Supporting Information

Mechanism of Transition-Metal (Cu or Pd)-Catalyzed Synthesis of Benzimidazoles from Amidines: Theoretical Investigation

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Complete Reference for Ref (25):

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, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision C.01*, Gaussian, Inc., Wallingford, CT, 2010.

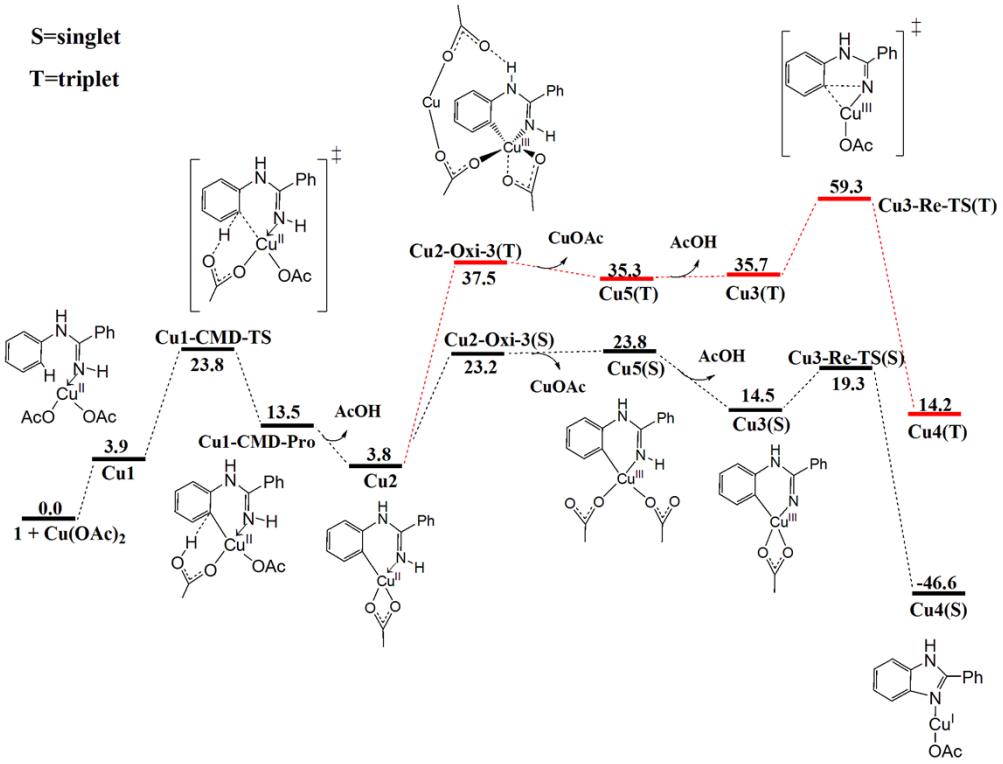

Figure S1. Calculated energy profiles calculated for Cu-CMD(II)-Oxi(III)1 pathway. Solvent-corrected free energies are given in kcal/mol.

Calculated imaginary frequencies of all transition states species

Cu1-CMD-TS	-1070.68
Cu2-Oxi-TS	-488.79
Cu3-Re-TS	-192.93
Cu1-Met-TS	-493.36
Cu1-Anag-TS	-1375.41
Cu7-FC-TS	-446.72
Cu9-Dep-TS	-1868.06
Cu7-CMD-TS	-1260.95
Cu8-CMD-TS	-281.55
Cu2-CN-TS	-550.41
Cu5-CN-TS	-259.84
Cu9-Cup-TS	-382.69
Cu1-Dep-TS	-672.31
Cu7-Dep-TS	-66.85
Pd1-Oxa-TS	-814.33
Pd1-Met-TS	-62.3
Pd1-Anag-TS	-1031.47
Pd2-Oxi-TS	-709.88
Pd6-Dep-TS	-862.07
Pd4-Re-TS	-336.02
Pd13-Cup-TS	-388.21
Pd13-Dep-TS	-620.72
Pd7-Oxi-TS	-782.65
Pd3-Oxi-TS	-561.85
Pd11-Oxi-TS	-736.98
Pd11-Met-TS	-75.84
Pd11-Anag-TS	-1045.63
Pd11-FC-TS	-342.92
Pd1-Dep-TS	-724.09
Pd2-CN-TS	-389.08
Pd6-CN-TS	-304.86
Cu3-Re-TS(T)	-535.74

Cartesian coordinates and electronic energies

1

E= -612.0025104au

H	-2.610518	1.929295	1.071983
C	-2.889339	0.994885	0.594780
C	-1.900831	0.228874	-0.047745
C	-4.212464	0.548497	0.644440
C	-0.491052	0.742919	-0.111938
C	-2.265300	-0.992138	-0.643941
C	-4.567297	-0.667921	0.047754
H	-4.963560	1.144221	1.153142
N	0.460279	-0.243063	0.108354
N	-0.167149	1.968884	-0.345784
C	-3.591392	-1.435125	-0.598348
H	-1.518344	-1.578356	-1.170677
H	-5.595366	-1.013442	0.085135
C	1.869641	-0.169756	0.077863
H	0.091127	-1.119549	0.443994
H	-3.862794	-2.372457	-1.073517
C	2.574011	-1.347139	0.406306
C	2.590181	0.988581	-0.269228
C	3.967161	-1.372060	0.386452
H	2.021106	-2.244425	0.675355
C	3.988695	0.945109	-0.287489
H	2.046487	1.892804	-0.506355
C	4.686704	-0.222631	0.036790
H	4.489469	-2.288526	0.643089
H	4.535444	1.844338	-0.556841
H	5.771542	-0.238669	0.020373
H	-1.008804	2.511459	-0.537844

AcOH

E= -229.0482842au

O	-0.794184	-1.044612	0.000011
C	-0.088082	0.129861	-0.000009
O	-0.631863	1.214509	0.000005
C	1.396905	-0.124120	0.000001
H	1.929649	0.826410	0.000360
H	1.680362	-0.708173	0.881783
H	1.680470	-0.707536	-0.882156
H	-1.735042	-0.804326	-0.000064

2

E= -610.8145567au

C	1.792334	-0.704787	0.002909
C	1.859162	0.714907	-0.002418
C	3.072148	1.412350	-0.005532
C	4.238872	0.646376	-0.003079
C	4.193101	-0.766720	0.002374
C	2.981017	-1.455842	0.005445
C	-0.254640	-0.025114	0.000776
H	3.112491	2.496632	-0.009617
H	5.202114	1.146119	-0.005353
H	5.125099	-1.322830	0.004179
H	2.942495	-2.539725	0.009602
N	0.476874	-1.128262	0.004720
N	0.533695	1.119205	-0.003272
C	-1.720785	0.002789	0.000557
C	-2.420111	-1.220290	-0.006045
C	-2.454219	1.204104	0.006860
C	-3.814590	-1.236950	-0.006745
H	-1.848504	-2.140875	-0.010561
C	-3.851375	1.183323	0.005974
H	-1.947663	2.164996	0.013782
C	-4.537294	-0.036266	-0.000931
H	-4.340039	-2.186544	-0.011959
H	-4.402509	2.118274	0.011043
H	-5.622379	-0.051205	-0.001581
H	0.203193	2.071280	-0.010534

H_2O

E= -76.4178778au

O	0.000000	0.000000	0.118537

H	0.000000	−0.759405	−0.474150
H	0.000000	0.759405	−0.474150

CuOAc

E= -424.6037512au

Cu	−1.310695	−0.002365	0.000820
O	0.447890	−1.110490	−0.002054
C	1.074276	0.007363	−0.002927
O	0.447128	1.122120	−0.001923
C	2.587245	−0.001194	0.001428
H	2.978814	1.014095	−0.057987
H	2.947296	−0.481885	0.917354
H	2.954778	−0.593681	−0.842326

$CuOAc_2$

E= -653.0878094au

Cu	−0.000015	0.000818	−0.006491
O	1.686596	−1.091118	−0.005147
O	−1.687952	1.093969	−0.008425
C	2.359679	0.003120	−0.004100
O	1.687877	1.096477	−0.004197
C	−2.359721	−0.000040	−0.008707
O	−1.686602	−1.093639	−0.007929
C	−3.855706	−0.002069	0.020570
H	−4.198421	−0.070691	1.060310
H	−4.245809	0.922514	−0.408426
H	−4.243661	−0.868639	−0.518955
C	3.855787	−0.002121	0.018173
H	4.238307	−0.738875	−0.693411
H	4.245433	0.989101	−0.216364
H	4.204993	−0.295978	1.015045

CuOAc·AcOH

E= -653.7183503au

Cu	0.082102	−1.149604	−0.000024
O	1.927762	−0.775381	−0.000233
O	−1.381266	1.466375	0.000382
C	2.099168	0.507387	−0.000378
O	1.166083	1.359333	−0.000440
C	−2.173264	0.426054	0.000483
O	−1.794622	−0.773957	0.000369
C	3.536805	0.983520	0.000242
H	4.052687	0.595912	0.885094
H	4.057344	0.585372	−0.877062
H	3.580766	2.072700	−0.005755
C	−3.639726	0.754939	−0.000227
H	−3.882480	1.366428	0.874902
H	−3.885011	1.348514	−0.887094
H	−4.231441	−0.159528	0.009259
H	−0.354368	1.286768	0.000003

Cu1

E= -1265.1116893au

C	−1.136804	−1.368041	−1.691487
C	−0.520519	−2.123146	−0.678036
C	−1.191919	−3.224061	−0.124417
C	−2.471739	−3.562872	−0.568461
C	−3.098703	−2.800360	−1.560349
C	−2.425190	−1.706438	−2.117476
C	1.418864	−0.631324	−0.092553
H	−0.718624	−3.799219	0.665942
H	−2.980586	−4.416283	−0.132096
H	−4.097304	−3.056426	−1.897774
H	−2.897787	−1.113562	−2.894028
N	0.764499	0.486832	−0.157384
N	0.806829	−1.853473	−0.243676
C	2.892680	−0.683314	0.136010
C	3.502605	0.294624	0.942858
C	3.685845	−1.687908	−0.448780
C	4.880656	0.261830	1.165713
H	2.895456	1.068733	1.399972
C	5.064952	−1.716389	−0.223336
H	3.231656	−2.420853	−1.107953
C	5.664140	−0.744099	0.586108
H	5.341246	1.017581	1.792808
H	5.670915	−2.487521	−0.687506
H	6.734966	−0.766862	0.760101
H	−0.611264	−0.535683	−2.146005

Cu	-1.097939	1.043000	0.257005
O	-3.027228	1.151963	0.954835
C	-2.773439	0.170319	1.731682
O	-1.589426	-0.327165	1.702177
C	-3.822404	-0.401845	2.641570
H	-4.722490	0.213777	2.623271
H	-4.070501	-1.418757	2.317334
H	-3.435241	-0.468471	3.663046
H	1.317640	1.352127	-0.173167
H	1.303303	-2.636972	0.157479
O	-1.074468	2.662322	-0.776886
C	-0.037145	3.461224	-0.825496
O	1.081279	3.227937	-0.332642
C	-0.310343	4.765721	-1.562345
H	0.589275	5.382861	-1.578986
H	-0.635888	4.553828	-2.586445
H	-1.124329	5.307219	-1.068839

Cu1-CMD-TS

E= -1265.0765168au

C	-1.024878	1.495025	0.374515
C	0.115022	2.149792	-0.149821
C	0.055272	3.476200	-0.612401
C	-1.155278	4.168188	-0.577577
C	-2.310189	3.541387	-0.089686
C	-2.234571	2.225837	0.373488
C	1.649126	0.182992	-0.367466
H	0.946484	3.957132	-1.008782
H	-1.198071	5.191224	-0.937706
H	-3.253501	4.077389	-0.069534
H	-3.127751	1.740961	0.756178
N	0.704264	-0.696244	-0.523036
N	1.385772	1.513141	-0.189255
C	3.096472	-0.179570	-0.395587
C	3.565074	-1.116934	-1.333264
C	3.998467	0.396560	0.517338
C	4.916798	-1.468613	-1.359262
H	2.876451	-1.548806	-2.052793
C	5.349397	0.037390	0.490195
H	3.636816	1.091508	1.268726
C	5.811260	-0.892640	-0.448434
H	5.272038	-2.185342	-2.092025
H	6.036484	0.474847	1.206844
H	6.860234	-1.169093	-0.468650
H	-0.826040	0.724023	1.438821
Cu	-1.273248	-0.533932	-0.325011
O	-3.258366	-0.558412	-0.745710
C	-3.095092	-1.617129	-1.454365
O	-1.909193	-2.058893	-1.619701
C	-4.281964	-2.331842	-2.038042
H	-4.700553	-3.010850	-1.285185
H	-5.059417	-1.615723	-2.314805
H	-3.981911	-2.922600	-2.905837
H	1.046666	-1.650285	-0.573114
H	2.178553	2.125703	-0.322887
O	-1.336433	-1.679352	1.553385
C	-0.965575	-1.065390	2.587039
O	-0.617556	0.180897	2.608235
C	-0.930592	-1.788571	3.921743
H	-1.005222	-2.866682	3.770489
H	-0.012852	-1.542168	4.463735
H	-1.774577	-1.455494	4.537726

Cu1-CMD-Pro

E= -1265.0959844au

C	-0.885038	1.410512	-0.633627
C	0.358477	2.065282	-0.513768
C	0.466544	3.467801	-0.606030
C	-0.670878	4.242247	-0.827495
C	-1.918526	3.621553	-0.963639
C	-2.010732	2.226360	-0.870453
C	1.827528	0.025361	-0.298065
H	1.438918	3.947511	-0.508448
H	-0.581856	5.321821	-0.896764
H	-2.807915	4.217711	-1.144203
H	-2.979143	1.746338	-0.988750
N	0.892585	-0.862338	-0.483117
N	1.581424	1.365700	-0.300299

C	3.255294	-0.356754	-0.071740
C	3.826932	-1.395320	-0.827825
C	4.034343	0.297473	0.899820
C	5.156843	-1.768900	-0.618456
H	3.235924	-1.890483	-1.591830
C	5.363664	-0.082057	1.108892
H	3.591402	1.074792	1.515040
C	5.927999	-1.113377	0.349396
H	5.591907	-2.564858	-1.213552
H	5.953132	0.419091	1.869575
H	6.960016	-1.406196	0.511981
H	-1.790139	1.173635	1.381514
Cu	-1.067041	-0.565962	-0.644363
O	-3.097484	-0.836477	-0.976631
C	-2.871894	-2.085657	-1.161413
O	-1.671894	-2.515699	-1.106560
C	-4.019627	-3.032509	-1.402969
H	-4.431454	-3.356343	-0.439091
H	-4.816571	-2.532808	-1.958795
H	-3.675790	-3.917097	-1.942905
H	1.217883	-1.818313	-0.379602
H	2.407493	1.947293	-0.284429
O	-1.501169	-1.105287	1.856098
C	-2.006226	-0.278640	2.602492
O	-2.134973	1.028549	2.289326
C	-2.557955	-0.588923	3.971014
H	-2.374503	-1.635398	4.213565
H	-2.094378	0.057633	4.722813
H	-3.635112	-0.390390	3.989667

Cu2

E= -1036.038946au

C	1.313995	1.357781	-0.038329
C	0.079357	2.028629	-0.093346
C	-1.432834	0.015957	-0.017697
H	3.442928	1.653078	-0.002879
C	2.477105	2.149411	-0.043960
C	0.007781	3.435991	-0.157307
C	1.177766	4.190966	-0.163425
C	2.421261	3.546732	-0.105339
H	-0.960633	3.931686	-0.200334
H	1.120336	5.273843	-0.212450
H	3.336972	4.130607	-0.109891
N	-1.172151	1.345472	-0.091270
N	-0.488674	-0.886440	0.031437
Cu	1.468583	-0.599073	0.026895
C	-2.881118	-0.354042	-0.001853
C	-3.328182	-1.453333	-0.756243
C	-3.805173	0.372385	0.771033
C	-4.677444	-1.815664	-0.741200
H	-2.623269	-2.005028	-1.370183
C	-5.153884	0.004349	0.786131
H	-3.464389	1.199463	1.386552
C	-5.592963	-1.088076	0.029172
H	-5.014502	-2.659041	-1.334563
H	-5.857108	0.562519	1.395299
H	-6.640068	-1.371974	0.041012
H	-1.982316	1.930799	-0.233974
O	3.511638	-0.945431	0.051350
C	3.274795	-2.204462	0.096850
O	2.062322	-2.607131	0.104536
C	4.418400	-3.183996	0.157913
H	5.157495	-2.945021	-0.612683
H	4.920834	-3.101225	1.128723
H	4.056982	-4.204940	0.027285
H	-0.841254	-1.830153	0.155460

Cu2-Oxi-1

E= -1689.1263076au

C	-1.633973	1.788713	0.351193
C	-0.344349	2.072494	0.806354
C	0.335316	-0.226398	1.116849
H	-3.508224	2.540760	-0.423667
C	-2.510591	2.785695	-0.081095
C	0.066305	3.426629	0.834121
C	-0.793662	4.430310	0.402262
C	-2.080046	4.118985	-0.056644
H	1.069033	3.654690	1.176945

