Conformational study of [Cu($CF_3COCHCO(C_4H_3X)$)$_2$] (X = O or S), a combined experimental and DFT study.

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Supplementary Information

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1 Figures (DFT optimized structures)

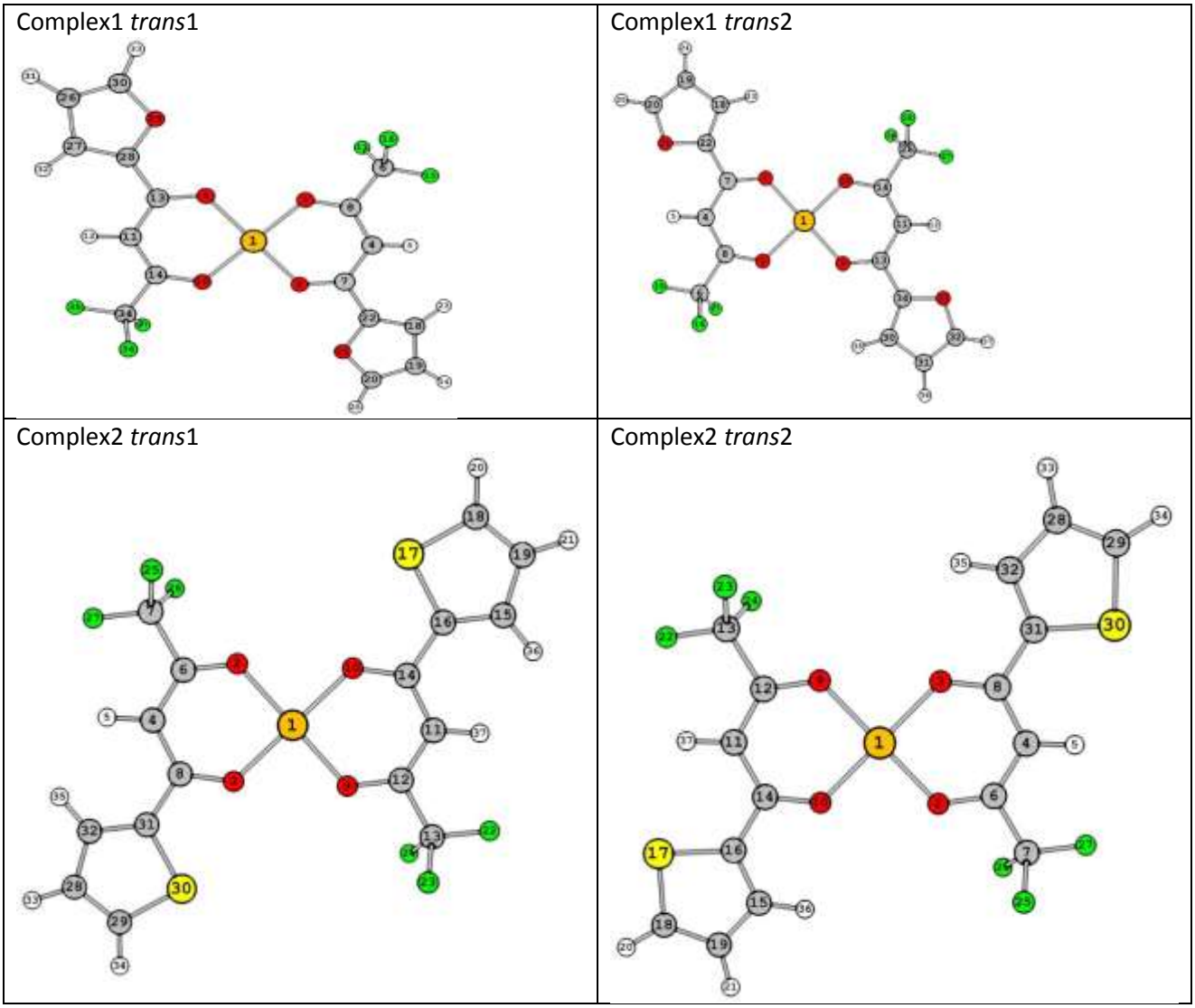


Fig S1 :The optimized main conformer structures of *bis*(2-fuyltrifluoroacetonato-O,O')-copper(II) (Complex 1) and *bis*(2-thenoyltrifluoroacetonato-O,O')-copper(II) (Complex 2) with atom numbering.

2 Crystallographic Details

Table S1. Crystal data and structure refinement for **1** and **2**.

