Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Racemic metal phosphonates based on 1-phosphonomethyl-2-benzimidazol-piperidine

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Table S1. Hydrogen bond lengths (Å) and angles (°) for **1**.

D-H...A	d(D-H)	d(D..A)	<DHA
O3W-H3WB...O3	0.850	2.728(3)	134.1
O2W-H2WA...O3W	0.850	2.681(3)	161.5
O2W-H2WB...O3A	0.850	2.712(3)	146.1
O4W-H4WB...O1C	0.850	2.894(3)	168.4
O3W-H3WA...O3D	0.850	2.806(3)	135.9
O1W-H1WA...O4WE	0.850	2.784(3)	146.3
N3-H3C...O6WF	0.850	2.852(5)	142.2
O4W-H4WA...O2WG	0.850	2.837(3)	168.4
O6W-H6WA...O4WG	0.850	2.859(5)	132.8
O6W-H6WB...N2H	0.850	3.266(5)	160.8

Symmetry codes: A: x+1, y, z; B: x-1, y, z; C: x+1, y-1, z; D: -x, -y+1,- z+1; E: x, y+1, z; F: x, y, z-1;G: -x+1, -y+1, -z+1; H: -x+1, -y+2, -z+1.

Table S2. Hydrogen bond lengths (Å) and angles (°) for **3**.

D-H...A	d(D-H)	d(D..A)	<DHA
O1W-H1X...O3C	0.850	2.971(6)	118.00
O1W-H1Y...O2WD	0.850	2.954(6)	111.00
O2W-H2X...O1WD	0.860	2.954(6)	109.00
O2W-H2Y...O2E	0.840	2.761(7)	140.00
N3-H3C...O2F	0.860	2.692(6)	159.00

Symmetry codes: C: x, 1+y, z; D: -x, 1-y, 1-z; E: 1-x, 1/2+y, 3/2-z ; F: 1-x, -y, 1-z.

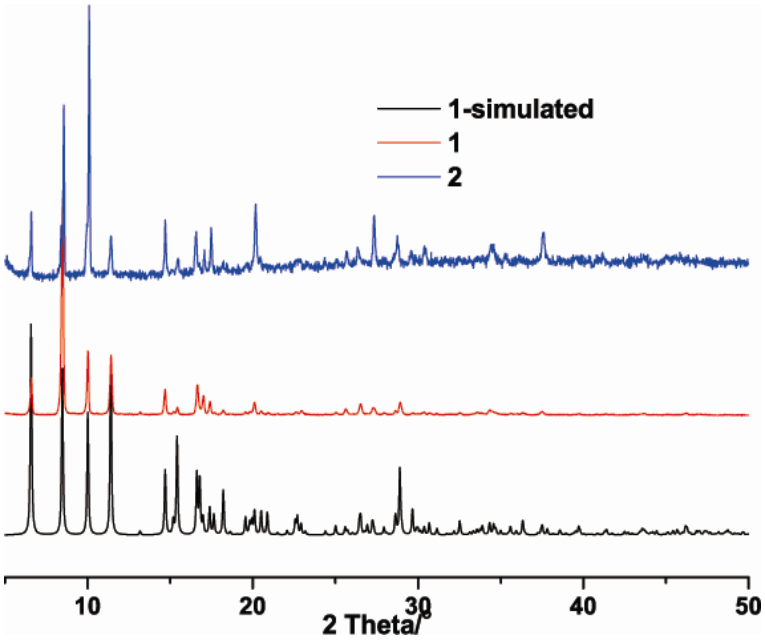

Fig. S1 Powder XRD patterns for compounds **1**, **2** and **1**-simulated from single crystal data.