H	-0.459044	5.462024	0.422140
H	-2.751152	4.900619	-0.396621
N	0.561468	1.100631	1.252166
N	-0.797242	-0.706288	0.652727
Cu	-2.437132	0.049551	0.344284
C	1.388998	-1.190231	1.560382
C	0.991251	-2.491769	1.928616
C	2.750254	-0.835283	1.650616
C	1.935835	-3.421971	2.364177
H	-0.054757	-2.767154	1.882059
C	3.687654	-1.774253	2.089387
H	3.088652	0.155773	1.369492
C	3.287401	-3.067366	2.444504
H	1.614471	-4.419025	2.645735
H	4.733366	-1.491544	2.149410
H	4.021211	-3.790539	2.785681
H	1.547651	1.425591	1.290700
O	-4.301946	0.509544	0.027821
C	-4.649889	-0.743763	0.041627
O	-3.725771	-1.591072	0.228407
C	-6.083870	-1.127706	-0.149385
H	-6.687404	-0.727775	0.672959
H	-6.466792	-0.691113	-1.077428
H	-6.183638	-2.213105	-0.181174
H	-0.695354	-1.627636	0.017195
O	1.043836	-1.709531	-2.207613
C	0.234468	-2.653024	-1.902469
O	-0.531838	-2.702530	-0.894585
C	0.202690	-3.826141	-2.868701
H	-0.037156	-3.467629	-3.875204
H	1.194834	-4.288121	-2.916431
H	-0.533795	-4.565485	-2.552877
Cu	1.890756	-0.140223	-1.638844
O	2.928370	1.402685	-1.465653
C	3.335696	2.206803	-0.543474
O	3.006585	2.181633	0.671999
C	4.312493	3.272927	-1.021735
H	4.604207	3.924212	-0.196749
H	5.201580	2.795067	-1.447373
H	3.851874	3.865749	-1.819288

Cu2-Oxi-TS

E= -1689.1298254au

C	1.592756	1.799488	-0.362633
C	0.297719	2.061193	-0.816893
C	-0.325589	-0.253203	-1.102175
H	3.455115	2.591238	0.400232
C	2.452524	2.816980	0.058668
C	-0.134753	3.408014	-0.858749
C	0.710059	4.429671	-0.439005
C	2.001738	4.143008	0.021471
H	-1.140802	3.617462	-1.203575
H	0.359639	5.455948	-0.470021
H	2.661363	4.938983	0.350658
N	-0.590228	1.068073	-1.248008
N	0.806259	-0.712045	-0.624902
Cu	2.430878	0.078549	-0.341378
C	-1.355928	-1.246714	-1.544335
C	-0.922009	-2.536208	-1.913416
C	-2.727259	-0.932986	-1.626721
C	-1.840893	-3.495238	-2.342085
H	0.133153	-2.776499	-1.873827
C	-3.639343	-1.900363	-2.058537
H	-3.092069	0.049804	-1.349637
C	-3.203133	-3.181560	-2.414211
H	-1.491505	-4.482296	-2.625903
H	-4.693253	-1.648564	-2.113783
H	-3.917096	-3.926651	-2.750364
H	-1.583313	1.371026	-1.292348
O	4.297246	0.569308	-0.038270
C	4.663523	-0.677455	-0.036050
O	3.755010	-1.545407	-0.203228
C	6.107237	-1.034324	0.144139
H	6.682225	-0.695497	-0.725240
H	6.512761	-0.523762	1.023020
H	6.219833	-2.113505	0.253497
H	0.712028	-1.667401	0.101853
O	-1.000149	-1.667350	2.202208

C	-0.171240	-2.593657	1.933877
O	0.620717	-2.643045	0.933239
C	-0.120928	-3.759351	2.902620
H	0.676344	-4.452031	2.632917
H	0.033817	-3.386408	3.919931
H	-1.083097	-4.283488	2.891015
Cu	-1.902694	-0.120595	1.633937
O	-2.984848	1.388053	1.458909
C	-3.396576	2.159385	0.509194
O	-3.056694	2.101685	-0.701161
C	-4.391210	3.224846	0.949179
H	-4.696159	3.838522	0.100538
H	-5.270283	2.748487	1.396454
H	-3.938674	3.856656	1.721125

Cu2-Oxi-2

E= -1689.1290626au

C	1.534184	1.825403	-0.429521
C	0.208864	2.027794	-0.828059
C	-0.253439	-0.324514	-1.137482
H	3.380284	2.725286	0.243731
C	2.353527	2.896947	-0.055673
C	-0.299619	3.347723	-0.853756
C	0.509474	4.414893	-0.478912
C	1.834936	4.197785	-0.079386
H	-1.328508	3.503620	-1.157704
H	0.105535	5.421801	-0.499256
H	2.467057	5.030046	0.212487
N	-0.633020	0.982733	-1.221148
N	0.908523	-0.733449	-0.719083
Cu	2.460482	0.150891	-0.385935
C	-1.238148	-1.376187	-1.570589
C	-0.736546	-2.635871	-1.954694
C	-2.627779	-1.150316	-1.608553
C	-1.605522	-3.651589	-2.356575
H	0.334190	-2.801477	-1.947950
C	-3.490977	-2.174785	-2.012733
H	-3.049018	-0.191214	-1.327085
C	-2.987202	-3.425700	-2.384451
H	-1.203440	-4.613968	-2.656020
H	-4.559762	-1.988693	-2.036449
H	-3.662939	-4.214217	-2.700023
H	-1.634942	1.219295	-1.281974
O	4.310652	0.716476	-0.020803
C	4.729222	-0.510013	0.027302
O	3.876655	-1.430963	-0.143724
C	6.185486	-0.789338	0.263652
H	6.770671	-0.444641	-0.596606
H	6.536649	-0.235322	1.139667
H	6.349472	-1.858093	0.406317
H	0.824928	-1.860622	0.399994
O	-0.881803	-1.507627	2.178283
C	-0.056222	-2.439237	2.091085
O	0.817720	-2.595981	1.128900
C	0.004014	-3.510643	3.148155
H	-0.720894	-3.306417	3.935456
H	-0.205102	-4.485864	2.695709
H	1.012821	-3.559517	3.570018
Cu	-1.977440	-0.061363	1.615972
O	-3.225585	1.304627	1.455021
C	-3.637410	2.000628	0.441088
O	-3.228205	1.901003	-0.739448
C	-4.719651	3.015733	0.780300
H	-5.043188	3.543513	-0.117710
H	-5.573625	2.508756	1.241753
H	-4.335551	3.733869	1.513150

Cu3

E= -1035.3977942au

C	1.254357	1.273839	-0.023878
C	0.108067	2.077267	-0.082087
C	-1.398879	0.162399	0.002703
H	3.410041	1.233920	0.018362
C	2.526736	1.859555	-0.029172
C	0.246671	3.480170	-0.160377
C	1.512498	4.058202	-0.174533
C	2.655969	3.252386	-0.106783
H	-0.642464	4.103383	-0.203180

H	1.607189	5.137543	-0.235230
H	3.644702	3.699146	-0.116947
N	-1.172913	1.524344	-0.058977
N	-0.496380	-0.744953	0.068148
Cu	1.312052	-0.648304	0.051098
C	-2.840679	-0.251745	0.002950
C	-3.205486	-1.470297	-0.594326
C	-3.828593	0.544292	0.609491
C	-4.542105	-1.874639	-0.602489
H	-2.434530	-2.084786	-1.044355
C	-5.165874	0.134693	0.599005
H	-3.554438	1.461104	1.122824
C	-5.526101	-1.072352	-0.010456
H	-4.816168	-2.814260	-1.070778
H	-5.920932	0.751523	1.075549
H	-6.564087	-1.388879	-0.018023
H	-1.959371	2.123680	-0.260412
O	3.257248	-0.968059	0.091824
C	3.110035	-2.257305	0.079298
O	1.934993	-2.720774	0.047277
C	4.328132	-3.137896	0.109400
H	4.998123	-2.876735	-0.716261
H	4.880637	-2.974021	1.041246
H	4.040415	-4.187291	0.035872

Cu3-Re-TS

E= -1035.386265au

Cu	-1.310742	-0.628612	-0.189654
H	2.109177	-2.226728	-0.211014
C	2.965345	-1.565956	-0.137771
C	2.748462	-0.181127	-0.028536
C	4.266253	-2.073443	-0.144617
C	1.350849	0.336062	-0.022010
C	3.852214	0.686501	0.060221
C	5.362140	-1.206900	-0.043722
H	4.424679	-3.143744	-0.224557
N	1.096799	1.508686	0.661040
N	0.422598	-0.269011	-0.689881
C	5.152480	0.173500	0.055601
H	3.704890	1.762038	0.092525
H	6.372170	-1.603689	-0.047298
C	-0.135699	2.099274	0.400115
H	1.812380	1.970631	1.202440
H	5.998562	0.850167	0.117462
C	-0.437029	3.437768	0.712692
C	-1.053012	1.311385	-0.307974
C	-1.628307	3.989710	0.247042
H	0.269336	4.038218	1.278075
C	-2.224611	1.886456	-0.823092
C	-2.509391	3.227015	-0.535565
H	-1.864025	5.023657	0.475871
H	-2.935631	1.292213	-1.386050
H	-3.430204	3.666653	-0.904140
O	-1.755452	-2.727348	0.222251
C	-2.959328	-2.335773	0.256838
O	-3.225010	-1.084894	0.063105
C	-4.096164	-3.290026	0.521511
H	-4.809758	-3.256960	-0.308650
H	-3.722131	-4.306865	0.645836
H	-4.635211	-2.982312	1.424125

Cu4

E= -1035.490846au

C	-2.184173	-0.650491	-0.023693
C	-3.042505	0.452099	0.186255
C	-0.904154	1.131305	0.029988
H	-2.056518	-2.802049	-0.268868
C	-2.707598	-1.949921	-0.105424
C	-4.426459	0.307665	0.327918
C	-4.934034	-0.989279	0.249161
C	-4.086844	-2.100012	0.034537
H	-5.077825	1.159037	0.491245
H	-6.001625	-1.149042	0.354112
H	-4.522557	-3.091677	-0.021635
N	-2.200590	1.556777	0.203986
N	-0.870189	-0.198331	-0.118738
Cu	0.669144	-1.328183	-0.370276
C	0.226250	2.064272	0.006406

C	1.512277	1.657097	0.411715
C	0.025389	3.393879	-0.421811
C	2.571678	2.568309	0.382580
H	1.709166	0.645485	0.757341
C	1.087816	4.298198	-0.439796
H	-0.949137	3.711438	-0.782387
C	2.365189	3.887326	-0.036715
H	3.555250	2.234790	0.694172
H	0.923523	5.315287	-0.780225
H	3.192105	4.589783	-0.055133
H	-2.457955	2.503150	0.437828
O	2.147991	-2.441769	-0.578519
C	3.125569	-2.092091	0.219979
O	3.078647	-1.132330	1.010893
C	4.366253	-2.967928	0.115169
H	4.109656	-4.005912	0.354027
H	4.744023	-2.957221	-0.913081
H	5.141139	-2.614670	0.797257

Cu2-Oxi-3

E= -1689.1425048au

C	-1.205158	-1.015217	1.395196
C	0.166096	-0.987522	1.642517
C	0.498086	1.281717	0.912755
H	-3.114384	-1.956239	1.750296
C	-2.047319	-1.975119	1.943431
C	0.734535	-2.043762	2.387443
C	-0.086045	-3.043470	2.907124
C	-1.473250	-3.004409	2.706999
H	1.804955	-2.042983	2.562811
H	0.355085	-3.848233	3.485469
H	-2.109414	-3.781184	3.118488
N	0.993009	0.064313	1.201312
N	-0.805935	1.492155	0.949789
Cu	-2.023417	0.249780	0.192336
C	1.452879	2.369754	0.578867
C	1.070689	3.371338	-0.334083
C	2.733225	2.411674	1.161006
C	1.954274	4.405025	-0.651162
H	0.102193	3.319424	-0.822307
C	3.611052	3.449506	0.839855
H	3.039527	1.641880	1.859246
C	3.223826	4.448298	-0.061920
H	1.656937	5.167145	-1.363448
H	4.595438	3.478134	1.294389
H	3.909541	5.252239	-0.308677
H	1.988224	-0.179618	0.977751
O	-4.265212	0.868657	0.717921
C	-4.065326	1.634152	-0.252857
O	-2.895196	1.678356	-0.835505
C	-5.147794	2.525116	-0.817313
H	-5.451164	2.151715	-1.802317
H	-6.014013	2.533004	-0.153940
H	-4.770727	3.543053	-0.956069
H	-1.107979	2.436884	0.737225
O	3.135742	-1.738180	-1.419291
C	3.871344	-1.424769	-0.399994
O	3.487835	-0.822653	0.632805
C	5.327973	-1.845624	-0.519983
H	5.877645	-1.585426	0.385418
H	5.390234	-2.924483	-0.696539
H	5.784414	-1.349737	-1.383680
Cu	1.312233	-1.400259	-1.600031
O	-0.521488	-0.986333	-1.677496
C	-1.651789	-1.583467	-1.720559
O	-2.615263	-1.228656	-0.964800
C	-1.879610	-2.726607	-2.681905
H	-1.578217	-2.426481	-3.690248
H	-1.254881	-3.578507	-2.388861
H	-2.926064	-3.031180	-2.681148

Cu5

E= -1264.4521052au

C	0.819740	1.726537	-0.368511
C	-0.398509	2.334346	-0.032413
C	-0.487771	3.740211	0.035865
C	0.617666	4.530297	-0.262883
C	1.820288	3.924535	-0.644140

C	1.918388	2.528133	-0.692825
C	-1.810050	0.316853	-0.104208
H	-1.435144	4.201677	0.303831
H	0.538486	5.610808	-0.207932
H	2.686931	4.531225	-0.885720
H	2.860842	2.058057	-0.945292
N	-0.845096	-0.411764	-0.589022
N	-1.587230	1.609184	0.228050
C	-3.182868	-0.216659	0.102726
C	-3.350691	-1.521690	0.599322
C	-4.313714	0.563470	-0.199712
C	-4.634811	-2.035748	0.794380
H	-2.479826	-2.115950	0.857325
C	-5.595717	0.042668	-0.005193
H	-4.193195	1.556927	-0.621122
C	-5.758087	-1.255718	0.493154
H	-4.757800	-3.038966	1.187670
H	-6.464331	0.644011	-0.251380
H	-6.754297	-1.657751	0.644363
Cu	1.028998	-0.216741	-0.433449
O	2.863779	-0.056580	-0.152649
C	3.045018	-0.136727	1.162534
O	2.120832	-0.054260	1.972592
C	4.488226	-0.369738	1.558154
H	4.700475	-1.433496	1.406901
H	5.172008	0.210995	0.933873
H	4.625824	-0.119385	2.611373
H	-1.062453	-1.365276	-0.863901
H	-2.339667	2.103895	0.685555
O	2.626011	-2.941155	0.498332
C	1.885074	-3.011412	-0.475353
O	1.045946	-2.074365	-0.894915
C	1.833730	-4.259331	-1.359678
H	2.209317	-4.016658	-2.360265
H	2.447955	-5.047189	-0.920303
H	0.802187	-4.608659	-1.472360

Cu1-Met-TS

E= -1265.0684052au

C	-1.244475	1.462702	0.263920
C	-0.106485	2.154421	-0.214373
C	-0.180929	3.515562	-0.558603
C	-1.397372	4.190570	-0.461322
C	-2.550250	3.516905	-0.030277
C	-2.466381	2.169694	0.323922
C	1.415848	0.213186	-0.592703
H	0.704223	4.033161	-0.918260
H	-1.448831	5.240343	-0.732008
H	-3.496028	4.044432	0.035463
H	-3.348200	1.643392	0.676134
N	0.476927	-0.652295	-0.868876
N	1.152884	1.521904	-0.339410
C	2.862974	-0.152379	-0.622837
C	3.409431	-0.745442	-1.774240
C	3.672102	0.080252	0.504064
C	4.764478	-1.086691	-1.806299
H	2.781108	-0.919173	-2.642658
C	5.025866	-0.269572	0.462721
H	3.216339	0.461628	1.411860
C	5.574480	-0.845685	-0.689527
H	5.186615	-1.535030	-2.699663
H	5.647639	-0.105086	1.336606
H	6.625929	-1.113378	-0.715210
H	-1.068086	0.577154	1.140067
Cu	-1.439772	-0.553762	-0.468307
O	-3.435698	-0.809574	-0.448628
C	-3.281850	-2.017343	-0.859413
O	-2.091785	-2.419339	-1.101001
C	-4.463504	-2.929104	-1.015430
H	-4.736501	-3.337723	-0.034919
H	-5.323707	-2.372530	-1.395576
H	-4.221441	-3.758208	-1.682490
H	0.842626	-1.586621	-1.021792
H	1.966633	2.110799	-0.228771
O	-0.991279	-0.488160	2.042908
C	0.184726	-0.604655	2.612606
O	1.154842	0.137382	2.390458