	1	**2**
CCDC Identifier	1937196	1937195
Emp. formula	$C_{16}H_8O_6F_6Cu$	$C_{16}H_8O_4F_6S_2Cu$
Form. weight (g.mol^{-1})	473.76	505.88
Temperature (K)	150(2)	150(2)
Crystal system	triclinic	monoclinic
Space group	*P-1*	*P2$_1$/c*
Crystal description	Green plate	Green plate
a (Å)	5.7274(4)	10.556(3)
b (Å)	7.3615(4)	11.061(3)
c (Å)	10.6484(6)	7.867(2)
α (°)	86.982(2)	90
β (°)	74.855(2)	105.227(9)
γ (°)	75.881(2)	90
Volume (Å^3)	420.25(4)	886.3(4)
Z	1	2
Abs. coeff. (m.mm^{-1})	1.398	1.551
2θ data range for data collection (º)	5.706 to 49.386	5.436 to 49.4
F(000)	235	502
Independent refl.	1432	1505
Completeness (%)	99.9	99.8
Data/Restr/Para	1432/10/164	1505/0/134
Goodness of fit on F^2	1.168	1.087
Final R$_1$ indexes	0.0215	0.0363
wR$_2$ indices (all data)	0.0545	0.0883
Largest diffraction peak and hole (e.Å^{-3})	0.23/-0.26	0.54/-0.34

Table S2. Bond lengths for **1** and **2**.

1			**2**		
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Cu1	O1	1.9216(13)	Cu1	O1	1.909(2)
Cu1	O2	1.9127(13)	Cu1	O2	1.917(2)
F1	C1	1.336(13)	O1	C2	1.270(4)
F2	C1	1.329(13)	C1	F1	1.327(4)
F3	C1	1.344(13)	C1	F2	1.338(4)
O1	C2	1.278(2)	C1	C2	1.526(5)
O2	C4	1.273(2)	C1	F3	1.335(4)
O3	C5	1.372(2)	O2	C4	1.258(4)
O3	C8	1.359(2)	C2	C3	1.365(5)
C1	C2	1.528(8)	C3	C4	1.402(5)
C2	C3	1.367(3)	C7	C8	1.353(5)
C2	C1A	1.524(12)	C7	C6A	1.502(7)
C3	C4	1.409(3)	C7	S1B	1.439(10)
C4	C5	1.452(3)	C8	S1A	1.669(4)
C5	C6	1.355(3)	C8	S1B	2.272(9)
C6	C7	1.415(3)	C8	C6B	1.65(4)
C7	C8	1.341(3)	C5	C4	1.469(4)
F3A	C1A	1.340(18)	C5	S1A	1.702(3)
C1A	F2A	1.326(19)	C5	C6A	1.584(6)
C1A	F1A	1.333(19)	C5	S1B	1.330(9)
			C5	C6B	1.35(4)
			S1B	C6B	2.16(4)

Table S3. Bond angles for **1** and **2**.

1				2			
Atom	**Atom**	**Atom**	**Angle/º**	**Atom**	**Atom**	**Atom**	**Angle/º**
O1[1]	Cu1	O1	180.0	O1	Cu1	O2	93.02(9)
O2[1]	Cu1	O1[1]	93.48(5)	O1	Cu1	O2[1]	86.98(9)
O2	Cu1	O1	93.49(5)	O2	Cu1	O2[1]	180.0
O2	Cu1	O1[1]	86.52(5)	C2	O1	Cu1	123.4(2)
O2[1]	Cu1	O1	86.51(5)	F1	C1	F2	108.2(3)
O2[1]	Cu1	O2	180.0	F1	C1	C2	111.0(3)
C2	O1	Cu1	123.61(12)	F1	C1	F3	107.1(3)
C4	O2	Cu1	126.44(12)	F2	C1	C2	110.6(3)
C8	O3	C5	105.71(15)	F3	C1	F2	106.2(3)
F1	C1	F3	107.5(12)	F3	C1	C2	113.6(3)
F1	C1	C2	109.1(13)	C4	O2	Cu1	127.4(2)
F2	C1	F1	106.9(13)	O1	C2	C1	111.5(3)
F2	C1	F3	106.8(11)	O1	C2	C3	129.5(3)
F2	C1	C2	111.3(11)	C3	C2	C1	119.0(3)
F3	C1	C2	114.8(12)	C2	C3	C4	122.2(3)
O1	C2	C1	111.9(7)	C8	C7	C6A	119.9(4)
O1	C2	C3	129.01(18)	C8	C7	S1B	108.9(4)
O1	C2	C1A	111.9(10)	C7	C8	S1A	114.0(3)
C3	C2	C1	119.1(7)	C7	C8	S1B	36.8(3)
C3	C2	C1A	119.1(10)	C7	C8	C6B	101.4(13)
C2	C3	C4	122.10(17)	C6B	C8	S1B	64.7(13)
O2	C4	C3	125.26(17)	C4	C5	S1A	118.1(3)
O2	C4	C5	114.81(17)	C4	C5	C6A	125.5(3)
C3	C4	C5	119.92(16)	C6A	C5	S1A	116.2(3)
O3	C5	C4	118.63(16)	S1B	C5	C4	131.0(5)
C6	C5	O3	110.04(16)	S1B	C5	C6B	107.8(19)
C6	C5	C4	131.29(18)	C6B	C5	C4	121.1(19)
C5	C6	C7	106.60(18)	O2	C4	C3	124.3(3)
C8	C7	C6	106.24(18)	O2	C4	C5	115.9(3)
C7	C8	O3	111.40(17)	C3	C4	C5	119.7(3)
F3A	C1A	C2	110.8(18)	C8	S1A	C5	91.93(18)
F2A	C1A	C2	113.8(19)	C7	C6A	C5	97.7(4)
F2A	C1A	F3A	107(2)	C7	S1B	C8	34.3(3)
F2A	C1A	F1A	106(2)	C7	S1B	C6B	77.8(12)
F1A	C1A	C2	110.4(17)	C5	S1B	C7	114.0(6)
F1A	C1A	F3A	108.9(19)	C5	S1B	C8	79.9(4)
				C5	S1B	C6B	36.4(12)
				C6B	S1B	C8	43.6(12)
				C8	C6B	S1B	71.7(15)
				C5	C6B	C8	107(3)
				C5	C6B	S1B	35.8(11)