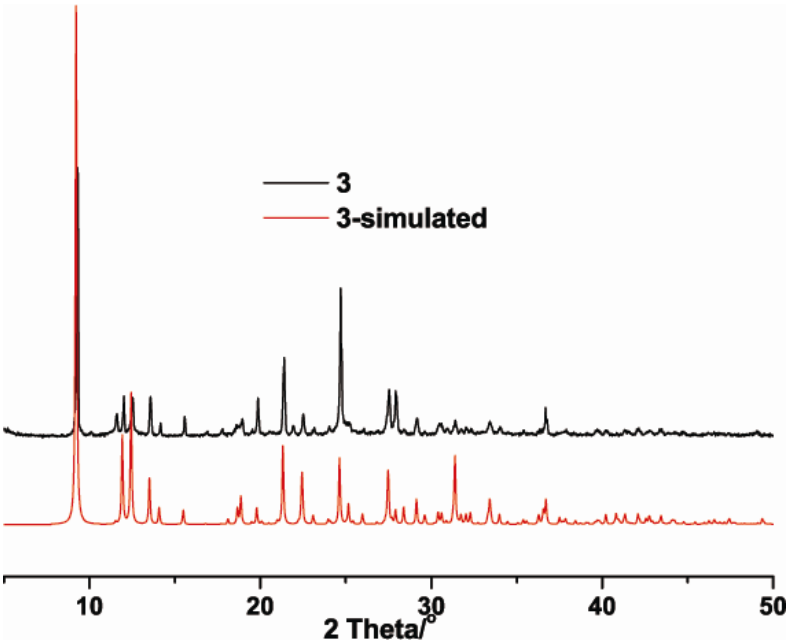

Fig. S2 Powder XRD patterns for compound **3** and **3**-simulated from single crystal data.

