

Magneto-structural Analysis of Hydroxido-bridged Cu^{II}₂ Complexes: Density Functional Theory and other Treatments

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Complexes:

1. [Cu(bipy)OH]₂(NO₃)₂
2. [Cu(bipy)OH]₂(ClO₄)₂
3. α-[Cu(dmaep)OH]₂(ClO₄)₂
4. β-[Cu(dmaep)OH]₂(ClO₄)₂
5. [Cu(eaep)OH]₂(ClO₄)₂
6. [Cu(tmen)OH]₂(ClO₄)₂
7. [Cu(tmen)OH]₂Br₂
8. [Cu(2miz)OH]₂(ClO₄)₂.2H₂O

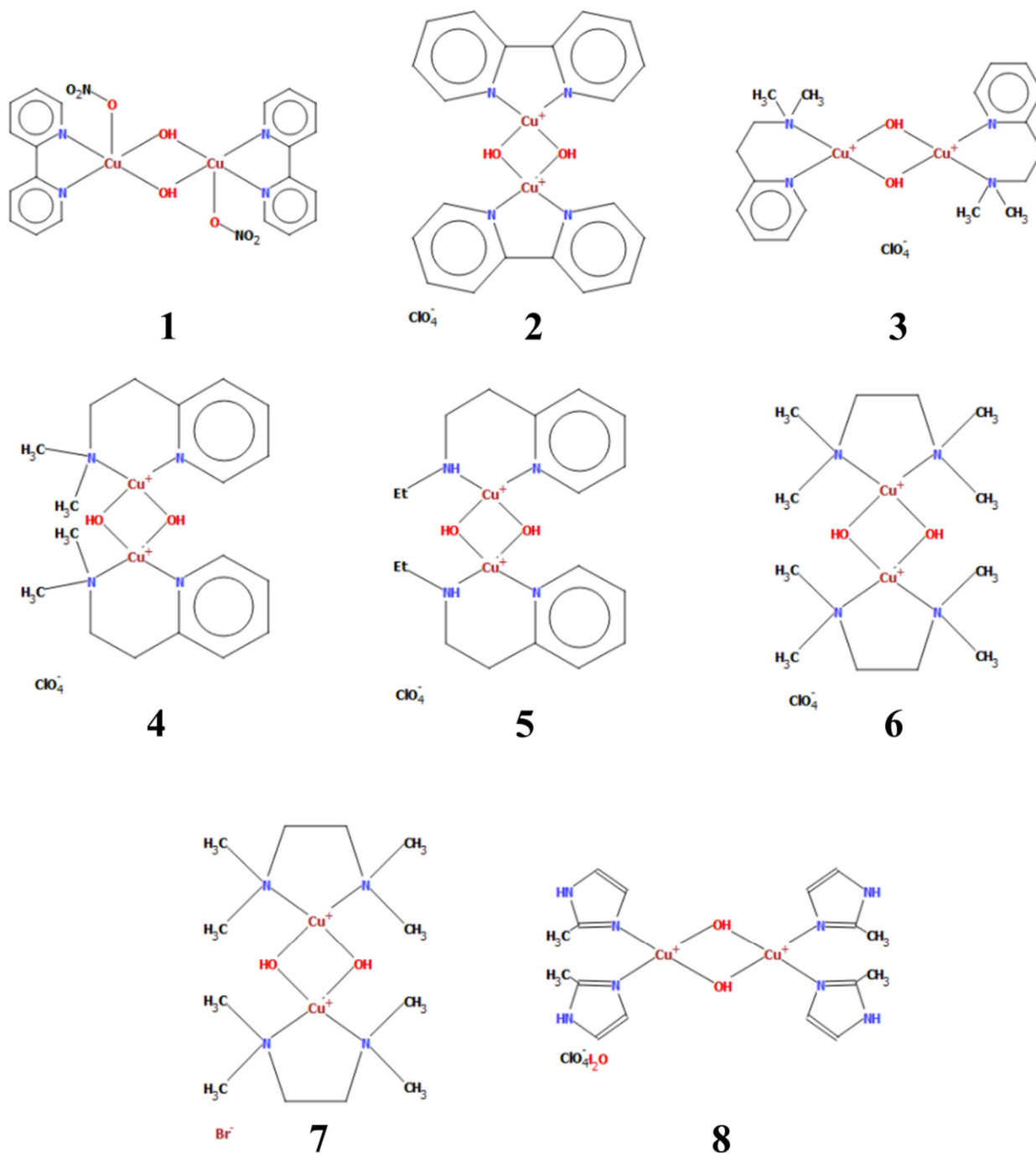


Figure S1. Molecular structures for Complex 1-8.

Table S1. Structural data from X-Ray crystallographic study.

	Complexes	$2J$ (exp)	Cu-Cu	Cu-O	Cu-N	\angle Cu-O-Cu	\angle OH-Cu ₂ O ₂
1	[Cu(bipy)OH] ₂ (NO ₃) ₂	172	2.847	1.922	1.999	95.6	126
2	[Cu(bipy)OH] ₂ (ClO ₄) ₂	93	2.871	1.919	1.99	96.9	146.5
3	α -[Cu(dmaep)OH] ₂ (ClO ₄) ₂	-4.8	2.938	1.942	2.037	98.4	117.3
4	β -[Cu(dmaep)OH] ₂ (ClO ₄) ₂	-201	2.935	1.91	2.035	100.4	139
5	[Cu(eaep)OH] ₂ (ClO ₄) ₂	-130	2.917	1.929 1.904	1.99 2.027	99.8 99.5	125
6	[Cu(tmen)OH] ₂ (ClO ₄) ₂	-360	2.966	1.929	2.014	101.6	
7	[Cu(tmen)OH] ₂ Br ₂	-509	3.000	1.902	2.03	104.1	
8	[Cu(2miz)OH] ₂ (ClO ₄) ₂ .2H ₂ O	-175	2.988	1.959	1.977	99.4	124.5

Table S2. Unit Cell data from Crystallographic study.

	Complexes	a	b	c	α	β	γ	Crystal System
1	[Cu(bipy)OH] ₂ (NO ₃) ₂	7.637	16.989	8.504	91.58	97.49	90.36	Body Centred
2	[Cu(bipy)OH] ₂ (ClO ₄) ₂	13.600	15.210	6.270	90	113.6	90	Monoclinic
3	α -[Cu(dmaep)OH] ₂ (ClO ₄) ₂	9.164	10.049	8.953	82.3	56.73	68.52	Triclinic
4	β -[Cu(dmaep)OH] ₂ (ClO ₄) ₂	7.266	16.500	10.851	90	82.43	90	Monoclinic
5	[Cu(eaep)OH] ₂ (ClO ₄) ₂	9.195	19.290	7.679	90	77	90	Monoclinic
6	[Cu(tmen)OH] ₂ (ClO ₄) ₂	7.707	14.996	11.627	90	109.13	90	Monoclinic
7	[Cu(tmen)OH] ₂ Br ₂	17.072	18.482	12.825	90	90	90	Orthorhombic
8	[Cu(2miz)OH] ₂ (ClO ₄) ₂ .2H ₂ O	14.93	13.725	7.481	90	103.4	90	Monoclinic