

Supplementary Information

Structural and theoretical study of copper(II) complex incorporating chalcone and 2,2'-bipyridine mixed ligands : A probable candidate for optical material

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SI 1: Selected bond lengths (Å) and bond angles (°) of **CuM**.

Cu(1)-O(1)	1.880(2)	O(1)-Cu(1)-O(2)	92.23(9)
Cu(1)-O(2)	1.9193(19)	O(1)-Cu(1)-O(3)	99.95(19)
Cu(1)-O(3)	2.443(8)	N(1)-Cu(1)-N(2)	81.02(11)
Cu(1)-N(1)	1.992(3)	O(2)-Cu(1)-N(1)	92.55(10)
Cu(1)-N(2)	2.002(3)	O(3)-Cu(1)-N(1)	81.4(2)
S(1)-C(24)	1.703(5)	C(20)-S(1)-(24)	90.8(2)

SI 2: Geometric features of π - π interactions obtained from **CuM**.

Cg(I)··· Cg(ring J)	Cg···Cg (Å)	α (°)	β (°)	γ (°)	Cg(I)···Prep (Å)	Cg(J)···Prep(Å)
Cg(4)-Cg(6) ^a	3.6783(19)	4.88	26.30	21.4	-3.4239(14)	-3.2975(11)

Symmetry transformation^a = -X,-Y,1-Z; Cg(4) = center of gravity of the ring N(1)-C(1)-C(2)-C(3)-C(4)-C(5); Cg(6) = center of gravity of the ring C(11)-C(12)-C(13)-C(14)- C(15)-C(16).