Electronic Supplementary Information

Toward a mechanistic understanding of oxidative homocoupling: the Glaser–Hay reaction

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Table S1. Computed potential energies, enthalpies, free energies and dispersion correction terms for all the species involved in the catalytic cycles (in Hartrees).

Species	Potential	Enthalpy	Free energy	Dispersion
Phenylacetylene	-308.076609	-307.963100	-308.000964	-0.004231
Diphenyldiacetylene	-614.994097	-614.784693	-614.840135	-0.009103
O_2	-150.236349	-150.229615	-150.252925	-0.000001
H_2O	-76.380900	-76.356823	-76.378306	-0.000004
TMEDA	-347.371068	-347.145162	-347.190952	-0.011080
TMEDA-H^+	-347.843450	-347.601824	-347.647779	-0.012538
$[Fe(CN)_6]^{3-}$	-1820.623761	-1820.560194	-1820.615095	-0.008841
$[Fe(CN)_6]^{4-}$	-1820.765989	-1820.703054	-1820.756364	-0.008848
G1	-544.632739	-544.401947	-544.451771	-0.016987
G2	-852.764499	-852.417613	-852.483578	-0.029129
DP_TS	-1200.116501	-1199.545258	-1199.638877	-0.047954
G3	-852.289850	-851.954905	-852.023633	-0.023680
G4	-1704.583454	-1703.912235	-1704.028188	-0.064477
G5 (O16)	-1704.303944	-1703.626756	-1703.733259	-0.070199
RedEl_TS	-1704.292304	-1703.617346	-1703.724353	-0.068613
NH_3	-56.511871	-56.474881	-56.497793	-0.000017
DP_TS-NH_3	-909.253106	-908.871636	-908.946675	-0.027978
OH^-	-75.858236	-75.846758	-75.866347	0.000000
DP_TS-OH^-	-928.627826	-928.271280	-928.345091	-0.028344
G2-*p*F-Phenylacetylene	-951.949721	-951.610075	-951.678028	-0.029534
DP_TS-*p*F-Phenylacetylene	-1299.302346	-1298.738111	-1298.834019	-0.048617
G2-*p*Me-Phenylacetylene	-892.036460	-891.661397	-891.730372	-0.030836
DP_TS-*p*Me-Phenylacetylene	-1239.388683	-1238.789437	-1238.884475	-0.049468
G1’	-544.473346	-544.241250	-544.290268	-0.017690
G2’	-852.568338	-852.220944	-852.288122	-0.028240

DP_TS’	-1199.950183	-1199.377050	-1199.472487	-0.044945
G3’	-852.135562	-851.798707	-851.865688	-0.024733
O4	-1002.526278	-1002.182337	-1002.255008	-0.028790
O5	-1854.833632	-1854.152278	-1854.269971	-0.065396
O6	-1854.834450	-1854.152981	-1854.271199	-0.061477
O7	-1855.297757	-1854.600007	-1854.717081	-0.062345
O8	-1855.310415	-1854.615085	-1854.730722	-0.069054
O9	-1855.305268	-1854.610517	-1854.725853	-0.072512
O10	-1855.307775	-1854.613188	-1854.730294	-0.067988
O11	-1855.767485	-1855.057259	-1855.175492	-0.069788
O12	-1855.772433	-1855.062694	-1855.176076	-0.075707
O13	-927.898358	-927.545279	-927.613204	-0.028618
O14	-1780.197782	-1779.508445	-1779.622771	-0.071448
O15	-1780.206929	-1779.517973	-1779.632752	-0.074538

Table S2. Computed potential energy, enthalpy and free energy profiles (in kcal/mol) for the catalytic cycles, dispersion corrections are included.

Species	Potential	Enthalpy	Free energy
G1	0.0	0.0	0.0
G2	-39.6	-38.0	-24.3
DP_TS	-32.5	-31.8	-6.8
G3	-35.7	-31.7	-19.9
G4	-42.2 (-84.4)	-37.8 (-75.6)	-19.2 (-38.4)
G5 (O16)	-45.5 (-91.0)	-39.7 (-79.4)	-17.2 (-34.4)
RedEl_TS	-41.4 (-82.8)	-33.2 (-72.4)	-13.9 (-27.8)
G1’	0.0	0.0	0.0
G2’	-15.5	-14.4	-2.0
DP_TS’	-26.8	-24.8	-1.4
G3’	-39.1	-34.7	-22.3
G5	-55.9 (-111.8)	-50.4 (-100.8)	-29.4 (-58.8)
RedEl_TS	-51.7 (-103.4)	-47.0 (-94.0)	-26.1 (-52.2)
G1	0.0	0.0	0.0
G2	-39.6	-38.0	-24.3
DP_TS	-32.5	-31.8	-6.8
G3	-35.7	-31.7	-19.9
O4	-38.9	-33.5	-9.5
O5	-46.8 (-93.6)	-41.3 (-82.6)	-16.0 (-32.0)
O6	-45.9 (-91.8)	-40.3 (-80.6)	-15.2 (-30.4)
O7	-42.8 (-85.6)	-37.1 (-74.2)	-11.6 (-23.2)
O8	-48.9 (-97.8)	-44.0 (-88.0)	-18.0 (-36.0)
O9	-48.4 (-96.8)	-43.6 (-87.2)	-17.5 (-35.0)
O10	-47.7 (-95.4)	-43.0 (-86.0)	-17.5 (-35.0)

O11	-43.9 (-87.8)	-39.2 (-78.4)	-14.0 (-82.0)
O12	-47.3 (-94.6)	-42.8 (-85.6)	-16.0 (-32.0)
O13	-49.1	-45.7	-26.0
O14	-55.2 (-110.4)	-51.2 (-102.4)	-24.5 (-49.0)
O15	-51.4 (-102.8)	-47.3 (-94.6)	-28.6 (-57.2)
G5	-55.1 (-110.2)	-52.2 (-104.4)	-33.7 (-67.4)
RedEl_TS	-51.0 (-102.0)	-48.8 (-97.6)	-30.4 (-60.8)

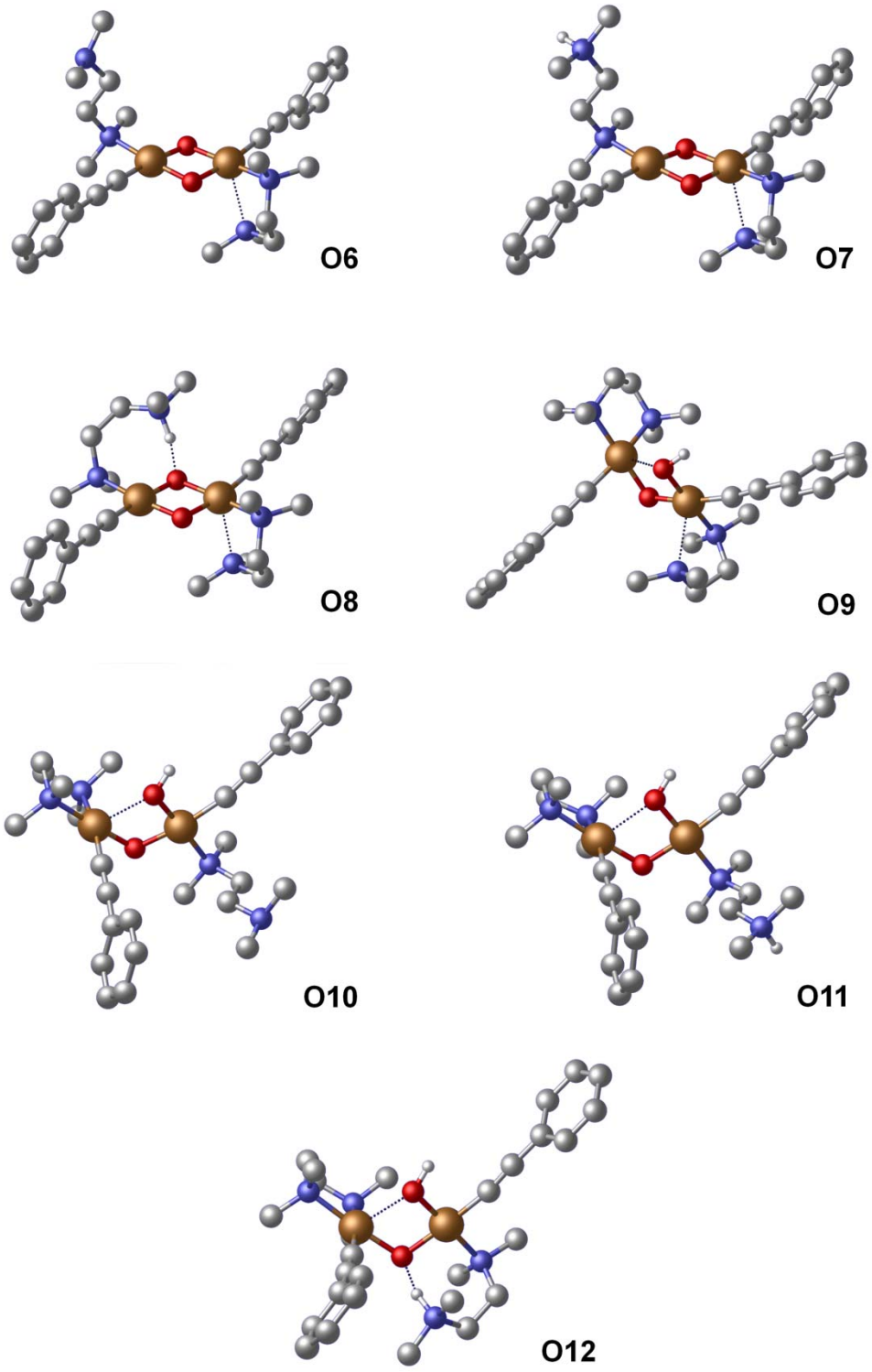
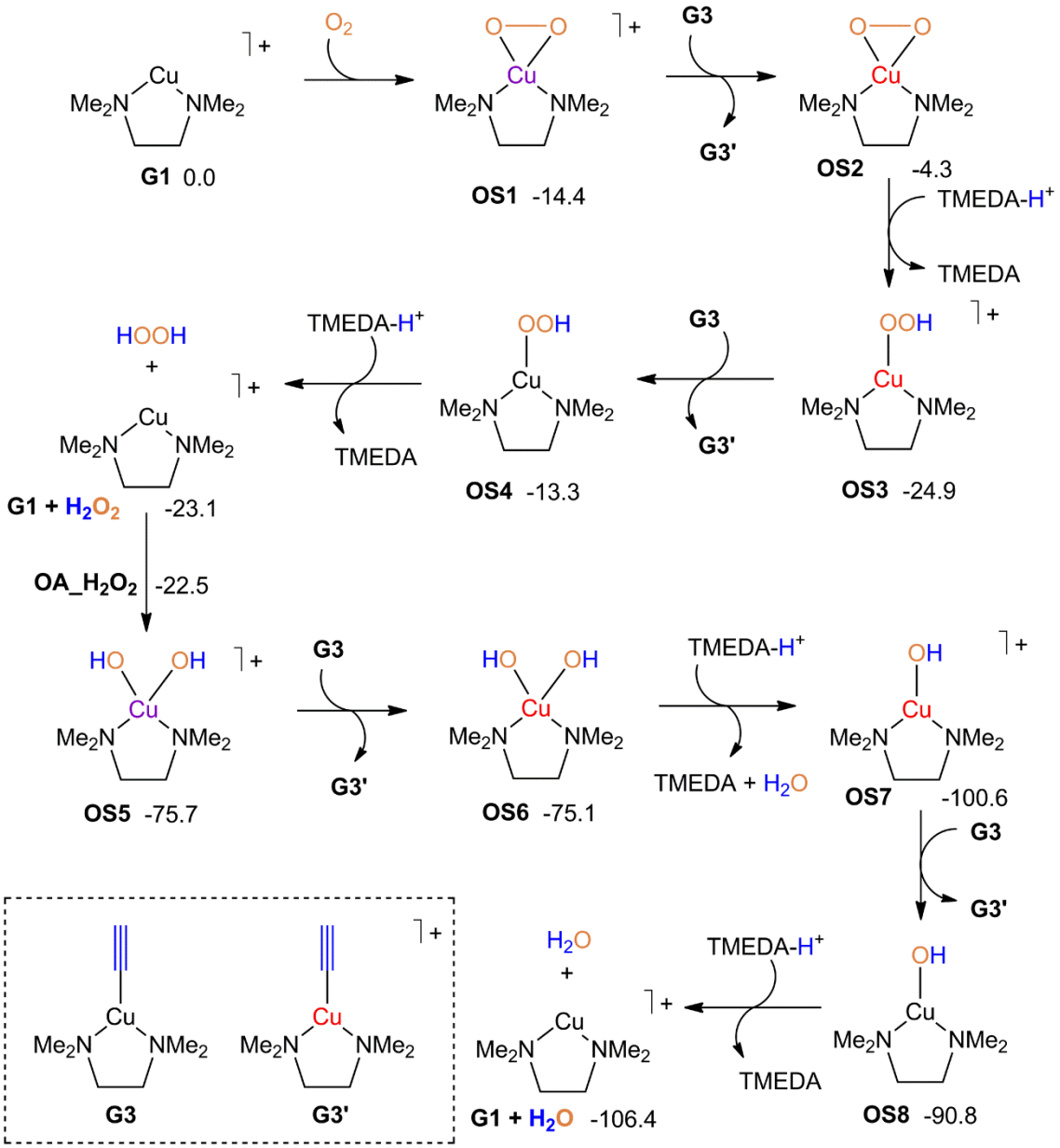


Figure S1. Detailed structures of intermediates **O6-O12**.

Outer-sphere catalytic cycle

An alternative reaction pathway, based on outer-sphere mononuclear oxidations, has also been computed since it is known that some Cu/O_2 species act in this fashion. This catalytic cycle consists mainly of a sequence of one-electron transfers and protonation of the derived oxygenated species (Scheme S1).



Scheme S1. Proposed outer-sphere mechanism for the Glaser-Hay coupling including the computed free energy values in kcal/mol (Cu(I), Cu(II), Cu(III); for clarity phenylacetylene is depicted as ≡).

The catalytic cycle starts with the 2-electron-transfer from **G1** to dioxygen to yield the copper (III)-η^2-peroxo intermediate **OS1**. This stage involves also a spin-crossing from triplet to singlet, probably through a low-energy minimum energy crossing point (MECP). In **OS1** the O–O distance has been elongated to 1.39 Å, matching the experimentally determined distance for this kind of peroxo complexes. This complex is then capable to act as an outer-sphere oxidant for other copper (I) species such as **G3**, which can be obtained by acetylene coordination to **G1** and subsequent deprotonation with a free TMEDA ligand; it has to be remembered that the barrier for this process is 17.5 kcal/mol. The electron transfer between **OS1** and **G3** affords the copper (II) species **G3'** and the η^2-peroxocopper (II) **OS2**, this process requires only 10.1 kcal/mol. The peroxo moiety is then protonated by a TMEDA-H^+, obtained in the formation of **G3**, to yield the η^1-hydroperoxocopper (II) intermediate **OS3**. This latter compound can, in turn, oxidize another equivalent of **G3** to **G3'** giving rise to the η^1-hydroperoxocopper (I) complex **OS4**; again, the barrier for this electron-transfer is quite low (11.5 kcal/mol). The protonation of **OS4** yields hydrogen peroxide and the starting catalyst **G1**; those two reactants can then undergo oxidative addition to form the dihydroxycopper (III) complex **OS5**. As may be seen the free energy of the transition state mediating this stage (**OA_H_2O_2**) is less than 1 kcal/mol higher than the separated reactants, indicating that this process should be very fast. **OS5** is another species capable of oxidizing **G3** to **G3'**, in fact, this stage requires only 0.6 kcal/mol and forms the dihydroxycopper (II) intermediate **OS6**. Adding a proton to **OS6** delivers a first water molecule and the hydroxycopper (II) **OS7**, which can again oxidize another unit of **G3** to **G3'**; this last oxidation requires only 9.8 kcal/mol and affords the hydroxycopper (I) species **OS8**. Finally, the protonation of the hydroxyl forms the second water molecule and regenerates the starting catalyst **G1**. The formation of diphenyldiacetylene from two **G3'** units is quite straightforward as described in the main text (Scheme 4).

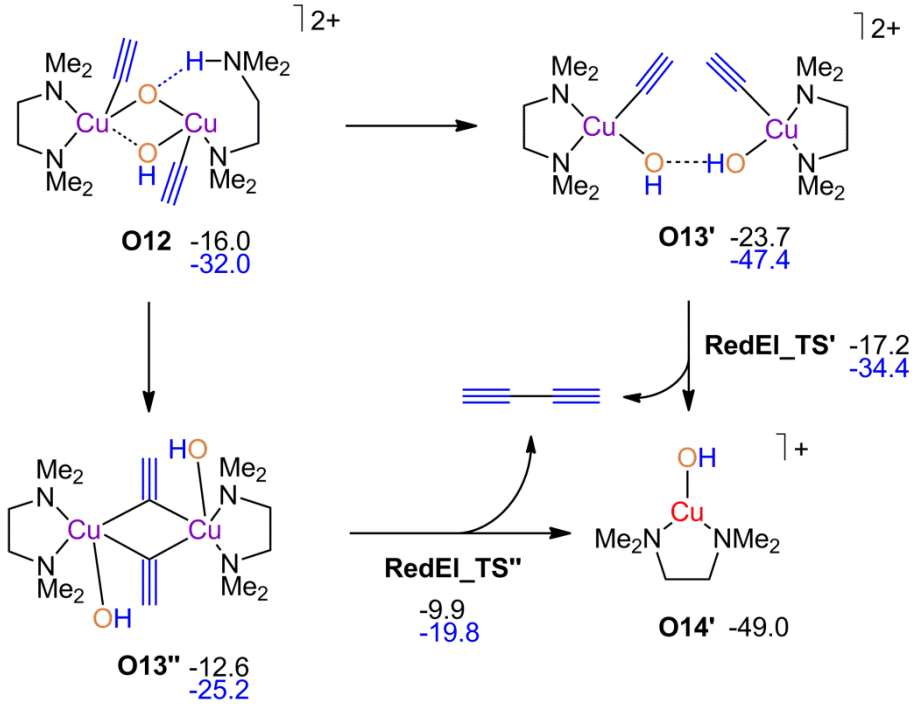
Once computed the inner- and outer-sphere mechanisms is possible to compare them in free energy terms. For both, the major barrier corresponds to the terminal alkyne deprotonation (17.5 kcal/mol) and thus it is not easy to state which one should be preferred. In terms of oxidation barriers the inner-sphere seems to be somehow favoured since the barrier is just 10.3 kcal/mol (computed between **G3** and **O4**); for the outer-sphere mechanism described here the free energy differences for the electron transfers are: -14.4, 10.1, 11.6, 0.6 and 9.8 kcal/mol. The highest increase in energy is therefore 11.6 kcal/mol, already higher than the 10.3 kcal/mol in the inner sphere mechanism. Moreover, there should be also a small barrier associated to the electron transfer, that could be estimated through Marcus theory, that would further increase the gap in favor of the inner sphere mechanism reported in the main text.

