-2.364130	0.456993
C	-2.738435	-3.572533	0.739640
C	-3.930766	-3.430163	-1.372553
H	-3.484826	-1.710099	-2.612343
H	-1.325362	-1.974248	1.163750
H	-2.513532	-4.100207	1.679238
H	-4.646118	-3.848847	-2.097409
H	-4.177653	-5.055791	0.053794

Cc-1Ph

81

E(SCF) -3242.691976

C	-0.147495	0.113794	-0.137721
Ru	0.041548	0.314401	2.029552
Cl	0.556206	-2.101063	2.019861
C	-1.669556	-0.048852	2.499150
C	1.102875	-0.035411	3.949575
C	0.654454	1.291907	3.957516
Cl	-0.481068	2.697819	1.703972
H	-2.413227	0.768783	2.642923
H	-2.012205	-1.093664	2.669741
H	-0.254273	1.584727	4.504202
H	0.580346	-0.829354	4.501832
H	2.143165	-0.270998	3.670816
H	1.330645	2.120642	3.704443
P	1.419258	0.223369	-0.844557
P	-1.578999	-0.202586	-1.051828
C	2.662140	0.405092	0.518028
C	4.613212	0.868290	2.502817
C	3.572474	-0.615045	0.872591
C	2.740200	1.663433	1.162157
C	3.714008	1.886493	2.152413
C	4.539242	-0.381374	1.861157
H	3.532082	-1.593488	0.376657
H	2.038056	2.468722	0.897387
H	3.767694	2.869278	2.644853
H	5.241724	-1.184237	2.131456
H	5.377382	1.046994	3.274865
C	1.975208	-1.229101	-1.856437
C	2.796607	-3.541609	-3.249945
C	2.464188	-1.128526	-3.175141
C	1.871893	-2.502347	-1.248258
C	2.293964	-3.647661	-1.941365
C	2.869783	-2.282851	-3.867140
H	2.518947	-0.151922	-3.675944
H	1.459189	-2.583717	-0.224769

H	2.223589	-4.632130	-1.453288
H	3.242965	-2.193336	-4.898921
H	3.122341	-4.442374	-3.792957
C	1.802831	1.740989	-1.848841
C	2.367974	4.132561	-3.230889
C	0.810274	2.728393	-1.993014
C	3.096586	1.974535	-2.368905
C	3.372744	3.161920	-3.063892
C	1.091857	3.918588	-2.686826
H	-0.171882	2.574618	-1.521148
H	3.899441	1.236839	-2.215697
H	4.381856	3.336203	-3.468163
H	0.309810	4.686390	-2.788043
H	2.588887	5.065573	-3.771955
C	-1.216524	-0.855169	-2.752569
C	-0.645265	-1.778794	-5.361689
C	-0.885382	0.056287	-3.781000
C	-1.257431	-2.233691	-3.047226
C	-0.972548	-2.690341	-4.344575
C	-0.600280	-0.404371	-5.075942
H	-0.865492	1.136791	-3.577371
H	-1.526641	-2.957225	-2.264805
H	-1.013726	-3.768701	-4.560386
H	-0.349069	0.318936	-5.866843
H	-0.429485	-2.139785	-6.379023
C	-2.769651	1.178345	-1.463677
C	-4.637161	3.210976	-2.058432
C	-2.795348	2.361030	-0.700714
C	-3.691779	1.015940	-2.525390
C	-4.617635	2.028775	-2.820214
C	-3.727734	3.371085	-1.001582
H	-2.076230	2.499516	0.128644
H	-3.691192	0.094783	-3.127628
H	-5.327183	1.893319	-3.651309
H	-3.735388	4.291184	-0.396754
H	-5.362852	4.005486	-2.292440
C	-2.685276	-1.453110	-0.253398
C	-4.310283	-3.456654	0.894140
C	-4.076306	-1.251432	-0.114058
C	-2.112993	-2.660029	0.205944
C	-2.925309	-3.655986	0.771099
C	-4.881742	-2.249391	0.458796
H	-4.536086	-0.309957	-0.444478
H	-1.021386	-2.788801	0.188067
H	-2.462786	-4.585073	1.137370
H	-5.963433	-2.077067	0.568577

