

## *Supporting Information*

# **Synthesis, Crystal Structure, Magnetic Study and Magneto-structural Correlation of Three Cu(II) Complexes formed via Pyridine bis(hydrazone) based ligand**

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**Table S1.** Hydrogen bonding distances (Å) and symmetry operations for the complex **1**

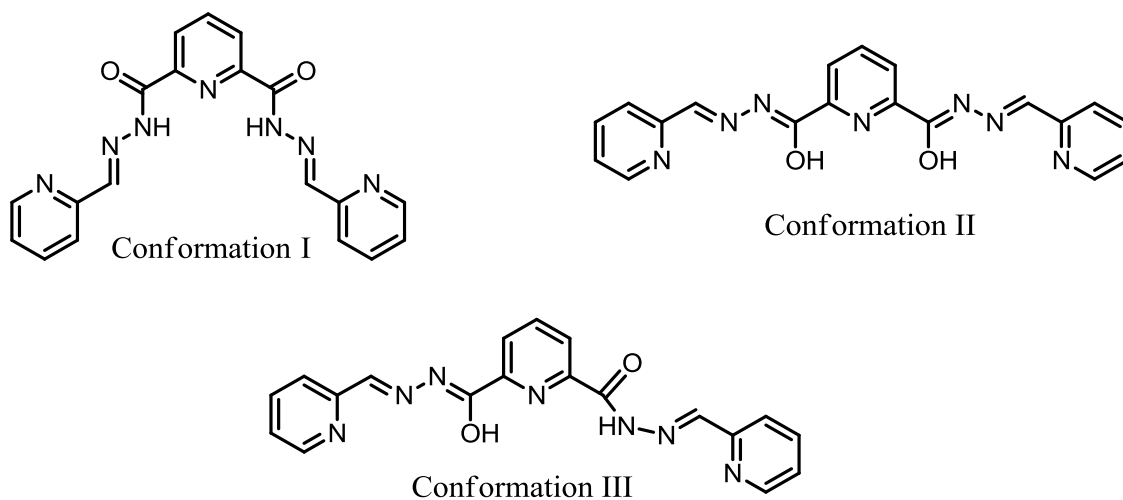
D...A	Symmetry operation	D...A(Å)
O4...O24	x-1,y,z	2.73(9)
O3...O20	-x+1,-y+1,-z+1	2.60(7)
O22...O19	-x+2,-y+1,-z+1	2.80(9)
O14...O15	-x+2,-y,-z+1	2.97(2)
O53...O7	x+1,y,z	2.60(1)
O15...O31	x,y-1,z	2.53(3)
O6...O54	-x+1,-y+1,-z+1	2.61(7)
O6...O17	-x+1,-y+1,-z+1	2.64(6)
O53...O32	-x+1,-y+1,-z+1	2.92(3)
O20...O16	x,y+1,z	2.76(1)
O17...O51	-x+1,-y+1,-z	2.91(9)
O19...O10	-x+2,-y+1,-z	2.58(9)
O10...O41	x+1,y,z	2.74(7)
O39...O13	x-1,y,z	2.95(8)
O29...O5	-x+1,-y+1,-z+1	3.00(2)
O29...O4	-x+1,-y+1,-z+1	2.96(2)

(D: donor, A:acceptor)

**Table S2.** Hydrogen bonding distances (Å) and symmetry operations for the complex **2**

D-H...A	Symmetry operation	D...A(Å)
O6...O3	x,y,z-1	2.72(1)
O5...O4	---	2.93(2)
O6...O5	x,y,z+1	2.75(1)

(D: donor, A:acceptor)