Table S3. Computed potential energies, enthalpies, free energies and dispersion correction terms (in Hartrees) for the outer-sphere catalytic cycle.

Species	Potential	Enthalpy	Free energy	Dispersion
OS1	-694.912111	-694.671500	-694.724661	-0.020024
OS2	-695.046531	-694.808456	-694.866349	-0.019163
OS3	-695.520425	-695.268675	-695.325293	-0.019569
OS4	-695.654253	-695.404699	-695.463318	-0.020052
H_2O_2	-151.460359	-151.430832	-151.456559	-0.000170
OA_H_2O_2	-696.105737	-695.845574	-695.903083	-0.021476
OS5	-696.194779	-695.932025	-695.986514	-0.022896
OS6	-696.345198	-696.085114	-696.143161	-0.022135
OS7	-620.429391	-620.182199	-620.234971	-0.019362
OS8	-620.566560	-620.321972	-620.377707	-0.017857

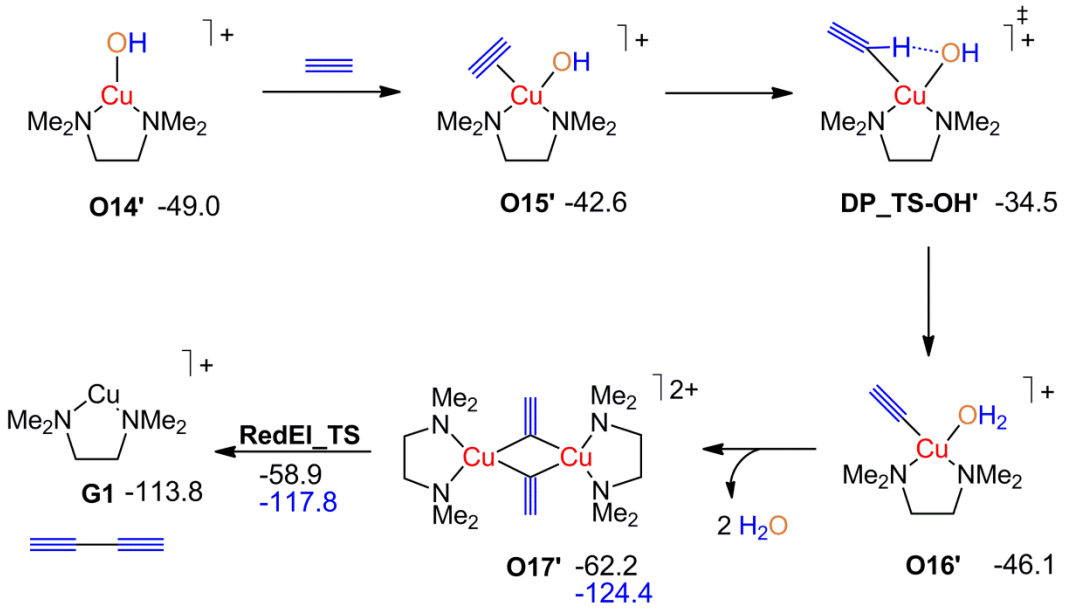
Alternative mechanisms for diphenyldiacetylene formation

A couple of alternative pathways have been found and analyzed, both of them involving a bimetallic reductive elimination from Cu(III) intermediates. These mechanisms are described in Scheme S2 and S3.



Scheme S2. Proposed alternative mechanisms for the Glaser Hay coupling including the computed free energy values in kcal/mol (Cu(II), Cu(III); for clarity phenylacetylene is depicted as ≡).

In Scheme S2, after the proton is transferred from the nitrogen to the bridging oxygen in **O12** the dinuclear complex is not stable anymore and rearranges into **O13'**, where both alkynyl groups act as bridging ligands, or into **O13''** where a hydrogen bond interaction is established between both hydroxyl groups. Bimetallic reductive elimination from either compound is quite easy, forming a first diphenyldiacetylene molecule and the copper (II) intermediate **O14'**. After that, the reaction follows the pathway shown in Scheme S3 where a second molecule of diphenyldiacetylene is formed and the catalyst is recovered.



Scheme S3. Proposed alternative mechanism for the product formation in the Glaser-Hay coupling including the computed free energy values in kcal/mol (Cu(I), Cu(II); for clarity phenylacetylene is depicted as ≡).

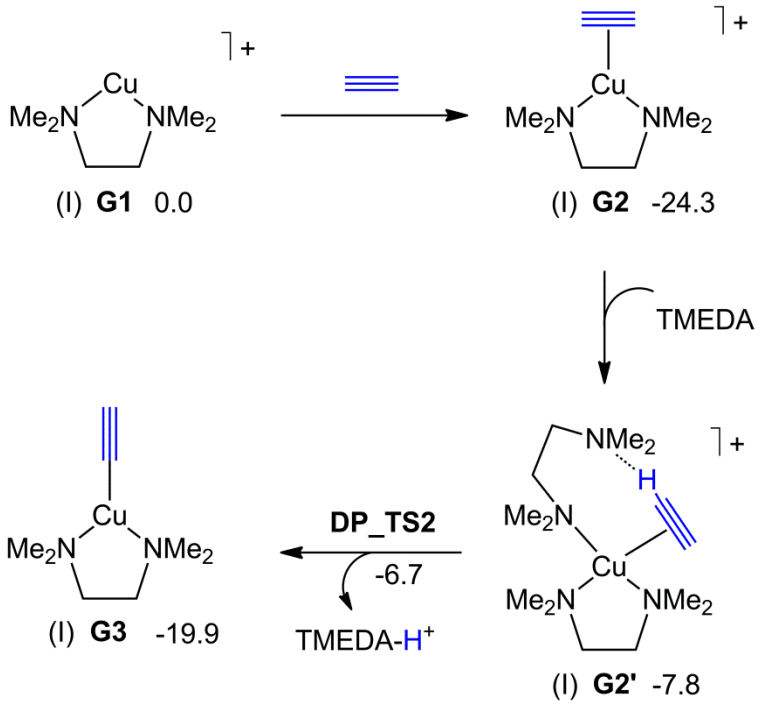
Complex **O14'** can easily coordinate a free alkyne to form **O15'**, then the intramolecular deprotonation happens with an energy requirement of less than 10 kcal/mol to yield the copper (II)–σ–acetylide–H_2O **O16'**. This latter intermediate is able to dimerize to form **O17'** (the same complex as **G5**) by liberating two molecules of water. In fact, the optimization of the dinuclear species where the water molecules remained on the copper atoms always ended up with their dissociation along the formation of the bimetallic complex. Once **O17'** is formed, a reductive elimination that requires less than 7 kcal/mol, the same as **RedEl_TS** in the outer sphere mechanism, produces the second diphenyldiacetylene molecule and regenerates the initial copper (I) catalyst.

Table S4. Computed potential energies, enthalpies, free energies and dispersion correction terms (in Hartrees) for the alternative pathways.

Species	Potential	Enthalpy	Free energy	Dispersion
O13’	-1855.799260	-1855.091562	-1855.205391	-0.070853
RedEl_TS’	-1855.774432	-1855.067731	-1855.178994	-0.076709
O14’	-620.429360	-620.182152	-620.234562	-0.019343
O13’’	-1855.749385	-1855.044092	-1855.161144	-0.079984
RedEl_TS’’	-1855.742761	-1855.037839	-1855.151319	-0.080964
O15’	-928.508727	-928.146521	-928.217891	-0.031001
DP_TS-OH’	-928.492964	-928.135776	-928.206332	-0.029629
O16’	-928.517040	-928.153459	-928.225472	-0.029053

Alternative intramolecular deprotonation

This alternative pathway, depicted in Scheme S4, consists in the coordination of TMEDA to **G2** to form intermediate G2', which is substantially higher in free energy than the separated counterparts. Nevertheless, the intramolecular deprotonation affords a barrier that is very close to the one proposed in the main text, suggesting that both pathways could be operating.



Scheme S4. Alternative intramolecular deprotonation mechanism including the computed free energy values in kcal/mol (for clarity phenylacetylene is depicted as ≡).

Optimized geometries

Phenylacetylene

C	3.250962	0.000004	0.000002
H	4.328734	0.000022	0.000005
C	2.027329	-0.000013	-0.000001
C	0.597380	-0.000005	0.000000
C	-0.119663	-1.221882	0.000000
C	-0.119652	1.221877	0.000000
C	-1.519061	-1.215391	0.000000
H	0.431149	-2.167473	0.000000
C	-1.519051	1.215397	0.000000
H	0.431165	2.167465	0.000000
C	-2.222634	0.000007	0.000000
H	-2.063564	-2.165311	0.000000
H	-2.063544	2.165323	0.000000
H	-3.317602	0.000010	0.000000

Diphenyldiacetylene

C	0.677808	-0.000121	-0.000102
C	1.915102	-0.000097	-0.000063
C	-0.677808	-0.000015	-0.000025
C	-1.915102	0.000034	0.000026
C	-3.335504	0.000023	0.000019
C	-4.054538	0.865129	0.866121
C	-4.054518	-0.865092	-0.866088
C	-5.452744	0.859406	0.860389
H	-3.503525	1.533036	1.534914
C	-5.452725	-0.859387	-0.860370
H	-3.503491	-1.532993	-1.534875
C	-6.155933	0.000005	0.000006
H	-5.997540	1.530548	1.532351
H	-5.997505	-1.530536	-1.532338
H	-7.250775	-0.000002	0.000001
C	3.335504	-0.000041	-0.000024
C	4.054516	0.866140	-0.865068
C	4.054540	-0.866167	0.865055
C	5.452722	0.860468	-0.859321
H	3.503486	1.534947	-1.532946
C	5.452747	-0.860388	0.859375
H	3.503530	-1.535015	1.532909
C	6.155933	0.000068	0.000045
H	5.997501	1.532492	-1.530416
H	5.997544	-1.532369	1.530496
H	7.250775	0.000111	0.000072

O_2

O	0.000000	0.000000	0.614021
O	0.000000	0.000000	-0.614021

H_2O

O	0.000000	0.000000	0.123172
H	0.000000	0.761276	-0.492687
H	0.000000	-0.761276	-0.492687

TMEDA

C	0.703041	0.307856	0.931681
C	-0.703043	-0.307939	0.931651
H	0.630991	1.404563	1.050976
H	1.216661	-0.071119	1.851687
H	-0.630992	-1.404657	1.050846
H	-1.216665	0.070952	1.851691
N	-1.497764	-0.053784	-0.275012
N	1.497765	0.053811	-0.275003
C	1.681057	-1.371716	-0.534831
H	0.708194	-1.851693	-0.731769
H	2.308500	-1.499221	-1.434156
H	2.177129	-1.915357	0.306666
C	2.789713	0.727080	-0.173257
H	3.357986	0.588750	-1.110016
H	2.636854	1.809929	-0.018475
H	3.421365	0.349617	0.668490
C	-1.681060	1.371765	-0.534711
H	-0.708197	1.851763	-0.731609
H	-2.308505	1.499350	-1.434023
H	-2.177130	1.915331	0.306836
C	-2.789710	-0.727068	-0.173328
H	-3.421362	-0.349689	0.668456
H	-3.357985	-0.588650	-1.110073
H	-2.636847	-1.809931	-0.018652

TMEDA-H^+

C	0.677296	0.271605	1.139708
C	-0.730657	-0.342975	1.080664
H	0.635760	1.364029	1.261343
H	1.291074	-0.154928	1.946451
H	-0.662272	-1.441071	1.155704
H	-1.317321	0.013465	1.952354
N	-1.352811	-0.007367	-0.212223
H	0.505546	0.007793	-0.835399
N	1.347543	0.002384	-0.187740
C	1.982978	-1.350081	-0.255746
H	1.247249	-2.113020	0.032703
H	2.315822	-1.525147	-1.288374
H	2.840571	-1.369158	0.432481
C	2.299665	1.077173	-0.595640
H	2.709837	0.823901	-1.583821
H	1.755687	2.030693	-0.644887
H	3.108700	1.136069	0.147221
C	-1.936781	1.340462	-0.212864
H	-1.181189	2.089165	0.076544
H	-2.287824	1.585465	-1.229093
H	-2.797152	1.425224	0.487123
C	-2.345158	-1.002875	-0.631107
H	-3.216820	-1.056550	0.057512
H	-2.717323	-0.740996	-1.635934
H	-1.877539	-1.999903	-0.682269

$[Fe(CN)_6]^{3-}$

Fe	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.925760
C	0.000000	1.934524	0.000000
C	-1.934524	0.000000	0.000000
C	1.934524	0.000000	0.000000
C	0.000000	-1.934524	0.000000
C	0.000000	0.000000	-1.925760
N	0.000000	0.000000	3.113291
N	3.120881	0.000000	0.000000
N	0.000000	-3.120881	0.000000
N	0.000000	3.120881	0.000000
N	-3.120881	0.000000	0.000000
N	0.000000	0.000000	-3.113291

$[Fe(CN)_6]^{4-}$

Fe	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.914115
C	0.000000	1.914115	0.000000
C	-1.914115	0.000000	0.000000
C	1.914115	0.000000	0.000000
C	0.000000	-1.914115	0.000000
C	0.000000	0.000000	-1.914115
N	0.000000	0.000000	3.108955
N	3.108955	0.000000	0.000000
N	0.000000	-3.108955	0.000000
N	0.000000	3.108955	0.000000
N	-3.108955	0.000000	0.000000
N	0.000000	0.000000	-3.108955

G1

Cu	-0.000003	-1.181400	-0.000004
C	0.685349	1.412035	-0.346595
C	-0.685344	1.412034	0.346600
H	0.556323	1.414203	-1.441388
H	1.224212	2.342947	-0.073716
H	-0.556319	1.414198	1.441393
H	-1.224206	2.342948	0.073725
N	-1.513935	0.214422	0.001520
N	1.513938	0.214420	-0.001520
C	2.579622	0.023609	-1.011121
H	3.256652	0.902662	-1.050772
H	3.171721	-0.867235	-0.748572
H	2.126675	-0.125884	-2.003859
C	2.130197	0.361208	1.337995
H	2.696502	-0.552235	1.577550
H	2.820379	1.230713	1.360446
H	1.353554	0.503045	2.104952
C	-2.130199	0.361220	-1.337992
H	-1.353558	0.503061	-2.104951
H	-2.696506	-0.552221	-1.577551
H	-2.820379	1.230726	-1.360434
C	-2.579616	0.023605	1.011123
H	-3.256645	0.902658	1.050782
H	-3.171716	-0.867237	0.748572
H	-2.126666	-0.125894	2.003860

G2

Cu	-0.757578	-0.500483	0.007956
C	-2.254116	1.887187	0.292165
C	-3.186046	0.885691	-0.385656
H	-2.384629	1.852582	1.386007
H	-2.498274	2.915286	-0.039857
H	-3.098220	0.959361	-1.482151
H	-4.238211	1.108419	-0.119354
N	-2.833698	-0.513431	-0.004249
N	-0.822236	1.569993	0.001224
C	1.035733	-1.461156	0.010470
C	0.046056	-2.253549	0.006417
H	-0.377329	-3.255086	0.002642
C	-3.400265	-1.471532	-0.980889
H	-3.117143	-2.495664	-0.691768
H	-4.506182	-1.400340	-1.009130
H	-2.998672	-1.257236	-1.983693
C	-3.329858	-0.844847	1.353491
H	-4.436627	-0.789487	1.389197
H	-3.012237	-1.866565	1.614101
H	-2.912096	-0.147520	2.095512
C	-0.432986	2.061454	-1.344256
H	-0.514690	3.165897	-1.394993
H	0.608619	1.767976	-1.548683
H	-1.082084	1.619115	-2.115326
C	0.055647	2.191476	1.020972
H	1.105500	1.948352	0.795370
H	-0.063848	3.293488	1.026206
H	-0.198751	1.795840	2.016757
C	2.332497	-0.837525	0.006369
C	2.975171	-0.533256	-1.220201
C	2.976891	-0.514424	1.226926
C	4.237274	0.071714	-1.218108
H	2.477845	-0.780185	-2.163429
C	4.239228	0.090109	1.213523
H	2.480628	-0.745008	2.174816
C	4.872804	0.385206	-0.005120
H	4.728473	0.298289	-2.170048
H	4.731785	0.331499	2.161112
H	5.859262	0.859767	-0.009460

DP_TS

Cu	-1.229171	-0.653345	-0.180883
C	-3.909499	-1.563831	0.225515
C	-3.189541	-1.886919	1.536325
H	-4.372477	-0.564669	0.282946
H	-4.724419	-2.298528	0.060135

H	-2.764502	-2.903488	1.496709
H	-3.922021	-1.868256	2.370057
N	-2.069923	-0.942988	1.792457
N	-2.975144	-1.551209	-0.936004
C	1.665689	-0.655740	-0.359619
C	0.550647	-0.083798	-0.506856
H	0.313304	1.038134	-1.018930
N	0.212986	2.273996	-1.879803
C	0.140253	3.560997	-1.136990
H	0.343552	4.388348	-1.847030
H	-0.898921	3.682252	-0.789734
C	1.104250	3.654445	0.052587
H	1.331777	4.731172	0.235592
H	2.063263	3.176368	-0.211319
N	0.594292	3.007754	1.272792
C	1.694347	2.685540	2.184261
H	1.294092	2.183093	3.082233
H	2.401639	1.997335	1.690032
H	2.262513	3.585219	2.521927
C	-0.379849	3.861354	1.957538
H	-1.233874	4.087687	1.297244
H	-0.770623	3.338553	2.847344
H	0.062090	4.831115	2.291492
C	1.400092	2.195626	-2.748844
H	1.445005	1.194657	-3.207854
H	1.359047	2.960857	-3.548380
H	2.314036	2.348239	-2.154264
C	-1.017974	2.026541	-2.647244
H	-0.928382	1.062193	-3.174249
H	-1.875443	1.980646	-1.955357
H	-1.200036	2.824609	-3.393517
C	-3.601092	-0.844803	-2.075309
H	-2.901191	-0.831564	-2.925617
H	-4.537727	-1.349389	-2.392694
H	-3.836450	0.191609	-1.785630
C	-2.630606	-2.930661	-1.354680
H	-3.538465	-3.488106	-1.667369
H	-1.927197	-2.886143	-2.201145
H	-2.145466	-3.473621	-0.529000
C	-1.099054	-1.524834	2.738962
H	-0.266256	-0.817969	2.884844
H	-1.564853	-1.735019	3.725189
H	-0.697064	-2.464641	2.327081
C	-2.565143	0.345723	2.319574
H	-3.060649	0.212106	3.305038
H	-1.717124	1.039201	2.434259
H	-3.288522	0.793672	1.620081
C	2.916588	-1.300278	-0.174437
C	3.703534	-1.033719	0.980974
C	3.413147	-2.218113	-1.141882
C	4.940850	-1.660705	1.153901
H	3.326706	-0.331175	1.731163
C	4.648378	-2.844775	-0.952734
H	2.814720	-2.427824	-2.034171
C	5.416751	-2.568138	0.191596
H	5.537482	-1.444363	2.046229
H	5.017753	-3.551534	-1.703098
H	6.384556	-3.060111	0.333441

