Supporting Information

Computational characterization of a mechanism for the copper-catalyzed aerobic oxidative trifluoromethylation of terminal alkynes

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Table of contents Page

Computational details

All the structures have been fully optimized in N,N-dimethylformamide using the Gaussian09 package,[1] with the PBE density functional.[2, 3] The standard 6-31+G(d)[4-6] basis set was used for all H, B, C, N, O and F atoms; the Stuttgart triple zeta basis set (SDD),[7, 8] along with the associated ECP to describe the 10 core electron, was employed for Cu. Solvation free energies are computed with the (IEF-PCM) continuum dielectric solvation model[9, 10] using the radii and non-electrostatic terms for Truhlar and coworkers' SMD solvation model.[11] In all cases frequency calculations were carried out to ensure the nature of stationary points and transition states, and allowing the calculation of free energies at 25ºC for all the species involved in the catalytic cycles.

Additional single point calculations on the previously optimized geometries were employed to obtain improved solvated free energy values with larger basis sets. The the aug-cc-pVTZ basis set including polarization and the associated electron core potential[12] was employed for Cu while the 6-311+G** all-electron basis set[5] was used for all the other atoms.

The empirical dispersion terms, included in the calculation of free energies, were computed for the optimized geometries using the DFT-D3 package[13] of Grimme using the corresponding PBE-D[14-16] functional.

Unless otherwise stated all the free energy values correspond to those obtained with the large basis set including solvation and dispersion corrections.

Along the reaction pathways mononuclear and dinuclear species coexist, it is not easy to assign a unique origin of energies for both species at the same time since for the latter that spot would correspond to two separated monomers and hence the energy for the dinuclear species would be "doubled". Throughout the paper all the energies have been calculated regarding to the mononuclear starting copper complex.

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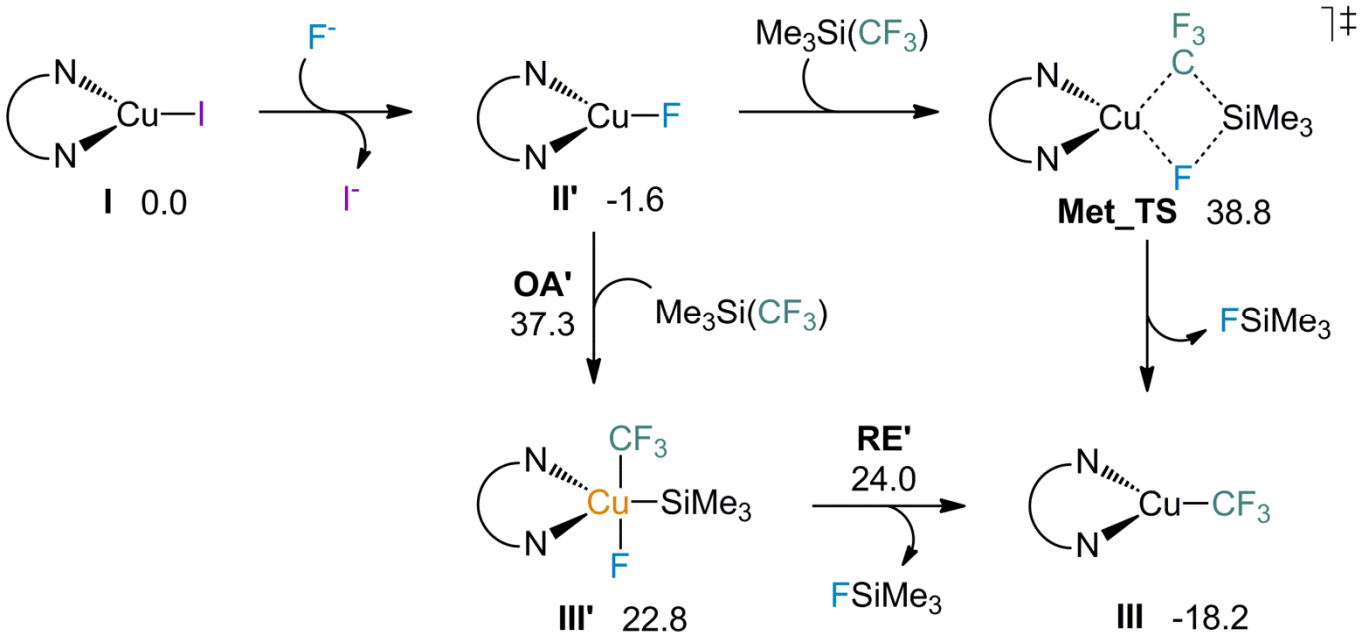
Alternative pathways to form the Cu-CF_3 bond

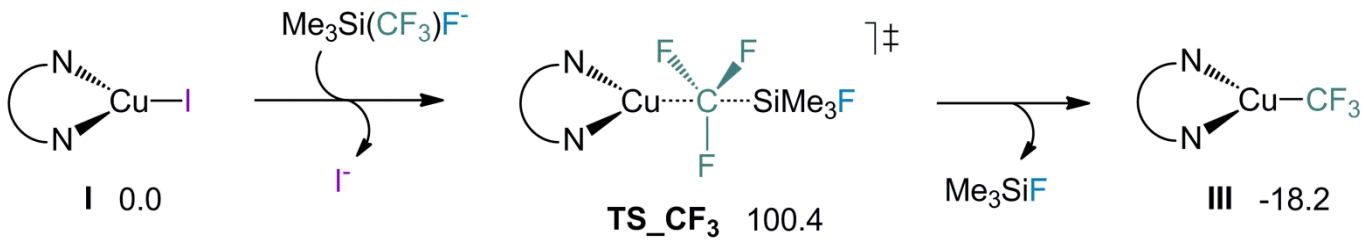
Three alternative pathways to form the Cu-CF_3 bond have been explored. The first one consists in the σ-bond metathesis between **II'** and $Me_3Si(CF_3)$; the second one implies the oxidative addition of $Me_3Si(CF_3)$ onto **II'** and subsequent reductive elimination of Me_3SiF (Scheme S1).



Scheme S1. σ-bond metathesis and oxidative addition/reductive elimination pathways leading to the formation of **III** (Cu(I), Cu(III); free energies in kcal/mol).

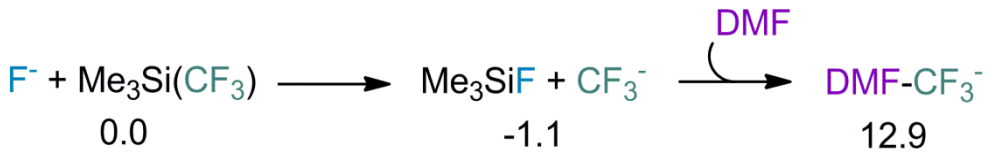
In both pathways in Scheme S1 the reaction starts with the replacement of iodide by fluoride, this step is slightly exergonic indicating that there may not be a barrier mediating this stage. As may be observed the transition state for the σ-bond metathesis (**Met_TS**) is very high in energy (40.4 kcal/mol) and, thus, this possible route can be ruled out. In the second pathway, the reaction proceeds by the oxidative addition of $Me_3Si(CF_3)$ onto the copper-fluoride intermediate **II'** to yield the copper (III) complex **III'** which may, in turn, reductively eliminate Me_3SiF delivering the active catalyst **II**. Unfortunately, the barrier for the oxidative addition process is very high (38.9 kcal/mol) preventing the reaction to proceed through this pathway.

The last studied pathway (Scheme S2) involves the substitution of the iodide by $Me_3Si(CF_3)F^-$ and direct trifluoromethyl group transfer in a S_N2-like fashion, with the CF_3 group inverting its configuration. As may be seen the energy of the transition state is even higher (more than 100 kcal/mol) than those found previously, probably due to the unfavorable planarization of the CF_3 moiety.



Scheme S2. Oxidative addition/reductive elimination pathway leading to the formation of **III** (Cu(I), Cu(III); free energies in kcal/mol).

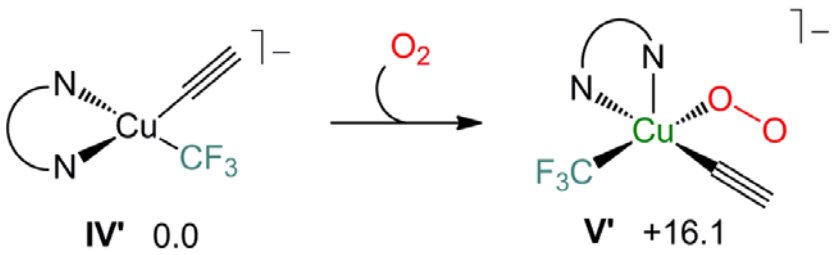
Additionally, the potential formation of an adduct between the CF_3^- group (obtained through the mechanism described in the main text) and a solvent molecule has been studied. However, 14.0 kcal/mol are required to bring both groups together (Scheme S3), indicating that this process is not favored.



