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Supporting Information

Computational study of the effects of the ancillary ligands on Copper(I)-ethylene interaction.

Stéphanie HALBERT[1,2]*, Hélène GERARD[1,2].

1. Sorbonne Universités, UPMC Univ Paris 06, UMR 7616, Laboratoire de Chimie Théorique, F-75005, Paris, France
2. CNRS, UMR 7616, Laboratoire de Chimie Théorique, F-75005, Paris, France UPMC Université Paris 06

Figure S1: Correlation C=C bond distances (Å) *vs* HHCC dihedral angle (°) for ethylene-Cu complexes.
Figure S2: C=C *vs* Cu-C distances (in Å) as function of the number of ligands binding sites in addition to ethylene (n=1, 2 or 3).
Figure S3: Correlation of Cu→ethylene back-donation computed with CDA (noted b) and NBO (noted π*) analysis for ethylene-Cu complexes (complex **25** is not included).
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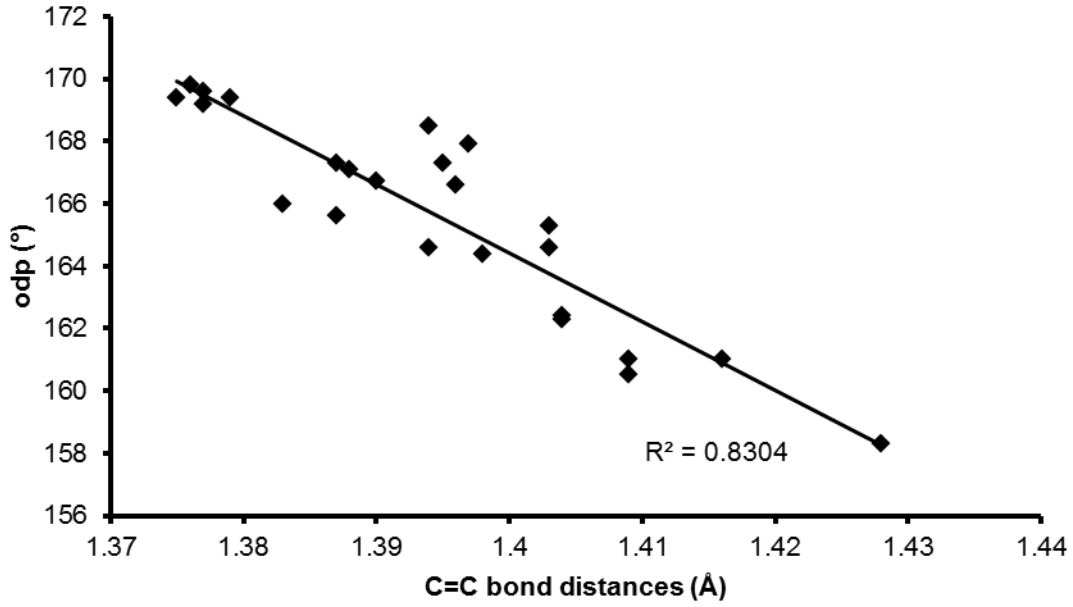
Figure S14: Ethylene→Cu donation (d) and Cu→Ethylene back-donation (b) (CDA analysis) of the complexes plotted against C=C bond distances (in Å).
Chart S1: Schematic representation of $[Cu(tme)(C_2H_4)]^+$ complex.
Table S1: Calculated and experimental geometries (distances in Å, angles in degrees) for $[Cu(tme)(C_2H_4)]^+$ system. A comparison of different functionals (PW91, B3LYP, B3PW91, PBEPBE, M06) and second order Moller Plesset level (MP2).

Cartesian coordinates.

Corresponding Author

* Email: halbert@lct.jussieu.fr



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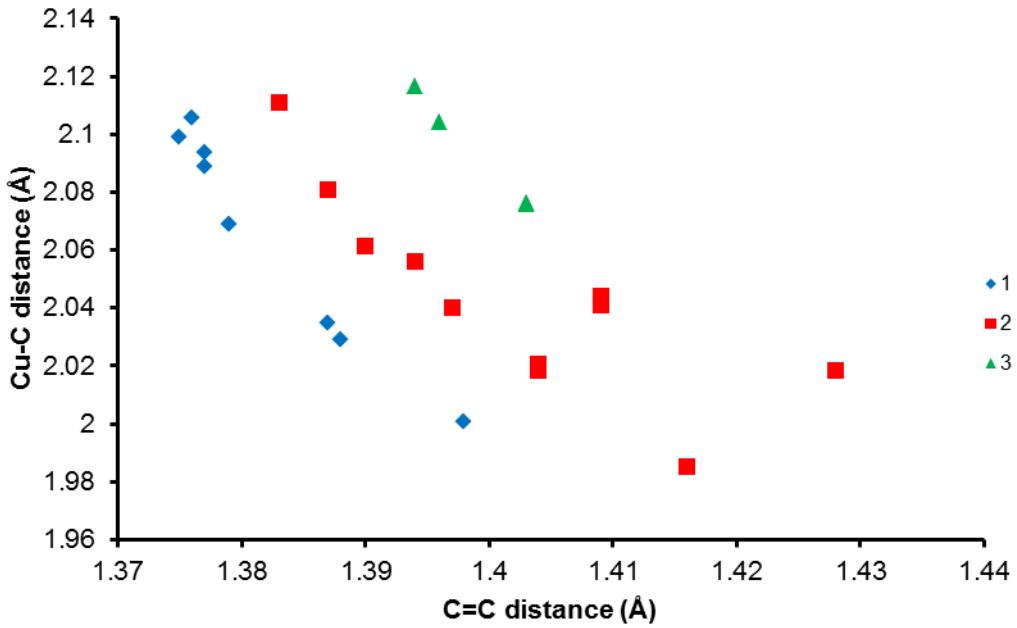

Figure S2: C=C *vs* Cu-C distances (in Å) as a function of the number of ligands binding sites in addition to ethylene (n=1, 2 or 3).

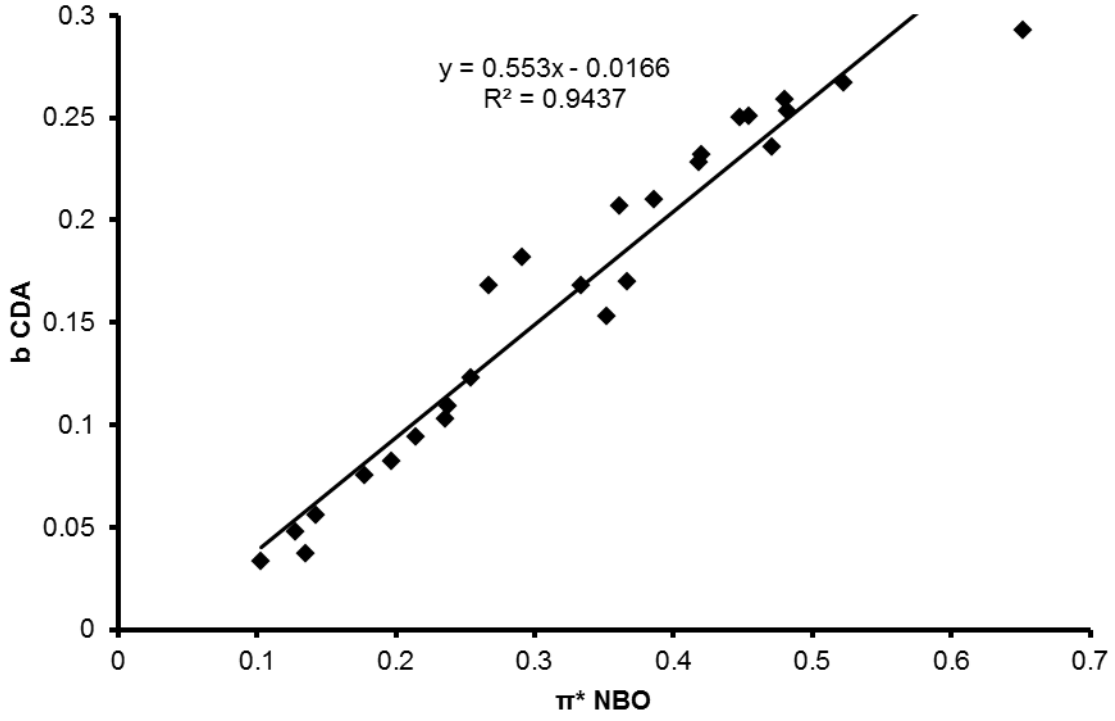

Figure S3: Correlation of Cu→ethylene back-donation computed with CDA (noted b) and NBO (noted π*) analysis for ethylene-Cu complexes (complex **25** is not included).

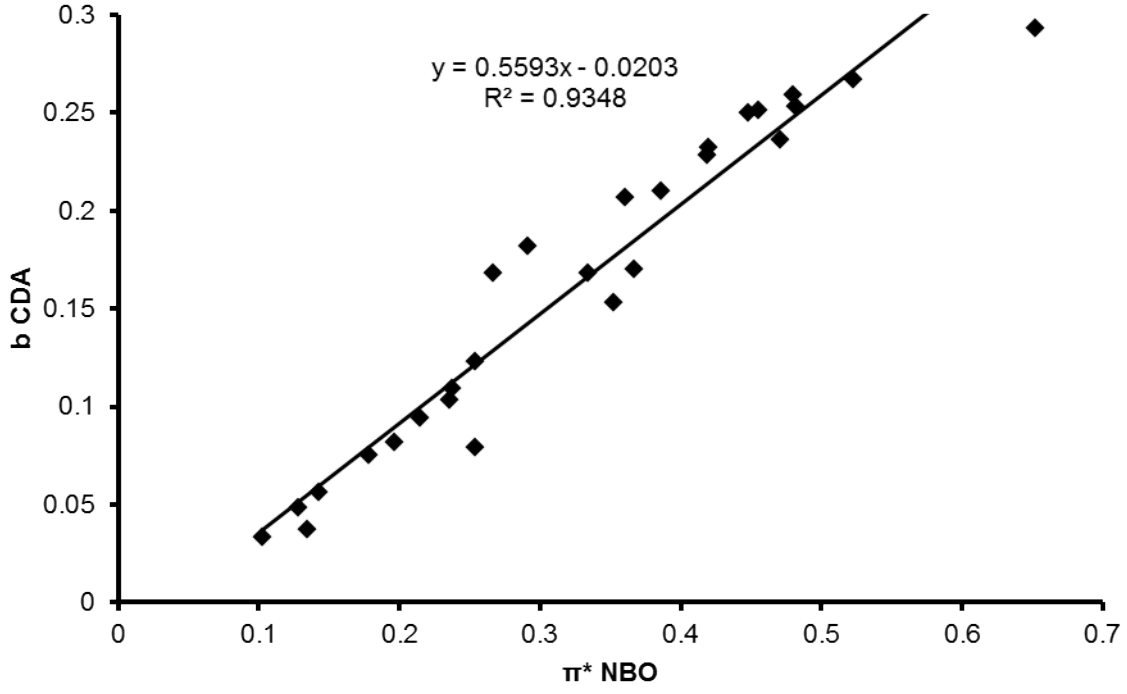

Figure S4: Correlation of Cu→ethylene back-donation computed with CDA (noted b) and NBO (noted π*) analysis for all complexes (complex **25** is included).

