Supporting information for

Exploration of a new building block for the construction of cyano-bridged solvatomagnetic assemblies: $[Ni(cyclam)]^{3+}$

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Table S1. Crystallographic data for **1** and **2**

	1	**2**
Empirical formula	$C_{16}H_{36}CrN_{10}NiO_6$	$C_{16}H_{36}FeN_{10}NiO_6$
Formula weight	575.26	579.11
Temperature / K	120(2)	120(2)
Crystal system	monoclinic	monoclinic
Space group	*C*2/m	*C*2/m
a /Å	10.5579(5)	10.2754(3)
b /Å	16.3314(6)	16.2306(4)
c /Å	8.8748(4)	8.8043(3)
α / º	90	90
β / º	112.254(3)	111.265(3)
γ / º	90	90
Volume / $Å^3$	1416.26(11)	1368.37(7)
Z	2	2
Density (calc.) / Mg/m^3	1.349	1.406
Absorption coeff. / mm^{-1}	1.094	1.066
F(000)	604	608
Crystal size / mm	0.12 x 0.12 x 0.07	0.31 x 0.22 x 0.13
Theta range / º	3.52-24.81	3.53-28.67
Reflections collected	6570	8656
R_{int}	0.063	0.037
Independent reflections	1265	1722
Parameters	95	98
GOF on F^2	1.077	1.066
R indices [I>2σ(I)]	R1 =0.0367 wR2 =0.0618	R1 =0.0307 wR2 =0.0654
R indices (all data)	R1 =0.0585 wR2 =0.0679	R1 =0.0462 wR2 =0.0731

Table S2. Crystallographic data for **1d** and **2d**

	1d	**2d**
Empirical formula	$C_{16}H_{29}CrN_{10}NiO_{2.5}$	$C_{16}H_{30}FeN_{10}NiO_3$
Formula weight	512.15	525.01
Temperature / K	298	298
Crystal system	monoclinic	monoclinic
Space group	$P\ 2_1$	$P\ 2_1$
a /Å	9.8002(14)	9.8927
b /Å	11.9983(17)	12.1549
c /Å	10.1260(11)	10.1774
α / º	90	90
β / º	102.646(19)	102.013
γ / º	90	90
Volume / $Å^3$	1161.8(3)	1197.0
Z	2	2
Rp (Rietveld)	0.1852	
Rwp (Rietveld)	0.1839	

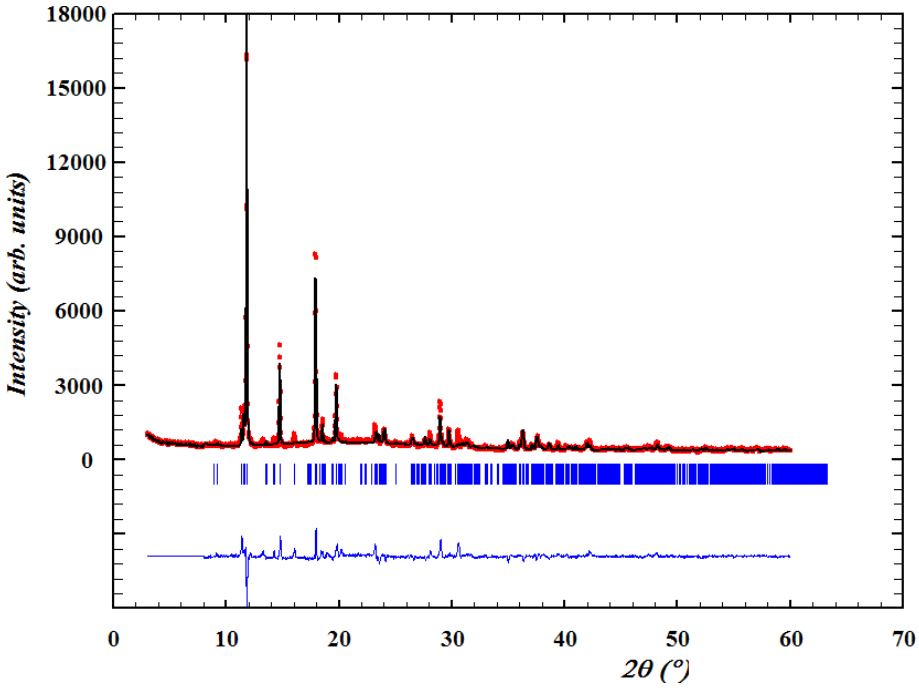

Figure S1. The Rietveld plot for **1d**.