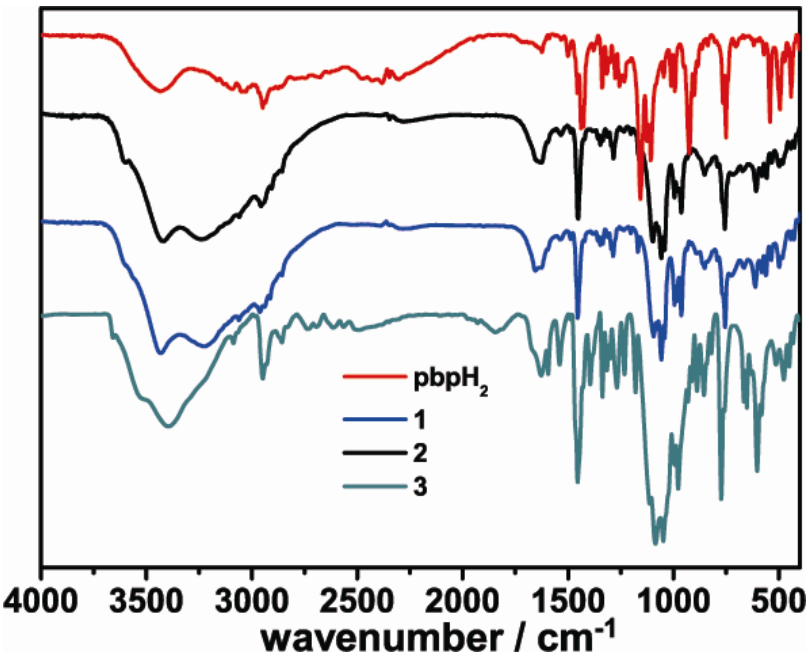

Fig. S3. The IR spectra of compounds **1- 3.**

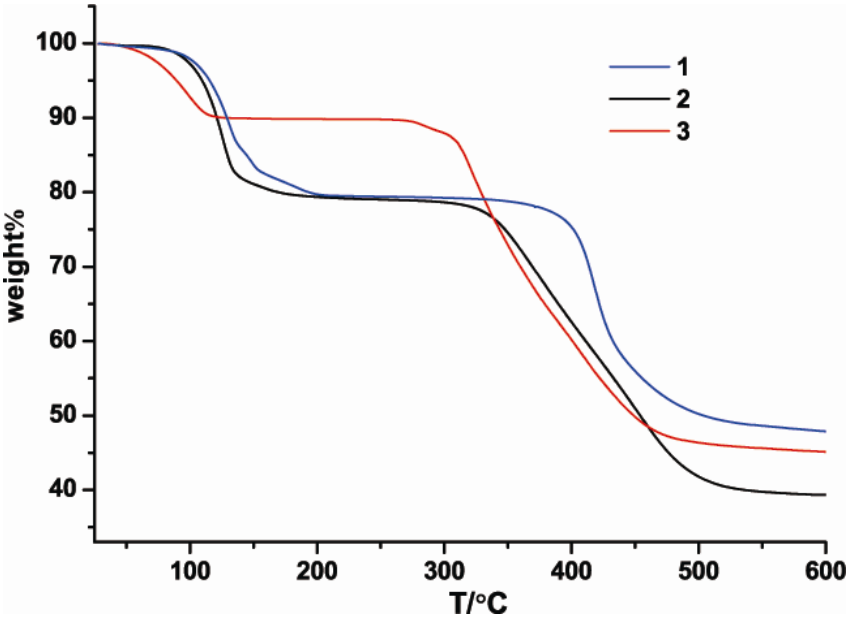

Fig. S4. Thermal analyses of compounds **1-3**.

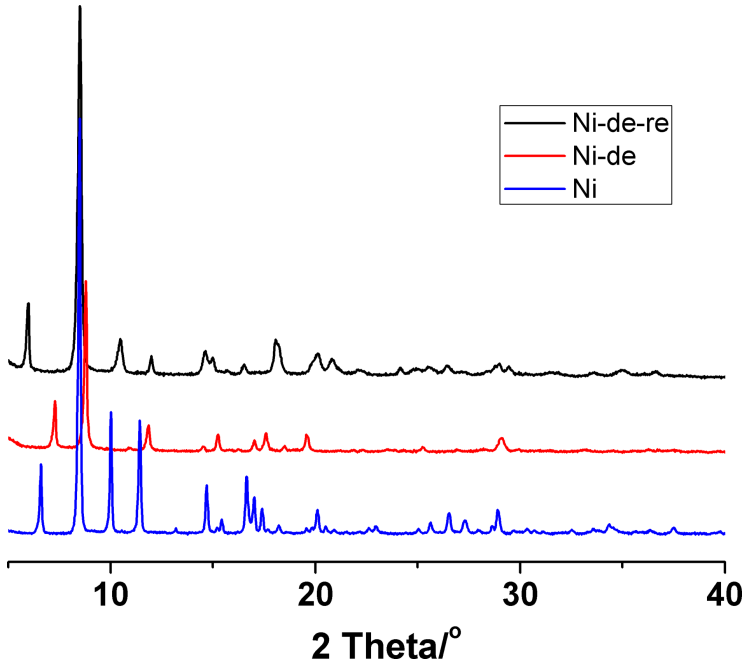

Fig. S5. Powder XRD patterns for compound **1** before dehydration (blue), after dehydration (red) and rehydration (black).

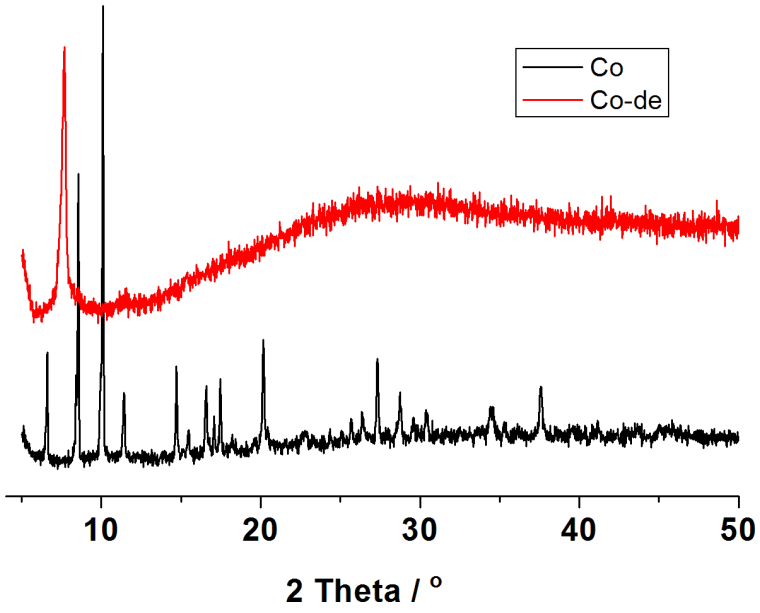

Fig. S6. Powder XRD patterns for compound **2** before dehydration (black), and after dehydration (red).