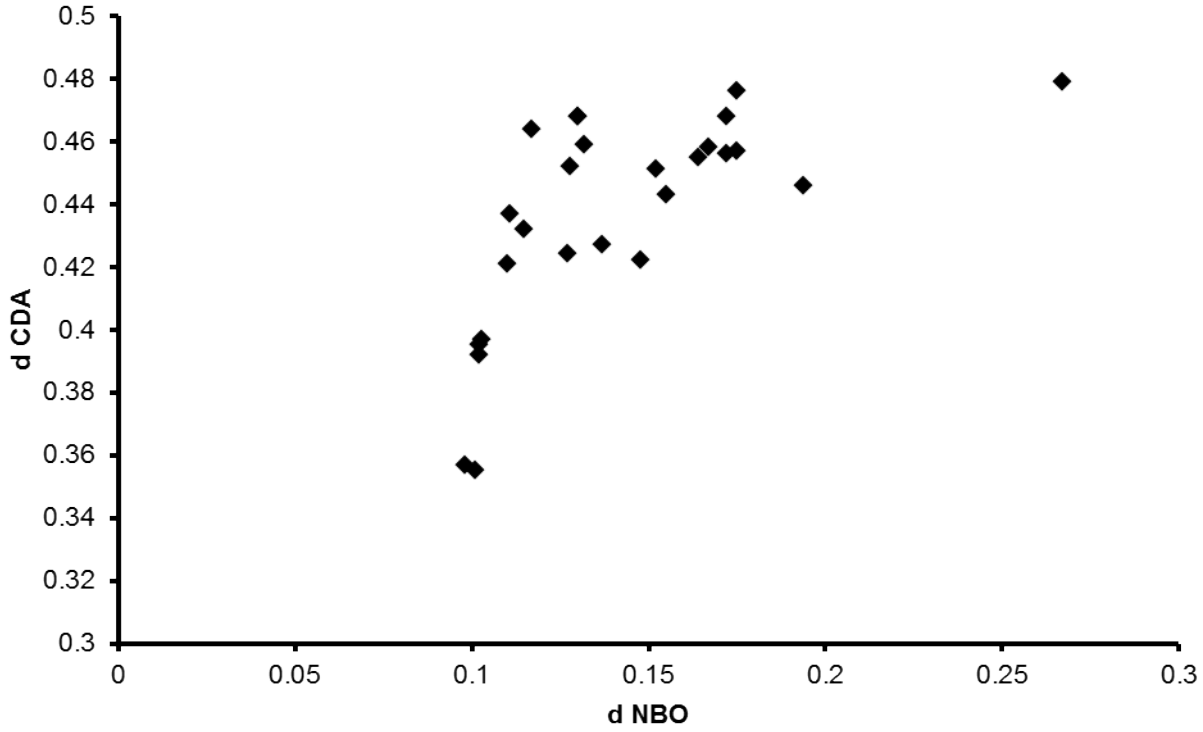

Figure S5: Ethylene→Cu donation (b) computed with CDA and NBO analysis for all complexes (complex **25** is not included).

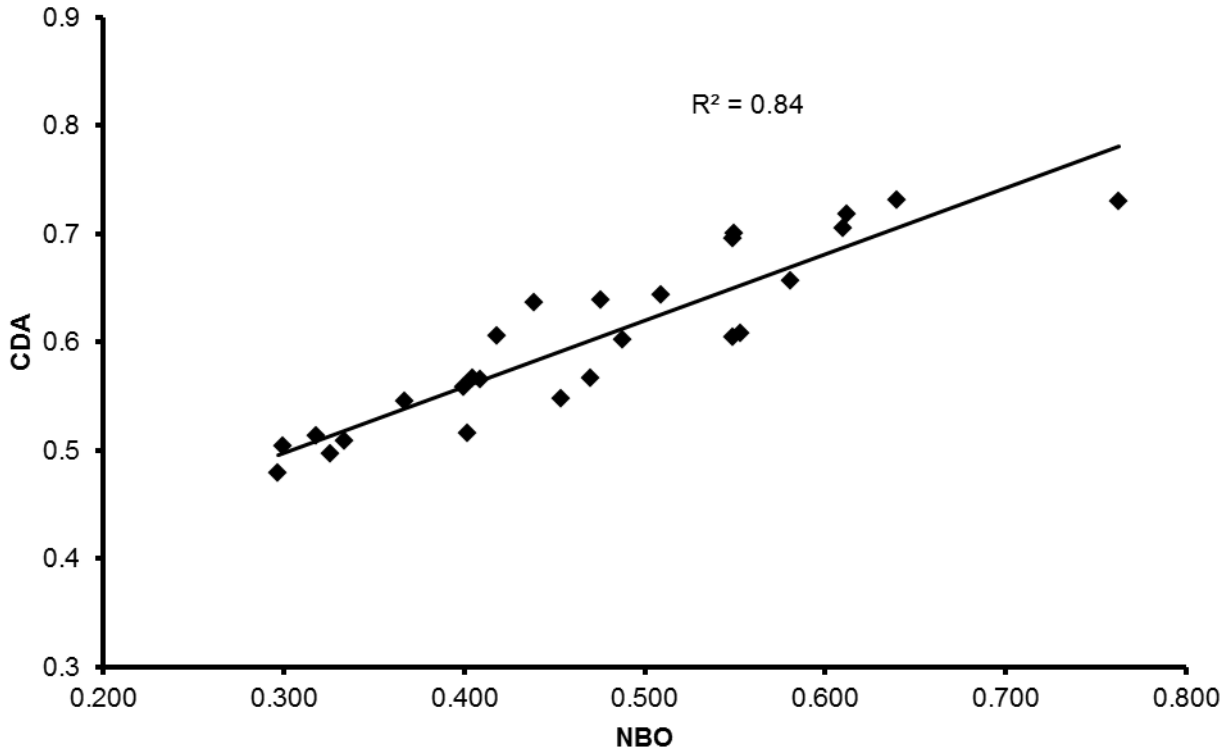

Figure S6: Total electron transfer (donation + back-donation) computed with CDA and NBO analysis for all complexes (complex **25** is not included).

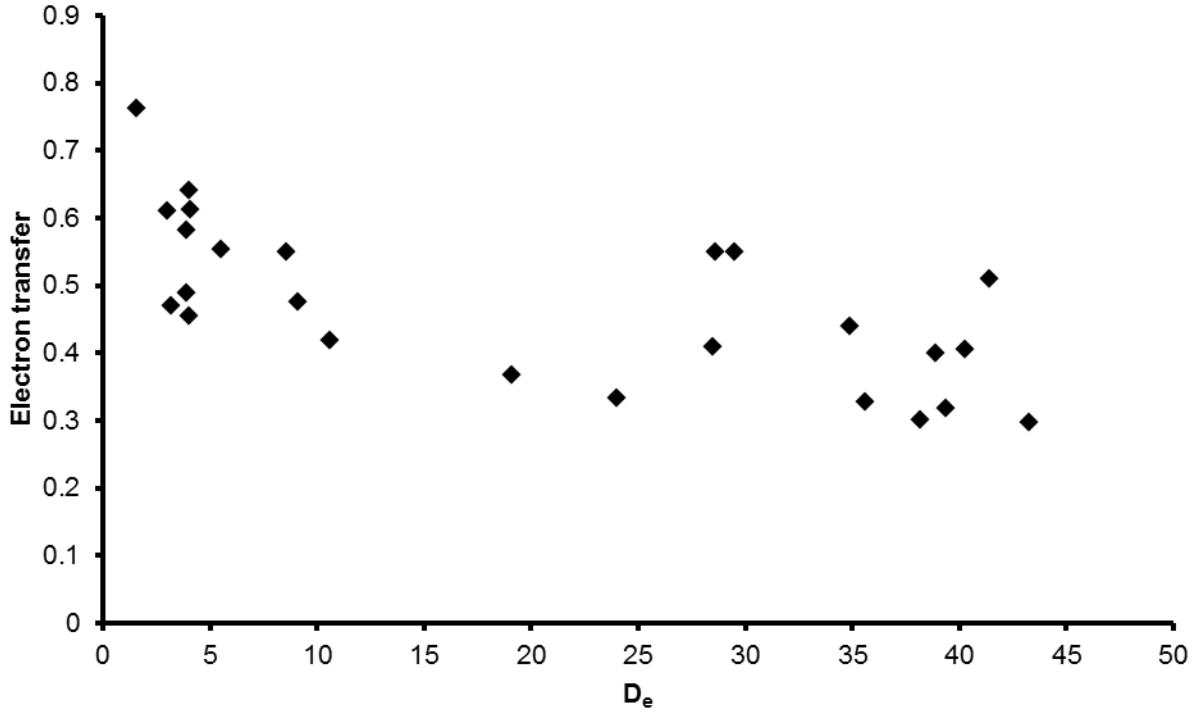

Figure S7: Total electron transfer (donation + back-donation) computed with NBO analysis of the complexes plotted against Bond Dissociation Energies (in kcal/mol).

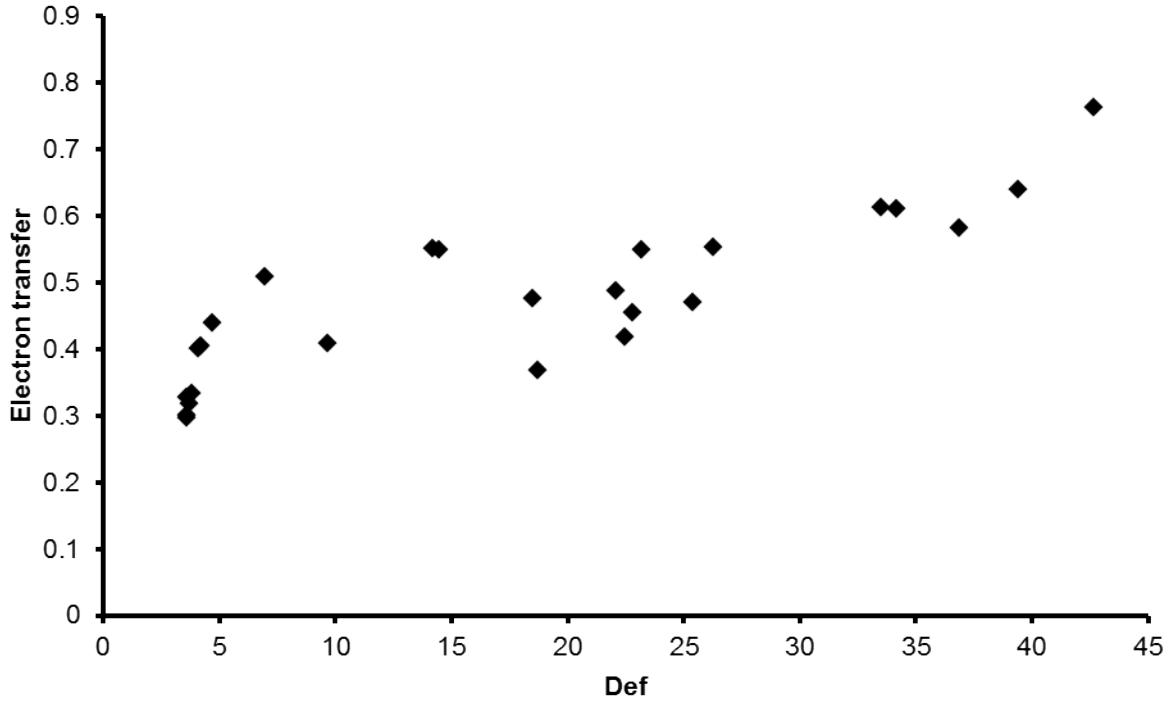

Figure S8: Total electron transfer (donation + back-donation) computed with NBO analysis of the complexes plotted against Deformation Energies (in kcal/mol).

