

Electronic Supplementary Information

Understanding the Reaction Mechanisms of Pd-Catalysed Oxidation of Alcohols and Domino Oxidation-Arylation Reactions Using Phenyl Chloride as Oxidant

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Complete Reference for Ref (22):

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, **2009**.

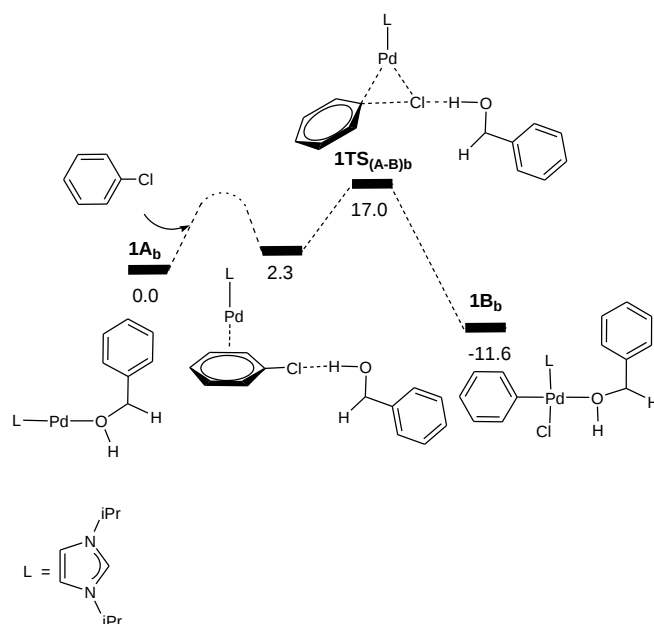


Figure S1. The energy profile calculated for the oxidative addition step for phenyl chloride to **1A** with the full NHC ligand.

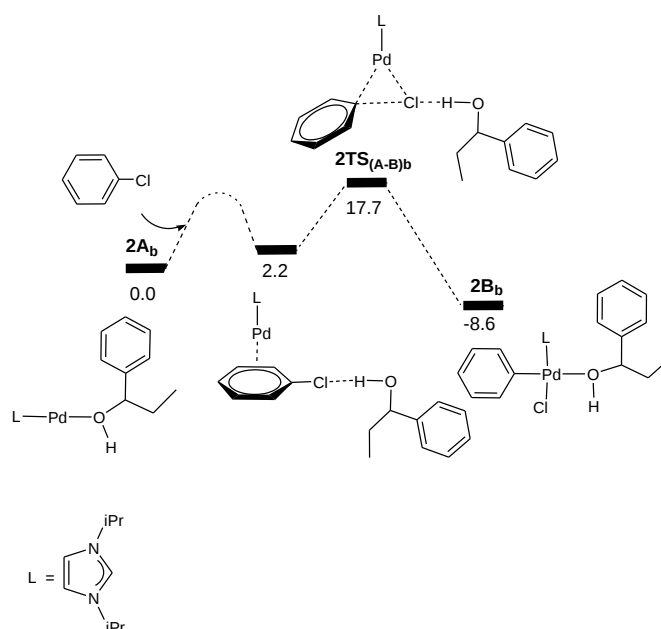
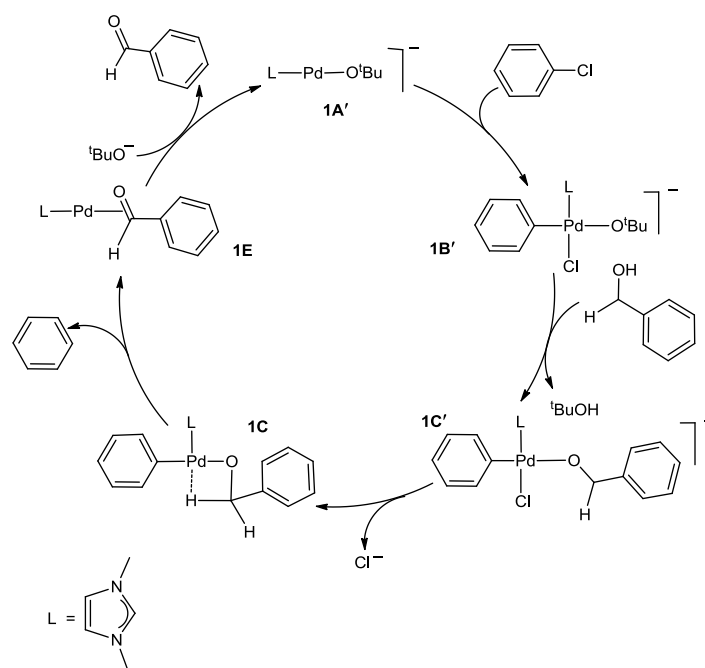


Figure S2. The energy profile calculated for the oxidative addition step for phenyl chloride to **2A** with the full NHC ligand

Comments on Figures S1 and S2

Because of the steric effect, with the full NHC ligand, ligand dissociation/association is involved, unlike the situation with the model NHC ligand in which no ligand dissociation/association is involved (see the main text). Since the relative free energies of **1TS(A-B)** with respect to **1A** + PhCl and **2TS(A-B)** with respect to **2A** + PhCl are most important in our discussion, the mechanistic details involving the ligand dissociation/association in the transformations do not affect the conclusions we have made.



Scheme S1. The proposed mechanism of the oxidation reactions of alcohols considering $[\text{LPd(0)(O}^t\text{Bu)}]^-$ as the active species.

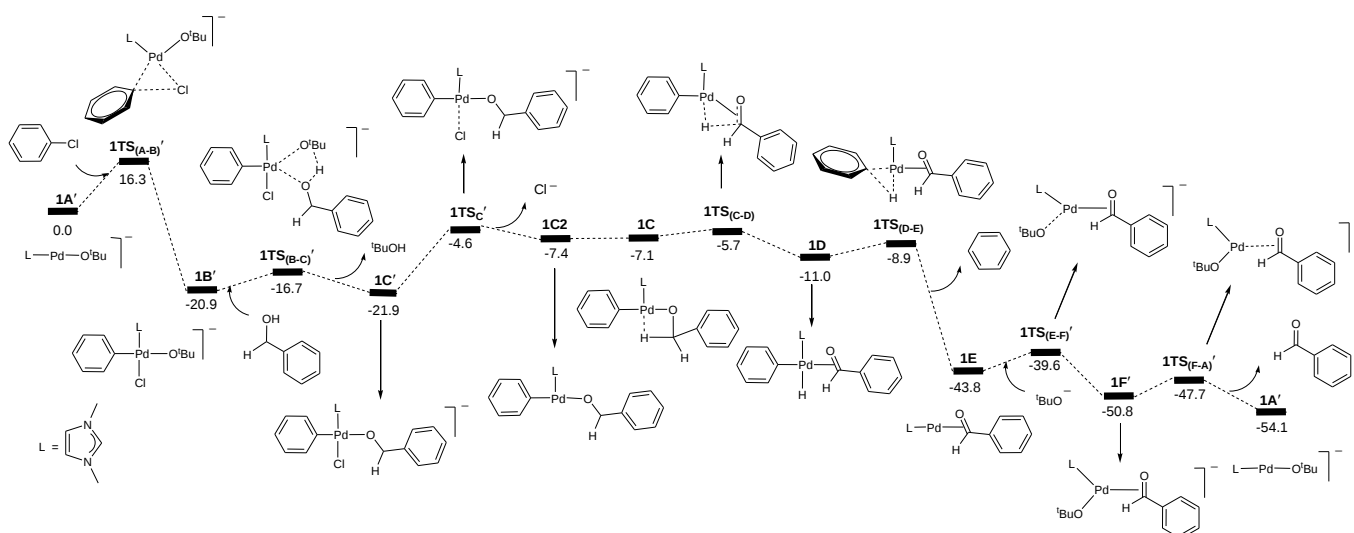


Figure S3. Energy profile calculated for the oxidation reaction of PhCH_2OH ($\text{PhCH}_2\text{OH} + \text{PhCl} + {}^t\text{BuO}^- \rightarrow \text{PhCHO} + \text{PhH} + {}^t\text{BuOH} + \text{Cl}^-$) considering $[\text{LPd(O}^t\text{Bu)}]^-$ as the active species. The relative free energies are given in kcal/mol.

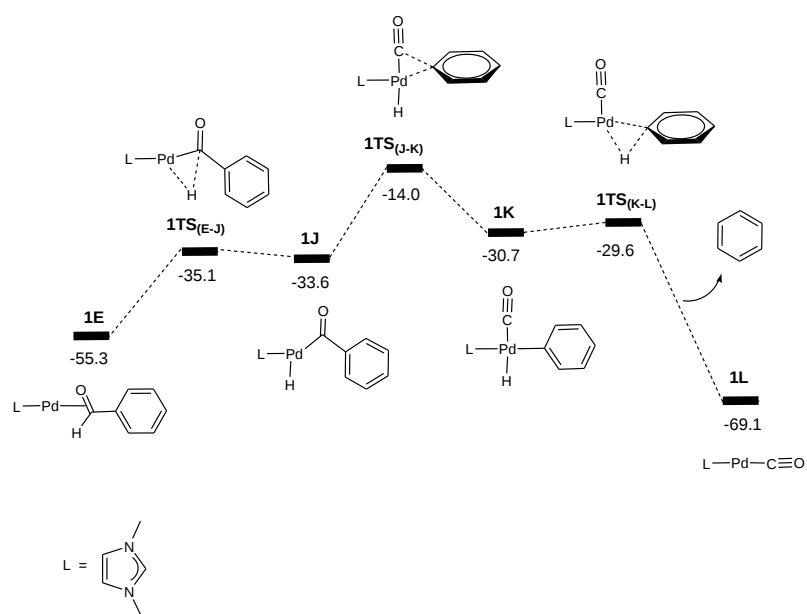


Figure S4. The energy profile calculated for the decarbonylation of LPd(0)(PhCHO) (**1E**) .

Cartesian coordinates and electronic energies for all of the calculated structures

1A

scf done: -778.365988

Pd	-0.866914	-0.143704	-0.172813
C	-2.818134	0.036514	-0.042737
N	-3.748010	-0.948689	0.190310
C	-5.037856	-0.439336	0.235427
H	-5.901917	-1.062717	0.409423
C	-4.936342	0.896522	0.025368
H	-5.694819	1.663385	-0.020483
N	-3.586630	1.171989	-0.142061
O	1.345648	-0.323969	-0.345996
C	2.178861	0.169378	0.725552
H	1.888681	1.192070	0.993970
C	3.645191	0.097917	0.367084
C	4.478760	1.208553	0.540115
C	4.191626	-1.089503	-0.143018
C	5.836977	1.135951	0.221098
H	4.062638	2.136017	0.927777
C	5.544876	-1.161302	-0.469418
H	3.546286	-1.951530	-0.289103
C	6.371906	-0.048948	-0.285450
H	6.472744	2.006121	0.361240
H	5.956947	-2.085919	-0.865071
H	7.427125	-0.106658	-0.538828
H	1.546630	0.186855	-1.148056
C	-3.413760	-2.351659	0.374226
H	-3.940019	-2.969496	-0.361809
H	-2.334987	-2.446181	0.232658
H	-3.683086	-2.683580	1.383344
C	-3.046198	2.497895	-0.391543
H	-3.287298	3.173690	0.436791
H	-1.962739	2.389579	-0.476035
H	-3.451076	2.909529	-1.322986
H	1.935378	-0.478705	1.571705

1TS_(A-B)

scf done: -1024.943148

C	1.414682	1.575305	-0.044967
N	2.110034	2.466925	-0.817007
C	2.832554	3.362681	-0.040375
C	2.589887	3.034414	1.253463
N	1.722697	1.951830	1.232650
Pd	0.307165	-0.056042	-0.656753
C	2.094293	2.474231	-2.272253
C	1.240979	1.262523	2.422592
C	1.455016	-1.790776	-0.149897
C	0.713817	-2.472146	0.840729
C	1.311579	-2.766166	2.067914
C	2.657839	-2.473202	2.298233
C	3.413298	-1.888314	1.270757
C	2.837901	-1.575317	0.043773
H	3.438758	4.146181	-0.469177
H	2.947411	3.473230	2.172655
H	3.102868	2.312246	-2.667106
H	1.442121	1.661496	-2.597289
H	1.709353	3.429025	-2.646318
H	2.010932	0.595867	2.822514
H	0.953366	1.995761	3.182324
H	0.374197	0.666519	2.135078
H	-0.314391	-2.756799	0.646282
H	0.719864	-3.256002	2.838190
H	3.123633	-2.730693	3.245101
H	4.470883	-1.684087	1.423532
H	3.428859	-1.141059	-0.755087
O	-1.773848	-1.081659	-1.473178
H	-1.327414	-1.841531	-1.890979
C	-2.872752	-1.541127	-0.682384
H	-2.523676	-2.169309	0.149549
Cl	0.990476	-2.382870	-2.020633
C	-3.648751	-0.363284	-0.142201
C	-4.269164	-0.447285	1.109474
C	-3.798632	0.806500	-0.897817
C	-5.035535	0.612865	1.597095
H	-4.151555	-1.347903	1.708779
C	-4.556611	1.870326	-0.407145

