Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

A novel large Ni-azido circle with co-ligands–tridentate (NNO) Schiff bases: hexagonal structure and ferromagnetic property

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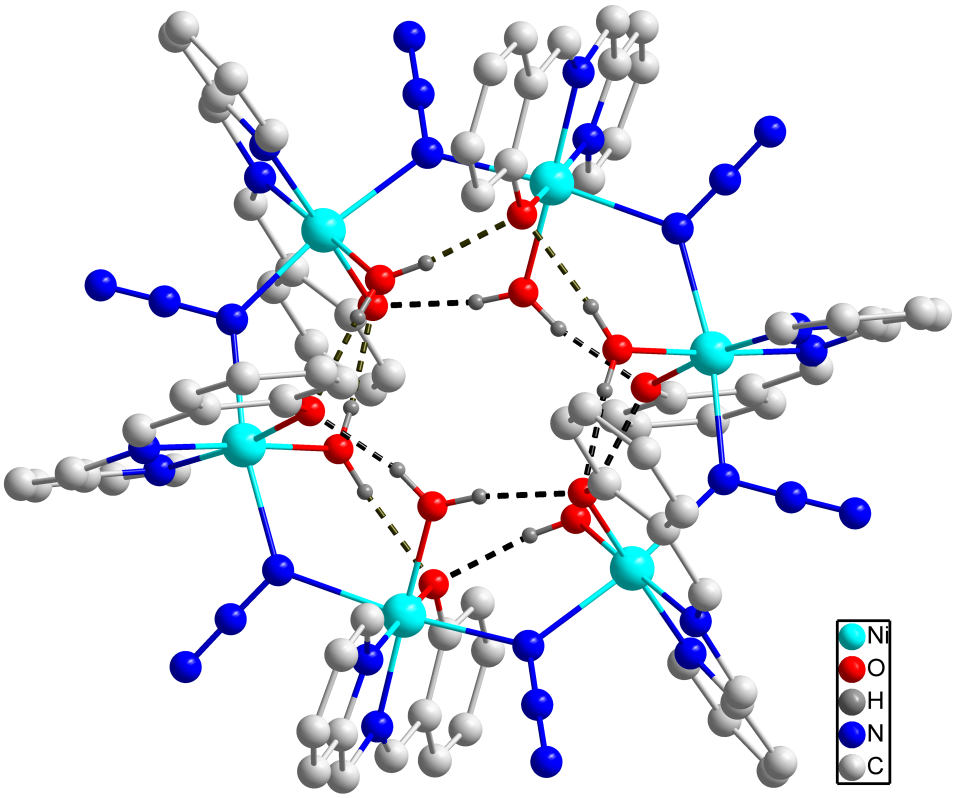

Fig.s1 Perspective view of complex **1**. All hydrogen atoms excepted H2A, H2C, H4A, H4C, H6A, H6B and solvent water molecules are omitted for clarity. Hydrogen bonds are showed as dash line.