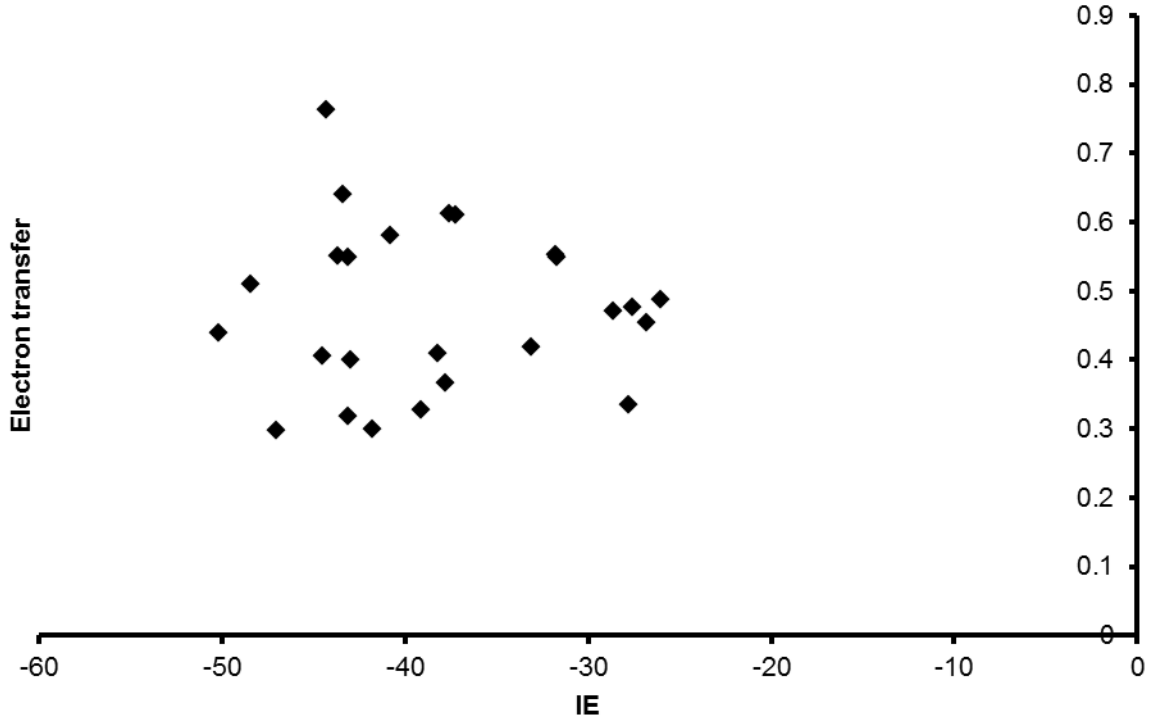

Figure S9: Total electron transfer (donation + back-donation) computed with NBO analysis of the complexes plotted against Interaction Energies (in kcal/mol).

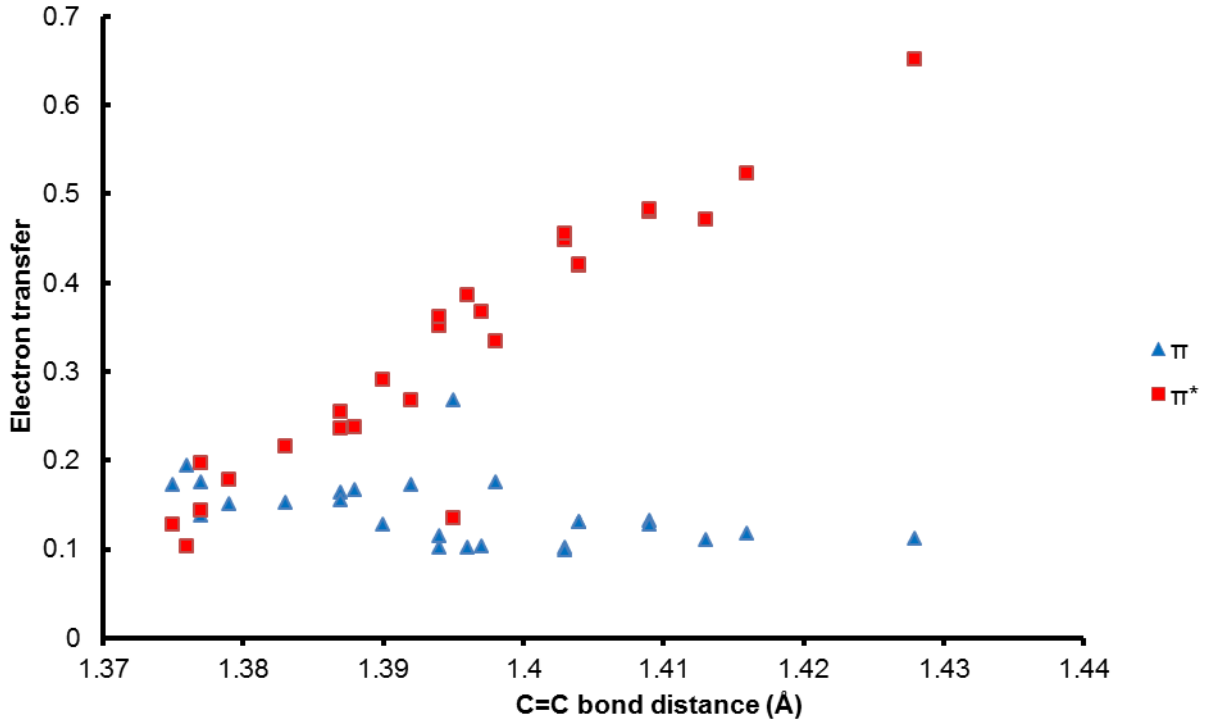

Figure S10: Ethylene→Cu donation and Cu→Ethylene back-donation (defining by the electron occupancies of π and π* NBO molecular orbital of the ethylene) of the complexes plotted against C=C bond distance (in Å).

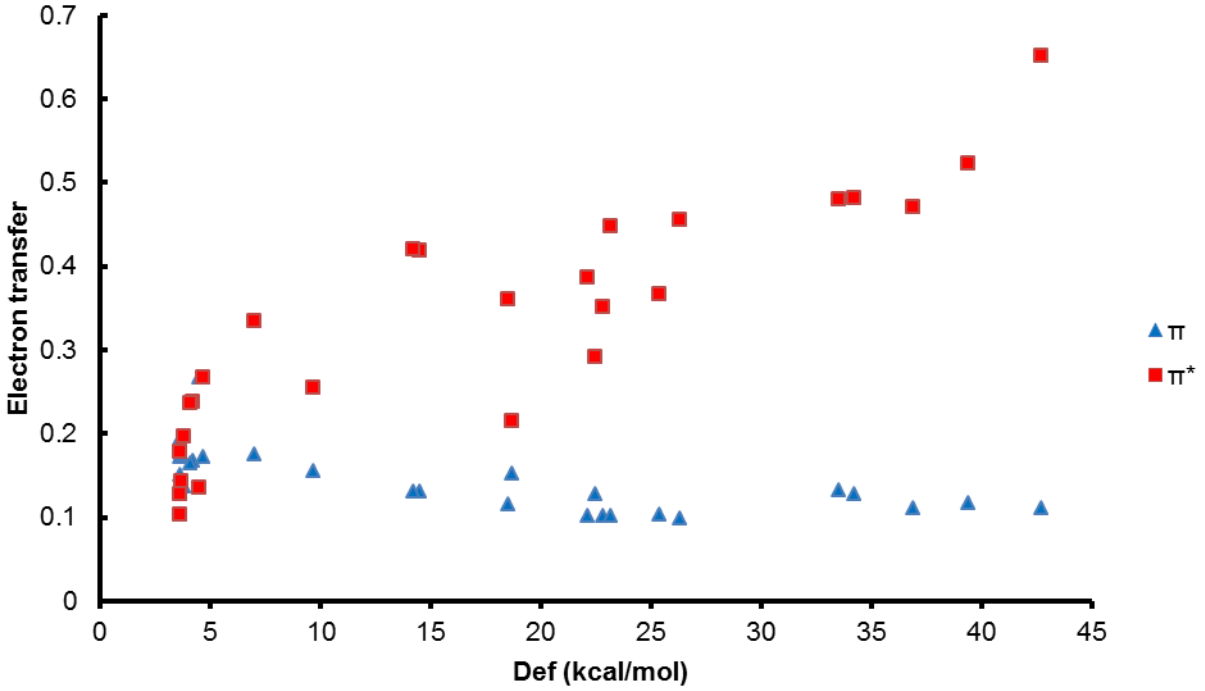

Figure S11: Ethylene→Cu donation and Cu→Ethylene back-donation (defining by the electron occupancies of π and π* NBO molecular orbital of the ethylene) of the complexes plotted against Deformation Energies (in kcal/mol).

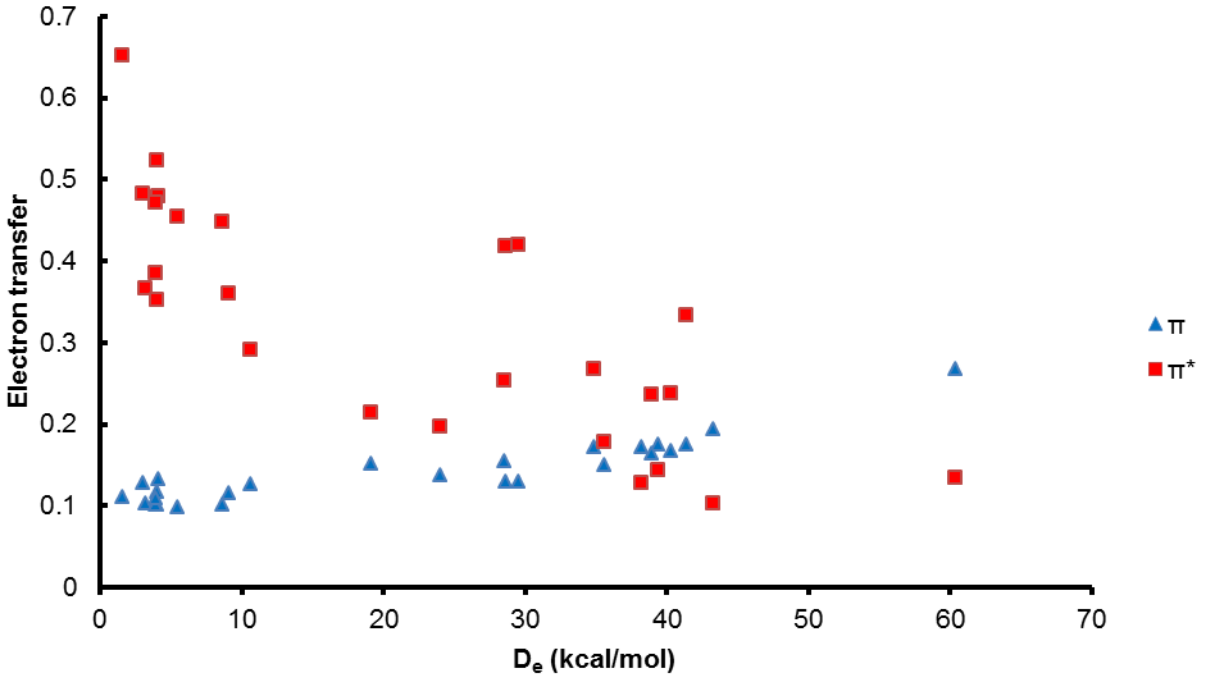

Figure S12: Ethylene→Cu donation and Cu→Ethylene back-donation (defining by the electron occupancies of π and π* NBO molecular orbital of the ethylene) of the complexes plotted against Bond Dissociation Energies (in kcal/mol).