G3

Cu	1.021612	-0.059053	-0.050653
C	-0.806635	-0.085670	-0.072156
N	2.694209	-1.409939	0.006041
N	2.540974	1.480635	0.018020
C	3.897699	-0.581352	-0.268106
C	3.792858	0.785173	0.409534
H	4.820494	-1.097487	0.069716
H	3.972429	-0.457566	-1.361417
H	4.685518	1.396188	0.158592
H	3.775632	0.664852	1.505651
C	-2.058181	-0.070004	-0.049641
C	2.576908	-2.493408	-0.991559
H	3.461344	-3.165642	-0.970447
H	1.675959	-3.089802	-0.776018
H	2.481655	-2.059793	-2.000089
C	2.753300	-1.999436	1.361492
H	1.834439	-2.578782	1.544453
H	3.631424	-2.672120	1.467609
H	2.820292	-1.207202	2.123377
C	2.656219	2.074052	-1.331267
H	2.890074	1.296879	-2.075475
H	1.695018	2.537481	-1.605227
H	3.452109	2.848935	-1.362024
C	2.212755	2.541418	0.990988
H	3.014056	3.309336	1.044645
H	1.273467	3.032444	0.689723
H	2.075613	2.097687	1.990342
C	-3.483699	-0.045845	-0.019842
C	-4.245803	-0.028368	-1.221625
C	-4.191437	-0.035668	1.214961
C	-5.644447	0.000630	-1.184462
H	-3.721277	-0.036380	-2.183009
C	-5.590232	-0.006811	1.240802
H	-3.624209	-0.049237	2.151748
C	-6.327191	0.011532	0.044060
H	-6.207419	0.014672	-2.124447
H	-6.110630	0.001462	2.205099
H	-7.421718	0.034279	0.068618

G4

Cu	-0.050506	-1.091047	-0.031493
Cu	0.056242	1.237443	-0.042199
C	0.056590	-3.970056	-0.500437
H	-0.274868	-4.916439	-0.979040
H	1.150694	-4.032784	-0.374203
C	-0.619580	-3.831329	0.865388
H	-0.416150	-4.743536	1.467046
H	-1.713170	-3.761718	0.739496
N	-0.223750	-2.807244	-1.381280
N	-0.173283	-2.611192	1.581482
C	1.686816	0.009320	-0.069050
C	2.939338	-0.119398	-0.087143
C	-1.683979	0.245171	-0.071495
C	-2.939855	0.157537	-0.086421
N	0.183181	2.793402	1.559130
N	0.214736	2.962996	-1.409660
C	0.627625	4.002962	0.825772
C	-0.061478	4.129871	-0.534014
H	0.434546	4.922803	1.419562
H	1.719642	3.927266	0.689605
H	0.261481	5.074524	-1.022221
H	-1.154600	4.189626	-0.397856
C	0.768918	-2.739230	-2.471576
H	0.744416	-3.651645	-3.106939
H	0.551364	-1.864297	-3.105427
H	1.779578	-2.625298	-2.048408
C	-1.575159	-2.904688	-1.969566
H	-1.774196	-2.005872	-2.574288
H	-1.665715	-3.803134	-2.618731
H	-2.337602	-2.962491	-1.178375
C	1.149506	-2.814969	2.204177
H	1.894399	-3.102164	1.446478
H	1.480169	-1.873345	2.670705
H	1.110165	-3.608078	2.983066
C	-1.143473	-2.239775	2.627940
H	-1.242706	-3.034710	3.399585
H	-0.807202	-1.312577	3.120373
H	-2.130681	-2.058398	2.174196
C	1.559795	3.063489	-2.010896
H	2.329986	3.122473	-1.227236
H	1.755148	2.164764	-2.617093
H	1.643070	3.961495	-2.661877
C	-0.785988	2.890471	-2.491913
H	-0.765123	3.799036	-3.133025
H	-0.574971	2.011754	-3.122951
H	-1.793520	2.780283	-2.060435
C	1.160708	2.434923	2.603124
H	1.271192	3.241688	3.361029
H	0.824693	1.517697	3.114260
H	2.142493	2.240055	2.143002
C	-1.133018	3.010840	2.190310
H	-1.464061	2.076868	2.671868
H	-1.084719	3.813606	2.958974
H	-1.883127	3.291045	1.435152
C	4.358682	-0.251835	-0.105292
C	5.108931	-0.302319	1.104676
C	5.075796	-0.326718	-1.333828
C	6.502776	-0.422885	1.081247
H	4.576823	-0.244497	2.060330
C	6.469804	-0.447236	-1.345635
H	4.517896	-0.288087	-2.275616
C	7.193209	-0.495418	-0.141181
H	7.056300	-0.459527	2.026181
H	6.997663	-0.503329	-2.304202
H	8.284097	-0.588991	-0.155062
C	-4.361869	0.055502	-0.102880
C	-5.111831	0.018482	1.107756
C	-5.081565	-0.003764	-1.330703
C	-6.507746	-0.075628	1.085579
H	-4.578205	0.066392	2.063138
C	-6.477648	-0.097568	-1.341281
H	-4.523923	0.025150	-2.272992
C	-7.200678	-0.133498	-0.136200
H	-7.060958	-0.102493	2.031025
H	-7.007423	-0.142024	-2.299402
H	-8.293202	-0.205849	-0.149078

G5

Cu	-0.098439	-0.767639	1.275732
Cu	0.098721	-0.767569	-1.275722
C	-0.901953	-2.530514	3.369629
H	-1.568656	-2.802669	4.210482
H	-0.674657	-3.453344	2.810515
C	0.370423	-1.887042	3.891875
H	0.926409	-2.600247	4.529534
H	0.138164	-1.003125	4.506293
N	-1.611273	-1.604377	2.435193
N	1.234851	-1.437340	2.758266
C	-1.238893	0.077095	-0.115077
C	-2.093607	0.987218	-0.104404
C	1.239102	0.077057	0.114787
C	2.093293	0.987688	0.104426
N	1.611557	-1.604591	-2.435061
N	-1.234437	-1.437330	-2.758314
C	0.902225	-2.531000	-3.369206
C	-0.370059	-1.887589	-3.891733
H	1.568955	-2.803500	-4.209928
H	0.674819	-3.453619	-2.809790
H	-0.926128	-2.601006	-4.529078
H	-0.137697	-1.003964	-4.506533
C	-2.633597	-2.359570	1.671112
H	-3.372144	-2.805801	2.364997
H	-3.151007	-1.676132	0.983041
H	-2.146324	-3.163326	1.098552
C	-2.271752	-0.496299	3.171319
H	-2.786421	0.155834	2.450073
H	-3.011338	-0.903067	3.887493
H	-1.526808	0.100498	3.718058
C	2.000388	-2.574373	2.189774
H	1.313850	-3.348434	1.813830
H	2.619495	-2.207685	1.358470
H	2.654746	-3.018274	2.965317
C	2.174429	-0.394912	3.231376
H	2.793902	-0.791185	4.058964
H	2.831477	-0.090558	2.404546
H	1.609039	0.480049	3.587785
C	-2.000264	-2.574013	-2.189520
H	-1.313897	-3.348159	-1.813425
H	-2.619227	-2.206964	-1.358275
H	-2.654759	-3.017923	-2.964939
C	-2.173729	-0.394801	-3.231754
H	-2.793238	-0.791144	-4.059279
H	-2.830761	-0.090109	-2.405037
H	-1.608111	0.479934	-3.588354
C	2.633949	-2.359539	-1.670827
H	3.372532	-2.805833	-2.364629
H	3.151284	-1.675918	-0.982880
H	2.146728	-3.163223	-1.098124

C	2.271921	-0.496652	-3.171504
H	2.786608	0.155676	-2.450447
H	3.011467	-0.903546	-3.887647
H	1.526880	0.099962	-3.718306
C	-3.089555	2.004063	-0.106873
C	-4.470670	1.671244	-0.122881
C	-2.711495	3.373708	-0.095540
C	-5.437740	2.681792	-0.128278
H	-4.769670	0.618366	-0.131076
C	-3.689559	4.373346	-0.100836
H	-1.648614	3.635656	-0.083395
C	-5.052987	4.033031	-0.117416
H	-6.499168	2.413596	-0.140974
H	-3.386661	5.425416	-0.092399
H	-5.814370	4.819703	-0.121892
C	3.089018	2.004745	0.106915
C	4.470192	1.672161	0.122811
C	2.710719	3.374323	0.095584
C	5.437089	2.682873	0.128065
H	4.769377	0.619336	0.131003
C	3.688613	4.374130	0.100744
H	1.647790	3.636083	0.083528
C	5.052102	4.034044	0.117187
H	6.498563	2.414856	0.140663
H	3.385540	5.426148	0.092300
H	5.813358	4.820840	0.121545

RedEl_TS

Cu	0.018857	-0.700865	1.372867
Cu	0.039534	-0.865065	-1.307675
C	-0.729482	-2.255560	3.657789
H	-1.268567	-2.338328	4.621294
H	-0.737182	-3.251959	3.187058
C	0.702171	-1.789268	3.900468
H	1.236578	-2.521525	4.536667
H	0.708029	-0.820890	4.426860
N	-1.444603	-1.318675	2.741387
N	1.429536	-1.598235	2.609610
C	-0.925137	0.272244	-0.042164
C	-1.857339	1.115662	-0.097835
C	0.958682	0.288215	-0.033903
C	1.851834	1.174976	-0.045410
N	1.505800	-1.644642	-2.568612
N	-1.368278	-1.848214	-2.485590
C	0.798193	-2.686213	-3.371673
C	-0.616960	-2.236536	-3.716895
H	1.362405	-2.904502	-4.299072
H	0.777521	-3.609798	-2.770120
H	-1.151296	-3.044993	-4.252392
H	-0.592983	-1.355965	-4.379338
C	-2.608988	-1.988757	2.118938
H	-3.337050	-2.304938	2.891788
H	-3.102327	-1.286873	1.428614
H	-2.270183	-2.873745	1.558279
C	-1.904346	-0.106254	3.462939
H	-2.373059	0.584409	2.744571
H	-2.644127	-0.379538	4.240845
H	-1.052425	0.402651	3.939579
C	1.820953	-2.900943	2.016415
H	0.929748	-3.508577	1.797511
H	2.367835	-2.719940	1.078997
H	2.475772	-3.462211	2.712466
C	2.638416	-0.771224	2.824148
H	3.331512	-1.270330	3.529532
H	3.151149	-0.619912	1.862010
H	2.348042	0.208805	3.233699
C	-1.828466	-3.045499	-1.741410
H	-0.970187	-3.671833	-1.453548
H	-2.355763	-2.724461	-0.830009
H	-2.517908	-3.648240	-2.365540
C	-2.534355	-1.010100	-2.842867
H	-3.227443	-1.569990	-3.500839
H	-3.067908	-0.716462	-1.926266
H	-2.190817	-0.103701	-3.365253
C	2.680280	-2.232352	-1.886136
H	3.412693	-2.608294	-2.627469
H	3.163742	-1.461181	-1.266852
H	2.357487	-3.067808	-1.246488
C	1.957105	-0.520096	-3.426582
H	2.449147	0.237011	-2.796737
H	2.676246	-0.882339	-4.187319
H	1.099071	-0.053169	-3.933916
C	2.834084	2.196290	-0.037505
C	4.219597	1.882739	-0.112852
C	2.440067	3.561054	0.052743
C	5.172830	2.904880	-0.096437
H	4.529320	0.835351	-0.183640
C	3.406037	4.571135	0.068384
H	1.375673	3.808521	0.112014
C	4.772223	4.248997	-0.005676
H	6.236525	2.652325	-0.154177
H	3.091787	5.617490	0.139206
H	5.524057	5.044631	0.007548
C	-2.905130	2.066759	-0.172267
C	-4.252785	1.686743	0.080633
C	-2.621463	3.421402	-0.503513
C	-5.276463	2.635377	0.003863
H	-4.478004	0.646632	0.336602
C	-3.657231	4.357084	-0.577777
H	-1.587183	3.720159	-0.700641
C	-4.984682	3.970321	-0.324980
H	-6.309719	2.332131	0.201531
H	-3.427891	5.396482	-0.834026
H	-5.790692	4.708770	-0.383783

NH_3

N	-0.000036	0.000004	-0.127922
H	0.416445	0.838960	0.298459
H	0.518568	-0.780026	0.298436
H	-0.934759	-0.058962	0.298562

DP_TS-NH_3

Cu	1.084296	0.261043	-0.129408
C	3.776904	-0.517113	0.395670
C	2.969943	-1.816879	0.455518
H	4.152767	-0.350554	-0.627612
H	4.658106	-0.596700	1.064642
H	2.629229	-2.005164	1.487145
H	3.619029	-2.667417	0.161292
N	1.760909	-1.750313	-0.409261
N	2.945961	0.665733	0.761053
C	-1.861410	0.584995	-0.254162
C	-0.664850	0.886354	-0.501574
H	-0.204262	1.902599	-1.081097
C	3.579473	1.908027	0.266832
H	2.949836	2.770008	0.539973
H	4.587727	2.052174	0.708655
H	3.673361	1.864887	-0.830059
C	2.769456	0.759330	2.229491
H	3.747576	0.884382	2.739629
H	2.129530	1.625362	2.461970
H	2.279534	-0.147935	2.615122
C	0.760936	-2.751936	0.012092
H	-0.135671	-2.659506	-0.621663
H	1.157155	-3.785179	-0.078672
H	0.474705	-2.569556	1.060312
C	2.106986	-1.964294	-1.831384
H	2.531507	-2.978220	-1.990154
H	1.199384	-1.856741	-2.446453
H	2.844477	-1.217070	-2.163859
C	-3.206544	0.229690	0.020665
C	-4.001932	-0.409219	-0.971390
C	-3.787655	0.510181	1.288716
C	-5.330531	-0.747677	-0.699590
H	-3.560543	-0.628815	-1.948632
C	-5.114508	0.156934	1.550232
H	-3.181640	1.002649	2.055656
C	-5.890655	-0.469417	0.559433
H	-5.933465	-1.236105	-1.472157
H	-5.549393	0.374157	2.531347
H	-6.930498	-0.740863	0.768438
N	0.156332	3.188984	-1.823229
H	0.302688	3.017950	-2.826259
H	-0.584366	3.895962	-1.732311
H	1.022540	3.594772	-1.445664

OH^-

O	0.000000	0.000000	0.109034
H	0.000000	0.000000	-0.872269

DP_TS-OH^-

Cu	1.332627	-0.637764	-0.164636
C	3.346707	1.438722	0.547506
C	2.260170	2.061761	-0.332064
H	3.070351	1.529473	1.611653
H	4.289377	2.012460	0.408599
H	2.549312	1.999793	-1.394426
H	2.151615	3.137046	-0.079829
N	0.945026	1.370591	-0.193209
N	3.536755	0.004095	0.251973
C	-2.017252	-1.182073	0.000271
C	-0.883922	-1.716642	-0.041013
H	0.393640	-2.507580	-0.172851
C	0.058420	1.762818	-1.313587
H	-0.901633	1.231806	-1.218463
H	-0.131015	2.856781	-1.305520
H	0.528980	1.486002	-2.270172
C	0.290480	1.740057	1.085597
H	0.109914	2.834384	1.131383
H	-0.671345	1.210400	1.162967
H	0.920768	1.443656	1.937618
C	4.328783	-0.195901	-0.971917
H	3.846450	0.302196	-1.828504
H	5.361366	0.206887	-0.867600
H	4.393266	-1.273804	-1.193594
C	4.174256	-0.689799	1.379974
H	3.546389	-0.589300	2.280853
H	4.273997	-1.760963	1.140232
H	5.186588	-0.285585	1.605379
C	-3.317027	-0.596208	0.051256
C	-3.948339	-0.315277	1.296090
C	-4.030595	-0.286136	-1.141144
C	-5.227430	0.250131	1.340289
H	-3.417180	-0.550532	2.224523
C	-5.309521	0.278807	-1.085191
H	-3.563651	-0.497290	-2.109113
C	-5.917643	0.550736	0.152908
H	-5.692222	0.455982	2.311051
H	-5.838321	0.508622	-2.017007
H	-6.919036	0.991905	0.192095
O	1.497009	-2.693296	-0.229011
H	1.675157	-2.929597	-1.167943

G2-*p*F-Phenylacetylene

Cu	-1.089738	-0.510332	0.005056
C	-2.457326	1.949511	0.316519
C	-3.454137	1.010013	-0.356716
H	-2.570664	1.908891	1.412221
H	-2.647945	2.993908	0.000064
H	-3.382721	1.096646	-1.453317
H	-4.487421	1.286064	-0.067345
N	-3.171421	-0.411565	-0.001912
N	-1.050814	1.556833	-0.002705
C	0.659649	-1.552154	0.009808
C	-0.366094	-2.297728	0.005137
H	-0.829390	-3.281495	0.002770
C	-3.791888	-1.323343	-0.990245
H	-3.563658	-2.365475	-0.717144
H	-4.892412	-1.192597	-1.013802
H	-3.382133	-1.117291	-1.991436
C	-3.673765	-0.740344	1.354331
H	-4.776100	-0.630518	1.400628
H	-3.405266	-1.780693	1.595755
H	-3.216553	-0.077157	2.104368
C	-0.665454	2.022619	-1.358468
H	-0.708113	3.128840	-1.417701
H	0.361576	1.690160	-1.576356

H	-1.341479	1.596909	-2.115778
C	-0.124278	2.141374	0.995540
H	0.908736	1.851030	0.749547
H	-0.193934	3.247747	0.997902
H	-0.376169	1.761488	1.998156
C	1.980350	-0.984359	0.007785
C	2.640550	-0.710878	-1.217313
C	2.632370	-0.675989	1.228689
C	3.922024	-0.152979	-1.223534
H	2.142434	-0.943579	-2.163191
C	3.914131	-0.118588	1.227350
H	2.127218	-0.879274	2.177610
C	4.536696	0.134312	0.000084
H	4.445984	0.058413	-2.159852
H	4.431951	0.119572	2.160661
F	5.777457	0.678039	-0.003539