H	-4.944084	-4.237182	1.342937

D-1Ph

81

E(SCF)	-3242.710001		
C	-0.062443	-0.131318	0.003586
Ru	-0.429923	-0.583388	1.941794
Cl	1.672324	-1.743964	2.099732
C	-1.239029	-2.090217	2.943064
C	-0.828987	-1.108000	4.117407
C	-0.102714	0.241855	3.720435
Cl	-2.559045	0.566615	2.002451
H	-2.334838	-2.197403	2.834948
H	-0.678764	-3.044285	2.964227
H	-0.695443	1.139246	3.981443
H	-1.765406	-0.822066	4.633268
H	-0.122173	-1.667956	4.759456
H	0.950922	0.270528	4.058720
P	1.591946	-0.193763	-0.602564
P	-1.488189	0.147083	-0.998625
C	2.815883	0.764283	0.407480
C	4.676928	2.398030	1.761829
C	4.144983	0.871649	-0.058773
C	2.420594	1.507614	1.533663
C	3.346820	2.320229	2.206421
C	5.072725	1.673262	0.625446
H	4.460754	0.343821	-0.971206
H	1.383117	1.436389	1.892444
H	3.023836	2.892513	3.089460
H	6.108282	1.739815	0.258085
H	5.402982	3.031492	2.294210
C	2.323496	-1.849008	-1.007170
C	3.324172	-4.389253	-1.731449
C	1.608698	-2.671528	-1.901698
C	3.535876	-2.319090	-0.460438
C	4.033664	-3.577413	-0.828460
C	2.107455	-3.935183	-2.262867
H	0.652848	-2.325923	-2.321888
H	4.072336	-1.717526	0.285764
H	4.977633	-3.934758	-0.389315
H	1.536345	-4.566297	-2.961059
H	3.714987	-5.379997	-2.009741
C	1.809484	0.776558	-2.178488
C	2.347757	2.435952	-4.402547
C	1.557028	2.166887	-2.116725
C	2.342639	0.230532	-3.362948

C	2.605411	1.057972	-4.469197
C	1.821658	2.989086	-3.221283
H	1.163927	2.611991	-1.190318
H	2.562593	-0.844296	-3.426471
H	3.022233	0.617075	-5.387641
H	1.624884	4.070126	-3.154789
H	2.565220	3.082332	-5.266817
C	-1.304077	-0.149162	-2.837163
C	-1.115322	-0.613648	-5.627295
C	-1.054612	0.914988	-3.731454
C	-1.470169	-1.449295	-3.367510
C	-1.369299	-1.679487	-4.749482
C	-0.962715	0.684063	-5.112820
H	-0.934435	1.937574	-3.350755
H	-1.714391	-2.289058	-2.701395
H	-1.509112	-2.698920	-5.140547
H	-0.770192	1.529842	-5.789880
H	-1.046837	-0.792532	-6.711339
C	-2.184393	1.862757	-0.966196
C	-3.143604	4.514476	-0.924569
C	-1.631596	2.804312	-0.075762
C	-3.216576	2.261216	-1.843991
C	-3.699461	3.580910	-1.814465
C	-2.104752	4.125378	-0.061732
H	-0.839130	2.481288	0.614456
H	-3.638396	1.550810	-2.570442
H	-4.508861	3.879982	-2.497967
H	-1.667590	4.852011	0.639835
H	-3.519554	5.549052	-0.905254
C	-2.804385	-1.089612	-0.598040
C	-4.730904	-3.103066	-0.164038
C	-4.177270	-0.787593	-0.686846
C	-2.400784	-2.402686	-0.278587
C	-3.363344	-3.404828	-0.066166
C	-5.133372	-1.791382	-0.469005
H	-4.507872	0.240545	-0.887062
H	-1.330437	-2.635520	-0.166550
H	-3.036352	-4.424339	0.189432
H	-6.203736	-1.540247	-0.522466
H	-5.484666	-3.886252	0.009907