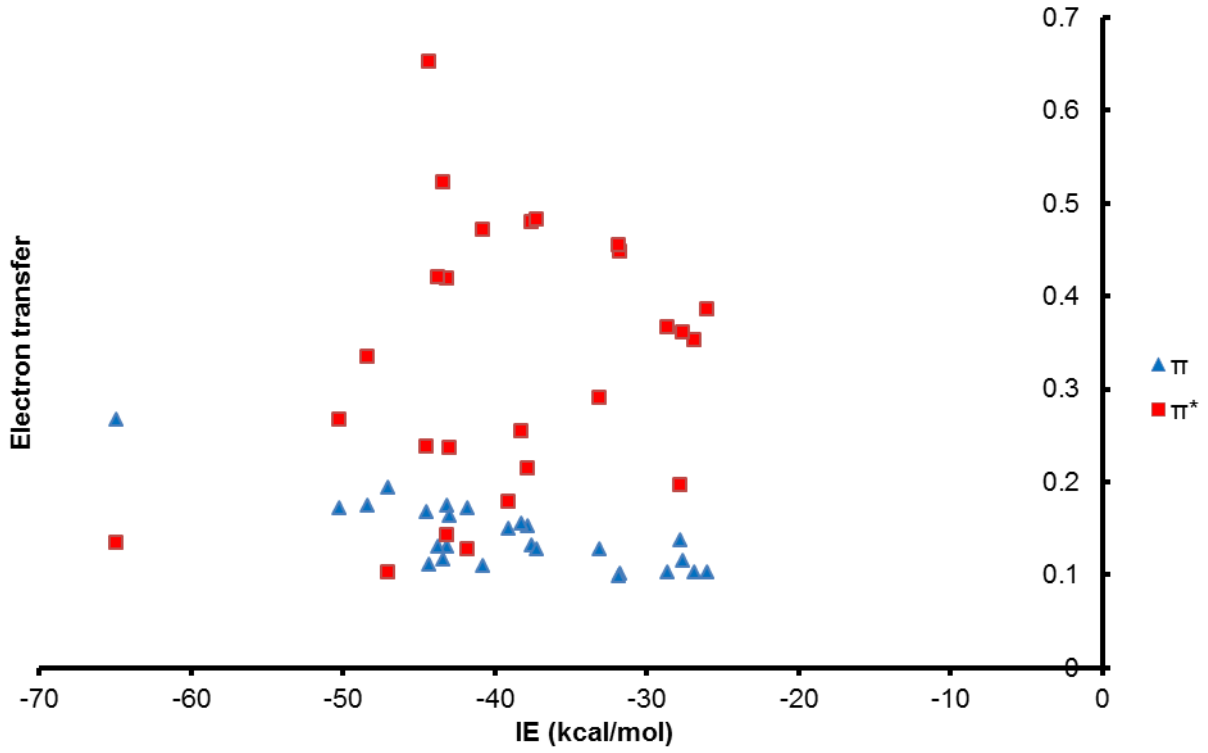

Figure S13: Ethylene→Cu donation and Cu→Ethylene back-donation (defining by the electron occupancies of π and π* NBO molecular orbital of the ethylene) of the complexes plotted against Interaction Energies (in kcal/mol).

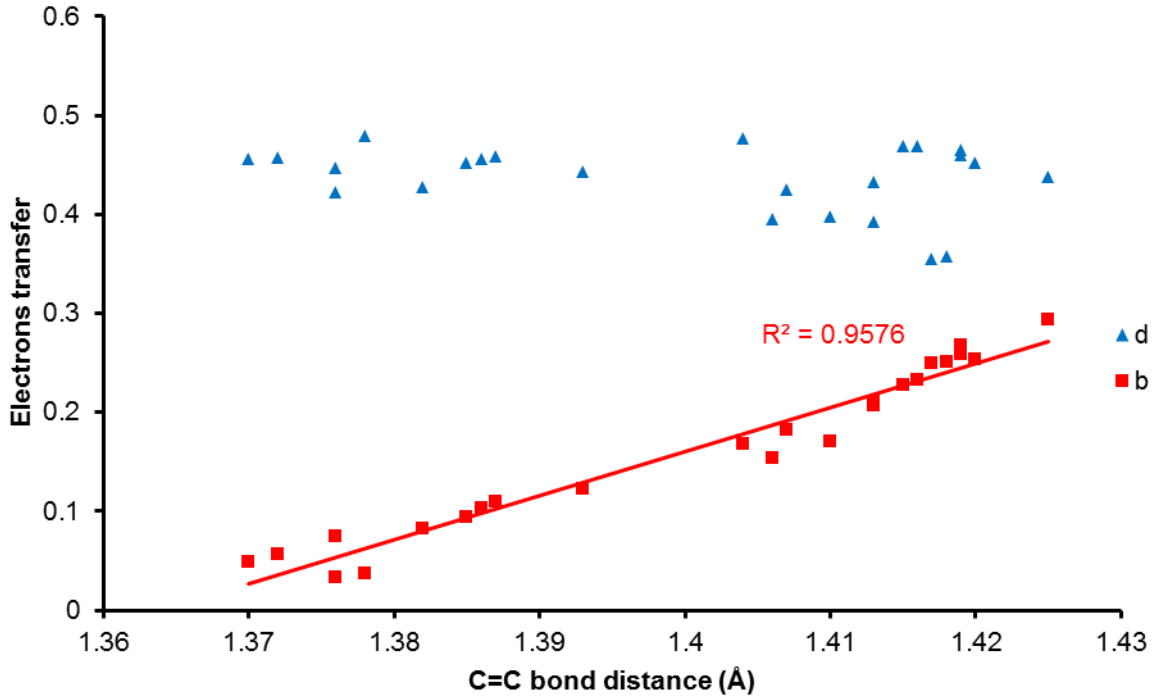

Figure S14: Ethylene→Cu donation (d) and Cu→Ethylene back-donation (b) (CDA analysis) of the complexes plotted against C=C bond distances (in Å).

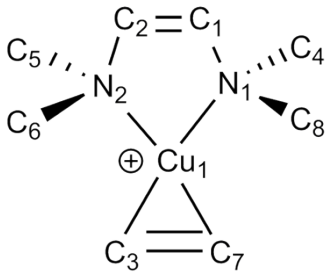

Chart S1: Schematic representation of $[Cu(tme)(C_2H_4)]^+$ complex, used to compare different methods.

	$Cu\text{-}C_7$ $Cu\text{-}C_3$	$Cu\text{-}N_1$ $Cu\text{-}N_2$	$C_3{=}C_7$	$C_1\text{-}N_1$ $C_2\text{-}N_2$	$C_4\text{-}N_1$ $C_8\text{-}N_1$	$C_5\text{-}N_2$ $C_6\text{-}N_2$	$C_2\text{-}C_1$	$C_7\text{-}Cu\text{-}C_3$	$C_7\text{-}Cu\text{-}N_2$ $C_3\text{-}Cu\text{-}N_2$	$C_7\text{-}Cu\text{-}N_1$ $C_3\text{-}Cu\text{-}N_1$	$N_1\text{-}Cu\text{-}N_2$
Experiment	1.95(1) 1.969(9)	2.010(6) 2.037(7)	1.36(1)	1.44(1) 1.44(2)	1.49(1) 1.49(2)	1.50(1) 1.46(1)	1.38(2)	40.6(4)	156.3(4) 115.5(4)	115.5(4) 156.3(4)	88.7(3)
PW91PW91	2.005 (*2.012*) 2.005 (*2.012*)	2.048 (*2.060*) 2.048 (*2.060*)	1.399 (*1.399*)	1.455 (*1.454*) 1.455 (*1.454*)	1.497 (*1.497*) 1.497 (*1.496*)	1.497 (*1.497*) 1.497 (*1.497*)	1.339 (*1.339*)	40.8 (40.7)	155.7 (156.4) 114.8 (115.7)	115.1 (115.6) 155.9 (156.3)	88.3 (88.0)
B3LYP	2.051 2.051	2.084 2.084	1.381	1.451 1.451	1.494 1.494	1.494 1.494	1.331	39.3	155.9 116.6	116.6 155.9	87.5
B3PW91	2.019 2.018	2.057 2.057	1.383	1.446 1.446	1.486 1.486	1.486 1.486	1.330	40.1	156.0 116.0	116.0 156.0	88.0
PBEPBE	2.004 2.004	2.051 2.051	1.400	1.456 1.456	1.497 1.497	1.497 1.497	1.340	40.9	156.3 115.4	115.4 156.3	88.2
M06	2.021 2.020	2.051 2.051	1.378	1.442 1.442	1.480 1.480	1.480 1.480	1.329	39.9	156.1 116.3	116.3 156.1	87.6
MP2	1.895 (*1.943*) 1.895 (*1.943*)	1.941 (*1.982*) 1.941 (*1.982*)	1.419 (*1.414*)	1.449 (*1.450*) 1.449 (*1.450*)	1.489 (*1.493*) 1.489 (*1.493*)	1.489 (*1.493*) 1.489 (*1.493*)	1.335 (*1.338*)	44.0 (*42.7*)	157.0 (*156.6*) 113.0 (*114.0*)	113.0 (*113.9*) 156.9 (*156.6*)	90.1 (*89.4*)

Table S1: Calculated and experimental geometries (distances in Å, angles in degrees) for $[Cu(tme)(C_2H_4)]^+$ system. A comparison of different functionals (PW91, B3LYP, B3PW91, PBEPBE, M06) and second order Moller Plesset level (MP2).

Cartesian coordinates :

PW91

7
1 scf done: -275.726304

C	-2.208352	-1.268246	-0.234828
H	-1.942723	-1.703343	-1.205983
H	-2.461738	-1.967874	0.570917
C	-2.475753	0.095153	-0.110004
H	-2.425994	0.760794	-0.980312
H	-2.944682	0.496246	0.796749
Cu	-0.532320	-0.282701	0.399137

22
2 scf done: -580.566008

C	-0.067102	-0.167449	0.726024
C	1.774344	0.795922	-0.183490
C	-0.233657	1.191464	0.794984
H	-1.051876	1.785747	1.189453
H	-0.712902	-0.977609	1.049798
N	1.160699	-0.387714	0.127406
N	0.897832	1.759614	0.236948
C	1.717307	-1.717772	-0.128643
H	2.691766	-1.601691	-0.618808
H	1.851540	-2.259021	0.818118
H	1.047043	-2.286177	-0.788058
Cu	3.470251	1.043391	-1.019547
C	4.917895	1.298183	-2.504327
C	5.529954	1.288405	-1.271335
H	4.644851	2.237578	-2.996816
H	4.849480	0.390161	-3.112962
H	5.763099	2.219657	-0.744107
H	5.967552	0.372208	-0.860659
C	1.111295	3.203390	0.115828
H	1.092013	3.671231	1.109754
H	2.091999	3.376094	-0.344284
H	0.331565	3.648209	-0.517802

24
3 scf done: -581.762009

C	-0.200089	-0.255323	0.587348
C	1.761862	0.781993	-0.178782
C	-0.222674	1.232199	0.992220
H	-0.131302	1.378680	2.082379
H	-0.959635	-0.501697	-0.174674
N	1.152294	-0.403620	0.002840
N	0.985602	1.761506	0.319518
C	1.598803	-1.690240	-0.505322
H	2.617572	-1.589855	-0.904001
H	1.608051	-2.437486	0.303202
H	0.934459	-2.047086	-1.310366
Cu	3.471609	1.037818	-1.019351
C	5.226666	0.654101	-2.104577
C	5.242225	1.958348	-1.669969
H	4.872359	0.394475	-3.108007
H	5.728326	-0.138196	-1.538470
H	4.901763	2.775102	-2.315631
H	5.755437	2.242496	-0.744917
C	1.337936	3.166961	0.435470
H	1.501308	3.446250	1.490053
H	2.260402	3.358165	-0.129723
H	0.534561	3.796542	0.022827
H	-1.121502	1.762978	0.645120
H	-0.329468	-0.939106	1.439295

15
4 scf done: -962.055662

C	-1.862728	-1.098911	0.522132
H	-1.596636	-2.160039	0.486922
H	-2.069244	-0.681096	1.512420
C	-2.207244	-0.411735	-0.627502
H	-2.222802	-0.912990	-1.600344
H	-2.697094	0.565544	-0.574217
Cu	-0.170671	-0.059402	-0.188142
P	1.489508	-0.587677	1.290666
H	1.164315	-1.112467	2.567821
H	2.411274	-1.579348	0.865081
H	2.408178	0.419924	1.683599
P	0.483288	1.325665	-1.886578
H	0.427780	0.792855	-3.200445
H	-0.276552	2.506647	-2.088908
H	1.786683	1.885628	-1.923741

11
5 scf done: -618.911114

C	-2.295088	-1.270657	-0.257622
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H	-2.478805	-1.964378	0.570701
C	-2.570579	0.072210	-0.137874
H	-2.551979	0.735712	-1.009954
H	-2.981894	0.487171	0.789358
Cu	-0.537842	-0.254306	0.303118
P	1.589298	0.126609	0.860779
H	1.965647	1.483975	1.009310
H	2.044116	-0.422403	2.084455
H	2.579879	-0.337768	-0.038631