C	0.286646	-1.758569	3.606881
H	1.282675	-1.787163	4.052629
H	-0.467524	-1.641163	4.392465
H	0.080766	-2.708574	3.100602

Cu1-Anag-Im

E= -1265.0953538au

Cu	1.029891	-0.656951	-0.654994
O	0.568003	-1.730767	1.861975
C	0.816195	-2.679688	1.104069
O	0.990096	-2.560974	-0.193097
C	0.970088	-4.102500	1.621345
H	0.480483	-4.815823	0.952663
H	2.036151	-4.355703	1.653660
H	0.556108	-4.177935	2.628397
H	-3.204424	-0.928166	-2.114333
C	-3.841008	-0.587933	-1.303571
C	-3.285093	0.147377	-0.241254
C	-5.212124	-0.852861	-1.332866
C	-1.818122	0.420190	-0.214408
C	-4.120880	0.610544	0.791291
C	-6.039863	-0.390042	-0.302252
H	-5.634332	-1.412821	-2.160428
N	-1.469791	1.669152	0.211422
N	-0.942062	-0.471772	-0.586093
C	-5.491883	0.339207	0.759410
H	-3.693477	1.144874	1.633787
H	-7.104222	-0.598993	-0.325517
C	-0.152008	2.188891	0.399665
H	-2.217331	2.349450	0.204162
H	-6.127685	0.686396	1.566897
C	0.131021	3.472676	-0.093538
C	0.821110	1.468641	1.114594
C	1.389893	4.037020	0.122079
H	-0.627298	4.018045	-0.648267
C	2.089278	2.038251	1.300998
C	2.373831	3.317438	0.811810
H	1.604263	5.030413	-0.258234
H	2.848040	1.459237	1.812980
H	3.355991	3.751412	0.965934
H	0.593755	0.495847	1.548756
O	2.695535	-0.420916	-1.435682
C	3.794059	-0.427895	-0.695810
C	5.070575	-0.302394	-1.513684
O	3.797790	-0.530743	0.530845
H	5.932811	-0.216035	-0.850552
H	5.186477	-1.185424	-2.152031
H	5.015466	0.570593	-2.172416
H	-1.366458	-1.379781	-0.747521

Cu1-Anag-TS

E= -1265.0629691au

Cu	1.003051	-0.509859	-0.736041
O	0.834434	-0.710818	2.188487
C	1.108274	-1.897254	1.747975
O	1.113977	-2.223489	0.527969
C	1.466715	-2.931908	2.792005
H	1.246873	-3.936103	2.423984
H	2.543286	-2.865831	2.991883
H	0.935898	-2.738527	3.727025
H	-3.272131	-1.145758	-2.229105
C	-3.887728	-0.856440	-1.383137
C	-3.319359	-0.123939	-0.325459
C	-5.245937	-1.181904	-1.362228
C	-1.865863	0.211747	-0.353836
C	-4.129277	0.273541	0.754142
C	-6.048097	-0.783320	-0.285567
H	-5.678678	-1.738404	-2.186702
N	-1.547560	1.465252	0.070869
N	-0.964423	-0.634164	-0.775144
C	-5.487297	-0.057901	0.772048
H	-3.690451	0.804059	1.593486
H	-7.102374	-1.038853	-0.270175
C	-0.262833	2.057427	0.225633
H	-2.331517	2.097446	0.159980
H	-6.102367	0.239770	1.614610
C	-0.221329	3.463237	0.182385
C	0.899411	1.284755	0.467666

C	0.991877	4.125134	0.364051
H	-1.129477	4.031655	-0.005697
C	2.112721	1.996519	0.624965
C	2.166331	3.391281	0.585173
H	1.021219	5.209601	0.327567
H	3.014310	1.415915	0.797291
H	3.110588	3.907241	0.726615
H	0.826631	0.175538	1.286883
O	2.659764	-0.539997	-1.583969
C	3.809796	-0.740663	-0.963357
C	4.936154	-1.141825	-1.906056
O	3.978526	-0.611595	0.249826
H	5.872462	-1.224311	-1.351798
H	4.702138	-2.103483	-2.376306
H	5.040247	-0.402688	-2.707345
H	-1.346236	-1.562710	-0.924022

Cu7

E= -1036.0215178au

H	-1.422777	1.714368	-1.295998
C	-0.911566	2.489183	-0.736208
C	0.260003	2.171141	-0.028619
C	-1.411253	3.793517	-0.717647
C	0.779888	0.759081	-0.041383
C	0.914702	3.174123	0.709624
C	-0.751200	4.791450	0.010414
H	-2.314429	4.029690	-1.270257
N	2.162679	0.665045	-0.072584
N	-0.018937	-0.237945	-0.010954
C	0.409774	4.478236	0.726353
H	1.793463	2.930617	1.299073
H	-1.142782	5.803355	0.025207
C	2.987388	-0.481672	-0.058653
H	2.638635	1.534471	-0.268440
H	0.915550	5.243342	1.306441
C	4.369699	-0.278415	-0.246291
C	2.504551	-1.785602	0.147476
C	5.252568	-1.356493	-0.228139
H	4.747652	0.728458	-0.405972
C	3.403084	-2.858135	0.164326
H	1.444548	-1.951148	0.288372
C	4.773998	-2.656537	-0.022392
H	6.313358	-1.180745	-0.375398
H	3.018498	-3.860907	0.323766
H	5.459652	-3.497016	-0.009568
Cu	-1.631675	-1.051973	0.038765
O	-2.905445	-2.619245	0.065527
C	-3.892774	-1.799915	0.050013
O	-3.655001	-0.544698	0.026877
C	-5.305426	-2.319602	0.076103
H	-5.428333	-3.103676	-0.676923
H	-5.510810	-2.771351	1.053465
H	-6.016884	-1.512541	-0.102270

Cu7-FC-TS

E= -1035.9848106au

C	2.526421	-0.799499	-0.765246
C	3.068157	0.350276	-0.083186
C	4.150220	0.249594	0.786237
C	4.686257	-1.017496	1.057197
C	4.109674	-2.178246	0.491817
C	3.061232	-2.083005	-0.410695
C	0.865731	1.039648	-0.244536
H	4.530720	1.129188	1.296217
H	5.522667	-1.109209	1.741364
H	4.520191	-3.151078	0.740916
H	2.673847	-2.968522	-0.903450
N	0.646553	-0.219795	-0.418130
N	2.217123	1.452653	-0.202406
C	-0.170218	2.088369	-0.079629
C	-1.428116	1.776849	0.470617
C	0.101253	3.410235	-0.488433
C	-2.391351	2.779605	0.610869
H	-1.669048	0.766715	0.790252
C	-0.868717	4.404849	-0.344175
H	1.052037	3.652228	-0.953617
C	-2.116678	4.092285	0.208651
H	-3.356018	2.525359	1.036186

H	-0.654265	5.417162	-0.671175
H	-2.870298	4.865305	0.319722
H	2.424194	2.297057	0.316471
H	2.212286	-0.673353	-1.801222
Cu	-0.840347	-1.345336	-0.516875
O	-3.035595	-1.074391	1.098840
C	-3.212185	-2.049122	0.344450
O	-2.351327	-2.443404	-0.559691
C	-4.481592	-2.884911	0.418016
H	-4.228476	-3.925741	0.648019
H	-5.153046	-2.492268	1.183124
H	-4.985620	-2.882332	-0.554616

Cu9

E= -1036.0107062au

C	2.204323	-0.731766	-0.554676
C	3.082115	0.395951	-0.082174
C	4.353817	0.211628	0.403638
C	4.777081	-1.117717	0.653761
C	3.851633	-2.202863	0.561320
C	2.579078	-2.044786	0.071049
C	0.930015	1.096069	-0.181653
H	4.986774	1.050853	0.674182
H	5.777989	-1.298419	1.028206
H	4.164648	-3.177759	0.922648
H	1.871902	-2.866253	0.019116
N	0.825135	-0.196767	-0.378578
N	2.259215	1.522005	-0.118986
C	-0.159881	2.071068	-0.035601
C	-1.417071	1.686345	0.469035
C	0.057642	3.415059	-0.406466
C	-2.434240	2.636225	0.595379
H	-1.623325	0.663149	0.772610
C	-0.964332	4.356193	-0.274208
H	1.008613	3.714678	-0.836832
C	-2.213209	3.968858	0.228772
H	-3.396784	2.322011	0.983274
H	-0.791078	5.384812	-0.572849
H	-3.008217	4.700686	0.329155
H	2.493832	2.383081	0.357214
H	2.323482	-0.840054	-1.659653
Cu	-0.742176	-1.287728	-0.511087
O	-3.030023	-1.076184	1.066916
C	-3.153793	-2.025750	0.272257
O	-2.248025	-2.378983	-0.605848
C	-4.410945	-2.883835	0.257693
H	-4.150408	-3.928458	0.460578
H	-5.122606	-2.530586	1.005513
H	-4.871171	-2.853046	-0.735987

Cu9-Dep-Re

E= -1265.0685925au

C	-0.793548	-1.919300	-0.142293
C	-2.260047	-2.232913	-0.009794
C	-2.821400	-3.422936	-0.401780
C	-2.011889	-4.325906	-1.136005
C	-0.712319	-3.933431	-1.581768
C	-0.126545	-2.752979	-1.197320
C	-1.965949	0.007450	0.100246
H	-3.873450	-3.635679	-0.237319
H	-2.421574	-5.279458	-1.448972
H	-0.181449	-4.591973	-2.262884
H	0.870090	-2.470189	-1.515110
N	-0.781985	-0.416492	-0.262220
N	-2.852635	-1.029783	0.388024
C	-2.407951	1.406177	0.218057
C	-1.870610	2.402351	-0.617689
C	-3.385202	1.756841	1.169902
C	-2.302245	3.724955	-0.498712
H	-1.127599	2.136941	-1.358366
C	-3.812588	3.081805	1.284630
H	-3.779545	1.002435	1.843561
C	-3.273352	4.068542	0.450966
H	-1.883801	4.484205	-1.148070
H	-4.556695	3.344453	2.029197
H	-3.604248	5.097725	0.541821
H	-3.850553	-0.874704	0.328814
H	-0.259353	-2.114914	0.816155

O	1.374273	-2.034170	2.323684
C	2.329885	-1.447892	1.842241
O	2.365702	-1.157164	0.519321
C	3.543881	-1.018719	2.643619
H	4.417136	-1.609257	2.342260
H	3.786021	0.031027	2.450620
H	3.354029	-1.175038	3.705573
Cu	0.853219	0.547442	-0.568487
O	2.262341	1.715804	-1.017154
C	3.525083	1.585309	-0.783716
O	4.070341	0.610925	-0.200109
H	3.129355	-0.523298	0.257856
C	4.396315	2.732710	-1.268864
H	5.448632	2.528762	-1.066664
H	4.245278	2.884897	-2.342976
H	4.096349	3.656630	-0.766272

Cu9-Dep-TS

E= -1265.0560103au

C	-1.275239	-1.521031	-0.479661
C	-2.701069	-1.480137	-0.151020
C	-3.541588	-2.554132	-0.293021
C	-3.013156	-3.729936	-0.914655
C	-1.708808	-3.723921	-1.452542
C	-0.850905	-2.634941	-1.332497
C	-1.813137	0.615516	-0.121692
H	-4.584094	-2.506795	0.005619
H	-3.646900	-4.601063	-1.035857
H	-1.370203	-4.596287	-2.005845
H	0.146900	-2.644736	-1.759303
N	-0.841456	-0.158923	-0.582721
N	-2.936965	-0.147043	0.246599
C	-1.772147	2.056402	0.096565
C	-0.859967	2.880036	-0.602309
C	-2.677178	2.666986	0.995611
C	-0.846968	4.258388	-0.397774
H	-0.182970	2.433328	-1.323670
C	-2.663022	4.049513	1.189671
H	-3.360147	2.051265	1.571785
C	-1.749778	4.853780	0.496909
H	-0.141664	4.874275	-0.946966
H	-3.359174	4.498671	1.891242
H	-1.741208	5.928105	0.648627
H	-3.860890	0.262262	0.192424
H	-0.615589	-1.846683	0.710725
O	-0.016667	-2.150595	1.774059
C	1.232793	-1.886366	1.778496
O	1.847959	-1.368977	0.787717
C	2.008057	-2.246897	3.028591
H	2.572079	-3.170347	2.849685
H	2.727646	-1.459692	3.271834
H	1.329908	-2.409208	3.866910
Cu	1.051585	0.197611	-0.713280
O	2.862115	0.846468	-1.053293
C	3.956802	0.554615	-0.525105
O	4.115790	-0.356321	0.408518
H	3.227236	-0.824178	0.648089
C	5.224746	1.247511	-0.942878
H	5.723114	1.674866	-0.067101
H	5.913877	0.519618	-1.384886
H	5.004872	2.030727	-1.667471

Cu9-Dep-Pro

E= -1265.0765486au

C	-0.375657	-1.912499	-0.746387
C	-1.466173	-2.710350	-0.289803
C	-1.429335	-4.100949	-0.320222
C	-0.260366	-4.719876	-0.818971
C	0.821734	-3.956795	-1.263681
C	0.792825	-2.540697	-1.220957
C	-1.983688	-0.495582	-0.100179
H	-2.267281	-4.695657	0.027991
H	-0.209763	-5.802901	-0.858858
H	1.704508	-4.453400	-1.654801
H	1.603659	-1.952319	-1.639227
N	-0.695202	-0.573610	-0.615953
N	-2.428015	-1.811134	0.150965
C	-2.744223	0.665822	0.189595

C	-2.359401	1.962106	-0.280262
C	-3.943125	0.591910	0.971525
C	-3.114578	3.090260	0.020883
H	-1.495938	2.059592	-0.929166
C	-4.686580	1.728998	1.258522
H	-4.256164	-0.361613	1.387875
C	-4.286833	2.995539	0.791917
H	-2.798873	4.055448	-0.362093
H	-5.585515	1.636619	1.862316
H	-4.872686	3.879547	1.019381
H	-3.408387	-2.039208	0.220254
H	1.661100	-2.423136	0.630563
O	2.109220	-2.294796	1.511612
C	2.711270	-1.112161	1.565082
O	2.705660	-0.320189	0.612981
C	3.367755	-0.841654	2.891032
H	3.948031	-1.710861	3.211473
H	4.011121	0.036257	2.827281
H	2.595408	-0.666766	3.649256
Cu	0.542069	0.849213	-0.764823
O	1.667688	2.386673	-0.997500
C	2.738860	2.831807	-0.544603
O	3.555157	2.155132	0.247555
H	3.230759	1.222872	0.427618
C	3.211490	4.220402	-0.865610
H	3.321400	4.798957	0.058319
H	4.196438	4.179736	-1.342807
H	2.499035	4.710615	-1.525041

Cu6

E= -806.9102136au

C	-2.333558	-0.256714	-0.024686
C	-1.486025	0.869991	0.097667
C	0.783056	-0.291607	-0.015482
H	-4.394356	-0.893592	-0.104656
C	-3.724180	-0.043169	-0.010267
C	-2.042155	2.162623	0.239178
C	-3.422205	2.340846	0.256704
C	-4.273913	1.235746	0.129838
H	-1.384956	3.024827	0.331205
H	-3.832420	3.339872	0.367038
H	-5.351175	1.369705	0.142669
N	-0.070969	0.804603	0.085704
N	0.438950	-1.526209	-0.118249
Cu	-1.373979	-1.904895	-0.181766
C	2.243250	0.069366	-0.000683
C	3.154494	-0.796853	0.627524
C	2.723117	1.233501	-0.627265
C	4.517654	-0.493725	0.646147
H	2.779113	-1.699164	1.096508
C	4.089675	1.532814	-0.609100
H	2.038929	1.886792	-1.160533
C	4.989230	0.673349	0.031136
H	5.211718	-1.165509	1.140981
H	4.450471	2.429415	-1.103074
H	6.048947	0.907204	0.045730
H	0.392611	1.676641	0.298892

Cu7-CMD-TS

E= -1035.9768588au

Cu	1.086010	-0.932392	-0.850606
O	2.727224	-0.887472	1.456612
C	3.180967	-1.793377	0.656099
O	2.744115	-1.969362	-0.524374
C	4.272541	-2.692226	1.183179
H	3.841307	-3.403260	1.897925
H	4.734010	-3.247686	0.366102
H	5.021727	-2.103130	1.718547
H	-3.131845	-1.184286	-1.863376
C	-3.645980	-0.849995	-0.969448
C	-2.907555	-0.192116	0.029807
C	-5.016219	-1.063702	-0.807802
C	-1.434226	0.013988	-0.168561
C	-3.561379	0.229177	1.201907
C	-5.665421	-0.631659	0.356436
H	-5.578312	-1.565612	-1.588809
N	-0.929226	1.174549	0.449207
N	-0.743759	-0.820701	-0.844480

C	-4.933895	0.009914	1.361722
H	-2.996045	0.692257	2.004722
H	-6.730423	-0.799549	0.480812
C	0.343060	1.735616	0.209505
H	-1.644717	1.852140	0.679572
H	-5.426845	0.330890	2.273876
C	0.422697	3.144011	0.182937
C	1.503886	0.944316	-0.004845
C	1.624301	3.781162	-0.118416
H	-0.469862	3.736770	0.368496
C	2.694133	1.634125	-0.347817
C	2.769115	3.025972	-0.407985
H	1.663052	4.865788	-0.143070
H	3.594215	1.049458	-0.524522
H	3.702459	3.518470	-0.660643
H	1.991033	-0.096385	0.826645