H	-3.308118	0.880202	-1.863025
C	-5.180256	1.776267	0.839432
H	-5.510743	0.532467	2.571339
H	-4.660864	2.775140	-1.000481
H	-5.771214	2.605618	1.219158
H	-3.528442	-2.163031	-1.311953

1B

scf done: -1025.015835

C	-0.590094	1.530492	-0.259970
N	0.105401	2.285270	0.633696
C	-0.220986	3.628458	0.508851
C	-1.142556	3.714119	-0.483798
N	-1.358945	2.422557	-0.939883
H	0.220954	4.389646	1.132921
H	-1.660021	4.565667	-0.897657
O	1.382826	-0.538041	-1.975908
C	2.755536	-0.152246	-1.859332
H	2.798687	0.897326	-2.165760
C	3.367167	-0.307435	-0.479785
C	3.026856	-1.374400	0.363286
C	4.330260	0.615926	-0.050726
C	3.636527	-1.504203	1.613605
H	2.271752	-2.094348	0.058462
C	4.946695	0.479981	1.195012
H	4.602389	1.447734	-0.698401
C	4.597262	-0.581248	2.033312
H	3.358330	-2.333214	2.258894
H	5.693387	1.203997	1.511376
H	5.070896	-0.688238	3.005625
H	1.282512	-1.518165	-1.980819
C	-2.278528	2.059265	-2.015520
H	-1.725605	1.826947	-2.929883
H	-2.857907	1.186646	-1.710959
H	-2.951312	2.899892	-2.199441
C	1.055973	1.759770	1.609064
H	1.058327	0.672526	1.531605
H	2.063129	2.130153	1.399780
H	0.755237	2.058730	2.617698
Pd	-0.477829	-0.453529	-0.558558
C	-2.170663	-0.635882	0.474506
C	-3.284920	-1.196125	-0.168668
C	-2.282405	-0.273276	1.823255
C	-4.484703	-1.383599	0.525740
H	-3.210458	-1.519940	-1.202493
C	-3.480937	-0.472953	2.517740
H	-1.435174	0.157661	2.349671
C	-4.588089	-1.022764	1.870521
H	-5.335718	-1.826513	0.012867
H	-3.545343	-0.194364	3.567530
H	-5.519781	-1.174442	2.409655
Cl	-0.229067	-2.823134	-1.008185
H	3.335490	-0.725401	-2.597025

1C

scf done: -1009.382220

C	-0.074948	1.794643	-0.452759
N	0.929897	2.522241	0.107296
C	0.574067	3.858316	0.199150
C	-0.673201	3.969250	-0.323170
N	-1.056877	2.696621	-0.720785
H	1.238145	4.602114	0.611278
H	-1.310169	4.829100	-0.460867
O	1.957381	-0.310110	-1.582024
C	-2.348339	2.401845	-1.336660
H	-2.284929	1.439379	-1.839557
H	-3.130379	2.349935	-0.574452
H	-2.583688	3.186459	-2.061020
C	2.209389	1.974665	0.565314
H	2.435821	1.080871	-0.021474
H	2.986013	2.727765	0.409333
H	2.154137	1.727053	1.630397
Pd	0.025361	-0.161284	-0.774560
C	-1.801777	-0.510134	0.013084
C	-2.694503	-1.318729	-0.716983
C	-2.212020	-0.081856	1.288453
C	-3.935864	-1.693478	-0.191333
H	-2.424208	-1.667685	-1.712906
C	-3.452101	-0.454232	1.818296

H	-1.555854	0.548876	1.884909	C	-2.234887	-0.622986	-1.350080
C	-4.320515	-1.260595	1.079169	H	3.211501	-2.763168	2.621358
H	-4.602550	-2.322476	-0.777852	H	3.025334	-4.241143	0.281231
H	-3.739499	-0.113774	2.811306	H	0.098570	2.841198	0.780341
H	-5.285629	-1.548685	1.488637	H	3.023091	0.605238	-1.455004
C	1.799505	-1.657128	-1.682745	H	1.794819	4.557272	1.275535
H	0.751469	-1.983806	-1.235604	H	4.701506	2.344098	-0.993965
H	2.486571	-2.235766	-1.033778	H	4.112783	4.331741	0.389007
C	1.808315	-2.233920	-3.094401	C	1.724510	-0.403566	2.529249
C	1.805102	-3.619075	-3.297294	C	1.433799	-2.994163	-1.655407
C	1.831148	-1.381571	-4.201117	H	1.277638	0.470522	2.058670
C	1.814398	-4.146375	-4.588816	H	1.070295	-0.773804	3.325958
H	1.797707	-4.289892	-2.439118	H	2.692489	-0.125568	2.956065
C	1.843540	-1.907467	-5.494925	H	1.321777	-4.081777	-1.682908
H	1.850826	-0.311321	-4.022770	H	0.493658	-2.526788	-1.945693
C	1.832695	-3.289760	-5.693240	H	2.227844	-2.696382	-2.348342
H	1.811237	-5.223832	-4.734469	H	-0.622996	1.292647	-1.408223
H	1.865611	-1.236431	-6.350444	H	-2.269383	-0.194494	-2.364623
H	1.843444	-3.698469	-6.700494	Pd	0.113841	0.078385	-0.660660
1TS (c-d)				C	-3.269273	-0.142058	-0.411308
scf done: -1009.373163				C	-3.417390	-0.735565	0.852138
Pd	-0.306807	-0.142734	0.220262	C	-4.139316	0.883660	-0.806323
C	-1.900450	-1.373817	-0.256469	C	-4.421691	-0.299036	1.710574
N	-2.792963	-1.335308	-1.284033	H	-2.738671	-1.534044	1.135047
C	-3.701873	-2.380305	-1.199450	C	-5.143630	1.320352	0.055281
C	-3.374021	-3.093026	-0.092658	H	-4.017040	1.341859	-1.785089
N	-2.269804	-2.468981	0.467191	C	-5.284200	0.729845	1.314177
C	-1.378380	1.555625	0.035867	H	-4.537892	-0.757655	2.688819
C	-0.936842	2.609243	-0.787001	H	-5.814004	2.118596	-0.250644
C	-2.592457	1.737232	0.722496	H	-6.067238	1.069484	1.986986
C	-1.683743	3.783862	-0.929253	1TS (d-e)			
C	-3.334641	2.915957	0.592550	scf done: -1009.371969			
C	-2.886732	3.944106	-0.239042	C	1.592098	-1.350711	0.307872
O	1.264080	-1.642564	0.643511	N	2.234280	-1.206855	1.501938
C	2.006971	-0.619186	0.835836	C	3.172836	-2.208791	1.704707
C	3.071209	-0.236983	-0.145113	C	3.128524	-3.004562	0.606665
C	4.018502	0.737140	0.191793	N	2.159129	-2.469502	-0.228708
C	3.158480	-0.889593	-1.380858	C	0.881514	1.827880	-0.455294
C	5.035969	1.067845	-0.702267	C	0.437537	2.685248	0.568621
C	4.176471	-0.560047	-2.273803	C	2.027375	2.207145	-1.177722
C	5.115218	0.420493	-1.938256	C	1.147833	3.843789	0.899101
H	1.015682	0.778723	0.677298	C	2.733230	3.367323	-0.849833
H	-4.482710	-2.525028	-1.930108	C	2.302556	4.189208	0.194829
H	-3.819854	-3.975190	0.340410	O	-1.188634	-1.892523	-1.132506
H	0.004906	2.518304	-1.322558	C	-1.952195	-0.915914	-1.357931
H	-2.971545	0.949799	1.369887	H	3.774077	-2.268075	2.599128
H	-1.316798	4.579000	-1.575513	H	3.693218	-3.887599	0.349007
H	-4.268105	3.027353	1.141293	H	-0.474174	2.447483	1.111359
H	-3.464904	4.858978	-0.344315	H	2.375877	1.588494	-2.000216
H	3.952008	1.240732	1.154280	H	0.787869	4.483002	1.702809
H	2.425314	-1.654159	-1.617482	H	3.624267	3.630547	-1.416286
H	5.766547	1.827117	-0.436287	H	2.850645	5.093990	0.445272
H	4.241988	-1.069086	-3.231965	C	1.934963	-0.168532	2.480338
H	5.908424	0.676214	-2.635908	C	1.831808	-3.007064	-1.545984
C	-2.778790	-0.371406	-2.379811	H	1.410506	0.642447	1.976983
C	-1.614377	-2.910613	1.696776	H	1.309925	-0.567863	3.286586
H	-2.072908	0.419772	-2.135300	H	2.867671	0.214586	2.904386
H	-2.480174	-0.864982	-3.310535	H	1.876248	-4.099362	-1.509488
H	-3.775451	0.062351	-2.501128	H	0.821262	-2.693752	-1.807578
H	-1.636342	-4.003041	1.738313	H	2.542041	-2.643822	-2.296659
H	-0.578698	-2.568566	1.685005	H	-0.428916	1.268828	-1.344793
H	-2.130900	-2.506280	2.573631	Pd	0.111805	-0.076562	-0.652610
H	2.206761	-0.297385	1.871039	C	-3.005695	-0.483587	-0.406993
1D				C	-3.890560	0.545018	-0.761154
scf done: -1009.377737				C	-3.156504	-1.130968	0.829323
C	1.334755	-1.415885	0.277162	C	-4.905614	0.931297	0.111621
N	1.914672	-1.428949	1.509787	H	-3.771999	1.045497	-1.719832
C	2.680937	-2.570075	1.701561	C	-4.171415	-0.743299	1.700565
C	2.585008	-3.295817	0.559345	H	-2.473069	-1.936055	1.080313
N	1.758001	-2.579761	-0.293714	C	-5.046303	0.288978	1.345417
C	1.428707	1.569919	-0.355842	H	-5.586315	1.731115	-0.167255
C	1.109412	2.709199	0.404377	H	-4.286579	-1.247274	2.656694
C	2.738422	1.466163	-0.855200	H	-5.838340	0.588924	2.026552
C	2.069963	3.688736	0.679962	H	-2.024152	-0.499980	-2.376065
C	3.695473	2.451957	-0.592565	1E			
C	3.368483	3.566431	0.182318	scf done: -777.176847			
O	-1.464434	-1.572291	-1.101025	Pd	-0.506327	-1.066882	-0.278671

C	-1.933672	0.358539	-0.071062
N	-3.239064	0.200762	0.310450
C	-3.919770	1.408816	0.316250
C	-3.029129	2.356922	-0.070883
N	-1.829505	1.702848	-0.306295
O	1.152843	-2.392958	-0.250930
C	1.443495	-1.525857	0.636341
C	2.432143	-0.441181	0.411971
C	2.779362	0.419221	1.464735
C	3.058709	-0.284595	-0.835863
C	3.719226	1.430916	1.271602
C	4.000434	0.722880	-1.025737
C	4.331491	1.586799	0.025095
H	-4.960887	1.487315	0.590090
H	-3.143157	3.422915	-0.196609
H	2.304025	0.292161	2.435408
H	2.792325	-0.967149	-1.636949
H	3.979168	2.093854	2.093021
H	4.483789	0.835957	-1.992962
H	5.067879	2.371870	-0.125942
C	-3.835804	-1.078934	0.667004
H	-4.579394	-1.380041	-0.078485
H	-3.033605	-1.818662	0.700972
H	-4.314812	-1.010618	1.649041
C	-0.606373	2.365815	-0.738916
H	0.174342	1.607792	-0.814120
H	-0.755032	2.837950	-1.715549
H	-0.308802	3.126778	-0.010156
H	1.206962	-1.730795	1.694780