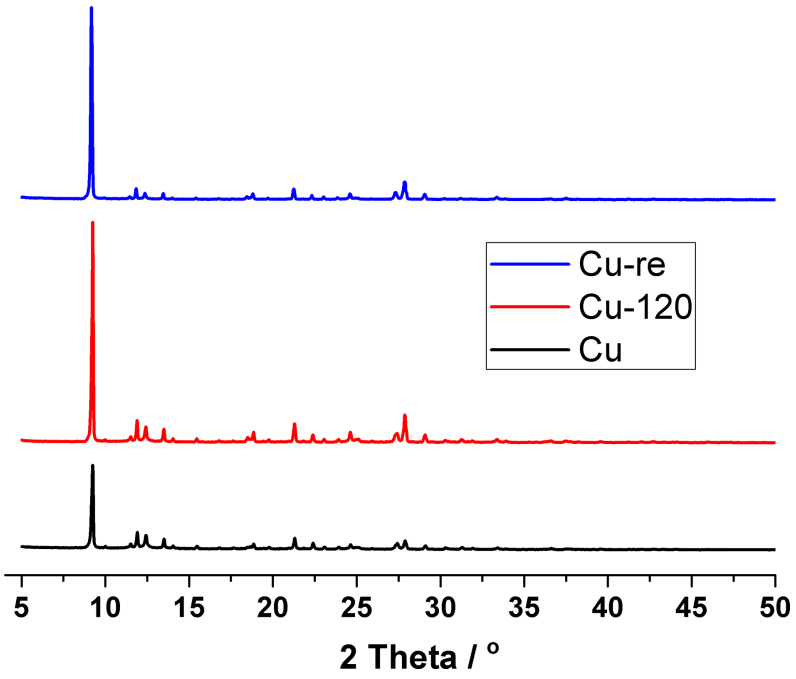

Fig. S7. Powder XRD patterns for compound **3** before dehydration (black), after dehydration (red) and rehydration (blue).

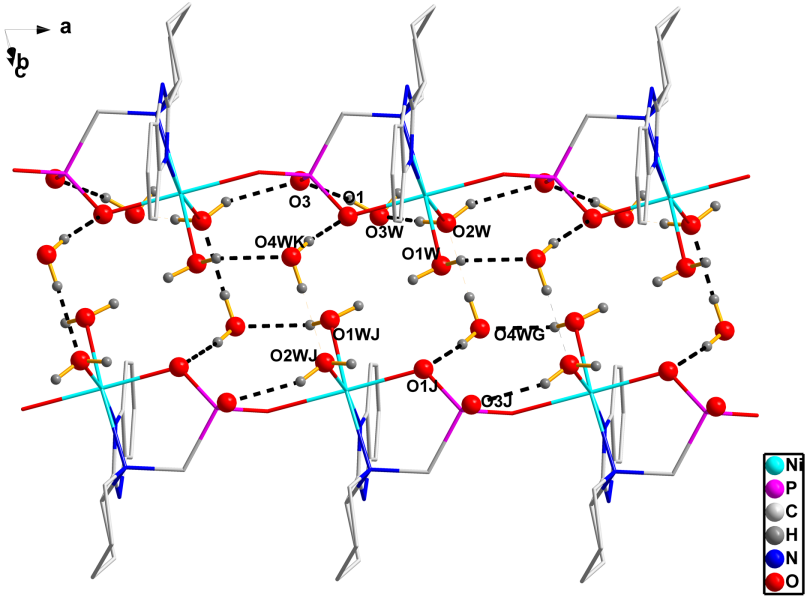

Fig. S8. The supramolecular double-chain in structure **1**. The hydrogen bond interactions are highlighted with dotted lines.