Cu8-CMD-TS

E= -1264.4056379au

Cu	1.132878	-0.613256	-0.251129
O	0.621396	-0.016815	2.754228
C	0.908574	-1.251555	2.611339
O	1.273508	-1.778973	1.509847
C	0.786057	-2.160885	3.820473
H	1.598312	-2.892992	3.824205
H	0.795754	-1.576481	4.742935
H	-0.159845	-2.713437	3.762349
H	-2.651926	-1.689991	-1.705934
C	-3.410491	-1.121917	-1.179920
C	-3.018341	-0.040102	-0.373015
C	-4.762791	-1.450480	-1.297356
C	-1.560626	0.297632	-0.251474
C	-3.991094	0.695551	0.327987
C	-5.731705	-0.709309	-0.608732
H	-5.060242	-2.282817	-1.926424
N	-1.280381	1.662614	-0.203954
N	-0.721869	-0.666819	-0.238717
C	-5.343335	0.360648	0.205760
H	-3.694048	1.501123	0.992691
H	-6.781606	-0.967125	-0.702139
C	-0.007038	2.189720	-0.062434
H	-2.040173	2.288978	-0.429824
H	-6.088952	0.927886	0.753267
C	0.232591	3.525420	-0.446967
C	1.043685	1.393292	0.474376
C	1.521763	4.040703	-0.372050
H	-0.579248	4.132134	-0.837000
C	2.353808	1.948751	0.505419
C	2.594046	3.252036	0.093644
H	1.703828	5.061482	-0.692955
H	3.160808	1.337271	0.893578
H	3.593145	3.670166	0.143828
H	0.788633	0.712021	1.431326
O	1.646268	-1.725268	-2.049481
C	2.847927	-1.499843	-1.711028
C	4.012459	-2.085042	-2.458148
O	3.059338	-0.764816	-0.669732
H	4.816375	-1.349113	-2.546812
H	4.406582	-2.943030	-1.900632
H	3.697858	-2.422969	-3.447159

Cu2-CN-TS

E= -1035.9605843au

Cu	1.304933	-0.897444	-0.422758
H	-2.400868	-2.377679	0.448163
C	-3.207996	-1.658798	0.348483
C	-2.920657	-0.336875	-0.074855
C	-4.521568	-2.058900	0.589355
C	-1.546720	0.060544	-0.318167
C	-4.004828	0.554392	-0.271538
C	-5.583446	-1.166719	0.388789
H	-4.720440	-3.074765	0.915003
N	-1.202540	1.225626	-0.978472
N	-0.459981	-0.523752	0.265275
C	-5.315778	0.139222	-0.047006
H	-3.819876	1.584985	-0.558337
H	-6.605418	-1.484688	0.564892
C	-0.092681	1.890356	-0.417937

H	-1.898416	1.738575	-1.498614
H	-6.131905	0.839152	-0.195065
C	0.236489	3.241625	-0.603341
C	0.676063	1.106897	0.440704
C	1.315180	3.766324	0.115741
H	-0.345920	3.871095	-1.269905
C	1.723119	1.616553	1.200636
C	2.047119	2.972365	1.013567
H	1.580538	4.810143	-0.015390
H	2.313522	0.976702	1.847419
H	2.887508	3.398080	1.552328
O	3.294195	-1.337313	1.209126
C	3.744718	-1.533142	0.061220
O	3.021080	-1.418239	-1.021667
C	5.194527	-1.928271	-0.166051
H	5.685009	-1.191427	-0.811478
H	5.724511	-1.996928	0.785064
H	5.239783	-2.892355	-0.684351
H	-0.696892	-1.037164	1.115346

Cu5-CN-TS

E= -1264.4341768au

Cu	1.063898	-0.453439	-0.313048
H	-2.608461	-1.652973	0.268022
C	-3.346063	-0.879408	0.083383
C	-2.942194	0.460522	-0.076622
C	-4.702098	-1.209619	0.024314
C	-1.510072	0.820621	-0.039228
C	-3.921512	1.456804	-0.274756
C	-5.666802	-0.219612	-0.193135
H	-5.002491	-2.244299	0.148319
N	-1.083674	1.984460	-0.610132
N	-0.560140	0.138759	0.577914
C	-5.272936	1.116646	-0.337015
H	-3.642933	2.504356	-0.338695
H	-6.718084	-0.483625	-0.240141
C	0.193757	2.398708	-0.235425
H	-1.712852	2.580809	-1.126331
H	-6.016780	1.892463	-0.483668
C	0.652368	3.726929	-0.289553
C	0.966629	1.411796	0.393089
C	1.826408	4.051141	0.384460
H	0.070441	4.487201	-0.801125
C	2.091006	1.747465	1.161539
C	2.520803	3.076657	1.128787
H	2.189811	5.072646	0.364189
H	2.661016	0.978287	1.667045
H	3.422999	3.349866	1.665478
O	3.297062	-1.064821	0.813279
C	3.604037	-0.871493	-0.384041
O	2.750003	-0.439261	-1.267646
C	5.007272	-1.144237	-0.898925
H	4.989595	-2.023816	-1.553404
H	5.366200	-0.299565	-1.495575
H	5.682836	-1.331464	-0.065078
H	-0.764832	-0.800889	1.061209
O	-0.803003	-2.395484	1.260702
C	-0.101634	-2.969865	0.368549
O	0.574996	-2.361054	-0.536209
C	-0.035133	-4.486640	0.355379
H	0.958634	-4.802474	0.693916
H	-0.790528	-4.911919	1.018207
H	-0.166404	-4.860931	-0.664260

Cu9-Cup-TS

E= -1265.0351433au

C	-0.453234	-0.929348	2.460307
C	-0.929871	-0.271690	1.358882
C	-0.335180	-0.380290	0.013584
C	0.838139	-1.271406	-0.051199
C	1.245065	-2.000874	1.105182
C	0.693814	-1.770271	2.354440
H	-0.986684	-0.862483	3.405666
H	-0.213486	0.546104	-0.553449
H	1.172169	-1.608914	-1.030746
H	2.062329	-2.711089	0.990770
H	1.080113	-2.266488	3.237514
N	-2.277156	0.185348	1.195569

H	-2.896101	0.267336	1.992425
C	-2.782142	-0.290024	0.014403
Cu	2.604262	0.051916	-0.034058
O	1.950865	1.659576	0.823114
O	1.228553	2.063807	-1.263991
C	-4.217339	-0.203419	-0.288698
C	-4.837161	-1.197150	-1.070211
C	-4.981069	0.875449	0.198164
C	-6.201511	-1.114925	-1.352030
H	-4.256294	-2.040709	-1.429112
C	-6.344840	0.953182	-0.092232
H	-4.500575	1.664741	0.767378
C	-6.957879	-0.040630	-0.865178
H	-6.675351	-1.888713	-1.946237
H	-6.925544	1.792151	0.275680
H	-8.017220	0.022844	-1.089799
N	-1.846676	-0.809309	-0.747872
H	-2.014676	-0.990913	-1.729366
C	1.468411	2.443891	-0.097542
C	1.214663	3.878960	0.337089
H	0.654041	3.898953	1.277083
H	2.174021	4.376286	0.520497
H	0.671543	4.420831	-0.439218
O	3.702794	-1.382377	-0.935849
C	4.793895	-0.699730	-0.810685
O	4.757115	0.424494	-0.231904
C	6.076148	-1.259136	-1.373448
H	6.223871	-2.285502	-1.022921
H	6.012675	-1.293228	-2.467216
H	6.924337	-0.638584	-1.081092

Cu1-Dep-TS

E= -1918.1578921au

C	0.708021	-1.391196	-0.356029
C	-0.455144	-1.072747	-1.131735
C	-1.074592	-2.064420	-1.924385
C	-0.533190	-3.341869	-1.984523
C	0.619605	-3.677549	-1.244705
C	1.236854	-2.711423	-0.467721
C	-0.508628	1.322791	-0.684330
H	-1.963307	-1.806336	-2.487322
H	-1.004044	-4.087434	-2.617024
H	1.022032	-4.683295	-1.291375
H	2.128014	-2.948140	0.100167
N	0.781594	1.392751	-0.475700
N	-1.098327	0.161239	-1.058964
C	-1.360730	2.538245	-0.583063
C	-0.846593	3.777072	-1.011809
C	-2.656363	2.475053	-0.039893
C	-1.617548	4.934966	-0.895122
H	0.138865	3.826947	-1.464101
C	-3.419269	3.639376	0.080505
H	-3.063321	1.527456	0.291716
C	-2.903652	4.868941	-0.345031
H	-1.219281	5.883211	-1.239620
H	-4.415315	3.584344	0.506307
H	-3.501750	5.769536	-0.253451
H	0.527800	-1.039914	0.861127
Cu	2.123084	0.091756	-0.133372
O	3.514846	-1.117040	0.138799
C	4.078723	-1.316143	-1.051777
O	3.546475	-0.957340	-2.102132
C	5.424108	-2.005080	-0.974593
H	6.165722	-1.248401	-0.698408
H	5.430197	-2.786864	-0.210671
H	5.678423	-2.421327	-1.950909
H	1.125761	2.275569	-0.107395
H	-2.124504	0.146843	-1.318828
O	-1.613581	-1.343204	2.720052
C	-0.431934	-0.966236	3.002074
O	0.482578	-0.661990	2.163723
C	-0.056399	-0.902797	4.469380
H	-0.946759	-0.778962	5.087637
H	0.437184	-1.840837	4.752072
H	0.651070	-0.089446	4.644057
O	5.215859	1.206592	-0.349072
C	4.431528	1.808528	0.367951
O	3.122732	1.599098	0.478654

C	4.876073	2.958221	1.278392
H	4.735851	2.670674	2.325832
H	5.928721	3.176902	1.092706
H	4.270005	3.850487	1.094681
Cu	-2.828945	-1.316060	1.294430
O	-4.292364	-1.338790	0.146564
C	-4.494850	-0.840985	-1.028352
O	-3.665424	-0.178360	-1.702604
C	-5.874407	-1.110310	-1.606547
H	-5.983014	-0.627545	-2.578300
H	-6.026341	-2.190242	-1.711535
H	-6.643568	-0.742683	-0.919389

Cu7-Dep-TS

E= -1689.0979115au

C	1.325017	-1.384479	-0.457608
C	0.030504	-1.443554	-1.084669
C	-0.457564	-2.689483	-1.564319
C	0.368602	-3.797815	-1.551472
C	1.692291	-3.734779	-1.040740
C	2.166082	-2.550881	-0.516671
C	-0.308890	0.942655	-0.942099
H	-1.460262	-2.734466	-1.971649
H	-0.000158	-4.734652	-1.957175
H	2.315085	-4.622241	-1.044399
H	3.161392	-2.488849	-0.092083
N	0.913118	1.267238	-0.735670
N	-0.779344	-0.350013	-1.175140
C	-1.331938	2.038840	-0.988666
C	-1.114204	3.204694	-0.232798
C	-2.474814	1.936622	-1.801026
C	-2.038073	4.250058	-0.277828
H	-0.227273	3.273947	0.385273
C	-3.394607	2.989213	-1.840952
H	-2.656295	1.048868	-2.394526
C	-3.180562	4.144943	-1.081373
H	-1.868404	5.143105	0.314359
H	-4.276723	2.903106	-2.466632
H	-3.898571	4.958017	-1.115210
H	1.223326	-0.979162	0.685945
Cu	2.438849	0.270292	-0.576392
H	-1.826032	-0.554629	-1.200403
O	-0.651704	0.216057	2.686648
C	0.619726	0.171618	2.809014
O	1.428368	-0.468939	2.068828
C	1.216566	1.003872	3.931705
H	1.535395	1.972045	3.525766
H	0.477241	1.181297	4.714273
H	2.098597	0.507548	4.342395
O	4.265013	-0.451200	-0.461354
C	4.794684	0.732607	-0.421650
O	4.014852	1.728150	-0.485887
C	6.283747	0.876806	-0.301681
H	6.627494	0.404729	0.625047
H	6.775871	0.360417	-1.132613
H	6.566008	1.930225	-0.303124
Cu	-1.981981	-0.669155	1.720070
O	-3.496794	-1.484470	0.992955
C	-3.913885	-1.561645	-0.223048
O	-3.290305	-1.167475	-1.246324
C	-5.286618	-2.190968	-0.394749
H	-5.311125	-3.170750	0.092946
H	-6.039752	-1.565892	0.097924
H	-5.533240	-2.293127	-1.452247

Cu8

E= -1264.4316204au

Cu	0.974448	-0.813623	-0.832632
O	-0.054230	-2.441875	1.787612
C	0.512985	-3.063193	0.893204
O	1.085207	-2.541591	-0.180070
C	0.646535	-4.583789	0.915683
H	1.692084	-4.876389	0.780674
H	0.267654	-4.968117	1.863802
H	0.073903	-5.013105	0.086512
H	-2.839706	0.098013	-2.225673
C	-3.476328	0.296039	-1.371380
C	-2.892667	0.451689	-0.103391

C	-4.862007	0.402624	-1.516984
C	-1.396082	0.341843	0.056744
C	-3.704199	0.690228	1.020064
C	-5.670008	0.653899	-0.400894
H	-5.310067	0.290073	-2.498688
N	-0.852812	1.316772	0.876496
N	-0.879955	-0.653220	-0.565439
C	-5.089759	0.795422	0.866020
H	-3.254077	0.770501	2.003881
H	-6.746164	0.733472	-0.516247
C	0.508546	1.497274	1.261794
H	-1.435836	2.138764	0.952815
H	-5.714763	0.977376	1.734231
C	1.095392	2.762816	1.099776
C	1.231213	0.453738	1.861684
C	2.405673	2.984652	1.528559
H	0.530560	3.560476	0.626275
C	2.555498	0.681732	2.258993
C	3.145064	1.940792	2.099850
H	2.850839	3.967247	1.408180
H	3.116297	-0.128702	2.713969
H	4.166621	2.110704	2.423746
H	0.752745	-0.509153	2.027505
O	1.203936	0.888839	-1.753498
C	2.439010	0.607116	-2.041090
C	3.279741	1.609389	-2.770064
O	2.877906	-0.523060	-1.669783
H	3.447781	2.480988	-2.127644
H	4.239882	1.169327	-3.042479
H	2.758422	1.956600	-3.667413

HCl

E= -460.7929763au

H	0.000000	0.000000	-1.220430
Cl	0.000000	0.000000	0.071790

$PdCl_2(PhCN)_2$

E= -1696.0949686au

Pd	0.000002	0.000193	-0.000040
Cl	0.000111	2.361611	-0.000074
Cl	-0.000107	-2.361225	-0.000034
C	-3.146183	0.000292	-0.000323
N	-1.989662	0.000270	-0.000310
C	-4.574818	0.000025	-0.000114
C	-5.274233	-1.224322	0.000089
C	-5.274684	1.224113	-0.000135
C	-6.669435	-1.215829	0.000270
H	-4.723639	-2.158243	0.000099
C	-6.669883	1.215104	0.000044
H	-4.724435	2.158237	-0.000297
C	-7.366627	-0.000491	0.000248
H	-7.211712	-2.154836	0.000425
H	-7.212506	2.153911	0.000025
H	-8.451558	-0.000691	0.000389
C	3.146180	0.000087	0.000347
N	1.989659	0.000121	0.000247
C	4.574815	-0.000083	0.000166
C	5.274312	-1.224383	0.000008
C	5.274599	1.224052	0.000195
C	6.669513	-1.215795	-0.000137
H	4.723781	-2.158341	-0.000001
C	6.669798	1.215137	0.000053
H	4.724287	2.158139	0.000330
C	7.366624	-0.000411	-0.000117
H	7.211853	-2.154766	-0.000262
H	7.212358	2.153981	0.000074
H	8.451554	-0.000538	-0.000228

$PdCl_2PhCN$

E= -1371.6136144au

Pd	-2.028426	-0.000002	-0.000132
Cl	-2.220799	-2.302248	0.000063
Cl	-2.220819	2.302243	-0.000355
C	1.087251	0.000013	0.000101
N	-0.069893	0.000005	-0.000001
C	2.514478	0.000008	0.000175
C	3.213080	1.225562	0.000233
C	3.213070	-1.225552	0.000192

C	4.607869	1.216076	0.000310
H	2.663939	2.160300	0.000220
C	4.607858	-1.216079	0.000268
H	2.663920	-2.160286	0.000146
C	5.304119	-0.000004	0.000327
H	5.150628	2.154564	0.000357
H	5.150609	-2.154571	0.000281
H	6.388880	-0.000009	0.000385

PhCN

E= -324.430859au

C	-2.050318	0.000186	-0.000179
N	-3.213097	-0.000122	0.000169
C	-0.615006	0.000384	-0.000034
C	0.091012	-1.219071	-0.000035
C	0.091593	1.219447	-0.000034
C	1.487252	-1.213490	0.000016
H	-0.457151	-2.154575	-0.000089
C	1.487688	1.213143	0.000016
H	-0.456157	2.155207	-0.000088
C	2.187069	-0.000369	0.000063
H	2.028022	-2.153848	0.000012
H	2.029092	2.153138	0.000011
H	3.272130	-0.000444	0.000089

Pd1

E= -1983.6815592au

H	-3.402861	-2.478020	-0.914461
C	-4.290307	-1.923922	-0.625677
C	-4.159053	-0.609491	-0.141870
C	-5.558023	-2.491777	-0.774713
C	-2.798663	-0.017579	0.015187
C	-5.310814	0.128702	0.185152
C	-6.701949	-1.755124	-0.442652
H	-5.653357	-3.501872	-1.158654
N	-2.684833	1.283047	-0.381040
N	-1.821845	-0.725731	0.509379
C	-6.576494	-0.445523	0.036924
H	-5.211220	1.133711	0.582659
H	-7.685556	-2.198649	-0.557981
C	-1.619840	2.207961	-0.168438
H	-3.394039	1.583253	-1.035750
H	-7.461055	0.123425	0.303490
C	-1.322429	3.117971	-1.194065
C	-0.942763	2.280652	1.058625
C	-0.351105	4.100839	-0.995878
H	-1.835253	3.039652	-2.147939
C	0.037509	3.261549	1.240603
H	-1.166054	1.582265	1.856891
C	0.335040	4.174137	0.222020
H	-0.124509	4.798955	-1.795028
H	0.564724	3.306657	2.187974
H	1.094511	4.934016	0.374674
H	-2.126783	-1.612397	0.894644
Pd	0.184027	-0.626658	0.322256
Cl	0.380034	-0.745390	2.684986
Cl	-0.050954	-0.647262	-2.038985
C	3.335524	-0.630773	-0.021991
N	2.187558	-0.625640	0.122075
C	4.752891	-0.634495	-0.208854
C	5.285617	-0.532997	-1.510324
C	5.609068	-0.738785	0.906230
C	6.669725	-0.535588	-1.687515
H	4.615983	-0.454777	-2.359370
C	6.991017	-0.740358	0.712570
H	5.187377	-0.817108	1.901933
C	7.521676	-0.638767	-0.580081
H	7.082844	-0.457872	-2.687182
H	7.652665	-0.820825	1.568025
H	8.597070	-0.640591	-0.724109