1TS (E-A)

scf done: -1123.945460

Pd	0.004143	0.150918	-0.418326
C	0.959422	1.844155	0.088076
N	1.647678	2.107138	1.242244
C	2.204782	3.377713	1.225830
C	1.860986	3.938806	0.039640
N	1.106189	2.994167	-0.642181
O	0.571156	-1.729574	-2.152032
C	1.484107	-1.012799	-1.640812
H	2.785264	3.766129	2.048820
H	2.078091	4.913320	-0.370629
C	-2.773801	-1.571703	-1.135798
H	-2.691461	-0.986916	-2.062060
O	-1.494721	-1.732574	-0.521864
H	-0.854870	-2.082040	-1.188416
C	1.795301	1.160194	2.339530
H	1.105629	0.334782	2.156556
H	2.816613	0.769205	2.378544
H	1.548795	1.647981	3.287837
C	0.520408	3.207813	-1.957472
H	1.297683	3.471949	-2.682203
H	0.039152	2.275277	-2.257581
H	-0.226150	4.008384	-1.920090
H	1.913526	-0.189434	-2.240592
H	-3.164081	-2.565602	-1.408635
C	-3.730847	-0.897284	-0.180596
C	-4.749885	-0.071801	-0.669980
C	-3.643022	-1.119503	1.199692
C	-5.671676	0.514574	0.199158
H	-4.821999	0.115265	-1.739599
C	-4.558542	-0.526866	2.070511
H	-2.848205	-1.751238	1.583307
C	-5.577653	0.289080	1.573771
H	-6.456763	1.153729	-0.196847
H	-4.476396	-0.704023	3.140016
H	-6.290678	0.749003	2.253117
C	2.407104	-1.531950	-0.584307
C	2.144291	-2.748706	0.064175
C	3.589941	-0.840900	-0.277537
C	3.029360	-3.245017	1.019092
H	1.243971	-3.295135	-0.198615
C	4.479645	-1.340787	0.671966
H	3.808514	0.092355	-0.793074
C	4.198547	-2.543016	1.329497
H	2.813946	-4.187064	1.517172
H	5.397329	-0.800834	0.893161
H	4.891816	-2.935903	2.068696

PhCH₂OH

scf done: -346.763698

O	-1.737596	-1.757252	-0.581507
C	-1.340514	-0.392260	-0.597775
H	-1.603198	0.091944	-1.552486
C	0.134180	-0.181433	-0.308578
C	0.835786	0.875811	-0.899892
C	0.810818	-1.033468	0.574097
C	2.184538	1.087490	-0.607601
H	0.323526	1.536745	-1.596530
C	2.160627	-0.828304	0.862156
H	0.269228	-1.859730	1.025661
C	2.851089	0.234465	0.274284
H	2.716258	1.911985	-1.075578
H	2.674171	-1.497643	1.547722
H	3.902420	0.394104	0.498588
H	-1.178920	-2.228114	-1.220486
H	-1.951612	0.085335	0.177633

PhCHO

scf done: -345.566491

O	1.675775	1.780012	-0.115811
C	1.243046	0.651550	-0.252195
C	-0.182465	0.272515	-0.125361
C	-0.568287	-1.062541	-0.303230
C	-1.148584	1.246608	0.172505
C	-1.909674	-1.425761	-0.185049
C	-2.486065	0.883618	0.290158
C	-2.866782	-0.452376	0.111425
H	0.185668	-1.812531	-0.533789
H	-0.824066	2.274153	0.305658
H	-2.209003	-2.460948	-0.323039
H	-3.236224	1.635058	0.520659
H	-3.912548	-0.733451	0.203845
H	1.927386	-0.193930	-0.489695

2A

scf done: -856.997683

Pd	-1.096821	-0.173135	-0.248667
C	-3.048432	0.045093	-0.154911
N	-4.005156	-0.929639	0.001079
C	-5.285083	-0.395027	0.033247
H	-6.166862	-1.007285	0.147697
C	-5.149676	0.947261	-0.104494
H	-5.890470	1.732058	-0.132476
N	-3.790088	1.200791	-0.218129
O	1.111318	-0.407299	-0.442676
C	2.031985	0.254520	0.464511
H	1.752960	1.314806	0.535198
C	1.827348	-0.400323	1.834502
H	0.748779	-0.383806	2.038148
H	2.125686	-1.454083	1.766615
C	2.593384	0.299147	2.960814
H	2.285483	1.347481	3.060594
H	2.398817	-0.193939	3.919098
H	3.675190	0.281950	2.787736
C	3.446638	0.143931	-0.071521
C	4.284450	1.264917	-0.111918
C	3.940030	-1.086877	-0.531189
C	5.592942	1.160953	-0.589746
H	3.908959	2.226391	0.231524
C	5.243349	-1.190754	-1.015709
H	3.291419	-1.958341	-0.516936
C	6.074872	-0.067451	-1.043571
H	6.230822	2.040550	-0.613954
H	5.611703	-2.149239	-1.372055
H	7.090625	-0.149745	-1.421026
H	1.277658	-0.075380	-1.340659
C	-3.705774	-2.347770	0.115157
H	-4.201943	-2.909622	-0.684062
H	-2.622691	-2.455194	0.024227
H	-4.034852	-2.734376	1.086335
C	-3.214441	2.525737	-0.377928
H	-3.425694	3.147189	0.499763
H	-2.135478	2.393813	-0.483976
H	-3.618879	3.013850	-1.271732

2TS (A-B)

scf done: -1103.574445

C	1.996926	1.365661	-0.290754	H	5.278203	-0.030129	-2.456687
N	2.814225	1.983213	-1.199232	H	5.582252	-0.725471	-0.855354
C	3.731547	2.819735	-0.577561	H	1.320515	-1.783214	-1.169090
C	3.490812	2.733542	0.754856	C	-2.208854	1.316051	-2.728363
N	2.430791	1.852453	0.910773	H	-1.461069	0.949559	-3.437232
Pd	0.564709	-0.079822	-0.630998	H	-2.767459	0.471752	-2.322846
C	2.732033	1.786510	-2.638869	H	-2.893548	1.997137	-3.238826
C	1.881995	1.445747	2.197867	C	0.270118	2.293520	1.424153
C	1.402186	-1.910963	0.104530	H	0.345572	1.228683	1.644324
C	0.608278	-2.288548	1.210376	H	1.278032	2.704294	1.323757
C	1.212774	-2.509121	2.449493	H	-0.257510	2.802758	2.236306
C	2.601118	-2.446285	2.592159	Pd	-0.666600	-0.546298	-0.323385
C	3.389400	-2.171487	1.464380	C	-2.508685	-0.609339	0.432982
C	2.810327	-1.937345	0.221900	C	-3.459930	-1.414893	-0.211869
H	4.456068	3.399531	-1.129050	C	-2.884449	0.078193	1.594302
H	3.968459	3.219727	1.591965	C	-4.758434	-1.524567	0.296312
H	3.667328	1.364930	-3.022198	H	-3.181584	-1.986464	-1.092251
H	1.914435	1.088670	-2.828850	C	-4.181456	-0.042919	2.106263
H	2.530970	2.737340	-3.144074	H	-2.169317	0.706450	2.117957
H	2.507672	0.676351	2.659945	C	-5.124856	-0.839439	1.456399
H	1.812219	2.315283	2.858513	H	-5.479959	-2.159988	-0.212742
H	0.888348	1.032076	2.022140	H	-4.451294	0.490854	3.015196
H	-0.464334	-2.399097	1.093721	H	-6.133081	-0.930378	1.852604
H	0.587307	-2.760995	3.303234	Cl	-0.249419	-2.922948	-0.085347
H	3.066415	-2.647009	3.552936				
H	4.473657	-2.151793	1.551826				
H	3.423269	-1.744906	-0.651753	2C			
O	-1.694926	-0.774288	-1.248524	scf done: -1088.013097			
H	-1.432057	-1.660295	-1.562794	C	-1.536411	-1.315805	0.221233
C	-2.830169	-0.893492	-0.373655	N	-1.851967	-2.486991	-0.396249
H	-2.543309	-1.462014	0.524685	C	-2.811176	-3.178663	0.326179
C	-3.956162	-1.657138	-1.097324	C	-3.093456	-2.429342	1.421361
H	-3.540210	-2.609603	-1.457344	N	-2.307139	-1.288651	1.341580
H	-4.245635	-1.082367	-1.985932	H	-3.202157	-4.129225	-0.001921
Cl	0.733175	-2.677335	-1.637346	H	-3.767164	-2.604015	2.245722
C	-3.234030	0.503218	0.050827	O	1.393061	-1.400286	-0.894579
C	-3.561569	0.775999	1.383712	C	-2.255686	-0.271782	2.388275
C	-3.317059	1.537685	-0.891847	H	-1.814859	0.632932	1.973795
C	-3.975189	2.052991	1.770604	H	-3.271495	-0.057692	2.730948
H	-3.489299	-0.015782	2.126214	H	-1.653089	-0.627034	3.230442
C	-3.723019	2.814930	-0.506366	C	-1.272266	-2.948703	-1.659420
H	-3.044008	1.338820	-1.923640	H	-0.256884	-2.552746	-1.740039
C	-4.056640	3.076246	0.825523	H	-1.245357	-4.041290	-1.650442
H	-4.226137	2.247509	2.810135	H	-1.881277	-2.608764	-2.503377
H	-3.777414	3.609207	-1.246455	Pd	-0.161224	-0.055963	-0.455036
H	-4.373289	4.072156	1.124155	C	-1.360261	1.562716	-0.293757
C	-5.181114	-1.940675	-0.222515	C	-0.844199	2.711211	0.338757
H	-5.651641	-1.013022	0.119233	C	-2.636752	1.663442	-0.876833
H	-5.929517	-2.513326	-0.780687	C	-1.563857	3.911070	0.372152
H	-4.910309	-2.526150	0.664963	H	0.135685	2.677384	0.813253
				C	-3.358119	2.861187	-0.847535
				H	-3.077684	0.798882	-1.368652
2B				C	-2.825029	3.990075	-0.221351
scf done: -1103.646517				H	-1.137105	4.782734	0.864217
C	-0.922717	1.427355	-0.596600	H	-4.339630	2.912015	-1.315048
N	-0.471665	2.451892	0.176944	H	-3.386690	4.920661	-0.195502
C	-0.822812	3.678311	-0.369794	C	2.166090	-0.349284	-1.296319
C	-1.510756	3.413718	-1.509326	H	1.521232	0.646364	-1.277687
N	-1.565652	2.033364	-1.630389	C	3.339155	-0.039423	-0.357308
H	-0.560545	4.614421	0.098286	C	4.089376	1.136997	-0.490291
H	-1.963607	4.074178	-2.232458	C	3.678980	-0.946605	0.651393
O	1.399493	-0.826821	-1.396288	C	5.160428	1.399872	0.364433
C	2.748186	-0.364461	-1.188675	H	3.830876	1.859874	-1.261926
H	2.819217	0.556643	-1.779088	C	4.753663	-0.687896	1.505245
C	3.047637	-0.026656	0.263311	H	3.081915	-1.846948	0.750427
C	2.648929	-0.873946	1.308327	C	5.498047	0.484972	1.365354
C	3.768288	1.134425	0.574094	H	5.729475	2.319450	0.251374
C	2.964464	-0.558157	2.631467	H	5.008566	-1.403637	2.283384
H	2.067104	-1.767390	1.096162	H	6.332388	0.687851	2.032050
C	4.093095	1.445762	1.897142	C	2.587925	-0.451803	-2.786530
H	4.080624	1.800890	-0.227696	H	1.667038	-0.508092	-3.379896
C	3.688638	0.599072	2.931046	H	3.113582	0.462432	-3.090962
H	2.641751	-1.221145	3.429830	C	3.459812	-1.681221	-3.057935
H	4.657877	2.348178	2.117856	H	3.698688	-1.761378	-4.124740
H	3.935424	0.838324	3.962128	H	4.403158	-1.629938	-2.503201
C	3.720075	-1.402963	-1.780977	H	2.936207	-2.591703	-2.750432
H	3.358610	-1.647462	-2.787594				
H	3.650867	-2.322657	-1.183284	2TS (c-b)			
C	5.178200	-0.939024	-1.850194	scf done: -1088.000074			
H	5.803851	-1.712504	-2.308215	Pd	-0.278103	-0.109703	0.300867

[illegible]