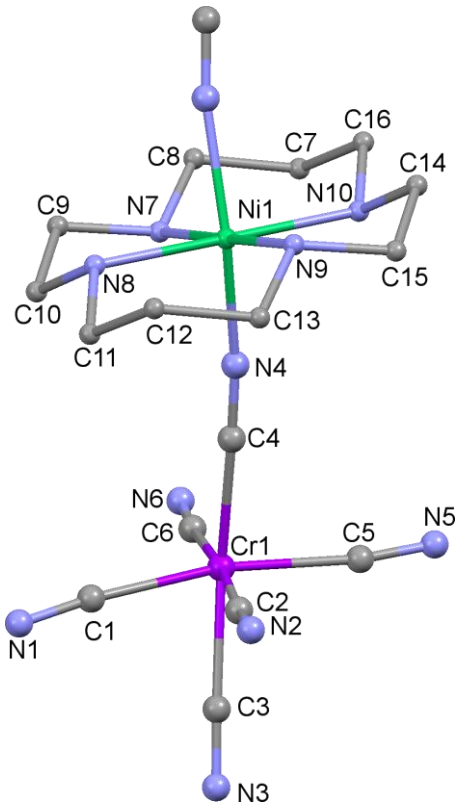

Figure S2. Structure of **1d** with atom numbering; thermal spheres at 50% probability.

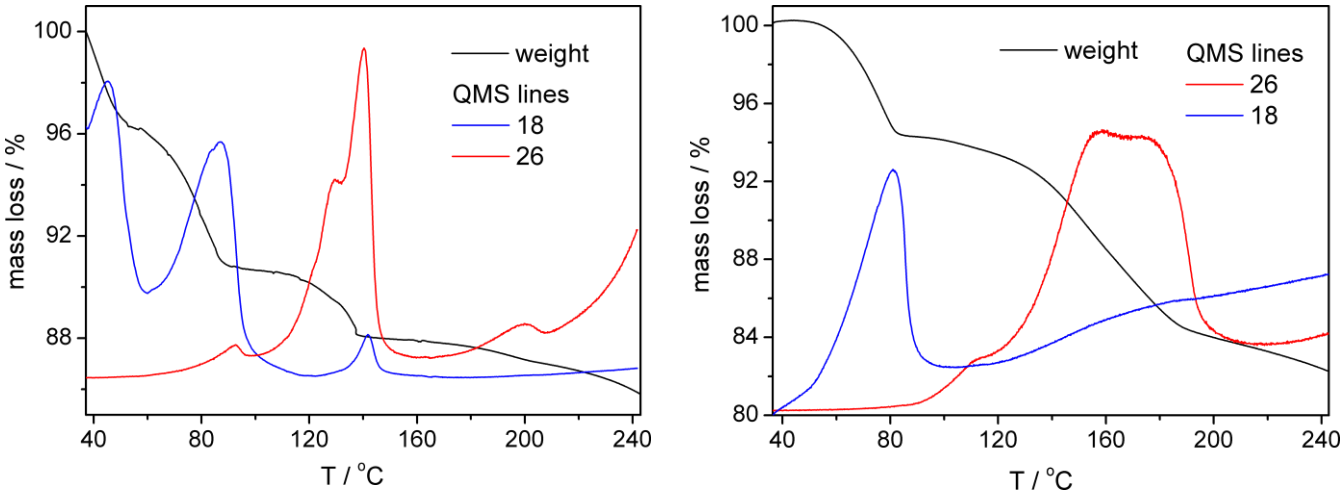

Figure S3. Thermogravimetric analysis of **1** (left) and **2** (right).