Scheme S3. Formation of an adduct between CF_3^- and a solvent DMF molecule (free energies in kcal/mol).

Alternative pathway for aerobic oxidation of (phen)Cu(CF_3)alkynyl

An alternative pathway for the aerobic oxidation was computed (Scheme S4); this process implies the addition of O_2 to the hypothetical (phen)Cu(CF_3)alkynyl species **IV'** (generated by the deprotonation of a Cu-coordinated terminal alkyne) to deliver the intermediate **V'**. This latter compound seems to be, in principle, a copper (II) complex since the O–O distance has been elongated to 1.34 Å, corresponding to a superoxo ligand and thus indicating that just one electron has been transferred from the metal to the O_2 moiety. As may be seen, the aerobic oxidation of **IV'** is not very high (16.1 kcal/mol) but affords a copper (II) intermediate which does not allow to reductively eliminate the product and recover the starting copper (I) catalyst. In addition, if the reductive elimination was possible, the barrier should be added to the one mediating the transformation between **IV'** and **V'**, surely affording an overall energy barrier higher than the one proposed in the main text.



Scheme S4. Aerobic oxidation of the hypothetical (phen)Cu(CF_3)alkynyl species (Cu(I), Cu(II); free energies in kcal/mol relative to **IV'**).

Table S1. Computed free energy values and dispersion corrections terms for all the species involved in the catalytic cycles (in Hartrees).

Species	Free energy	Dispersion correction
PhCCH	-307.999059	-0.004231
$Me_3Si(CF_3)$	-746.330805	-0.006246
F^-	-99.944342	0.000000
$Me_3Si(CF_3)F^-$	-846.271861	-0.008270
Me_3SiF	-508.748750	-0.004001
CF_3^-	-337.530141	-0.000275
$PhCCCF_3$	-644.838856	-0.005508
I^-	-295.894330	0.000000
O_2	-150.256524	-0.000001
OH^-	-75.866502	0.000000
$Me_3Si(CF_3)OH^-$	-822.214906	-0.009130
Me_3SiOH	-484.709283	-0.004642
I	-1064.117291	-0.014071
II	-1401.664839	-0.017942
III	-1105.780082	-0.014641
IV	-1256.028218	-0.017451
V	-2361.789322	-0.039325
TS_OO	-2361.775066	-0.040789
VI	-2361.805644	-0.043023
VII	-2669.791641	-0.054149
DPTS1	-2669.781453	-0.056044
VIII	-2669.787614	-0.057935
IX	-2977.773010	-0.073060
DPTS2	-2977.765689	-0.074033
X	-1488.906750	-0.027050
RETS	-1488.883378	-0.027031
XI	-844.121247	-0.013813
II’	-868.170822	-0.013093
Met_TS	-1614.427976	-0.028592
OA’	-1614.428823	-0.030233
III’	-1614.453489	-0.028570
RE’	-1614.452180	-0.027985
TS_CF_3	-1614.336278	-0.022207
CF_3-DMF	-585.725767	-0.007862
IV’	-1413.301264	-0.022542
V’	-1563.527359	-0.027304

Optimized geometries

PhCCH

C	-3.254336	0.000004	-0.000001
H	-4.333564	0.000022	0.000000
C	-2.028692	-0.000014	-0.000002
C	-0.597882	-0.000006	0.000000
C	0.119483	-1.222938	0.000000
C	0.119471	1.222932	0.000000
C	1.520467	-1.216483	0.000001
H	-0.430662	-2.169618	0.000000
C	1.520456	1.216491	0.000001
H	-0.430683	2.169607	0.000000
C	2.225105	0.000008	0.000001
H	2.064954	-2.167057	0.000001
H	2.064932	2.167070	0.000001
H	3.320595	0.000013	0.000002

$Me_3Si(CF_3)$

Si	-0.885009	0.000894	-0.000060
C	-1.392226	-0.899112	1.598736
H	-1.013644	-1.936479	1.611344
H	-1.007415	-0.377511	2.492889
C	-1.392002	1.835622	-0.020999
H	-2.493586	1.925284	-0.025572
H	-1.011879	2.365825	0.870157
C	-1.392737	-0.936013	-1.577295
H	-1.013791	-0.431643	-2.483764
H	-2.494559	-0.982371	-1.651422
C	1.097985	-0.000038	-0.000098
F	1.645434	0.613451	-1.112104
F	1.643122	-1.270605	0.024394
F	1.645644	0.655482	1.087410
H	-1.005684	2.347014	-0.920407
H	-1.009256	-1.971643	-1.569411
H	-2.493983	-0.938701	1.677663

$Me_3Si(CF_3)F^-$

C	0.866410	-0.505993	1.859158
H	-0.121394	-0.612121	2.339861
H	1.402756	-1.466998	1.962948
C	0.870073	1.865924	-0.500823
H	1.274453	2.455595	0.343542
H	-0.103507	2.301102	-0.783996
C	-1.320703	-0.001215	-0.002254
F	-1.928679	0.312150	-1.229523
F	-1.911602	0.911221	0.889752
F	-1.918033	-1.224475	0.347205
Si	0.785582	-0.000459	-0.005004
C	0.883358	-1.362676	-1.373244
H	-0.098797	-1.686897	-1.758902
H	1.483400	-0.995399	-2.225397
F	2.753486	0.005706	0.013649
H	1.566470	1.995916	-1.348426
H	1.403533	-2.251189	-0.970547
H	1.443568	0.248761	2.424201

Me_3SiF

C	-1.639051	-0.807323	-0.526120
H	-1.721465	-0.839396	-1.628297
H	-1.709761	-1.843855	-0.150543
C	0.118960	1.823380	-0.521092
H	-0.735473	2.402911	-0.128135
H	0.113041	1.915818	-1.622979
Si	-0.000153	-0.000531	-0.014834
C	1.521241	-1.012404	-0.525076
H	1.600583	-1.054842	-1.627014
H	2.450468	-0.558185	-0.136770
F	-0.001015	-0.003665	1.708166
H	1.052115	2.283262	-0.149138
H	1.458015	-2.049508	-0.149663
H	-2.503141	-0.237708	-0.139546

CF_3^-

C	-0.000207	-0.000494	0.558714
F	0.958505	-0.853815	-0.124200
F	-1.219107	-0.402526	-0.124242
F	0.260740	1.256670	-0.124034

$PhCCCF_3$

C	-1.330725	0.000723	-0.003700
C	-0.105042	0.000382	0.001294
C	1.318912	0.000190	0.001394
C	2.029841	1.227123	0.000944
C	2.029392	-1.227008	0.001007
C	3.429607	1.218187	-0.000072
H	1.477346	2.171972	0.001303
C	3.429162	-1.218593	-0.000022
H	1.476541	-2.171649	0.001413
C	4.131058	-0.000333	-0.000634
H	3.975871	2.167331	-0.000524
H	3.975073	-2.167940	-0.000449
H	5.226432	-0.000533	-0.001523
C	-2.775755	0.000121	-0.001317
F	-3.297845	-1.074454	-0.678625
F	-3.297658	1.125801	-0.589201
F	-3.301159	-0.051784	1.268539

O_2

O	0.000000	0.000000	0.614229
O	0.000000	0.000000	-0.614229

OH

O	0.000000	0.000000	0.109033
H	0.000000	0.000000	-0.872262

$Me_3Si(CF_3)OH^-$

C	-0.779942	1.937125	-0.124762
H	0.010943	2.355708	0.522294
H	-0.543125	2.231115	-1.165041
C	-0.875341	-0.873207	1.738030
H	-1.115482	-0.140698	2.532002
H	0.090715	-1.344283	1.991198
C	1.333299	-0.007323	0.002794
F	1.965030	-1.276662	0.050910
F	1.974093	0.677294	1.068396
F	1.939124	0.581666	-1.138019
Si	-0.911859	0.008852	0.008873
C	-0.846774	-1.126881	-1.567823
H	0.106327	-1.668472	-1.697291
H	-1.663027	-1.873129	-1.540702
H	-1.659114	-1.652774	1.775297
H	-1.010182	-0.506540	-2.469899
H	-1.744425	2.400726	0.145645
O	-2.797519	0.170993	-0.033862
H	-3.218127	-0.712503	-0.067844