O	1.207410	-2.311787	-0.083212
C	1.470476	-1.458778	0.832648
C	2.412432	-0.328405	0.526320
C	2.685510	0.702968	1.441501
C	3.069876	-0.312639	-0.717138
C	3.574459	1.727867	1.115346
C	3.960318	0.707767	-1.039088
C	4.215268	1.736055	-0.125456
H	-4.995844	1.488874	0.407261
H	-3.155318	3.448293	-0.258230
H	2.191991	0.717539	2.408359
H	2.862933	-1.117169	-1.414960
H	3.768821	2.520031	1.834227
H	4.462096	0.700882	-2.003567
H	4.911057	2.532415	-0.376600
C	-3.847681	-1.064195	0.545872
H	-4.541675	-1.368421	-0.244906
H	-3.040538	-1.795276	0.623092
H	-4.386046	-1.007674	1.497591
C	-0.578035	2.422228	-0.646944
H	0.219178	1.677832	-0.652517
H	-0.665015	2.873755	-1.640695
H	-0.346963	3.202063	0.086016
C	1.244952	-1.861231	2.289048
H	0.995260	-0.990792	2.905085
H	0.381266	-2.531428	2.309303
C	2.477751	-2.581902	2.870155
H	3.356898	-1.928424	2.882885
H	2.283149	-2.909053	3.897931
H	2.720674	-3.466483	2.271616

2TS_(E-A)

scf done: -1281.196990

Pd	0.086020	0.261642	0.194616
C	1.209229	1.867107	-0.208051
N	1.272970	3.046606	0.494347
C	2.151618	3.946960	-0.091444
C	2.655689	3.336337	-1.192185
N	2.074418	2.078111	-1.250666
O	0.485572	-2.393574	0.619220
C	1.474576	-1.733202	1.028168
C	1.624353	-1.506042	2.543051
C	1.738976	-0.079507	3.097250
C	2.693481	-1.670755	0.149089
C	3.907632	-1.091404	0.553078
C	2.643587	-2.314823	-1.100401
C	5.028438	-1.131758	-0.277102
C	3.763375	-2.361840	-1.925740
C	4.962475	-1.765456	-1.520553
H	2.332743	4.929638	0.317043
H	3.360252	3.683474	-1.932699
H	0.751047	-1.990449	2.991862
H	2.503028	-2.089233	2.858271
H	0.830230	0.484439	2.868661
H	1.869957	-0.116556	4.186120
H	2.580880	0.474811	2.672614
H	3.984867	-0.604596	1.518843
H	1.710459	-2.782386	-1.395269
H	5.958487	-0.676144	0.053519
H	3.706248	-2.870761	-2.884881
H	5.839280	-1.805418	-2.161793
C	-2.787113	-1.445965	-0.171170
H	-2.294677	-1.637396	-1.136219
C	-3.515110	-2.731750	0.268796
H	-4.008508	-2.537197	1.229678
H	-2.751492	-3.500219	0.453979
C	-4.528606	-3.257449	-0.752339
H	-4.049047	-3.471079	-1.715863
H	-4.987996	-4.186962	-0.398579
H	-5.329210	-2.532068	-0.931169
C	-3.721254	-0.263402	-0.328868
C	-4.114994	0.174773	-1.598082
C	-4.232344	0.393082	0.799870
C	-5.008381	1.239239	-1.742328
H	-3.715204	-0.317977	-2.481620
C	-5.119535	1.459722	0.658893
H	-3.916956	0.070638	1.787599
C	-5.513481	1.884676	-0.613164
H	-5.302272	1.566779	-2.736290

H	-5.504449	1.961755	1.543149
H	-6.205360	2.715945	-0.721955
O	-1.796306	-1.100737	0.809725
H	-1.161832	-1.849491	0.903191
C	0.494597	3.332271	1.689334
H	-0.242395	2.534469	1.798253
H	1.136512	3.362714	2.576876
H	-0.017413	4.294096	1.581469
C	2.334229	1.110568	-2.306005
H	3.378522	0.784905	-2.283179
H	1.686493	0.251932	-2.128589
H	2.106404	1.549984	-3.283289

PhEtCHOH

scf done: -425.395403

O	-1.694531	-1.839238	-0.559126
C	-1.364515	-0.449672	-0.538876
H	-1.620771	0.008734	-1.510028
C	-2.249388	0.194445	0.538778
H	-1.992734	-0.261113	1.503921
H	-1.981577	1.256186	0.609564
C	-3.747656	0.040482	0.260959
H	-4.024747	-1.015745	0.202003
H	-4.341375	0.509472	1.053766
H	-4.025007	0.515289	-0.688786
C	0.116054	-0.217814	-0.275775
C	0.777290	0.879125	-0.841942
C	0.835238	-1.082305	0.559997
C	2.126376	1.115586	-0.573277
H	0.231645	1.551299	-1.501670
C	2.185572	-0.850738	0.826790
H	0.327010	-1.940410	0.990267
C	2.834934	0.249771	0.262819
H	2.625814	1.970065	-1.022738
H	2.731753	-1.530772	1.475698
H	3.886825	0.428849	0.469172
H	-1.118679	-2.267261	-1.212342

PhEtCO

scf done: -424.199729

O	1.464229	-1.807334	-1.194089
C	1.741227	-1.320146	-0.106886
C	2.408825	0.022586	-0.026265
C	2.732234	0.649838	1.187211
C	2.720391	0.673061	-1.231987
C	3.354613	1.898800	1.193692
C	3.339187	1.919132	-1.225820
C	3.658515	2.535033	-0.011223
H	2.501816	0.170172	2.133188
H	2.463105	0.175287	-2.161171
H	3.600697	2.374998	2.138859
H	3.574387	2.413059	-2.164743
H	4.142045	3.508362	-0.004721
C	1.445499	-2.099679	1.170436
H	1.067072	-1.438414	1.958407
H	0.652566	-2.810898	0.921401
C	2.687191	-2.863593	1.671422
H	3.503054	-2.183286	1.938387
H	2.438225	-3.458566	2.556558
H	3.055522	-3.544451	0.896873

2TS_(E-F)

scf done: -1102.373846

C	0.176612	1.823699	0.203457
N	-0.132960	2.946605	-0.507901
C	0.020533	4.093256	0.257864
C	0.447758	3.688530	1.480591
N	0.532400	2.303744	1.430588
Pd	0.195473	-0.132551	-0.532946
C	-0.608406	2.933384	-1.888716
C	1.018728	1.474510	2.524535
C	2.269380	-0.548783	-0.621723
C	2.494852	-1.898725	-0.322477
C	3.590967	-2.234510	0.478839
C	4.482962	-1.255541	0.921705
C	4.278497	0.077735	0.549807
C	3.186517	0.440338	-0.240300
H	-0.186452	5.079464	-0.128553
H	0.698281	4.253326	2.365495

H	-0.333356	3.875734	-2.369516
H	-0.134426	2.103711	-2.415443
H	-1.696003	2.813042	-1.921395
H	2.111141	1.510029	2.581014
H	0.589206	1.821023	3.469149
H	0.712493	0.446597	2.331244
H	1.812496	-2.656134	-0.688888
H	3.752136	-3.278474	0.737449
H	5.342609	-1.529630	1.526698
H	4.982446	0.846091	0.862095
H	3.045651	1.467405	-0.556643
Cl	1.608694	-0.259259	-2.700681
O	-0.682096	-2.212173	-0.610059
C	-1.273630	-1.735698	0.402321
C	-2.615628	-1.082896	0.223628
C	-3.329423	-0.496078	1.283353
C	-3.200996	-1.095405	-1.056303
C	-4.581488	0.077525	1.065040
C	-4.451325	-0.522748	-1.271510
C	-5.146772	0.069402	-0.212405
H	-2.905930	-0.476050	2.282713
H	-2.653549	-1.565995	-1.866195
H	-5.118026	0.529918	1.895142
H	-4.889671	-0.544188	-2.265990
H	-6.124202	0.514153	-0.379691
C	-0.823546	-2.182869	1.790469
H	0.257589	-2.344074	1.744222
H	-1.012131	-1.408687	2.542047
C	-1.525998	-3.491227	2.204744
H	-1.321642	-4.282174	1.475599
H	-1.165515	-3.827133	3.183444
H	-2.611738	-3.360144	2.268924

2F

scf done: -1102.440676

C	1.019498	1.241380	0.055324
N	1.416464	2.014300	-0.990994
C	1.206963	3.359919	-0.725007
C	0.671844	3.434122	0.519650
N	0.566253	2.130116	0.983462
C	2.980301	-0.773421	0.239085
C	3.662766	-1.551291	-0.709047
C	3.727568	-0.039140	1.170801
C	5.061113	-1.581624	-0.727211
C	5.126354	-0.084174	1.158708
C	5.798793	-0.849692	0.205473
O	-1.345464	-0.522935	0.224574
C	-2.385699	-1.132042	-0.049752
H	1.463124	4.133253	-1.432600
H	0.375524	4.284606	1.114090
H	3.105289	-2.161619	-1.412088
H	3.226538	0.567870	1.919986
H	5.572483	-2.195023	-1.466062
H	5.687717	0.484897	1.896980
H	6.885454	-0.881608	0.193599
C	1.950575	1.498996	-2.248568
C	0.028068	1.761129	2.288617
H	2.480834	0.568386	-2.048471
H	1.141636	1.315617	-2.962787
H	2.645557	2.231815	-2.666050
H	-1.058987	1.883211	2.304565
H	0.271595	0.714089	2.472208
H	0.479916	2.386713	3.063732
Pd	0.988446	-0.767543	0.242787
C	-3.667957	-0.358191	-0.085294
C	-3.617925	1.040528	0.048951
C	-4.917973	-0.979078	-0.244341
C	-4.784371	1.798087	0.023927
H	-2.648302	1.513665	0.160903
C	-6.088018	-0.219964	-0.259827
H	-4.984858	-2.056504	-0.347845
C	-6.023994	1.168295	-0.127751
H	-4.732143	2.879131	0.121291
H	-7.048920	-0.712844	-0.377372
H	-6.936110	1.758768	-0.145300
C	-2.388138	-2.619261	-0.314409
H	-3.128398	-2.863306	-1.084345
H	-1.392758	-2.895710	-0.670720
C	-2.668704	-3.422543	0.975410

H	-3.623492	-3.149188	1.439315
H	-2.694805	-4.490358	0.737237
H	-1.858640	-3.262781	1.691229
Cl	0.928644	-3.170615	0.517300

2G

scf done: -1202.556744

C	0.882625	1.585742	0.246687
N	1.287371	2.532186	-0.645979
C	1.128157	3.810963	-0.131111
C	0.605667	3.668336	1.112773
N	0.464835	2.304513	1.328138
Pd	0.839443	-0.434080	0.040479
C	1.860724	2.247583	-1.957293
C	-0.099259	1.715773	2.536462
C	2.823211	-0.505869	-0.164134
C	3.361883	-1.363932	-1.138588
C	4.743924	-1.444644	-1.335903
C	5.617933	-0.682312	-0.557400
C	5.096054	0.163299	0.422646
C	3.712101	0.257044	0.611901
H	1.399967	4.694711	-0.687756
H	0.325839	4.402840	1.852335
H	2.935641	2.450828	-1.954575
H	1.700823	1.192914	-2.175712
H	1.368611	2.865109	-2.714763
H	0.335584	2.195555	3.418182
H	-1.186971	1.834835	2.551585
H	0.144613	0.652942	2.538560
H	2.691849	-1.991296	-1.717812
H	5.138350	-2.114624	-2.097612
H	6.692630	-0.750525	-0.708973
H	5.764917	0.755908	1.044175
H	3.332392	0.929555	1.376733
O	-1.513109	-0.180786	0.182760
C	-2.486716	-0.916453	-0.025257
C	-3.807347	-0.276453	-0.319619
C	-4.997205	-1.016761	-0.413903
C	-3.858612	1.117651	-0.495384
C	-6.209088	-0.377086	-0.674199
C	-5.066149	1.753932	-0.763732
C	-6.245654	1.007116	-0.852299
H	-4.983455	-2.092722	-0.277290
H	-2.933881	1.680083	-0.421934
H	-7.123625	-0.959764	-0.740532
H	-5.092526	2.831006	-0.905508
H	-7.189702	1.503389	-1.061062
C	-2.349094	-2.416009	0.060984
H	-3.056517	-2.913306	-0.610735
H	-1.315976	-2.647718	-0.241120
C	-2.562664	-2.904357	1.510904
H	-3.566603	-2.673267	1.887472
H	-2.421625	-3.988703	1.559015
H	-1.828982	-2.441830	2.178676
O	0.679548	-2.424483	-0.286708
C	1.251191	-3.348232	0.590447
H	2.347444	-3.245843	0.671370
H	0.846300	-3.296337	1.622256
H	1.053490	-4.372784	0.225560