[1]1-X, 1-Y, 1-Z

Table S4. Torsion angles for **1** and **2**.

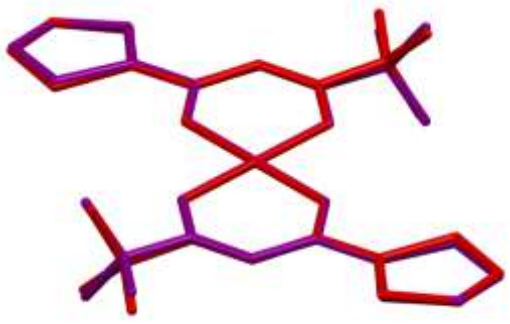
1					2				
A	**B**	**C**	**D**	**Angle/º**	**A**	**B**	**C**	**D**	**Angle/º**
Cu1	O1	C2	C1	-178.0(7)	Cu1	O1	C2	C1	-178.4(2)
Cu1	O1	C2	C3	1.5(3)	Cu1	O1	C2	C3	2.4(5)
Cu1	O1	C2	C1A	-180.0(11)	Cu1	O2	C4	C3	3.9(5)
Cu1	O2	C4	C3	-3.6(3)	Cu1	O2	C4	C5	-176.2(2)
Cu1	O2	C4	C5	175.55(11)	O1	C2	C3	C4	0.4(6)
F1	C1	C2	O1	-68.1(14)	C1	C2	C3	C4	-178.7(3)
F1	C1	C2	C3	112.4(13)	F1	C1	C2	O1	51.6(4)
F2	C1	C2	O1	49.6(15)	F1	C1	C2	C3	-129.1(3)
F2	C1	C2	C3	-129.9(12)	F2	C1	C2	O1	-68.5(4)

F3	C1	C2	O1	171.1(11)	F2	C1	C2	C3	110.8(4)
F3	C1	C2	C3	-8.4(16)	C2	C3	C4	O2	-3.9(5)
O1	C2	C3	C4	-0.7(3)	C2	C3	C4	C5	176.2(3)
O1	C2	C1A	F3A	66(2)	F3	C1	C2	O1	172.3(3)
O1	C2	C1A	F2A	-55(2)	F3	C1	C2	C3	-8.4(5)
O1	C2	C1A	F1A	-174(2)	C7	C8	S1A	C5	-0.7(3)
O2	C4	C5	O3	-170.92(15)	C7	C8	C6B	C5	-3(3)
O2	C4	C5	C6	6.8(3)	C7	C8	C6B	S1B	-3.6(11)
O3	C5	C6	C7	0.8(2)	C8	C7	C6A	C5	5.2(5)
C1	C2	C3	C4	178.7(7)	C8	C7	S1B	C5	-6.7(8)
C2	C3	C4	O2	1.8(3)	C8	C7	S1B	C6B	-4.2(13)
C2	C3	C4	C5	-177.36(17)	C4	C5	S1A	C8	179.7(3)
C3	C2	C1A	F3A	-116(2)	C4	C5	C6A	C7	179.2(3)
C3	C2	C1A	F2A	124(2)	C4	C5	S1B	C7	-177.2(4)
C3	C2	C1A	F1A	5(3)	C4	C5	S1B	C8	179.0(4)
C3	C4	C5	O3	8.3(3)	C4	C5	S1B	C6B	179(2)
C3	C4	C5	C6	-174.04(19)	C4	C5	C6B	C8	-179.3(11)
C4	C5	C6	C7	-177.02(19)	C4	C5	C6B	S1B	-178.9(18)
C5	O3	C8	C7	0.7(2)	S1A	C5	C4	O2	-4.4(4)
C5	C6	C7	C8	-0.4(2)	S1A	C5	C4	C3	175.5(3)
C6	C7	C8	O3	-0.2(2)	S1A	C5	C6A	C7	-5.5(4)
C8	O3	C5	C4	177.23(16)	C6A	C7	C8	S1A	-3.1(5)
C8	O3	C5	C6	-0.9(2)	C6A	C5	C4	O2	170.8(4)
C1A	C2	C3	C4	-179.1(12)	C6A	C5	C4	C3	-9.3(5)
					C6A	C5	S1A	C8	4.0(3)
					S1B	C7	C8	C6B	5.5(17)
					S1B	C8	C6B	C5	0.3(17)
					S1B	C5	C4	O2	179.2(6)
					S1B	C5	C4	C3	-0.9(7)
					S1B	C5	C6B	C8	0(3)
					C6B	C5	C4	O2	-2(2)
					C6B	C5	C4	C3	178(2)
					C6B	C5	S1B	C7	4(2)
					C6B	C5	S1B	C8	0(2)