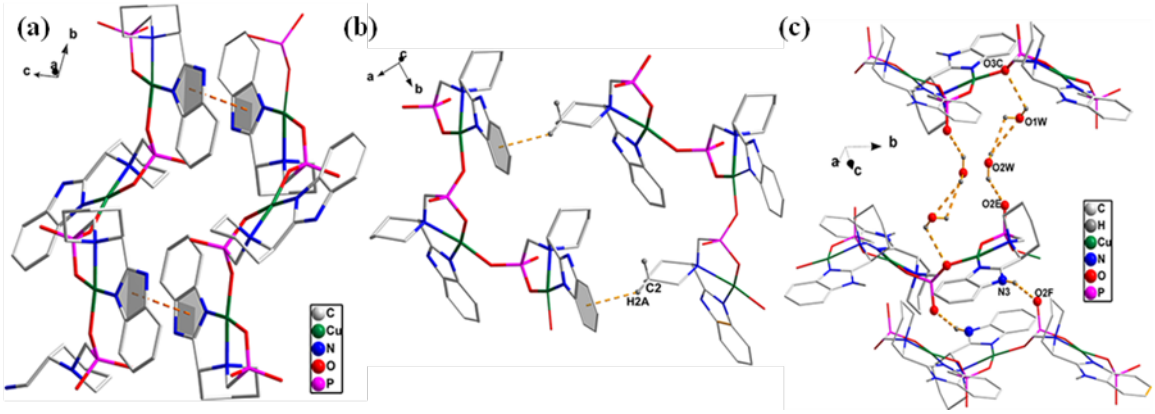

Fig. S9. (a) The inter-chain π-π stacking in structure **3** along the *c*-axis. (b) The C-H ··· π interactions along the *a*-axis. (c) The hydrogen bond interactions between the chains are highlighted with dotted lines. Symmetry codes: A: 1-x, y-0.5,0.5-z ;C: x,1+y,z; D: -x,1-y,1-z; E: 1-x,1/2+y,3/2-z ; F: 1-x,-y,1-z.