**Chart S1.** Existence of different conformations of the ligand (H<sub>2</sub>L).

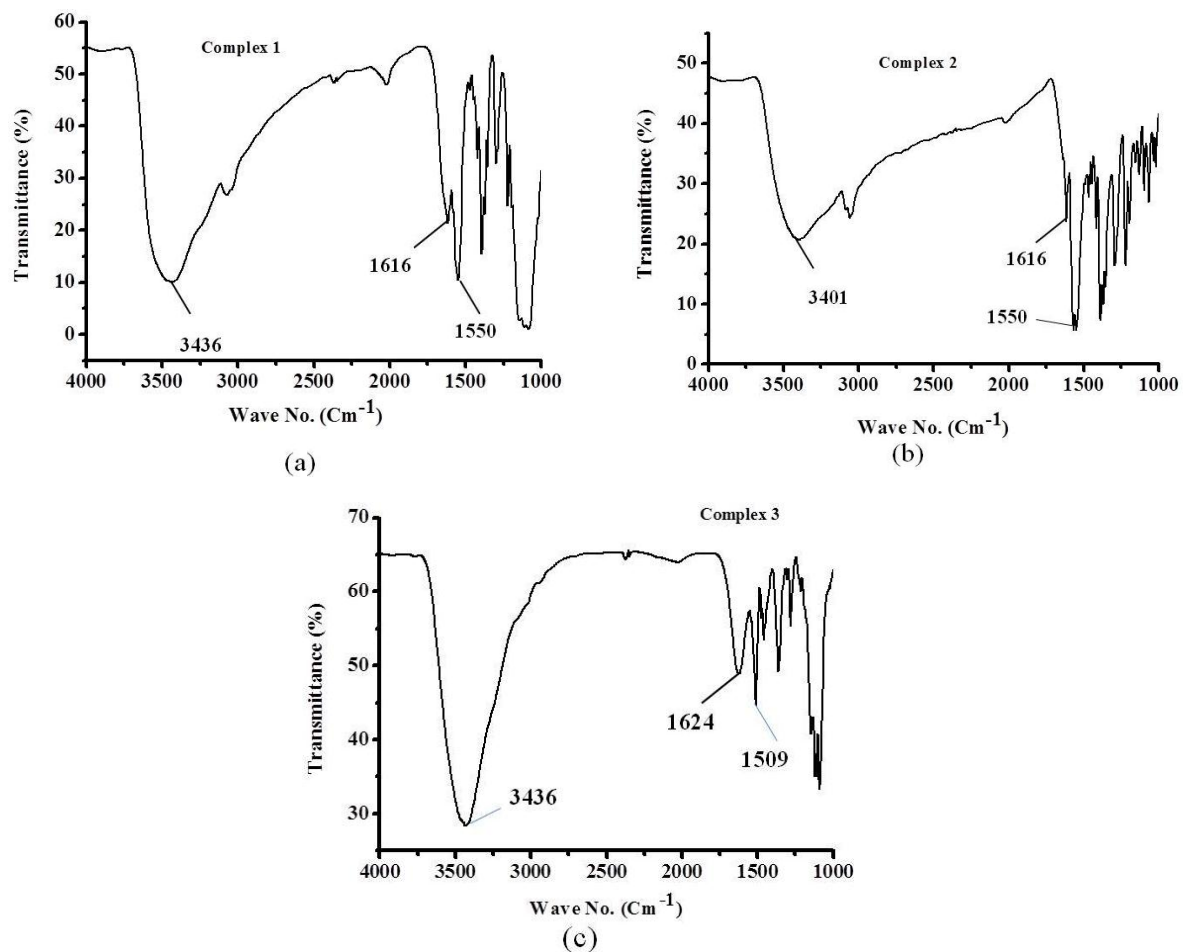


Fig. S1. IR spectra of (a) complex 1, (b) complex 2 and (c) complex 3 in solutions.