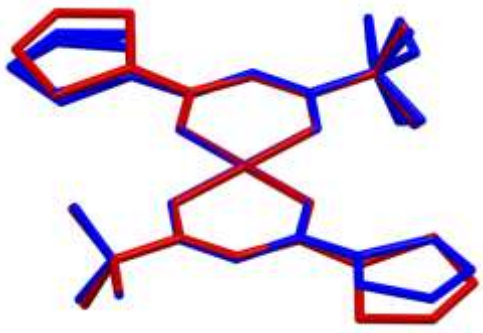
Table S5. Atomic occupancy for **2**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
S1A	0.846(4)	C6A	0.846(4)	H6A	0.846(4)
S1B	0.154(4)	C6B	0.154(4)	H6B	0.154(4)

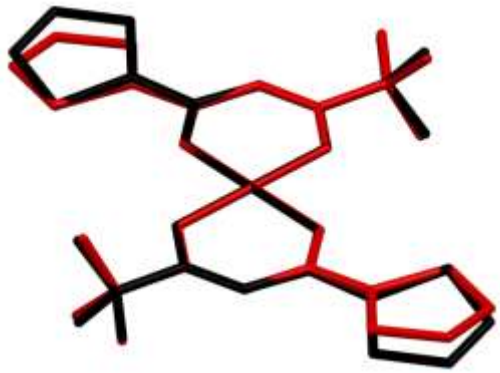
3 Figures (Structure overlays)



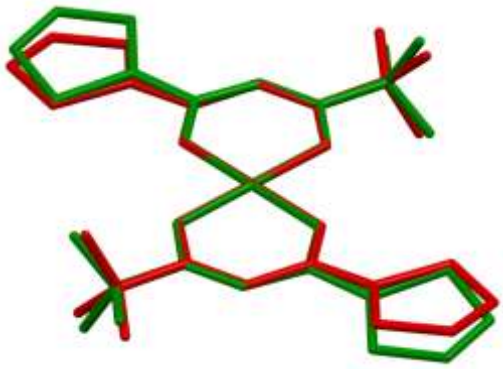
2 – TFTBCU (RMS = 6.62×10^{-3})



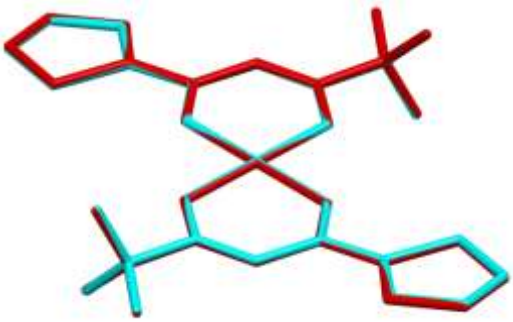
2 – TFTBCU01 (RMS = 5.73×10^{-3})



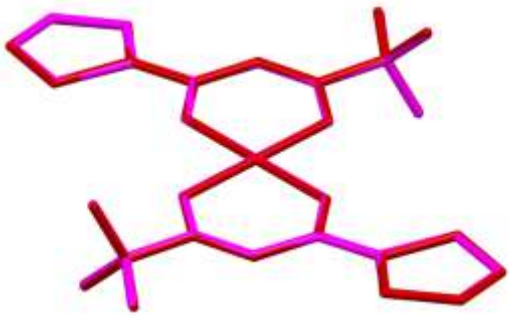
2 – TFTBCU02 (RMS = 3.82×10^{-3})