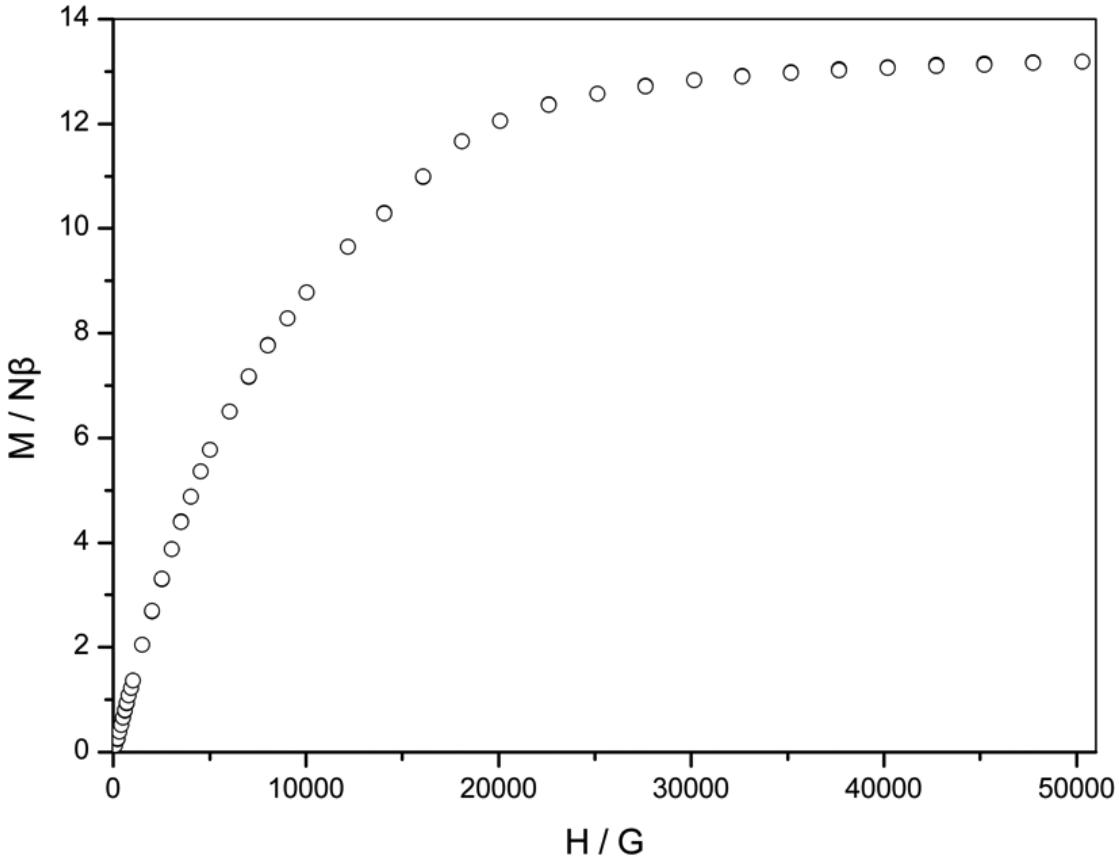

Fig. s2. Plot of the reduced magnetization for **1** (*M*/Nβ) vs *H* at 1.9K.

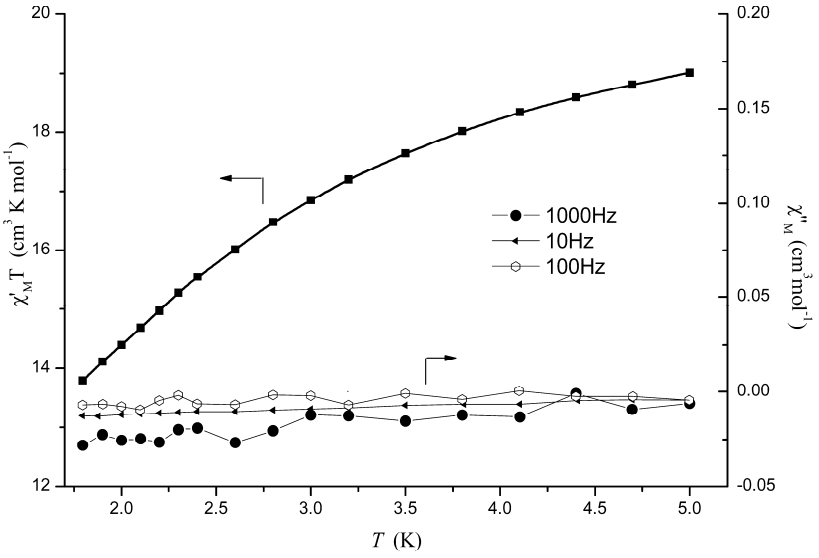

Fig. s3. Plot of temperature dependence of the in-phase $\chi'_M T$-T and out-of-phase χ''_M-T ac magnetic susceptibilities.