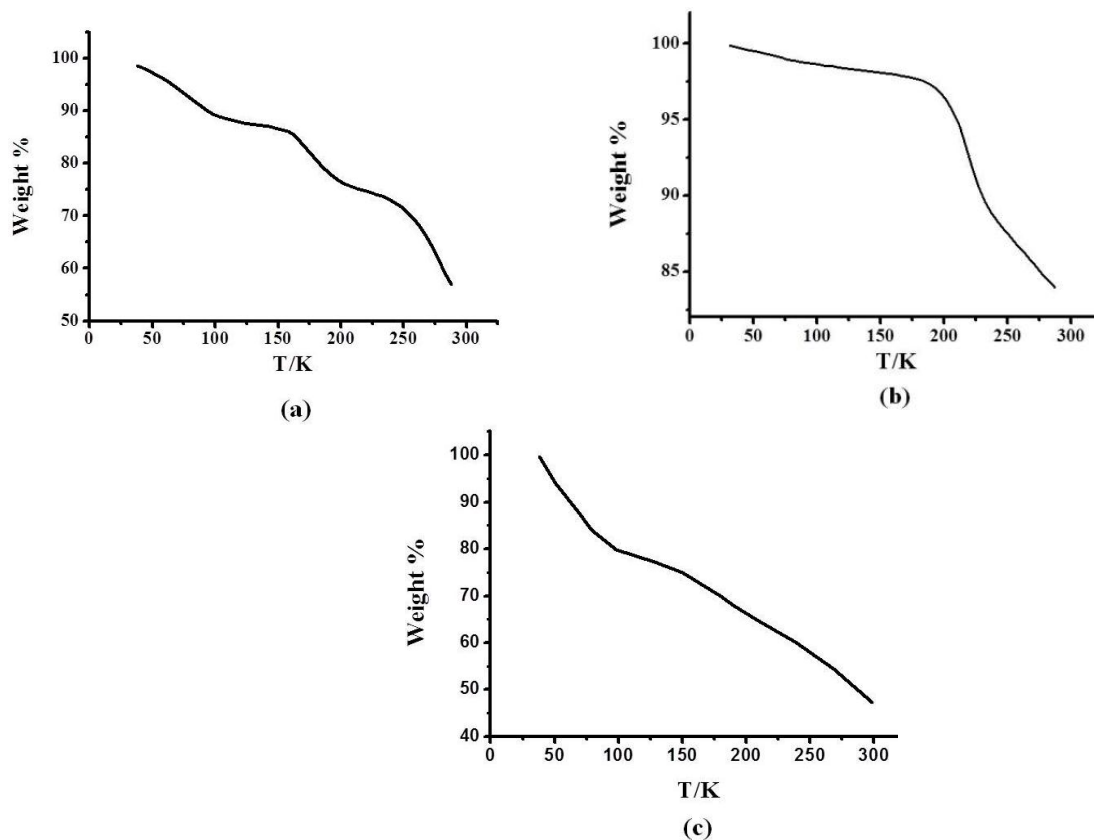


Fig. S2. TG analysis of (a) complex 1, (b) complex 2 and (c) complex 3

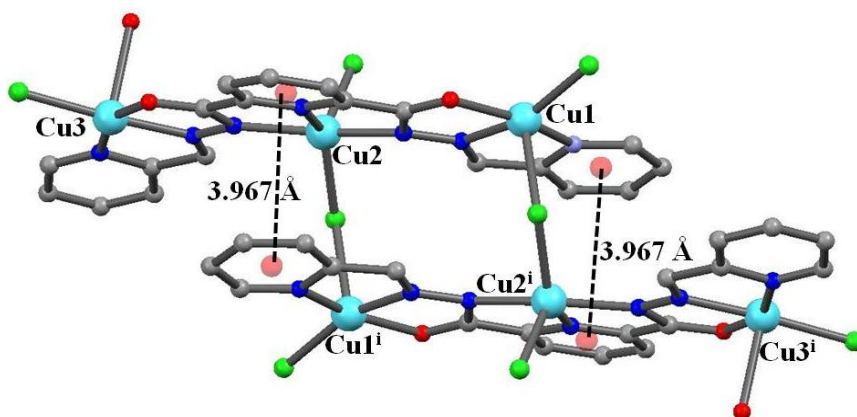


Fig. S3.  $\pi$ - $\pi$  stacking between pyridine ring of opposite trimeric unit of complex 2 where 'i' denotes atom generated by center of inversion (-x, -y, -z).