DP_TS-*p*F-Phenylacetylene

Cu	1.200569	-0.839203	-0.032497
C	3.070360	-3.045658	0.116499
C	3.261869	-2.393664	-1.254944
H	3.763192	-2.600632	0.850231
H	3.317393	-4.125628	0.045974
H	2.609176	-2.876853	-2.001053
H	4.309654	-2.538491	-1.589697
N	2.915037	-0.943289	-1.235574
N	1.688822	-2.849465	0.628826
C	-1.611374	-0.112181	0.249725
C	-0.382061	0.067886	0.472361
H	0.152208	1.020928	1.067047
N	0.576500	2.131877	2.039196
C	1.147665	3.347554	1.401596
H	1.138967	4.173317	2.142321
H	2.204246	3.133849	1.170742
C	0.415825	3.783298	0.124191
H	0.518042	4.888571	0.013368
H	-0.664216	3.582008	0.230752
N	0.891947	3.086356	-1.083355
C	-0.117591	3.140384	-2.143338
H	0.254585	2.607856	-3.035709
H	-1.042269	2.642737	-1.803665
H	-0.373470	4.182547	-2.450286
C	2.148778	3.664798	-1.566040
H	2.925379	3.621039	-0.783815
H	2.511457	3.091658	-2.436602
H	2.036684	4.731835	-1.875579
C	-0.652274	2.422231	2.796703
H	-1.089768	1.474832	3.151909
H	-0.440787	3.072309	3.668779
H	-1.387482	2.923860	2.148325
C	1.566207	1.448896	2.886326
H	1.106264	0.550693	3.331354
H	2.427041	1.141595	2.268483
H	1.927637	2.104250	3.703573
C	1.643783	-3.023171	2.093598
H	0.617291	-2.838233	2.449793
H	1.943167	-4.050060	2.393275
H	2.323039	-2.300462	2.573846
C	0.738923	-3.784745	-0.007766
H	0.982929	-4.838658	0.244781
H	-0.281233	-3.560332	0.343318
H	0.760907	-3.668792	-1.102520
C	2.663409	-0.462181	-2.612214
H	2.389717	0.604148	-2.577037
H	3.563316	-0.582258	-3.251189
H	1.830123	-1.030093	-3.056103
C	4.007400	-0.143770	-0.634386
H	4.942597	-0.244443	-1.224422
H	3.710216	0.916536	-0.613978
H	4.202815	-0.472807	0.397665
C	-2.988035	-0.325842	-0.008796
C	-3.568714	0.082950	-1.243151
C	-3.822031	-0.948430	0.962975
C	-4.924550	-0.125809	-1.499724
H	-2.939386	0.563360	-1.998427
C	-5.180550	-1.150953	0.715366
H	-3.388479	-1.267277	1.915573
C	-5.708215	-0.738147	-0.514089
H	-5.380853	0.180527	-2.445212
H	-5.831606	-1.624964	1.455221
F	-7.024900	-0.938957	-0.759068

G2-*p*Me-Phenylacetylene

Cu	-1.114217	-0.510588	0.005507
C	-2.463045	1.960821	0.319206
C	-3.467194	1.030546	-0.356034
H	-2.577558	1.919543	1.414770
H	-2.645001	3.007268	0.004157
H	-3.394583	1.118766	-1.452446
H	-4.498299	1.314982	-0.066688
N	-3.196989	-0.393997	-0.003813
N	-1.059649	1.557434	0.000745
C	0.628398	-1.566938	0.008582
C	-0.404368	-2.303127	0.003536
H	-0.875494	-3.283110	-0.000685
C	-3.825356	-1.298338	-0.993814
H	-3.607801	-2.343056	-0.721810
H	-4.924586	-1.156832	-1.018478
H	-3.412579	-1.095316	-1.994392
C	-3.701641	-0.720866	1.351895
H	-4.802841	-0.600036	1.399635
H	-3.443283	-1.764420	1.590595
H	-3.237134	-0.064291	2.103264
C	-0.669047	2.019858	-1.354589
H	-0.705614	3.126288	-1.415081
H	0.356648	1.681445	-1.569650
H	-1.345553	1.596835	-2.112966
C	-0.129459	2.134513	0.999886
H	0.901483	1.835936	0.755107
H	-0.190322	3.241478	1.002301
H	-0.385516	1.756603	2.002217
C	1.951948	-1.006685	0.006730
C	2.614248	-0.727507	-1.215068
C	2.611806	-0.706058	1.224451
C	3.899074	-0.177100	-1.208460
H	2.112003	-0.947702	-2.162475
C	3.897075	-0.156573	1.210490
H	2.106825	-0.906784	2.174713
C	4.567490	0.116312	-0.000857
H	4.397793	0.030449	-2.161995
H	4.393986	0.067920	2.161132
C	5.966315	0.679382	-0.004667
H	6.718377	-0.132774	0.000703
H	6.155071	1.289023	-0.904452
H	6.155283	1.301348	0.886574

DP_TS-*p*Me-Phenylacetylene

Cu	1.278922	-0.813435	-0.017839
C	3.482696	-2.678292	0.032483
C	3.251216	-2.327406	-1.438825
H	4.229344	-1.995924	0.472011
H	3.894240	-3.706757	0.104338
H	2.542284	-3.039943	-1.892157
H	4.208022	-2.413828	-1.994127
N	2.672721	-0.963560	-1.595301
N	2.235477	-2.550058	0.831946
C	-1.539825	-0.191894	0.287985
C	-0.319768	0.070705	0.478166
H	0.174013	1.070209	1.080481
N	0.556000	2.151547	2.024875
C	0.958957	3.432823	1.383122
H	0.938512	4.231167	2.152274
H	2.006795	3.323271	1.059273
C	0.083451	3.837801	0.189991
H	0.103003	4.949801	0.100015
H	-0.966501	3.563483	0.391931
N	0.486400	3.197127	-1.072757
C	-0.616155	3.220905	-2.036526
H	-0.302909	2.717966	-2.968075
H	-1.484487	2.678354	-1.624719
H	-0.944377	4.254567	-2.300968
C	1.662580	3.853706	-1.649335
H	2.510554	3.825800	-0.944660
H	1.968148	3.326183	-2.569162
H	1.470380	4.922461	-1.910192
C	-0.636058	2.304496	2.877558
H	-0.945561	1.312883	3.245867
H	-0.425173	2.963738	3.741703
H	-1.463843	2.733620	2.292014
C	1.670286	1.550942	2.777057
H	1.335632	0.599594	3.222252
H	2.508394	1.351893	2.088267
H	2.020725	2.220345	3.586595
C	2.553318	-2.441064	2.269686
H	1.618186	-2.325833	2.841176
H	3.085162	-3.343915	2.638586
H	3.190024	-1.559086	2.443474
C	1.337926	-3.705294	0.615307
H	1.819952	-4.653389	0.935749
H	0.414266	-3.559305	1.197914
H	1.066168	-3.786696	-0.448669
C	2.034183	-0.828091	-2.922725
H	1.602181	0.181045	-3.016294
H	2.767434	-0.979920	-3.742836
H	1.226448	-1.570793	-3.022158
C	3.714457	0.078390	-1.445605
H	4.491494	-0.018428	-2.233242
H	3.245858	1.071861	-1.526514
H	4.197675	-0.001310	-0.459416
C	-2.907849	-0.492504	0.061481
C	-3.542786	-0.138130	-1.160090
C	-3.683764	-1.156971	1.052675
C	-4.890065	-0.439849	-1.374011
H	-2.961784	0.370101	-1.936470
C	-5.029235	-1.445550	0.824698
H	-3.210874	-1.439426	1.998863
C	-5.660574	-1.094708	-0.390124
H	-5.359417	-0.162244	-2.324627
H	-5.608505	-1.958009	1.601348
C	-7.119017	-1.403153	-0.614551
H	-7.760986	-0.776506	0.032879
H	-7.416624	-1.219464	-1.659997
H	-7.350620	-2.454525	-0.367223

G1’

Cu	0.000000	1.140164	0.000001
C	-0.683655	-1.518076	-0.336503
C	0.683655	-1.518077	0.336498
H	-0.585353	-1.560168	-1.432100
H	-1.277477	-2.390622	-0.009548
H	0.585353	-1.560174	1.432095
H	1.277477	-2.390623	0.009538
N	1.423864	-0.255927	0.003804
N	-1.423864	-0.255926	-0.003804
C	-2.438724	0.076859	-1.033410
H	-3.205474	-0.720243	-1.068847
H	-2.924099	1.028380	-0.766744
H	-1.954358	0.162840	-2.017009
C	-2.042198	-0.287730	1.348456
H	-2.489452	0.694945	1.560778
H	-2.832790	-1.061161	1.366804
H	-1.287283	-0.521169	2.112841
C	2.042200	-0.287726	-1.348456
H	1.287286	-0.521165	-2.112842
H	2.489451	0.694951	-1.560775
H	2.832794	-1.061154	-1.366805
C	2.438722	0.076856	1.033412
H	3.205472	-0.720247	1.068848
H	2.924098	1.028377	0.766750
H	1.954356	0.162834	2.017010

G2’

Cu	0.698660	-0.210973	-0.263118
C	2.850334	1.585941	0.071682
C	3.267197	0.317597	0.799013
H	3.212649	1.583386	-0.968002
H	3.266626	2.476980	0.575824
H	2.976919	0.356237	1.860490

H	4.363211	0.180979	0.750750
N	2.595065	-0.879671	0.195090
N	1.357608	1.675530	0.027393
C	-1.340392	-1.468147	-0.481349
C	-0.231814	-1.985077	-0.744335
H	0.382403	-2.816841	-1.074824
C	2.539134	-2.000473	1.162583
H	2.028377	-2.860826	0.705924
H	3.568683	-2.296144	1.440804
H	1.995641	-1.680544	2.064269
C	3.229502	-1.305863	-1.077988
H	4.267385	-1.630532	-0.873658
H	2.663111	-2.147781	-1.502103
H	3.244104	-0.475052	-1.798095
C	0.774916	2.141940	1.313330
H	1.104187	3.179095	1.515000
H	-0.323049	2.118431	1.240572
H	1.099336	1.490776	2.138058
C	0.893912	2.528271	-1.093579
H	-0.207371	2.532598	-1.112278
H	1.256471	3.565285	-0.958332
H	1.280045	2.129335	-2.043770
C	-2.544078	-0.786706	-0.184804
C	-3.078645	-0.815565	1.133708
C	-3.232329	-0.093375	-1.220487
C	-4.277110	-0.154121	1.402667
H	-2.544645	-1.356678	1.920218
C	-4.431466	0.558137	-0.932033
H	-2.816099	-0.086956	-2.231949
C	-4.952142	0.530796	0.374988
H	-4.691905	-0.170653	2.414749
H	-4.965902	1.088950	-1.725340
H	-5.892129	1.047027	0.594359

DP_TS’

Cu	1.639285	-0.724514	-0.199541
C	3.488994	-2.805752	0.219669
C	3.389121	-2.107118	1.571030
H	2.756473	-3.625968	0.148195
H	4.498096	-3.238780	0.084086
H	4.168370	-1.334897	1.669069
H	3.531979	-2.835608	2.391244
N	2.065383	-1.428679	1.714573
N	3.188747	-1.843136	-0.884520
C	0.319547	1.566147	-0.255355
C	-0.019815	0.357657	-0.357683
H	-1.025159	-0.291484	-0.608876
N	-2.325176	-0.993677	-0.968079
C	-3.358671	-0.358139	-0.127227
H	-3.021110	-0.426526	0.921893
H	-3.383580	0.709936	-0.404287
C	-4.770533	-0.975954	-0.237248
H	-4.741490	-2.015452	0.128324
H	-5.097429	-1.006682	-1.300074
N	-5.726679	-0.231127	0.580300
C	-6.242253	0.980483	-0.040911
H	-6.805683	1.568398	0.703209
H	-5.415632	1.602753	-0.420389
H	-6.923791	0.756736	-0.894040
C	-6.758720	-1.041336	1.209591
H	-6.295839	-1.865051	1.778036
H	-7.344202	-0.416333	1.905397
H	-7.466707	-1.483518	0.470903
C	-2.482785	-0.764090	-2.411652
H	-1.561046	-1.086937	-2.925800
H	-3.334653	-1.327494	-2.836441
H	-2.635180	0.312090	-2.593403
C	-2.058279	-2.402294	-0.646698
H	-1.113843	-2.705415	-1.132485
H	-1.954528	-2.516484	0.444627
H	-2.862194	-3.074314	-1.002839
C	2.800300	-2.556271	-2.124490
H	2.549440	-1.818165	-2.902269
H	3.635581	-3.188139	-2.484675
H	1.924451	-3.192289	-1.924532
C	4.332931	-0.937440	-1.156833
H	5.203527	-1.522177	-1.512354
H	4.042396	-0.213151	-1.933313
H	4.614212	-0.391969	-0.243570
C	2.132670	-0.301454	2.670816
H	1.144649	0.179087	2.736098
H	2.422108	-0.667461	3.675429
H	2.876721	0.431843	2.324231
C	0.988266	-2.372822	2.092074
H	1.194232	-2.798056	3.093936
H	0.029232	-1.833683	2.119054
H	0.923733	-3.192536	1.361339
C	0.729895	2.917278	-0.133438
C	0.487464	3.634636	1.069818
C	1.374306	3.568629	-1.221167
C	0.884761	4.969758	1.174751
H	-0.012223	3.131844	1.903207
C	1.767936	4.902933	-1.098656
H	1.553378	3.014748	-2.147774
C	1.524403	5.604347	0.095431
H	0.695905	5.520819	2.101236
H	2.264116	5.401577	-1.936984
H	1.833271	6.650800	0.184425

G3’

Cu	1.127566	-0.308333	-0.007522
C	3.566341	1.152794	0.334018
C	3.942532	-0.161103	-0.337838
H	3.639253	1.068577	1.429791
H	4.245826	1.964256	0.011335
H	3.958474	-0.051408	-1.433795
H	4.948253	-0.490466	-0.016004
N	2.925294	-1.206670	-0.004929
N	2.154320	1.511699	0.007087
C	-0.735370	-0.135351	-0.004409
C	-1.980768	-0.076191	-0.002871
C	1.573921	2.411883	1.027697
H	2.158784	3.351092	1.080635
H	0.534622	2.647660	0.755582
H	1.593908	1.916193	2.010100
C	2.015264	2.095962	-1.347838
H	0.949975	2.280578	-1.551140
H	2.571007	3.052300	-1.401431
H	2.411434	1.404654	-2.106135
C	3.137610	-1.769701	1.353871
H	3.131960	-0.966104	2.105557
H	2.326526	-2.478631	1.580763
H	4.108107	-2.300778	1.396608
C	2.928304	-2.295999	-1.011682
H	3.914835	-2.798369	-1.034307
H	2.156076	-3.034595	-0.745664
H	2.709973	-1.878121	-2.006395
C	-3.405117	-0.081368	-0.000803
C	-4.130706	-0.082224	-1.222825
C	-4.126650	-0.099865	1.223486
C	-5.528649	-0.102950	-1.214152
H	-3.581597	-0.069830	-2.169569
C	-5.524622	-0.120416	1.219180
H	-3.574409	-0.101308	2.168483
C	-6.230438	-0.122976	0.003605
H	-6.075832	-0.105511	-2.162545
H	-6.068621	-0.136808	2.169268
H	-7.325174	-0.141898	0.005280

O4

Cu	-1.225386	-0.268023	-0.793664
O	-2.716628	-1.018600	-1.669374
O	-1.569051	-1.732963	-1.952331
C	-2.879525	1.329474	0.932609
C	-2.284428	0.381650	1.974889
H	-3.805474	0.905159	0.511321
H	-3.138954	2.294797	1.410125
H	-1.339529	0.795272	2.365024
H	-2.987932	0.316210	2.833120
N	-1.999314	-0.949147	1.404846
N	-1.948548	1.585025	-0.208564
C	0.633534	-0.167257	-0.543354
C	1.861041	-0.124860	-0.367160
C	-2.689362	2.168223	-1.357384
H	-3.139004	3.137835	-1.066901
H	-1.989764	2.332827	-2.191685
H	-3.481518	1.477747	-1.680921
C	-0.866152	2.520504	0.185328
H	-0.187873	2.667809	-0.667523
H	-1.305431	3.493582	0.479529
H	-0.290764	2.108275	1.025190
C	-3.212117	-1.779185	1.336810
H	-3.992131	-1.279671	0.743582
H	-2.973028	-2.735026	0.843996
H	-3.613773	-1.992404	2.352360
C	-0.967253	-1.649074	2.184707
H	-1.291819	-1.841138	3.231219
H	-0.746072	-2.617755	1.706206
H	-0.042146	-1.051057	2.202733
C	3.272837	-0.049684	-0.148410
C	3.823792	0.966679	0.675559
C	4.155174	-0.987167	-0.745497
C	5.204877	1.037847	0.891904
H	3.153731	1.696485	1.141875
C	5.535101	-0.907801	-0.523051
H	3.743154	-1.775456	-1.383799
C	6.066965	0.102597	0.295312
H	5.611058	1.829013	1.531414
H	6.200263	-1.640841	-0.992118
H	7.146774	0.160693	0.467588

O5

Cu	-1.180355	0.691648	0.384661
Cu	1.137727	-0.705192	-0.426266
O	-0.688180	-0.842968	-0.526535
O	0.649417	0.856189	0.444122
C	2.086240	-3.443895	-0.790087
C	1.341138	-3.780722	0.503167
H	3.100640	-3.076731	-0.565437
H	2.182160	-4.360738	-1.405686
H	0.299979	-4.061799	0.274165
H	1.819425	-4.685085	0.944018
N	1.324135	-2.657607	1.450063
N	1.419021	-2.393283	-1.618830
C	2.291600	-2.040016	-2.768656
H	2.414123	-2.918611	-3.431257
H	1.825394	-1.220347	-3.336930
H	3.272998	-1.712067	-2.399166
C	0.120200	-2.872897	-2.150338
H	-0.272288	-2.131806	-2.860621
H	0.269498	-3.838485	-2.672169
H	-0.610218	-2.990663	-1.338737
C	2.546741	-2.609045	2.254002
H	3.435003	-2.571857	1.602966
H	2.545257	-1.696834	2.874821
H	2.643627	-3.493292	2.927263
C	0.143873	-2.686388	2.314595
H	0.103724	-3.591122	2.965325
H	0.150876	-1.796038	2.967699
H	-0.767774	-2.649222	1.696402
N	-1.356979	2.362887	1.612753
N	-1.359800	2.721347	-1.443804
C	-0.764649	3.506803	0.852588
C	-2.734383	2.674432	2.068725
C	-0.518569	2.082275	2.806864
C	-1.471577	3.814408	-0.469218
C	-2.466848	2.733664	-2.402024
C	-0.074888	2.747559	-2.144930
H	0.292302	3.249751	0.676720
H	-0.799117	4.405892	1.500545
H	-3.405860	2.814808	1.212458
H	-3.110313	1.838867	2.676067
H	-2.718606	3.595972	2.683051
H	-0.483235	2.974504	3.462115
H	-0.958256	1.240290	3.364233
H	0.495629	1.812602	2.477650
H	-2.541643	4.009066	-0.287208
H	-1.043889	4.764805	-0.864711