2TS_g

scf done: -1320.48752884

C	-1.06296700	-1.95117000	0.40709700
N	-1.39496600	-2.88684800	-0.52213700
C	-1.68207400	-4.10418100	0.07923400
C	-1.51678300	-3.92701100	1.41408900
N	-1.13554200	-2.60665000	1.59641300
Pd	-0.50382200	-0.04590300	-0.18942400
C	-1.44976100	-2.65557700	-1.96152600
C	-0.81305800	-2.00276300	2.88842100
C	-2.35498600	0.33972400	-0.48414900
C	-2.61361900	0.53013100	-1.85176900
C	-3.90614600	0.80705700	-2.31307700
C	-4.97196500	0.89591500	-1.41578400
C	-4.73272400	0.70293600	-0.05403200
C	-3.44053200	0.42085900	0.40390500
H	-1.96235000	-4.97573700	-0.49144300
H	-1.62205200	-4.61494700	2.23845200
H	-2.45125500	-2.34103000	-2.26573400

H	-0.73894700	-1.86930700	-2.21438900	C	5.50039400	-0.48443100	-1.42959800
H	-1.17441600	-3.57825800	-2.47898300	C	3.63950900	-1.74141500	-2.30096400
H	-0.69700500	-2.80091700	3.62518400	C	4.96175200	-1.31069500	-2.41935900
H	0.12041300	-1.44737100	2.79123500	H	5.17579100	0.53185100	0.42553600
H	-1.61552700	-1.33125600	3.20663800	H	1.84172200	-1.68737200	-1.10374700
H	-1.79948500	0.48090200	-2.57063900	H	6.53431400	-0.15466500	-1.49882700
H	-4.07561000	0.95920700	-3.37717500	H	3.21075300	-2.39395000	-3.05842500
H	-5.97546100	1.11274800	-1.77315400	H	5.56937600	-1.62201100	-3.26532600
H	-5.55280500	0.76920600	0.65802200	C	2.84755000	0.91997700	1.77902500
H	-3.28238000	0.27220100	1.46936300	H	3.79609400	1.42727800	1.62915700
O	1.50427500	-0.75669600	0.99399700	H	1.38484700	1.70861600	0.46129300
C	2.47379400	0.06099400	0.83767700	C	2.09800400	1.25658900	3.03953700
C	3.53508700	-0.32062800	-0.15392900	H	2.56524900	0.79361000	3.92378200
C	4.79355600	0.30075900	-0.20095100	H	2.07912800	2.33790800	3.23354500
C	3.27431000	-1.37360900	-1.04647600	H	1.06521700	0.89759900	2.99539000
C	5.75479400	-0.10637900	-1.12604100	O	0.54631200	1.87578700	-0.04109100
C	4.23172800	-1.77870500	-1.97322900	C	0.18622500	3.29022300	0.07665500
C	5.47617400	-1.14404800	-2.01789100	C	1.48899500	4.08815800	0.22443000
H	5.03408500	1.09380800	0.49948200	H	1.27139700	5.16088300	0.26902800
H	2.30786100	-1.86264800	-0.99044500	H	2.02330500	3.81356300	1.14083900
H	6.72480700	0.38357200	-1.14622000	H	2.15115900	3.90669200	-0.62900600
H	4.01075600	-2.59091400	-2.66136400	C	-0.72297900	3.48327800	1.29538100
H	6.22606400	-1.46037800	-2.73844200	H	-0.99744700	4.53905200	1.40683000
C	2.46542200	1.34223200	1.46164800	H	-1.64040500	2.89807100	1.18303800
H	3.35293800	1.95355500	1.30379400	H	-0.21512900	3.16352100	2.21169100
H	1.45403200	1.78503400	0.66890800	C	-0.52762700	3.67766300	-1.21902000
C	1.84195600	1.49478000	2.84436100	H	-1.44287000	3.09695300	-1.35146600
H	2.49416000	1.09268100	3.63283400	H	-0.79125200	4.74139600	-1.19778300
H	1.66097900	2.55068300	3.07631900	H	0.12499000	3.49960500	-2.08041900
H	0.88208600	0.97452000	2.90315400				
O	0.33809100	1.90868100	0.06355200				
C	-0.14095800	3.25633700	-0.03773100	2H			
C	1.04996400	4.20923800	0.18990700	scf done: -1086.825440			
H	0.73589000	5.25145400	0.05981700	C	1.423439	-1.728444	-1.000245
H	1.45709000	4.10492600	1.20153100	N	2.745213	-2.029429	-0.870361
H	1.85153200	4.00116600	-0.52766000	C	3.177213	-2.849478	-1.902883
C	-0.69510800	3.49215800	-1.45177400	C	2.102577	-3.070945	-2.700984
H	-1.56527700	2.86048300	-1.64142800	N	1.040435	-2.384715	-2.133528
H	-0.99571800	4.53953200	-1.58261100	Pd	0.125887	-0.593230	0.141517
H	0.07301600	3.25785700	-2.19774600	C	3.607342	-1.604940	0.228213
C	-1.22379800	3.51722900	1.02178700	C	-0.309069	-2.349163	-2.693909
H	-2.08003000	2.85531000	0.86415200	C	1.408088	0.941245	0.394351
H	-0.82373800	3.33093300	2.02535800	C	1.747957	1.389932	1.683779
H	-1.57704100	4.55545700	0.98078100	C	2.620620	2.468195	1.869491
				C	3.166179	3.132503	0.769152
				C	2.833275	2.705008	-0.517735
2G2				C	1.970429	1.618761	-0.701398
scf done: -1320.50046525				H	4.193914	-3.205294	-1.968598
C	-1.18771600	-1.91966200	0.43437800	H	1.999162	-3.649655	-3.605962
N	-1.64502200	-2.81266600	-0.48298200	H	4.455696	-1.034794	-0.161499
C	-2.00569300	-4.00493200	0.12844700	H	3.029365	-0.969414	0.895321
C	-1.76008500	-3.85279600	1.45396800	H	3.974173	-2.481616	0.771589
N	-1.25539000	-2.57325900	1.62349000	H	-0.388247	-1.566318	-3.455386
Pd	-0.47548400	-0.08663500	0.19057700	H	-0.531024	-3.318216	-3.148878
C	-1.74639600	-2.57106900	-1.91842300	H	-1.020887	-2.154081	-1.890302
C	-0.81367400	-2.01442600	2.90251100	H	1.327881	0.898004	2.558399
C	-2.28575300	0.46850200	-0.50791900	H	2.867550	2.792335	2.878655
C	-2.48268100	0.76360200	-1.86861600	H	3.840235	3.973426	0.912706
C	-3.72220700	1.20471600	-2.34690900	H	3.248478	3.215165	-1.384949
C	-4.80042000	1.35836600	-1.47273900	H	1.736319	1.300376	-1.714808
C	-4.62668200	1.06442100	-0.11901800	O	-1.816233	-1.785259	0.322540
C	-3.38702200	0.61780200	0.35333000	C	-1.793125	-0.949423	1.306231
H	-2.38535300	-4.84522700	-0.43143900	C	-1.775366	-1.497675	2.702479
H	-1.88198300	-4.53569800	2.28011200	C	-2.026113	-0.699444	3.828936
H	-2.72939600	-2.16933900	-2.17629100	C	-1.547261	-2.870976	2.883833
H	-0.98220100	-1.84997100	-2.20570200	C	-2.022096	-1.256535	5.108065
H	-1.57730000	-3.51287700	-2.44676200	C	-1.545183	-3.427686	4.160532
H	-0.63246900	-2.83980300	3.59495900	C	-1.778177	-2.620905	5.278203
H	0.11131300	-1.46134600	2.72845500	H	-2.243054	0.357288	3.707386
H	-1.58424400	-1.35767500	3.31772700	H	-1.377061	-3.482244	2.003946
H	-1.65619200	0.66540500	-2.56966400	H	-2.218916	-0.626065	5.971289
H	-3.84182700	1.43199700	-3.40445100	H	-1.363248	-4.492029	4.286463
H	-5.76357800	1.70125500	-1.84237400	H	-1.778537	-3.054785	6.274853
H	-5.45817400	1.17804800	0.57371100	C	-1.624510	0.442421	1.023221
H	-3.28241800	0.38801100	1.41156800	H	-1.433049	1.097665	1.869159
O	1.37732200	-0.79079000	1.06928800	C	-2.310865	1.101995	-0.157444
C	2.49859500	-0.10538400	0.93643900	H	-3.265046	1.551227	0.160841
C	3.38370300	-0.49717300	-0.21828000	H	-1.701670	1.903727	-0.587355
C	4.72339200	-0.08774600	-0.34247000	H	-2.531904	0.372666	-0.941351
C	2.86475800	-1.34435100	-1.21089200				

2TS_(H-T)				C	-0.370116	1.651780	1.571736
scf done: -1086.790800				C	0.990645	2.070774	1.086378
C	1.200924	-1.838469	0.054015	C	1.309260	2.277523	-0.264859
N	1.690147	-2.478555	-1.049141	C	1.987161	2.268525	2.056874
C	2.750974	-3.311965	-0.728662	C	2.596002	2.670049	-0.634749
C	2.938028	-3.196361	0.611036	C	3.268536	2.671315	1.688720
N	1.988529	-2.296329	1.069088	C	3.576781	2.872642	0.339526
Pd	-0.451757	-0.520574	0.145184	H	0.567508	2.093082	-1.034025
C	1.168670	-2.302130	-2.397415	H	1.728874	2.100806	3.097378
C	1.827982	-1.914879	2.470714	H	2.833295	2.815960	-1.685154
C	-2.331450	0.216214	-0.096555	H	4.026835	2.831645	2.450817
C	-2.658997	0.736456	-1.362296	H	4.575948	3.187329	0.049205
C	-3.913110	0.495686	-1.927673	C	-1.611959	1.881607	0.695129
C	-4.870630	-0.245986	-1.230519	H	-1.316087	2.408456	-0.216828
C	-4.564613	-0.745505	0.037247	C	-2.589069	2.794702	1.473184
C	-3.312277	-0.503960	0.609190	H	-2.126921	3.762708	1.701320
H	3.275526	-3.896212	-1.469192	H	-3.490786	2.973654	0.878348
H	3.656532	-3.663558	1.267135	H	-2.875215	2.320735	2.415935
H	0.751654	-3.242269	-2.773444	2TS_(T-B)			
H	0.381552	-1.547514	-2.355222	scf done: -1511.037159			
H	1.963000	-1.963143	-3.070114	C	-0.806376	-2.266998	-0.152558
H	1.146870	-2.605969	2.978179	N	-1.438757	-3.182982	0.645672
H	2.804750	-1.950671	2.961275	C	-2.539248	-3.748298	0.014178
H	1.432864	-0.898464	2.525422	C	-2.612544	-3.175333	-1.213245
H	-1.928788	1.321629	-1.914816	C	-1.553551	-2.284767	-1.298888
H	-4.143792	0.894303	-2.913034	N	1.004811	-1.209508	0.057349
H	-5.849694	-0.424009	-1.667421	Pd	-0.962521	-3.593147	1.956018
H	-5.304412	-1.320085	0.589916	C	-1.268482	-1.463464	-2.469797
H	-3.096194	-0.879770	1.604902	H	-3.154481	-4.502097	0.481955
O	0.867938	1.199358	2.346051	H	-3.314096	-3.320815	-2.020424
C	0.366673	1.488338	1.244619	H	-0.570327	-4.615856	1.921394
C	1.258609	2.096951	0.181144	H	-0.166842	-2.910701	2.251769
C	0.796011	2.641896	-1.027024	H	-1.775955	-3.545380	2.687733
C	2.634112	2.154213	0.455387	H	-1.442493	-2.052040	-3.375772
C	1.683931	3.214095	-1.938234	H	-1.906973	-0.574979	-2.485115
C	3.523206	2.720318	-0.455181	H	-0.219563	-1.166052	-2.425514
C	3.051680	3.252616	-1.658296	C	-0.950251	1.489398	2.117374
H	-0.261763	2.626337	-1.266700	C	-1.303891	0.617260	3.157758
H	2.978410	1.749595	1.401009	C	-0.399425	-0.328252	3.643116
H	1.305464	3.634176	-2.866771	C	0.883932	-0.412864	3.098143
H	4.585278	2.753113	-0.224831	C	1.254673	0.453506	2.058551
H	3.742465	3.700061	-2.368367	C	0.335551	1.394057	1.567495
C	-1.130636	1.472154	1.052945	O	-1.366111	3.384845	-0.521568
H	-1.445017	2.271978	0.387586	C	-2.060318	2.625556	0.138642
C	-1.870737	1.508185	2.380901	C	-3.081829	1.757852	-0.537788
H	-1.530612	2.379058	2.956182	C	-3.727792	0.689126	0.101831
H	-2.951052	1.582736	2.238285	C	-3.405202	2.050922	-1.873403
H	-1.648473	0.626362	2.986509	C	-4.682857	-0.066630	-0.579686
2I				C	-4.368430	1.306036	-2.548354
scf done: -1086.845195				C	-5.010874	0.245060	-1.900859
C	1.001670	-1.854229	-0.931032	C	-1.920934	2.582699	1.671258
N	1.170850	-2.492924	-2.131274	C	-1.481236	3.962448	2.197413
C	2.467791	-2.959153	-2.287555	H	-2.292619	0.694208	3.606325
C	3.141219	-2.610765	-1.161767	H	-0.691168	-0.985306	4.458635
N	2.237298	-1.944253	-0.348852	H	1.605564	-1.120357	3.497410
Pd	-0.686083	-0.956572	-0.189288	H	2.279824	0.480635	1.706817
C	0.111219	-2.671925	-3.112290	H	0.640041	2.071251	0.775069
C	2.566386	-1.382968	0.954457	H	-3.468694	0.425276	1.121521
C	-2.312269	0.589524	0.264529	H	-2.890682	2.875169	-2.356497
C	-3.061702	0.608458	-0.945758	H	-5.167530	-0.900095	-0.079297
C	-3.992180	-0.380700	-1.238674	H	-4.621757	1.550589	-3.576491
C	-4.180742	-1.457801	-0.356720	H	-5.764912	-0.336070	-2.425631
C	-3.425030	-1.532470	0.806877	H	-2.903953	2.348655	2.096068
C	-2.501477	-0.512673	1.141191	H	-2.217840	4.731152	1.938348
H	2.791518	-3.494174	-3.167486	H	-1.376233	3.932086	3.286670
H	4.167325	-2.779663	-0.871988	H	-0.524351	4.253882	1.758311
H	-0.075033	-3.737565	-3.284327	O	2.351667	-1.404949	-1.646729
H	-0.788311	-2.202895	-2.709269	C	3.062607	-0.762408	-0.795998
H	0.382242	-2.195023	-4.060541	C	3.196044	0.721576	-0.931326
H	3.070873	-2.136530	1.567969	C	4.090599	-1.555077	0.010856
H	3.212027	-0.505652	0.846860	C	4.062416	1.488463	-0.128864
H	1.632375	-1.082965	1.431619	C	2.435689	1.391905	-1.910024
H	-2.935629	1.449467	-1.624532	C	5.394287	-1.783528	-0.778404
H	-4.570767	-0.320322	-2.157058	C	4.147377	2.873140	-0.285091
H	-4.907166	-2.232315	-0.587880	C	2.517423	2.772806	-2.060238
H	-3.565145	-2.358341	1.499210	C	3.372607	3.523898	-1.246222
H	-2.058859	-0.491711	2.131485	H	4.316875	-1.064964	0.965713
O	-0.502218	1.237250	2.718538	H	3.634235	-2.522996	0.246421

