Electronic Supplementary Information File

Azido bridged binuclear copper (II) Schiff base compound: synthesis, structure and electrical properties

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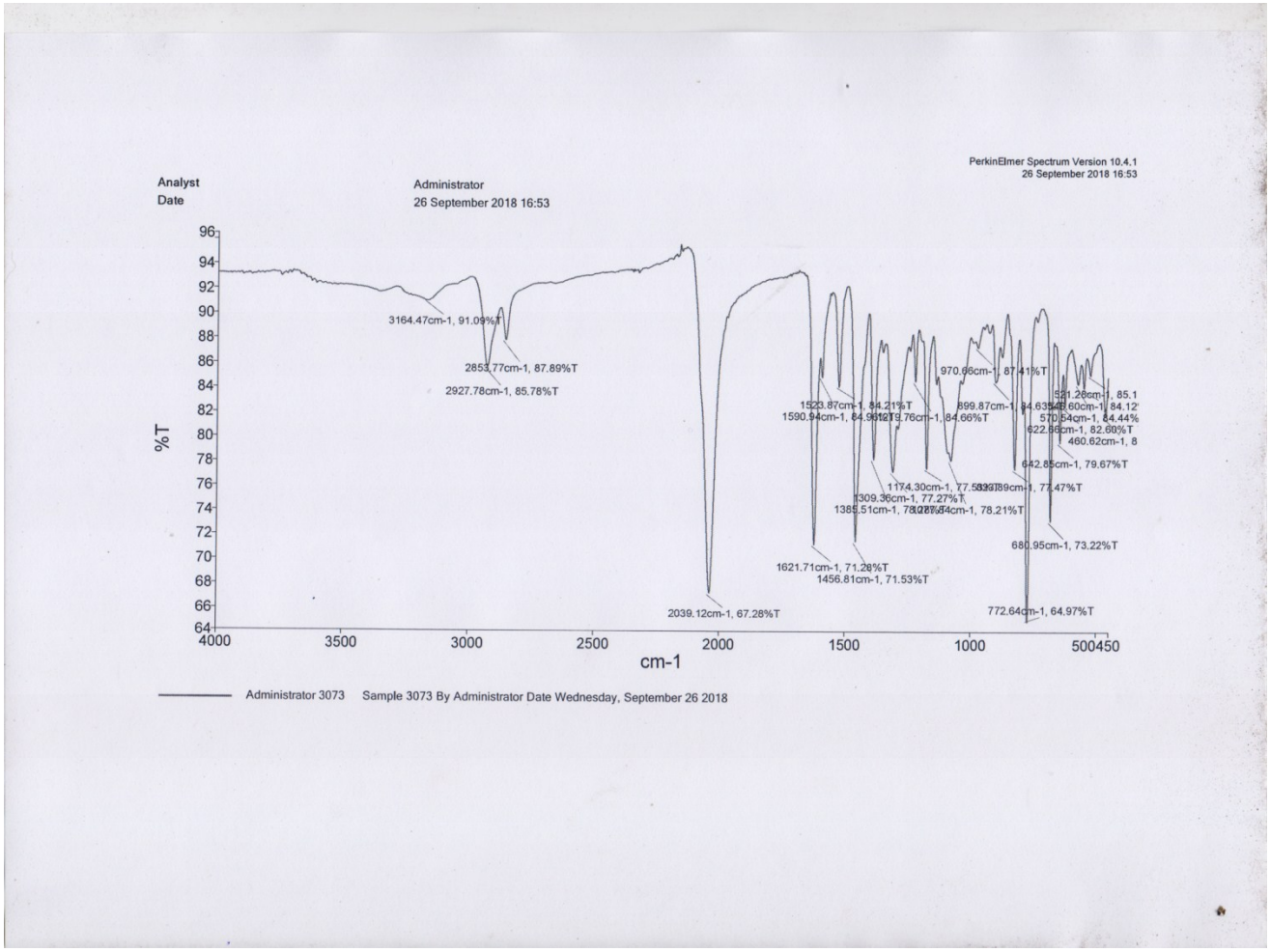