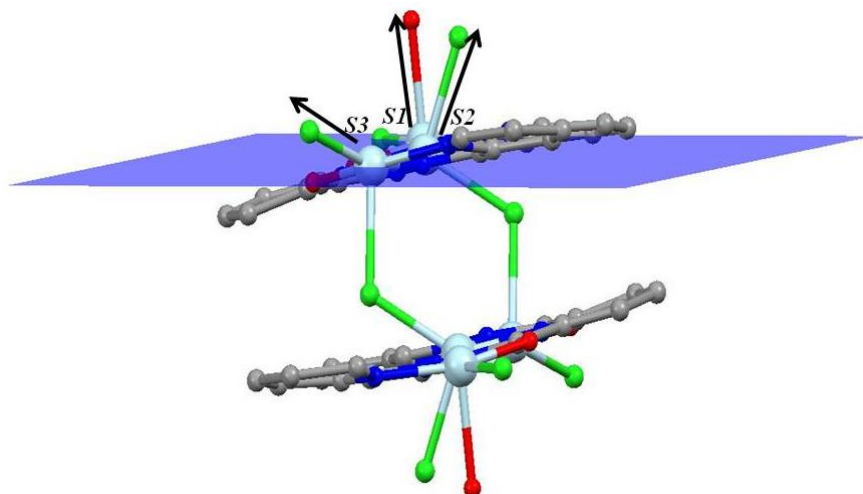


Fig. S4. Illustration of the canting of spins with different orientations of complex 2.

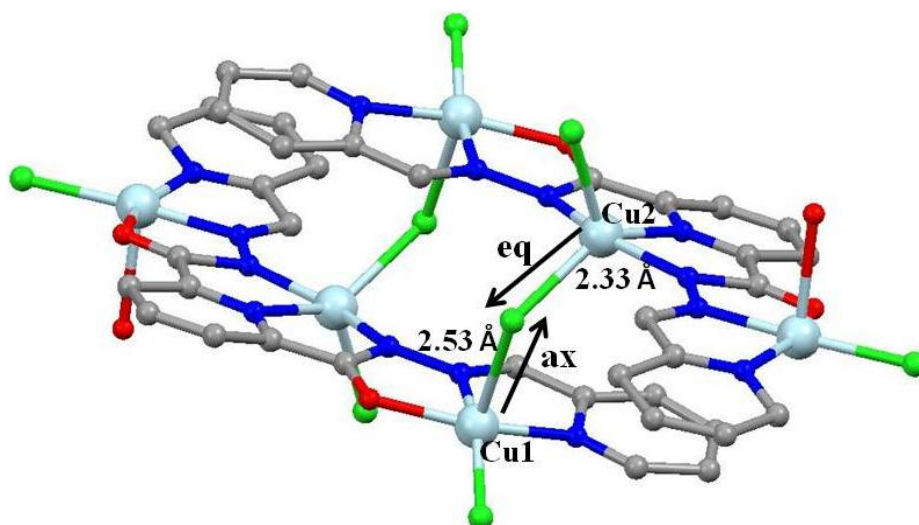


Fig. S5. Axial (ax)-equatorial(eq) interactions of Cu(II) centres through chloro-bridging of complex 2.

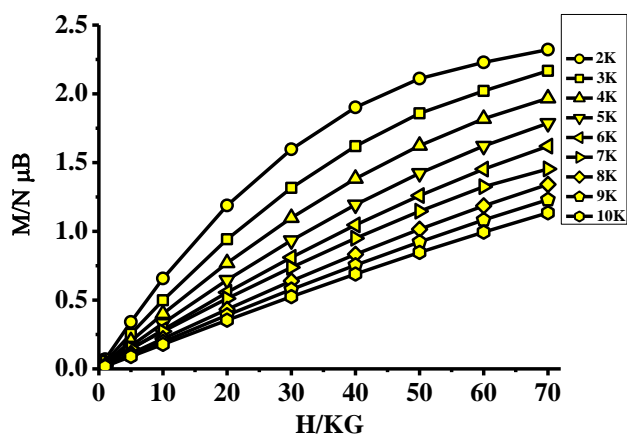


Fig. S6. Field-dependencies of isothermal normalized magnetization for complex 1.