Me_3SiOH

C	0.941891	1.565409	-0.533662
H	1.035635	1.602671	-1.635091
H	0.419001	2.482162	-0.206068
C	0.944798	-1.563079	-0.535164
H	1.967074	-1.579356	-0.114487
H	1.036342	-1.600206	-1.636788
Si	-0.004233	0.000050	0.008203
C	-1.795547	-0.001332	-0.627312
H	-1.817289	-0.000467	-1.732471
H	-2.340126	-0.897072	-0.278082
H	0.424789	-2.481081	-0.206504
H	-2.342061	0.892666	-0.276652
H	1.963271	1.584294	-0.110913
O	-0.188322	-0.000876	1.754485
H	0.672351	-0.003286	2.223170

I

Cu	-0.907018	-0.000017	0.079408
N	0.657932	1.355642	0.075012
N	0.657923	-1.355633	0.074949
C	0.640855	2.696647	0.081264
C	1.814909	3.478522	0.028324
C	3.050226	2.845700	-0.032972
C	4.337240	0.686797	-0.096593
C	4.337237	-0.686804	-0.096577
C	3.050215	-2.845702	-0.032930
C	1.814894	-3.478517	0.028340
C	0.640840	-2.696639	0.081216
C	1.868582	0.722950	0.017706
C	3.106327	1.427832	-0.038015
C	3.106321	-1.427834	-0.037996
C	1.868579	-0.722946	0.017696
H	-0.345697	3.168202	0.130092
H	1.735446	4.568941	0.035649
H	3.979827	3.422544	-0.076396
H	5.277953	1.245127	-0.142628
H	5.277949	-1.245138	-0.142596
H	3.979815	-3.422550	-0.076323
H	1.735427	-4.568936	0.035680
H	-0.345717	-3.168189	0.129983
I	-3.434337	0.000008	-0.052128

II

Cu	-0.775753	0.091876	0.709213
N	0.794855	1.378206	0.087488
N	0.782401	-1.294203	0.460457
C	0.784616	2.706471	-0.105087
C	1.947807	3.454302	-0.382275
C	3.173575	2.801483	-0.464334
C	4.439886	0.632473	-0.349558
C	4.431681	-0.729640	-0.171620
C	3.142508	-2.839677	0.279830
C	1.910932	-3.434887	0.533369
C	0.758120	-2.627544	0.618866
C	1.994964	0.727808	0.002753
C	3.224510	1.397742	-0.273158
C	3.208402	-1.434909	0.102019
C	1.987400	-0.702307	0.195507
H	-0.192146	3.196788	-0.035836
H	1.870345	4.535200	-0.529353
H	4.095687	3.352567	-0.676826
H	5.375362	1.162293	-0.558262
H	5.360325	-1.306439	-0.236459
H	4.057816	-3.436815	0.212523
H	1.821267	-4.516044	0.671075
H	-0.221263	-3.071698	0.825118
C	-2.148801	0.333650	2.032098
F	-1.697677	0.682494	3.320087
F	-2.965937	-0.788340	2.284620
F	-3.096057	1.341191	1.756092
I	-2.151092	-0.301815	-1.932688

III

Cu	-1.399125	-0.020370	0.090124

N	0.208197	1.339558	0.098301
N	0.227919	-1.350215	0.096234
C	0.173232	2.679731	0.107848
C	1.338164	3.477861	0.043459
C	2.582075	2.861116	-0.034872
C	3.893018	0.710823	-0.117900
C	3.903337	-0.664676	-0.117874
C	2.625723	-2.834852	-0.035398
C	1.391469	-3.470704	0.042261
C	0.214110	-2.690956	0.105656
C	1.425913	0.726451	0.025797
C	2.656060	1.443208	-0.043937
C	2.677652	-1.415976	-0.044258
C	1.436585	-0.718260	0.025305
H	-0.818784	3.139769	0.167652
H	1.244833	4.567855	0.054620
H	3.503396	3.451557	-0.088368
H	4.830181	1.275456	-0.175074
H	4.848869	-1.215127	-0.175135
H	3.556107	-3.410977	-0.088518
H	1.315122	-4.562015	0.053419
H	-0.770427	-3.166698	0.164529
C	-3.302367	-0.006483	-0.068612
F	-3.880557	1.109375	-0.741763
F	-4.027557	-0.014816	1.153934
F	-3.900475	-1.094356	-0.769207

IV

Cu	-1.269306	-0.267388	-0.029201
O	-1.043997	-1.264907	2.694105
O	-1.965036	-1.118364	1.820937
C	-3.064447	0.234494	-0.609780
F	-3.781137	1.095173	0.243102
F	-3.072827	0.932470	-1.837787
F	-3.981062	-0.810951	-0.838649
C	1.147655	3.553797	0.313755
C	2.437666	3.055934	0.166438
C	0.056086	2.655188	0.297064
H	0.963036	4.624652	0.440900
C	2.633198	1.658930	0.003590
H	3.305037	3.725334	0.173259
N	0.208763	1.334342	0.147951
H	-0.972613	3.016361	0.406871
C	3.927773	1.051433	-0.155772
C	1.468951	0.835265	0.001923
C	4.056262	-0.309493	-0.305713
H	4.811607	1.698806	-0.153825
C	1.604381	-0.594750	-0.162395
C	2.901146	-1.167756	-0.312662
H	5.043921	-0.767869	-0.425650
N	0.461868	-1.345601	-0.172827
C	2.978250	-2.576615	-0.466122
C	0.566407	-2.674158	-0.324192
C	1.808915	-3.328675	-0.469532
H	3.957275	-3.054553	-0.581967
H	-0.370762	-3.239467	-0.331106
H	1.831982	-4.415822	-0.587458

V

Cu	1.595978	0.676643	-0.688935
Cu	-1.596853	-0.677964	0.691224
O	-0.292030	0.154608	-0.647041
O	0.291352	-0.156460	0.649487
C	-1.816649	-1.642161	2.388489
C	1.814569	1.641035	-2.386379
F	1.344205	0.973325	-3.529532
F	3.142008	1.954210	-2.725130
F	1.167209	2.889071	-2.454772
F	-3.144368	-1.954873	2.726540
F	-1.346628	-0.974657	3.531898
F	-1.169756	-2.890444	2.457177
H	-4.376575	-3.781834	-2.399611
C	-4.371779	-2.813740	-1.890658
C	-3.244063	-2.435518	-1.131245
C	-5.454893	-1.945871	-1.974233
N	-3.168391	-1.261781	-0.487550
H	-2.377313	-3.097957	-1.040390
C	-5.404996	-0.699008	-1.299032
H	-6.346733	-2.210330	-2.553088
C	-4.222403	-0.395851	-0.559368
C	-6.482604	0.254220	-1.329691
C	-4.121944	0.864315	0.147104
C	-6.389779	1.450256	-0.658227
H	-7.382193	0.003679	-1.902507
N	-2.977268	1.110695	0.841564
C	-5.211362	1.785914	0.095278
H	-7.214058	2.171514	-0.685351
C	-2.868285	2.269078	1.500012
C	-5.062377	3.006792	0.804217
C	-3.887751	3.249465	1.507467
H	-1.932233	2.431375	2.047331
H	-5.874226	3.742688	0.788773
H	-3.739868	4.180388	2.063203
C	4.371458	2.813381	1.891507
C	5.455641	1.946656	1.973062
C	3.243246	2.434533	1.133144
H	4.375809	3.781083	2.401209
C	5.406288	0.700261	1.296958
H	6.347925	2.211664	2.550981
N	3.168043	1.261181	0.488688
H	2.375698	3.096130	1.043787
C	6.485145	-0.251617	1.325220
C	4.223060	0.396316	0.558635
C	6.392866	-1.447190	0.652858
H	7.385233	-0.000424	1.896968
C	4.123051	-0.863512	-0.148498
C	5.213746	-1.783722	-0.099157
H	7.218122	-2.167397	0.678126
N	2.977595	-1.110832	-0.841347
C	5.065183	-3.004267	-0.808761
C	2.869045	-2.268856	-1.500500
C	3.889734	-3.247944	-1.510283
H	5.877987	-3.739144	-0.795125
H	1.932317	-2.431949	-2.046425
H	3.742135	-4.178666	-2.066430