Pd1-Anag-Im

E= -1659.2206158au

C	1.164458	1.489006	-0.960482
C	0.312156	1.948207	0.077322
C	-1.546935	0.318959	-0.090993
H	3.166987	1.529560	-1.751660
C	2.514785	1.893381	-0.967271

C	0.811756	2.810207	1.063343
C	2.150553	3.210207	1.025933
C	3.009045	2.743839	0.023456
H	0.161073	3.151698	1.862541
H	2.528344	3.871636	1.798339
H	4.052738	3.034110	0.019027
N	-1.063942	1.598960	0.089709
N	-0.738178	-0.679372	-0.272212
C	-3.024688	0.167192	-0.044685
C	-3.591760	-0.979589	0.541711
C	-3.865952	1.158667	-0.583637
C	-4.979371	-1.131067	0.584128
H	-2.949786	-1.734205	0.985299
C	-5.253697	1.000259	-0.539697
H	-3.434430	2.030870	-1.064226
C	-5.812420	-0.143031	0.044052
H	-5.409180	-2.014022	1.044495
H	-5.896216	1.762181	-0.968020
H	-6.890012	-0.263880	0.077862
H	-1.674646	2.218028	0.606329
H	0.740581	1.001245	-1.834429
Pd	1.310142	-0.804395	-0.128661
Cl	3.605449	-1.011266	0.096851
Cl	0.971642	-3.068982	0.245721
H	-1.185248	-1.575395	-0.442453

Pd1-Anag-TS

E= -1659.1771863au

C	-1.637069	1.076550	-0.023080
C	-0.540579	1.938988	0.223608
C	1.368084	0.373725	-0.091592
H	-3.690352	1.034804	-0.679090
C	-2.840637	1.674459	-0.463071
C	-0.692375	3.334805	0.148979
C	-1.913712	3.894317	-0.224885
C	-2.986716	3.060977	-0.558700
H	0.161672	3.978507	0.342981
H	-2.017093	4.972857	-0.278615
H	-3.933307	3.485494	-0.875354
N	0.772315	1.458339	0.488462
N	0.662809	-0.524670	-0.718748
C	2.847656	0.269543	0.028097
C	3.429804	-0.986753	0.278939
C	3.671410	1.401315	-0.113684
C	4.817304	-1.104164	0.390588
H	2.795979	-1.858325	0.410813
C	5.058820	1.276772	-0.003972
H	3.235987	2.368108	-0.348894
C	5.633086	0.025309	0.250246
H	5.259037	-2.073671	0.593362
H	5.689760	2.150557	-0.127114
H	6.710413	-0.069287	0.336228
H	1.395864	2.098277	0.960753
Pd	-1.209038	-0.975500	-0.182926
H	-2.344941	0.084744	0.899216
Cl	-3.285926	-1.114172	1.185297
Cl	-0.606053	-3.235885	-0.546040
H	1.180067	-1.298850	-1.123893

Pd1-Met-TS

E= -1983.6347493au

H	-4.253069	-1.594867	-1.553216
C	-4.681177	-1.461874	-0.564608
C	-4.046442	-0.621839	0.368038
C	-5.876122	-2.102047	-0.228323
C	-2.765013	0.048503	0.016010
C	-4.618889	-0.433502	1.639516
C	-6.443905	-1.912433	1.037783
H	-6.364510	-2.743373	-0.953991
N	-2.650084	1.354544	0.400688
N	-1.837335	-0.567257	-0.659628
C	-5.812982	-1.080340	1.970003
H	-4.109041	0.177008	2.377937
H	-7.370193	-2.413943	1.297538
C	-1.567477	2.230486	0.137524
H	-3.520785	1.796089	0.664490
H	-6.241161	-0.945397	2.957440
C	-1.871355	3.551934	-0.226383

C	-0.222230	1.813459	0.282129
C	-0.842293	4.462126	-0.470614
H	-2.907605	3.858426	-0.336715
C	0.796932	2.760309	0.027268
C	0.498837	4.067276	-0.352215
H	-1.087142	5.479157	-0.758828
H	1.824997	2.452307	0.176853
H	1.294442	4.780438	-0.537534
H	-2.024953	-1.547746	-0.846489
Pd	0.100354	-0.164481	-0.896343
Cl	0.149389	-2.033268	-2.322151
Cl	0.902114	-0.414022	2.263295
C	3.190192	-0.234862	-0.557261
N	2.130685	-0.006600	-0.967213
C	4.452034	-0.513553	0.049923
C	4.474778	-0.734111	1.444883
C	5.633537	-0.574978	-0.715480
C	5.696459	-1.013413	2.060616
H	3.540934	-0.689702	2.002846
C	6.842960	-0.854628	-0.079497
H	5.595603	-0.409575	-1.786608
C	6.874764	-1.072708	1.305169
H	5.725490	-1.187921	3.130528
H	7.757554	-0.905535	-0.660232
H	7.818988	-1.291921	1.793332
H	0.050088	0.948986	0.981161

Pd1-Oxa-TS

E= -1983.5903788au

C	-0.559570	1.983641	-0.314163
C	-1.943318	2.241920	-0.339610
C	-2.793594	-0.102505	-0.097341
H	1.393753	2.887233	-0.303840
C	0.326998	3.072977	-0.309995
C	-2.414401	3.567856	-0.345271
C	-1.521783	4.636847	-0.330071
C	-0.144572	4.388648	-0.310388
H	-3.485742	3.752384	-0.349387
H	-1.898650	5.653793	-0.332323
H	0.560527	5.213004	-0.297274
N	-2.929786	1.220993	-0.378780
N	-1.642113	-0.643858	0.150098
C	-4.037116	-0.920858	-0.087833
C	-4.018863	-2.211869	-0.645658
C	-5.223494	-0.422419	0.480037
C	-5.178918	-2.990230	-0.639670
H	-3.107791	-2.592399	-1.097102
C	-6.379784	-1.207074	0.483061
H	-5.232592	0.553969	0.955070
C	-6.359969	-2.489607	-0.078310
H	-5.160930	-3.982804	-1.076344
H	-7.288838	-0.823974	0.934253
H	-7.258674	-3.097335	-0.073451
H	-3.859714	1.516894	-0.639039
Pd	0.178705	0.063650	-0.032453
H	-0.173444	0.776551	-1.392801
Cl	0.785590	-2.296926	-0.704629
C	3.301567	0.203568	-0.153654
N	2.180426	0.488481	-0.175745
C	4.647714	-0.270940	-0.148447
C	5.735618	0.599296	0.055785
C	4.853431	-1.652960	-0.348547
C	7.031591	0.082686	0.054938
H	5.561542	1.657453	0.215818
C	6.156762	-2.151391	-0.344313
H	3.995600	-2.301522	-0.494434
C	7.242366	-1.288339	-0.145009
H	7.875015	0.745780	0.212993
H	6.323932	-3.212268	-0.493639
H	8.252817	-1.683754	-0.142217
Cl	0.468324	-0.305685	2.449510
H	-1.617444	-1.621310	0.421313

Pd1-Oxa-1

E= -1983.6016215au

C	-0.476895	1.864672	-0.144447
C	-1.814673	2.193271	-0.405608

C	-2.821548	-0.076589	-0.171776
H	1.478093	2.664756	0.258083
C	0.450663	2.900923	0.013893
C	-2.199257	3.541199	-0.551359
C	-1.261990	4.561025	-0.418112
C	0.067517	4.239948	-0.123872
H	-3.240615	3.779780	-0.755169
H	-1.568938	5.595319	-0.530021
H	0.805770	5.025105	0.002621
N	-2.855028	1.230654	-0.523425
N	-1.713539	-0.670957	0.155559
C	-4.111787	-0.817969	-0.178380
C	-4.153094	-2.137589	-0.663136
C	-5.287479	-0.216144	0.305592
C	-5.359517	-2.841834	-0.668390
H	-3.250379	-2.598968	-1.051154
C	-6.490707	-0.926500	0.297896
H	-5.253812	0.784877	0.724704
C	-6.529083	-2.238189	-0.190395
H	-5.386567	-3.857006	-1.049118
H	-7.391930	-0.462580	0.684280
H	-7.464189	-2.788264	-0.193790
H	-3.745191	1.576150	-0.852667
Pd	0.148758	-0.068205	-0.015855
H	-0.030774	-0.128551	-1.536012
Cl	0.720648	-2.492082	-0.171392
C	3.293418	0.067394	-0.266731
N	2.160039	0.296442	-0.252328
C	4.666306	-0.325710	-0.271043
C	5.699576	0.625419	-0.374321
C	4.959462	-1.702022	-0.164764
C	7.026670	0.194983	-0.372213
H	5.459978	1.680022	-0.451581
C	6.292565	-2.114135	-0.164199
H	4.146001	-2.414966	-0.082061
C	7.323175	-1.170666	-0.267914
H	7.827850	0.921660	-0.449728
H	6.526137	-3.169667	-0.080681
H	8.357395	-1.498777	-0.265708
Cl	0.388844	0.135642	2.459692
H	-1.753285	-1.633899	0.473260

Pd3

E= -1522.8575693au

H	3.383653	-2.419197	1.236357
C	4.240667	-2.015546	0.706793
C	4.125302	-0.790970	0.024995
C	5.460283	-2.696727	0.725892
C	2.817680	-0.075885	0.005252
C	5.247030	-0.262859	-0.639981
C	6.574765	-2.164746	0.065839
H	5.541300	-3.637407	1.260034
N	2.862846	1.274001	0.129420
N	1.690790	-0.712828	-0.120736
C	6.464974	-0.948404	-0.618094
H	5.158391	0.660527	-1.204383
H	7.520708	-2.695962	0.081380
C	1.787264	2.202527	0.100426
H	3.771131	1.664386	0.335834
H	7.321803	-0.539789	-1.143569
C	2.171702	3.558193	0.175399
C	0.429213	1.825178	0.007438
C	1.216898	4.568298	0.152149
H	3.227989	3.810781	0.246739
C	-0.509541	2.879176	-0.021712
C	-0.135902	4.224452	0.049442
H	1.523565	5.607521	0.210343
H	-1.563290	2.639529	-0.097617
H	-0.897008	4.998606	0.027071
H	1.749829	-1.715941	-0.267279
Pd	-0.189263	-0.090146	-0.070916
Cl	-0.802540	-2.478316	-0.180398
C	-3.336838	0.079704	0.002247
N	-2.196829	0.287772	-0.016309
C	-4.712521	-0.306466	0.017866
C	-5.016254	-1.683470	-0.045641
C	-5.741930	0.651752	0.094130
C	-6.351790	-2.087979	-0.032198

H	-4.206325	-2.403145	-0.103632
C	-7.071980	0.229787	0.106442
H	-5.496031	1.706743	0.142704
C	-7.377432	-1.136323	0.043462
H	-6.591478	-3.144498	-0.080881
H	-7.868553	0.963506	0.164928
H	-8.413595	-1.458347	0.053358

Pd2

E= -1198.3884354au

C	1.759739	0.902054	-0.028151
C	0.747541	1.871912	-0.094957
C	-1.171380	0.286315	-0.006944
H	3.897452	0.592790	0.021122
C	3.096407	1.330347	-0.031528
C	1.070067	3.241072	-0.170731
C	2.402999	3.645741	-0.176195
C	3.424796	2.689143	-0.105475
H	0.274813	3.981380	-0.222904
H	2.644785	4.701578	-0.234443
H	4.465106	2.997417	-0.108766
N	-0.628425	1.525521	-0.096058
N	-0.440272	-0.791810	0.075279
C	-2.659342	0.208346	-0.009477
C	-3.304746	-0.798505	-0.749901
C	-3.428100	1.123921	0.732467
C	-4.699200	-0.883867	-0.749673
H	-2.717822	-1.493123	-1.342478
C	-4.822755	1.032928	0.729309
H	-2.937936	1.878572	1.339996
C	-5.460364	0.030965	-0.011925
H	-5.189810	-1.658100	-1.329552
H	-5.408758	1.734651	1.313252
H	-6.542988	-0.038181	-0.012457
H	-1.279356	2.278865	-0.268768
Pd	1.523910	-1.050756	0.050763
Cl	1.728950	-3.423684	0.145937
H	-0.950571	-1.656645	0.213542

Pd2-Oxi-1

E= -1851.4765426au

C	-2.437015	0.871262	0.282461
C	-1.336837	1.688885	0.674146
C	0.347039	-0.070283	1.038102
H	-4.478495	0.878577	-0.399631
C	-3.638639	1.488130	-0.098078
C	-1.486972	3.112552	0.682558
C	-2.682718	3.694100	0.315203
C	-3.765496	2.880869	-0.075722
H	-0.631519	3.716561	0.961476
H	-2.785373	4.773228	0.324967
H	-4.709846	3.331644	-0.362100
N	-0.094756	1.229081	1.065651
N	-0.411233	-1.006788	0.524365
C	1.677713	-0.392979	1.629652
C	1.897059	-1.712584	2.079201
C	2.698878	0.564757	1.800618
C	3.110751	-2.068489	2.667928
H	1.117802	-2.457177	1.978000
C	3.910639	0.198105	2.391387
H	2.571110	1.584541	1.458124
C	4.123405	-1.115327	2.824401
H	3.260327	-3.086859	3.009683
H	4.690067	0.943419	2.509039
H	5.066262	-1.392030	3.284656
H	0.656882	1.969351	1.025447
H	0.121881	-1.878946	0.147895
O	1.967256	-1.641693	-2.053001
C	1.541129	-2.777722	-1.627091
O	0.778639	-2.973341	-0.640239
C	2.014980	-3.982872	-2.422923
H	1.690639	-4.908840	-1.947087
H	1.607183	-3.932374	-3.438762
H	3.105900	-3.965915	-2.509517
O	2.039142	2.043193	-1.612344
C	2.013960	3.085669	-0.862952
O	1.622910	3.133280	0.339353
C	2.511737	4.364445	-1.518051

H	3.562029	4.244526	-1.805971
H	1.945745	4.555171	-2.435777
H	2.413405	5.210618	-0.837076
Pd	-2.340696	-1.081591	0.182712
Cl	-4.536416	-1.762816	-0.001225
Cu	1.891991	0.176444	-1.635606

Pd2-Oxi-TS

E= -1851.4751531au

C	-2.350445	1.001482	0.293734
C	-1.192742	1.721516	0.702156
C	0.319539	-0.197221	1.021536
H	-4.382976	1.184092	-0.392518
C	-3.497584	1.719822	-0.079219
C	-1.225528	3.150459	0.741605
C	-2.371377	3.832700	0.384776
C	-3.513780	3.117240	-0.026323
H	-0.325526	3.678621	1.034492
H	-2.388177	4.916241	0.418188
H	-4.418608	3.648570	-0.302374
N	0.003151	1.141735	1.081156
N	-0.496841	-1.062307	0.480356
C	1.621121	-0.648260	1.604624
C	1.715645	-1.991220	2.025913
C	2.731179	0.202300	1.783860
C	2.893859	-2.476274	2.594715
H	0.860035	-2.646766	1.919568
C	3.907747	-0.292935	2.353766
H	2.697957	1.239086	1.469527
C	3.996293	-1.629341	2.758252
H	2.946379	-3.510528	2.917702
H	4.756563	0.371106	2.478941
H	4.911876	-2.005352	3.203044
H	0.808294	1.812048	1.102096
H	0.041516	-2.038482	-0.133626
O	1.774008	-1.585038	-2.075559
C	1.277417	-2.710349	-1.775928
O	0.461278	-2.947326	-0.810883
C	1.641106	-3.896123	-2.641314
H	1.690353	-4.805481	-2.038739
H	0.860831	-4.039112	-3.399131
H	2.589440	-3.719872	-3.150711
O	2.287081	2.066222	-1.553309
C	2.309367	3.028768	-0.696480
O	1.906476	2.974093	0.497182
C	2.883824	4.335293	-1.222019
H	3.906594	4.172715	-1.578220
H	2.294607	4.678847	-2.079150
H	2.881139	5.097889	-0.442400
Pd	-2.412643	-0.953799	0.172324
Cu	1.917314	0.239233	-1.623294
Cl	-4.658801	-1.489612	-0.012353

Pd2-Oxi-2

E= -1851.4762977au

C	-2.296499	1.113900	0.277424
C	-1.093173	1.755719	0.675101
C	0.252941	-0.276143	1.041586
H	-4.308151	1.429172	-0.421390
C	-3.387347	1.906807	-0.115018
C	-1.020979	3.181674	0.692504
C	-2.115260	3.939420	0.321200
C	-3.304243	3.302444	-0.083781
H	-0.087314	3.649285	0.983486
H	-2.054194	5.021893	0.339654
H	-4.168467	3.893258	-0.369305
N	0.056192	1.088119	1.064736
N	-0.622803	-1.092446	0.522097
C	1.522008	-0.820886	1.625666
C	1.534208	-2.181204	1.998392
C	2.680425	-0.047071	1.840466
C	2.676658	-2.757408	2.554832
H	0.637800	-2.774903	1.864730
C	3.822284	-0.633291	2.396643
H	2.714448	1.001670	1.568498
C	3.828157	-1.985826	2.753033
H	2.663899	-3.803469	2.842577
H	4.708222	-0.025961	2.550263