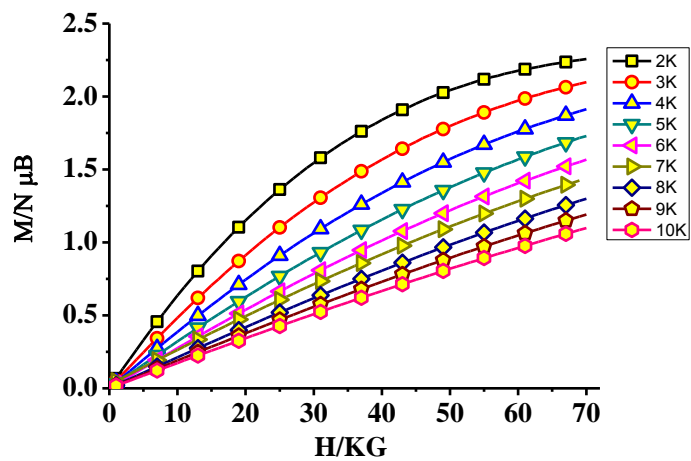


Fig. S7. Field-dependencies of isothermal normalized magnetizations for complex 2.

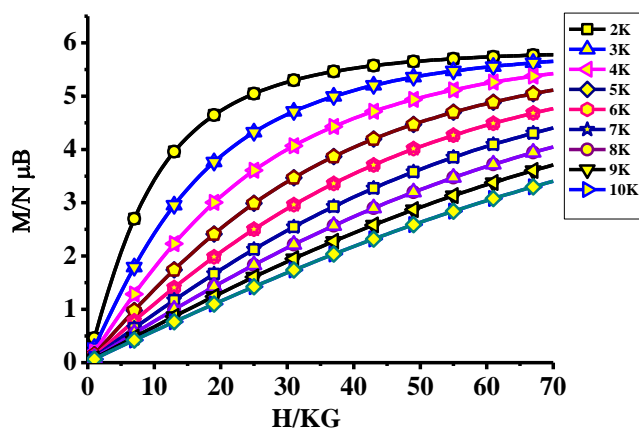


Fig. S8. Field-dependencies of isothermal normalized magnetizations for complex 3.

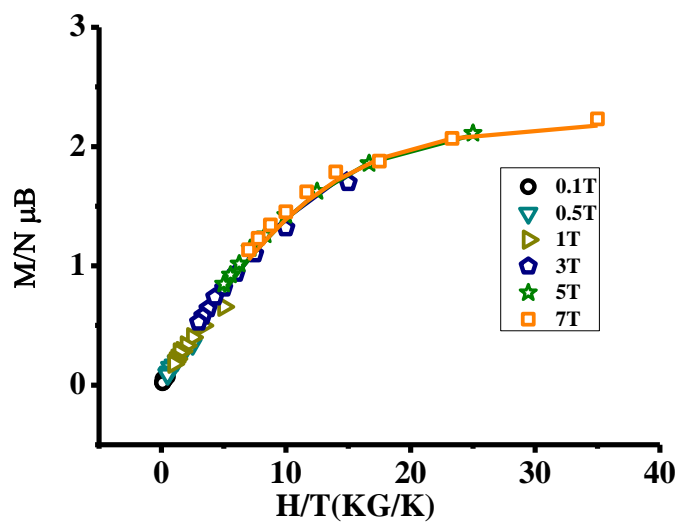


Fig. S9.  $M/N\mu_B$  vs  $H/T$  plots for complex 1.

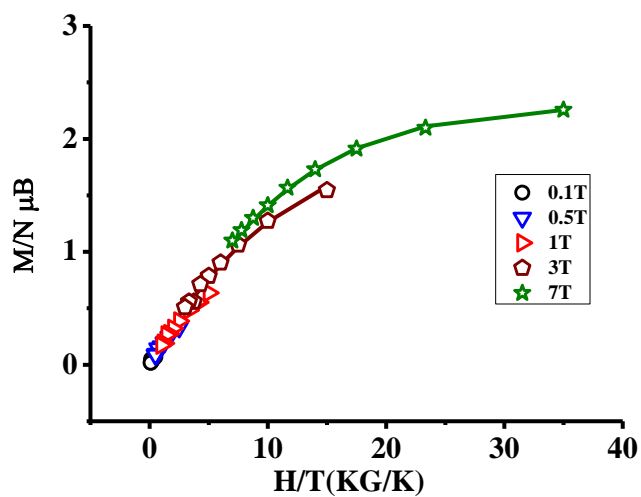


Fig. S10.  $M/N\mu_B$  vs  $H/T$  plots for complex 2.