Reaction IV

Ab-2Mes

107

E(SCF) -3026.032522

C	3.323151	1.044833	0.067048

C	2.546683	-0.143910	0.127593
C	3.135860	-1.393369	0.461777
C	4.509535	-1.416238	0.774911
C	5.307886	-0.257055	0.737186
C	4.692193	0.960543	0.390151
N	1.189256	-0.114376	-0.351578
C	0.034059	0.090721	0.346581
N	-0.997859	0.036579	-0.549549
C	-0.554117	-0.201839	-1.939348
C	0.969429	-0.337890	-1.797198
Ru	-0.111608	0.406541	2.370815
C	-1.911860	0.577639	2.496740
C	-2.404933	0.202726	-0.315725
C	-2.980007	1.495178	-0.440752
C	-4.375605	1.616129	-0.295408
C	-5.202653	0.503473	-0.048705
C	-4.599644	-0.766457	0.038837
C	-3.210138	-0.947152	-0.098539
C	-2.124432	2.709468	-0.698689
C	-6.693722	0.668373	0.136377
C	-2.597336	-2.321183	0.000907
C	2.333651	-2.669913	0.458823
C	6.794966	-0.329508	1.001242
C	2.718814	2.359941	-0.354988
P	0.353524	0.729404	4.779896
C	2.207885	0.616255	5.107467
C	3.016622	1.792232	4.519011
C	4.501904	1.680503	4.909936
C	5.106631	0.331673	4.492472
C	4.280473	-0.848052	5.026913
C	2.798400	-0.728865	4.629996
C	-0.365247	-0.636661	5.868959
C	0.267663	-0.872747	7.257781
C	-0.294682	-2.158091	7.897986
C	-1.828585	-2.135918	7.986201
C	-2.462463	-1.855911	6.614732
C	-1.902245	-0.566344	5.988803
C	-0.091153	2.432293	5.463748
C	-1.552302	2.862738	5.215774
C	-1.753918	4.344080	5.583527
C	-1.334849	4.639453	7.031997
C	0.107250	4.181412	7.297978
C	0.312011	2.698778	6.930225
Cl	0.206824	2.797963	2.084803
Cl	-0.259051	-1.988042	2.761807
H	1.529102	0.413560	-2.392627

H	1.343092	-1.341382	-2.091799
H	-1.033335	-1.116508	-2.346917
H	-0.852555	0.647455	-2.590086
H	-2.570292	-0.299054	2.693410
H	-2.422453	1.562214	2.397104
H	-5.230681	-1.653234	0.213912
H	-4.829169	2.616794	-0.385248
H	5.299898	1.879047	0.344184
H	4.972696	-2.382496	1.033667
H	2.976866	-3.538974	0.695239
H	1.504854	-2.629459	1.199665
H	1.867011	-2.859061	-0.531111
H	3.491715	3.150597	-0.403894
H	2.244848	2.291699	-1.356999
H	1.924593	2.683141	0.353849
H	7.044883	-1.127669	1.727964
H	7.351487	-0.555677	0.065714
H	7.190451	0.629018	1.391153
H	-2.750259	3.612074	-0.835330
H	-1.420916	2.892296	0.144415
H	-1.501288	2.591454	-1.610010
H	-3.378902	-3.093678	0.133195
H	-2.018932	-2.582808	-0.910404
H	-1.889516	-2.384114	0.857430
H	-7.075891	1.563416	-0.393097
H	-7.252043	-0.215825	-0.230550
H	-6.949835	0.790691	1.211228
H	-0.144730	-1.523464	5.229851
H	-2.189950	0.298068	6.627633
H	-2.359117	-0.395687	4.993041
H	-3.567469	-1.783972	6.705271
H	-2.256995	-2.705238	5.926128
H	-2.141799	-1.342364	8.702788
H	-2.205354	-3.094966	8.401587
H	0.150873	-2.301091	8.905890
H	0.024283	-3.032923	7.288024
H	0.056795	-0.010285	7.926771
H	1.371384	-0.954536	7.189299
H	2.310526	0.659890	6.215821
H	2.910185	1.795535	3.412459
H	2.615162	2.765529	4.866418
H	5.072625	2.518253	4.455382
H	4.597193	1.803373	6.013313
H	5.128132	0.276956	3.382539
H	6.160654	0.256231	4.836019
H	4.692425	-1.810056	4.654493