H	4.681890	1.006773	0.621722
H	1.786637	0.800830	-2.546614
H	5.885577	-0.834735	-1.022111
H	6.099631	-2.392803	-0.200981
H	5.180630	-2.304727	-1.717478
H	4.824360	3.442964	0.346748
H	1.913221	3.268519	-2.815661
H	3.436424	4.602175	-1.364862

CH₃CH (Ph) C (O) Ph

scf done: -655.245219

O	1.635111	-1.559301	1.573560
C	1.977559	-0.452190	1.181383
C	3.035767	-0.319138	0.126076
C	3.380515	0.903091	-0.472007
C	3.707057	-1.486816	-0.274413
C	4.376142	0.954584	-1.447785
C	4.705459	-1.433531	-1.241989
C	5.042586	-0.210860	-1.831284
H	2.860057	1.814422	-0.198594
H	3.425653	-2.424896	0.192563
H	4.629991	1.904769	-1.909613
H	5.221405	-2.342313	-1.539913
H	5.820916	-0.167553	-2.588640
C	1.317200	0.809805	1.765688
H	2.085516	1.587176	1.855339
C	0.750357	0.522112	3.167130
H	1.544393	0.201081	3.849964
H	0.281737	1.424083	3.573719
H	0.003490	-0.274240	3.126268
C	0.234869	1.331431	0.821298
C	0.158559	2.695822	0.510389
C	-0.727899	0.465848	0.281790
C	-0.851950	3.186754	-0.318424
H	0.893265	0.381947	0.927506
C	-1.737418	0.954377	-0.548524
H	-0.682488	-0.595276	0.511791
C	-1.803121	2.315903	-0.852497
H	-0.894693	4.248776	-0.545951
H	-2.473094	0.268427	-0.960333
H	-2.589142	2.694770	-1.500155

1A'

scf done: -664.68851745

Pd	0.14045600	-0.30504100	-0.00276600
C	-1.77094000	0.01972200	0.00001500
N	-2.81649700	-0.90098700	0.00114700
C	-4.06228700	-0.28858100	0.00251100
H	-4.98701500	-0.84796000	0.00352500
C	-3.84060300	1.04943200	0.00219200
H	-4.53568700	1.87694000	0.00286300
N	-2.46395200	1.22776100	0.00075900
O	2.15072000	-0.78880200	-0.00713000
C	3.23619800	0.05182100	0.00122700
C	-2.59866400	-2.33146300	0.00111200
H	-3.03591500	-2.79769200	-0.89268000
H	-1.51408800	-2.47819200	0.00034300
H	-3.03463700	-2.79749900	0.89563400
C	-1.79543200	2.51098700	-0.00043100
H	-2.05613800	3.09322300	0.89422200
H	-0.72206000	2.29575800	-0.00178100
H	-2.05840100	3.09270200	-0.89476300
C	3.25684000	0.97437600	-1.24943000
C	2.34802300	1.58769300	-1.25587900
H	4.13749200	1.63686200	-1.28610300
H	3.24649600	0.35733400	-2.15669800
C	3.25883600	0.94690500	1.27168700
H	3.24934600	0.31026300	2.16531900
H	4.13993900	1.60792000	1.32158700
H	2.35047000	1.56056200	1.29274900
C	4.52586100	-0.81596700	-0.00916700
H	4.52877400	-1.45323700	-0.90236700
H	5.45188400	-0.21953700	-0.00246000
H	4.52907500	-1.47362600	0.86912400

1TS_(A-B)'

scf done: -911.28295417

C	1.04952500	1.51689100	0.13261200
N	0.76838600	2.60121000	0.91441400

C	1.72706700	3.59259700	0.77890600
C	2.64644300	3.12242200	-0.10236200
N	2.22478100	1.85702000	-0.47817000
H	1.67477800	4.52466900	1.32109600
H	3.55557900	3.56359100	-0.48227100
O	1.64821800	-1.51645400	-0.59378800
C	1.98319500	-2.54963000	0.26413700
C	2.92315300	1.01050700	-1.44356600
H	2.65338800	-0.03716300	-1.23246500
H	2.63413200	1.28576000	-2.46495500
H	4.00228900	1.16087700	-1.32489000
C	-0.43450600	2.73056600	1.72724700
H	-0.57192700	1.81867400	2.31038700
H	-0.30859500	3.58196600	2.40349500
H	-1.30189200	2.87671500	1.07511800
Pd	-0.05860800	-0.19539000	-0.23154900
C	-2.01011400	0.16895500	-0.18891300
C	-2.74032900	0.06269400	1.03434000
C	-2.15256900	-0.89630600	-1.13726000
C	-3.50904200	-1.05590600	1.30548300
H	-2.69114000	0.87201300	1.75619700
C	-2.96748500	-2.01220800	-0.84122900
H	-1.78020500	-0.76779300	-2.14979500
C	-3.63569400	-2.10632200	0.36931300
H	-4.02230300	-1.12618300	2.26456100
H	-3.08099200	-2.79494200	-1.59054400
H	-4.25560400	-2.97072900	0.59700500
Cl	-2.52939400	2.17965300	-1.05603900
C	2.37924800	-2.01366300	1.66596500
H	1.52922200	-1.47764600	2.10468600
H	2.68715700	-2.81109200	2.35977600
H	3.20914800	-1.30179300	1.56868800
C	3.19648200	-3.30418600	-0.33871200
H	3.52140200	-4.15543300	0.27853700
H	2.93567300	-3.67770100	-1.33638000
H	4.04419100	-2.61597700	-0.44994700
C	0.81115200	-3.55101700	0.42755000
H	-0.07068000	-3.03224600	0.82224600
H	0.53964200	-3.96296900	-0.55217500
H	1.05535100	-4.38707500	1.10105700

1B'

scf done: -911.35050585

C	-0.16187200	1.53180100	0.06100600
N	-0.84960400	2.22252400	1.01638900
C	-0.79490500	3.59016800	0.78520600
C	-0.05221000	3.76113500	-0.33819300
N	0.32702400	2.49893800	-0.76465900
H	-1.26798000	4.30544900	1.44060200
H	0.25061600	4.65759600	-0.85761200
O	2.18784100	0.14483500	-0.16072700
C	3.32182800	-0.53421100	0.27227300
C	1.17428600	2.22115600	-1.92525100
H	1.81810100	1.37521100	-1.64823400
H	0.55709000	1.98693400	-2.79956000
H	1.77546000	3.11191300	-2.13374400
C	-1.56531600	1.60940800	2.12557900
H	-1.21375400	0.58346700	2.22592500
H	-1.35986100	2.16888000	3.04467500
H	-2.64212400	1.59501700	1.93036200
Pd	0.11947100	-0.43949100	-0.12874400
C	-1.89466900	-0.71401400	-0.18177400
C	-2.74415200	0.05465700	-1.00343900
C	-2.52200100	-1.68292800	0.62888600
C	-4.13299300	-0.12696400	-1.01953000
H	-2.31661800	0.81616700	-1.65356400
C	-3.90845600	-1.86172100	0.62926100
H	-1.90511300	-2.32768300	1.24790900
C	-4.72720300	-1.08385600	-0.19535500
H	-4.75043400	0.48471200	-1.67800700
H	-4.35258900	-2.62233700	1.27170200
H	-5.80683800	-1.22666500	-0.19968200
Cl	0.42126300	-2.84635900	-0.34347700
C	4.43900600	0.52412800	0.46962400
H	4.11701500	1.26886700	1.20867000
H	5.38586000	0.07947200	0.81141600
H	4.62803200	1.04852000	-0.47624100
C	3.78821400	-1.56421500	-0.78578000

H	4.71588800	-2.08026900	-0.49167800
H	2.99815200	-2.30450200	-0.93922200
H	3.97041800	-1.05066100	-1.73974400
C	3.08645400	-1.25591300	1.62008100
H	2.76546300	-0.52711300	2.37670900
H	2.29815100	-2.00518700	1.50148600
H	3.99721100	-1.75383400	1.98732500