Fig. S1: IR Spectra of Complex**1**

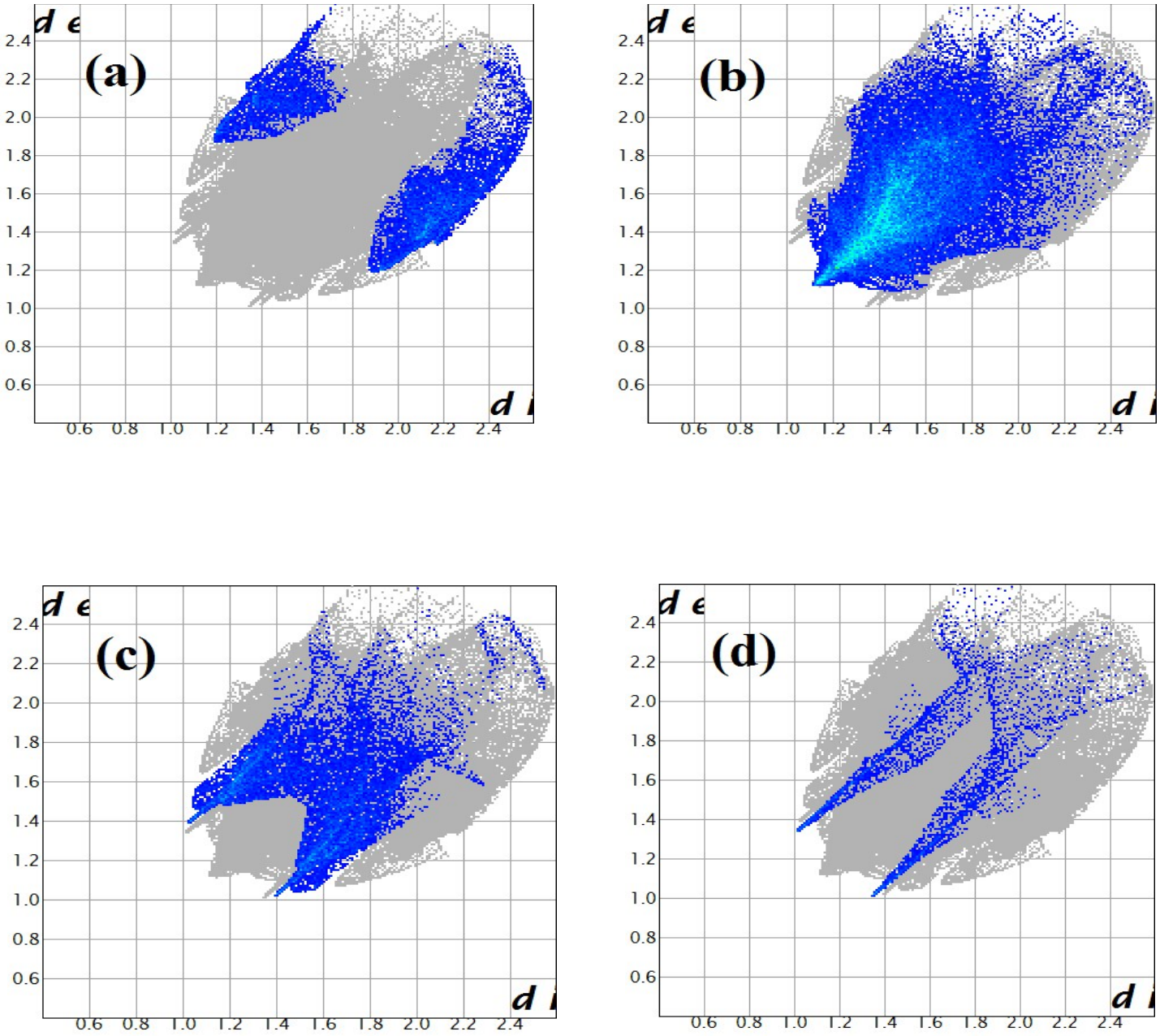
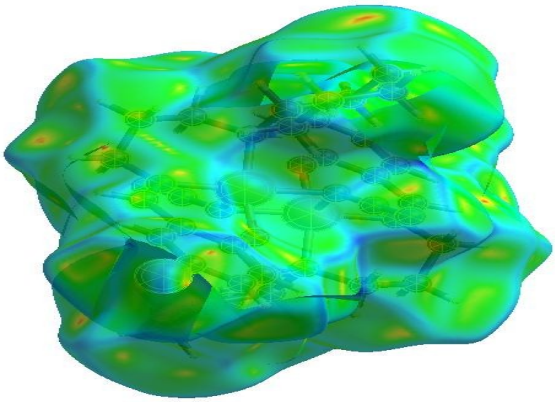
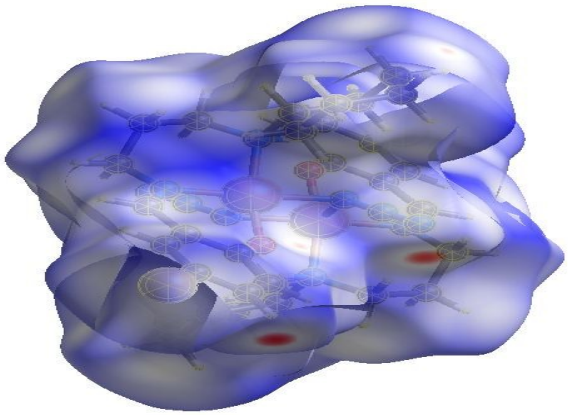