45
6 scf done: -1730.005046

C	-6.221232	-0.172168	3.628183
C	-5.226465	-0.388300	2.687531
C	-4.907964	0.610591	1.720321
C	-5.649466	1.848991	1.740240
C	-6.661057	2.039828	2.724486
C	-6.942424	1.050384	3.651436
H	-6.451562	-0.948701	4.360874
C	-3.883608	0.418058	0.727831
C	-5.351645	2.853740	0.777982
H	-7.213003	2.983327	2.734237
C	-4.375624	2.653174	-0.180242
C	-3.637699	1.433561	-0.206579
H	-5.905893	3.795492	0.805157
H	-4.162190	3.438416	-0.909743
C	-3.080862	-0.849434	0.732283
C	-2.031418	-1.019402	1.702362
C	-3.352129	-1.887058	-0.170257
C	-1.685742	0.002973	2.635117
C	-1.292714	-2.259236	1.734979
C	-2.615865	-3.107343	-0.132519
C	-0.668469	-0.192601	3.555982
C	-0.257727	-2.428550	2.698593
C	-1.616901	-3.286898	0.805995
H	-2.848940	-3.909672	-0.836971
C	0.049335	-1.416837	3.592760
H	-0.417538	0.601597	4.262497
H	0.291626	-3.373395	2.718807
H	-1.064357	-4.229313	0.843053
H	-7.719988	1.207232	4.401972
H	0.844634	-1.557349	4.327784
P	-2.494663	1.141818	-1.607101
H	-2.126343	2.463504	-1.973321

H	-1.276677	0.710178	-1.016081
P	-4.531109	-1.628052	-1.547001
H	-4.909996	-2.957781	-1.870951
H	-5.732698	-1.180092	-0.934913
H	-2.233326	0.947451	2.622020
H	-4.675817	-1.331027	2.685409
Cu	-3.529405	-0.263412	-3.090026
C	-3.984189	-0.832295	-5.039470
H	-3.618884	-1.857824	-5.150131
H	-5.062812	-0.687816	-5.154278
C	-3.110297	0.244973	-5.064012
H	-3.477568	1.266733	-5.200022
H	-2.033922	0.096377	-5.193809

8

7 scf done: -375.866301

C	-2.146044	-1.253925	-0.222782
H	-1.939975	-1.703313	-1.199508
H	-2.365599	-1.949602	0.593605
C	-2.418869	0.105292	-0.100783
H	-2.432819	0.760564	-0.977724
H	-2.857622	0.513741	0.815421
Cu	-0.492774	-0.254059	0.313631
F	1.178460	0.079954	0.778141

8

8 scf done: -736.240631

C	-2.193673	-1.259130	-0.232445
H	-1.968322	-1.707061	-1.205516
H	-2.398610	-1.954698	0.587640
C	-2.475519	0.094190	-0.112833
H	-2.479911	0.751130	-0.988459
H	-2.910775	0.503174	0.804566
Cu	-0.520267	-0.247285	0.310116
Cl	1.471834	0.118331	0.836930

8

9 scf done: -2847.612867

C	-2.210084	-1.261975	-0.236534
H	-1.984607	-1.710110	-1.209374
H	-2.410906	-1.956692	0.585265
C	-2.493075	0.090579	-0.117159
H	-2.498606	0.747111	-0.992998
H	-2.924660	0.499892	0.801736
Cu	-0.531212	-0.248110	0.306187
Br	1.577907	0.137957	0.862878

11

10 scf done: -315.892367

C	-2.235978	-1.259746	-0.242746
H	-1.990787	-1.706816	-1.210941
H	-2.422816	-1.955401	0.580991
C	-2.510826	0.084093	-0.122737
H	-2.492445	0.749144	-0.991520
H	-2.924489	0.500772	0.800674
Cu	-0.490700	-0.249286	0.317578
C	1.329430	0.071350	0.797431
H	2.015065	-0.172227	-0.031956
H	1.474803	1.136709	1.050494
H	1.625121	-0.524203	1.677977

12

11 scf done: -391.111300

C	-2.235690	-1.286093	-0.318324
H	-1.896291	-1.706129	-1.270608
H	-2.539059	-2.009851	0.444688
C	-2.579115	0.064256	-0.208719
H	-2.516476	0.734055	-1.072368
H	-3.159849	0.432116	0.643068
Cu	-0.707547	-0.234425	0.431015
O	0.940646	0.153134	0.955075
C	1.442837	0.168600	2.274862
H	1.953644	1.132681	2.469240
H	0.672258	0.035176	3.059718
H	2.195937	-0.634233	2.406774

9

12 scf done: -368.836516

C	-2.202296	-1.256224	-0.233970
H	-1.956875	-1.702562	-1.203044
H	-2.388730	-1.951020	0.591296
C	-2.482241	0.088515	-0.115211
H	-2.467649	0.751449	-0.986335
H	-2.899563	0.503116	0.808109
Cu	-0.486385	-0.241004	0.319393
C	1.278581	0.080927	0.785339
N	2.402669	0.285366	1.081413

28

13 scf done: -621.827065

C	0.155887	-0.250682	0.924512
C	1.729940	1.076168	-0.224991
C	-0.535756	1.028057	0.428603
H	-1.105026	1.549474	1.213691
H	-0.393640	-1.170769	0.672815
N	1.444719	-0.182611	0.211034
N	0.617034	1.828034	-0.017226
C	2.454698	-1.199256	0.428857
H	3.319896	-0.973484	-0.208940
H	2.789756	-1.221868	1.483059
H	2.059682	-2.192915	0.162251
Cu	3.434648	1.760451	-0.825264
C	3.783194	1.165796	-2.781097
C	4.831228	1.946787	-2.255603
H	3.024040	1.607961	-3.432731
H	3.859946	0.075215	-2.823732
H	4.916161	3.009804	-2.499677
H	5.749518	1.482369	-1.883753
C	0.440400	3.164341	-0.548873
H	-0.121464	3.785136	0.167326
H	1.434377	3.608731	-0.700987
H	-0.104221	3.155339	-1.511955
C	4.268609	2.782813	0.662281
H	4.878462	3.632522	0.311020
H	3.517180	3.163126	1.376421
H	4.940968	2.103055	1.218536
H	-1.216243	0.827644	-0.422619
H	0.325093	-0.232011	2.019474

26

14 scf done: -620.628447

C	0.046268	-0.254028	0.618292
C	1.727456	1.047804	-0.234226
C	-0.464869	1.000450	0.425527
H	-1.459393	1.396832	0.603828
H	-0.413317	-1.155305	1.011226
N	1.373784	-0.205798	0.204746
N	0.571042	1.774732	-0.083949
C	2.307086	-1.321247	0.282446
H	3.151120	-1.101481	-0.383983
H	2.682369	-1.450083	1.309557
H	1.812924	-2.247479	-0.044999
Cu	3.453981	1.766361	-0.761997
C	4.102393	0.848669	-2.515797

C	4.995573	1.829723	-2.042836
H	3.391456	1.072418	-3.316076
H	4.300416	-0.214492	-2.348333
H	5.010236	2.833240	-2.478645
H	5.900263	1.550160	-1.494629
C	0.464242	3.182482	-0.449730
H	1.474814	3.614426	-0.414961
H	0.050117	3.295485	-1.463745
H	-0.183832	3.703594	0.269111
C	4.028463	3.167732	0.533778
H	4.216584	4.133953	0.030833
H	3.297188	3.336814	1.344222
H	4.981104	2.863078	1.003767

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15 scf done: -1770.054088

C	-6.011137	-0.334605	4.111263
C	-5.091634	-0.505778	3.087789
C	-5.057609	0.386767	1.975298
C	-6.005397	1.472905	1.939564
C	-6.932519	1.623731	3.009776
C	-6.939211	0.738988	4.076169
H	-6.021728	-1.032404	4.952144
C	-4.124968	0.226418	0.891857
C	-5.992370	2.364301	0.829088
H	-7.645804	2.452150	2.971643
C	-5.097645	2.189175	-0.208762
C	-4.152672	1.120262	-0.187960
H	-6.705408	3.193521	0.807493
H	-5.108740	2.880497	-1.055726
C	-3.126749	-0.891258	0.915879
C	-1.937986	-0.767415	1.717101
C	-3.333168	-2.043066	0.144327
C	-1.664350	0.393306	2.500677
C	-0.973724	-1.838986	1.721363
C	-2.364646	-3.090188	0.154870
C	-0.503732	0.488698	3.253136
C	0.205756	-1.711294	2.509599
C	-1.222846	-2.993479	0.926949
H	-2.528965	-3.977670	-0.460554
C	0.439879	-0.571709	3.261983
H	-0.313694	1.388007	3.844183
H	0.929202	-2.531703	2.504965
H	-0.490166	-3.805611	0.928879
H	-7.658267	0.863491	4.889310
H	1.350294	-0.485015	3.859841
P	-3.141783	0.788501	-1.691377
H	-3.050404	2.122500	-2.191753
H	-1.827728	0.727720	-1.138343
P	-4.758882	-2.125334	-1.027796
H	-4.791605	-3.541752	-1.197664
H	-5.833731	-2.080814	-0.073040
H	-2.384222	1.214604	2.500197
H	-4.380828	-1.334268	3.122578
Cu	-3.930955	-0.921702	-3.019143
C	-2.478494	-2.170224	-3.550562
H	-2.879191	-3.139617	-3.894833
H	-1.909618	-1.728758	-4.387590
H	-1.769145	-2.360913	-2.726818
C	-5.675890	0.061569	-3.839883
H	-6.516211	-0.142278	-3.172768
C	-5.162099	-0.924078	-4.680371
H	-5.594028	-1.928253	-4.703732
H	-4.510062	-0.667746	-5.519357
H	-5.432795	1.114935	-4.002375

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16 scf done: -735.157357

C	-0.087906	-0.248583	0.502392
C	1.787842	0.980222	-0.222544
C	-0.427239	1.250390	0.520045
H	-0.837778	1.593868	1.481272
H	-0.826111	-0.858273	-0.040947
N	1.216944	-0.253122	-0.188316
N	0.892611	1.863822	0.262932
C	1.921625	-1.500544	-0.397952
H	2.857474	-1.282557	-0.926518
H	2.157375	-1.997974	0.562004
H	1.310466	-2.188440	-1.005270
C	1.067401	3.330809	0.266198
H	0.342475	3.707755	1.011692
C	2.484911	3.709407	0.776834
H	2.584975	3.247992	1.791513
H	2.453410	4.812677	0.940290
O	3.531386	3.389511	-0.071889
Cu	3.542910	1.618045	-0.805284
C	4.689777	0.405188	-1.975233
C	5.314119	1.640212	-1.740771
H	4.160845	0.211223	-2.913891
H	4.997470	-0.483042	-1.413288
H	5.254817	2.454810	-2.468403
H	6.076179	1.751140	-0.964182
C	0.752425	3.933727	-1.109735
H	-0.227423	3.604387	-1.491565
H	0.743317	5.032881	-1.044210
H	1.536062	3.643621	-1.825600
H	0.024195	-0.665533	1.522284
H	-1.137386	1.526849	-0.281447

28

17 scf done: -733.963127

C	-0.084104	-0.142704	0.417820
C	1.783069	0.982852	-0.262369
C	-0.314542	1.195927	0.599175
H	-1.183022	1.719726	0.986019
H	-0.709476	-1.006447	0.619342
N	1.196555	-0.249214	-0.109015
N	0.831435	1.858717	0.188502
C	1.851694	-1.510377	-0.431367
H	2.784771	-1.274351	-0.956643
H	2.080969	-2.074802	0.485499
H	1.205475	-2.118719	-1.081293
C	1.008385	3.333246	0.213443
H	0.260502	3.701390	0.938214
C	2.419274	3.694525	0.757847
H	2.503467	3.208163	1.762260
H	2.381453	4.793032	0.949718
O	3.474596	3.398170	-0.085814
Cu	3.532996	1.622804	-0.824469
C	4.727117	0.412065	-1.944948
C	5.332712	1.654504	-1.699265
H	4.235335	0.206226	-2.901104
H	5.020630	-0.469016	-1.364285
H	5.294261	2.460779	-2.437602
H	6.066887	1.778230	-0.898129
C	0.736416	3.929550	-1.170515
H	-0.243172	3.616355	-1.564060
H	0.754712	5.028391	-1.105975
H	1.527161	3.620262	-1.869582