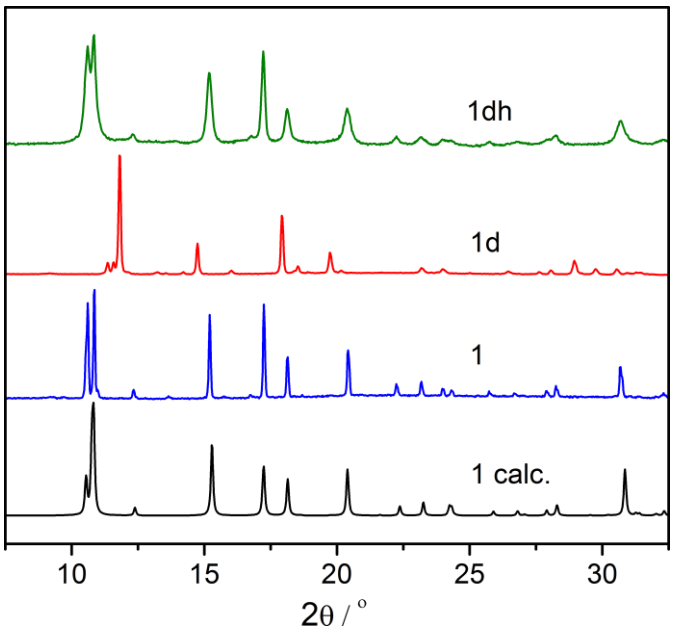

Figure S4. PXRD patterns for as synthesised fully hydrated **1**, partly dehydrated **1d** and rehydrated **1dh** in comparison to the pattern generated from the single-crystal structure of **1**.

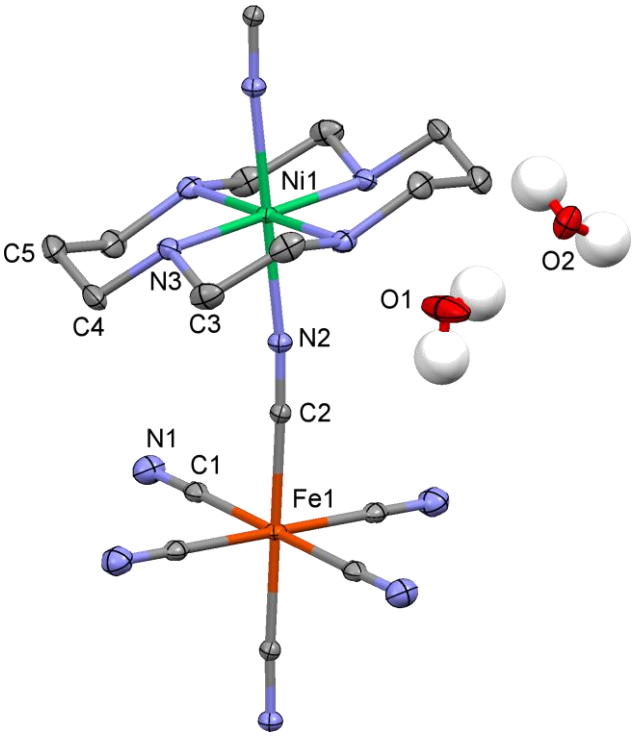

Figure S5. Structure of **2** with atom numbering; thermal ellipsoids at 50% probability; hydrogen atoms on cyclam ring omitted for clarity.