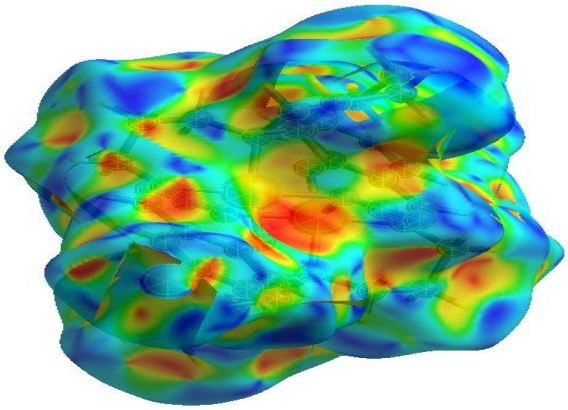
Fig. S2 (A): Decomposed fingerprint plot of complex **1**: (a) Br···H/H···Br contacts; (b) H···H contacts; (c) N···H/H···N contacts; (d) O···H/H···O contacts.



(a)



(b)



(c)

Fig. S2 (B): (a) Curvedness (b) Dnorm (c) Shape index

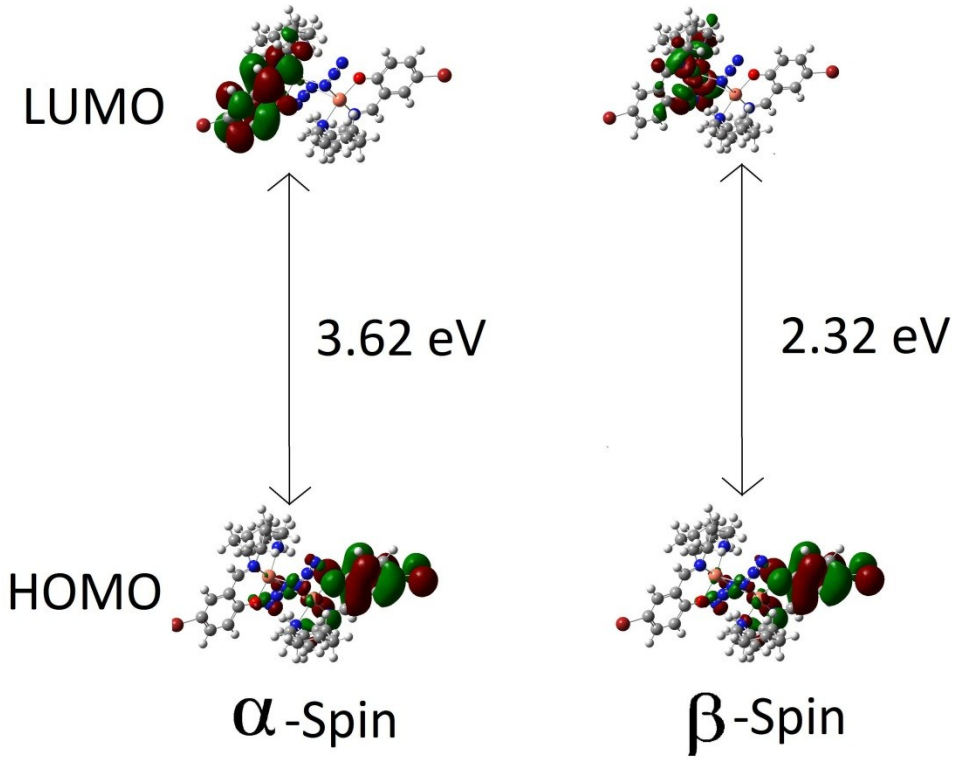


Fig. S3 DFT computed energy of MOs in the triplet state and the energy difference between HOMO and LUMO of the compound **1**.