H	4.359656	-0.885316	6.137836
H	2.700833	-0.797314	3.524123
H	2.223055	-1.586802	5.033040
H	0.526338	3.079359	4.799927
H	-0.310882	2.071871	7.605649
H	1.366923	2.410251	7.119019
H	0.379656	4.346444	8.362576
H	0.807339	4.803427	6.695907
H	-2.020956	4.105898	7.728989
H	-1.444429	5.721902	7.257100
H	-2.814877	4.630626	5.420472
H	-1.151455	4.968389	4.886586
H	-2.245246	2.238795	5.820101
H	-1.806842	2.705518	4.150399

B-2Mes

55

E(SCF) -1979.380876

C	3.319272	-0.543126	0.376364
C	2.415772	0.455671	-0.074178
C	2.839733	1.801021	-0.250936
C	4.146704	2.143940	0.138375
C	5.042429	1.197057	0.670983
C	4.613565	-0.139503	0.760811
N	1.087066	0.094616	-0.497721
C	0.870351	-0.431756	-1.857067
C	-0.655321	-0.361752	-2.001837
N	-1.105754	-0.192668	-0.606607
C	-0.075796	0.131212	0.244039
C	-2.515287	-0.209771	-0.343107
C	-3.140444	-1.440961	-0.022759
C	-4.534115	-1.442647	0.177911
C	-5.309557	-0.271965	0.061167
C	-4.651354	0.932290	-0.256863
C	-3.259440	0.990802	-0.465200
Ru	-0.083352	0.432481	2.152981
Cl	0.609574	2.649110	2.307408
C	-2.330835	-2.705166	0.134008
C	-6.808701	-0.314864	0.249087
C	-2.574821	2.307701	-0.745802
C	1.930465	2.845466	-0.850168
C	6.420368	1.608231	1.134653
C	2.958348	-2.009035	0.383737
Cl	0.399090	-1.780019	2.725127
C	-1.833493	0.567969	2.585510
H	1.408329	0.184103	-2.605264

H	1.252705	-1.473651	-1.934228
H	-1.092144	-1.279810	-2.443095
H	-0.987046	0.500791	-2.623061
H	-2.732761	0.566376	1.940988
H	-2.011717	0.687865	3.685455
H	-5.028142	-2.392976	0.438455
H	-5.237483	1.862121	-0.339620
H	4.475818	3.188663	0.015302
H	5.313192	-0.906502	1.131141
H	3.667110	-2.584146	1.009848
H	1.940418	-2.186798	0.780322
H	3.013430	-2.434481	-0.642529
H	2.511329	3.726012	-1.185772
H	1.361805	2.455765	-1.718461
H	1.191233	3.186657	-0.095894
H	7.129377	0.757184	1.121856
H	6.839317	2.418741	0.505241
H	6.386754	1.992225	2.177181
H	-3.312981	3.126838	-0.837672
H	-1.867080	2.571250	0.068387
H	-1.984233	2.281685	-1.685139
H	-2.982577	-3.564396	0.381971
H	-1.779291	-2.959658	-0.795685
H	-1.570210	-2.599331	0.936286
H	-7.218133	0.681366	0.507011
H	-7.316852	-0.648841	-0.681432
H	-7.099620	-1.025338	1.048413

Ca-2Mes

61

E(SCF)	-2057.946775		
C	-2.989178	-1.533758	-0.125637
C	-2.437181	-0.262789	-0.435753
C	-3.250671	0.897419	-0.528244
C	-4.620865	0.767419	-0.230301
C	-5.196737	-0.465479	0.130688
C	-4.366157	-1.601580	0.162581
N	-1.036205	-0.165012	-0.766537
C	-0.562143	-0.348160	-2.157042
C	0.961441	-0.132916	-2.038337
N	1.155638	0.097373	-0.588865
C	-0.016039	0.078043	0.091486
C	2.469358	0.324568	-0.037422
C	2.985951	1.646617	0.001261
C	4.283094	1.832327	0.517769
C	5.072736	0.757710	0.968537