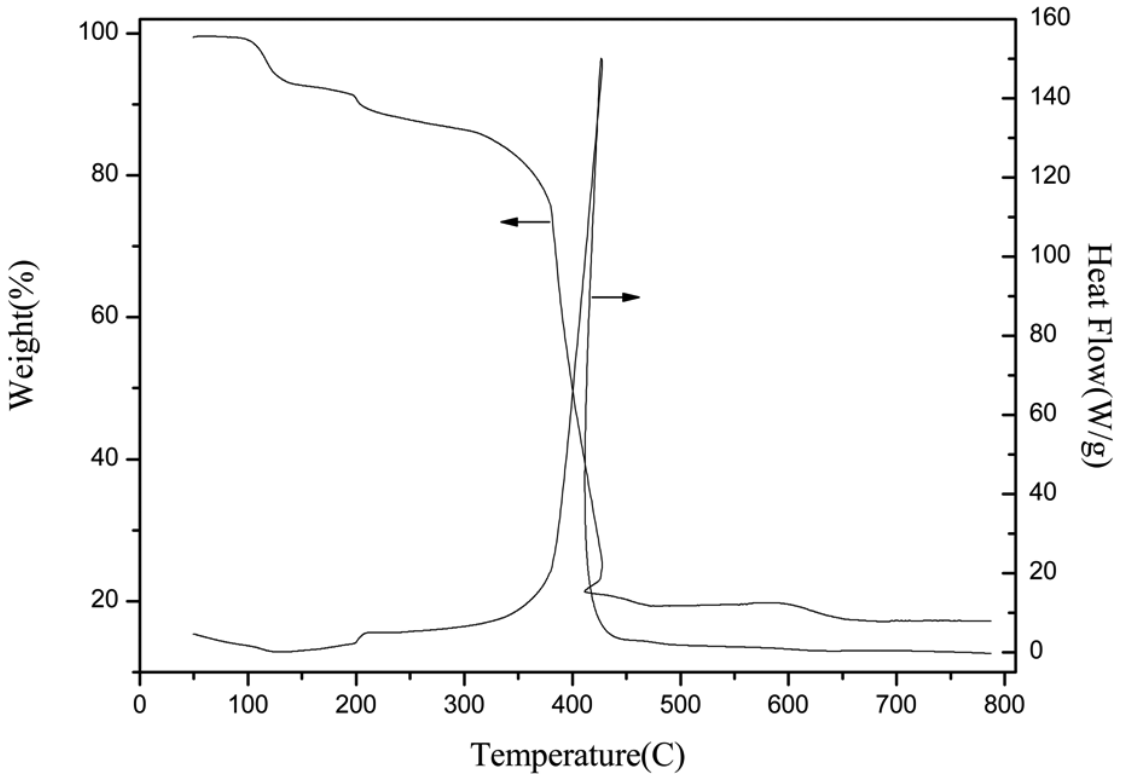

Fig. s4. The TG-DSC curves of complex **1**.H_2O precursor under a nitrogen atmosphere with a heating rate of 10 /min without the ball-milled precursor.

The result of TG-DSC indicated that it lost the H_2O molecular outer the ring above 99.6□, with a mass loss of approximately 1.01% (calculated loss of 0.9%), and with another mass loss about 5.78% from 99.6□ to 141.7□, which should be the six coordinated water(calculated loss of 5.41%). Above 141.7□, it lost the six azido molecules, the mass loss of about 12.57%(calculated loss of 12.62%), further, it lost mass of 63.11% above 355.6□, what means the six Schiff bases were gone(calculated loss of 63.44%). The residual is about 17.53%, which coincide with the Nickel dioxide (NiO, calculated of 17.63%).

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Table s1. Hydrogen bonds of complex **1**

D-H…A	d(D-H)	d(H…A)	d(D…A)	< (DHA)
O(6)-H(6A)...O(3)	0.85	1.83	2.671(4)	170.2
O(2)-H(2A)...O(3)	0.85	1.95	2.779(4)	166.3
O(4)-H(4A)...O(1)	0.85	1.78	2.610(4)	166.5
O(4)-H(4C)...O(5)	0.85	1.85	2.689(4)	170.6
O(6)-H(6B)...O(1)#1	0.85	1.85	2.685(4)	166.4
O(2)-H(2C)...O(5)#1	0.85	1.85	2.679(4)	165.9

Symmetry transformations used to generate equivalent atoms: #1 1-x, -y, 1-z