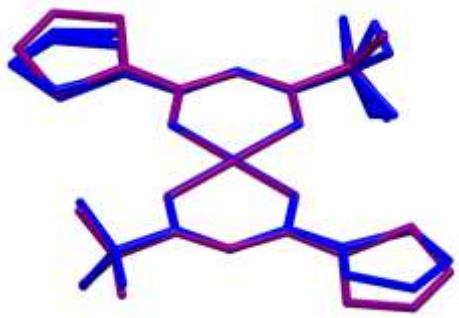
2 – TFTBCU03 (RMS = 1.11×10^{-2})



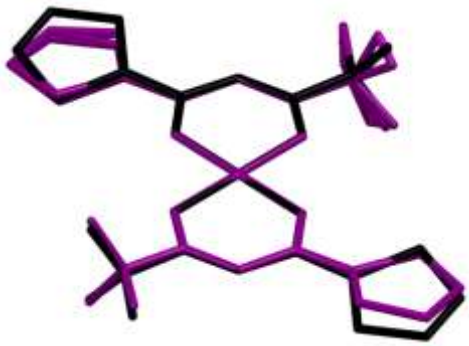
2 – TFTBCU04 (RMS = 3.87×10^{-3})



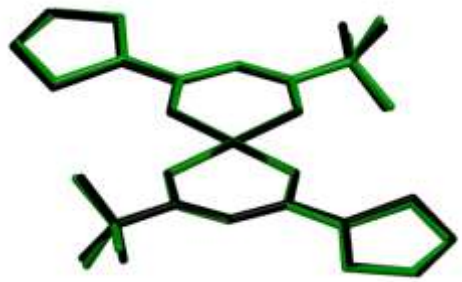
2 – TFTBCU05 (RMS = 5.17×10^{-2})



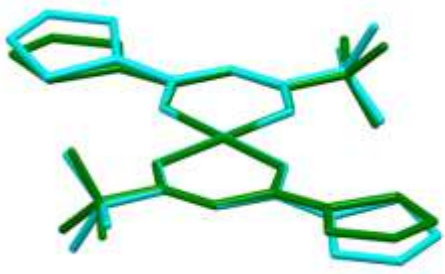
TFTBCU-TFTBCU01 (RMS = 8.76×10^{-3})



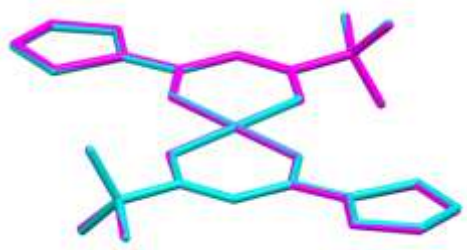
TFTBCU01-TFTBCU02 (RMS = 8.17×10^{-3})



TFTBCU02-TFTBCU03 (RMS = 8.16×10^{-3})



TFTBCU03-TFTBCU04 (RMS = 1.35×10^{-2})



TFTBCU04-TFTBCU05 (RMS = 2.67×10^{-3})

4 Optimized coordinates

4.1 Complex 1 cis 1

Cu	0.000001000	-0.273660000	-0.019797000
O	1.340367000	1.113077000	-0.018523000
O	1.340479000	-1.652749000	-0.017989000
C	3.282634000	-0.263822000	0.023931000
H	4.359800000	-0.283219000	0.046678000
C	3.390569000	-2.778158000	0.006792000
C	2.600189000	0.979421000	0.003999000
C	2.593691000	-1.463408000	0.007564000
O	-1.340643000	-1.652736000	-0.018875000
O	-1.340281000	1.113090000	-0.018321000
C	-3.282676000	-0.263636000	0.023564000
H	-4.359844000	-0.282934000	0.046242000
C	-2.593827000	-1.463276000	0.006840000
C	-3.390810000	-2.777970000	0.006035000
C	-2.600134000	0.979540000	0.004098000
F	4.723718000	-2.578209000	0.100605000
F	3.165192000	-3.461625000	-1.128136000
F	3.025659000	-3.554706000	1.038445000
F	-3.164619000	-3.462079000	-1.128289000
F	-4.724020000	-2.577895000	0.098757000
F	-3.026721000	-3.553974000	1.038453000
C	4.745126000	2.454133000	0.023001000
C	4.898408000	3.866556000	0.014321000
C	3.633332000	4.377392000	-0.006266000
O	2.714373000	3.390075000	-0.010885000
C	3.394234000	2.204956000	0.007111000
H	5.532967000	1.718867000	0.038460000
H	5.819036000	4.427300000	0.021960000
H	3.243385000	5.381520000	-0.019205000
C	-4.744926000	2.454439000	0.023363000
C	-4.898070000	3.866888000	0.015236000
C	-3.632934000	4.377594000	-0.004987000
O	-2.714083000	3.390198000	-0.009851000
C	-3.394064000	2.205129000	0.007584000
H	-5.532856000	1.719256000	0.038375000
H	-5.818644000	4.427717000	0.022970000
H	-3.242898000	5.381695000	-0.017442000