1TS_(a-c)'

scf done: -1258.12871618

C	-1.38385300	-0.69402500	1.38725200
N	-0.96950000	-1.89227000	1.87708800
C	-1.42913400	-2.08393800	3.17054000
C	-2.14944800	-0.98031000	3.50098200
N	-2.11459800	-0.14461000	2.39621300
H	-1.19644200	-2.97345100	3.73527800
H	-2.66628400	-0.71467300	4.41028800
O	0.75005800	1.47601000	1.00279200
C	1.39177900	2.73104400	0.80322500
C	-2.70935800	1.18420100	2.32017800
H	-1.92207300	1.92140500	2.14970700
H	-3.42187400	1.22266900	1.49306100
H	-3.22227400	1.39212700	3.26367700
C	-0.10079800	-2.81778300	1.14623700
H	-0.68145800	-3.36555200	0.39656200
H	0.69318500	-2.21230400	0.67237100
H	0.32034900	-3.52818000	1.86396800
Pd	-1.00488200	-0.16888900	-0.37950500
C	-2.83758400	-0.36357000	-0.97062400
C	-3.76146800	0.62475200	-1.35879300
C	-3.25567300	-1.70354700	-1.03857000
C	-5.04900400	0.28518700	-1.78624800
H	-3.45730800	1.66686700	-1.35899100
C	-4.53971800	-2.04566400	-1.47845500
H	-2.57111100	-2.49867200	-0.75488600
C	-5.44755800	-1.05244100	-1.84913300
H	-5.73967600	1.07315900	-2.08441800
H	-4.82861500	-3.09496100	-1.52858400
H	-6.44782200	1.31609300	-2.18771700
Cl	-0.60240300	-1.30921800	-2.46682500
O	1.64031500	-0.66924300	0.10661000
C	2.36991800	-0.82999300	-1.04727600
H	2.24170200	0.00536900	-1.76411600
C	3.87650000	-1.00618100	-0.81287400
C	4.77862600	-1.09912000	-1.88339100
C	4.38180000	-1.09594400	0.48841400
C	6.14413000	-1.28022200	-1.66142500
H	4.40118200	-1.02577600	-2.90315700
C	5.74860000	-1.27651400	0.71800600
H	3.66541000	-1.01859800	1.30095900
C	6.63748400	-1.37094600	-0.35506200
H	6.82767600	-1.34752300	-2.50651100
H	6.12282800	-1.34269000	1.73883800
H	7.70255800	-1.50991000	-0.17889400
H	1.30966800	0.66608900	0.64303800
C	2.29784400	2.70204900	-0.43945600
H	1.70774500	2.43651300	-1.32180500
H	2.76737900	3.68169300	-0.60404700
H	3.09653300	1.96161500	-0.31719300
C	2.22555000	3.04780800	2.06235700
H	1.58168700	3.04851100	2.95041900
H	2.99782100	2.28275200	2.20472200
H	2.72044200	4.02649600	1.99047500
C	0.28773300	3.78316300	0.61738200
H	-0.37372000	3.79995200	1.49391600
H	0.71072200	4.78905200	0.49247900
H	-0.30869100	3.53484700	-0.26609800
H	2.04337500	-1.73030400	-1.61800500

1C'

scf done: -1024.45306648

C	-0.75063400	1.55285200	0.08230200
N	-0.99602600	1.95672700	1.36325300
C	-1.18311200	3.33019900	1.43013300
C	-1.06110900	3.80018800	0.16230400
N	-0.79446300	2.70631600	-0.64515300
H	-1.37588400	3.84052500	2.36136500
H	-1.14180700	4.80120300	-0.23320900
O	1.40442000	0.54581000	-1.53594100

C	2.37501900	1.14641000	-0.77643300
H	1.98264500	1.87953400	-0.02802000
C	3.30608100	0.20556700	-0.00105700
C	3.21749700	-1.18143800	-0.16373200
C	4.28073100	0.72096200	0.86607900
C	4.08643800	-2.02916100	0.53108800
H	2.45096000	-1.57609700	-0.82544500
C	5.15183700	-0.12276000	1.55667900
H	4.35658800	1.80110200	1.00085200
C	5.05675600	-1.50844100	1.39047100
H	3.99965700	-3.10616000	0.39925200
H	5.90163900	0.29727400	2.22617200
H	5.73060700	-2.17255100	1.92925900
C	-0.56937700	2.75640100	-2.09033700
H	0.20399500	2.00926800	-2.31552800
H	-1.49628100	2.53096600	-2.62853300
H	-0.23047400	3.76306900	-2.35461200
C	-0.95959000	1.07682400	2.52411900
H	-1.30084000	0.08693300	2.22228300
H	0.05939900	1.00558500	2.91914200
H	-1.62445200	1.47733200	3.29548600
Pd	-0.37771900	-0.26145200	-0.66816400
C	-2.14001200	-0.95334300	0.07224400
C	-3.36707000	-0.28746100	-0.12163500
C	-2.18587300	-2.14042200	0.83338300
C	-4.56969700	-0.77219800	0.40706000
H	-3.39269000	0.63236400	-0.70393100
C	-3.38019400	-2.62220100	1.37882700
H	-1.27141800	-2.70943200	0.97440400
C	-4.58299900	-1.94135300	1.16952100
H	-5.49792300	-0.23028200	0.22417100
H	-3.37249400	-3.54333800	1.96151600
H	-5.51441000	-2.31945000	1.58823500
Cl	0.04797800	-2.43472300	-1.65257400
H	3.04255700	1.75771300	-1.42882000

1TS_c'

scf done: -1024.41364527

C	-1.15583100	-1.19927900	-0.82269700
N	-1.64953000	-1.04980400	-2.08672800
C	-2.34272400	-2.18611600	-2.47720000
C	-2.26751900	-3.05968900	-1.43976700
N	-1.53319200	-2.44827200	-0.44196600
H	-2.80963100	-2.26903700	-3.44639900
H	-2.66210800	-4.05716000	-1.32481500
O	1.38510300	-1.30591000	0.98202500
C	2.42131000	-1.60681500	0.12550600
H	2.08874200	-1.79884200	-0.91783100
C	3.53130000	-0.55211300	0.04987900
C	3.63077900	0.44394900	1.02733900
C	4.48853200	-0.57921900	-0.97401000
C	4.65710900	1.39119000	0.98126000
H	2.88541400	0.45421100	1.81705600
C	5.51663700	0.36333400	-1.02474900
H	4.42193100	-1.34688700	-1.74512100
C	5.60490000	1.35621900	-0.04416100
H	4.71607900	2.16016100	1.74918100
H	6.24548700	0.32965500	-1.83288700
H	6.40158700	2.09627500	-0.08297600
C	-1.23683800	-3.04775900	0.86956300
H	-0.17652800	-2.89020900	1.08043000
H	-1.82073800	-2.52677200	1.64699100
H	-1.47938600	-4.11314200	0.80848200
C	-1.50305200	0.13639000	-2.91756700
H	-2.27944100	0.87068900	-2.69006200
H	-0.53212100	0.58978000	-2.72188200
H	-1.56601000	-0.16374100	-3.96811700
Pd	-0.13149500	-0.01787400	0.38097800
C	-1.33949700	1.54331300	-0.00890500
C	-2.62397400	1.68049800	0.54784700
C	-0.81395500	2.62286600	-0.74404100
C	-3.34835700	2.86444300	0.37213200
H	-3.01299300	0.87554900	1.17128000
C	-1.53847800	3.81015300	-0.91145400
H	0.17671400	2.54644100	-1.19311900
C	-2.81523400	3.93099900	-0.35942700
H	-4.33608800	2.95757000	0.82214100
H	-1.10482000	4.63533700	-1.47587500
H	-3.38575200	4.84913800	-0.49142200

Cl	-2.39009100	-0.72741000	3.01014200
H	2.91752200	-2.55124000	0.44492600

1C2

scf done: -1009.38467777

C	1.30206500	-1.31307000	0.30635600
N	1.76702300	-1.26105000	1.58413900
C	2.48481600	-2.41020200	1.88512300
C	2.47144000	-3.18613400	0.77208500
N	1.73816500	-2.50427700	-0.18547300
H	2.92684200	-2.57024600	2.85615400
H	2.91398000	-4.15012900	0.57513700
O	-1.17435200	-1.37065300	-1.54634300
C	-2.28364300	-1.78496900	-0.81247700
H	-2.01195700	-2.50289600	-0.01208400
C	-3.08018600	-0.65103300	-0.17200800
C	-3.25912000	0.56042700	-0.85663400
C	-3.66420300	-0.79273500	1.09255900
C	-3.99698300	1.60126200	-0.28961600
H	-2.81747600	0.67296700	-1.84334500
C	-4.40663000	0.24427000	1.66326100
H	-3.53318700	-1.72603000	1.63797800
C	-4.57382000	1.44718400	0.97428800
H	-4.12875400	2.53148800	-0.83750600
H	-4.84884000	0.11507500	2.64848300
H	-5.14811200	2.25698000	1.41712000
C	1.46930800	-2.99508900	-1.54080400
H	0.47059300	-2.65158600	-1.83302800
H	2.22402400	-2.61679400	-2.23742500
H	1.50719200	-4.08712100	-1.52444700
C	1.47130100	-0.21657700	2.56076400
H	1.20971800	0.69595200	2.02826700
H	0.63855100	-0.52282500	3.20195600
H	2.35883400	-0.03986000	3.17382600
Pd	0.17345400	-0.07549600	-0.71552400
C	1.34716600	1.50623500	-0.30137200
C	2.73142000	1.60233400	-0.52688800
C	0.66392400	2.67131000	0.09819300
C	3.40230800	2.82146100	-0.38829500
H	3.29614700	0.72148700	-0.82500700
C	1.33324900	3.89252700	0.23771300
H	-0.40680400	2.63285700	0.29986700
C	2.70613900	3.97023900	-0.00433400
H	4.47202800	2.87427200	-0.58116400
H	0.78128100	4.77964900	0.54131800
H	3.22936700	4.91662700	0.10769700
H	-2.96511300	-2.33921000	-1.48695900

1TS_(E-F)'

scf done: -1010.24519028

Pd	-0.42850500	-0.59729100	-0.51285100
C	0.31327300	1.28842600	-0.32560500
N	1.42526500	1.79875000	-0.91888000
C	1.71382900	3.06090100	-0.44109800
C	0.74611800	3.38001700	0.45833700
N	-0.10410200	2.28668300	0.51748800
O	-1.60375200	-2.34132200	-0.84889800
C	-2.31413600	-1.31815600	-1.17439700
C	-3.44565200	-0.84483300	-0.32807500
C	-4.29373300	0.18092100	-0.77639800
C	-3.71345400	-1.44531500	0.91443100
C	-5.36513100	0.61390700	0.00407100
C	-4.78586300	-1.01527300	1.69162500
C	-5.61626200	0.01944100	1.24428000
H	2.58644200	3.60708500	-0.76424100
H	0.59421300	4.26698900	1.05463100
H	-4.09884300	0.64429400	-1.74205500
H	-3.06017700	-2.24741500	1.24405100
H	-6.00825000	1.41441600	-0.35612800
H	-4.97963100	-1.48840500	2.65216000
H	-6.45265900	0.35437200	1.85351500
C	2.31982400	1.03535200	-1.79431000
H	2.75302000	1.72429100	-2.52958000
H	3.08705900	0.54959400	-1.13595800
H	1.71405900	0.28448500	-2.30755300
C	-1.26411300	2.19428700	1.38455400
H	-1.96472500	3.01317400	1.18158100
H	-1.75366200	1.23956600	1.18761400
H	-0.96149400	2.23434700	2.43729700

O	3.74076100	-0.00178700	0.42570600
C	4.73785100	-0.88786200	0.64474700
C	4.55655000	-2.19885900	-0.18684900
H	5.34376600	-2.95411200	-0.02086700
H	3.58641000	-2.64735800	0.06295800
H	4.54133400	-1.95268600	-1.25748300
C	4.79870600	-1.28902500	2.15390600
H	5.61086200	-1.99300700	2.40314200
H	4.92589200	-0.38232000	2.76014600
H	3.84273900	-1.74584300	2.44103900
C	6.12525100	-0.27078900	0.26186700
H	6.12091400	-0.00408000	-0.80401200
H	6.27238300	0.65572500	0.83273500
H	6.98746300	-0.93416400	0.44611700
H	-2.39843500	-1.03556300	-2.23921500

1F'

scf done: -1010.27624892

Pd	0.36880000	-0.20112600	-0.35569800
C	0.49158400	1.79134900	-0.00622300
N	1.55459700	2.60574900	-0.29834500
C	1.32870100	3.91157600	0.10615900
C	0.10027900	3.93780300	0.68324400
N	-0.39554400	2.64276900	0.60760700
O	-0.45383600	-2.00628100	-1.06231400
C	-1.29887000	-1.03043000	-1.32473800
C	-2.59438400	-0.94524900	-0.60563000
C	-3.61165400	-0.06891600	-1.03405500
C	-2.86005000	-1.75841800	0.51519100
C	-4.82818100	0.01419600	-0.35863500
C	-4.07589300	-1.67486200	1.18897800
C	-5.07182800	-0.78653500	-0.76299200
H	2.05777800	4.69473600	-0.04047000
H	-0.44945000	4.74421200	1.14558900
H	-3.43111400	0.55577200	-1.90836800
H	-2.08420900	-2.45530700	0.82854000
H	-5.59535800	0.70246400	-0.71176300
H	-4.25522600	-2.31276500	2.05350900
H	-6.02167400	-0.72511000	1.29017700
C	2.77074600	2.13048600	-0.95479700
H	3.60634300	2.76696400	-0.64313600
H	2.93228700	1.09076600	-0.62751500
C	2.66342800	2.18761600	-2.04534200
C	-1.67620900	2.22411300	1.14989900
H	-2.49604800	2.78021500	0.68112200
H	-1.79395200	1.16143600	0.93863500
H	-1.70452500	2.38731900	2.23394400
O	2.41941100	-0.46624500	0.43365100
C	2.97915800	-1.73165200	0.50253900
C	3.11216900	-2.37033000	-0.90502900
H	3.58587900	-3.36466700	-0.88082600
H	2.11759200	-2.46433600	-1.35426200
H	3.71930300	-1.71806400	-1.54768100
C	2.12980800	-2.67299200	1.39544700
H	2.57507500	-3.67490900	1.50193700
H	2.02569000	-2.23228100	2.39547000
H	1.12917900	-2.77858100	0.96176500
C	4.39311200	-1.59700400	1.12813900
H	5.01502300	-0.94276100	0.50305600
H	4.31391500	-1.13479600	2.12020000
H	4.90885000	-2.56389700	1.23438200
H	-1.35249700	-0.65545100	-2.36326200