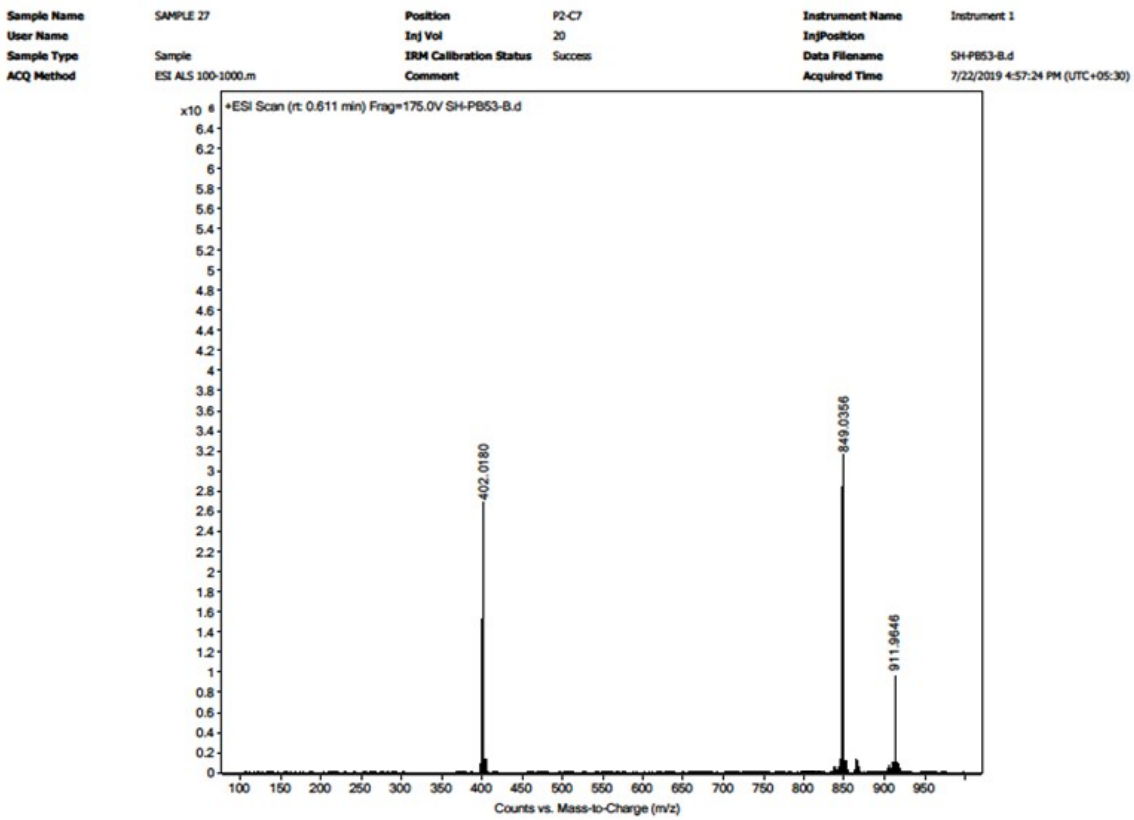


Fig.S4(a) ESI MS spectra of complex**1** in 1:1 methanol and acetonitrile mixture.