H	-2.489756	3.656153	-3.028542
H	-2.375273	1.865426	-3.077235
H	-3.428168	2.653623	-1.867190
H	-0.006728	1.874077	-2.816361
H	0.052569	3.672638	-2.755056
H	0.751884	2.673720	-1.422047
C	-3.017463	0.250774	0.287465
C	-4.196047	-0.122845	0.170083
C	2.980894	-0.280831	-0.296296
C	4.156926	0.097373	-0.166852
C	-5.563530	-0.524399	0.045281
C	-6.290567	-0.265276	-1.146478
C	-6.228905	-1.186578	1.110410
C	-7.629796	-0.655585	-1.263297
H	-5.789437	0.245235	-1.975530
C	-7.568416	-1.572920	0.983843
H	-5.679930	-1.393282	2.035037
C	-8.275754	-1.310243	-0.201187
H	-8.173825	-0.446430	-2.190849
H	-8.063811	-2.082818	1.817229
H	-9.323711	-1.613293	-0.296240
C	5.521906	0.503309	-0.028116
C	6.197654	1.161070	-1.089423
C	6.235695	0.253064	1.173412
C	7.534566	1.551748	-0.949849
H	5.658549	1.360777	-2.021368
C	7.572515	0.647606	1.303353
H	5.726156	-0.253288	1.999814
C	8.228815	1.297745	0.244826
H	8.038193	2.058306	-1.780320
H	8.106495	0.445526	2.238273
H	9.274791	1.604227	0.350172

O6

Cu	1.352064	-0.753705	0.390515
Cu	-1.014766	0.370902	-0.638301
O	0.794095	0.626438	-0.718491
O	-0.457039	-1.092573	0.331292
C	-2.349177	2.945903	-1.075634
C	-1.878494	3.355250	0.326367
H	-3.301025	2.397478	-1.016280
H	-2.502519	3.848707	-1.698759
H	-1.583467	2.439852	0.899422
H	-0.980764	3.991158	0.246216
N	-1.390536	2.046608	-1.789071
C	-2.004462	1.574856	-3.058756
H	-2.207062	2.437295	-3.722052
H	-1.308591	0.885628	-3.561932
H	-2.943867	1.048587	-2.836978
C	-0.128797	2.760833	-2.104724
H	0.523789	2.101515	-2.693484
H	-0.364786	3.669479	-2.691926
H	0.397132	3.037922	-1.182227
C	-2.324550	4.925132	2.103765
H	-1.562380	5.610833	1.695153
H	-3.112623	5.530944	2.584261
H	-1.843345	4.302609	2.896382
C	-3.976932	3.278293	1.554919
H	-3.609555	2.554327	2.322718
H	-4.751168	3.910133	2.023707
H	-4.457616	2.700812	0.748672
N	1.566024	-2.210565	1.861393
N	1.862463	-2.943283	-1.091605
C	1.128506	-3.493766	1.230925
C	2.924951	-2.328410	2.444439
C	0.616907	-1.841108	2.942697
C	1.963406	-3.904109	0.015914
C	3.057001	-2.963428	-1.939105
C	0.659918	-3.169419	-1.897112
H	0.072090	-3.358056	0.947619
H	1.182084	-4.293103	1.997182
H	3.668142	-2.531220	1.663083
H	3.185392	-1.382297	2.939482
H	2.934602	-3.147520	3.189880
H	0.593163	-2.638177	3.710923
H	0.951181	-0.900045	3.407093
H	-0.383347	-1.700291	2.507470
H	3.024401	-3.996536	0.301858
H	1.632232	-4.922648	-0.290608
H	3.211033	-3.944512	-2.445409
H	2.965119	-2.187558	-2.718540
H	3.951096	-2.738306	-1.334216
H	0.587113	-2.387237	-2.672284
H	0.673894	-4.164235	-2.400641
H	-0.238425	-3.095419	-1.265068
C	3.135836	-0.139467	0.362429
C	4.279475	0.330905	0.251657
C	-2.843090	-0.092346	-0.435061
C	-4.002532	-0.495665	-0.249503
C	5.607991	0.846109	0.125042
C	6.332628	0.685730	-1.085470
C	6.236490	1.523820	1.202511
C	7.634097	1.185951	-1.208609
H	5.859262	0.164957	-1.924314
C	7.538556	2.020671	1.069364
H	5.689119	1.655299	2.141703
C	8.243953	1.854931	-0.134164
H	8.176456	1.052227	-2.150915
H	8.006245	2.540951	1.912253
H	9.262394	2.244622	-0.234127
C	-5.351698	-0.927806	-0.050289
C	-6.051030	-1.619019	-1.074059
C	-6.024104	-0.670294	1.173150
C	-7.372692	-2.035469	-0.876997
H	-5.542502	-1.823965	-2.021832
C	-7.346039	-1.091129	1.360250
H	-5.495226	-0.137619	1.970350
C	-8.026702	-1.774502	0.338743
H	-7.895968	-2.567622	-1.678757
H	-7.849095	-0.883788	2.310938
H	-9.060893	-2.101398	0.489194
N	-2.910277	4.128939	1.025289

O7

Cu	1.365095	-0.788245	0.389772
Cu	-1.003658	0.335898	-0.636026
O	0.802444	0.594764	-0.715975
O	-0.447117	-1.120026	0.340423
C	-2.327354	2.921241	-1.078581
C	-1.835954	3.281369	0.324110
H	-3.279125	2.373419	-1.023488
H	-2.471819	3.836569	-1.686583
H	-1.728400	2.378480	0.948592
H	-0.875530	3.816707	0.297236
N	-1.368673	2.024330	-1.788967
C	-1.997152	1.553649	-3.054392
H	-2.207423	2.416371	-3.714443
H	-1.301839	0.867784	-3.561625
H	-2.931555	1.022729	-2.823670
C	-0.107266	2.734593	-2.120925
H	0.534010	2.065702	-2.710714
H	-0.345184	3.638964	-2.713154
H	0.434001	3.013911	-1.208108
C	-2.194816	4.657177	2.344458
H	-1.226757	5.132556	2.135437
H	-2.883909	5.376147	2.807971
H	-2.063984	3.776387	2.988730
C	-4.156170	3.603699	1.266834
H	-4.030166	2.643934	1.787736
H	-4.736969	4.304030	1.882538
H	-4.655574	3.459332	0.300268
N	1.587547	-2.241983	1.859048
N	1.865238	-2.949431	-1.097481
C	1.156566	-3.526038	1.225200
C	2.948805	-2.353200	2.438788
C	0.639087	-1.880918	2.943651
C	1.985407	-3.919414	0.000740
C	3.054405	-2.949368	-1.953633
C	0.660427	-3.184728	-1.897870
H	0.096303	-3.399995	0.951731
H	1.224782	-4.328724	1.986513
H	3.690495	-2.555276	1.655903
H	3.206856	-1.405134	2.931249
H	2.962615	-3.170738	3.185652
H	0.620984	-2.681520	3.708164
H	0.970871	-0.940764	3.411679
H	-0.363323	-1.743661	2.512143
H	3.049594	-4.003540	0.276955
H	1.661216	-4.938032	-0.311726
H	3.214807	-3.924961	-2.467863
H	2.948234	-2.168816	-2.726495
H	3.949917	-2.719079	-1.353053
H	0.570334	-2.395034	-2.663570
H	0.687154	-4.173238	-2.412540
H	-0.234890	-3.132907	-1.259389
C	3.142485	-0.162223	0.359650
C	4.279499	0.323683	0.249445
C	-2.836670	-0.109552	-0.421082
C	-3.995723	-0.510741	-0.227748
C	5.600351	0.857831	0.121158
C	6.318068	0.723510	-1.096571
C	6.226914	1.529554	1.203406
C	7.611464	1.243559	-1.222158
H	5.846052	0.206903	-1.938710
C	7.520926	2.046338	1.067655
H	5.684907	1.640197	2.148383
C	8.219555	1.906662	-0.143088
H	8.148964	1.129715	-2.169786
H	7.987807	2.561424	1.914142
H	9.231724	2.311819	-0.244964
C	-5.341977	-0.954433	-0.032926
C	-6.041748	-1.619182	-1.073820
C	-6.009023	-0.739221	1.201256
C	-7.359236	-2.050889	-0.882455
H	-5.536566	-1.792396	-2.029639
C	-7.327061	-1.174633	1.382438
H	-5.479225	-0.230072	2.013095
C	-8.008318	-1.831221	0.344014
H	-7.882842	-2.563118	-1.696768
H	-7.826163	-1.000992	2.341867
H	-9.039206	-2.170243	0.489916
H	-2.920544	5.044115	0.455821
N	-2.795238	4.201169	1.045257

O8

Cu	-0.880920	-0.910858	-0.174004
Cu	1.315721	0.713251	0.519426
O	-0.535409	0.763703	0.612294
O	0.963609	-0.931526	-0.217813
C	1.259244	3.649905	0.349157
C	-0.142929	3.893006	-0.205135
H	1.988645	3.448314	-0.451448
H	1.549589	4.612095	0.815609
H	-0.859639	4.102891	0.602809
H	-0.085684	4.790149	-0.844549
N	1.444660	2.583752	1.393157
C	2.788687	2.793390	2.006068
H	2.789626	3.756066	2.551061
H	2.998882	1.973056	2.706607
H	3.556346	2.809513	1.220998
C	0.428590	2.671850	2.475194
H	0.709322	1.968159	3.273095
H	0.409951	3.700131	2.882936
H	-0.564714	2.394246	2.095879
C	0.043386	2.489309	-2.266232
H	1.042879	2.131756	-1.977243
H	-0.476126	1.695522	-2.822470
H	0.126569	3.396762	-2.884484
C	-2.161313	3.133765	-1.386211
H	-2.179570	4.055368	-1.988756
H	-2.590011	2.298400	-1.957617
H	-2.729307	3.277908	-0.455507
N	-0.902276	-2.689117	-1.235577
N	-0.915840	-2.577884	1.807596
C	-0.243159	-3.679278	-0.328353
C	-2.241484	-3.161582	-1.670407
C	-0.060051	-2.470376	-2.439040
C	-0.938718	-3.825947	1.027188

C	-2.055826	-2.492867	2.727603
C	0.343060	-2.428421	2.546237
H	0.797428	-3.341718	-0.197717
H	-0.228108	-4.660057	-0.842866
H	-2.909071	-3.287173	-0.808924
H	-2.680002	-2.422603	-2.354939
H	-2.127173	-4.128866	-2.196429
H	0.072571	-3.427487	-2.979082
H	-0.560462	-1.745940	-3.100350
H	0.917686	-2.073370	-2.128857
H	-1.988868	-4.128272	0.882745
H	-0.443087	-4.659435	1.572318
H	-2.046660	-3.302567	3.491909
H	-2.027338	-1.523670	3.254044
H	-3.000228	-2.552213	2.162279
H	0.349031	-1.456319	3.068108
H	0.476632	-3.234491	3.303385
H	1.195153	-2.441721	1.849908
C	-2.731310	-0.572582	-0.227645
C	-3.926829	-0.240510	-0.235145
C	3.151291	0.456038	0.205828
C	4.320717	0.158123	-0.080662
C	-5.309610	0.124589	-0.271540
C	-6.008228	0.453244	0.919423
C	-6.014777	0.161857	-1.502967
C	-7.362312	0.805561	0.874432
H	-5.475326	0.426909	1.875506
C	-7.368504	0.515878	-1.537014
H	-5.486101	-0.089821	-2.428277
C	-8.048638	0.838572	-0.350893
H	-7.886249	1.055210	1.803345
H	-7.896577	0.539018	-2.496311
H	-9.107886	1.114225	-0.381121
C	5.679813	-0.161604	-0.389664
C	6.492776	-0.850618	0.547827
C	6.243819	0.201065	-1.640475
C	7.821742	-1.163460	0.239431
H	6.067961	-1.135987	1.515713
C	7.574043	-0.116524	-1.938213
H	5.625502	0.731466	-2.371964
C	8.368715	-0.798938	-1.002112
H	8.434847	-1.695959	0.974373
H	7.992824	0.170442	-2.908714
H	9.408766	-1.045879	-1.239093
H	-0.754348	1.887828	-0.410546
N	-0.748785	2.796198	-1.040681

O9

Cu	1.387805	1.652611	0.010085
Cu	-0.875952	-0.109944	0.718022
O	0.748645	0.520313	1.327184
O	-0.420043	0.498088	-1.006465
C	-1.794901	-2.115832	2.608688
C	-0.728121	-3.050494	2.034915
H	-2.716265	-2.157946	2.007559
H	-2.037259	-2.431690	3.642148
H	0.203149	-2.959019	2.617215
H	-1.085101	-4.094612	2.176398
N	-0.429256	-2.765649	0.623873
N	-1.374765	-0.678554	2.661648
C	-2.511467	0.161789	3.125558
H	-2.772545	-0.116234	4.164160
H	-2.213712	1.221102	3.098732
H	-3.377733	0.005904	2.469083
C	-0.241763	-0.495374	3.604017
H	-0.028516	0.575444	3.713930
H	-0.529957	-0.914586	4.587132
H	0.661231	-0.996816	3.235134
C	-1.356417	-3.467451	-0.270968
H	-2.398241	-3.218911	-0.017393
H	-1.173965	-3.154122	-1.312794
H	-1.231639	-4.573068	-0.208917
C	0.954193	-3.112859	0.282403
H	1.163603	-4.199959	0.410507
H	1.145975	-2.849828	-0.770986
H	1.650250	-2.541343	0.915696
N	2.059688	2.856852	-1.496936
N	0.428073	3.346871	0.768372
C	1.187694	4.075923	-1.446323
C	3.489561	3.207191	-1.279922
C	1.898999	2.176817	-2.807688
C	0.985898	4.500886	-0.006260
C	0.780350	3.455381	2.202390
C	-1.045271	3.274556	0.626941
H	0.226610	3.811996	-1.916369
H	1.649556	4.883409	-2.044195
H	3.622328	3.682957	-0.297664
H	4.089555	2.287486	-1.314851
H	3.820817	3.902246	-2.073606
H	2.132093	2.888503	-3.621690
H	2.583822	1.318908	-2.857429
H	0.862657	1.821996	-2.909504
H	1.940076	4.791443	0.460538
H	0.303176	5.367979	0.056960
H	0.339142	4.372788	2.636986
H	0.389407	2.570685	2.725100
H	1.875520	3.488582	2.312758
H	-1.412401	2.364340	1.127204
H	-1.508646	4.161061	1.100868
H	-1.331815	3.240050	-0.434125
C	2.614351	0.302496	-0.341185
C	3.460928	-0.588567	-0.489903
C	-2.620290	-0.421740	0.076717
C	-3.725415	-0.499748	-0.479622
C	4.466468	-1.584012	-0.693600
C	5.496192	-1.774155	0.264393
C	4.449295	-2.409010	-1.848303
C	6.473085	-2.757069	0.068848
H	5.516784	-1.143875	1.159383
C	5.430426	-3.390467	-2.031998
H	3.659239	-2.270032	-2.593316
C	6.445426	-3.569103	-1.077245
H	7.260958	-2.890793	0.817737
H	5.402410	-4.019732	-2.927918
H	7.211462	-4.337221	-1.225436
C	-5.006841	-0.640052	-1.101395
C	-6.099410	0.179044	-0.716688
C	-5.207362	-1.606883	-2.120789
C	-7.346804	0.034122	-1.335443
H	-5.956323	0.927706	0.069322
C	-6.458801	-1.743661	-2.732555
H	-4.370409	-2.244144	-2.424414
C	-7.532823	-0.925682	-2.344203
H	-8.179792	0.675096	-1.027560
H	-6.595891	-2.494160	-3.518335
H	-8.510020	-1.035632	-2.825757
H	-1.281441	0.786558	-1.386490

O10

Cu	-1.797693	-1.770279	0.008111
Cu	0.745037	-0.371399	0.760294
O	-0.894506	-0.936423	1.377185
O	0.328012	-1.064844	-0.918304
C	1.586091	1.919463	2.312294
C	0.626900	2.726021	1.426204
H	2.574570	1.835094	1.838369
H	1.705405	2.417045	3.293488
H	0.435751	2.154848	0.481355
H	-0.344015	2.838876	1.936949
N	1.145341	4.069826	1.159290
N	1.119947	0.517357	2.571141
C	2.197509	-0.262617	3.242787
H	2.415382	0.192150	4.226887
H	1.854924	-1.298233	3.389548
H	3.102305	-0.255770	2.619507
C	-0.076343	0.521273	3.454695
H	-0.384288	-0.513046	3.657690
H	0.199314	1.020165	4.403315
H	-0.907825	1.053276	2.978244
C	0.070188	4.963570	0.724928
H	-0.715681	5.011149	1.498509
H	0.474959	5.980050	0.578720
H	-0.406313	4.642838	-0.232689
C	2.224603	4.068138	0.170288
H	1.893516	3.693146	-0.828692
H	2.601968	5.097189	0.040839
H	3.068065	3.442810	0.506116
N	-2.734092	-2.711879	-1.532756
N	-1.344092	-3.646122	0.737501
C	-2.237815	-4.127702	-1.493879
C	-4.205121	-2.643017	-1.321367
C	-2.380714	-2.092750	-2.836074
C	-2.174419	-4.605659	-0.057817
C	-1.718116	-3.680887	2.170502
C	0.104103	-3.930294	0.595265
H	-1.239018	-4.138580	-1.958805
H	-2.904345	-4.767127	-2.101588
H	-4.472417	-3.073129	-0.345400
H	-4.516693	-1.589403	-1.347361
H	-4.717880	-3.204764	-2.124102
H	-2.819151	-2.691673	-3.655980
H	-2.777738	-1.068884	-2.870100
H	-1.286163	-2.065445	-2.941359
H	-3.178160	-4.636465	0.394017
H	-1.745840	-5.622654	0.003098
H	-1.498626	-4.678070	2.596661
H	-1.135997	-2.911056	2.698971
H	-2.792663	-3.464768	2.275804
H	0.670643	-3.158149	1.136135
H	0.327615	-4.924349	1.026541
H	0.397869	-3.911502	-0.463419
C	-2.467077	-0.079504	-0.399031
C	-2.887091	1.070709	-0.583567
C	2.509207	-0.109752	0.144485
C	3.620581	-0.109507	-0.404644
C	-3.422484	2.372851	-0.830381
C	-4.363345	2.946342	0.064154
C	-3.019999	3.120278	-1.968024
C	-4.881583	4.224157	-0.175717
H	-4.679660	2.377319	0.944449
C	-3.542929	4.398926	-2.195895
H	-2.295963	2.685693	-2.664467
C	-4.475170	4.955583	-1.304148
H	-5.607895	4.651697	0.523584
H	-3.222599	4.963343	-3.078091
H	-4.883518	5.954731	-1.488306
C	4.921815	-0.098165	-0.999168
C	5.916134	-1.016121	-0.573303
C	5.238876	0.821145	-2.032402
C	7.183085	-1.014380	-1.167951
H	5.680003	-1.728383	0.223863
C	6.509657	0.814185	-2.619510
H	4.477955	1.533453	-2.367193
C	7.485521	-0.101526	-2.191922
H	7.939245	-1.730719	-0.829495
H	6.739443	1.528100	-3.417523
H	8.477648	-0.103852	-2.655055
H	1.192740	-1.326953	-1.308883