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18 scf done: -1170.779810

C	-1.198832	1.428537	0.698042

C	-0.265041	1.427774	-0.376212
C	-0.374020	2.398922	-1.392555
C	-1.386343	3.363495	-1.356482
C	-2.310076	3.362678	-0.299945
C	-2.214870	2.400097	0.716729
H	0.350333	2.389999	-2.212177
H	-1.455691	4.113528	-2.147539
H	-3.103665	4.112510	-0.262139
H	-2.938427	2.410460	1.536426
P	-1.174048	0.098655	1.968244
H	-0.106402	0.398472	2.851226
H	-2.243830	0.631001	2.770756
C	0.797587	0.424302	-0.414451
N	0.939176	-0.373276	0.588513
C	1.937228	-1.409540	0.590429
H	2.591062	-1.379270	-0.302106
H	2.576491	-1.274409	1.479895
C	1.398240	-2.880115	0.715465
O	2.256814	-3.758971	0.573985
O	0.142423	-3.089506	0.965070
H	1.451168	0.381762	-1.307017
Cu	-1.436203	-2.012819	1.181807
C	-3.476336	-2.224541	0.948126
C	-2.827088	-3.372163	0.507207
H	-3.807672	-1.457612	0.241001
H	-3.911122	-2.171840	1.951098
H	-2.592953	-3.524555	-0.550050
H	-2.691655	-4.240337	1.158212

9

19 scf done: -475.772286

C	-2.246135	0.430922	1.207318
H	-2.552790	-0.355024	1.905620
H	-2.234631	1.446155	1.617808
C	-2.236162	0.206360	-0.187210
H	-2.534357	-0.759881	-0.607796
H	-2.216506	1.041143	-0.895832
Cu	-0.417385	0.003899	0.574136
F	0.685129	-0.429327	-0.905660
F	0.660761	0.056715	2.132580

9

20 scf done: -1196.535408

C	-2.308477	0.439978	1.197298
H	-2.575287	-0.352191	1.902636
H	-2.254148	1.449756	1.613987
C	-2.298511	0.217788	-0.181419
H	-2.556569	-0.756661	-0.605876
H	-2.236198	1.045436	-0.893691
Cu	-0.415690	0.002839	0.574278
Cl	0.764574	-0.501784	-1.282386
Cl	0.733805	0.105222	2.514339

9

21 scf done: -5419.284704

C	-2.318752	0.442848	1.195453
H	-2.581214	-0.348291	1.903249
H	-2.259028	1.452783	1.610569
C	-2.309133	0.218257	-0.180162
H	-2.562657	-0.757933	-0.602910
H	-2.241458	1.043306	-0.894607
Cu	-0.409461	0.001925	0.574741
Br	0.811961	-0.524012	-1.408411
Br	0.777665	0.112079	2.643042

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22 scf done: -355.800991

C	-1.239005	-1.869263	0.106390
H	-0.571684	-2.571877	0.619003
H	-2.202966	-1.707611	0.602780
C	-1.078829	-1.592593	-1.285139
H	-0.285000	-2.077174	-1.865404
H	-1.917000	-1.214297	-1.881960
Cu	-0.299379	-0.103556	-0.167403
C	0.090764	0.642195	1.650074
H	-0.315059	0.072382	2.509437
H	1.190957	0.708173	1.774993
H	-0.302628	1.677191	1.707274
C	0.428994	1.259557	-1.441101
H	1.493439	1.449855	-1.195662
H	0.365390	1.003555	-2.517321
H	-0.113097	2.214560	-1.285351

17

23 scf done: -506.249758

C	-1.755209	-0.803402	0.899408
H	-1.514894	-1.806801	1.269943
H	-2.019070	-0.073878	1.673948
C	-2.107894	-0.589752	-0.455457
H	-2.149894	-1.422841	-1.166724
H	-2.653681	0.310153	-0.762144
Cu	-0.208672	-0.110591	-0.133551
O	1.275600	0.046685	1.072827
C	1.131294	-0.302991	2.401781
H	0.868708	-1.383132	2.578765
H	2.087530	-0.133356	2.960131
H	0.349566	0.282811	2.960564
O	0.539026	0.493659	-1.793072
C	-0.242928	0.554211	-2.930674
H	-1.122928	1.252393	-2.860288
H	0.357890	0.919034	-3.802954
H	-0.676861	-0.431656	-3.256789

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24 scf done: -1210.702625

C	-1.011139	1.202591	0.848081
C	-0.390188	1.195838	-0.436085
C	-0.840759	2.088172	-1.433845
C	-1.883173	2.985805	-1.185610
C	-2.504728	2.989940	0.074960
C	-2.071449	2.102035	1.070774
H	-0.356576	2.064110	-2.415599
H	-2.215490	3.672777	-1.968849
H	-3.326923	3.680565	0.282818
H	-2.568954	2.104495	2.045211
P	-0.590601	-0.083935	2.104803
H	0.620705	0.421736	2.668408
H	-1.455772	0.466063	3.125986
C	0.699954	0.269849	-0.723368
N	1.222688	-0.432887	0.224686
C	2.239915	-1.399665	-0.067395
H	2.600371	-1.340592	-1.114040
H	3.097342	-1.222398	0.605405
C	1.855607	-2.927718	0.212125
O	2.674895	-3.723430	-0.310243
O	0.845988	-3.170471	0.936084
H	1.046944	0.191363	-1.775023
Cu	-1.102590	-2.238346	1.629985
C	-2.393515	-2.328813	0.122216
H	-2.196381	-1.545081	-0.632951
H	-2.292153	-3.311344	-0.373950
H	-3.443901	-2.220648	0.452877
C	-1.555166	-3.857001	2.814348
H	-1.192554	-4.677895	2.189461

C	-0.657290	-3.088246	3.557177
H	-1.009566	-2.427238	4.355293
H	0.416127	-3.281493	3.500857
H	-2.629898	-3.832615	3.016554

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25 scf done: -775.039858

C	-0.200071	-0.065605	0.727514
C	1.690019	1.047269	-0.157603
C	-0.575736	1.387038	0.405763
H	-1.069180	1.907520	1.243333
H	-0.931675	-0.802823	0.355389
N	1.093984	-0.186020	0.041141
N	0.740542	1.979695	0.114133
C	1.878488	-1.388643	0.219589
H	2.868465	-1.209444	-0.225481
H	2.026456	-1.623774	1.293144
H	1.387996	-2.251530	-0.267246
C	0.853803	3.419034	-0.177801
H	0.027875	3.899536	0.386427
C	2.205583	4.016805	0.362253
H	2.207863	3.757996	1.466143
H	2.022609	5.138546	0.329149
O	3.304011	3.627052	-0.315570
Cu	3.578867	1.395781	-0.348344
C	4.244784	1.558854	-2.351915
C	5.299137	1.512146	-1.427953
H	3.838994	2.521310	-2.672010
H	3.952176	0.673187	-2.925343
H	5.742413	2.439853	-1.054006
H	5.882984	0.598246	-1.277303
C	0.692523	3.686602	-1.680642
H	-0.218122	3.220744	-2.096835
H	0.645771	4.772934	-1.866182
H	1.580548	3.286666	-2.192423
C	4.429191	0.807098	1.398557
H	5.035141	-0.115283	1.293276
H	5.102867	1.621487	1.724002
H	3.689339	0.637069	2.204448
H	-0.075181	-0.222018	1.821956
H	-1.239788	1.452309	-0.481509

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26 scf done: -773.845314

C	-0.232863	0.066372	0.703032
C	1.671785	1.054394	-0.133339
C	-0.499412	1.398621	0.515308
H	-1.398607	1.975803	0.711958
H	-0.856539	-0.737012	1.084367
N	1.085568	-0.120728	0.306810
N	0.657567	1.979157	0.009212
C	1.809500	-1.379036	0.342244
H	2.881464	-1.126538	0.308878
H	1.584526	-1.920433	1.274802
H	1.549809	-2.016489	-0.521246
C	0.790472	3.417747	-0.300667
H	-0.086970	3.901334	0.173690
C	2.093340	4.023414	0.347465
H	2.001715	3.775491	1.451035
H	1.903334	5.143258	0.289690
O	3.243625	3.636494	-0.233528
Cu	3.570875	1.397418	-0.348419
C	4.217501	1.643887	-2.358867
C	5.272768	1.561368	-1.437995
H	3.817989	2.619337	-2.645709
H	3.921933	0.780394	-2.963414
H	5.721720	2.474690	-1.035642
H	5.859324	0.643587	-1.326396
C	0.764590	3.634475	-1.815344
H	-0.147257	3.216020	-2.275231
H	0.814505	4.713986	-2.033656
H	1.652282	3.154420	-2.250991
C	4.452837	0.754391	1.366683
H	5.110115	-0.128959	1.231512
H	5.083959	1.586666	1.730980
H	3.719611	0.514925	2.161820

22

27 scf done: -547.182207

C	1.084944	0.917431	0.739032
C	0.764928	0.593471	-0.641093
C	0.783278	-0.921265	-0.781142
H	-0.117333	-1.450028	-0.434022
H	0.999498	-1.243219	-1.809159
C	1.308657	-0.389352	1.484966
H	1.966537	-0.265360	2.356173
H	0.402624	-0.924478	1.807221
C	1.759280	1.320761	-1.533445
C	2.285902	1.851128	0.732938
H	2.074647	2.910574	0.522675
H	1.552089	2.385120	-1.721475
C	1.960632	-1.123283	0.249832
H	2.208887	-2.180353	0.440331
C	2.960713	1.172532	-0.521394
H	3.886057	1.671633	-0.852861
C	3.220140	-0.336804	-0.227595
H	3.621517	-0.816783	-1.137002
H	4.009903	-0.422840	0.538734
H	1.897552	0.818895	-2.500975
H	2.863747	1.791724	1.665478
Cu	-0.763031	1.556752	0.250663

Ethylene

6

scf done: -78.551868

C	-0.219809	-0.034294	0.000000
H	0.298738	-0.996964	0.000000
H	-1.312759	-0.067069	0.000000
C	0.450272	1.126899	0.000000
H	-0.068274	2.089569	0.000000
H	1.543223	1.159674	0.000000

Strained olefin

21

scf done: -349.952751

C	1.080911	0.907085	0.701390
C	0.777843	0.600662	-0.604676
C	0.786297	-0.914917	-0.766025
H	-0.128021	-1.436245	-0.433437
H	1.006432	-1.234384	-1.796980
C	1.304312	-0.390395	1.468855
H	1.966013	-0.263482	2.340234
H	0.390899	-0.911355	1.804331
C	1.761205	1.323636	-1.517255
C	2.280801	1.846739	0.717665
H	2.058275	2.910462	0.524124
H	1.536646	2.385848	-1.716176
C	1.956438	-1.140679	0.254960
H	2.231576	-2.199638	0.439735
C	2.970974	1.187071	-0.527348
H	3.915627	1.665664	-0.858595
C	3.220118	-0.336942	-0.227497
H	3.620089	-0.817213	-1.138904
H	4.009202	-0.421790	0.541504

H	1.899530	0.816466	-2.485170
H	2.859516	1.782835	1.652661

MP2

7

1 scf done: -274.608776

C	-2.225876	-1.262200	-0.239224
H	-1.949181	-1.688644	-1.197591
H	-2.462919	-1.950859	0.564788
C	-2.490131	0.084088	-0.115971
H	-2.426617	0.743682	-0.974915
H	-2.940387	0.481533	0.787458
Cu	-0.496452	-0.277570	0.411131

22

2 scf done: -578.615408

C	-0.070071	-0.165345	0.676439
C	1.782145	0.794686	-0.199005
C	-0.228410	1.195099	0.758136
H	-1.042331	1.787130	1.140306
H	-0.715884	-0.968851	0.986806
N	1.152101	-0.380894	0.091960
N	0.906011	1.752056	0.224584
C	1.722228	-1.711724	-0.122051
H	0.949141	-2.369763	-0.509390
H	2.522501	-1.631370	-0.850932
H	2.111037	-2.104568	0.814515
Cu	3.472415	1.039520	-1.001065
C	4.924602	1.303350	-2.450250
C	5.515682	1.282065	-1.212519
H	4.663882	2.240162	-2.929025
H	4.868381	0.407585	-3.057981
H	5.736601	2.201717	-0.683053
H	5.940867	0.369096	-0.811870
C	1.104493	3.194245	0.074079
H	2.162236	3.382947	-0.079956
H	0.534178	3.561226	-0.776049
H	0.779936	3.692925	0.983309