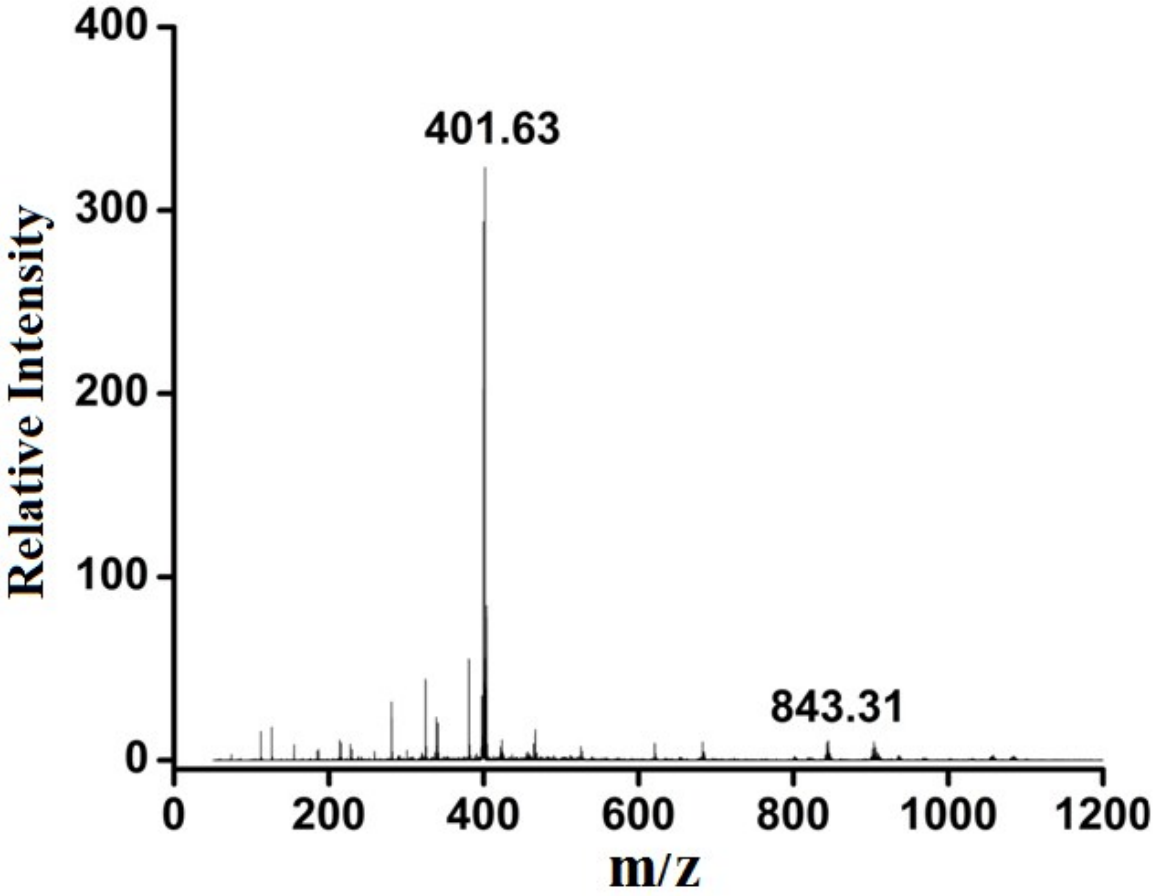


Fig.S4(b) ESI MS spectra of complex**1**before deposition.