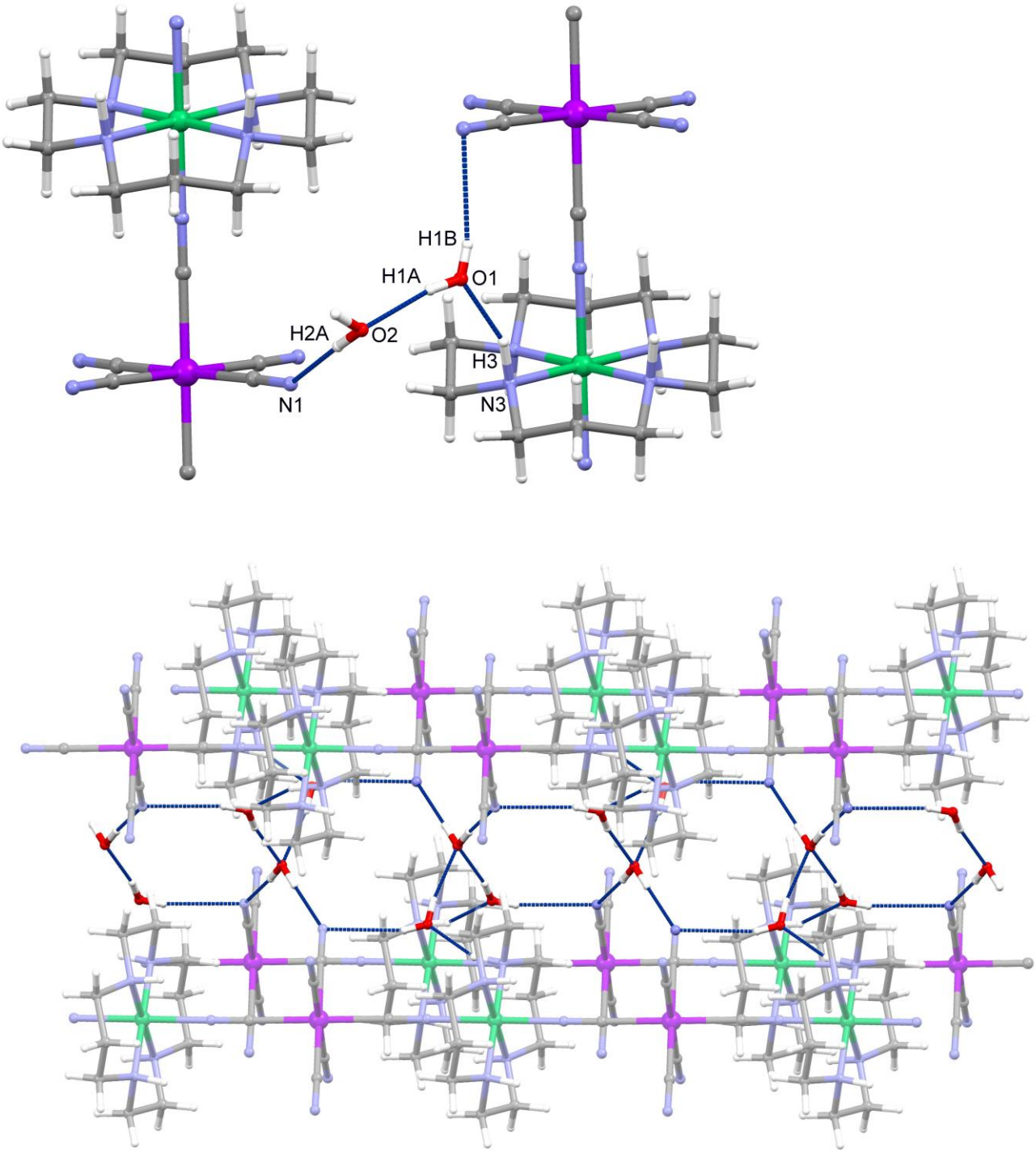

Figure S6. Hydrogen bonds in the structure of **1**: detail view with atom numbering (top); view of the net (bottom).