C	4.543741	-0.542969	0.866206
C	3.253607	-0.790868	0.359141
C	2.185165	2.826201	-0.488990
C	2.735049	-2.202292	0.250411
C	6.445683	0.993792	1.554408
Ru	-0.209643	0.365392	2.071343
Cl	0.062262	-1.983001	2.532620
C	-2.680637	2.234600	-0.928017
C	-6.663020	-0.564234	0.483338
C	-2.142905	-2.781201	-0.099823
C	-1.680299	0.396663	3.389141
C	-0.428316	0.691241	4.313357
C	0.983752	0.746094	3.598186
Cl	-0.499978	2.740144	1.793018
H	1.318287	0.745089	-2.616419
H	1.548593	-1.014534	-2.368694
H	-0.826363	-1.363223	-2.520785
H	-1.050656	0.387497	-2.828843
H	-2.153580	-0.581826	3.587952
H	-2.372814	1.253139	3.300336
H	-4.802347	-2.582887	0.410882
H	-5.258899	1.663996	-0.293223
H	4.690160	2.855827	0.557598
H	5.157069	-1.402350	1.182653
H	3.536459	-2.933315	0.469600
H	1.900245	-2.370471	0.966543
H	2.342811	-2.425536	-0.763564
H	2.807185	3.741278	-0.510402
H	1.788989	2.664402	-1.513090
H	1.309634	3.012295	0.172073
H	7.123811	0.137645	1.367323
H	6.917024	1.906740	1.139710
H	6.388079	1.128273	2.656357
H	-3.487941	2.975733	-1.082080
H	-1.994605	2.620302	-0.141518
H	-2.094472	2.173801	-1.868546
H	-2.774420	-3.681361	0.025020
H	-1.558126	-2.907295	-1.034708
H	-1.411886	-2.746311	0.738288
H	-7.266955	0.188903	-0.060588
H	-7.072906	-1.568048	0.255235
H	-6.822025	-0.386245	1.569046
H	1.438457	1.753181	3.599141
H	-0.594472	1.688333	4.762773
H	-0.377921	-0.132738	5.049760
H	1.655992	-0.081950	3.887011

Cb-2Mes

61

E(SCF) -2057.916960

C	-2.938852	-1.639968	-0.671603
C	-2.427938	-0.337117	-0.903210
C	-3.278706	0.794799	-0.971563
C	-4.659053	0.595198	-0.774968
C	-5.204561	-0.679221	-0.526049
C	-4.327321	-1.780603	-0.482956
N	-1.023087	-0.174920	-1.162588
C	-0.580185	-0.280591	-2.573315
C	0.940189	-0.088232	-2.470842
N	1.155417	0.053770	-1.015190
C	-0.000109	0.011819	-0.286467
C	2.506401	0.205630	-0.531474
C	3.091038	1.500065	-0.462790
C	4.400065	1.612382	0.046065
C	5.157407	0.490785	0.428737
C	4.591526	-0.781991	0.227991
C	3.287027	-0.955235	-0.271245
C	2.419613	2.728391	-1.029593
C	2.814784	-2.346426	-0.622159
C	6.536000	0.645454	1.027305
Ru	0.031314	0.277099	1.800991
Cl	0.746847	-2.014096	1.842680
C	-2.723592	2.176997	-1.213693
C	-6.685849	-0.856381	-0.282931
C	-2.021836	-2.835743	-0.586061
C	-1.734584	0.052290	2.163631
C	0.254136	1.293937	3.870758
C	0.484807	-0.057480	4.046868
Cl	0.071352	2.608414	1.227254
H	1.297795	0.820580	-2.998515
H	1.514598	-0.953686	-2.860726
H	-0.868137	-1.269373	-2.988038
H	-1.077692	0.496903	-3.188907
H	-2.120495	0.164138	3.206207
H	-2.502798	-0.205926	1.409756
H	-4.733603	-2.787735	-0.294283
H	-5.328417	1.469921	-0.817415
H	4.845766	2.617475	0.126197
H	5.188854	-1.680074	0.455641
H	3.213650	-3.092146	0.091749
H	1.715411	-2.435987	-0.606379
H	3.188551	-2.626400	-1.632574

H	2.670896	3.628726	-0.436590
H	2.783193	2.907091	-2.066170
H	1.319760	2.643862	-1.040503
H	7.194013	-0.207467	0.767215
H	7.027821	1.579088	0.689476
H	6.482285	0.687768	2.136786
H	-3.529024	2.935515	-1.189137
H	-1.960763	2.446608	-0.451910
H	-2.225917	2.254266	-2.204101
H	-2.598529	-3.763026	-0.406737
H	-1.441303	-2.980385	-1.521957
H	-1.278079	-2.721208	0.232410
H	-7.282634	-0.089149	-0.814665
H	-7.037441	-1.855372	-0.608471
H	-6.924847	-0.763360	0.798644
H	1.505848	-0.467802	4.054371
H	1.083894	2.003388	3.733956
H	-0.719557	1.751398	4.105920
H	-0.294934	-0.734298	4.429153