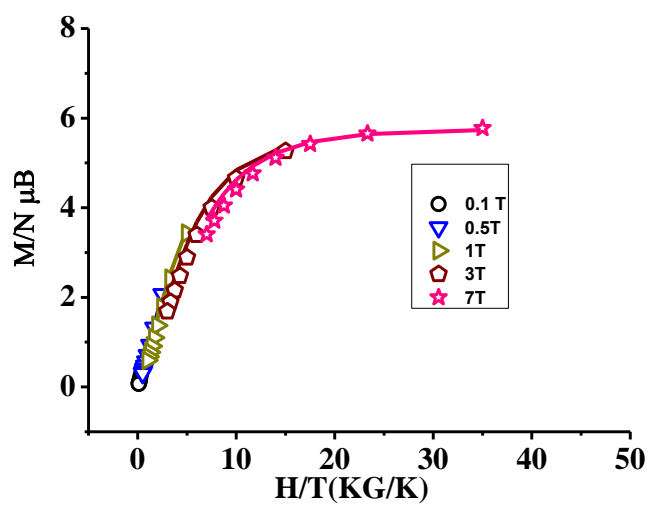


Fig. S11.  $M/N\mu_B$  vs  $H/T$  plots for complex 3.

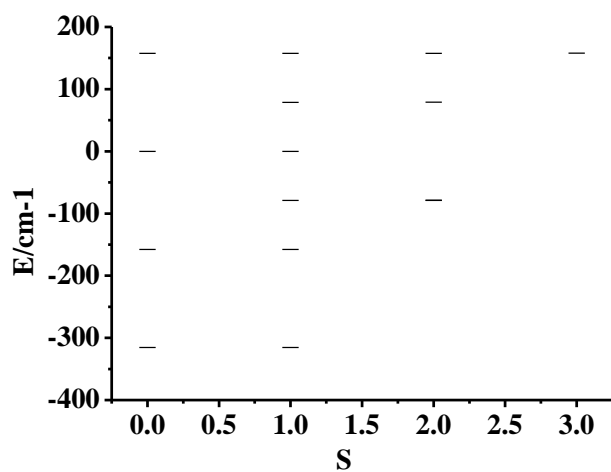


Fig. S12. Energy spectrum vs total spin (S) for complex 1.

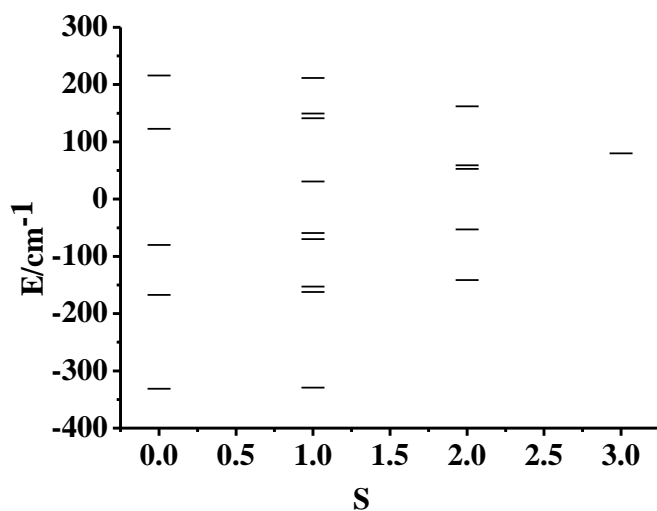


Fig. S13. Energy spectrum vs total spin (S) for complex 2.