O11

Cu	-1.876139	-1.732166	-0.021927
Cu	0.735383	-0.470653	0.768681
O	-0.960163	-0.898331	1.341623
O	0.349996	-1.228174	-0.883102
C	1.555477	1.841827	2.296021
C	0.555687	2.619022	1.436911
H	2.524590	1.757640	1.784425
H	1.704764	2.349183	3.269479
H	0.477841	2.197172	0.421197
H	-0.443461	2.645096	1.895412
N	1.096556	0.443663	2.571991
C	2.196549	-0.306149	3.248674
H	2.400141	0.159194	4.230551
H	1.876378	-1.347999	3.397659
H	3.100529	-0.281196	2.625230
C	-0.088577	0.438524	3.472647
H	-0.336452	-0.599229	3.732246
H	0.172046	0.997403	4.391279

H	-0.955822	0.894163	2.981266
C	-0.125981	4.859458	0.624291
H	-1.047237	4.733278	1.209271
H	0.179249	5.914639	0.610798
H	-0.263869	4.485020	-0.399968
C	2.263311	4.236581	0.527817
H	2.157606	3.753207	-0.454191
H	2.445154	5.313827	0.409687
H	3.083372	3.782655	1.098928
N	-2.796423	-2.674173	-1.565888
N	-1.576794	-3.602444	0.803010
C	-2.405326	-4.118172	-1.446247
C	-4.268626	-2.498882	-1.438326
C	-2.333032	-2.134431	-2.870945
C	-2.439919	-4.535001	0.009265
C	-2.011863	-3.551047	2.217685
C	-0.147674	-3.988447	0.735315
H	-1.390388	-4.220397	-1.861800
H	-3.089316	-4.734598	-2.058029
H	-4.615617	-2.872397	-0.463826
H	-4.507345	-1.429178	-1.519068
H	-4.774832	-3.057272	-2.247510
H	-2.760801	-2.742284	-3.689630
H	-2.665488	-1.091992	-2.970176
H	-1.234403	-2.176951	-2.912644
H	-3.461657	-4.474909	0.415507
H	-2.088365	-5.575597	0.132548
H	-1.882500	-4.542581	2.691373
H	-1.398790	-2.803099	2.742243
H	-3.072133	-3.257965	2.267611
H	0.445590	-3.240870	1.281504
H	-0.010756	-4.982084	1.202320
H	0.193918	-4.020117	-0.308413
C	-2.412131	-0.017532	-0.513553
C	-2.749387	1.157513	-0.710293
C	2.510166	-0.247285	0.171985
C	3.610481	-0.261683	-0.399858
C	-3.170233	2.501559	-0.950524
C	-3.985543	3.177037	-0.004804
C	-2.763675	3.194848	-2.120447
C	-4.373957	4.503917	-0.223881
H	-4.306624	2.648348	0.898735
C	-3.156241	4.522915	-2.327213
H	-2.139325	2.680095	-2.857997
C	-3.960089	5.182630	-1.382485
H	-5.004144	5.010837	0.514516
H	-2.834488	5.045572	-3.234276
H	-4.266375	6.220239	-1.550030
C	4.904222	-0.271344	-1.010190
C	5.905361	-1.169031	-0.556798
C	5.205854	0.601364	-2.087219
C	7.164176	-1.192108	-1.167437
H	5.680143	-1.846083	0.273449
C	6.468929	0.570027	-2.689725
H	4.438945	1.295757	-2.445444
C	7.451673	-0.324657	-2.234377
H	7.925696	-1.892409	-0.808298
H	6.687249	1.247294	-3.522159
H	8.437533	-0.346488	-2.710000
H	1.219389	-1.525428	-1.237730
H	1.105467	4.455686	2.224797
N	0.970955	4.064370	1.274803

O12

Cu	-1.426377	-1.567171	-0.375685
Cu	1.120657	-0.364758	0.714178
O	-0.579617	-1.002352	1.191509
O	0.558341	-0.290653	-1.047880
C	1.357878	0.787640	3.405229
C	-0.112173	1.054445	3.706216
H	1.821585	1.611378	2.840761
H	1.854338	0.749362	4.394841
H	-0.572770	0.221999	4.258497
H	-0.150728	1.948403	4.350327
N	1.707118	-0.491875	2.700267
C	3.188339	-0.667306	2.795981
H	3.451690	-0.833002	3.856798
H	3.490560	-1.540629	2.201208
H	3.696211	0.229874	2.421320
C	1.077685	-1.672353	3.351480
H	1.469191	-2.582574	2.875437
H	1.346737	-1.673530	4.424416
H	-0.012287	-1.643798	3.234515
C	-0.517949	2.473328	1.691659
H	0.404545	2.166030	1.174621
H	-1.285040	2.713162	0.944512
H	-0.328384	3.340936	2.341189
C	-2.404150	1.582685	3.019341
H	-2.400730	2.467649	3.673291
H	-3.055785	1.750357	2.151356
H	-2.741162	0.697152	3.578625
N	-2.218205	-2.130798	-2.166426
N	-0.734473	-3.504188	-0.179243
C	-1.515587	-3.414947	-2.505397
C	-3.687326	-2.325511	-2.017304
C	-1.944583	-1.129586	-3.231222
C	-1.407846	-4.282818	-1.272578
C	-1.170651	-4.005464	1.147058
C	0.741999	-3.598135	-0.291604
H	-0.519332	-3.146760	-2.892287
H	-2.069880	-3.926824	-3.313306
H	-3.902846	-3.030378	-1.202003
H	-4.148683	-1.355538	-1.786440
H	-4.097222	-2.720139	-2.964979
H	-2.257011	-1.551398	-4.204335
H	-2.508340	-0.211150	-3.023051
H	-0.867657	-0.906419	-3.253922
H	-2.401031	-4.586208	-0.907993
H	-0.834776	-5.202765	-1.486954
H	-0.909742	-5.076054	1.245657
H	-0.665295	-3.427957	1.931954
H	-2.261246	-3.886140	1.243882
H	1.209158	-2.963348	0.477109
H	1.053372	-4.647274	-0.129489
H	1.074786	-3.267644	-1.285658
C	-2.327398	0.058784	-0.416059
C	-2.954864	1.118167	-0.532288
C	2.756352	0.323015	0.111215
C	3.750371	0.755162	-0.488475
C	-3.683268	2.335371	-0.722896
C	-5.009364	2.479136	-0.241369
C	-3.079209	3.424070	-1.404658
C	-5.705566	3.677715	-0.439501
H	-5.483307	1.643643	0.283347
C	-3.786272	4.617058	-1.596922
H	-2.057046	3.318826	-1.782172
C	-5.099249	4.749490	-1.115659
H	-6.729662	3.774847	-0.064044
H	-3.308208	5.448167	-2.126311
H	-5.648576	5.684256	-1.268917
C	4.951835	1.228857	-1.101336
C	5.907012	0.307339	-1.603516
C	5.209762	2.618281	-1.222180
C	7.081055	0.767181	-2.209873
H	5.713611	-0.766393	-1.512747
C	6.388911	3.065881	-1.828714
H	4.477650	3.335141	-0.836959
C	7.327469	2.145474	-2.324319
H	7.808712	0.044897	-2.594699
H	6.577217	4.141047	-1.915292
H	8.248231	2.501331	-2.797763
H	1.379741	-0.224190	-1.589047
H	-1.018985	0.446451	1.913251
N	-1.012268	1.336495	2.528587

O13

Cu	-1.182723	-0.406403	-0.046157
C	-3.794578	0.667770	-0.262222
C	-3.001967	1.652581	0.567682
H	-3.765057	0.929448	-1.331292
H	-4.853171	0.643002	0.053872
H	-3.099567	1.440141	1.643031
H	-3.338010	2.690088	0.390986
N	-1.540782	1.549798	0.224025
N	-3.190791	-0.695212	-0.112887
C	1.903832	-0.232334	0.001401
C	0.667430	-0.235050	0.032036
C	-0.739602	2.162150	1.318982
H	-1.063871	3.210812	1.450123
H	-0.908731	1.604938	2.252079
H	0.325249	2.131500	1.054431
C	-1.229012	2.222360	-1.069471
H	-1.506781	3.289445	-0.994850
H	-0.151557	2.130132	-1.265644
H	-1.789795	1.753971	-1.891299
C	-3.586144	-1.570041	-1.240986
H	-3.298514	-1.094843	-2.190599
H	-3.072665	-2.536579	-1.139693
H	-4.680858	-1.724632	-1.218584
C	-3.556416	-1.336724	1.178900
H	-3.250617	-0.703491	2.024501
H	-4.650148	-1.493906	1.213631
H	-3.041046	-2.305687	1.245172
O	-0.948656	-2.195629	-0.323951
H	0.021854	-2.358336	-0.280945
C	3.332074	-0.167370	-0.009456
C	4.103004	-1.173918	0.625686
C	3.999425	0.902533	-0.658330
C	5.500862	-1.107619	0.607247
H	3.593727	-2.002004	1.128746
C	5.397667	0.957486	-0.670953
H	3.409567	1.682562	-1.150091
C	6.152885	-0.044680	-0.039556
H	6.084831	-1.891390	1.100980
H	5.900924	1.788135	-1.176671
H	7.246698	0.002433	-0.051430

O14

Cu	-1.921822	0.627307	-0.614241
Cu	-0.464600	-1.121418	0.640954
C	-2.716773	2.158978	-2.932976
C	-3.749366	1.042789	-2.861953
H	-3.064882	3.045749	-2.379443
H	-2.553958	2.462023	-3.985642
H	-3.440668	0.188483	-3.485933
H	-4.721904	1.404423	-3.250857
N	-3.884209	0.553050	-1.465772
N	-1.419785	1.742019	-2.321253
C	2.288387	-1.344835	-0.837175
C	1.189224	-1.339609	-0.256059
C	-4.710694	1.462291	-0.639429
H	-5.754676	1.488175	-1.011771
H	-4.710002	1.099769	0.401018
H	-4.298911	2.483365	-0.658082
C	-4.465618	-0.803672	-1.432957
H	-4.469645	-1.160426	-0.392001
H	-5.502225	-0.797950	-1.825812
H	-3.851303	-1.481910	-2.046076
C	-0.676733	0.806320	-3.202057
H	-1.276709	-0.094649	-3.400671
H	-0.435069	1.297950	-4.165318
H	0.256601	0.506853	-2.701304
C	-0.593512	2.943177	-2.068564
H	-1.104047	3.597045	-1.344412
H	0.380123	2.641115	-1.659837
H	-0.437268	3.499181	-3.013638
C	3.558880	-1.393669	-1.491956
C	4.752101	-1.103439	-0.778609
C	3.658874	-1.723920	-2.869391
C	5.993885	-1.140452	-1.423330
H	4.689024	-0.847587	0.284235
C	4.905760	-1.757720	-3.504543
H	2.746827	-1.950454	-3.431545
C	6.078245	-1.466877	-2.787225
H	6.902876	-0.912640	-0.856150
H	4.962351	-2.013426	-4.568165
H	7.051504	-1.494799	-3.288076

O	-2.428084	-0.620156	0.894081
H	-2.368067	-0.034950	1.683179
H	-1.034447	0.481178	3.586237
C	-1.059214	-0.591724	3.842717
N	-0.066714	-1.316848	3.033899
H	-2.073451	-0.978195	3.651303
H	-0.855390	-0.695041	4.931323
C	-0.188531	-2.779023	3.234320
C	1.282420	-0.844748	3.381004
C	-1.258294	-3.380761	2.325229
H	0.792014	-3.237305	3.024603
H	-0.434730	-3.021118	4.290411
H	2.029256	-1.347974	2.745718
H	1.346074	0.240957	3.200200
H	1.531733	-1.037811	4.447638
H	-2.223157	-2.871295	2.483724
H	-1.402673	-4.452984	2.571724
N	-0.923628	-3.243954	0.880543
C	0.176174	-4.156020	0.496570
C	-2.112685	-3.552242	0.057257
H	-0.115143	-5.207410	0.693401
H	0.390419	-4.034654	-0.575239
H	1.089928	-3.922453	1.060133
H	-1.854416	-3.437034	-1.007878
H	-2.449012	-4.594623	0.231634
H	-2.924647	-2.858029	0.316987
C	-0.245050	0.833526	0.399011
C	0.433709	1.766594	0.879340
C	1.247865	2.831680	1.354959
C	2.431865	3.192043	0.652328
C	0.912236	3.553561	2.533283
C	3.241462	4.234583	1.114541
H	2.704711	2.638044	-0.251658
C	1.732191	4.593258	2.985184
H	0.003786	3.286781	3.083277
C	2.897650	4.940364	2.280327
H	4.149757	4.496919	0.561533
H	1.459223	5.138874	3.894781
H	3.534698	5.755715	2.638138

O15

Cu	-0.023864	-0.282264	1.506857
Cu	-0.135735	1.546834	-0.193978
C	2.029124	-1.899688	2.811717
C	0.881989	-2.908857	2.796270
H	2.605990	-1.963241	1.874208
H	2.720608	-2.135643	3.646066
H	0.267368	-2.795772	3.704502
H	1.311526	-3.933757	2.826725
N	0.007019	-2.730290	1.620381
N	1.559741	-0.490185	2.948817
C	-2.346927	-0.490839	-0.450599
C	-1.380252	0.051709	0.123894
C	0.553608	-3.407559	0.437851
H	0.576833	-4.512359	0.571544
H	-0.071410	-3.172945	-0.439769
H	1.577615	-3.059993	0.231989
C	-1.351254	-3.218183	1.895083
H	-1.973695	-3.088918	0.993970
H	-1.360414	-4.295238	2.173063
H	-1.789122	-2.620528	2.709990
C	1.058974	-0.230614	4.318818
H	0.162537	-0.828902	4.521750
H	1.852241	-0.464536	5.056900
H	0.786162	0.831174	4.404068
C	2.691574	0.431819	2.692613
H	3.093188	0.255659	1.685095
H	2.335183	1.471617	2.765198
H	3.493151	0.274760	3.441974
C	-3.473961	-1.073458	-1.097089
C	-4.783605	-0.895721	-0.573345
C	-3.311326	-1.847121	-2.278586
C	-5.885786	-1.473139	-1.212504
H	-4.918827	-0.305865	0.339009
C	-4.422081	-2.418848	-2.907937
H	-2.306287	-1.990513	-2.688556
C	-5.711681	-2.235291	-2.380292
H	-6.888205	-1.328886	-0.795745
H	-4.280751	-3.011836	-3.817682
H	-6.577507	-2.685480	-2.876593
O	-1.331297	-0.081744	2.869459
H	-2.170592	-0.022625	2.364621
H	1.835566	1.879751	-2.467867
C	1.371686	2.860446	-2.281460
N	1.219923	3.049877	-0.817406
H	0.389779	2.887520	-2.778231
H	2.014771	3.655483	-2.709012
C	0.554174	4.346638	-0.504845
C	2.557858	3.017309	-0.185037
C	-0.936242	4.279775	-0.802144
H	0.730186	4.558604	0.562658
H	1.019745	5.165523	-1.088273
H	2.454500	3.120173	0.906375
H	3.044997	2.059077	-0.415671
H	3.185584	3.845717	-0.569440
H	-1.109834	4.147973	-1.882333
H	-1.425379	5.226476	-0.498453
N	-1.570313	3.125116	-0.104842
C	-1.762320	3.408675	1.338942
C	-2.880659	2.832848	-0.724878
H	-2.468132	4.252251	1.477360
H	-2.157672	2.509165	1.835216
H	-0.801018	3.669101	1.808290
H	-3.360576	2.000236	-0.191692
H	-3.538098	3.723500	-0.674304
H	-2.737262	2.549461	-1.779422
C	1.151448	-0.029098	-0.050136
C	1.978394	-0.488014	-0.866337
C	2.945088	-1.012836	-1.772360
C	4.332352	-0.763692	-1.588578
C	2.536245	-1.805236	-2.879707
C	5.270633	-1.289170	-2.483444
H	4.659007	-0.157833	-0.737138
C	3.484716	-2.323485	-3.767869
H	1.470186	-2.005600	-3.027683
C	4.853375	-2.069184	-3.575313
H	6.335956	-1.088687	-2.327681
H	3.153719	-2.931768	-4.616269
H	5.591690	-2.477634	-4.272953

OS1

Cu	-0.000022	0.736822	-0.000046
O	-0.695441	2.461687	-0.009350
O	0.695186	2.461789	0.009390
C	-0.680493	-1.917591	-0.339401
C	0.680649	-1.917512	0.339506
H	-0.576626	-1.954216	-1.434918
H	-1.279652	-2.790504	-0.022892
H	0.576784	-1.954069	1.435026
H	1.279874	-2.790403	0.023059
N	1.416056	-0.650847	0.001814
N	-1.415997	-0.650957	-0.001802
C	-2.459270	-0.362566	-1.022480
H	-3.173351	-1.205480	-1.069795
H	-2.999016	0.553488	-0.740863
H	-1.983910	-0.227027	-2.005394
C	-2.037717	-0.718916	1.351080
H	-2.523736	0.242707	1.572283
H	-2.794709	-1.524649	1.363173
H	-1.275222	-0.923139	2.116538
C	2.037782	-0.718863	-1.351065
H	1.275292	-0.923139	-2.116514
H	2.523775	0.242763	-1.572313
H	2.794794	-1.524578	-1.363119
C	2.459312	-0.362316	1.022470
H	3.173458	-1.205173	1.069825
H	2.998985	0.553764	0.740800
H	1.983947	-0.226764	2.005379