4.2 Complex 1 cis 2

Cu	0.000012000	-0.224560000	0.025464000
O	-1.337907000	1.163474000	0.026529000
O	-1.340427000	-1.604386000	0.020921000
C	-3.284177000	-0.218390000	-0.024982000
H	-4.361354000	-0.223164000	-0.050350000
C	-3.386943000	-2.736364000	-0.008225000
C	-2.602465000	1.020120000	-0.000919000
C	-2.593057000	-1.419134000	-0.007608000
O	1.340460000	-1.604400000	0.021629000
O	1.337928000	1.163471000	0.026162000
C	3.284216000	-0.218406000	-0.024277000
H	4.361397000	-0.223193000	-0.049376000
C	2.593091000	-1.419145000	-0.006924000
C	3.386915000	-2.736409000	-0.008165000
C	2.602491000	1.020116000	-0.000799000
F	-4.717938000	-2.540586000	-0.111557000
F	-3.165096000	-3.414533000	1.130962000
F	-3.010743000	-3.514728000	-1.034700000
F	3.163227000	-3.416454000	1.129458000
F	4.718086000	-2.540565000	-0.109114000
F	3.012260000	-3.513036000	-1.036610000
C	-2.970099000	3.568404000	0.018547000
C	-4.156076000	4.353210000	0.003389000
C	-5.193384000	3.467991000	-0.027598000
O	-4.738155000	2.194230000	-0.032501000
C	-3.369255000	2.258546000	-0.004150000
H	-1.946668000	3.903682000	0.043110000
H	-4.233752000	5.428422000	0.013983000
H	-6.264153000	3.583963000	-0.048061000
C	2.970101000	3.568413000	0.017860000
C	4.156088000	4.353224000	0.002880000
C	5.193413000	3.468015000	-0.027460000
O	4.738182000	2.194239000	-0.032136000
C	3.369267000	2.258556000	-0.004246000
H	1.946677000	3.903747000	0.041933000
H	4.233734000	5.428440000	0.013146000
H	6.264193000	3.583952000	-0.047559000

4.3 Complex 1 trans 1

Cu	0.000028000	-0.000015000	0.000102000
O	-1.726428000	0.856832000	0.000054000
O	-0.800932000	-1.748273000	0.000412000
C	-3.097087000	-1.089985000	-0.000117000
H	-4.106118000	-1.468340000	-0.000307000
C	-2.354807000	-3.494486000	0.000199000
C	-2.869534000	0.310877000	-0.000091000
C	-2.046229000	-1.988846000	0.000146000
O	1.726443000	-0.856814000	-0.000069000
O	0.800932000	1.748265000	0.000013000

C	3.097094000	1.089988000	0.000268000
H	4.106120000	1.468360000	0.000372000
C	2.869557000	-0.310874000	0.000052000
C	2.046226000	1.988838000	0.000157000
F	-3.680317000	-3.755801000	-0.000114000
F	-1.828533000	-4.083878000	1.086798000
F	-1.827981000	-4.084075000	-1.086017000
C	-5.383068000	0.988305000	-0.000287000
C	-5.995992000	2.269853000	-0.000361000
C	-4.971635000	3.171724000	-0.000334000
O	-3.777715000	2.545206000	-0.000243000
C	-4.025736000	1.201724000	-0.000212000
H	-5.882268000	0.033144000	-0.000283000
H	-7.050492000	2.493580000	-0.000425000
H	-4.936352000	4.248435000	-0.000369000
C	5.996019000	-2.269827000	-0.000397000
C	5.383083000	-0.988286000	-0.000144000
C	4.025753000	-1.201713000	-0.000134000
O	3.777746000	-2.545191000	-0.000363000
C	4.971671000	-3.171705000	-0.000526000
H	7.050519000	-2.493550000	-0.000479000
H	5.882273000	-0.033119000	0.000000000
H	4.936393000	-4.248416000	-0.000719000
C	2.354761000	3.494475000	0.000176000
F	3.680262000	3.755837000	0.000336000
F	1.828054000	4.083992000	1.086489000
F	1.828325000	4.083902000	-1.086332000