Cc-2Mes

61

E(SCF)	-2057.926421		
C	-3.107764	-1.559332	-0.184108
C	-2.550115	-0.268454	-0.382575
C	-3.371441	0.887365	-0.461140
C	-4.755342	0.730065	-0.252298
C	-5.338718	-0.525315	0.003364
C	-4.498355	-1.654535	0.017683
N	-1.138152	-0.145691	-0.644255
C	-0.664209	-0.252049	-2.045541
C	0.860123	-0.069098	-1.919874
N	1.047918	0.106620	-0.463710
C	-0.120702	0.058295	0.228413
C	2.362177	0.307098	0.100347
C	2.894989	1.624352	0.174259
C	4.181086	1.786629	0.726099
C	4.956450	0.695314	1.161120
C	4.431559	-0.599157	0.986784
C	3.152183	-0.825813	0.442352
C	2.140876	2.820073	-0.348525
C	2.670188	-2.234131	0.205903
C	6.314585	0.906245	1.788690
Ru	-0.088808	0.290624	2.280197
Cl	0.037132	-2.152011	2.407402
C	-2.796039	2.247090	-0.767263

C	-6.821275	-0.655430	0.265295
C	-2.252141	-2.800804	-0.195739
C	-1.862612	0.138021	2.624131
C	0.856408	1.299003	4.064316
C	1.004464	-0.077200	4.220216
Cl	-0.483807	2.671042	1.861505
H	1.234582	0.821283	-2.466276
H	1.432110	-0.949810	-2.278199
H	-0.947593	-1.238144	-2.467744
H	-1.143396	0.530759	-2.668604
H	-2.516899	1.035699	2.638163
H	-2.312907	-0.851587	2.852249
H	-4.936669	-2.652278	0.182833
H	-5.397603	1.624501	-0.301153
H	4.594431	2.805760	0.798204
H	5.043516	-1.472364	1.265504
H	3.468299	-2.964377	0.438885
H	1.786532	-2.463736	0.840587
H	2.369020	-2.393078	-0.850830
H	2.762137	3.733369	-0.281569
H	1.852254	2.689671	-1.412752
H	1.206846	2.986871	0.231126
H	6.993254	0.052462	1.593448
H	6.800302	1.829061	1.414410
H	6.228634	1.007904	2.892255
H	-3.594435	3.012587	-0.802722
H	-2.050618	2.549259	0.000269
H	-2.277768	2.262818	-1.749952
H	-2.871093	-3.705748	-0.045229
H	-1.716414	-2.922382	-1.161490
H	-1.480190	-2.763739	0.603500
H	-7.400457	0.131043	-0.257887
H	-7.208917	-1.642753	-0.055047
H	-7.042068	-0.555119	1.350150
H	1.935542	-0.586437	3.925272
H	1.666594	1.914163	3.641997
H	0.059892	1.857788	4.577082
H	0.331054	-0.663294	4.862574