OS2

Cu	0.000008	0.823456	-0.000036
O	-0.735562	2.602058	-0.049563
O	0.735634	2.602035	0.049580
C	-0.686862	-1.946844	-0.335694
C	0.686815	-1.946835	0.335791
H	-0.575904	-1.977808	-1.432113
H	-1.253629	-2.851170	-0.033991
H	0.575857	-1.977715	1.432212
H	1.253562	-2.851197	0.034156
N	1.443617	-0.710043	0.000004
N	-1.443635	-0.710010	0.000001
C	-2.513357	-0.472627	-0.993265
H	-3.240434	-1.310770	-1.009592
H	-3.047295	0.455870	-0.736620
H	-2.068624	-0.361859	-1.995108
C	-2.041762	-0.797058	1.351889
H	-2.543538	0.154626	1.587590
H	-2.784963	-1.619912	1.403154
H	-1.261144	-0.975562	2.107215
C	2.041747	-0.797208	-1.351875
H	1.261132	-0.975778	-2.107188
H	2.543525	0.154456	-1.587657
H	2.784947	-1.620067	-1.403066
C	2.513339	-0.472605	0.993255
H	3.240396	-1.310764	1.009653
H	3.047300	0.455858	0.736538
H	2.068603	-0.361746	1.995087

OS3

Cu	0.461204	-0.520829	-0.175908
O	2.139519	-1.164838	-0.605954
O	2.904256	-1.489313	0.563848
H	3.821106	-1.370207	0.214256
C	-2.007389	0.597146	0.585816
C	-1.253904	1.738520	-0.090919
H	-1.819620	0.597909	1.671821
H	-3.097113	0.710287	0.430712
H	-1.496940	1.782387	-1.164652
H	-1.540928	2.707739	0.360180
N	0.221238	1.534010	0.024663
N	-1.541950	-0.719840	0.052014
C	-1.860782	-1.814778	1.000508
H	-2.954177	-1.884976	1.162459
H	-1.497064	-2.767907	0.585943
H	-1.362538	-1.623404	1.963679
C	-2.147728	-1.014758	-1.272260
H	-1.730721	-1.957752	-1.658171
H	-3.246382	-1.114867	-1.175125
H	-1.921031	-0.206373	-1.982908
C	0.728455	1.929142	1.360620
H	0.210004	1.363229	2.149258
H	1.806377	1.713353	1.417575
H	0.565132	3.012279	1.526439
C	0.942467	2.278400	-1.033777
H	0.739332	3.364191	-0.950404
H	2.024212	2.106484	-0.926677
H	0.613498	1.923647	-2.022860

OS4

Cu	-0.158866	-0.940728	0.038328
O	-1.590801	-2.080947	0.078707
O	-2.856289	-1.274042	-0.151104
H	-3.037989	-1.006463	0.776846
C	1.680002	1.172810	-0.530475
C	0.602062	2.025453	0.142372
H	1.488755	1.104649	-1.614362
H	2.672610	1.650486	-0.396252
H	0.822863	2.134075	1.217706
H	0.636171	3.048331	-0.295088
N	-0.731279	1.413874	0.010993
N	1.718062	-0.226961	-0.006682
C	2.564821	-1.053530	-0.905480
H	3.600550	-0.655697	-0.946945
H	2.592973	-2.087897	-0.529987
H	2.136251	-1.051980	-1.919689
C	2.307650	-0.262250	1.357047
H	2.347470	-1.306351	1.703574
H	3.335059	0.158513	1.348030

H	1.687521	0.313871	2.059160
C	-1.327805	1.662325	-1.307751
H	-0.649318	1.319716	-2.106363
H	-2.264044	1.086619	-1.385184
H	-1.544061	2.742932	-1.473711
C	-1.641843	1.863416	1.069084
H	-1.842001	2.958838	1.029066
H	-2.601568	1.330885	0.964847
H	-1.214197	1.622746	2.057066

H_2O_2

O	0.000000	0.732877	-0.065560
H	0.772148	0.900093	0.524481
O	0.000000	-0.732877	-0.065560
H	-0.772148	-0.900093	0.524481

$OA\_H_2O_2$

Cu	0.216919	-0.753920	-0.259785
C	-1.749466	1.252950	-0.032734
C	-0.527823	1.914448	0.601389
H	-1.816855	1.506946	-1.102641
H	-2.673728	1.614012	0.457574
H	-0.503500	1.715399	1.685482
H	-0.595013	3.013459	0.466666
N	0.733843	1.385192	0.022919
N	-1.676210	-0.239510	0.063436
C	0.999274	1.929079	-1.324129
H	1.159006	3.026783	-1.283437
H	1.906110	1.455146	-1.734852
H	0.157016	1.716398	-2.000354
C	1.880188	1.660585	0.909497
H	2.786915	1.199135	0.487616
H	2.052846	2.752517	1.010418
H	1.691538	1.231972	1.905052
C	-2.032357	-0.714205	1.428063
H	-1.350597	-0.278243	2.173939
H	-3.073071	-0.425762	1.672879
H	-1.943762	-1.811221	1.460821
C	-2.585532	-0.864515	-0.930923
H	-2.294839	-0.546814	-1.943823
H	-2.508207	-1.960003	-0.855089
H	-3.633647	-0.562240	-0.738651
O	1.719358	-1.737171	-0.806179
H	2.428191	-1.114536	-1.104555
O	2.109345	-1.653984	0.982587
H	1.982196	-2.629848	1.053998

OS5

Cu	0.001141	0.776139	-0.001075
O	-1.312811	2.048361	0.062851
H	-0.971230	2.775573	-0.506637
O	1.308505	2.052424	-0.053699
H	0.918663	2.808707	0.442315
C	0.686496	-1.926208	-0.382614
C	-0.671924	-1.954558	0.286202
H	0.596227	-1.937533	-1.479668
H	1.299866	-2.794468	-0.080469
H	-0.576258	-2.044665	1.378916
H	-1.279684	-2.803107	-0.075373
N	-1.388862	-0.667323	0.001250
N	1.393970	-0.659229	-0.004408
C	-2.429394	-0.406730	1.025442
H	-3.187470	-1.210434	0.985216
H	-1.966304	-0.387008	2.023172
H	-2.901539	0.562418	0.812011
C	-2.000447	-0.649468	-1.354986
H	-2.778372	-1.432502	-1.412263
H	-2.452182	0.339448	-1.517517
H	-1.237479	-0.834715	-2.125270
C	2.486931	-0.367525	-0.962622
H	2.074069	-0.304431	-1.980550
H	2.953941	0.588437	-0.688210
H	3.235510	-1.179599	-0.915024
C	1.932685	-0.702487	1.381776
H	1.125196	-0.891654	2.103999
H	2.685878	-1.508345	1.453825
H	2.400692	0.267298	1.602397

OS6

Cu	0.103423	-1.353032	0.006989
O	1.558540	-0.123971	-0.118927
H	1.185674	0.706458	0.246428
O	-1.311681	-0.079730	0.141855
H	-0.905315	0.745501	-0.198780
C	-0.535245	-4.189902	0.470173
C	0.638472	-4.196969	-0.505628
H	-0.171243	-4.257648	1.508676
H	-1.183804	-5.071114	0.289101
H	0.272578	-4.216721	-1.545576
H	1.252050	-5.108469	-0.353964
N	1.458637	-2.969668	-0.343096
N	-1.307084	-2.926822	0.347328
C	2.275512	-2.713817	-1.545832
H	3.010278	-3.528660	-1.713594
H	1.619139	-2.636259	-2.427704
H	2.802965	-1.758129	-1.410033
C	2.341010	-3.053424	0.840405
H	3.083070	-3.871239	0.726270
H	2.859939	-2.089722	0.951913
H	1.747061	-3.237489	1.749306
C	-2.093724	-2.663705	1.568752
H	-1.420175	-2.627285	2.440320
H	-2.587792	-1.686888	1.459944
H	-2.856018	-3.453322	1.734424
C	-2.210425	-2.950043	-0.823264
H	-1.638622	-3.147311	-1.743730
H	-2.987406	-3.734755	-0.710142
H	-2.684952	-1.961387	-0.912274

OS7

Cu	-0.097116	0.949041	-0.017109
O	-0.920806	2.571337	-0.095872
H	-1.147845	2.829077	0.825532
C	-0.333403	-1.859962	0.374039
C	1.014385	-1.648431	-0.300877
H	-0.228306	-1.850031	1.470617
H	-0.766866	-2.835115	0.082631
H	0.922379	-1.736966	-1.395118
H	1.745377	-2.404730	0.040454
N	1.516412	-0.271984	-0.000095
N	-1.267909	-0.754038	0.005379
C	2.499604	0.171770	-1.017262
H	3.376887	-0.503579	-1.029287
H	2.026778	0.170844	-2.011289
H	2.834750	1.191918	-0.772686
C	2.122712	-0.194335	1.354377
H	3.016577	-0.845483	1.408710
H	2.418244	0.846754	1.556522
H	1.396223	-0.514279	2.116292
C	-2.361655	-0.628149	0.996457
H	-1.935651	-0.419815	1.989848
H	-3.027353	0.196267	0.700214
H	-2.945744	-1.567995	1.039919
C	-1.828587	-0.931569	-1.356917
H	-1.019509	-0.986100	-2.100363
H	-2.425226	-1.863397	-1.400030
H	-2.475758	-0.074057	-1.594709

OS8

Cu	0.792081	-0.716632	-0.365747
O	-0.909353	-0.219996	-0.754453
H	-0.950374	0.712170	-0.448357
N	2.564873	-1.482357	-0.030338
N	2.546933	1.636983	0.159411
C	3.680338	-0.551586	-0.399398
C	3.718011	0.776106	0.359489
H	4.642513	-1.074668	-0.213806
H	3.605862	-0.380164	-1.485867
H	4.660901	1.291338	0.052497
H	3.813758	0.581722	1.441577
C	2.691487	-2.697345	-0.883305
H	3.668482	-3.194607	-0.710745
H	1.880166	-3.400479	-0.640805
H	2.614681	-2.411279	-1.943800
C	2.676517	-1.897896	1.393865
H	1.910633	-2.659864	1.604710
H	3.680405	-2.325638	1.595645
H	2.506170	-1.038848	2.058607
C	2.514408	2.218731	-1.183208
H	2.474228	1.426706	-1.949320
H	1.606019	2.835483	-1.292846
H	3.401578	2.863883	-1.391992
C	2.507138	2.695525	1.169544
H	3.385740	3.382586	1.118888
H	1.595173	3.301852	1.032199
H	2.477623	2.250013	2.178842

O13’

Cu	1.763694	-1.662001	-0.807380
Cu	-2.769228	0.095042	0.031216
C	3.226858	-3.780965	0.380941
C	4.258641	-2.872707	-0.247878
H	3.044967	-3.509892	1.432576
H	3.554645	-4.835900	0.351598
H	4.498198	-3.186716	-1.275276
H	5.197793	-2.869423	0.334285
N	3.725262	-1.468803	-0.322417
N	1.929937	-3.634970	-0.354979
C	1.525626	1.332826	-1.575238
C	1.601625	0.140802	-1.250354
C	4.527554	-0.700964	-1.313026
H	5.591908	-0.746559	-1.018077
H	4.401532	-1.148927	-2.309845
H	4.191013	0.343216	-1.328984
C	3.772262	-0.790389	1.004723
H	4.817860	-0.770796	1.362902
H	3.398370	0.236699	0.891304
H	3.144439	-1.325325	1.732409
C	0.804351	-4.118647	0.477171
H	0.792734	-3.571662	1.432017
H	-0.136919	-3.939713	-0.061160
H	0.930385	-5.200323	0.669629
C	1.937589	-4.354335	-1.658141
H	2.756346	-3.991169	-2.296226
H	2.068440	-5.437481	-1.477502
H	0.977156	-4.177031	-2.163063
O	-0.002793	-1.931038	-1.157320
H	-0.468978	-1.062921	-1.312776
C	1.493643	2.714376	-1.947715
C	0.657807	3.154106	-3.005605
C	2.299157	3.663389	-1.267900
C	0.631891	4.505808	-3.368127
H	0.036359	2.425623	-3.535955
C	2.263069	5.012899	-1.638690
H	2.947206	3.329478	-0.451373
C	1.431653	5.438919	-2.687611
H	-0.016357	4.832192	-4.188020
H	2.889756	5.736048	-1.106394
H	1.407672	6.495178	-2.974619
C	-5.438788	-0.568367	-0.610775
C	-5.185252	-1.149186	0.761909
H	-5.858621	0.447452	-0.550140
H	-6.145852	-1.196046	-1.182847
H	-4.826951	-2.188059	0.695529
H	-6.102333	-1.143269	1.377646
N	-4.117504	-0.354844	1.464057
N	-4.137239	-0.476082	-1.348959
C	-0.549895	1.096770	1.940987
C	-1.495848	0.708795	1.244490
C	-3.538641	-1.172223	2.563525
H	-4.354467	-1.482037	3.242008
H	-3.053263	-2.063689	2.139043
H	-2.802264	-0.574298	3.116100
C	-4.647119	0.930848	2.000284
H	-5.451933	0.711932	2.725311
H	-3.829238	1.471134	2.496842
H	-5.046246	1.547973	1.182414
C	-4.233426	0.502964	-2.457912
H	-4.520935	1.485965	-2.054956

H	-3.256985	0.576552	-2.956582
H	-4.997483	0.159790	-3.179757
C	-3.698706	-1.797016	-1.873460
H	-3.636042	-2.533006	-1.057982
H	-4.426104	-2.149582	-2.627607
H	-2.710738	-1.684683	-2.342876
O	-1.562849	0.417631	-1.322403
H	-0.785280	0.885374	-0.932272
C	0.503605	1.542899	2.798403
C	0.841798	0.811651	3.966026
C	1.235621	2.717138	2.486114
C	1.887566	1.243400	4.790025
H	0.276214	-0.091831	4.215754
C	2.279224	3.138723	3.318423
H	0.977715	3.287061	1.587980
C	2.609537	2.405498	4.470433
H	2.138154	0.670899	5.689207
H	2.836860	4.047051	3.067001
H	3.425272	2.740648	5.119229

RedEl_TS’

Cu	-0.427011	-2.012070	-0.425515
Cu	1.903036	0.730588	0.938549
C	-0.412929	-4.041769	-2.468811
C	-1.779539	-3.387933	-2.500393
H	0.263967	-3.590133	-3.210389
H	-0.492771	-5.119825	-2.701763
H	-2.482098	-3.904604	-1.827265
H	-2.205933	-3.410096	-3.520448
N	-1.689816	-1.963633	-2.034029
N	0.198239	-3.854229	-1.118580
C	-2.043747	-0.167200	1.190745
C	-1.097731	-0.425599	0.401878
C	-3.062107	-1.466496	-1.756878
H	-3.680017	-1.592052	-2.665336
H	-3.502456	-2.044420	-0.930786
H	-3.020367	-0.404062	-1.484255
C	-1.043751	-1.090844	-3.050496
H	-1.636631	-1.110886	-3.984461
H	-1.009144	-0.062275	-2.663695
H	-0.020643	-1.432225	-3.264626
C	1.672110	-3.959749	-1.184953
H	2.059296	-3.238121	-1.920114
H	2.086181	-3.734728	-0.191837
H	1.960684	-4.983573	-1.489669
C	-0.330179	-4.833327	-0.132503
H	-1.425858	-4.757650	-0.065149
H	-0.054970	-5.859043	-0.443020
H	0.109542	-4.611231	0.850389
O	0.861341	-2.115342	0.890968
H	0.739690	-1.364824	1.534523
C	-3.129695	0.143199	2.039205
C	-3.024789	-0.054212	3.447172
C	-4.349171	0.647846	1.501720
C	-4.105799	0.241961	4.279091
H	-2.087624	-0.436814	3.863521
C	-5.422224	0.934783	2.348171
H	-4.433552	0.804745	0.422046
C	-5.306514	0.734636	3.735544
H	-4.015491	0.088128	5.359181
H	-6.355844	1.320493	1.926383
H	-6.150636	0.964767	4.393373
C	4.741630	1.048491	1.266567
C	4.513323	0.449928	-0.105071
H	4.813438	2.145788	1.216736
H	5.680030	0.668248	1.710157
H	4.484559	-0.650317	-0.053925
H	5.316311	0.740265	-0.807557
N	3.189243	0.904045	-0.648312
N	3.584647	0.706303	2.149763
C	-0.169207	1.980007	-0.806162
C	0.271834	1.054091	-0.077040
C	2.799647	0.026462	-1.780573
H	3.594969	0.042688	-2.549416
H	2.663510	-1.001204	-1.411621
H	1.861769	0.394748	-2.217401
C	3.243211	2.317121	-1.101751
H	3.984285	2.412637	-1.917135
H	2.251838	2.612903	-1.473242
H	3.526781	2.977743	-0.270073
C	3.433431	1.705083	3.234265
H	3.272538	2.701911	2.794908
H	2.567525	1.430284	3.852237
H	4.348702	1.721844	3.856199
C	3.717575	-0.653898	2.725834
H	3.858932	-1.394378	1.924901
H	4.589053	-0.682262	3.407133
H	2.802583	-0.892123	3.286352
O	0.912239	0.317540	2.451903
H	-0.025419	0.489171	2.208038
C	-0.712638	3.017890	-1.595917
C	-0.490512	3.067872	-3.002521
C	-1.499619	4.038457	-0.986377
C	-1.041112	4.100984	-3.764177
H	0.113709	2.289401	-3.478455
C	-2.039727	5.066039	-1.762623
H	-1.673929	4.004804	0.093527
C	-1.814786	5.102627	-3.150544
H	-0.865003	4.129270	-4.844312
H	-2.641628	5.845284	-1.284068
H	-2.241324	5.911027	-3.752831

O14’

Cu	-0.095553	0.947501	-0.004099
N	1.513161	-0.280841	0.007785
N	-1.273309	-0.749785	-0.003055
C	1.003462	-1.652676	0.318247
C	-0.343551	-1.863914	-0.358167
H	1.731888	-2.414756	-0.015533
H	0.909049	-1.732595	1.412896
H	-0.782470	-2.834449	-0.059506
H	-0.234438	-1.863902	-1.454512
C	2.492184	0.166687	1.027397
H	3.365266	-0.513844	1.051199
H	2.834947	1.182609	0.776024
H	2.013333	0.177390	2.018489
C	2.127023	-0.216733	-1.344145
H	2.433758	0.820139	-1.550738
H	3.014651	-0.876962	-1.390542
H	1.400364	-0.533976	-2.107066
C	-1.835449	-0.905367	1.361911
H	-1.027615	-0.958080	2.106640
H	-2.474869	-0.038386	1.587229
H	-2.441589	-1.830418	1.416496
C	-2.365842	-0.630952	-0.996975
H	-2.954324	-1.568468	-1.029170
H	-3.027056	0.201069	-0.712831
H	-1.938003	-0.436931	-1.992476
O	-0.884336	2.589955	-0.104034
H	-1.123092	2.856510	0.811840