1TS_(F-A)'

scf done: -1010.25825770

Pd	-0.61107100	-0.35806000	0.05169000
C	0.93162000	-1.59668800	0.22284900
N	1.27700100	-2.67403800	-0.57038000
C	2.43830800	-3.29511300	-0.12686600
C	2.85295700	-2.60717400	0.96623100
N	1.93514000	-1.58585300	1.16966400
O	-0.85283800	1.42283700	-1.75582900
C	0.26846100	0.87691900	-1.50667100
C	1.36048300	1.65500800	-0.82296000
C	2.70330300	1.24856200	-0.88574100
C	1.05742900	2.85504400	-0.15759200
C	3.71033800	1.99621300	-0.27492500
C	2.06066100	3.60015000	0.45826800
C	3.39423200	3.17578300	0.40898600

H	2.85583500	-4.16349800	-0.61495400
H	3.70567800	-2.75769600	1.61191000
H	2.95125300	0.32974000	-1.41582600
H	0.01879900	3.17088700	-0.14052300
H	4.74591500	1.66410500	-0.33733900
H	1.80574300	4.52224400	0.97835100
H	4.17744000	3.76175700	0.88599900
C	0.49540200	-3.09705600	-1.71695200
H	0.25059800	-4.16378900	-1.64226100
H	-0.42345900	-2.50521300	-1.71172600
H	1.03709100	-2.91719000	-2.65386300
C	2.01317100	-0.59613100	2.23084100
H	2.76380200	0.16773500	2.00093600
H	1.03202500	-0.11963600	2.29737500
H	2.25972900	-1.08561000	3.18051600
O	-2.48225700	0.00479900	0.99970100
C	-3.68330400	0.30373300	0.39146900
C	-3.85300700	-0.42639900	-0.96839700
H	-4.82234900	-0.21610400	-1.44915700
H	-3.04897900	-0.11231600	-1.64324100
H	-3.77330200	-1.51065000	-0.81228800
C	-3.77842800	1.83330200	0.13902900
H	-4.72117100	2.13410900	-0.34637200
H	-3.69976400	2.36555800	1.09641300
H	-2.93770600	2.13481400	-0.49401700
C	-4.83855800	-0.12902500	1.33428500
H	-4.77806900	-1.20989500	1.51655200
H	-4.73229100	0.37885400	2.30126900
H	-5.83652700	0.10066700	0.92829200
H	0.67633200	0.11726100	-2.21087400

1TS (E-J)

scf done: -777.1450962

Pd	0.36261000	-0.08315300	-1.12456900
C	2.04960500	0.13983000	0.11784400
N	2.77830700	1.25345800	0.41931700
C	3.81541000	0.96326600	1.29301800
C	3.73869300	-0.36745500	1.55234800
N	2.66091400	-0.85171500	0.82801600
O	-1.23686200	-2.28040300	-0.53442600
C	-1.30104000	-1.07034900	-0.61771500
C	-2.42591500	-0.28510200	-0.00634700
C	-2.65814400	1.05735800	-0.32408000
C	-3.26108900	-0.93296900	0.91767200
C	-3.71157200	1.74820100	0.27489800
C	-4.30733500	-0.23991400	1.52154200
C	-4.53454400	1.10241800	1.20098900
H	4.50217100	1.71516600	1.65074000
H	4.34509500	-1.00007200	2.18252500
H	-2.01063000	1.54365500	-1.04868300
H	-3.07420300	-1.97844300	1.14208100
H	-3.89259300	2.78865900	0.01800300
H	-4.95025500	-0.74449600	2.23822100
H	-5.35389400	1.64194900	1.66936200
C	2.50104400	2.58036400	-0.11486000
H	3.29685800	2.89576100	-0.79761700
H	1.55492000	2.53147700	-0.65662200
H	2.41629700	3.30431200	0.70145000
C	2.23859000	-2.24991000	0.82243700
H	1.29367300	-2.32474400	0.28269100
H	2.99179900	-2.87063700	0.32674000
H	2.10101500	-2.59934200	1.85026400
H	-0.94220600	-0.32162800	-2.11136300

1J

scf done: -777.149374

Pd	-0.36990800	-0.25914600	-1.30094400
C	-1.93552700	0.24448300	0.07872100
N	-2.72633100	-0.62012200	0.77426000
C	-3.63799100	0.05287800	1.57158800
C	-3.41703900	1.37942600	1.38064100
N	-2.37655100	1.47516600	0.46902200
O	0.67051500	-2.13925400	0.42821000
C	0.96017000	-1.09496100	-0.11725000
C	2.23721200	-0.36823000	0.19819300
C	2.69892500	0.71230900	-0.56145400
C	2.97626800	-0.79743800	1.31359900
C	3.88527500	1.35761600	-0.21244200
C	4.15735100	-0.14811900	1.66355700

C	4.61397700	0.93142200	0.90068800
H	-4.34827000	-0.46146500	2.20079800
H	-3.89432300	2.24589600	1.81225900
H	2.12617100	1.01901000	-1.43171100
H	2.60775200	-1.64244700	1.88643700
H	4.244430100	2.19022000	-0.81170100
H	4.72510100	-0.48375000	2.52759600
H	5.53784000	1.43613000	1.17203600
C	-2.64239600	-2.07607600	0.66243400
H	-3.30247200	-2.43708200	-0.13251400
H	-1.61009700	-2.35358200	0.44330300
H	-2.94620500	-2.52241100	1.61306500
C	-1.81560000	2.73311600	-0.00686000
H	-0.94823200	2.49885700	-0.62617400
H	-2.55290200	3.28287400	-0.60110900
H	-1.50112200	3.35051200	0.84027900
H	0.75050100	-0.63189900	-2.40627000

1TS (J-K)

scf done: -777.11335

Pd	-0.04293800	-0.18191500	-0.18012300
C	-2.05289900	-0.12080400	-0.10229900
N	-2.92124600	-1.16247200	0.02272900
C	-4.23566200	-0.71901300	0.01407800
C	-4.19282100	0.62962000	-0.12451300
N	-2.85156000	0.98098300	-0.18454100
O	1.10998200	1.97946900	1.73307900
C	0.85126300	1.08197000	1.00507900
H	-5.07121900	-1.39432900	0.11314300
H	-4.98357700	1.36083300	-0.18837300
C	-2.52077000	-2.55626500	0.17313400
H	-1.57593300	-2.69293300	-0.35742800
H	-2.38845300	-2.80954000	1.22992500
H	-3.29232700	-3.19788900	-0.26055900
C	-2.36533900	2.34358600	-0.36518900
H	-1.43856400	2.46625300	-0.19662200
H	-2.17609900	2.55100500	-1.42307700
H	-3.11719400	3.04120200	0.01196900
C	2.16909900	0.21367200	0.20243700
C	2.85716700	0.84278800	-0.84405900
C	2.80254400	-0.81746100	0.91345400
C	4.15226200	0.45366900	-1.17843100
H	2.37909400	1.65678500	-1.39179500
C	4.09877500	-1.21263600	0.58040800
H	2.28230900	-1.30318500	1.73575300
C	4.77253000	-0.57705600	-0.46590000
H	4.67855200	0.94546000	-1.99266200
H	4.58360400	-2.01279200	1.13406000
H	5.78341200	-0.88212500	-0.72411700
H	-0.17555000	-1.33135600	-1.37893900

1K

scf done: -777.11335

Pd	-0.05266300	0.00261000	-0.00987300
C	2.05622600	0.05303300	-0.16823900
N	2.85584700	1.15309800	-0.19012900
C	4.18625700	0.80791700	-0.38941600
C	4.22283300	-0.54361800	-0.49791900
N	2.91320400	-0.98616100	-0.35966000
O	-0.59866300	-0.76287500	2.97799700
C	-0.33257400	-0.49754500	1.89629800
H	4.97415200	1.54369300	-0.44011600
H	5.04813900	-1.21864300	-0.66506500
C	2.37124000	2.51819900	-0.02657900
H	1.28962900	2.51128500	-0.16835100
H	2.60805300	2.89654600	0.97331600
H	2.83145400	3.16592700	-0.77814400
C	2.50463000	-2.38331300	-0.42598900
H	1.41480900	-2.41676500	-0.40229200
H	2.85875500	-2.83494500	-1.35753900
H	2.90751800	-2.94274900	0.42463300
C	-2.10948000	0.06365200	-0.27858400
C	-2.81647000	-1.05450600	-0.74809800
C	-2.84961900	1.21495000	0.03327000
C	-4.20751400	-1.02791600	-0.89415700
H	-2.28139400	-1.96442000	-1.01293200
C	-4.24077800	1.24880000	-0.11214700
H	-2.34186400	2.10731900	0.39494800
C	-4.92708700	0.12537700	-0.57616000

H	-4.72857300	-1.91044900	-1.26081600
H	-4.78772400	2.15610100	0.13778100
H	-6.00828400	0.14885300	-0.69054700
H	-0.10219000	0.42247000	-1.54986100

1TS_(K-L)

scf done: -777.1358

Pd	-0.07547400	-0.05010000	0.17686100
C	2.02989300	0.06971800	-0.22363100
N	2.81896600	1.18063800	-0.22991900
C	4.13068500	0.87487800	-0.57045300
C	4.17040800	-0.46339200	-0.78664500
N	2.88182500	-0.93589700	-0.57013400
H	4.90512100	1.62440800	-0.62939700
H	4.98569400	-1.11007100	-1.07328000
C	2.34132600	2.51989600	0.08500200
H	2.59447500	3.21099500	-0.72499400
H	1.25690500	2.47063300	0.19305000
H	2.78517800	2.87848000	1.01968800
C	2.48387400	-2.33021300	-0.70439800
H	2.69106100	-2.68913900	-1.71753200
H	3.02080100	-2.95381700	0.01792100
H	1.41191800	-2.39154900	-0.51205400
H	-0.68098100	0.36779700	-1.26960800
C	-2.09673900	0.10936100	-0.41727700
C	-2.80660700	-1.02552600	-0.84321800
C	-2.82739100	1.27996000	-0.15438700
C	-4.19944700	-1.00615400	-0.95427200
H	-2.26912000	-1.93792300	-1.09133800
C	-4.22022900	1.30179100	-0.26482000
H	-2.30682300	2.18743800	0.14303000
C	-4.91464600	0.15705700	-0.66177300
H	-4.72623000	-1.90250300	-1.27544200
H	-4.76340000	2.21839700	-0.04370000
H	-5.99775900	0.17481100	-0.75389200
C	-0.20566000	-0.58353300	2.09432600
O	-0.33167400	-0.87245100	3.19894800

1L

scf done: -544.9538597

C	-0.99575200	-0.00004900	0.00041900
N	-1.83750100	1.07366200	-0.00007900
C	-3.16681800	0.68033600	-0.00072700
C	-3.16774800	-0.67745400	-0.00069800
N	-1.83901100	-1.07257600	0.00002300
Pd	1.10804000	-0.00086300	0.00017900
C	-1.39169900	2.46163200	0.00046600
C	-1.39517800	-2.46120400	0.00041700
H	-3.98228800	1.38748500	-0.00110500
H	-3.98417900	-1.38350600	-0.00112000
H	-1.75679900	2.97738600	0.89432300
H	-0.30043300	2.46031300	-0.00029800
H	-1.75808200	2.97843500	-0.89225100
H	-1.76205200	-2.97675100	0.89363400
H	-1.76107800	-2.97699000	-0.89306600
H	-0.30392200	-2.46141800	0.00115600
C	2.98941600	-0.00023000	-0.00049800
O	4.14265400	0.00111800	-0.00067500