H	4.716445	-2.432162	3.188153
H	0.903500	1.694867	1.106328
H	-0.045664	-2.210209	-0.366047
O	1.651428	-1.547059	-2.088526
C	1.117250	-2.667641	-1.940768
O	0.250596	-2.982345	-1.013845
C	1.448733	-3.794739	-2.882995
H	1.749909	-4.680027	-2.314898
H	0.555810	-4.066039	-3.457074
H	2.244611	-3.496884	-3.564770
O	2.564233	2.017877	-1.483407
C	2.596824	2.927578	-0.565597
O	2.123724	2.826688	0.595193
C	3.280902	4.220220	-0.982091
H	4.304813	4.009732	-1.308264
H	2.753429	4.657827	-1.836695
H	3.294635	4.930440	-0.154616
Pd	-2.505908	-0.837933	0.202528
Cl	-4.784060	-1.239649	-0.046760
Cu	2.000211	0.249247	-1.586025

Pd2-Oxi-3

E= -1851.4958808au

C	-1.613234	1.569527	-0.874039
C	-0.319036	2.153596	-0.677752
C	1.071413	0.198226	-1.209388
H	-3.700560	2.029811	-1.133911
C	-2.712831	2.444027	-0.978971
C	-0.184957	3.553345	-0.435975
C	-1.291517	4.373328	-0.509261
C	-2.560235	3.818253	-0.807376
H	0.801240	3.953667	-0.228044
H	-1.190064	5.440596	-0.346156
H	-3.428729	4.466439	-0.866438
N	0.876531	1.449914	-0.704528
N	0.050037	-0.552802	-1.538378
C	2.474541	-0.263679	-1.344865
C	2.791537	-1.614851	-1.104922
C	3.492660	0.633255	-1.715314
C	4.107428	-2.060471	-1.245806
H	2.021636	-2.300192	-0.763357
C	4.806029	0.180802	-1.856896
H	3.252312	1.673665	-1.903180
C	5.115261	-1.165134	-1.625306
H	4.347827	-3.099177	-1.046475
H	5.585788	0.876225	-2.147908
H	6.137261	-1.513133	-1.732850
H	1.625212	1.779161	0.003876
H	0.291463	-1.445518	-1.959106
O	1.104891	0.608554	2.504017
C	1.980930	1.540822	2.382308
O	2.382170	2.062859	1.303456
C	2.560456	2.059899	3.689447
H	3.275414	2.861828	3.502751
H	1.750758	2.424690	4.330344
H	3.053244	1.240813	4.224240
Cu	0.249817	-0.865887	1.721535
O	-0.389246	-2.581780	1.266463
C	-1.169148	-3.121658	0.407085
O	-1.751023	-2.538013	-0.559227
C	-1.433956	-4.606277	0.577774
H	-0.557997	-5.107628	0.994963
H	-2.265001	-4.733699	1.282336
H	-1.722396	-5.057584	-0.373078
Pd	-1.779605	-0.388531	-0.753873
Cl	-3.800745	-0.315155	0.380816

Pd6

E= -1426.8177057au

H	-2.878364	1.366984	0.837543
C	-3.474581	0.521250	0.513697
C	-2.845521	-0.643343	0.034844
C	-4.868688	0.592959	0.558765
C	-1.358386	-0.712932	-0.001152
C	-3.634603	-1.720188	-0.414064
C	-5.648241	-0.486730	0.126816
H	-5.344244	1.493774	0.930844
N	-0.796359	-1.946371	0.182016

N	-0.609080	0.330054	-0.192210
C	-5.028430	-1.641284	-0.365246
H	-3.171146	-2.602218	-0.847589
H	-6.730804	-0.425295	0.163063
C	0.546158	-2.316968	0.094550
H	-1.444971	-2.695014	0.391623
H	-5.627409	-2.471667	-0.723763
C	0.779895	-3.718402	0.153999
C	1.618342	-1.385990	-0.061331
C	2.058316	-4.218676	0.011789
H	-0.061941	-4.392621	0.292328
C	2.906608	-1.949451	-0.224489
C	3.129473	-3.323185	-0.191493
H	2.233924	-5.288139	0.050642
H	3.748458	-1.283154	-0.350818
H	4.138199	-3.705626	-0.308380
H	-1.058298	1.293069	-0.316089
Pd	1.338495	0.596814	-0.046428
Cl	3.557226	1.117512	0.399212
O	-1.223038	2.853631	-0.315295
C	-0.071231	3.359121	-0.199911
O	1.035936	2.705601	-0.105347
C	0.075306	4.872557	-0.174438
H	0.692059	5.196284	-1.019757
H	-0.904017	5.350654	-0.228029
H	0.593334	5.179760	0.739928

Pd6-Dep-TS

E= -1426.8152431au

H	-2.909694	1.218409	1.041002
C	-3.479720	0.393739	0.629577
C	-2.806879	-0.699077	0.053949
C	-4.875689	0.418671	0.663771
C	-1.313085	-0.715561	0.028318
C	-3.556187	-1.754219	-0.501064
C	-5.615574	-0.639712	0.122242
H	-5.384789	1.264572	1.113010
N	-0.735913	-1.955033	0.183403
N	-0.609558	0.358869	-0.129367
C	-4.953033	-1.723579	-0.465060
H	-3.056542	-2.578234	-1.003271
H	-6.699957	-0.615559	0.149042
C	0.608101	-2.300583	0.092072
H	-1.375269	-2.715955	0.380551
H	-5.520998	-2.535898	-0.906351
C	0.876731	-3.697233	0.140948
C	1.655513	-1.346403	-0.065969
C	2.166093	-4.164920	-0.014235
H	0.052400	-4.391768	0.283610
C	2.955788	-1.872075	-0.240008
C	3.212275	-3.242085	-0.218882
H	2.368562	-5.229912	0.016452
H	3.779678	-1.183869	-0.366799
H	4.229422	-3.597838	-0.346921
H	-1.085307	1.526736	-0.256953
Pd	1.335518	0.621346	-0.035080
Cl	3.545304	1.207729	0.426917
O	-1.300662	2.721972	-0.321480
C	-0.171825	3.347159	-0.228177
O	0.952399	2.783839	-0.111966
C	-0.226154	4.857165	-0.285236
H	0.742706	5.282544	-0.022822
H	-0.496688	5.172756	-1.299734
H	-1.001235	5.229653	0.391127

Pd4

E= -1197.7386363au

H	2.866449	-1.783562	1.231705
C	3.459506	-1.068696	0.673448
C	2.808568	0.007575	0.043051
C	4.845929	-1.200531	0.580601
C	1.327617	0.121881	0.153997
C	3.564476	0.934871	-0.698735
C	5.596421	-0.265943	-0.144959
H	5.341531	-2.029450	1.074739
N	0.806767	1.396610	0.115462
N	0.590864	-0.932010	0.306734
C	4.952705	0.798461	-0.787445

H	3.070861	1.735160	-1.242488
H	6.673957	-0.371305	-0.216621
C	-0.548387	1.739399	0.107300
H	1.462139	2.156348	0.259246
H	5.527790	1.512065	-1.368170
C	-0.852556	3.121832	0.175931
C	-1.584359	0.780858	0.031281
C	-2.170760	3.550726	0.168953
H	-0.041364	3.842407	0.242614
C	-2.914673	1.237558	0.052899
C	-3.205914	2.604560	0.104729
H	-2.396169	4.610453	0.217473
H	-3.721214	0.518925	0.002786
H	-4.241011	2.929208	0.087897
Pd	-1.271683	-1.182835	-0.011065
Cl	-3.382376	-2.125726	-0.323640

Pd4-Re-TS

E= -1197.7120705au

H	-2.377866	-1.930884	0.433274
C	-3.103081	-1.144099	0.260552
C	-2.651485	0.168312	0.032555
C	-4.470211	-1.426595	0.250316
C	-1.197662	0.452684	0.045356
C	-3.589670	1.192762	-0.194000
C	-5.399302	-0.406186	0.011113
H	-4.810009	-2.442162	0.422770
N	-0.694786	1.509565	-0.669653
N	-0.354583	-0.216010	0.787471
C	-4.956285	0.903520	-0.208869
H	-3.262147	2.220204	-0.321303
H	-6.461086	-0.628989	0.000074
C	0.637750	1.822752	-0.394576
H	-1.271660	2.064768	-1.284134
H	-5.673086	1.699693	-0.380080
C	1.211691	3.074333	-0.677759
C	1.343627	0.859627	0.350415
C	2.458485	3.382560	-0.140835
H	0.663640	3.803541	-1.266800
C	2.554803	1.215131	0.969881
C	3.112328	2.469374	0.704706
H	2.910389	4.345773	-0.351037
H	3.086702	0.503362	1.589176
H	4.073430	2.725085	1.137817
Pd	1.181305	-1.218951	0.126339
Cl	2.965961	-2.395800	-0.745248

Pd5

E= -1197.8112837au

H	-1.904534	-0.072623	1.130242
C	-2.169181	-1.010036	0.647890
C	-1.166013	-1.803068	0.057390
C	-3.499524	-1.434463	0.638882
C	0.229646	-1.358534	0.052906
C	-1.522695	-3.033596	-0.530140
C	-3.844684	-2.659261	0.055027
H	-4.262269	-0.810803	1.091841
N	1.289755	-2.237348	0.046414
N	0.669286	-0.097819	0.039019
C	-2.852702	-3.458017	-0.527302
H	-0.770494	-3.638889	-1.027571
H	-4.878789	-2.986990	0.049978
C	2.471517	-1.506926	0.049886
H	1.202449	-3.236166	0.161571
H	-3.116921	-4.402227	-0.991631
C	3.820567	-1.877604	0.059387
C	2.059250	-0.154272	0.038797
C	4.755945	-0.843226	0.052849
H	4.129677	-2.916886	0.070314
C	3.010997	0.877317	0.026977
C	4.356487	0.512884	0.035215
H	5.813437	-1.083923	0.060023
H	2.703540	1.917623	0.013442
H	5.117283	1.285782	0.028157
Pd	-0.487029	1.674927	-0.056314
Cl	-1.720059	3.631615	-0.149442

Pd7-Oxi-TS

E= -1751.2365574au

H	3.869595	-1.778800	0.915362
C	4.467289	-1.456305	0.070531
C	3.991425	-0.439403	-0.775080
C	5.709150	-2.047718	-0.174519
C	2.660413	0.198671	-0.512073
C	4.770165	-0.038722	-1.876569
C	6.484656	-1.640527	-1.267071
H	6.069989	-2.827945	0.487588
N	2.612916	1.564087	-0.739756
N	1.662351	-0.513942	-0.124858
C	6.009706	-0.638269	-2.120007
H	4.393334	0.710431	-2.566782
H	7.446691	-2.105636	-1.456162
C	1.669914	2.429030	-0.141516
H	3.504137	1.989878	-0.954596
H	6.596093	-0.330270	-2.979686
C	2.000284	3.799738	-0.074094
C	0.458442	1.969492	0.405196
C	1.157992	4.697753	0.574279
H	2.930660	4.147066	-0.517185
C	-0.360970	2.883106	1.087552
C	-0.022021	4.237805	1.173292
H	1.427443	5.747678	0.625261
H	-1.280644	2.534661	1.543941
H	-0.676348	4.927658	1.696691
H	1.624710	-1.544391	0.712985
Pd	-0.214539	0.101976	0.057395
Cl	-1.067529	-2.070295	-0.833963
C	-3.425829	0.391441	-0.161748
N	-2.315425	0.621906	0.075826
C	-4.750282	-0.022518	-0.504343
C	-4.910869	-1.313482	-1.051741
C	-5.860147	0.821823	-0.310009
C	-6.190590	-1.747166	-1.401542
H	-4.035245	-1.940559	-1.189627
C	-7.132062	0.370826	-0.665009
H	-5.721335	1.811400	0.111187
C	-7.297546	-0.909915	-1.209641
H	-6.322925	-2.737292	-1.823601
H	-7.991972	1.015270	-0.518375
H	-8.289265	-1.254344	-1.484242
O	1.461798	-2.215064	1.646286
C	0.489816	-1.793311	2.382485
O	-0.228202	-0.776421	2.148700
C	0.179561	-2.611139	3.615345
H	-0.411534	-3.483420	3.311926
H	1.104469	-2.971460	4.071714
H	-0.399693	-2.025519	4.330128

Pd3-Oxi-TS

E= -2175.9193177au

C	0.590042	1.866880	-0.294535
C	-0.740669	2.121780	-0.747384
C	-1.446215	-0.238863	-0.971511
H	2.369486	2.841875	0.434019
C	1.360596	2.990800	0.070579
C	-1.246351	3.455998	-0.839677
C	-0.449300	4.523781	-0.483384
C	0.863087	4.290807	-0.018804
H	-2.266223	3.604498	-1.175154
H	-0.832999	5.535588	-0.554821
H	1.489005	5.128196	0.274252
N	-1.619817	1.125776	-1.129487
N	-0.409342	-0.745052	-0.367017
C	-2.498224	-1.153559	-1.518110
C	-2.093815	-2.462043	-1.858417
C	-3.836574	-0.771773	-1.741092
C	-3.010099	-3.371546	-2.388354
H	-1.059026	-2.752938	-1.718539
C	-4.746391	-1.690318	-2.273941
H	-4.183930	0.224588	-1.492330
C	-4.340989	-2.990261	-2.595691
H	-2.680840	-4.372174	-2.647864
H	-5.775395	-1.385394	-2.434572
H	-5.052709	-3.696488	-3.011346
H	-2.604738	1.453113	-1.221226

H	-0.629113	-1.832774	0.368115
O	-2.447585	-1.694645	2.258233
C	-1.667598	-2.663185	2.023422
O	-0.807937	-2.740986	1.072014
C	-1.703796	-3.846094	2.965182
H	-1.515151	-4.771540	2.417009
H	-0.907418	-3.733217	3.711013
H	-2.662614	-3.892658	3.483287
O	-4.229669	1.463086	1.436116
C	-4.553481	2.254317	0.470039
O	-4.112559	2.211564	-0.708152
C	-5.568520	3.325581	0.843018
H	-6.485383	2.853836	1.212361
H	-5.172445	3.942550	1.656891
H	-5.798182	3.953436	-0.018842
Pd	1.367833	0.037032	-0.219888
Cl	2.372572	-2.179647	-0.467760
C	4.519998	0.537296	0.025676
N	3.367840	0.651779	-0.025823
C	5.919194	0.253476	0.076980
C	6.320535	-1.095836	-0.026781
C	6.873378	1.278454	0.226958
C	7.680120	-1.406279	0.022329
H	5.565113	-1.865868	-0.144574
C	8.228571	0.949638	0.274121
H	6.551915	2.311168	0.304658
C	8.631636	-0.388745	0.172552
H	7.996244	-2.440493	-0.056859
H	8.968793	1.733717	0.389574
H	9.687010	-0.637854	0.210103
Cu	-3.219139	-0.090074	1.648041

Pd8

E= -737.5219183au

C	-2.063513	0.160508	0.012210
C	-1.203170	1.270882	0.098813
C	0.937440	-0.027900	-0.006956
H	-4.125872	-0.491586	-0.039686
C	-3.453007	0.360993	0.029218
C	-1.754170	2.566865	0.212124
C	-3.134496	2.749852	0.235142
C	-3.994176	1.647521	0.141747
H	-1.091198	3.426115	0.277987
H	-3.539950	3.752598	0.323519
H	-5.070326	1.785546	0.158059
N	0.194130	1.146501	0.074834
N	0.487794	-1.229221	-0.098257
C	2.424187	0.178718	0.004934
C	3.247986	-0.768018	0.638153
C	3.015596	1.287948	-0.626567
C	4.634031	-0.598246	0.654761
H	2.787325	-1.626819	1.112191
C	4.404539	1.454491	-0.608308
H	2.398938	2.001547	-1.164799
C	5.217034	0.515105	0.035570
H	5.259517	-1.332180	1.152820
H	4.849750	2.310438	-1.105611
H	6.294366	0.645601	0.050222
H	0.719532	1.984617	0.280214
Pd	-1.367940	-1.666721	-0.126218

Pd9

E= -1061.9860672au

H	3.557288	-2.550248	0.992069
C	4.387894	-2.036878	0.521641
C	4.156283	-0.775709	-0.055448
C	5.660400	-2.610032	0.485042
C	2.774604	-0.192695	-0.005825
C	5.223575	-0.110211	-0.685646
C	6.722086	-1.935711	-0.133096
H	5.826228	-3.581516	0.940380
N	2.737716	1.202772	0.032174
N	1.751907	-0.960828	-0.009696
C	6.498057	-0.687025	-0.722169
H	5.055430	0.839926	-1.183891
H	7.711152	-2.382231	-0.159990
C	1.589556	1.999336	0.115192
H	3.616060	1.669311	0.208077