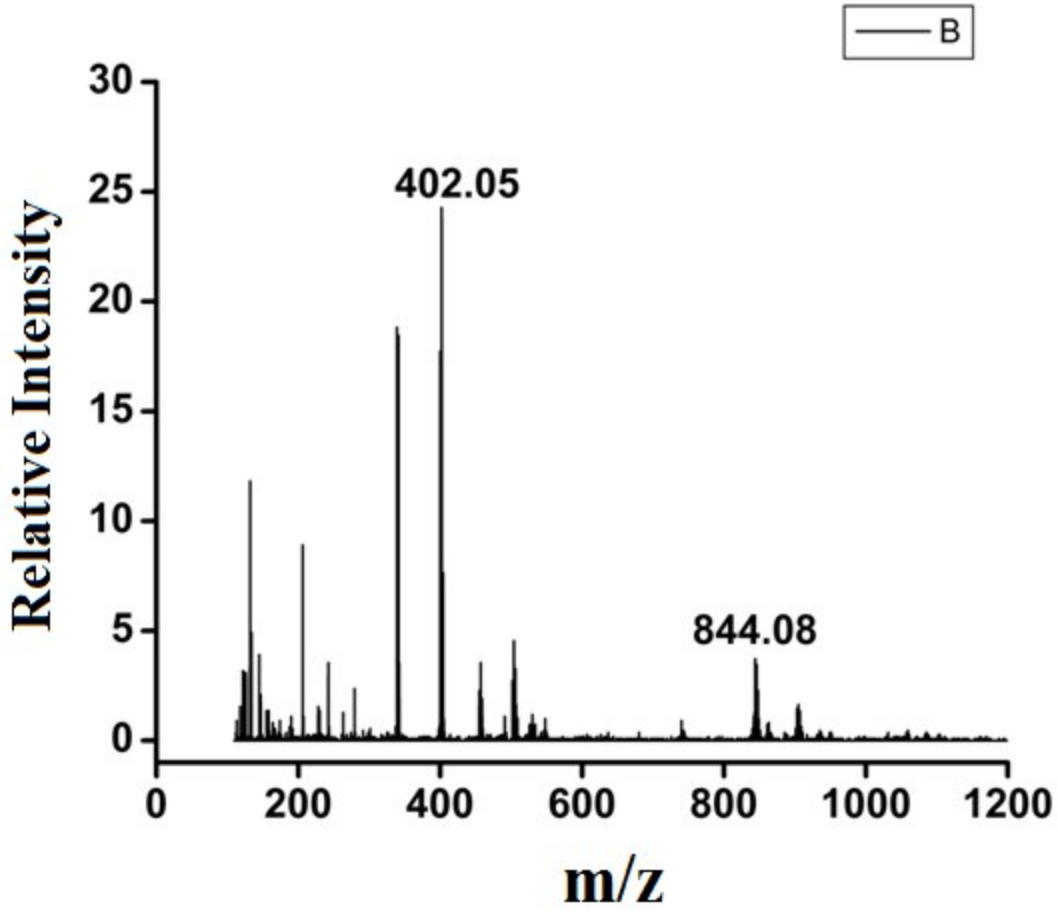


Fig.S4(c) ESI MS spectra of complex **1**after deposition.