TS_OO

Cu	-1.399299	0.427625	0.686845
Cu	1.443972	-0.583607	-0.712337
O	0.400729	-0.089456	0.797334
O	-0.362074	-0.077044	-0.828165
C	1.852171	-1.223672	-2.518711
C	-1.793307	0.979403	2.525953
F	-1.284304	0.123436	3.493905
F	-3.139848	1.098297	2.851572
F	-1.254640	2.224336	2.845250
F	3.197580	-1.222070	-2.872419
F	1.231647	-0.515922	-3.539219
F	1.449689	-2.544314	-2.719898
H	4.274536	-4.082184	1.778010
C	4.274313	-3.047914	1.424473
C	3.155062	-2.554976	0.723502
C	5.353537	-2.203549	1.651612
N	3.087082	-1.297374	0.264748
H	2.286395	-3.190906	0.526791
C	5.309980	-0.868232	1.176675
H	6.239068	-2.552425	2.192957
C	4.137573	-0.450986	0.476280
C	6.386670	0.063759	1.374275
C	4.050336	0.905086	-0.027052
C	6.307567	1.348252	0.896207
H	7.273984	-0.278212	1.916896
N	2.918348	1.266631	-0.687030
C	5.143787	1.799985	0.184149
H	7.132016	2.052592	1.048606
C	2.829163	2.511478	-1.161300
C	5.014466	3.114817	-0.333479
C	3.855021	3.472370	-1.009274
H	1.901199	2.764368	-1.688011
H	5.831281	3.830726	-0.193580
H	3.724207	4.477246	-1.420602
C	-4.084499	3.252811	-1.188256
C	-5.245072	2.521332	-1.406246
C	-2.975982	2.617000	-0.593054
H	-4.013799	4.307326	-1.467436
C	-5.291696	1.154626	-1.031537
H	-6.125882	2.983260	-1.864185
N	-2.993287	1.327100	-0.229514
H	-2.046613	3.162908	-0.402550
C	-6.454221	0.331821	-1.227051
C	-4.122307	0.589502	-0.438530
C	-6.457949	-0.988526	-0.850690
H	-7.338512	0.785931	-1.685811
C	-4.124501	-0.802580	-0.037103
C	-5.299209	-1.587608	-0.247409
H	-7.346893	-1.609814	-1.002214
N	-2.995533	-1.301150	0.533015
C	-5.254081	-2.944733	0.164034
C	-2.986973	-2.582195	0.909950
C	-4.095200	-3.444366	0.744089
H	-6.134476	-3.579695	0.019394
H	-2.059089	-2.947962	1.365380
H	-4.027443	-4.485428	1.071968

VI

Cu	1.139594	0.297742	-0.617965
Cu	-1.165631	-0.471131	0.699156
O	-0.483415	-0.431308	-1.036931
O	0.510515	0.115572	1.128490
C	-1.625737	-0.628265	2.602546
C	1.515043	0.607742	-2.519950
F	1.144757	-0.428105	-3.354728
F	2.843635	0.857378	-2.851984
F	0.828341	1.721450	-3.000533
F	-2.981165	-0.730766	2.901086
F	-1.181046	0.413914	3.391752
F	-1.064087	-1.771894	3.169557
H	-3.865810	-4.462638	-0.740920
C	-3.920075	-3.375903	-0.632140
C	-2.821712	-2.679608	-0.089090
C	-5.045839	-2.659870	-1.019572
N	-2.825830	-1.348455	0.072062
H	-1.914407	-3.205674	0.222779
C	-5.072148	-1.251032	-0.858214
H	-5.916558	-3.166781	-1.449604
C	-3.921150	-0.618480	-0.293463
C	-6.205388	-0.452144	-1.241003
C	-3.915569	0.819651	-0.102820
C	-6.201067	0.910765	-1.069612
H	-7.073365	-0.960822	-1.674249
N	-2.813054	1.386677	0.452503
C	-5.062817	1.577002	-0.497418
H	-7.067628	1.513770	-1.363087
C	-2.801209	2.709373	0.631596
C	-5.015019	2.981237	-0.292962
C	-3.881026	3.551552	0.272323
H	-1.894211	3.130877	1.083046

H	-5.874424	3.596269	-0.582786
H	-3.812037	4.630195	0.444145
C	3.662805	3.383063	0.775332
C	4.867887	2.759895	1.075037
C	2.610235	2.613329	0.240689
H	3.511935	4.452515	0.946745
C	5.018828	1.370204	0.834951
H	5.706321	3.325728	1.495650
N	2.731965	1.299047	0.005231
H	1.644168	3.065401	-0.003412
C	6.238497	0.664521	1.124105
C	3.906937	0.660690	0.283651
C	6.352710	-0.682089	0.877512
H	7.075075	1.230334	1.548156
C	4.025913	-0.759838	0.014815
C	5.255278	-1.423915	0.318592
H	7.283844	-1.214682	1.100913
N	2.954734	-1.399174	-0.522691
C	5.326359	-2.814824	0.041836
C	3.055243	-2.706700	-0.771339
C	4.223285	-3.460385	-0.503551
H	6.250586	-3.360902	0.262045
H	2.170055	-3.188477	-1.205302
H	4.244492	-4.531235	-0.728340

VII

Cu	-1.433304	-0.544097	-0.606893
Cu	0.757038	-1.210487	0.949596
O	-1.061432	-1.370838	1.023360
C	0.919763	-2.075076	2.702630
C	-1.585481	0.176247	-2.429379
F	-0.827362	1.304624	-2.664137
F	-2.863760	0.523880	-2.849984
F	-1.153887	-0.754723	-3.371627
F	2.176550	-2.578198	3.019255
F	0.065455	-3.140059	2.895684
F	0.631678	-1.187243	3.735617
H	4.747326	1.767070	1.745245
C	4.446387	0.830308	1.267985
C	3.116942	0.382343	1.402632
C	5.339464	0.071776	0.521881
N	2.684430	-0.757160	0.843226
H	2.380313	0.955613	1.972861
C	4.905358	-1.139953	-0.074006
H	6.377990	0.393420	0.387672
C	3.545617	-1.534620	0.121362
C	5.779898	-1.972071	-0.856231
C	3.073145	-2.783079	-0.445163
C	5.330501	-3.144876	-1.412808
H	6.815748	-1.644517	-0.996553
N	1.786375	-3.145911	-0.204612
C	3.974078	-3.580144	-1.218714
H	6.000836	-3.773381	-2.009637
C	1.343185	-4.293185	-0.722849
C	3.467533	-4.792299	-1.757731
C	2.147711	-5.150796	-1.511379
H	0.299246	-4.552806	-0.506338
H	4.125306	-5.430161	-2.358755
H	1.726277	-6.078217	-1.911325
C	-4.848459	-3.001946	-0.871185
C	-5.889762	-2.239737	-0.356261
C	-3.561387	-2.433932	-0.950041
H	-5.003799	-4.028591	-1.214181
C	-5.641541	-0.912163	0.076182
H	-6.903244	-2.648133	-0.278467
N	-3.305914	-1.180456	-0.547913
H	-2.713876	-3.000576	-1.346995
C	-6.675227	-0.071107	0.617528
C	-4.309165	-0.406074	-0.038756
C	-6.402735	1.211962	1.024968
H	-7.687469	-0.482160	0.696335
C	-4.017856	0.950126	0.384493
C	-5.074646	1.752206	0.918744
H	-7.194409	1.847840	1.436666
N	-2.744271	1.403106	0.247472
C	-4.746764	3.073880	1.320500
C	-2.470896	2.652144	0.632495
C	-3.441082	3.526754	1.178066
H	-5.528689	3.719395	1.736052
H	-1.433294	2.984452	0.502234
H	-3.154520	4.539999	1.476330
O	0.375370	-0.241715	-0.612830
H	0.860851	1.598870	-0.479268
C	1.244095	2.631437	-0.451357
C	1.676647	3.781024	-0.416026
C	2.176139	5.121533	-0.370974
C	2.743432	5.718264	-1.526049
C	2.110250	5.873328	0.830227
C	3.228995	7.031982	-1.475301
H	2.797432	5.143389	-2.456484
C	2.598537	7.186335	0.869168
H	1.673160	5.418579	1.725554
C	3.158746	7.770486	-0.280711
H	3.664514	7.481568	-2.374528
H	2.540858	7.756268	1.803097
H	3.538701	8.797367	-0.246253