24

3 scf done: -579.793459

C	-0.133671	-0.258132	0.670901
C	1.768152	0.785028	-0.182205
C	-0.243592	1.248353	0.899977
H	-0.100258	1.521561	1.948949
H	-0.805923	-0.609698	-0.116500
N	1.261597	-0.389927	0.213686
N	0.890658	1.754948	0.106231
C	1.796782	-1.702772	-0.106183
H	2.836936	-1.600265	-0.403661
H	1.741367	-2.341354	0.773646
H	1.229832	-2.161616	-0.918160
Cu	3.459704	1.035861	-1.019032
C	4.912296	1.227982	-2.497449
C	5.500584	1.361469	-1.267445
H	4.600202	2.097004	-3.065203
H	4.898349	0.272784	-3.009618
H	5.668930	2.339535	-0.831607
H	5.966279	0.515197	-0.775617
C	1.143336	3.184502	0.036910
H	1.341506	3.588499	1.031298
H	2.002220	3.363413	-0.604362
H	0.274902	3.686347	-0.386091
H	-1.181674	1.673040	0.547052
H	-0.301950	-0.846756	1.570965

15

4 scf done: -959.896776

C	-1.786201	-1.095664	0.504042
H	-1.526406	-2.147432	0.479026
H	-2.028386	-0.676123	1.473274
C	-2.127866	-0.426636	-0.659075
H	-2.139246	-0.945822	-1.610036
H	-2.646184	0.523983	-0.615430
Cu	-0.149356	-0.057130	-0.198095
P	1.447164	-0.556366	1.293805
H	1.068344	-1.044778	2.544037
H	2.344774	-1.548052	0.893481
H	2.337299	0.449782	1.671741
P	0.460324	1.304582	-1.872866
H	0.135585	0.892893	-3.165823
H	-0.123649	2.572226	-1.854367
H	1.801857	1.647136	-2.044950

11

5 scf done: -617.270065

C	-2.284745	-1.265460	-0.254360
H	-2.036190	-1.700892	-1.215885
H	-2.462730	-1.947544	0.569654
C	-2.559343	0.070689	-0.135330
H	-2.535238	0.724713	-0.999959
H	-2.961769	0.477918	0.785613
Cu	-0.523817	-0.250641	0.306527
P	1.581321	0.125961	0.858181
H	1.939076	1.464807	1.001877
H	2.012879	-0.421477	2.064159
H	2.544305	-0.337565	-0.035290

8

7 scf done: -374.527263

C	-2.105967	-1.247565	-0.211177
H	-1.927271	-1.689741	-1.184372
H	-2.356883	-1.935366	0.587910
C	-2.388055	0.116233	-0.090640
H	-2.431845	0.749896	-0.968778
H	-2.861572	0.504574	0.803523
Cu	-0.519946	-0.249363	0.311890
F	1.116295	0.049985	0.751645

8

8 scf done: -734.550244

C	-2.171610	-1.254949	-0.226381
H	-1.965102	-1.694766	-1.194774
H	-2.392411	-1.940547	0.582985
C	-2.453163	0.098119	-0.106913
H	-2.471723	0.739620	-0.979839
H	-2.898961	0.493631	0.797911
Cu	-0.543013	-0.251794	0.303519
Cl	1.420741	0.109337	0.823491

8

9 scf done: -2844.662930

C	-2.190987	-1.258009	-0.230805
H	-1.981422	-1.697658	-1.198581
H	-2.406585	-1.943101	0.580350
C	-2.473028	0.093483	-0.111665
H	-2.489336	0.735666	-0.984096
H	-2.914433	0.490014	0.794831
Cu	-0.553228	-0.252620	0.299499
Br	1.533776	0.130876	0.850468

11

10 scf done: -314.631029

C	-2.182301	-1.252352	-0.228797
H	-1.967338	-1.692697	-1.194897
H	-2.395625	-1.938886	0.581533
C	-2.458995	0.096068	-0.108531
H	-2.466864	0.742409	-0.977821
H	-2.895178	0.495932	0.798852
Cu	-0.519243	-0.252707	0.309873
C	1.282649	0.062631	0.784512
H	1.966771	-0.177254	-0.032041
H	1.432352	1.115985	1.036728
H	1.580149	-0.524739	1.655835

12

11 scf done: -389.688388

C	-2.094965	-1.289581	-0.394446
H	-1.786858	-1.541042	-1.402936
H	-2.315573	-2.126666	0.257691
C	-2.587902	-0.008207	-0.101291
H	-2.664598	0.741223	-0.880844
H	-3.195178	0.159582	0.780589
Cu	-0.729758	-0.182966	0.425414
O	0.840837	0.295504	0.973403
C	1.400232	0.212759	2.273437
H	2.417531	0.610219	2.245808
H	0.833108	0.797162	3.003845
H	1.454417	-0.818700	2.633751

9

12 scf done: -367.481107

C	-2.184413	-1.251678	-0.229044
H	-1.951462	-1.689615	-1.192219
H	-2.379404	-1.935836	0.588065
C	-2.463394	0.090699	-0.110372
H	-2.456565	0.740240	-0.977445
H	-2.884472	0.493824	0.802837
Cu	-0.505094	-0.245205	0.313392
C	1.245251	0.074690	0.776355
N	2.377063	0.281444	1.075421

28

13 scf done: -619.727535

C	0.241347	-0.221109	0.951142
C	1.758685	1.094967	-0.240422
C	-0.477998	1.019629	0.432724
H	-1.067409	1.531519	1.193040
H	-0.298193	-1.148815	0.762256
N	1.488613	-0.161758	0.180430
N	0.659575	1.837010	0.000843
C	2.529686	-1.146108	0.398266
H	3.329986	-0.957010	-0.312342
H	2.929950	-1.084501	1.414117
H	2.127881	-2.145662	0.232761
Cu	3.428685	1.748403	-0.863945
C	3.693877	1.199624	-2.760703
C	4.789275	1.947727	-2.256087
H	2.965244	1.671263	-3.410547
H	3.768231	0.121891	-2.856945
H	4.901521	2.995591	-2.511393
H	5.702522	1.446982	-1.954475
C	0.463597	3.160361	-0.553918
H	-0.117820	3.765006	0.141862
H	1.441558	3.614601	-0.692030
H	-0.061103	3.117881	-1.512530
C	4.147694	2.680876	0.686706
H	5.122181	3.148470	0.531583
H	3.453372	3.463892	1.011793
H	4.245838	1.986494	1.528664
H	-1.123861	0.786930	-0.421796
H	0.456156	-0.144928	2.023382

26

14 scf done: -618.544315

C	0.076462	-0.235222	0.589781
C	1.760812	1.058645	-0.232921
C	-0.420976	1.027811	0.418522
H	-1.402947	1.430225	0.598049
H	-0.386250	-1.131720	0.964721
N	1.392845	-0.189622	0.178318
N	0.618981	1.789037	-0.072420
C	2.322548	-1.307146	0.250216
H	3.093152	-1.143553	-0.496668
H	2.775956	-1.364197	1.238468
H	1.789165	-2.231085	0.036758
Cu	3.463302	1.748988	-0.771567
C	4.062919	0.822721	-2.439860
C	4.970511	1.828000	-2.014407
H	3.379445	1.015313	-3.259229
H	4.307419	-0.222383	-2.281291
H	4.981042	2.797317	-2.500855
H	5.891620	1.553973	-1.512280
C	0.525041	3.197991	-0.432753
H	1.529311	3.610907	-0.388652
H	0.119171	3.307499	-1.437278
H	-0.119401	3.707024	0.280787
C	3.933650	3.133604	0.523601
H	4.026974	4.116648	0.048721
H	3.217746	3.231933	1.346412
H	4.908970	2.915332	0.969252

49

15 scf done: -1765.661340

C	-5.926496	-0.328857	4.094318
C	-5.035854	-0.513186	3.054688
C	-5.019341	0.382874	1.951849
C	-5.994248	1.434020	1.901977
C	-6.884929	1.603363	2.993159
C	-6.866665	0.727225	4.059708
H	-5.923250	-1.016174	4.932159
C	-4.125385	0.209619	0.851163
C	-5.993226	2.323900	0.797595
H	-7.607637	2.411867	2.957438
C	-5.116660	2.145282	-0.252630
C	-4.153044	1.104104	-0.222642
H	-6.719884	3.129592	0.770309
H	-5.135431	2.833140	-1.091194
C	-3.129238	-0.891411	0.873952
C	-1.968663	-0.776539	1.698884
C	-3.350041	-2.053296	0.128373
C	-1.697215	0.394403	2.457440
C	-0.997616	-1.832336	1.688822
C	-2.384293	-3.092283	0.136942
C	-0.554691	0.480996	3.228900
C	0.158218	-1.716459	2.503460
C	-1.253678	-2.997049	0.922092
H	-2.555013	-3.984684	-0.454425
C	0.387224	-0.574001	3.243411
H	-0.364281	1.377459	3.807307
H	0.879805	-2.526720	2.504467
H	-0.524274	-3.800604	0.925775
H	-7.557377	0.860727	4.883746
H	1.277923	-0.492579	3.854945
P	-3.151262	0.748358	-1.709660
H	-3.119458	2.036433	-2.268716

H	-1.851169	0.726162	-1.176884
P	-4.736503	-2.104620	-1.066167
H	-4.845837	-3.497643	-1.206180
H	-5.826127	-1.919479	-0.190386
H	-2.414069	1.206558	2.449737
H	-4.318721	-1.324522	3.085625
Cu	-3.991858	-0.924121	-2.914421
C	-2.529481	-2.108616	-3.431309
H	-2.893032	-3.083486	-3.768877
H	-1.970627	-1.665786	-4.260287
H	-1.818997	-2.282386	-2.616891
C	-5.609814	0.032464	-3.707633
H	-6.515284	-0.203751	-3.162212
C	-5.046007	-0.911547	-4.594775
H	-5.509537	-1.883284	-4.721857
H	-4.407182	-0.586299	-5.407302
H	-5.417446	1.089299	-3.856279

30

16 scf done: -732.792324

C	-0.062557	-0.232861	0.468526
C	1.810506	0.992157	-0.200978
C	-0.423264	1.247897	0.428498
H	-0.909133	1.604225	1.335809
H	-0.781213	-0.870279	-0.045752
N	1.234426	-0.231929	-0.220306
N	0.904555	1.859888	0.268829
C	1.962788	-1.475592	-0.356955
H	2.894301	-1.269043	-0.870997
H	2.176532	-1.913583	0.622737
H	1.372349	-2.185604	-0.936420
C	1.080001	3.319382	0.290352
H	0.350541	3.685491	1.021582
C	2.481297	3.673564	0.808940
H	2.579362	3.193466	1.798760
H	2.466877	4.760933	0.989668
O	3.512027	3.346615	-0.061938
Cu	3.546636	1.639811	-0.782307
C	4.568173	0.421935	-1.939334
C	5.230283	1.660528	-1.762921
H	4.035506	0.213940	-2.861456
H	4.929616	-0.452068	-1.407273
H	5.168509	2.433712	-2.519962
H	6.050164	1.748960	-1.059957
C	0.789895	3.923696	-1.077294
H	-0.194634	3.631600	-1.445408
H	0.823799	5.011763	-1.015332
H	1.551995	3.597173	-1.781727
H	0.061809	-0.596103	1.495323
H	-1.053976	1.490794	-0.432297