4.4 Complex 1 trans 2

Cu	-0.000005000	-0.000062000	-0.001040000
O	-1.681852000	0.931723000	-0.001370000
O	-0.876275000	-1.714865000	-0.001417000
C	-3.141864000	-0.955927000	0.000443000
H	-4.171109000	-1.274986000	0.001448000
C	-2.504546000	-3.392262000	0.000365000
C	-2.850286000	0.429548000	-0.000374000
C	-2.130868000	-1.901217000	-0.000246000
O	1.681950000	-0.931700000	-0.000663000
O	0.876324000	1.714721000	-0.000562000
C	3.141951000	0.955933000	0.000198000
H	4.171178000	1.275053000	0.000602000
C	2.850395000	-0.429538000	-0.000146000
C	2.130909000	1.901166000	-0.000099000
F	-3.837328000	-3.597348000	0.001917000
F	-1.999429000	-4.003131000	1.086316000
F	-2.001921000	-4.003390000	-1.086612000
C	-3.926884000	2.764263000	-0.000559000
C	-5.286844000	3.179374000	0.000217000
C	-6.030882000	2.035816000	0.001198000
O	-5.233682000	0.942910000	0.001065000
C	-3.939135000	1.394626000	-0.000003000
H	-3.039136000	3.375087000	-0.001409000

H	-5.666007000	4.188551000	0.000072000
H	-7.090839000	1.843533000	0.002015000
C	2.504378000	3.392255000	0.000375000
F	3.837121000	3.597563000	0.000767000
F	2.000078000	4.002844000	1.086886000
F	2.000676000	4.003510000	-1.086025000
C	3.927082000	-2.764241000	-0.000169000
C	5.287083000	-3.179276000	0.000380000
C	6.031045000	-2.035686000	0.000803000
O	5.233791000	-0.942812000	0.000711000
C	3.939229000	-1.394626000	0.000128000
H	3.039415000	-3.375184000	-0.000635000
H	5.666245000	-4.188453000	0.000402000
H	7.090991000	-1.843329000	0.001235000

4.5 Complex 2 cis 1

Cu	-0.000009000	-0.553802000	-0.015756000
O	1.337893000	0.833199000	-0.013189000
O	1.343988000	-1.927726000	-0.014552000
C	3.284057000	-0.531798000	0.022618000
H	4.360814000	-0.554060000	0.042447000
C	3.396555000	-3.046470000	0.004555000
C	2.604838000	0.711527000	0.005839000
C	2.596030000	-1.733272000	0.007718000
O	-1.344055000	-1.927681000	-0.015983000
O	-1.337894000	0.833236000	-0.014622000
C	-3.284050000	-0.531742000	0.023345000
H	-4.360785000	-0.553912000	0.044387000
C	-2.596076000	-1.733232000	0.007665000
C	-3.396619000	-3.046409000	0.005097000
C	-2.604798000	0.711563000	0.005543000
F	4.729125000	-2.843641000	0.095705000
F	3.169777000	-3.729126000	-1.130368000
F	3.034991000	-3.823862000	1.036554000
F	-3.171046000	-3.728867000	-1.130196000
F	-4.729086000	-2.843564000	0.097682000
F	-3.033989000	-3.823997000	1.036564000
C	4.728980000	2.172939000	0.021841000
C	5.075301000	3.544522000	0.017133000
C	3.972636000	4.359640000	-0.000226000
S	2.496314000	3.472920000	-0.011151000
C	3.366792000	1.958673000	0.008115000
H	5.457478000	1.374063000	0.034271000
H	6.092137000	3.912886000	0.025928000
H	3.948707000	5.439019000	-0.007508000
C	-4.728952000	2.173049000	0.021878000
C	-5.075203000	3.544648000	0.016937000
C	-3.972496000	4.359700000	-0.000923000
S	-2.496238000	3.472880000	-0.012058000
C	-3.366776000	1.958727000	0.007853000
H	-5.457478000	1.374203000	0.034621000
H	-6.092020000	3.913059000	0.025906000

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H       -3.948539000      5.439076000     -0.008390000
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4.6 Complex 2 cis 2

```
Cu      -0.000014000     -0.443720000      0.027331000
O       -1.339540000      0.942787000      0.027851000
O       -1.341473000     -1.820182000      0.023672000
C       -3.281197000     -0.426763000     -0.023781000
H       -4.359187000     -0.451405000     -0.050430000
C       -3.391715000     -2.943419000     -0.007784000
C       -2.605123000      0.817979000      0.000528000
C       -2.592985000     -1.628901000     -0.005895000
O        1.341459000     -1.820190000      0.023323000
O        1.339538000      0.942767000      0.028125000
C        3.281197000     -0.426778000     -0.023650000
H        4.359187000     -0.451414000     -0.050230000
C        2.592975000     -1.628914000     -0.006027000
C        3.391694000     -2.943437000     -0.008069000
C        2.605118000      0.817962000      0.000733000
F       -4.723032000     -2.742452000     -0.108826000
F       -3.171259000     -3.624380000      1.129395000
F       -3.020454000     -3.720499000     -1.036539000
F        3.170966000     -3.624706000      1.128864000
F        4.723038000     -2.742457000     -0.108753000
F        3.020658000     -3.720236000     -1.037127000
C       -2.818639000      3.336744000      0.021776000
C       -3.789368000      4.366224000      0.014408000
C       -5.069803000      3.879334000     -0.015249000
S       -5.110784000      2.156397000     -0.034490000
C       -3.363760000      2.072819000     -0.002203000
H       -1.749048000      3.488760000      0.044079000
H       -3.556360000      5.422260000      0.030425000
H       -5.995797000      4.434093000     -0.026846000
C        2.818671000      3.336742000      0.022000000
C        3.789420000      4.366208000      0.014612000
C        5.069848000      3.879313000     -0.015072000
S        5.110825000      2.156359000     -0.034309000
C        3.363742000      2.072806000     -0.001984000
H        1.749082000      3.488780000      0.044318000
H        3.556427000      5.422249000      0.030632000
H        5.995846000      4.434067000     -0.026699000
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4.7 Complex 2 trans 1

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symmetry c1
Cu       0.000001000     -0.000001000      0.000144000
O       -0.466953000      1.865200000      0.000012000
O       -1.851387000     -0.523526000     -0.000073000
C       -2.846877000      1.635229000      0.000116000
H       -3.766881000      2.195633000      0.000196000
```