D-2Mes

61

E(SCF) -2057.946781

C	1.030348	3.235021	-1.051277
C	1.562382	1.924385	-1.175631
C	2.941836	1.660438	-0.967362
C	3.762471	2.729674	-0.557905

C	3.262714	4.032762	-0.375042
C	1.899683	4.263920	-0.641373
N	0.697502	0.860045	-1.623657
C	-0.000055	0.000024	-0.842417
N	-0.697679	-0.860030	-1.623552
C	-0.528380	-0.562021	-3.063843
C	0.528065	0.561981	-3.063918
C	-1.562433	-1.924425	-1.175420
C	-2.941928	-1.660650	-0.967204
C	-3.762426	-2.729961	-0.557674
C	-3.262497	-4.032967	-0.374687
C	-1.899426	-4.263959	-0.640957
C	-1.030226	-3.234977	-1.050941
Ru	0.000014	0.000093	1.166860
Cl	1.800570	-1.597077	1.258962
C	-3.528558	-0.287136	-1.174374
C	-4.160183	-5.150860	0.103338
C	0.419660	-3.530304	-1.339451
C	3.528289	0.286833	-1.174441
C	4.160542	5.150574	0.102906
C	-0.419485	3.530522	-1.339876
Cl	-1.800552	1.597318	1.258439
C	0.894065	1.008287	2.610737
C	-0.000005	0.000219	3.443109
C	-0.894287	-1.007748	2.610819
H	0.194892	1.468827	-3.608372
H	1.496227	0.240858	-3.503695
H	-0.195255	-1.468890	-3.608286
H	-1.496580	-0.240915	-3.503543
H	1.978415	0.821071	2.711806
H	0.579943	2.062836	2.712538
H	-0.694059	0.616292	4.045156
H	-1.978602	-0.820321	2.711857
H	-0.580355	-2.062343	2.712752
H	0.694135	-0.615891	4.045010
H	-4.833489	-2.533470	-0.387272
H	-1.493108	-5.283084	-0.535267
H	4.833503	2.533053	-0.387457
H	1.493495	5.283103	-0.535759
H	0.608762	-4.620633	-1.328451
H	0.735825	-3.142261	-2.330041
H	1.073869	-3.051937	-0.577151
H	-4.631758	-0.315731	-1.091916
H	-3.139791	0.431818	-0.419214
H	-3.277484	0.126156	-2.173555
H	-3.842661	-6.132585	-0.300823

H	-4.135010	-5.232325	1.211701
H	-5.216036	-4.981476	-0.186511
H	3.843139	6.132312	-0.301313
H	4.135386	5.232108	1.211263
H	5.216373	4.981042	-0.186938
H	4.631514	0.315343	-1.092271
H	3.139650	-0.431963	-0.419060
H	3.276911	-0.126621	-2.173475
H	-0.608484	4.620868	-1.328735
H	-0.735587	3.142668	-2.330564
H	-1.073798	3.052112	-0.577696

Fragments

1Ph

69

E(SCF) -2109.539519

C	0.169718	0.337843	-0.588703
P	1.693353	-0.110724	-1.078788
P	-1.373676	0.235516	-1.201838
C	2.853017	0.001498	0.365398
C	4.528789	0.207770	2.621777
C	4.243768	-0.195976	0.236916
C	2.308754	0.309045	1.626585
C	3.144245	0.411124	2.751369
C	5.077173	-0.095331	1.362965
H	4.685142	-0.426689	-0.744709
H	1.218937	0.469142	1.687565
H	2.711854	0.652874	3.734896
H	6.161957	-0.250722	1.256090
H	5.184454	0.289042	3.502704
C	2.504664	0.981645	-2.360282
C	3.667701	2.784417	-4.195963
C	2.028386	2.304512	-2.461369
C	3.567220	0.566899	-3.191179
C	4.143043	1.465234	-4.106489
C	2.609044	3.202883	-3.370856
H	1.188166	2.609801	-1.815899
H	3.940592	-0.467616	-3.138950
H	4.966400	1.130089	-4.756465
H	2.231584	4.235216	-3.438299
H	4.120535	3.486343	-4.913331
C	1.949132	-1.827267	-1.746385
C	2.049821	-4.484796	-2.708991
C	1.588229	-2.121497	-3.081107
C	2.348468	-2.883326	-0.897945
C	2.399143	-4.202617	-1.377560

C	1.642737	-3.440869	-3.557946
H	1.258933	-1.314480	-3.754052
H	2.626391	-2.670919	0.145817
H	2.717763	-5.015127	-0.706074
H	1.362578	-3.653706	-4.601094
H	2.092769	-5.518683	-3.084971
C	-1.634419	-0.275379	-2.970593
C	-1.730371	-1.079033	-5.679826
C	-1.239175	0.612821	-3.997841
C	-2.067922	-1.572618	-3.317140
C	-2.115936	-1.969932	-4.664888
C	-1.290574	0.214415	-5.342148
H	-0.885558	1.623665	-3.741351
H	-2.369887	-2.278509	-2.528981
H	-2.459082	-2.984282	-4.921336
H	-0.986148	0.918290	-6.132209
H	-1.771774	-1.390427	-6.735023
C	-2.262772	1.862950	-1.077376
C	-3.546098	4.354708	-0.756754
C	-1.781199	2.795455	-0.136448
C	-3.386384	2.191139	-1.865047
C	-4.023238	3.434256	-1.704947
C	-2.423195	4.033266	0.026326
H	-0.885178	2.528085	0.447748
H	-3.757050	1.484715	-2.624127
H	-4.894195	3.686420	-2.329732
H	-2.041692	4.754865	0.765518
H	-4.046141	5.327844	-0.632992
C	-2.456432	-0.932149	-0.232157
C	-3.971477	-2.744607	1.307716
C	-3.858773	-0.989843	-0.378066
C	-1.822259	-1.781151	0.693616
C	-2.575887	-2.686936	1.458894
C	-4.611751	-1.893758	0.389050
H	-4.373165	-0.324501	-1.087951
H	-0.727655	-1.700784	0.800375
H	-2.070726	-3.348342	2.180013
H	-5.706010	-1.931270	0.271974
H	-4.564410	-3.450482	1.909920