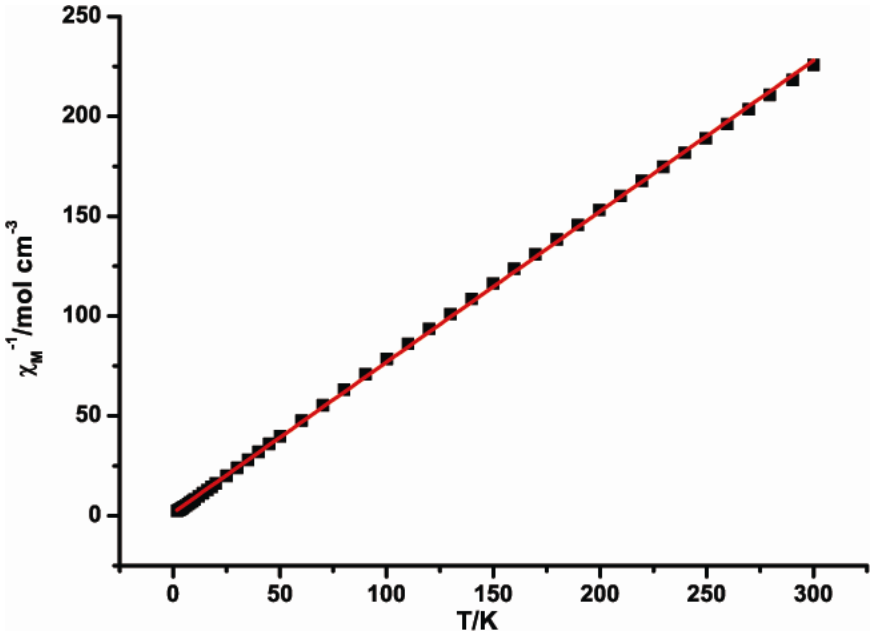

Fig. S10 Plot of the temperature dependence of $1/\chi_M$ for compound **1.**

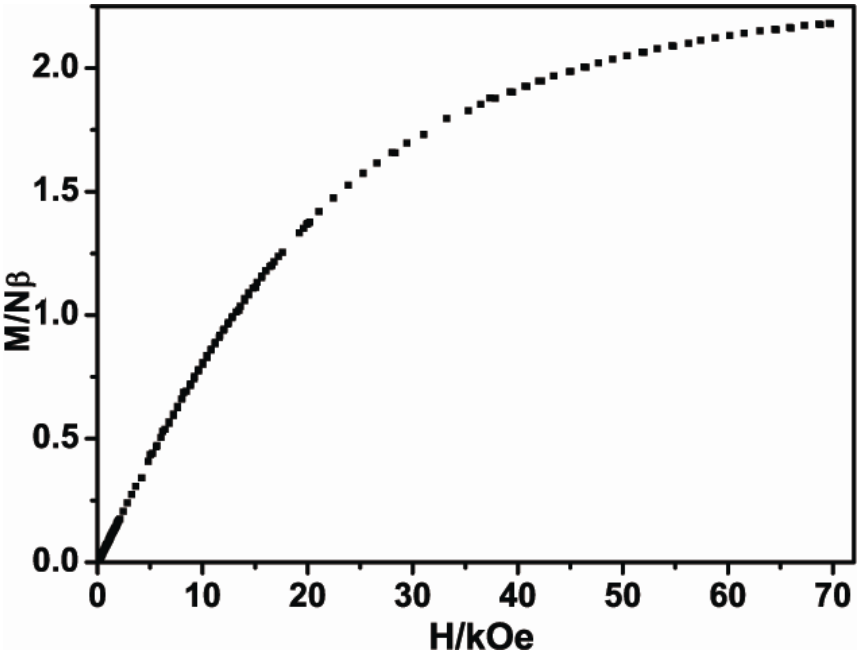

Fig. S11. The *M vs. H* plot for **1** measured at 1.8 K

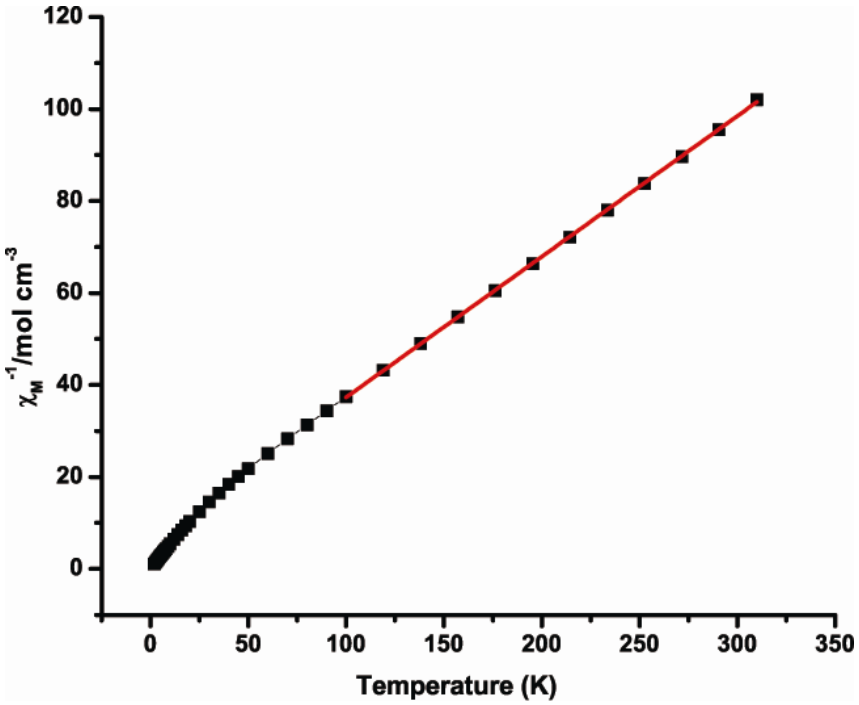

Fig. S12 Plot of the temperature dependence of $1/\chi_M$ for compound **2.**

