Electronic Supplementary Material (ESI) for Dalton Transactions

Spontaneous asymmetrical crystallization of a quartz-type framework from achrial precursors

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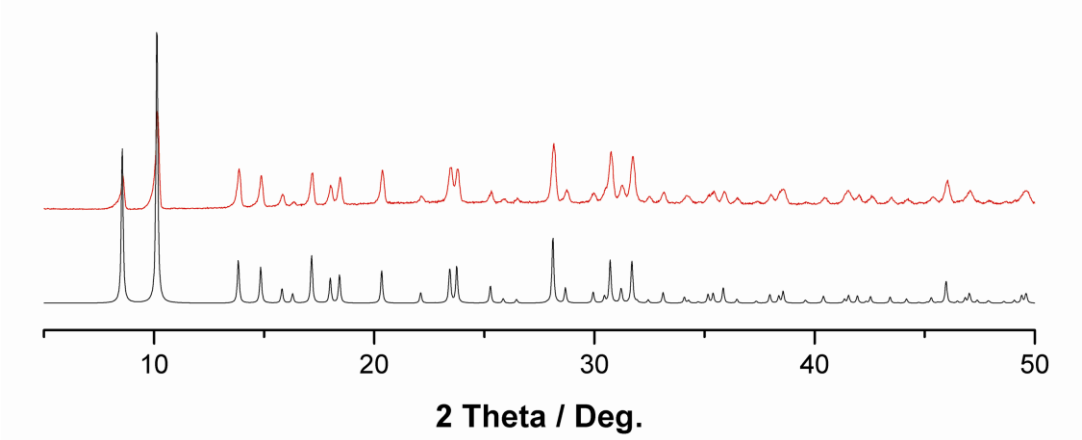

Figure S1. XPRD patterns for **1** (top, red) experimental at room temperature; (bottom, black) calculated on the basis of the structure determined by single-crystal X-ray diffraction.

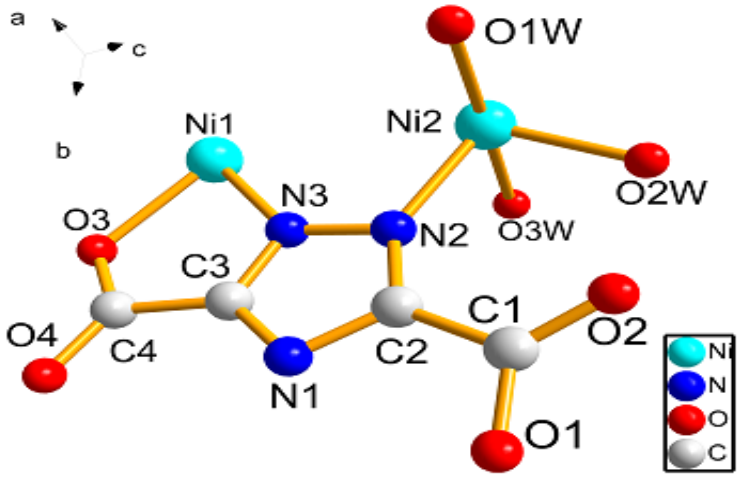

Figure S2. The crystallographic asymmetric unit in compound **1**. Hydrogen atoms are omitted for clarity.