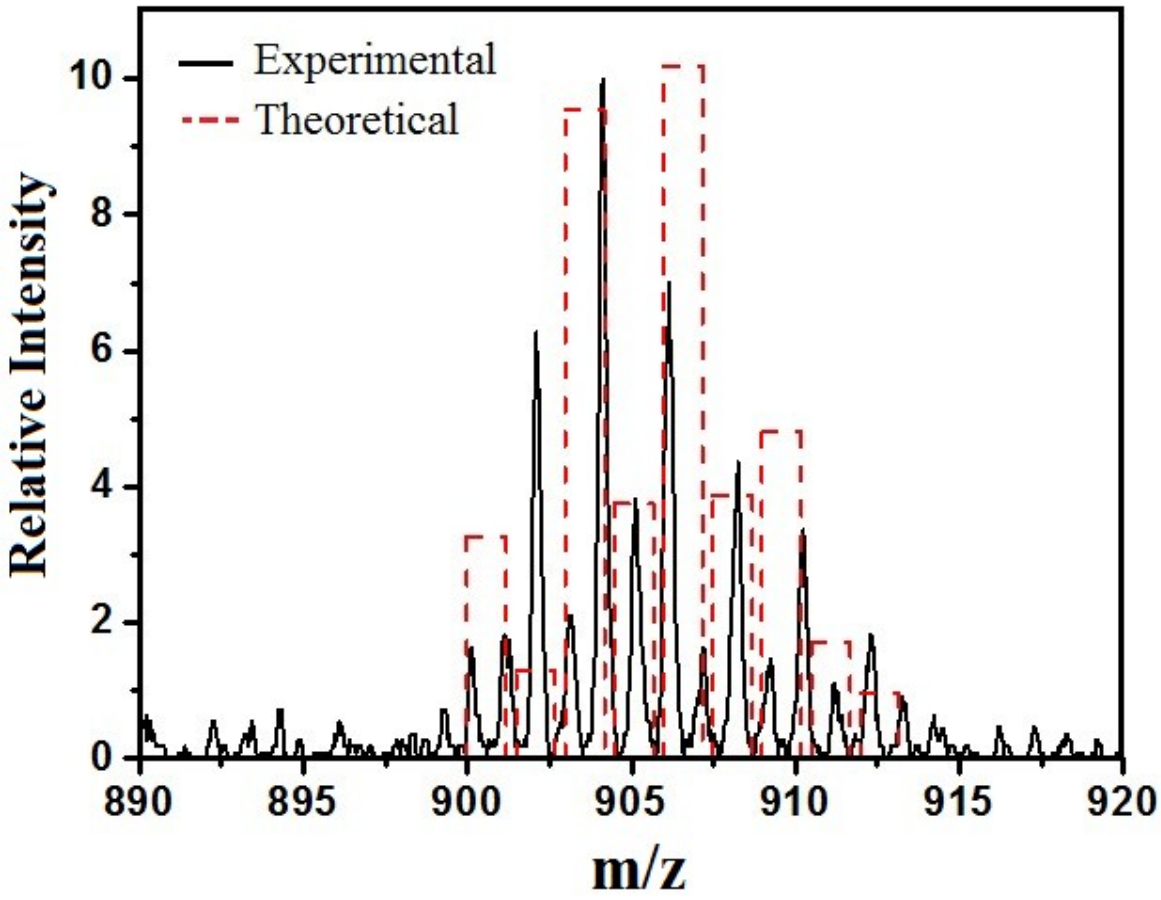


Fig.S4(d) Experimental isotopic pattern (black) of complex **1** with theoretical pattern (red) after deposition.