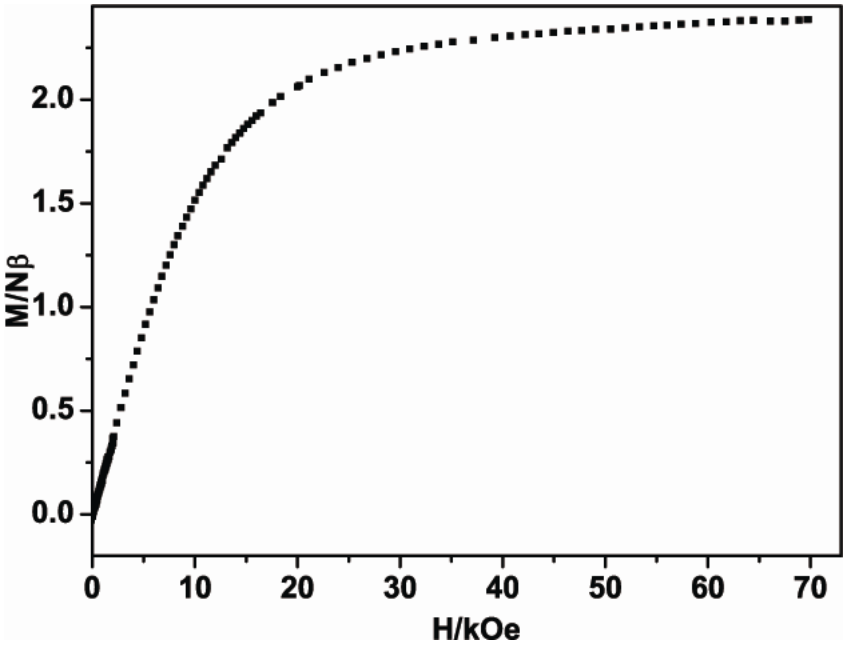

Fig. S13. The *M vs. H* plot for **2** measured at 1.8 K

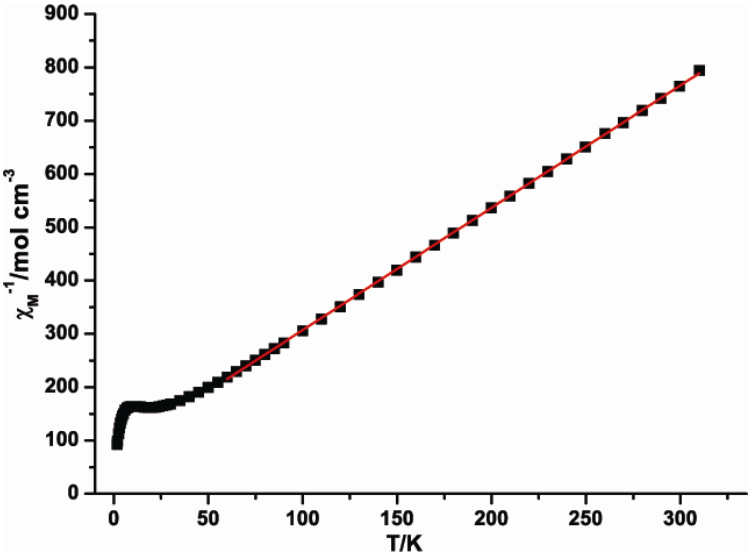

Fig. S14 Plot of the temperature dependence of $1/\chi_M$ for compound **3.**

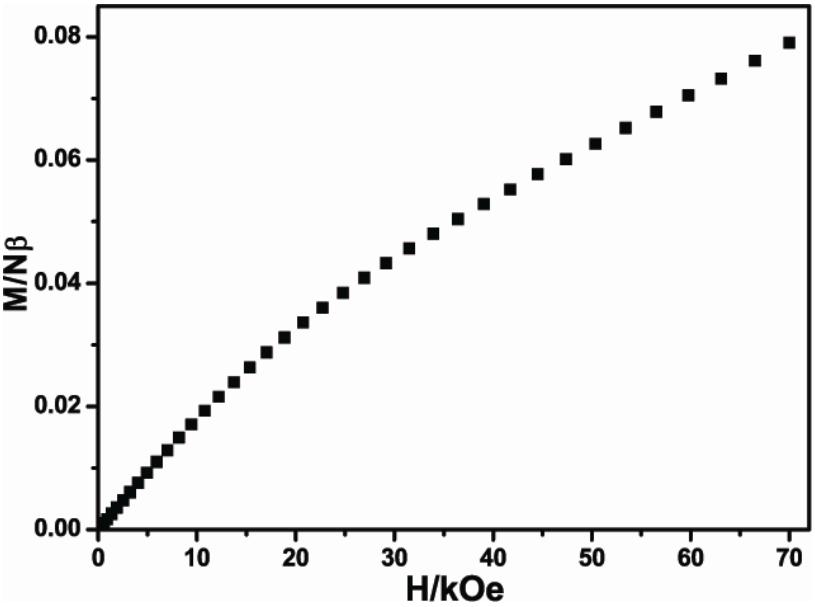

Fig. S15. The *M vs. H* plot for **3** measured at 1.8 K.