DPTS1

Cu	-1.455567	-0.549124	-0.621104
Cu	0.770974	-1.092355	0.954315
O	-1.042740	-1.267114	1.050263
C	0.904724	-1.915052	2.722248
C	-1.698555	-0.031583	-2.504101
F	-0.964537	1.064639	-2.895900
F	-2.995429	0.251212	-2.899965
F	-1.291586	-1.066392	-3.338234
F	2.155652	-2.413152	3.043967
F	0.046166	-2.968039	2.916870
F	0.612839	-1.000564	3.720409
H	4.745844	1.870115	1.922907
C	4.449968	0.950367	1.410730
C	3.116817	0.504096	1.510198
C	5.351864	0.215545	0.651545
N	2.692460	-0.615881	0.907276
H	2.371947	1.060606	2.085630
C	4.925026	-0.975645	0.010427
H	6.392328	0.540155	0.541896
C	3.563206	-1.374070	0.176752
C	5.806087	-1.784616	-0.788530
C	3.096203	-2.605432	-0.427765
C	5.360453	-2.938625	-1.386460
H	6.843600	-1.454499	-0.908694
N	1.808017	-2.975288	-0.204034
C	4.002362	-3.379489	-1.217202
H	6.035483	-3.548348	-1.997253
C	1.366915	-4.106391	-0.758488
C	3.498049	-4.574196	-1.795830
C	2.176326	-4.938636	-1.568774
H	0.322183	-4.372581	-0.554984
H	4.158635	-5.194332	-2.412020
H	1.756845	-5.852862	-1.999828
C	-4.876790	-3.018627	-0.572260
C	-5.885249	-2.207586	-0.065762
C	-3.588220	-2.477070	-0.751827
H	-5.058730	-4.064690	-0.833531
C	-5.604583	-0.855644	0.258871
H	-6.897578	-2.596907	0.087456
N	-3.306176	-1.200902	-0.453960
H	-2.765644	-3.081497	-1.144914
C	-6.599722	0.038198	0.787979
C	-4.275542	-0.377530	0.043184
C	-6.292216	1.343401	1.087355
H	-7.611530	-0.350478	0.946146
C	-3.948037	1.000299	0.351591
C	-4.965659	1.855518	0.876400
H	-7.054490	2.019193	1.490692
N	-2.677451	1.419815	0.118368
C	-4.599304	3.196883	1.164256
C	-2.365755	2.688545	0.395673
C	-3.296338	3.615289	0.923718
H	-5.349495	3.884499	1.570570
H	-1.330117	2.987548	0.190445
H	-2.981382	4.642231	1.133147
O	0.368737	-0.195446	-0.686856
H	0.704422	0.999691	-0.667235
C	1.176952	2.217727	-0.671968
C	1.625214	3.374277	-0.600251
C	2.129964	4.711049	-0.489827
C	2.754229	5.351680	-1.592720
C	2.016623	5.426318	0.732296
C	3.245427	6.659278	-1.472988
H	2.848458	4.811914	-2.541191
C	2.510317	6.733508	0.842504
H	1.537206	4.944182	1.591323
C	3.126480	7.356737	-0.257487
H	3.724133	7.136984	-2.335344
H	2.412900	7.268974	1.793779
H	3.510873	8.378781	-0.168190

VIII

Cu	1.229604	0.763284	-0.976145
Cu	-1.081734	-1.303830	-0.461872
O	-0.203400	0.232735	0.097726
O	0.420459	0.080603	-2.504642
H	0.984290	0.321459	-3.270625
C	0.473678	-2.268454	-0.172501
C	1.491923	-2.935573	0.054738
C	2.674949	-3.695664	0.321441
C	3.531483	-4.101514	-0.736627
C	3.018406	-4.063760	1.649921
C	4.687971	-4.847318	-0.470146
H	3.277689	-3.825192	-1.765806
C	4.176549	-4.810844	1.905370
H	2.366061	-3.758519	2.475435
C	5.017279	-5.206131	0.849381
H	5.336197	-5.151296	-1.299953
H	4.424002	-5.086076	2.936994
H	5.921697	-5.789907	1.053110
C	-1.927475	-2.967906	-1.169739
F	-1.429026	-3.288958	-2.423247
F	-3.300135	-2.893121	-1.351326
F	-1.754049	-4.101690	-0.400360
C	-2.680265	0.409049	-2.215000
C	-3.677836	0.013855	-0.132840
C	-3.749263	1.237767	-2.616777
H	-1.797939	0.242466	-2.842790
C	-4.791885	0.845162	-0.460277
C	-4.807031	1.454117	-1.741605
H	-3.725744	1.698799	-3.608437
H	-5.651078	2.093233	-2.023536
C	-3.615910	-0.623482	1.166014
C	-4.672702	-0.407557	2.102977
C	-4.559792	-1.049978	3.364059
C	-2.459938	-1.994795	2.630958
C	-3.451128	-1.845233	3.630239
H	-5.348279	-0.911255	4.112236
H	-1.573175	-2.615057	2.810586

H	-3.333475	-2.352713	4.592569
N	-2.658408	-0.188401	-1.016737
N	-2.537185	-1.404346	1.436176
C	2.853346	1.258950	-2.004365
F	2.664083	1.504268	-3.360280
F	3.783409	0.231168	-1.955254
F	3.523300	2.375576	-1.551171
C	1.980318	2.545373	1.194740
C	2.869953	0.378738	1.354021
C	2.571550	2.914858	2.442631
C	3.485620	0.670666	2.587373
H	2.955594	-0.609105	0.893339
C	3.335160	1.939576	3.133037
H	4.068403	-0.105890	3.090466
H	3.798957	2.200669	4.090472
C	1.199625	3.517910	0.454912
C	1.028904	4.829718	0.997169
C	0.253465	5.747136	0.239857
C	-0.056720	4.021404	-1.421113
C	-0.293930	5.342786	-0.971711
H	0.097629	6.762584	0.620965
H	-0.471546	3.675038	-2.375961
H	-0.897791	6.024503	-1.578566
N	0.666955	3.135572	-0.733970
N	2.145068	1.288071	0.689115
C	-5.783360	0.431671	1.741757
C	-5.839654	1.034485	0.507766
H	-6.584826	0.582260	2.473517
H	-6.686369	1.674264	0.235839
C	2.378464	4.246859	2.950516
C	1.634689	5.169615	2.256037
H	2.841866	4.506116	3.908579
H	1.491209	6.182364	2.648756

IX

Cu	-1.338923	-1.225265	-1.108892
Cu	-1.051629	1.832706	-0.387178
O	-1.689482	-0.052013	-2.501950
H	-2.144587	-0.550516	-3.214038
C	-2.673030	1.293383	0.330813
C	-3.757722	0.958073	0.824402
C	-5.003997	0.546367	1.395469
C	-6.106684	0.209128	0.566047
C	-5.166126	0.466737	2.804451
C	-7.325276	-0.192072	1.130709
H	-5.994582	0.266234	-0.522162
C	-6.389258	0.064801	3.358854
H	-4.323476	0.724684	3.455319
C	-7.474145	-0.266378	2.527347
H	-8.165050	-0.448036	0.474693
H	-6.495591	0.010684	4.448319
H	-8.428629	-0.579951	2.964183
C	-1.858689	3.635898	-0.647667
F	-2.799931	3.633903	-1.661735
F	-0.953195	4.618547	-1.012620
F	-2.496077	4.159754	0.457062
C	0.605090	2.066945	-2.793978
C	1.634732	2.910251	-0.867120
C	1.730400	2.384204	-3.583984
H	-0.274059	1.557738	-3.203735
C	2.813136	3.256879	-1.594476
C	2.833406	2.982171	-2.986182
H	1.716525	2.151672	-4.652731
H	3.722653	3.240005	-3.572049
C	1.570442	3.162674	0.557172
C	2.690609	3.757786	1.213566
C	2.578859	3.974407	2.612394
C	0.360212	3.019573	2.525900
C	1.412272	3.603317	3.271224
H	3.414651	4.429777	3.155359
H	-0.572591	2.716800	3.017241
H	1.295773	3.754455	4.348748
N	0.562641	2.333130	-1.482214
N	0.433690	2.805676	1.210173
C	-2.464471	-2.611617	-1.969020
F	-2.496786	-2.576863	-3.357978
F	-3.783176	-2.462066	-1.572766
F	-2.140056	-3.916344	-1.670091
C	-0.010933	-3.200431	0.557857
C	-1.971600	-2.303166	1.486637
C	0.234591	-3.971198	1.736366
C	-1.801761	-3.041133	2.675082
H	-2.818356	-1.625023	1.350847
C	-0.695913	-3.872592	2.801837
H	-2.541081	-2.942961	3.474880
H	-0.530094	-4.455597	3.714327
C	0.912790	-3.282574	-0.556342
C	2.053583	-4.137291	-0.454721
C	2.929667	-4.183532	-1.570940
C	1.492476	-2.596756	-2.689031
C	2.649776	-3.411935	-2.692464
H	3.816273	-4.826270	-1.532013
H	1.245661	-1.974191	-3.558005
H	3.305939	-3.423013	-3.568252
N	0.648854	-2.532835	-1.657241
N	-1.102971	-2.384654	0.470121
C	3.861606	4.101184	0.452360
C	3.919819	3.858931	-0.899443
H	4.708963	4.558984	0.974775
H	4.814175	4.118313	-1.476553
C	1.398160	-4.814519	1.800597
C	2.274732	-4.895842	0.746007
H	1.566456	-5.392510	2.715728
H	3.158369	-5.541379	0.801528
O	-0.399263	0.097314	-0.170071
H	1.389999	-0.120351	0.256963
C	2.442503	-0.285702	0.543206
C	3.617369	-0.473932	0.849769
C	4.987012	-0.700410	1.198161
C	5.340682	-1.099723	2.512403
C	6.010640	-0.534191	0.230247
C	6.683517	-1.325738	2.843880
H	4.555086	-1.229255	3.264350
C	7.350023	-0.763644	0.572716
H	5.743561	-0.226253	-0.786293
C	7.691893	-1.159846	1.877950
H	6.943861	-1.633332	3.862727
H	8.131109	-0.632907	-0.184435
H	8.740134	-1.338526	2.141414