H	7.310083	-0.165544	-1.219578
C	1.785923	3.398201	0.199778
C	0.277342	1.475311	0.111420
C	0.704958	4.269358	0.278992
H	2.800090	3.791186	0.197580
C	-0.798943	2.378008	0.185048
C	-0.599298	3.760339	0.270250
H	0.878958	5.338906	0.344708
H	-1.812713	1.994211	0.183127
H	-1.452222	4.429315	0.331541
Pd	-0.090585	-0.485909	0.010828
C	-3.352918	-0.611833	-0.039293
N	-2.195571	-0.508486	-0.014217
C	-4.777889	-0.732664	-0.071936
C	-5.484341	-0.408340	-1.248939
C	-5.473667	-1.175378	1.072333
C	-6.874305	-0.528278	-1.274021
H	-4.942562	-0.068863	-2.124562
C	-6.863646	-1.291054	1.032256
H	-4.923997	-1.422028	1.973731
C	-7.564441	-0.968724	-0.137190
H	-7.418157	-0.279058	-2.178536
H	-7.399338	-1.631543	1.911547
H	-8.645140	-1.060374	-0.162459

Pd10

E= -1198.3866292au

H	-2.467689	-0.584826	0.963935
C	-2.631358	0.423312	0.596188
C	-1.574274	1.103905	-0.035141
C	-3.890781	1.019457	0.699731
C	-0.206010	0.503745	-0.132137
C	-1.807121	2.385271	-0.572470
C	-4.115569	2.292638	0.162296
H	-4.699634	0.480487	1.181375
N	0.657712	0.993025	-1.149072
N	0.644925	0.364422	1.033597
C	-3.071860	2.971906	-0.476816
H	-0.993920	2.917192	-1.054136
H	-5.097961	2.748130	0.233824
C	1.981083	1.010058	-0.700353
H	0.414296	0.828467	-2.117157
H	-3.240216	3.958134	-0.897213
C	3.173336	1.307944	-1.362203
C	1.979354	0.704399	0.672543
C	4.350094	1.324263	-0.602508
H	3.189207	1.528450	-2.423379
C	3.142091	0.726385	1.435535
C	4.336740	1.048618	0.774875
H	5.290386	1.556930	-1.090145
H	3.132261	0.485623	2.493101
H	5.264513	1.073141	1.335328
H	0.279689	0.638731	1.939644
Pd	-0.064536	-1.517094	0.258547
Cl	-1.012654	-3.310452	-0.847485

Pd11-Oxi-TS

E= -1982.919214au

C	-0.605133	1.894528	-0.361249
C	-1.993375	2.162324	-0.316500
C	-2.743333	-0.211038	-0.141905
H	1.350205	2.784136	-0.490496
C	0.286613	2.978470	-0.452429
C	-2.459920	3.500793	-0.365512
C	-1.562540	4.551446	-0.451104
C	-0.179401	4.290944	-0.495429
H	-3.528534	3.691669	-0.317740
H	-1.927420	5.572339	-0.481426
H	0.526412	5.111566	-0.566145
N	-2.945156	1.159257	-0.229193
N	-1.628366	-0.855963	-0.142326
C	-4.000283	-1.023561	-0.038366
C	-4.034213	-2.305372	-0.614162
C	-5.130863	-0.542480	0.646667
C	-5.191832	-3.081229	-0.527418
H	-3.148325	-2.677729	-1.115117
C	-6.287546	-1.324256	0.730286
H	-5.101048	0.415743	1.158006

C	-6.322792	-2.591752	0.138831
H	-5.210848	-4.067897	-0.978149
H	-7.151580	-0.949492	1.269342
H	-7.220504	-3.197715	0.205833
H	-3.910957	1.454254	-0.298291
Pd	0.123424	-0.015332	-0.197740
H	-0.183141	0.579492	-1.588183
Cl	1.080263	-2.269021	-0.592890
C	3.374207	0.230450	-0.158490
N	2.268287	0.562967	-0.256944
C	4.701041	-0.290527	-0.053048
C	5.803910	0.555917	0.171559
C	4.874268	-1.685404	-0.176034
C	7.081065	0.002722	0.269796
H	5.655502	1.625674	0.268859
C	6.159022	-2.221089	-0.073223
H	4.004283	-2.312771	-0.342181
C	7.259048	-1.382028	0.147567
H	7.935160	0.648209	0.443225
H	6.300322	-3.292405	-0.163915
H	8.254732	-1.806142	0.226440
Cl	0.075455	0.504865	2.297960

Pd11-Met-TS

E= -1982.9603964au

H	4.148109	-1.180482	1.768206
C	4.170409	-1.649738	0.791195
C	3.420650	-1.094574	-0.261878
C	4.939602	-2.791632	0.561265
C	2.598693	0.111598	-0.026181
C	3.410244	-1.705059	-1.530924
C	4.950903	-3.387547	-0.706921
H	5.524939	-3.217957	1.368747
N	2.608475	1.096502	-0.965427
N	1.953779	0.261197	1.109330
C	4.181200	-2.849392	-1.746635
H	2.742017	-1.332159	-2.300295
H	5.545553	-4.278707	-0.879995
C	1.717590	2.200403	-0.948619
H	3.358371	1.079089	-1.646742
H	4.162127	-3.333483	-2.717023
C	2.207300	3.498191	-1.142094
C	0.335337	1.962949	-0.751857
C	1.321583	4.577414	-1.097995
H	3.269621	3.663206	-1.291048
C	-0.533939	3.071423	-0.696149
C	-0.045972	4.368686	-0.860260
H	1.700346	5.584753	-1.234698
H	-1.595514	2.898669	-0.558022
H	-0.723062	5.215108	-0.822808
Pd	0.017360	0.468269	1.122766
Cl	-0.098106	-0.582299	3.211778
Cl	-0.334695	-1.015769	-1.775913
C	-3.009521	0.011108	0.544573
N	-2.037381	0.487759	0.960299
C	-4.155743	-0.603987	-0.042434
C	-3.974424	-1.326708	-1.242357
C	-5.425357	-0.502381	0.561212
C	-5.081883	-1.942213	-1.828959
H	-2.977886	-1.395958	-1.674979
C	-6.517912	-1.123627	-0.043120
H	-5.543552	0.050482	1.486632
C	-6.346904	-1.841327	-1.235438
H	-4.954292	-2.503225	-2.748139
H	-7.498741	-1.052399	0.414117
H	-7.200944	-2.324524	-1.699112
H	-0.043253	0.934665	-1.029738

Pd11-Anag-TS

E= -1658.5021768au

C	-1.749226	0.920651	-0.054872
C	-0.819696	1.964756	0.199583
C	1.221022	0.667867	-0.208134
H	-3.760173	0.516807	-0.719522
C	-3.037928	1.296999	-0.500280
C	-1.219435	3.311428	0.157288
C	-2.523227	3.642808	-0.210093
C	-3.428966	2.636215	-0.569105

H	-0.495018	4.095706	0.358065
H	-2.822100	4.685013	-0.243629
H	-4.436675	2.891921	-0.877746
N	0.547995	1.686310	0.421340
N	0.594199	-0.165789	-0.993768
C	2.691748	0.556442	-0.028186
C	3.270428	-0.726822	-0.049548
C	3.506057	1.689974	0.148302
C	4.648947	-0.868060	0.122912
H	2.635565	-1.596833	-0.185070
C	4.884262	1.539244	0.318460
H	3.082792	2.690171	0.115304
C	5.456398	0.260936	0.309599
H	5.090370	-1.858542	0.114408
H	5.510242	2.415809	0.447098
H	6.527124	0.146749	0.442542
H	1.104276	2.387279	0.892909
Pd	-0.957036	-1.059207	-0.249757
H	-2.231836	-0.080139	0.920136
Cl	-2.877814	-1.414625	1.367588
Cl	-0.156220	-3.265885	-0.401954

Pd12

E= -1522.7903472au

H	-3.466537	-2.326577	-1.355705
C	-4.334381	-1.855840	-0.909092
C	-4.156750	-0.679881	-0.160302
C	-5.607419	-2.408228	-1.063416
C	-2.774307	-0.096443	0.002451
C	-5.274273	-0.078594	0.447170
C	-6.719469	-1.799428	-0.466551
H	-5.732836	-3.313861	-1.648386
N	-2.790656	1.303755	0.088811
N	-1.798654	-0.933366	0.031318
C	-6.548070	-0.637332	0.292509
H	-5.145009	0.801185	1.069319
H	-7.707897	-2.231600	-0.586307
C	-1.677806	2.184677	0.078853
H	-3.625881	1.700192	-0.322440
H	-7.401102	-0.169960	0.774460
C	-1.649501	3.229964	-0.865077
C	-0.651789	2.083638	1.033003
C	-0.606095	4.157021	-0.859618
H	-2.444946	3.307606	-1.601587
C	0.401583	3.008270	1.015604
H	-0.692852	1.318168	1.798659
C	0.429643	4.045011	0.077702
H	-0.598498	4.960333	-1.589630
H	1.189158	2.918088	1.757013
H	1.242458	4.764088	0.080143
Pd	0.078845	-0.621440	-0.167831
Cl	0.552260	-0.979899	2.155117
C	3.308474	-0.603608	-0.544210
N	2.149231	-0.587588	-0.577854
C	4.733867	-0.642320	-0.436507
C	5.546900	-0.361432	-1.552822
C	5.316406	-0.968457	0.806241
C	6.935345	-0.408072	-1.421128
H	5.089943	-0.112170	-2.503982
C	6.706385	-1.011194	0.921722
H	4.678315	-1.181941	1.656465
C	7.515308	-0.732163	-0.187618
H	7.563864	-0.192774	-2.278296
H	7.157362	-1.261998	1.875468
H	8.595398	-0.767394	-0.091378

Pd13

E= -1983.661915au

C	2.895945	-2.283862	-1.582445
C	2.582525	-1.572950	-0.408654
C	1.624534	-2.128218	0.508468
C	1.050122	-3.400688	0.199701
C	1.352080	-4.070242	-0.980583
C	2.287503	-3.503405	-1.860946
H	3.609559	-1.863321	-2.284501
H	1.627818	-1.762673	1.530097
H	0.389492	-3.843019	0.939089
H	0.892515	-5.028971	-1.207591

H	2.544325	-4.021037	-2.780499
N	3.210097	-0.354356	-0.213374
H	3.719015	-0.006958	-1.014610
C	3.039689	0.577142	0.817679
C	3.493037	1.956528	0.454436
C	4.264614	2.700854	1.363446
C	3.116369	2.536321	-0.771354
C	4.663833	4.002394	1.048422
H	4.564130	2.249626	2.304649
C	3.512688	3.842156	-1.078965
H	2.476787	1.983048	-1.453674
C	4.289656	4.574918	-0.173974
H	5.268937	4.566264	1.751013
H	3.205875	4.288993	-2.019125
H	4.598835	5.586485	-0.417006
N	2.544061	0.222189	1.947935
H	2.442791	1.035199	2.554728
Pd	-0.376497	-1.131618	0.161230
Cl	0.203603	-0.135580	-1.918241
Cl	-1.085766	-1.975485	2.259673
C	-3.218092	0.316560	-0.058465
N	-2.186622	-0.204260	0.001746
C	-4.495118	0.955621	-0.128602
C	-5.416931	0.792114	0.925603
C	-4.825568	1.743629	-1.249817
C	-6.662121	1.417593	0.851156
H	-5.150518	0.183290	1.782219
C	-6.074745	2.362663	-1.309381
H	-4.108131	1.861105	-2.054109
C	-6.991776	2.201115	-0.262507
H	-7.373807	1.293892	1.659971
H	-6.332627	2.969401	-2.170427
H	-7.961607	2.684741	-0.314582

Pd13-Cup-TS

E= -1983.6047236au

C	2.367350	2.630433	0.970690
C	2.425482	1.274894	0.828814
C	1.714151	0.556393	-0.231239
C	0.826492	1.373130	-1.092335
C	0.885298	2.818128	-0.935631
C	1.545266	3.419533	0.099205
H	2.998162	3.128158	1.703718
H	1.337550	-0.436292	-0.003049
H	0.708046	1.006413	-2.113264
H	0.326047	3.422093	-1.646399
H	1.486795	4.490584	0.252404
N	3.514394	0.448346	1.270953
H	4.156744	0.789226	1.975478
C	4.030789	-0.238501	0.194246
C	5.303778	-0.968674	0.317161
C	6.151569	-1.098518	-0.798625
C	5.679541	-1.542013	1.546990
C	7.360470	-1.786571	-0.682270
H	5.873090	-0.640024	-1.742003
C	6.888575	-2.233124	1.655109
H	5.011450	-1.476696	2.399644
C	7.731142	-2.355028	0.543376
H	8.013752	-1.876054	-1.543426
H	7.167957	-2.683115	2.601676
H	8.669520	-2.892421	0.630198
N	3.273670	-0.157027	-0.868228
H	3.390114	-0.809856	-1.634629
Pd	-1.125475	0.658469	-0.522422
Cl	-1.800278	2.614563	0.643438
Cl	-0.527438	-1.393286	-1.631526
C	-4.088469	-0.526701	0.070191
N	-3.022179	-0.120748	-0.126059
C	-5.409466	-1.018917	0.315169
C	-5.810445	-2.257486	-0.225000
C	-6.305840	-0.259521	1.094224
C	-7.102103	-2.727878	0.016447
H	-5.112443	-2.832200	-0.823318
C	-7.594179	-0.742912	1.327602
H	-5.986154	0.692431	1.502899
C	-7.993346	-1.973822	0.790855
H	-7.412912	-3.680330	-0.399011
H	-8.285700	-0.160068	1.926309

H	-8.996494	-2.344215	0.975145

Pd13-Cup-Pro

E= -1983.6382549au

C	-3.286138	3.356349	-0.178158
C	-3.235852	2.036870	-0.434007
C	-1.917042	1.286722	-0.422366
C	-0.959899	1.752323	0.672443
C	-0.993162	3.254690	0.726666
C	-2.050332	3.990221	0.292337
H	-4.206006	3.931211	-0.222725
H	-1.425285	1.404987	-1.402337
H	-1.257127	1.353786	1.658718
H	-0.166328	3.754220	1.223791
H	-2.041580	5.070443	0.396444
N	-4.238156	1.055589	-0.642296
H	-5.226459	1.227942	-0.517404
C	-3.704206	-0.184632	-0.441175
C	-4.493837	-1.413805	-0.362237
C	-3.985592	-2.523608	0.341957
C	-5.758510	-1.494191	-0.976746
C	-4.742923	-3.692413	0.432004
H	-3.017465	-2.466139	0.830587
C	-6.507247	-2.668024	-0.882750
H	-6.139688	-0.658757	-1.556010
C	-6.002069	-3.767572	-0.177059
H	-4.350963	-4.542058	0.979875
H	-7.476505	-2.728734	-1.365538
H	-6.585293	-4.679493	-0.105739
N	-2.395864	-0.102253	-0.298276
H	-1.739222	-0.842501	0.015467
Pd	0.844163	0.805045	0.414875
Cl	1.767591	2.728230	-0.608885
Cl	-0.127512	-1.306034	1.255133
C	3.818273	-0.589022	0.019289
N	2.747194	-0.176816	0.177309
C	5.151193	-1.069015	-0.186296
C	5.491937	-2.390730	0.164072
C	6.121151	-0.209283	-0.740773
C	6.796032	-2.843901	-0.041362
H	4.738712	-3.043482	0.590864
C	7.421363	-0.675868	-0.940293
H	5.846721	0.805494	-1.006118
C	7.760200	-1.989865	-0.592224
H	7.059935	-3.860828	0.228368
H	8.168775	-0.015412	-1.366393
H	8.772669	-2.347198	-0.749390

Pd13-Dep-TS

E= -1983.5993119au

C	-3.331073	-3.100494	0.398934
C	-3.126987	-1.756154	0.259658
C	-1.838510	-1.230358	-0.186419
C	-0.950377	-2.050016	-1.060726
C	-1.220628	-3.472986	-0.865426
C	-2.291301	-3.945468	-0.132460
H	-4.226181	-3.526856	0.833646
H	-1.190979	-1.259261	0.920824
H	-0.804678	-1.716344	-2.097996
H	-0.611662	-4.189519	-1.414946
H	-2.422688	-5.019579	-0.036209
N	-3.908938	-0.617522	0.497905
H	-4.876311	-0.624717	0.787571
C	-3.266177	0.508459	0.038082
C	-3.812782	1.860945	0.084881
C	-3.268106	2.862901	-0.743593
C	-4.878702	2.178728	0.949029
C	-3.789030	4.156202	-0.707599
H	-2.450522	2.628901	-1.417718
C	-5.396598	3.474342	0.975812
H	-5.279010	1.431924	1.627606
C	-4.855107	4.464776	0.147304
H	-3.365059	4.921609	-1.348029
H	-6.212023	3.713376	1.649693
H	-5.257540	5.471792	0.171625
N	-2.088181	0.153626	-0.446227
H	-1.284378	0.736590	-0.775316
Pd	0.951656	-1.648645	-0.436841

Cl	-0.113223	-1.480276	2.232218
Cl	0.660519	0.732775	-1.540386
C	3.864303	-0.358187	0.174139
N	3.049681	-1.178841	0.067591
C	4.794843	0.726497	0.248546
C	4.436375	1.958859	-0.337659
C	6.039094	0.576953	0.890840
C	5.329192	3.030095	-0.276418
H	3.470176	2.053435	-0.822794
C	6.920825	1.657836	0.942936
H	6.302241	-0.373878	1.340801
C	6.568317	2.882329	0.360618
H	5.057636	3.979684	-0.724910
H	7.879866	1.546137	1.437383
H	7.257534	3.719493	0.404564