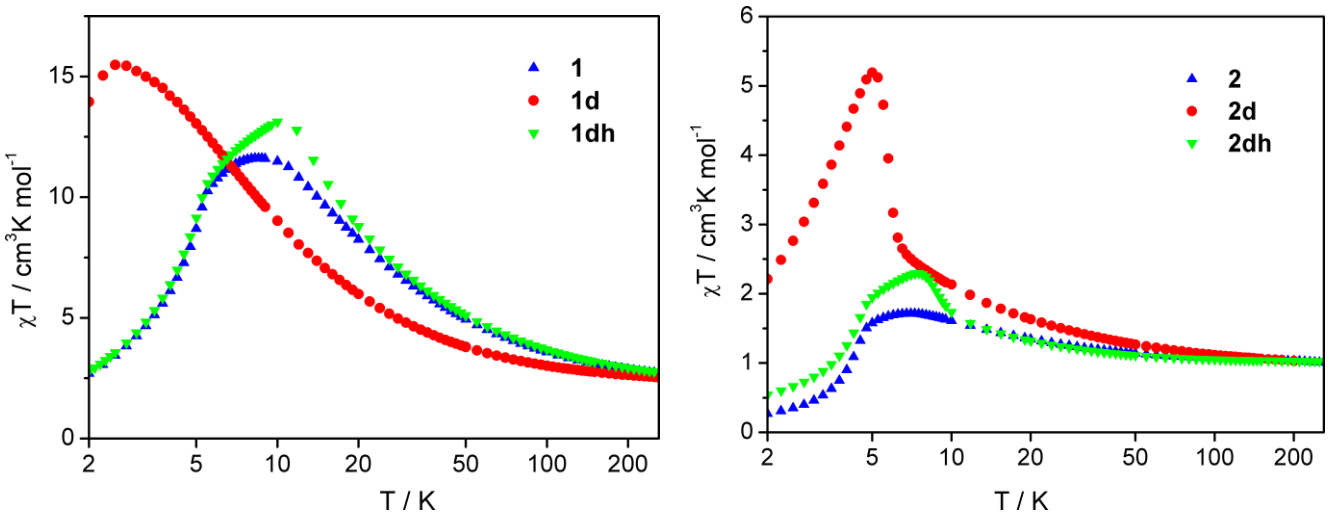

Figure S7. Magnetic susceptibility at 1kOe for fully hydrated, partly dehydrated (**d**) and rehydrated (**dh**) forms of NiCr and NiFe chains; temperature in logarithmic scale.

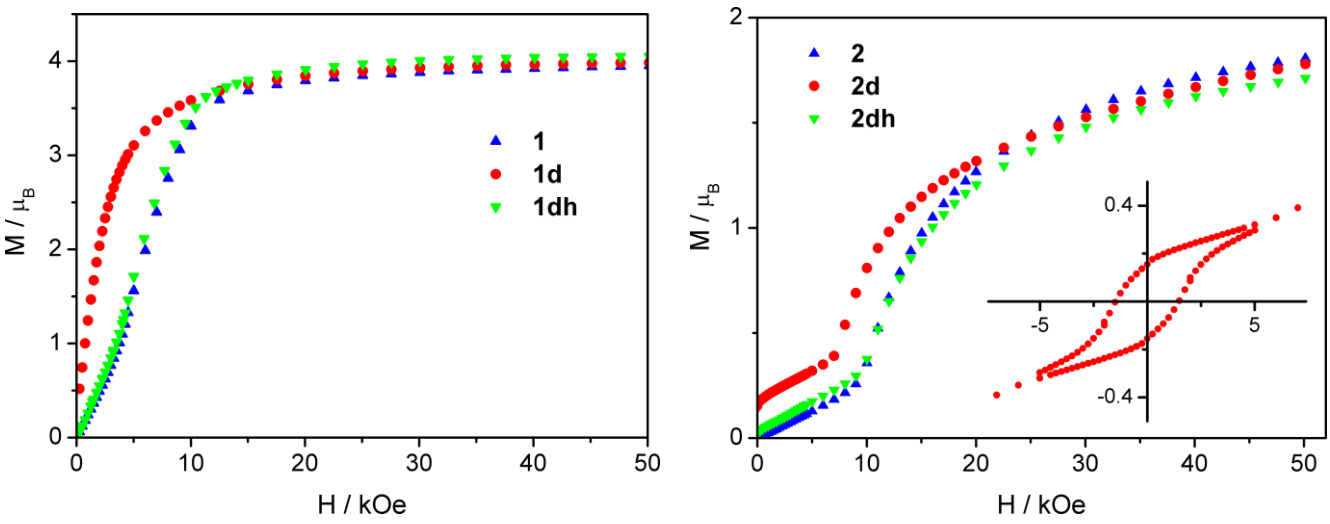

Figure S8. Field dependence of magnetisation measured at 2 K for fully hydrated, partly dehydrated (**d**) and rehydrated (**dh**) forms of NiCr and NiFe chains; inset in the right graph shows magnetic hysteresis for **2d**.