DPTS2

Cu	1.158763	1.284343	-1.094604
Cu	0.949319	-1.836859	-0.456950
O	1.346059	0.170244	-2.560892
H	1.754277	0.675273	-3.296351
C	2.623008	-1.318443	0.164655
C	3.733078	-1.004509	0.612497
C	5.002308	-0.613630	1.147205
C	6.076945	-0.262109	0.288268
C	5.212531	-0.571685	2.551206
C	7.316980	0.117247	0.820517
H	5.926494	-0.290503	-0.796363
C	6.456605	-0.191255	3.072919
H	4.390997	-0.841849	3.223615
C	7.513911	0.154891	2.212555
H	8.135510	0.384943	0.142840
H	6.601422	-0.165989	4.158937
H	8.484900	0.451812	2.623905
C	1.791519	-3.594891	-0.871849
F	2.638394	-3.492273	-1.954785
F	0.880134	-4.570940	-1.221492
F	2.521386	-4.155161	0.146342
C	-0.928723	-2.011509	-2.685986
C	-1.710586	-3.013236	-0.716217
C	-2.104872	-2.364947	-3.380147
H	-0.125742	-1.428959	-3.150699
C	-2.930326	-3.402785	-1.346695
C	-3.103169	-3.065511	-2.713651
H	-2.210847	-2.080190	-4.430844
H	-4.027299	-3.354750	-3.226299
C	-1.493556	-3.321037	0.680743
C	-2.507499	-4.011446	1.411245
C	-2.247081	-4.278057	2.781235
C	-0.105177	-3.186010	2.529079
C	-1.044552	-3.863511	3.342544
H	-2.998244	-4.805217	3.379963
H	0.853066	-2.847475	2.941497
H	-0.814975	-4.051442	4.395781
N	-0.740697	-2.340982	-1.401366
N	-0.320660	-2.921533	1.238316
C	2.278628	2.647343	-1.980020
F	2.146344	2.707885	-3.356941
F	3.611116	2.374064	-1.745962
F	2.083300	3.938149	-1.556036
C	0.061305	3.284182	0.700114
C	1.997110	2.214213	1.491350
C	-0.044541	4.052453	1.900247
C	1.958862	2.938354	2.699408
H	2.777785	1.475348	1.291743
C	0.937574	3.857810	2.904403
H	2.733604	2.763124	3.450884
H	0.878088	4.436480	3.832585
C	-0.918689	3.456295	-0.352612
C	-1.978823	4.395771	-0.169254
C	-2.915645	4.527608	-1.228108
C	-1.675780	2.855058	-2.454163
C	-2.763626	3.757350	-2.374930
H	-3.746186	5.235315	-1.127753
H	-1.531880	2.231620	-3.345200
H	-3.468411	3.834159	-3.208578
N	-0.780559	2.705217	-1.475942
N	1.077803	2.388637	0.532218
C	-3.723911	-4.396500	0.747438
C	-3.926348	-4.103301	-0.580120
H	-4.489202	-4.927281	1.324546
H	-4.855252	-4.394160	-1.082754
C	-1.128245	4.986738	2.045870
C	-2.060046	5.153346	1.049990
H	-1.190838	5.563997	2.974616
H	-2.882705	5.867298	1.168216
O	0.292895	-0.095564	-0.112117
H	-0.923851	0.022986	0.115791
C	-2.161513	0.204610	0.449521
C	-3.348341	0.424177	0.739450
C	-4.721533	0.678842	1.061496
C	-5.097441	1.104472	2.363045
C	-5.737730	0.517071	0.082576
C	-6.441687	1.358104	2.669430
H	-4.323837	1.232806	3.127995
C	-7.079126	0.774144	0.397792
H	-5.460951	0.189846	-0.925668
C	-7.438439	1.195529	1.690651
H	-6.712690	1.685047	3.679774
H	-7.848876	0.645145	-0.371629
H	-8.487778	1.395842	1.933691

X

Cu	0.088090	-0.495975	-0.226170
C	1.921097	-0.217123	-0.239223
C	3.149911	-0.079842	-0.286188
C	4.571816	0.077762	-0.346847
C	5.358703	-0.004789	0.831887
C	5.222452	0.314583	-1.586027
C	6.751141	0.141210	0.767193
H	4.866241	-0.186869	1.793136
C	6.615309	0.460905	-1.639654
H	4.624517	0.380340	-2.501342
C	7.385440	0.374320	-0.466074
H	7.344127	0.072374	1.686112
H	7.102827	0.642257	-2.604163
H	8.474112	0.487804	-0.512367
C	0.190385	-0.530819	1.745672
F	0.834554	0.541039	2.310271
F	0.840400	-1.660875	2.193797
F	-1.046521	-0.560514	2.354192
C	-1.922867	-2.589103	-0.375392
C	-2.833535	-0.431677	-0.309070
C	-3.197391	-3.170225	-0.537196
H	-1.018208	-3.202971	-0.335618
C	-4.157844	-0.940590	-0.472066
C	-4.315057	-2.345697	-0.586580
H	-3.283900	-4.257012	-0.621743
H	-5.319030	-2.765376	-0.712978
C	-2.621320	0.995412	-0.187022
C	-3.746197	1.874197	-0.229694
C	-3.483785	3.264106	-0.103205
C	-1.130326	2.745014	0.083275
C	-2.173478	3.701389	0.052649
H	-4.317149	3.975110	-0.129952
H	-0.086712	3.058998	0.205546
H	-1.937619	4.765331	0.151698
N	-1.755144	-1.264928	-0.265491
N	-1.344883	1.432550	-0.033212
O	0.077807	-0.569976	-2.103255
H	0.993893	-0.355201	-2.385077
C	-5.068018	1.331889	-0.395981
C	-5.265445	-0.023213	-0.513696
H	-5.916540	2.024310	-0.426873
H	-6.273080	-0.433462	-0.640772

RETS

Cu	0.041518	-0.773140	-0.555076
C	1.778532	-0.378133	-0.199577
C	2.978410	-0.043645	-0.212855
C	4.345373	0.342588	-0.259362
C	5.377687	-0.635343	-0.220287
C	4.706940	1.716326	-0.338043
C	6.722130	-0.245936	-0.256488
H	5.109301	-1.695410	-0.161808
C	6.055425	2.091460	-0.373744
H	3.919139	2.476392	-0.371080
C	7.068293	1.115644	-0.333144
H	7.506138	-1.010808	-0.225238
H	6.318262	3.153476	-0.434537
H	8.121705	1.414664	-0.362441
C	0.830982	-0.645977	1.490926
F	1.158325	0.532269	2.097804
F	1.631783	-1.629328	2.002874
F	-0.429843	-0.947187	2.024061
C	-2.209173	-2.752229	-0.455405
C	-2.875402	-0.521443	-0.319897
C	-3.546701	-3.201642	-0.415479
H	-1.378359	-3.461078	-0.529670
C	-4.255337	-0.884459	-0.284387
C	-4.571779	-2.266794	-0.330463
H	-3.755369	-4.274687	-0.452389
H	-5.620921	-2.580842	-0.300299
C	-2.501586	0.876451	-0.265418
C	-3.521986	1.872813	-0.196841
C	-3.102833	3.228561	-0.163287
C	-0.811905	2.463609	-0.248310
C	-1.745033	3.525583	-0.192794
H	-3.855093	4.023928	-0.116203
H	0.265999	2.665188	-0.265785
H	-1.389227	4.560039	-0.171051
N	-1.882166	-1.454051	-0.405434
N	-1.174402	1.177945	-0.282389
O	0.123381	-1.091793	-2.439772
H	1.063725	-0.947896	-2.680135
C	-4.903755	1.474396	-0.167348
C	-5.256236	0.146285	-0.205477
H	-5.670736	2.255029	-0.113226
H	-6.309463	-0.153940	-0.180472