O13’’

Cu	0.013312	1.314562	-0.862472
Cu	-0.013304	-1.253606	-0.921028
C	2.175809	3.196467	-1.345276
C	1.246607	3.996949	-0.423946
H	2.899217	2.615878	-0.751012
H	2.743007	3.904156	-1.980299
H	0.473459	4.511203	-1.016501
H	1.850880	4.777909	0.080801
N	0.571085	3.141348	0.571740
N	1.447423	2.241928	-2.220882
C	-2.223985	0.203913	0.679697
C	-1.273953	-0.058779	-0.102342
C	1.437090	2.851657	1.726958
H	1.626651	3.776427	2.310792
H	0.943294	2.115178	2.380035
H	2.402751	2.440786	1.397854
C	-0.698711	3.730086	1.029155
H	-1.162501	3.058984	1.770358
H	-0.529717	4.717667	1.507050
H	-1.375517	3.842395	0.169322
C	0.746714	2.934837	-3.322818
H	0.002506	3.640580	-2.932592
H	1.491410	3.479614	-3.935556
H	0.234039	2.191819	-3.950184
C	2.367543	1.232463	-2.796490
H	2.920998	0.726464	-1.994518
H	1.784990	0.492082	-3.364499
H	3.084083	1.730650	-3.477970
C	-3.316106	0.480790	1.521426
C	-4.616507	0.682405	0.968139
C	-3.133335	0.545123	2.935876
C	-5.695759	0.938552	1.811849
H	-4.751618	0.630504	-0.116096
C	-4.225051	0.800501	3.763467
H	-2.133979	0.391636	3.353366
C	-5.503338	0.996867	3.205525
H	-6.693310	1.091894	1.389669
H	-4.087455	0.848218	4.847695
H	-6.356000	1.197283	3.861888
O	-1.343863	2.276022	-1.649974
H	-2.171603	1.913022	-1.263055
H	-0.988222	-2.202345	2.256201
C	-1.453929	-2.927651	1.570671
N	-0.565045	-3.155563	0.419101
H	-2.424604	-2.530424	1.240151
H	-1.628362	-3.876644	2.119603
C	-1.212268	-3.970387	-0.626925
C	0.704056	-3.748236	0.871948
C	-2.148167	-3.137715	-1.512224
H	-0.422348	-4.434323	-1.237995
H	-1.805014	-4.789694	-0.172004
H	1.395571	-3.817068	0.019352
H	1.148009	-3.103228	1.647605
H	0.538614	-4.756919	1.304980
H	-2.879233	-2.595569	-0.891951
H	-2.704391	-3.819489	-2.184189
N	-1.430699	-2.130891	-2.336796
C	-0.713535	-2.756846	-3.468085
C	-2.365489	-1.109535	-2.866396
H	-1.444195	-3.291650	-4.106035
H	-0.219066	-1.973604	-4.060371
H	0.047420	-3.460820	-3.108013
H	-1.793292	-0.330392	-3.391289
H	-3.068603	-1.584542	-3.577627
H	-2.933578	-0.654973	-2.044261
C	1.258821	0.094942	-0.068546
O	1.353922	-2.185493	-1.727686
C	2.202966	-0.220929	0.700435
H	2.177977	-1.829983	-1.326009
C	3.295016	-0.560021	1.519749
C	4.599448	-0.688493	0.953985
C	3.110946	-0.760481	2.920912
C	5.681580	-1.005955	1.772764
H	4.735447	-0.531139	-0.119993
C	4.204939	-1.078959	3.723306
H	2.108796	-0.660953	3.347936
C	5.487407	-1.200711	3.153630
H	6.682174	-1.102392	1.341114
H	4.066466	-1.233442	4.797505
H	6.341954	-1.449588	3.790730

RedEl_TS’’

Cu	1.064163	-1.128284	-0.728414
Cu	-1.064156	1.128544	-0.728578
C	0.347589	-3.852940	-1.388789
C	1.536576	-4.018888	-0.434282
H	-0.599339	-3.820645	-0.826626
H	0.312642	-4.729352	-2.064617
H	2.482593	-3.997505	-0.997380
H	1.457404	-5.014858	0.045855
N	1.592228	-2.957157	0.595655
N	0.423557	-2.615209	-2.207592
C	1.704358	0.966169	0.654568
C	0.631481	0.828287	0.003613
C	0.662236	-3.227275	1.707789
H	0.975994	-4.135235	2.263095

H	0.659192	-2.370626	2.399780
H	-0.358740	-3.381937	1.330327
C	2.963628	-2.796161	1.118845
H	2.967997	-2.006214	1.886747
H	3.320897	-3.740374	1.579091
H	3.634674	-2.510332	0.295630
C	1.420032	-2.726958	-3.293827
H	2.424795	-2.886315	-2.883947
H	1.141906	-3.571552	-3.954435
H	1.423300	-1.794917	-3.877200
C	-0.895456	-2.281063	-2.792352
H	-1.656030	-2.219739	-2.002763
H	-0.828147	-1.315248	-3.315457
H	-1.187545	-3.064070	-3.519089
C	2.908502	1.195758	1.352292
C	4.058898	1.680386	0.663132
C	2.975932	0.950272	2.754843
C	5.243743	1.902212	1.365868
H	3.998589	1.882486	-0.410906
C	4.167281	1.184824	3.440552
H	2.088750	0.580858	3.277679
C	5.299843	1.656238	2.749834
H	6.127046	2.273907	0.838048
H	4.220090	0.998659	4.517397
H	6.231666	1.835672	3.295374
O	2.743647	-1.054952	-1.496532
H	3.268215	-0.457322	-0.917740
H	-0.659750	2.369505	2.400286
C	-0.662713	3.226549	1.708782
N	-1.592422	2.956985	0.596283
H	0.358331	3.381507	1.331622
H	-0.976658	4.134174	2.264529
C	-1.536416	4.019143	-0.433176
C	-2.963970	2.795734	1.118991
C	-0.347273	3.853447	-1.387553
H	-2.482340	3.998160	-0.996442
H	-1.457166	5.014897	0.047397
H	-3.634736	2.510158	0.295461
H	-2.968525	2.005499	1.886593
H	-3.321423	3.739752	1.579499
H	0.599554	3.820812	-0.825240
H	-0.312119	4.730139	-2.063007
N	-0.423224	2.616068	-2.206888
C	-1.419454	2.728399	-3.293287
C	0.895862	2.281978	-2.791539
H	-1.140695	3.572818	-3.953850
H	-1.423221	1.796350	-3.876636
H	-2.424185	2.888415	-2.883594
H	0.828496	1.316428	-3.315132
H	1.188239	3.065287	-3.517833
H	1.656256	2.220138	-2.001816
C	-0.631772	-0.828158	0.003200
O	-2.743453	1.055595	-1.497124
C	-1.704562	-0.966176	0.654287
H	-3.267737	0.456575	-0.919512
C	-2.908687	-1.196114	1.351921
C	-4.058824	-1.681264	0.662697
C	-2.976332	-0.950574	2.754453
C	-5.243629	-1.903553	1.365346
H	-3.998355	-1.883339	-0.411340
C	-4.167638	-1.185582	3.440077
H	-2.089338	-0.580786	3.277344
C	-5.299943	-1.657521	2.749294
H	-6.126737	-2.275643	0.837478
H	-4.220616	-0.999381	4.516907
H	-6.231733	-1.837320	3.294771

O15’

Cu	-0.993766	-0.341263	-0.494112
C	-3.444231	0.363080	0.876117
C	-2.461537	1.496712	1.127026
H	-4.063912	0.572212	-0.010608
H	-4.126972	0.253595	1.741165
H	-1.891519	1.318850	2.053103
H	-2.999954	2.456838	1.242682
N	-1.468999	1.602422	0.010040
N	-2.708308	-0.905312	0.625838
C	1.719865	0.129491	-1.200593
C	0.599542	0.183833	-1.762906
H	0.107194	0.368392	-2.716360
C	-0.308045	2.401451	0.475406
H	0.397666	2.541436	-0.355141
H	-0.648819	3.392723	0.831986
H	0.195879	1.872859	1.299361
C	-2.075604	2.262720	-1.175853
H	-2.405403	3.286589	-0.913819
H	-1.327588	2.320753	-1.981076
H	-2.941290	1.685912	-1.533840
C	-2.231097	-1.531646	1.879249
H	-1.603174	-0.828434	2.447881
H	-3.091288	-1.835797	2.508458
H	-1.630481	-2.416737	1.622872
C	-3.536298	-1.868681	-0.129241
H	-3.875617	-1.405140	-1.068814
H	-2.922607	-2.750123	-0.364335
H	-4.419450	-2.172463	0.467249
C	2.910038	0.007266	-0.453853
C	3.506421	1.150716	0.149673
C	3.540217	-1.263152	-0.321444
C	4.696679	1.016908	0.866819
H	3.025736	2.127278	0.040217
C	4.729231	-1.378175	0.400385
H	3.080421	-2.139320	-0.788478
C	5.309467	-0.242735	0.994370
H	5.153427	1.897828	1.328515
H	5.209675	-2.356290	0.501916
H	6.243515	-0.339886	1.556843
O	-0.667697	-2.132172	-0.882417
H	0.208612	-2.143558	-1.323262

DP_TS-OH’

Cu	1.310728	-0.563622	-0.096363
C	3.366555	1.289643	0.570076
C	2.304076	2.106361	-0.150951
H	3.182530	1.279373	1.656530
H	4.368890	1.728453	0.402100
H	2.527072	2.171211	-1.227591
H	2.270469	3.137436	0.248014
N	0.959058	1.463153	-0.008674
N	3.334432	-0.126212	0.100774
C	-1.852338	-0.967361	-0.101544
C	-0.667842	-1.351993	-0.147619
H	0.229659	-2.246644	-0.191445
C	0.059434	1.929654	-1.091936
H	-0.928848	1.463690	-0.972039
H	-0.048323	3.030560	-1.047546
H	0.481517	1.644739	-2.068045
C	0.355539	1.773361	1.313439
H	0.192440	2.864302	1.406321
H	-0.608142	1.250623	1.401813
H	1.020028	1.437840	2.123823
C	3.979013	-0.287586	-1.225521
H	3.489163	0.353137	-1.974290
H	5.051376	-0.018024	-1.163324
H	3.891088	-1.338016	-1.543582
C	3.979420	-1.022790	1.086207
H	3.475151	-0.921050	2.059858
H	3.885897	-2.062124	0.740001
H	5.049842	-0.762092	1.199031
C	-3.202831	-0.530159	-0.036146
C	-3.877393	-0.482518	1.213370
C	-3.895318	-0.142991	-1.214620
C	-5.207791	-0.058742	1.275459
H	-3.344595	-0.784272	2.120291
C	-5.224613	0.282915	-1.136803
H	-3.377972	-0.182466	-2.178065
C	-5.883491	0.324769	0.104058
H	-5.722214	-0.027359	2.241176
H	-5.752470	0.581624	-2.048140
H	-6.925514	0.656219	0.158147
O	1.540227	-2.580298	-0.112938
H	1.811081	-2.803684	-1.034518

O16’

Cu	1.166490	-0.377293	-0.008900
C	3.826534	0.549681	0.451230
C	3.140002	1.743746	-0.190991
H	3.728157	0.589927	1.548130
H	4.906081	0.544133	0.208545
H	3.286098	1.742376	-1.282645
H	3.561212	2.688554	0.202377
N	1.672250	1.694592	0.066353
N	3.191451	-0.725292	-0.007015
C	-1.975292	-0.161914	0.037010
C	-0.732974	-0.200608	0.042372
C	0.929427	2.455487	-0.961781
H	1.253150	3.514534	-0.956813
H	1.126445	2.020066	-1.953671
H	-0.147508	2.401656	-0.747002
C	1.323177	2.172887	1.423457
H	1.582174	3.245015	1.523062
H	0.242705	2.039962	1.582026
H	1.870586	1.597562	2.185523
C	3.565860	-1.822528	0.920968
H	3.164559	-1.611098	1.924498
H	3.159183	-2.775317	0.550859
H	4.667562	-1.912741	0.980533
C	3.619550	-1.078318	-1.386181
H	3.352954	-0.274060	-2.087655
H	4.714778	-1.237114	-1.413445
H	3.110378	-2.003087	-1.695699
C	-3.405265	-0.110827	0.021808
C	-4.103075	0.180463	-1.178927
C	-4.153857	-0.352624	1.202385
C	-5.501831	0.227502	-1.192796
H	-3.534344	0.367518	-2.095539
C	-5.552539	-0.301969	1.177689
H	-3.624828	-0.578265	2.133945
C	-6.232276	-0.013266	-0.017240
H	-6.025477	0.452339	-2.128118
H	-6.115841	-0.490389	2.097861
H	-7.326507	0.023664	-0.032425
H	-0.202263	-2.369552	-0.470257
O	0.761152	-2.571568	-0.358398
H	0.802747	-2.973025	0.541798

G2’

Cu	-0.776081	-0.576401	-0.108634
C	0.096393	-3.367938	0.186436
C	0.423733	-2.691601	1.518158
H	-0.927209	-3.778832	0.212238
H	0.788317	-4.224118	0.036386
H	1.442775	-2.272187	1.489099
H	0.406136	-3.453456	2.326149
N	-0.507893	-1.576396	1.833043
N	0.174806	-2.424943	-0.960610
C	1.613025	1.095912	-0.248056
C	0.356358	1.079588	-0.265886
H	-0.522798	1.802941	-0.219946
N	-1.796682	2.995187	0.207454
C	-3.112820	2.603438	-0.318683
H	-3.915459	3.219110	0.150349
H	-3.128640	2.845865	-1.394415
C	-3.525711	1.145349	-0.109464
H	-4.584658	1.089977	-0.444631
H	-3.518913	0.880474	0.961108
N	-2.760980	0.078817	-0.833177
C	-3.584754	-1.151675	-0.737994
H	-3.061692	-1.992241	-1.216804
H	-3.766938	-1.393915	0.320311
H	-4.566206	-1.013271	-1.241221
C	-2.588975	0.421411	-2.263457
H	-1.895393	1.269058	-2.373908
H	-2.160002	-0.447292	-2.788083
H	-3.558440	0.681025	-2.740523
C	-1.742317	2.959829	1.671263
H	-0.728291	3.237319	2.004854
H	-2.471096	3.660784	2.135501

H	-1.954809	1.942639	2.039287
C	-1.397569	4.312368	-0.298131
H	-0.378802	4.545792	0.055124
H	-1.392094	4.300040	-1.401154
H	-2.079854	5.123191	0.041341
C	-0.494969	-3.011569	-2.139816
H	-0.461376	-2.293168	-2.974816
H	0.004801	-3.950195	-2.462845
H	-1.545948	-3.241532	-1.906797
C	1.583273	-2.161292	-1.322756
H	2.088763	-3.094765	-1.651954
H	1.614941	-1.430613	-2.145986
H	2.133134	-1.742678	-0.468189
C	0.091246	-0.695527	2.856292
H	-0.603797	0.130045	3.080123
H	0.299815	-1.249344	3.796540
H	1.033648	-0.269948	2.476507
C	-1.792192	-2.098850	2.347992
H	-1.646669	-2.645430	3.304735
H	-2.483705	-1.258752	2.521475
H	-2.248650	-2.784920	1.618544
C	3.029683	1.034158	-0.212745
C	3.721313	1.013769	1.031643
C	3.790758	1.008739	-1.415269
C	5.117989	0.965038	1.064369
H	3.145230	1.038999	1.962373
C	5.187151	0.960440	-1.367248
H	3.269387	1.028450	-2.377485
C	5.856842	0.938107	-0.131358
H	5.635620	0.948740	2.029275
H	5.759154	0.940778	-2.300837
H	6.950571	0.900264	-0.100054

DP_TS2

Cu	-0.932552	-0.431199	-0.115460
C	-0.961249	-3.369162	0.097071
C	-0.860400	-2.859350	1.533648
H	-2.019651	-3.466377	-0.198469
H	-0.511346	-4.383387	0.038316
H	0.198654	-2.749525	1.821435
H	-1.308360	-3.608258	2.220878
N	-1.513703	-1.535390	1.708323
N	-0.308465	-2.448833	-0.869572
C	1.889186	0.650067	0.052632
C	0.637507	0.767386	0.084818
H	-0.147960	1.727802	0.272341
N	-0.923558	3.034887	0.543465
C	-1.985840	3.208984	-0.470264
H	-2.613500	4.084419	-0.197340
H	-1.491715	3.462087	-1.422653
C	-2.940250	2.029800	-0.662475
H	-3.750794	2.407289	-1.324934
H	-3.417453	1.751473	0.292064
N	-2.393000	0.777241	-1.265683
C	-3.557072	-0.109810	-1.503958
H	-3.218756	-1.062919	-1.937111
H	-4.071865	-0.309887	-0.551228
H	-4.281958	0.359301	-2.204588
C	-1.744417	1.062355	-2.565343
H	-0.814736	1.631371	-2.413781
H	-1.487324	0.109400	-3.054163
H	-2.418520	1.636405	-3.237591
C	-1.444901	2.936691	1.914272
H	-0.604443	2.756636	2.604084
H	-1.965948	3.867656	2.218367
H	-2.149098	2.094349	1.994956
C	0.081044	4.104942	0.439624
H	0.883914	3.920061	1.171818
H	0.515551	4.101346	-0.573471
H	-0.360581	5.102462	0.637661
C	-0.754676	-2.767944	-2.241557
H	-0.299292	-2.058001	-2.950663
H	-0.458379	-3.797854	-2.537332
H	-1.850899	-2.690962	-2.310881
C	1.160892	-2.593672	-0.817607
H	1.467740	-3.627797	-1.085512
H	1.621065	-1.890749	-1.528998
H	1.539791	-2.360539	0.188011
C	-1.000720	-0.889394	2.934629
H	-1.503364	0.080474	3.076152
H	-1.185730	-1.517081	3.832737
H	0.082774	-0.715119	2.835663
C	-2.978968	-1.691980	1.829279
H	-3.245543	-2.301332	2.720140
H	-3.446610	-0.699591	1.930807
H	-3.390565	-2.182525	0.934205
C	3.296085	0.461882	-0.002205
C	4.035149	0.134921	1.169358
C	4.000961	0.603978	-1.230590
C	5.420754	-0.043340	1.107418
H	3.504409	0.025218	2.120693
C	5.386744	0.423749	-1.278734
H	3.443282	0.856746	-2.138246
C	6.102941	0.099469	-0.113402
H	5.974450	-0.295387	2.018163
H	5.913441	0.536588	-2.232345
H	7.187802	-0.041779	-0.156286