28

17 scf done: -731.615209

C	-0.063335	-0.132094	0.352412
C	1.819222	1.001364	-0.232423
C	-0.303662	1.203428	0.547105
H	-1.178445	1.718784	0.904760
H	-0.687085	-0.993979	0.516051
N	1.225688	-0.224853	-0.120414
N	0.850275	1.862289	0.193751
C	1.890234	-1.484403	-0.424844
H	2.826538	-1.246892	-0.916107
H	2.083336	-2.038047	0.492554
H	1.261811	-2.078070	-1.085893
C	1.018933	3.328974	0.230167
H	0.275718	3.685545	0.950221
C	2.418318	3.678563	0.758871
H	2.518913	3.179850	1.739508
H	2.393579	4.761770	0.962105
O	3.447413	3.377449	-0.120702
Cu	3.546024	1.651031	-0.802303
C	4.632576	0.410420	-1.870610
C	5.271242	1.663792	-1.707296
H	4.148655	0.165232	-2.810374
H	4.978062	-0.440966	-1.292772
H	5.237748	2.407003	-2.495557
H	6.057535	1.786700	-0.971944
C	0.745451	3.917667	-1.144804
H	-0.240393	3.626910	-1.508833
H	0.793164	5.005461	-1.090333
H	1.508040	3.576358	-1.840893

29

18 scf done: -1167.691650

C	-1.231108	1.400011	0.899165
C	-0.536421	1.211360	-0.321966
C	-0.756439	2.087752	-1.394736
C	-1.656368	3.145854	-1.276513
C	-2.345524	3.336004	-0.076473
C	-2.139156	2.463790	0.996074
H	-0.215135	1.932168	-2.321915
H	-1.815226	3.819266	-2.109645
H	-3.048072	4.154209	0.024759
H	-2.687851	2.618679	1.918048
P	-1.119208	0.163779	2.244090
H	0.018425	0.484500	2.986507
H	-2.102493	0.715894	3.087313
C	0.432212	0.123151	-0.466907
N	0.820186	-0.514953	0.584001
C	1.768753	-1.606986	0.462677
H	1.920375	-1.913771	-0.580244
H	2.728980	-1.264924	0.852658
C	1.389615	-2.860929	1.291927
O	2.256847	-3.728168	1.383559
O	0.197780	-2.899982	1.828938
H	0.806153	-0.109664	-1.472320
Cu	-1.287814	-1.880827	1.328183
C	-2.999894	-1.810304	0.350366
C	-2.323652	-3.018937	0.102922
H	-2.981417	-1.011824	-0.383811
H	-3.825521	-1.782630	1.053181
H	-1.753683	-3.157133	-0.808481
H	-2.588093	-3.922146	0.640201

9

19 scf done: -474.201661

C	-2.217242	0.425741	1.211003
H	-2.560242	-0.347473	1.889907
H	-2.242242	1.435830	1.605360
C	-2.206730	0.200531	-0.188796
H	-2.541600	-0.747439	-0.595787
H	-2.223682	1.035865	-0.880424
Cu	-0.424608	0.004437	0.574225
F	0.673200	-0.413818	-0.823605
F	0.651070	0.047287	2.049080

9

20 scf done: -1194.274410

C	-2.267351	0.433619	1.205241
H	-2.590221	-0.343078	1.888454
H	-2.272074	1.441249	1.603923
C	-2.256757	0.209819	-0.186584
H	-2.571291	-0.742690	-0.596564
H	-2.253189	1.041644	-0.881090

Cu	-0.464916	0.011453	0.572905
Cl	0.778457	-0.489249	-1.180109
Cl	0.750842	0.087614	2.412991

9

21 scf done: -5414.503450

C	-2.280351	0.435816	1.202863
H	-2.595810	-0.341954	1.887879
H	-2.277508	1.442772	1.602538
C	-2.269847	0.212136	-0.185172
H	-2.576933	-0.742299	-0.595613
H	-2.258834	1.042457	-0.880968
Cu	-0.465245	0.011512	0.572898
Br	0.831255	-0.518840	-1.313560
Br	0.801198	0.099362	2.550098

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22 scf done: -354.399922

C	-1.225447	-1.835470	0.113813
H	-0.570993	-2.542929	0.612971
H	-2.185880	-1.680420	0.594948
C	-1.063902	-1.562084	-1.275482
H	-0.285238	-2.059276	-1.845083
H	-1.900073	-1.196673	-1.863071
Cu	-0.295813	-0.100898	-0.167701
C	0.072337	0.626154	1.622095
H	-0.254043	0.034717	2.486751
H	1.153404	0.786495	1.729794
H	-0.396151	1.615336	1.711812
C	0.426908	1.226034	-1.426444
H	1.496592	1.369221	-1.223261
H	0.327317	1.015017	-2.498590
H	-0.054121	2.195872	-1.241941

17

23 scf done: -504.518128

C	-1.736579	-0.794666	0.894505
H	-1.522640	-1.796352	1.252827
H	-2.027811	-0.080951	1.658267
C	-2.087247	-0.577138	-0.462736
H	-2.144917	-1.410359	-1.155523
H	-2.650057	0.305040	-0.750047
Cu	-0.215683	-0.104776	-0.129210
O	1.248137	0.054683	1.020220
C	1.117273	-0.297845	2.355217
H	0.843567	-1.358386	2.523243
H	2.067810	-0.147663	2.898398
H	0.361126	0.291015	2.911457
O	0.537903	0.495404	-1.729607
C	-0.234992	0.540849	-2.880359
H	-1.117884	1.206972	-2.811963
H	0.353624	0.916296	-3.736917
H	-0.634045	-0.441576	-3.202060

33

24 scf done: -1207.466030

C	-1.070599	1.195687	0.942524
C	-0.568314	1.128170	-0.379547
C	-1.054316	2.002586	-1.364015
C	-2.031746	2.948060	-1.061579
C	-2.537140	3.021394	0.239881
C	-2.066449	2.145991	1.221183
H	-0.661453	1.925560	-2.373054
H	-2.396829	3.620656	-1.829578
H	-3.303177	3.747932	0.487450
H	-2.479946	2.201326	2.222402
P	-0.634915	-0.090404	2.183128
H	0.566100	0.368799	2.738221
H	-1.494688	0.422687	3.186688
C	0.462648	0.148688	-0.721461
N	1.147150	-0.399189	0.219749
C	2.105122	-1.425799	-0.137554
H	2.100767	-1.638998	-1.214399
H	3.101823	-1.060660	0.127431
C	1.934953	-2.780250	0.626858
O	2.678294	-3.683671	0.192802
O	1.128770	-2.797961	1.616943
H	0.600545	-0.105893	-1.781063
Cu	-0.957074	-2.199649	1.640803
C	-1.583044	-2.337983	-0.198181
H	-0.752224	-2.713098	-0.806154
H	-2.416360	-3.037779	-0.324134
H	-1.902349	-1.381633	-0.631663
C	-1.625157	-3.834899	2.524679
H	-1.010217	-4.634796	2.129017
C	-1.096612	-2.968594	3.508449
H	-1.769527	-2.406415	4.148942
H	-0.085295	-3.112839	3.866398
H	-2.696970	-3.941504	2.399983

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25 scf done: -772.525022

C	-0.106046	-0.073392	0.693946
C	1.719076	1.070226	-0.212684
C	-0.517670	1.363507	0.402950
H	-1.025129	1.852187	1.236095
H	-0.845351	-0.813617	0.380652
N	1.124681	-0.166711	-0.090739
N	0.788578	1.974399	0.145525
C	1.952790	-1.346019	0.042463
H	2.816352	-1.215486	-0.604275
H	2.308579	-1.477593	1.069857
H	1.384071	-2.229051	-0.259693
C	0.920830	3.416807	-0.088981
H	0.150974	3.885894	0.539485
C	2.318485	3.934137	0.360988
H	2.420964	3.599170	1.421085
H	2.173639	5.044296	0.421767
O	3.326708	3.550878	-0.457571
Cu	3.555615	1.429350	-0.399275
C	4.178155	1.354235	-2.311523
C	5.259127	1.357825	-1.394641
H	3.859237	2.282509	-2.769145
H	3.896312	0.438754	-2.823099
H	5.766664	2.288401	-1.167118
H	5.814694	0.446171	-1.196277
C	0.681498	3.732881	-1.558592
H	-0.269525	3.330615	-1.917876
H	0.681412	4.813897	-1.712910
H	1.509603	3.301168	-2.116795
C	4.136712	1.066155	1.452845
H	5.056179	0.470317	1.515305
H	4.340492	2.043597	1.903528
H	3.389431	0.565243	2.084242
H	0.105825	-0.214305	1.763723
H	-1.160284	1.423192	-0.485209

32

26 scf done: -771.344353

C	-0.184487	0.048323	0.637191
C	1.710539	1.072897	-0.135470
C	-0.460422	1.382783	0.488070
H	-1.357063	1.945100	0.687393
H	-0.797393	-0.767781	0.981318

N	1.132366	-0.107897	0.258546
N	0.695958	1.975328	0.022039
C	1.881716	-1.350345	0.267357
H	2.926907	-1.077859	0.403642
H	1.538657	-1.974736	1.092259
H	1.756383	-1.888959	-0.673039
C	0.852950	3.414706	-0.238946
H	0.004715	3.894066	0.266768
C	2.185939	3.942666	0.372224
H	2.158934	3.614871	1.441192
H	2.023180	5.051710	0.409979
O	3.283581	3.565303	-0.317795
Cu	3.567062	1.438564	-0.374736
C	4.074384	1.484828	-2.330066
C	5.201388	1.438545	-1.470303
H	3.746982	2.439380	-2.722983
H	3.766748	0.601201	-2.880971
H	5.725144	2.355998	-1.224965
H	5.768939	0.519876	-1.354514
C	0.800905	3.666909	-1.735927
H	-0.133298	3.302723	-2.170490
H	0.889583	4.737277	-1.930244
H	1.648917	3.159205	-2.188185
C	4.291481	0.979545	1.408369
H	5.192368	0.351323	1.390739
H	4.565536	1.934339	1.870292
H	3.572465	0.488564	2.080298

22

27 scf done: -545.298117

C	1.092871	0.911244	0.731932
C	0.775491	0.590712	-0.635666
C	0.790188	-0.920436	-0.771582
H	-0.107938	-1.438804	-0.430909
H	1.007354	-1.235765	-1.791674
C	1.311189	-0.394093	1.473968
H	1.965063	-0.268219	2.336394
H	0.408495	-0.916984	1.795104
C	1.766170	1.320620	-1.523349
C	2.287211	1.846942	0.722230
H	2.069279	2.896395	0.515968
H	1.552808	2.374672	-1.710013
C	1.956062	-1.121284	0.249884
H	2.217061	-2.167052	0.434474
C	2.955951	1.174645	-0.520287
H	3.881846	1.655537	-0.847835
C	3.204576	-0.329578	-0.225390
H	3.598098	-0.804099	-1.129028
H	3.984657	-0.413613	0.536840
H	1.902080	0.818847	-2.480910
H	2.859946	1.786378	1.647152
Cu	-0.747293	1.550190	0.250576

Ethylene

6

scf done: -78.317282

C	-3.562755	-0.015462	0.000000
H	-3.048281	-0.965820	0.000000
H	-4.643013	-0.045586	0.000000
C	-2.895414	1.141016	0.000000
H	-3.409888	2.091374	0.000000
H	-1.815157	1.171140	0.000000

Constrained olefin

21

scf done: -348.968483

C	1.086866	0.904725	0.701764
C	0.783498	0.597967	-0.606577
C	0.794144	-0.908792	-0.760830
H	-0.112153	-1.420789	-0.428072
H	1.014124	-1.226433	-1.781136
C	1.308780	-0.388416	1.458570
H	1.965321	-0.264629	2.321088
H	0.401385	-0.901463	1.786681
C	1.765028	1.317832	-1.508040
C	2.279776	1.838120	0.711366
H	2.054540	2.889255	0.514879
H	1.540733	2.369994	-1.700114
C	1.954320	-1.131288	0.252689
H	2.232266	-2.178602	0.433796
C	2.963174	1.182402	-0.523797
H	3.901746	1.650199	-0.851165
C	3.205818	-0.330346	-0.225412
H	3.599924	-0.805659	-1.129460
H	3.986595	-0.414755	0.537355
H	1.904204	0.815006	-2.466225
H	2.855592	1.776430	1.636010