XI

Cu	-1.471634	-0.441847	0.074136
N	0.184425	1.375357	0.030479
N	0.194652	-1.375511	0.038260
C	0.168130	2.711588	0.031141
C	1.339263	3.504575	-0.000962
C	2.575499	2.869155	-0.035517
C	3.870415	0.720738	-0.070166
C	3.874622	-0.652804	-0.068918
C	2.625475	-2.819034	-0.029883
C	1.402433	-3.480127	0.008510
C	0.214342	-2.727139	0.042040
C	1.388998	0.742836	-0.002073
C	2.632447	1.450978	-0.036525
C	2.645685	-1.400989	-0.033090
C	1.396811	-0.706881	0.000973
H	-0.821993	3.184432	0.058638
H	1.260567	4.596238	0.001490
H	3.507544	3.444947	-0.061447
H	4.810165	1.283728	-0.097452
H	4.817421	-1.210285	-0.095426
H	3.570112	-3.372952	-0.056967
H	1.343303	-4.572430	0.012799
H	-0.760700	-3.221071	0.072790
O	-3.233798	0.080105	0.127123
H	-3.231436	1.061525	0.125086

II’

Cu	-1.357769	-0.023423	0.096146
N	0.207692	1.341548	0.068340
N	0.227249	-1.350187	0.068575
C	0.176369	2.683670	0.074951
C	1.342543	3.479433	0.024562
C	2.587854	2.861730	-0.034276
C	3.896697	0.710787	-0.095349
C	3.906690	-0.664638	-0.095757
C	2.630041	-2.834752	-0.035719
C	1.394060	-3.470895	0.023229
C	0.216112	-2.692993	0.074555
C	1.427751	0.727082	0.012617
C	2.659133	1.443940	-0.040012
C	2.680059	-1.416039	-0.040720
C	1.438347	-0.717366	0.012563
H	-0.815294	3.146086	0.122309
H	1.250103	4.569691	0.032318
H	3.510524	3.451003	-0.074894
H	4.834888	1.275110	-0.138291
H	4.852918	-1.215296	-0.139208
H	3.561343	-3.410256	-0.076945
H	1.317821	-4.562405	0.030493
H	-0.768314	-3.170306	0.122319
F	-3.256217	-0.016613	0.106744

Met_TS

Cu	0.479185	-0.374642	-0.197756
N	-0.755084	1.182242	-0.115399
N	-1.397748	-1.471526	-0.133891
C	-0.433184	2.486911	-0.073359
C	-1.397412	3.511703	0.025280
C	-2.745380	3.175354	0.074351
C	-4.493283	1.375369	0.070675
C	-4.818351	0.040755	0.022492
C	-4.072252	-2.356764	-0.098905
C	-3.020417	-3.263839	-0.162203
C	-1.693428	-2.776136	-0.174308
C	-2.080934	0.835907	-0.055937
C	-3.121526	1.807861	0.032055
C	-3.793389	-0.965193	-0.056700
C	-2.421806	-0.571579	-0.085261
H	0.633368	2.725185	-0.126273
H	-1.069280	4.554793	0.054929
H	-3.520469	3.946499	0.143506
H	-5.275498	2.139611	0.136378
H	-5.865228	-0.281280	0.047729
H	-5.112917	-2.698705	-0.079101
H	-3.201397	-4.342439	-0.194809
H	-0.842792	-3.466368	-0.212319
F	1.923822	-1.501681	-1.059974
Si	3.088303	0.100777	-0.670271
C	4.622902	-1.037163	-0.852165
C	2.412688	0.830195	-2.332006
C	2.191214	-0.297500	1.264782
C	3.802547	1.761552	0.084836
H	5.560068	-0.453279	-0.804972
H	4.652303	-1.795947	-0.050522
H	4.589074	-1.573286	-1.817195
H	2.159510	0.049904	-3.068339
H	3.193481	1.487739	-2.761432
H	1.516825	1.456000	-2.168130
F	1.603376	0.776568	1.922994
F	3.372265	-0.510629	2.033653
F	1.435774	-1.424214	1.662267
H	4.514690	2.183585	-0.651555
H	3.013991	2.519553	0.247863
H	4.346422	1.622170	1.035756

OA’

Cu	-0.643696	-0.325944	-0.596038
N	0.586909	1.280419	-0.202122
N	1.182308	-1.372897	-0.307062
C	0.292449	2.588212	-0.116255
C	1.260480	3.584930	0.128301
C	2.591749	3.217200	0.278006
C	4.298137	1.379803	0.329185
C	4.601694	0.042207	0.241146
C	3.820226	-2.328211	-0.070171
C	2.759417	-3.202169	-0.281697
C	1.450744	-2.681115	-0.394962
C	1.895514	0.903991	-0.034034
C	2.943264	1.845477	0.195882
C	3.568658	-0.934253	0.023146
C	2.214345	-0.504367	-0.109211
H	-0.755598	2.867732	-0.255250
H	0.947265	4.631447	0.185155
H	3.371639	3.965763	0.455040
H	5.085633	2.122102	0.499058
H	5.636414	-0.304256	0.338709
H	4.846980	-2.698444	0.024633
H	2.919655	-4.281652	-0.358747

H	0.593645	-3.342823	-0.561138
C	-1.861946	-0.897814	1.288218
F	-0.772097	-0.595836	2.097663
F	-1.803758	-2.264908	1.070990
F	-2.941365	-0.761597	2.168712
F	-1.426124	-1.385865	-2.055154
Si	-2.883981	0.576656	-0.298620
C	-2.642861	1.440495	-2.014997
H	-3.407650	2.241473	-2.069170
H	-1.653669	1.899221	-2.173292
H	-2.823092	0.713920	-2.822851
C	-3.115678	1.939725	1.034382
H	-2.203888	2.102248	1.634429
H	-3.375060	2.895135	0.543214
H	-3.932924	1.675879	1.727404
C	-4.401206	-0.565914	-0.497142
H	-5.209839	0.013883	-0.982042
H	-4.159755	-1.417950	-1.155801
H	-4.781183	-0.952449	0.462045

III’

Cu	-0.908925	-0.075231	-0.210343
N	0.851291	1.362947	-0.102652
N	0.893698	-1.364817	-0.123481
C	0.814313	2.698914	-0.091102
C	1.978299	3.502054	-0.112635
C	3.222190	2.882873	-0.145624
C	4.541610	0.744138	-0.189711
C	4.562185	-0.630376	-0.198662
C	3.309696	-2.808681	-0.183765
C	2.085902	-3.467044	-0.160991
C	0.897463	-2.701791	-0.130614
C	2.063624	0.744052	-0.136133
C	3.296800	1.465220	-0.157945
C	3.339933	-1.389423	-0.176978
C	2.085777	-0.705944	-0.146771
H	-0.180515	3.158625	-0.064023
H	1.885389	4.592190	-0.102664
H	4.146206	3.471567	-0.162181
H	5.475551	1.316935	-0.206490
H	5.512631	-1.174937	-0.222589
H	4.251643	-3.368028	-0.206574
H	2.026792	-4.559515	-0.165076
H	-0.082685	-3.191870	-0.111527
C	-1.261784	-0.058682	1.680558
F	-1.881427	1.075495	2.196514
F	-0.046031	-0.098553	2.367017
F	-1.964466	-1.132901	2.214447
F	-0.915078	-0.073845	-2.100580
Si	-3.265939	0.033831	-0.664562
C	-3.468857	1.708673	-1.564991
H	-4.515716	1.795367	-1.918010
H	-3.272172	2.554821	-0.883055
H	-2.798364	1.790112	-2.435427
C	-4.488829	-0.011249	0.809561
H	-4.337993	0.819993	1.516696
H	-5.505350	0.088711	0.378493
H	-4.448269	-0.964078	1.362073
C	-3.624345	-1.494727	-1.756366
H	-4.704482	-1.499741	-2.003942
H	-3.046489	-1.475720	-2.693640
H	-3.399958	-2.433097	-1.218876