Pd14

E= -1062.0397219au

C	-1.733647	-2.622574	1.606394
C	-2.318738	-1.574834	0.871350
C	-1.958492	-1.272502	-0.463932
C	-0.965222	-2.049918	-1.124485
C	-0.383055	-3.123884	-0.396946
C	-0.765320	-3.380887	0.962865
H	-2.024827	-2.835264	2.629650
H	-0.842024	-1.956156	-2.200688
H	0.195531	-3.883210	-0.922505
H	-0.300098	-4.212253	1.482977
N	-3.309608	-0.657791	1.175524
H	-3.793249	-0.577698	2.056255
C	-3.514093	0.129842	0.050443
C	-4.496502	1.213930	-0.015910
C	-4.621609	1.942242	-1.216239
C	-5.321564	1.555737	1.072838
C	-5.546869	2.980336	-1.320509
H	-3.982918	1.674792	-2.049750
C	-6.246990	2.596964	0.964309
H	-5.251589	1.016440	2.013264
C	-6.364426	3.313566	-0.231921
H	-5.631736	3.531748	-2.251568
H	-6.875280	2.847593	1.813214
H	-7.083852	4.121824	-0.315115
N	-2.714236	-0.227860	-0.945704
Pd	1.094230	-1.490680	-0.364424
C	3.713311	0.315994	-0.046452
N	2.739592	-0.312921	-0.163288
C	4.907516	1.089730	0.094050
C	5.110224	1.874990	1.248773
C	5.887008	1.068571	-0.921459
C	6.279178	2.625740	1.380031
H	4.354279	1.888320	2.025852
C	7.051223	1.824303	-0.777497
H	5.726391	0.463769	-1.806842
C	7.250071	2.602355	0.370391
H	6.432753	3.228682	2.268567
H	7.802650	1.806480	-1.559561
H	8.157127	3.188013	0.477459

Pd11-FC-TS

E= -1982.994865au

C	-2.671982	-1.985803	0.550720
C	-3.961457	-1.380993	0.332838
C	-5.022026	-2.087759	-0.231408
C	-4.801869	-3.400274	-0.666720
C	-3.515852	-3.983201	-0.575267
C	-2.467683	-3.301192	0.022822
C	-2.657406	0.535775	0.163896
H	-5.981481	-1.606074	-0.392440
H	-5.615001	-3.957238	-1.119438
H	-3.362003	-4.990588	-0.947555
H	-1.500831	-3.772570	0.159441
N	-1.736420	-0.328665	-0.096848
N	-3.916815	0.002470	0.507190
C	-2.549002	2.013565	0.123074
C	-1.745976	2.648645	-0.841232
C	-3.270006	2.788888	1.052436
C	-1.672601	4.043776	-0.871218
H	-1.192778	2.051242	-1.558298

C	-3.185059	4.182947	1.017793
H	-3.862694	2.301058	1.819842
C	-2.388652	4.813227	0.054149
H	-1.055162	4.528115	-1.620355
H	-3.731531	4.773808	1.745708
H	-2.323971	5.896338	0.027402
H	-4.733281	0.564284	0.299105
H	-2.107911	-1.725806	1.449975
Pd	0.239762	-0.265776	-0.077298
Cl	0.315560	0.102801	-2.422535
Cl	0.172324	-0.677697	2.264398
C	3.422671	-0.229425	0.013578
N	2.266589	-0.258750	-0.027788
C	4.850880	-0.194674	0.065045
C	5.508647	-0.268462	1.309936
C	5.593008	-0.086982	-1.128839
C	6.902969	-0.233804	1.352302
H	4.926515	-0.351386	2.220801
C	6.986767	-0.053883	-1.069830
H	5.075351	-0.030675	-2.079772
C	7.641617	-0.126948	0.166599
H	7.412351	-0.290272	2.307998
H	7.560839	0.028801	-1.986129
H	8.725566	-0.100693	0.206090

Pd1-Dep-TS

E= -2312.2811053au

C	1.160902	-1.184916	-0.705911
C	-0.066980	-0.791691	-1.336197
C	-0.676940	-1.603379	-2.324169
C	-0.063872	-2.783630	-2.718077
C	1.142486	-3.198281	-2.117508
C	1.732939	-2.414005	-1.131726
C	-0.282406	1.479540	-0.406883
H	-1.615205	-1.285341	-2.762496
H	-0.522583	-3.392241	-3.490009
H	1.604308	-4.132193	-2.418671
H	2.652300	-2.738614	-0.660429
N	1.016069	1.658810	-0.264888
N	-0.779403	0.345812	-0.958450
C	-1.240138	2.552646	-0.032897
C	-0.899658	3.899334	-0.266692
C	-2.467561	2.242740	0.580495
C	-1.775760	4.918746	0.109023
H	0.030218	4.149084	-0.768712
C	-3.335751	3.269213	0.959916
H	-2.737876	1.210947	0.771755
C	-2.993516	4.605896	0.725884
H	-1.511524	5.952514	-0.084786
H	-4.276562	3.023583	1.440233
H	-3.671872	5.399589	1.020481
H	1.079884	-1.049851	0.561723
H	-1.818269	0.305758	-1.186149
O	-0.968853	-2.212314	2.270018
C	0.158716	-1.740975	2.633288
O	0.929015	-1.013644	1.922179
C	0.644496	-2.098087	4.023372
H	-0.184669	-2.430907	4.648825
H	1.380088	-2.908224	3.947917
H	1.148418	-1.240832	4.476274
Cu	-2.289897	-1.792774	1.013036
O	-3.835748	-1.522117	0.011471
C	-4.122471	-0.808775	-1.025263
O	-3.344102	-0.010906	-1.610617
C	-5.537443	-0.980885	-1.550919
H	-6.257587	-0.776217	-0.751966
H	-5.717104	-0.312587	-2.393578
H	-5.691006	-2.019502	-1.863959
Pd	2.560755	0.417070	-0.267627
Cl	4.419510	-0.924099	-0.043513
Cl	3.890872	2.355973	-0.094003
H	1.283399	2.566982	0.108643

Pd2-CN-TS

E= -1198.3440696au

H	-2.348472	-1.891854	0.698258
C	-3.082790	-1.136950	0.436532
C	-2.651194	0.130623	-0.006678

C	-4.444924	-1.438008	0.486645
C	-1.222126	0.438800	-0.033551
C	-3.612404	1.082756	-0.407506
C	-5.391923	-0.489205	0.081916
H	-4.765700	-2.417760	0.823587
N	-0.675454	1.373803	-0.851303
N	-0.307405	-0.063848	0.822141
C	-4.971325	0.769658	-0.367632
H	-3.301571	2.077748	-0.711432
H	-6.449418	-0.728619	0.113758
C	0.621413	1.749752	-0.504395
H	-1.192419	1.789743	-1.613013
H	-5.703023	1.510330	-0.672257
C	1.245853	2.955834	-0.859139
C	1.195470	0.867974	0.455089
C	2.379409	3.343136	-0.152699
H	0.820156	3.591576	-1.629418
C	2.252668	1.351998	1.268718
C	2.850401	2.562401	0.927212
H	2.878970	4.271978	-0.403415
H	2.650878	0.742360	2.070418
H	3.715775	2.899471	1.488513
H	-0.655481	-0.432828	1.703492
Pd	1.295604	-1.110539	0.065688
Cl	2.977728	-2.507628	-0.743121

Pd6-CN-TS

E= -1426.7816233au

H	2.543505	1.523888	-0.021890
C	3.233318	0.695125	-0.134606
C	2.748675	-0.627897	-0.137992
C	4.602190	0.937830	-0.263416
C	1.300859	-0.877019	-0.015048
C	3.660597	-1.696174	-0.261514
C	5.500264	-0.126955	-0.402581
H	4.965558	1.959568	-0.258453
N	0.755767	-2.059497	-0.422915
N	0.433501	-0.051796	0.541875
C	5.026271	-1.444959	-0.397792
H	3.317448	-2.725154	-0.212585
H	6.562589	0.066918	-0.506823
C	-0.532287	-2.313034	0.060957
H	1.299751	-2.761102	-0.902718
H	5.719893	-2.274175	-0.486930
C	-1.092379	-3.592499	0.204677
C	-1.192082	-1.184504	0.587442
C	-2.248372	-3.735602	0.968610
H	-0.601706	-4.456423	-0.232826
C	-2.285288	-1.342667	1.456974
C	-2.818379	-2.624323	1.617753
H	-2.689499	-4.717963	1.094013
H	-2.750179	-0.484641	1.926862
H	-3.701032	-2.754894	2.234475
H	0.717774	0.856516	1.037363
Pd	-1.301158	0.543408	-0.497568
Cl	-3.180109	0.793603	-1.872017
O	0.803580	2.360202	1.449270
C	-0.143728	3.037669	0.960456
O	-1.108093	2.579319	0.240319
C	-0.203457	4.534953	1.227582
H	-0.232512	5.081767	0.279815
H	-1.124294	4.774719	1.769369
H	0.661860	4.846163	1.814310

Cu2-Oxi-3(T)

E= -1689.1136652au

C	-1.587349	-1.318006	1.031300
C	-0.180375	-1.443095	1.277173
C	0.435668	0.960637	0.994799
H	-3.432106	-2.410945	0.997637
C	-2.363779	-2.477581	1.180297
C	0.410073	-2.700728	1.637297
C	-0.398622	-3.806074	1.782967
C	-1.797466	-3.697438	1.561370
H	1.483436	-2.759664	1.782409
H	0.032123	-4.761355	2.062824
H	-2.426251	-4.574197	1.685600
N	0.703520	-0.388813	1.163293

N	-0.776758	1.400041	0.865224
Cu	-2.411638	0.339728	0.345931
C	1.622074	1.860428	0.970611
C	1.666357	2.898162	0.019797
C	2.673279	1.715504	1.893063
C	2.745760	3.784465	0.001516
H	0.878305	2.977430	-0.722363
C	3.745987	2.610674	1.873704
H	2.652746	0.915463	2.624249
C	3.783892	3.645366	0.931247
H	2.780674	4.574420	-0.741034
H	4.549934	2.499814	2.593360
H	4.620592	4.336114	0.917594
H	1.721966	-0.664171	1.120112
O	-4.459073	-0.091887	0.467571
C	-4.694462	1.144117	0.225047
O	-3.712169	1.954077	0.112819
C	-6.110186	1.622932	0.034345
H	-6.398396	1.487080	-1.015380
H	-6.797910	1.039885	0.651282
H	-6.188987	2.684986	0.275912
H	-0.826841	2.413305	0.784032
O	3.427269	-1.216308	-1.338678
C	3.869438	-1.490723	-0.154434
O	3.249256	-1.305728	0.924255
C	5.269430	-2.080540	-0.116897
H	5.551229	-2.334326	0.905638
H	5.314931	-2.972907	-0.749561
H	5.983336	-1.357299	-0.526251
Cu	1.750389	-0.491924	-1.714965
O	0.071869	0.284419	-1.919032
C	-1.058189	-0.127995	-2.403811
O	-2.148697	-0.018280	-1.797401
C	-1.052310	-0.748955	-3.794839
H	-0.531953	-0.087689	-4.495325
H	-0.509143	-1.701432	-3.773948
H	-2.071760	-0.926681	-4.137995

Cu5(T)

E= -1264.4335999au

C	1.104152	1.524256	-0.373728
C	-0.108689	2.209953	-0.315406
C	-0.100414	3.605715	-0.530746
C	1.093603	4.269420	-0.807099
C	2.297534	3.557639	-0.878624
C	2.300648	2.170960	-0.659379
C	-1.672487	0.276079	0.022380
H	-1.035607	4.160017	-0.486573
H	1.082867	5.341912	-0.971418
H	3.227332	4.072025	-1.099580
H	3.226742	1.607438	-0.699563
N	-0.771549	-0.655702	-0.045209
N	-1.362933	1.602180	-0.055758
C	-3.124196	-0.031934	0.194111
C	-3.515403	-1.041243	1.091500
C	-4.105213	0.662021	-0.537018
C	-4.868520	-1.346603	1.258096
H	-2.761937	-1.564349	1.671694
C	-5.457725	0.350277	-0.369580
H	-3.810847	1.415603	-1.261310
C	-5.841715	-0.651859	0.529230
H	-5.162562	-2.119900	1.959729
H	-6.207880	0.880963	-0.946462
H	-6.891903	-0.891527	0.659087
Cu	1.231684	-0.602698	0.036821
O	3.166673	-0.605988	0.711520
C	2.749646	-0.495018	1.920068
O	1.491681	-0.392142	2.116829
C	3.719328	-0.521828	3.067726
H	3.975557	-1.562264	3.301251
H	4.642020	-0.003507	2.794936
H	3.274279	-0.065654	3.953851
H	-1.137373	-1.602430	-0.064805
H	-2.126656	2.238407	0.122373
O	1.043304	-2.916993	-0.468357
C	1.408324	-2.513388	-1.601853
O	1.592147	-1.248888	-1.832541

C	1.674196	-3.466711	-2.746475
H	2.754073	-3.528401	-2.924511
H	1.295659	-4.460729	-2.502415
H	1.209908	-3.099023	-3.666165

Cu3(T)

E= -1035.3582819au

C	1.322757	1.312553	-0.056777
C	0.160455	2.108087	-0.121381
C	-1.432648	0.206305	-0.357792
H	3.464879	1.399373	0.092005
C	2.551600	1.985604	0.042731
C	0.221406	3.516156	-0.086329
C	1.456728	4.151382	0.017121
C	2.627977	3.385166	0.082304
H	-0.692548	4.104023	-0.144596
H	1.505609	5.235280	0.041613
H	3.593862	3.875247	0.160762
N	-1.136263	1.530768	-0.172527
N	-0.528622	-0.639274	-0.744725
Cu	1.343039	-0.689261	-0.101685
C	-2.838265	-0.223728	-0.117025
C	-3.363440	-1.300886	-0.853766
C	-3.637130	0.414043	0.849811
C	-4.677069	-1.720954	-0.636519
H	-2.737977	-1.787755	-1.593330
C	-4.952686	-0.008284	1.059338
H	-3.221611	1.210599	1.459294
C	-5.475247	-1.073579	0.315631
H	-5.079343	-2.548660	-1.210876
H	-5.563188	0.482932	1.809781
H	-6.496108	-1.401598	0.482081
H	-1.919403	2.172454	-0.192529
O	3.390000	-1.127437	-0.021103
C	3.068423	-2.338711	0.239460
O	1.826241	-2.639604	0.312913
C	4.126169	-3.393223	0.420310
H	4.364655	-3.839846	-0.552879
H	5.040060	-2.951411	0.823182
H	3.763062	-4.185789	1.077935

Cu3-Re-TS(T)

E=-1035.3158112au

Cu	-0.960420	-0.951472	-0.142673
H	2.022073	-1.255428	-0.965076
C	2.756483	-0.558335	-0.578126
C	2.335140	0.706519	-0.121056
C	4.104067	-0.913708	-0.516630
C	0.908551	1.077720	-0.198931
C	3.294860	1.608857	0.380343
C	5.052727	-0.012517	-0.013735
H	4.414892	-1.894610	-0.860633
N	0.375918	2.006293	0.667078
N	0.041342	0.526284	-1.029656
C	4.644107	1.250400	0.430246
H	3.001445	2.604970	0.698540
H	6.100769	-0.290662	0.027452
C	-1.021047	2.149636	0.488131
H	0.922446	2.550542	1.316857
H	5.374836	1.957469	0.809401
C	-1.733067	3.310482	0.726045
C	-1.570555	1.016076	-0.205850
C	-3.047230	3.424157	0.207646
H	-1.273834	4.145764	1.246719
C	-2.852705	1.215174	-0.808907
C	-3.566826	2.402365	-0.595701
H	-3.622758	4.324037	0.394710
H	-3.323311	0.407078	-1.361831
H	-4.556404	2.512366	-1.029763
O	-0.218632	-2.805293	-0.217704
C	-1.283536	-3.264139	0.346697
O	-2.202771	-2.437459	0.654989
C	-1.423149	-4.735711	0.610905
H	-1.498683	-5.273644	-0.340968
H	-0.532769	-5.108588	1.126287
H	-2.313049	-4.934491	1.209103

Cu4(T)

E= -1035.385621au

C	−2.111385	−0.696327	0.078817
C	−3.050529	0.389635	0.029038
C	−0.923431	1.201483	0.033585
H	−1.877049	−2.857951	0.192379
C	−2.579788	−2.033125	0.140700
C	−4.421026	0.171651	0.056780
C	−4.865320	−1.164583	0.120285
C	−3.956426	−2.245086	0.155860
H	−5.128692	0.991894	0.022346
H	−5.930873	−1.365605	0.142025
H	−4.340762	−3.257862	0.206120
N	−2.296863	1.550828	−0.068330
N	−0.840375	−0.228774	0.074503
Cu	0.684110	−1.300570	−0.265045
C	0.128817	2.108653	0.029122
C	1.497913	1.710608	0.296634
C	−0.111625	3.514614	−0.240951
C	2.518784	2.642083	0.266686
H	1.739592	0.689207	0.571361
C	0.929696	4.418507	−0.259034
H	−1.114277	3.848982	−0.486975
C	2.260892	4.002974	−0.008311
H	3.530549	2.312058	0.477407
H	0.727692	5.462031	−0.481031
H	3.069999	4.724630	−0.022557
H	−2.631425	2.434872	0.290459
O	2.099396	−2.462700	−0.515256
C	3.187046	−2.089519	0.125373
O	3.247568	−1.078559	0.841261
C	4.380126	−3.007942	−0.072812
H	4.140887	−4.012306	0.293649
H	4.607605	−3.098674	−1.140341
H	5.250039	−2.620815	0.459578