PMe3

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E(SCF)	-460.943192		
P	-0.015904	-0.000291	-0.008167
C	0.021067	0.006074	1.861848
C	1.211527	-1.374618	-0.329030

C	1.088906	1.472851	-0.336239
H	1.051789	0.052789	2.274282
H	-0.553440	0.876626	2.238456
H	-0.474226	-0.909975	2.243006
H	1.431993	-1.425389	-1.414645
H	2.166179	-1.240120	0.223454
H	0.762928	-2.345092	-0.034562
H	1.305067	1.536399	-1.422044
H	2.051183	1.423974	0.217250
H	0.558201	2.402705	-0.047308

PCy3

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E(SCF) -1046.610406

C	0.142111	2.717770	7.097257
C	-0.044597	2.453524	5.589810
C	-1.446079	2.916558	5.127791
C	-1.694142	4.395780	5.475490
C	-1.483657	4.672857	6.973184
C	-0.097780	4.200819	7.442323
P	0.402190	0.759912	4.849858
C	-0.315056	-0.602444	5.969893
C	0.176120	-0.762571	7.424092
C	-0.392987	-2.043329	8.065978
C	-1.928603	-2.077584	8.001475
C	-2.434194	-1.892582	6.561529
C	-1.859269	-0.618075	5.917091
C	2.258833	0.643491	5.239001
C	3.042984	1.744233	4.488169
C	4.564410	1.619505	4.687718
C	5.079275	0.228877	4.288027
C	4.316499	-0.874144	5.036278
C	2.794709	-0.750721	4.838699
H	0.020157	-1.511107	5.413589
H	-2.255297	0.268948	6.460534
H	-2.207204	-0.522190	4.866343
H	-3.544774	-1.863390	6.540932
H	-2.134594	-2.774413	5.950793
H	-2.337934	-1.261094	8.639294
H	-2.314262	-3.027464	8.429579
H	-0.047029	-2.128146	9.118664
H	0.015963	-2.931536	7.532416
H	-0.143811	0.113922	8.026053
H	1.285107	-0.781260	7.469019
H	2.424924	0.782545	6.332625
H	2.805412	1.675531	3.401782

H	2.711720	2.752253	4.814347
H	5.086370	2.410285	4.107380
H	4.809386	1.806707	5.757933
H	4.943047	0.089205	3.191572
H	6.170532	0.147169	4.479617
H	4.659012	-1.878200	4.705948
H	4.550463	-0.808283	6.123232
H	2.545121	-0.934066	3.768360
H	2.282279	-1.548173	5.416156
H	0.683306	3.106054	5.050678
H	-0.582409	2.098339	7.670053
H	1.154138	2.406706	7.432122
H	0.017668	4.362316	8.535793
H	0.686940	4.820834	6.951990
H	-2.266795	4.137028	7.556746
H	-1.620270	5.753610	7.191409
H	-2.718733	4.694353	5.166164
H	-0.994158	5.029399	4.884326
H	-2.225477	2.293607	5.619912
H	-1.558866	2.748136	4.035975

Ethene

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E(SCF) -78.528698

H	-0.027313	0.000000	0.074153
C	-0.000533	0.000000	1.176327
C	1.156704	0.000000	1.854241
H	-0.974872	0.000000	1.692071
H	1.183446	0.000000	2.956282
H	2.130999	0.000000	1.338426