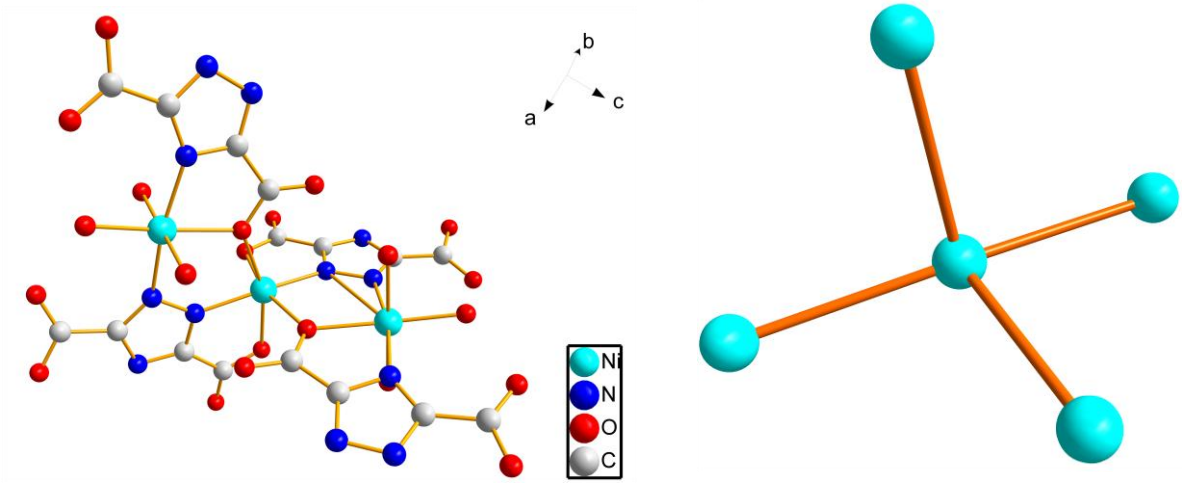

Figure S3. Left: the trinuclear SBU and tetrahedron building block in compound **1**; Right: the node (represent tinuclear SBU) and rod (represent ligand) of topology.

Table S1 A summary of the 10 structure determinations of 1 with the R factors and Flack absolute structure parameters for each refinement.

	Space group	a = b	c	R_1	wR_2	Flack parameter
1-1	$P3_121$	11.92450(10)	16.3020(5)	0.0444	0.1223	0.02(2)
1-2	$P3_121$	11.9265(5)	16.3060(11)	0.0529	0.1444	0.01(3)
1-3	$P3_121$	11.910(9)	16.306(13)	0.0556	0.1468	0.02(3)
1-4	$P3_121$	11.9386(5)	16.2986(15)	0.0958	0.2183	0.01(5)
1-5	$P3_121$	11.9130(8)	16.2942(19)	0.0898	0.1951	0.01(5)
1-6	$P3_121$	11.9224(4)	16.2261(11)	0.0657	0.1439	0.03(3)
1-7	$P3_121$	11.9250(4)	16.2715(10)	0.0401	0.1132	0.01(2)
1-8	$P3_121$	11.9298(4)	16.4486(8)	0.0527	0.1380	0.03(3)
1-9	$P3_121$	11.8921(6)	16.248(2)	0.0478	0.1304	0.01(3)
1-10	$P3_221$	11.9029(6)	16.2687(15)	0.0848	0.2255	0.04(5)

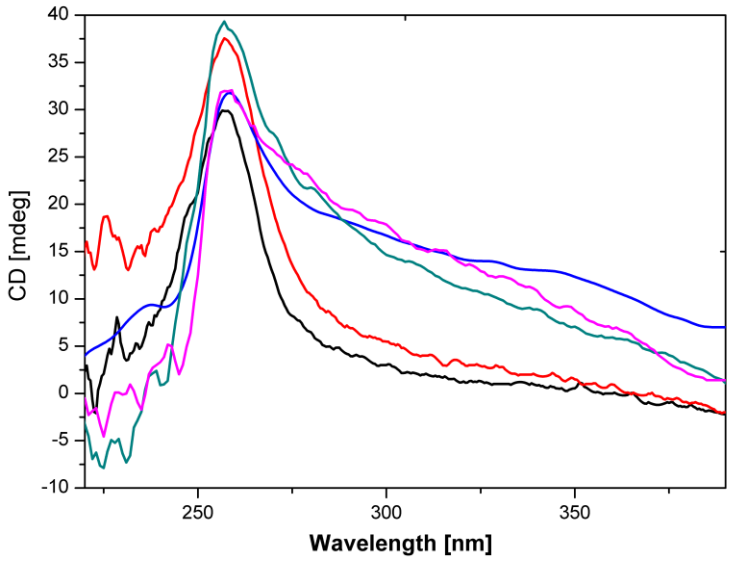

Figure S4. The solid-state CD spectra of each whole batch from 5 parallel products.

CD spectra of each whole batch from 5 parallel hydrothermal syntheses were measured in solid-state. The mixture of 0.6g sample and 1.2g dried KCl powder was grinded for 30 minute, and then 20 mg sample was picked out from the well-ground powder for use in CD measurement.

