Electronic supplementary information (ESI)

Long-range ordering or not: magnetic properties modulated by second ligands in flexible three-dimensional metal-organic frameworks

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Crystal Data Collection and Refinement

Diffraction intensity data were collected at 296 K on a Bruker APEX II diffractometer equipped with a CCD area detector and graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). Empirical absorption corrections were applied using the SADABS program.[1] The structures were solved by the direct method and refined by the full-matrix least-squares method on F^2, with all non-hydrogen atoms refined with anisotropic thermal parameters.[2] The hydrogen atoms attached to carbon atoms were placed in calculated positions and refined using the riding model. The ligands in **2** are heavily disordered (Fig. S1).

References:

1. G. M. Sheldrick, *Program for Empirical Absorption Correction of Area Detector Data;* University of Göttingen, Germany, 1996**.**

2. G. M. Sheldrick, *SHELXTL* Version 5.1. Bruker Analytical X-ray Instruments Inc., Madison, Wisconsin,USA, 1998.

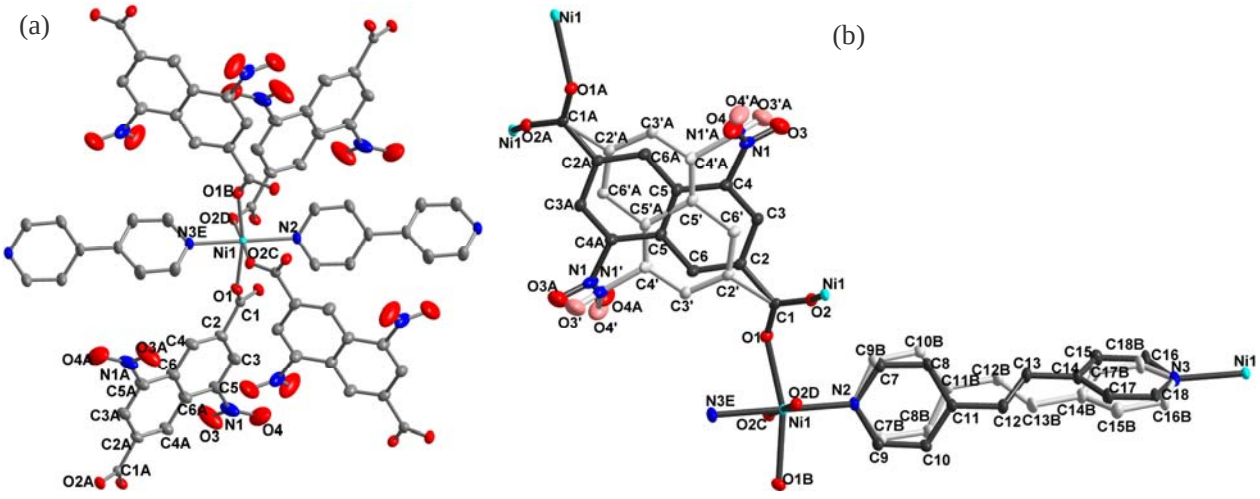

Fig. S1. Coordination geometry around the metal centers in **1** (a) and **2** (b). Symmetry code: A: 0.5-x, -0.5-y, -z, B: -x, y, 0.5-z, C: x, -y, 0.5+z, D: -x, -y, -z, E: x, -1+y, z. The ellipsoids are drawn at 30% probability. The disorder of the ligands in **2** is also shown: the 1,5-dinitronaphthalene moiety, located at an inversion center, is disordered over two independent positions with the occupancies refined to be 0.87 (the dark set) and 0.13 (the light gray set), and the bpe ligand is disordered over two symmetry-related positions with equal occupancies (0.5).

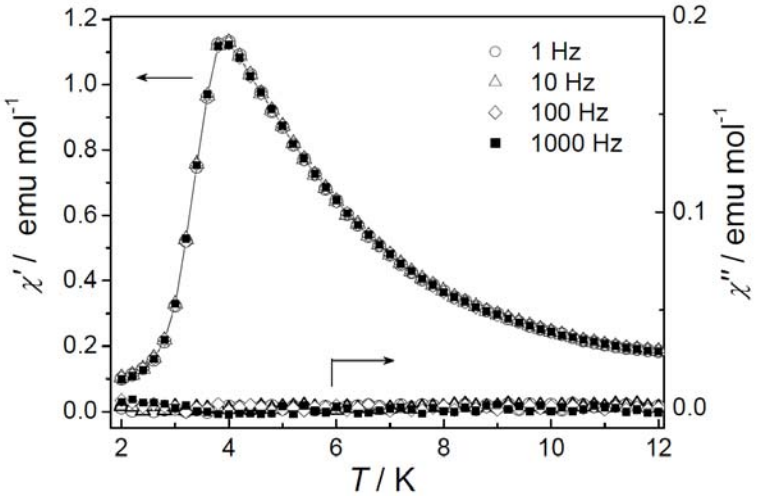

Fig. S2. Thermal dependence of the ac susceptibility of **1**, measured at different frequencies under $H_{dc} = 0$, $H_{ac} = 3.5$ Oe.

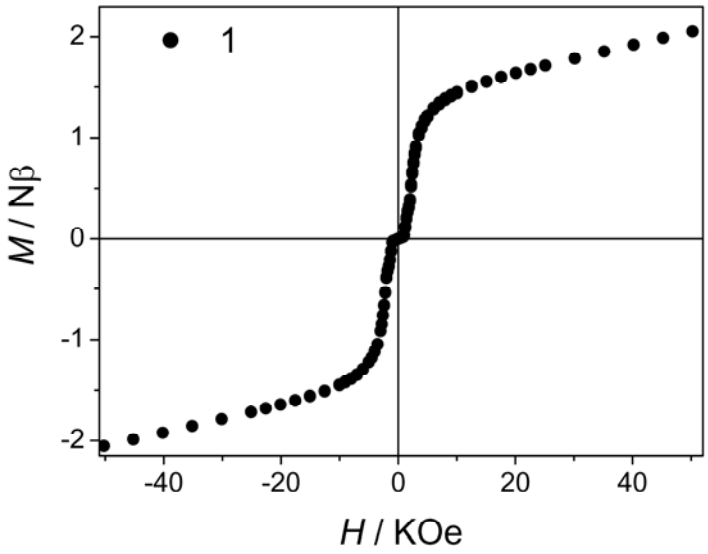

Fig. S3. Hysteresis measurement of **1** at 2 K.