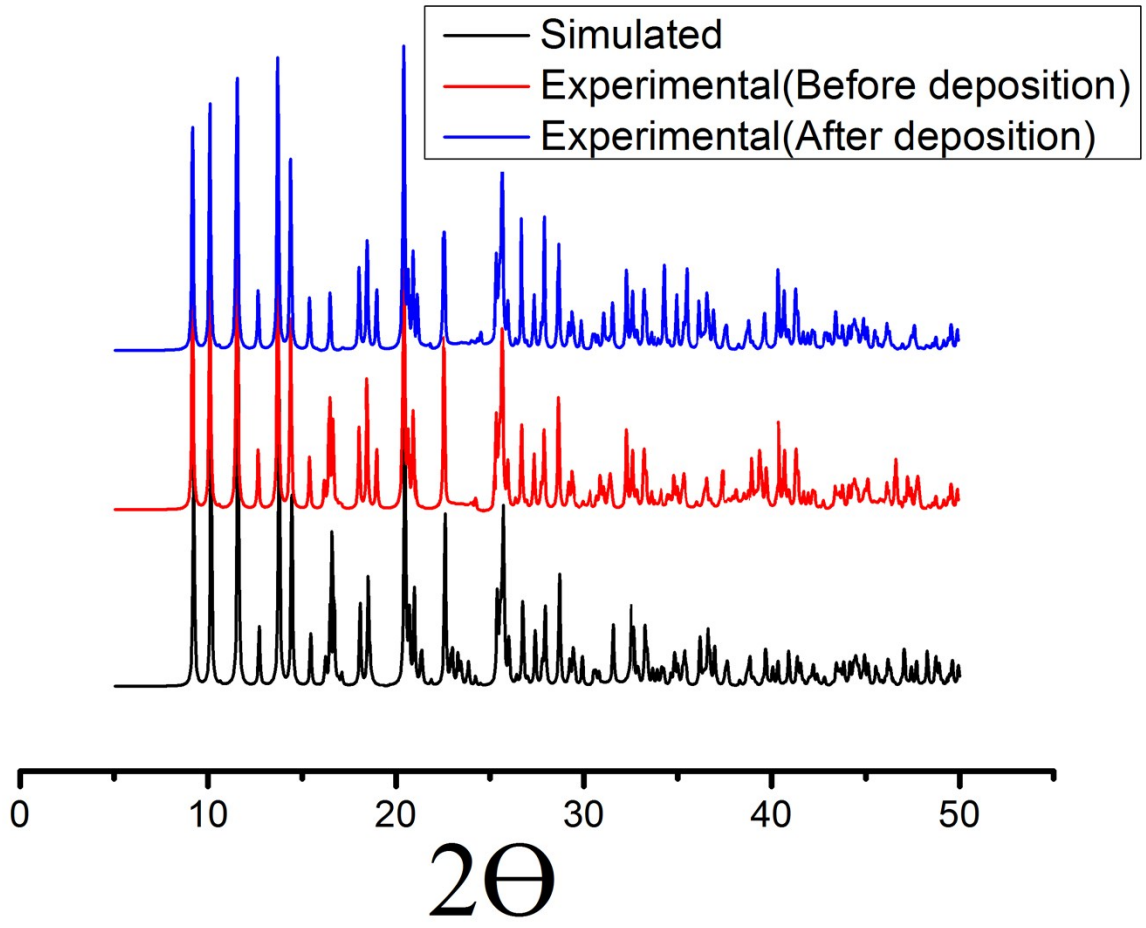


Fig.S5 Experimental (before and after deposition) and simulated PXRD patterns of the complex confirming purity of the bulk material.

Table S1: Bond distances (Å) and bond angles (◦) for complex 1

Bond distances (Å)			
Bond	X-ray	Bond	X-ray
Cu1A-O7A	1.926(6)	Cu1A-N20	2.275(8)
Cu1A-N9A	1.961(6)	Cu1A- N20A	2.037(7)

Cu1A-N13A	2.065(6)	N20-N21	1.22(1)
Bond angles (◦)			
Angle	X-Ray (◦)	Angle	X-Ray (◦)
Cu1-N20A-Cu1A	93.9(3)	N13-Cu1-N20	84.9(3)
O7A-Cu1A-N9A	91.7(3)	N13-Cu1-N20A	92.9(3)
O7A-Cu1A-N13A	167.0(3)	N20-Cu1-N20A	86.1(3)
O7A-Cu1A-N20	97.1(3)	Cu1A-N20-N21	129.6(6)
O7A-Cu1A-N20A	87.5(3)	N20-N21-N22	178.5(9)
N9-Cu1-N20A	100.8(3)	Cu1A-N20A-N21A	117.8(6)
Cu1-N20-N21	129.6(6)	N20A-N21A-N22A	178.5(9)