C	-1.648456000	2.326769000	0.000091000
C	-1.678168000	3.863859000	0.000129000
C	-2.885541000	0.217486000	0.000000000
O	0.466951000	-1.865202000	0.000291000
O	1.851387000	0.523530000	0.000329000
C	2.846875000	-1.635227000	-0.000212000
C	1.648454000	-2.326769000	-0.000023000
C	1.678169000	-3.863859000	-0.000132000
C	2.885539000	-0.217485000	0.000037000
C	5.455871000	-0.018401000	-0.000264000
C	4.169216000	0.479001000	-0.000017000
S	4.172854000	2.225652000	0.000168000
C	5.894102000	2.253328000	0.000152000
C	6.441715000	0.995542000	-0.000169000
H	6.413376000	3.199941000	0.000309000
H	7.506512000	0.806019000	-0.000290000
F	2.933123000	-4.362230000	-0.000600000
F	1.052841000	-4.347002000	1.086499000
F	1.052072000	-4.346890000	-1.086358000
F	-1.052261000	4.346936000	1.086445000
F	-1.052649000	4.346955000	-1.086413000
F	-2.933121000	4.362232000	0.000355000
C	-6.441715000	-0.995544000	-0.000041000
C	-5.894102000	-2.253329000	0.000196000
S	-4.172854000	-2.225652000	-0.000468000
C	-4.169217000	-0.479001000	-0.000107000
C	-5.455872000	0.018401000	-0.000213000
H	-7.506512000	-0.806021000	0.000066000
H	-6.413375000	-3.199943000	0.000444000
H	-5.686265000	1.074854000	-0.000234000
H	5.686263000	-1.074855000	-0.000455000
H	3.766879000	-2.195631000	-0.000497000

4.8 Complex 2 trans 2

Cu	-0.000065000	0.000107000	0.000337000
O	0.691759000	-1.794682000	0.000060000
O	1.771708000	0.745008000	0.000147000
C	3.024749000	-1.273395000	0.000484000
H	4.008116000	-1.716931000	0.000667000
C	1.920796000	-2.108187000	0.000357000
C	2.135920000	-3.630159000	0.000098000
C	2.888605000	0.138935000	0.000161000
O	-0.691720000	1.794870000	0.000693000
O	-1.771671000	-0.744975000	0.000292000
C	-3.024695000	1.273406000	-0.000282000
C	-1.920825000	2.108258000	0.000085000
C	-2.136051000	3.630208000	0.000203000
C	-2.888568000	-0.138950000	-0.000041000
C	-4.048356000	-2.380117000	0.000180000
C	-4.071177000	-1.003184000	-0.000151000
S	-5.717811000	-0.412076000	-0.000756000
C	-6.336705000	-2.020875000	-0.000534000

C	-5.338767000	-2.960067000	-0.000036000
H	-7.404428000	-2.180232000	-0.000784000
H	-5.525920000	-4.025245000	0.000146000
F	-3.440180000	3.975103000	-0.001841000
F	-1.572868000	4.183982000	1.087788000
F	-1.569243000	4.184780000	-1.085019000
F	1.569631000	-4.184700000	1.085619000
F	1.572117000	-4.183877000	-1.087189000
F	3.440020000	-3.975152000	0.001474000
C	5.339050000	2.959903000	-0.000756000
C	6.336903000	2.020657000	-0.000573000
S	5.717873000	0.411876000	-0.000194000
C	4.071245000	1.003141000	-0.000192000
C	4.048573000	2.380049000	-0.000533000
H	5.526236000	4.025076000	-0.001018000
H	7.404647000	2.179873000	-0.000680000
H	3.117229000	2.928786000	-0.000591000
H	-3.116939000	-2.928728000	0.000585000
H	-4.008134000	1.716786000	-0.000748000