RE’

Cu	-0.897527	-0.007818	-0.052711
N	0.873632	1.358070	-0.142028
N	0.879630	-1.365449	-0.140634
C	0.854575	2.695390	-0.142574
C	2.027412	3.483132	-0.199141
C	3.262674	2.848098	-0.252739
C	4.553887	0.692187	-0.302597
C	4.557097	-0.682542	-0.299495
C	3.276274	-2.844373	-0.241205
C	2.044006	-3.485112	-0.186833
C	0.867210	-2.702871	-0.136082
C	2.078369	0.723942	-0.199361
C	3.319212	1.429577	-0.253263
C	3.325900	-1.425610	-0.247725
C	2.081621	-0.725767	-0.197459
H	-0.133423	3.167723	-0.094983
H	1.948165	4.574377	-0.197674
H	4.193326	3.425041	-0.293801
H	5.494385	1.252974	-0.342167
H	5.500209	-1.239080	-0.336448
H	4.209789	-3.416946	-0.278441
H	1.970078	-4.576713	-0.180663
H	-0.118576	-3.179891	-0.089190
C	-1.223420	0.003458	1.838254
F	-1.870686	1.123274	2.366736
F	-0.000887	-0.009082	2.531416
F	-1.905811	-1.082803	2.389037
F	-1.264678	-0.000278	-1.934314
Si	-3.205996	-0.003373	-0.847286
C	-3.579860	1.646378	-1.734243
H	-4.676005	1.801629	-1.749910
H	-3.133527	2.500543	-1.194082
H	-3.205286	1.655671	-2.770772
C	-4.363893	-0.056052	0.697767
H	-4.214882	0.796615	1.379277
H	-5.399197	-0.004478	0.302228
H	-4.262405	-0.994235	1.267037
C	-3.595829	-1.592386	-1.834884
H	-4.690308	-1.759249	-1.828881
H	-3.251408	-1.526757	-2.879868
H	-3.124410	-2.476345	-1.368806

TS_CF_3

Cu	-0.616331	0.072197	-1.020317
N	-2.033720	1.409119	-0.574014
N	-1.977553	-1.331050	-0.631325
C	-2.063429	2.760465	-0.545694
C	-3.122559	3.498747	0.004489
C	-4.215370	2.818716	0.568317
C	-5.287892	0.625533	1.141791
C	-5.242674	-0.748596	1.144062
C	-4.040951	-2.872514	0.562066
C	-2.914488	-3.483530	-0.015595
C	-1.918824	-2.683732	-0.595165
C	-3.111256	0.721074	-0.025656
C	-4.223122	1.405648	0.565844
C	-4.134416	-1.461783	0.561749
C	-3.073471	-0.710373	-0.040148
H	-1.198573	3.267571	-0.987517
H	-3.081834	4.592310	-0.011425
H	-5.054538	3.365155	1.012802
H	-6.135521	1.155193	1.592036
H	-6.053095	-1.330607	1.598233
H	-4.840809	-3.469717	1.013504
H	-2.807434	-4.572635	-0.033790
H	-1.042022	-3.137928	-1.069369
F	7.365323	0.185297	0.695318
Si	5.665592	0.061651	0.427193
C	5.108294	1.820245	-0.014961
C	5.477565	-1.167244	-1.005277
C	1.652387	-0.148485	-0.179424
C	4.952165	-0.574875	2.065075
H	4.021039	1.840381	-0.212887
H	5.317897	2.524427	0.810249
H	5.626065	2.181367	-0.921674
H	5.966459	-0.791168	-1.921824
H	4.407503	-1.329375	-1.231378
H	5.921631	-2.146515	-0.751394
F	1.450216	-1.435128	0.239473
F	1.784186	0.106353	-1.533673
F	1.415735	0.885447	0.688214
H	3.861053	-0.728072	1.974900
H	5.407507	-1.541297	2.347379
H	5.128010	0.144132	2.885175

CF_3-DMF

O	0.104869	-1.847617	-0.714699
N	-1.480803	-0.104062	-0.348092
C	-1.917101	-0.686334	0.904439
H	-1.606556	-0.118063	1.817019
H	-3.023113	-0.773277	0.938747
H	-1.470054	-1.696101	0.945891
C	-1.833730	1.293184	-0.491245
H	-1.463195	1.964961	0.321605
H	-1.430492	1.679952	-1.447128
H	-2.937444	1.410712	-0.521259
C	-0.077127	-0.557307	-0.773192
H	0.022616	-0.033476	-1.798011
C	1.021117	0.186457	0.073154
F	2.285058	-0.135587	-0.365799
F	0.988874	-0.141886	1.404973
F	0.978952	1.572880	0.029540

IV’

Cu	-0.023837	0.678747	-0.455114
N	1.364000	-0.879436	-1.042598
N	1.434108	0.721619	1.135084
C	1.314704	-1.676252	-2.122330
C	2.285515	-2.661197	-2.404282
C	3.357963	-2.827260	-1.531156
C	4.518318	-2.099566	0.575942
C	4.559250	-1.278654	1.678012
C	3.525052	0.564907	3.036556
C	2.486305	1.480658	3.183417
C	1.464129	1.524888	2.211633
C	2.413377	-1.036969	-0.179309
C	3.447169	-2.003456	-0.380775
C	3.530691	-0.299374	1.912598
C	2.453139	-0.178702	0.981679
H	0.460396	-1.527011	-2.792588
H	2.181849	-3.279738	-3.301308
H	4.129380	-3.582651	-1.718617
H	5.305009	-2.843448	0.405671
H	5.379031	-1.356217	2.401237
H	4.333701	0.502846	3.773432
H	2.447403	2.162583	4.038720
H	0.634206	2.234107	2.307039
C	0.239070	2.304536	-1.589239
F	1.095378	2.199062	-2.730139
F	0.779033	3.460948	-0.943521
F	-0.941708	2.849084	-2.185192
C	-1.780045	0.066201	-0.033067
C	-2.979904	-0.242586	0.166621
C	-4.349787	-0.572686	0.406720
C	-5.079546	0.053252	1.458333
C	-5.035645	-1.530716	-0.393954
C	-6.423353	-0.265918	1.694185
H	-4.573234	0.795166	2.086003
C	-6.380319	-1.843392	-0.150955
H	-4.496867	-2.024845	-1.210380
C	-7.084708	-1.215559	0.893374
H	-6.959760	0.232507	2.510281
H	-6.883730	-2.583876	-0.783693

H	-8.135443	-1.463154	1.080779

V’

Cu	0.062087	-0.608415	0.042944
O	-0.067334	-1.114748	-1.923414
O	-0.197140	-2.437922	-2.063697
N	-1.149494	1.460675	-0.124471
N	-1.853603	-1.175805	-0.076119
C	-0.795218	2.748083	-0.120259
C	-1.726177	3.809201	-0.235958
C	-3.075803	3.507093	-0.377691
C	-4.857568	1.743808	-0.567417
C	-5.192021	0.407245	-0.612446
C	-4.493880	-2.011081	-0.544292
C	-3.468069	-2.936557	-0.406283
C	-2.148805	-2.485568	-0.163469
C	-2.472208	1.154271	-0.248332
C	-3.491071	2.149293	-0.396658
C	-4.195834	-0.617950	-0.471064
C	-2.835929	-0.244503	-0.256914
H	0.277747	2.956695	-0.024025
H	-1.374454	4.845489	-0.220318
H	-3.824764	4.300744	-0.480625
H	-5.626316	2.517534	-0.673453
H	-6.233357	0.100303	-0.763599
H	-5.528358	-2.332466	-0.708474
H	-3.664636	-4.012136	-0.458061
H	-1.332168	-3.187820	0.019095
C	1.921157	-0.333542	-0.170783
C	3.147892	-0.137622	-0.251397
C	4.555870	0.094073	-0.363923
C	5.082257	1.414611	-0.338724
C	5.466989	-0.987943	-0.506747
C	6.461128	1.638847	-0.453455
H	4.394625	2.260379	-0.228989
C	6.844564	-0.753910	-0.618990
H	5.079531	-2.012388	-0.529267
C	7.350806	0.558292	-0.593840
H	6.843431	2.665895	-0.432249
H	7.528231	-1.603719	-0.728169
H	8.428029	0.737224	-0.682750
C	0.098886	-0.481056	2.064105
F	0.711435	-1.595035	2.664491
F	0.797099	0.608098	2.595187
F	-1.141022	-0.410279	2.715181