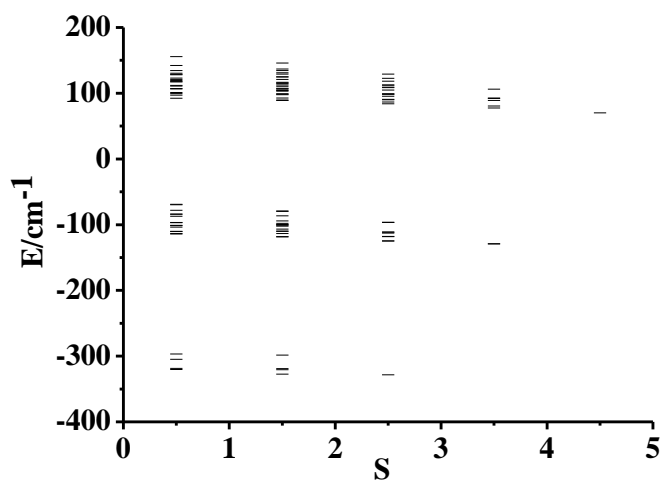
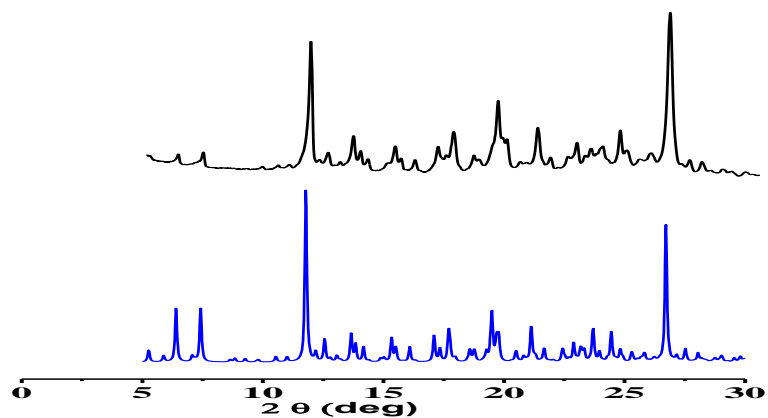
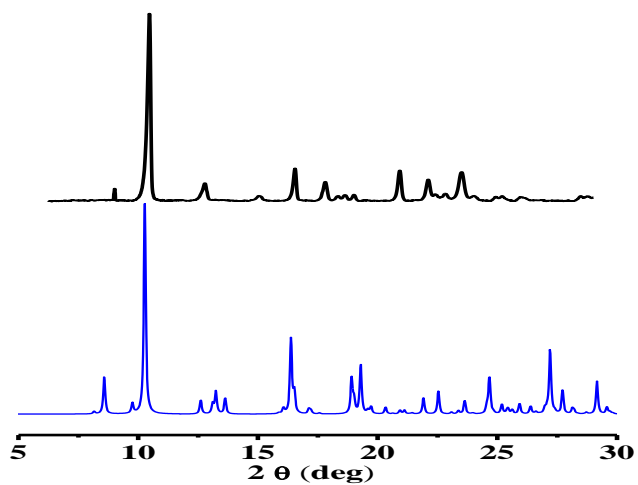


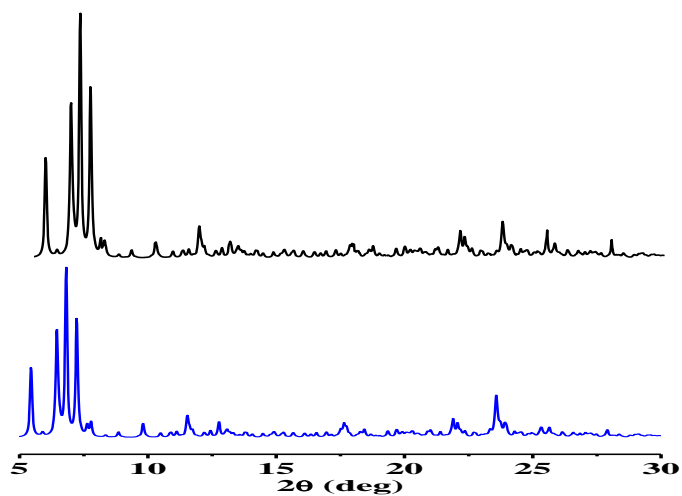
Fig. S14. Energy spectrum vs total spin (S) for complex 3.



**Fig. S15.** Experimental (black) and simulated (blue) powder XRD data for complex 1.



**Fig. S16.** Experimental (black) and simulated (blue) powder XRD data for complex 2.



**Fig. S17.** Experimental (black) and simulated (blue) powder XRD data for complex 3.