

ESI

A combined experimental and theoretical approach to structure, magnetic properties and DNA binding affinity of a homodinuclear Cu(II) complex

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Table 1S: Selected bond lengths (Å) and bond angles (°) of **1**.

Bond Lengths			Bond Angles			
Atom	Atom	Length	Atom	Atom	Atom	Angle
Cu1	O1	1.9166(14)	O2	Cu1	O1	94.26(6)
Cu1	O2	1.9342(13)	O2	Cu1	O1	169.71(6)
Cu1	N1	1.9654(17)	N1	Cu1	O1	171.37(6)
O1	C3	1.419(2)	N1	Cu1	O1	95.99(6)
O2	C4	1.279(2)	N1	Cu1	O2	93.78(6)
O3	C4	1.241(2)	C3	O1	Cu1	127.13(12)
N1	C1	1.482(3)	C3	O1	Cu1	128.86(12)
N1	H1a	0.9000	C4	O2	Cu1	114.62(12)
C4	C5	1.507(3)	C1	N1	Cu1	119.21(13)
C2	C1	1.514(3)	H1a	N1	Cu1	107.52(5)
C2	C3	1.518(3)	H1b	N1	Cu1	107.52(5)
C2	H2a	0.9700	H1b	N1	C1	107.52(11)
C3	H3b	0.9700	H1b	N1	H1a	107.0
C5	H5a	0.9600	H1c	C1	C2	109.28(11)

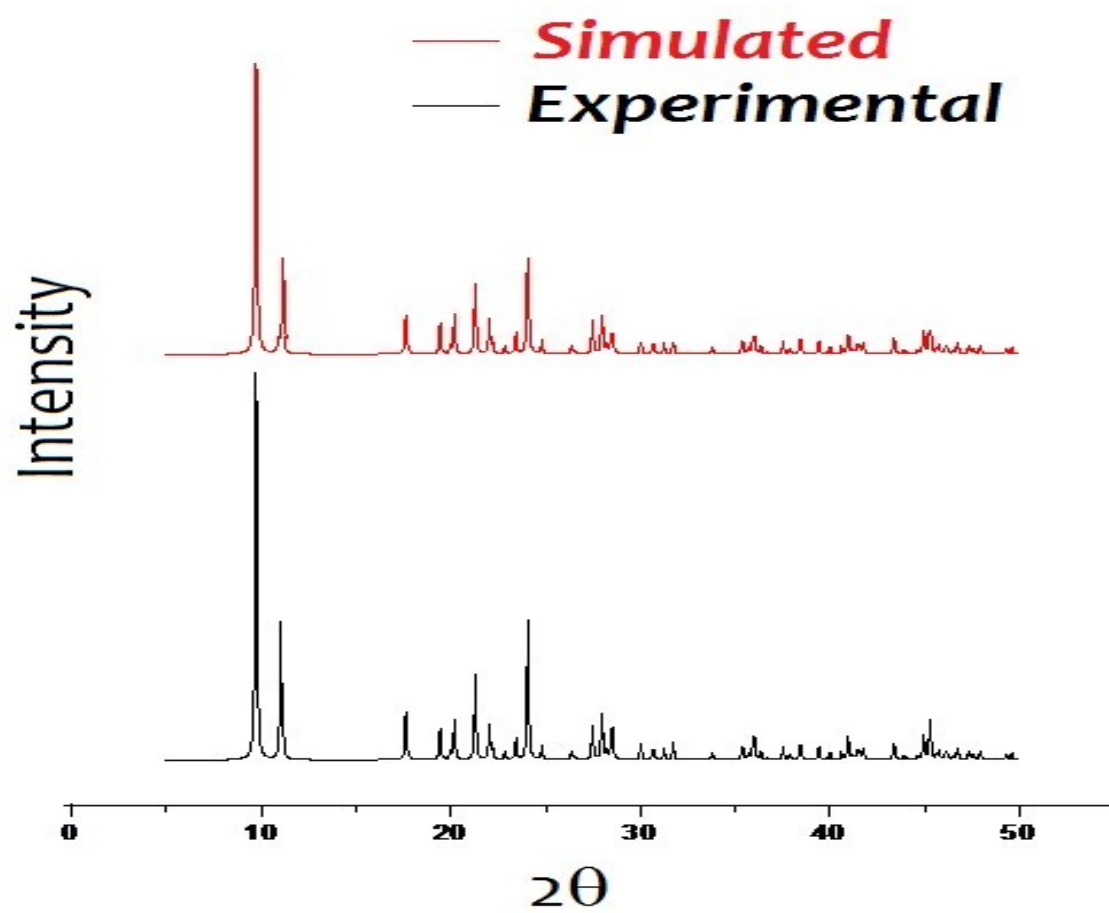


Fig. 1S. PXRD patterns (experimental and simulated) for **1**.

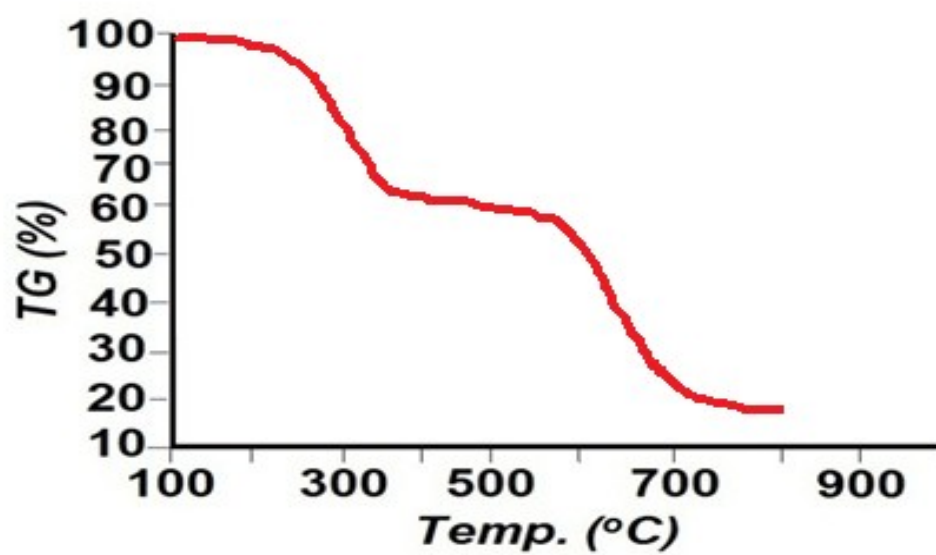


Fig. 2S. Thermogram for 1.