Figure S5. The image of green products.

Magnetic properties: Magnetic susceptibilities were measured for **1** with a Quantum Design MPMS-XL system.

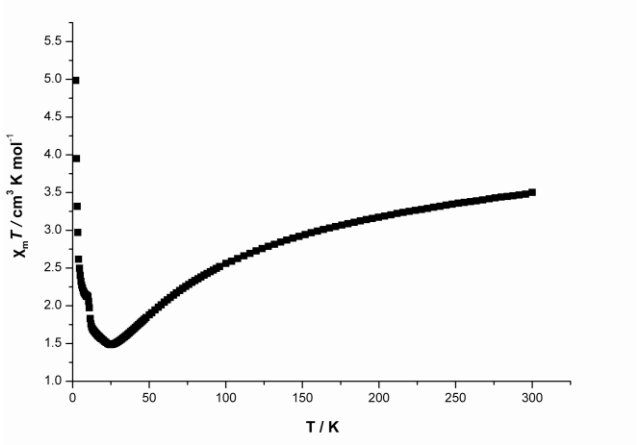

Figure S4. Plot of $\chi_m T$ *vs.* *T* for **1** at 1000 oe.

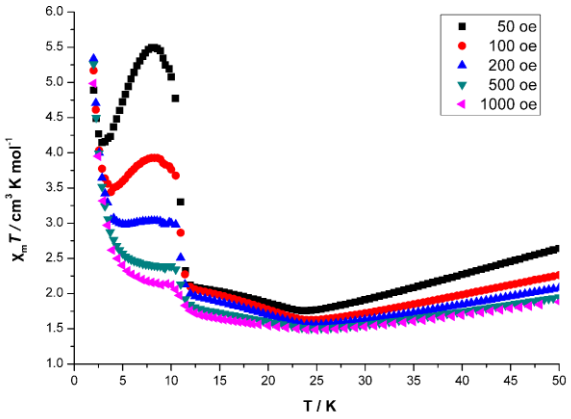

Figure S5. Plot of $\chi_m T$ *vs. T* under different fields at low temperature.

A plot of$\chi_m T$ *vs. T* per Ni3 unit under a applied field of 1000 oe for **1** is shown in Figure S1. Upon cooling, the $\chi_m T$ undergoes a gradual decrease down to 1.46 cm^3 K mol^{-1} around 25 K. Below 25 K, the $\chi_m T$ product increases rapidly to a sharp maximum of 4.98 cm^3 K mol^{-1} at 2 K. As shown in Figure S2, the$\chi_m T$ curve is field dependent and disappears at higher field. Such behavior can well be expected for a canted spin system.

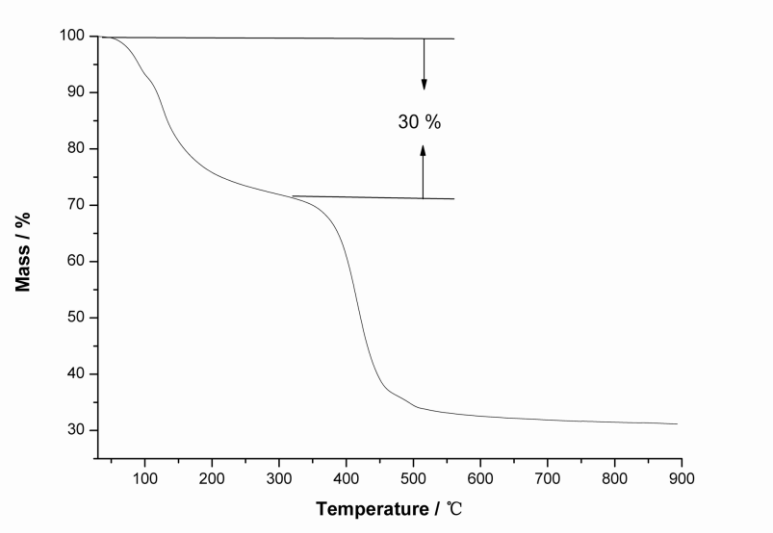

Figure S6. The TGA diagram of **1**. The weight of 30% is corresponding to the loss of uncoordinated and coordinated water molecules.