Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Conformational Control of Ligands to Create a Finite Metal–Organic Cluster and an Extended Metal–Organic Framework

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Table S1. Crystal data and structure refinement for **1**.

Empirical formula	$C_{60}H_{42}N_6O_{21}Cu_3$	
Formula weight	1373.66	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	*Pn*-3*n*	
Unit cell dimensions	a = 32.365(4) Å	α = 90°
	b = 32.365(4) Å	β = 90°
	c = 32.365(4) Å	γ = 90°
Volume	33902(7) $Å^3$	
Z	8	
Density (calculated)	0.538 Mg/m^3	
Absorption coefficient	0.402 mm^{-1}	
F(000)	5592	
Crystal size	0.50 x 0.49 x 0.43 mm^3	
Theta range for data collection	2.88 to 23.33°.	
Index ranges	-35<=h<=34, -35<=k<=30, -32<=l<=32	
Reflections collected	108634	
Independent reflections	4057 [R(int) = 0.2337]	
Completeness to theta = 23.33°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8460 and 0.8241	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4057 / 82 / 119	
Goodness-of-fit on F^2	1.341	
Final R indices [I>2sigma(I)]	R1 = 0.1515, wR2 = 0.4379	
R indices (all data)	R1 = 0.2465, wR2 = 0.4844	
Largest diff. peak and hole	0.619 and –0.335 $e \cdot Å^{-3}$	

Table S2. Crystal data and structure refinement for **2.**

Empirical formula	$C_{278}H_{340}N_{44}O_{94}Ni_{14}$	
Formula weight	6623.88	
Temperature	96(2) K	
Wavelength	0.80000 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 41.121(8) Å	α = 90°
	b = 20.457(4) Å	β = 106.71(3)°
	c = 39.436(8) Å	γ = 90°
Volume	31773(11) $Å^3$	
Z	4	
Density (calculated)	1.385 Mg/m^3	
Absorption coefficient	1.179 mm^{-1}	
F(000)	13840	
Crystal size	0.50 x 0.50 x 0.33 mm^3	
Theta range for data collection	1.63 to 28.00°	
Index ranges	-48<=h<=48, -23<=k<=23, -46<=l<=46	
Reflections collected	93568	
Independent reflections	26217 [R(int) = 0.0407]	
Completeness to theta = 28.00°	97.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6969 and 0.5901	
Refinement method	Full-matrix-block least-squares on F^2	
Data / restraints / parameters	26217 / 177 / 2303	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I)]	R1 = 0.0643, wR2 = 0.1933	
R indices (all data)	R1 = 0.0803, wR2 = 0.2031	
Largest diff. peak and hole	0.668 and –0.425 $e \cdot Å^{-3}$	

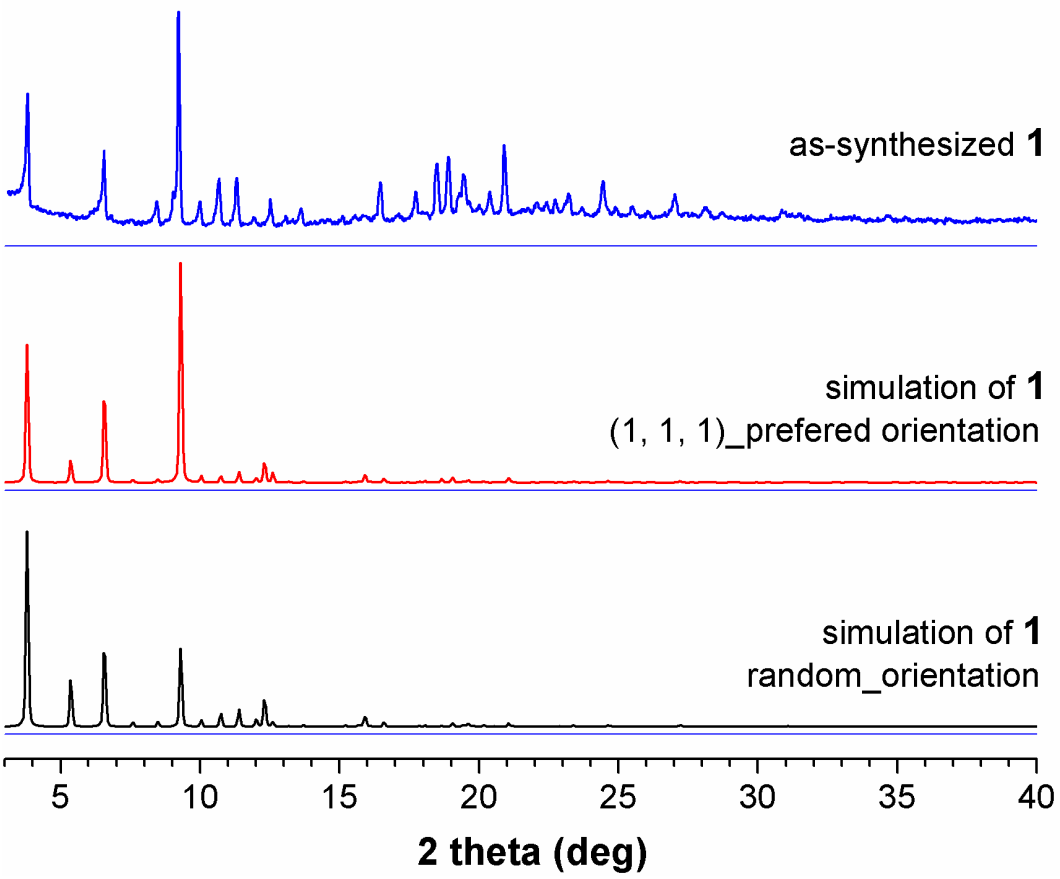

Fig. S1 PXRD patterns of **1**. (a) A simulated PXRD pattern from the single crystal structure of **1**, (b) from the single crystal structure of **1** with [1, 1, 1] preferred orientation, and (c) a PXRD pattern of the as-synthesized sample.

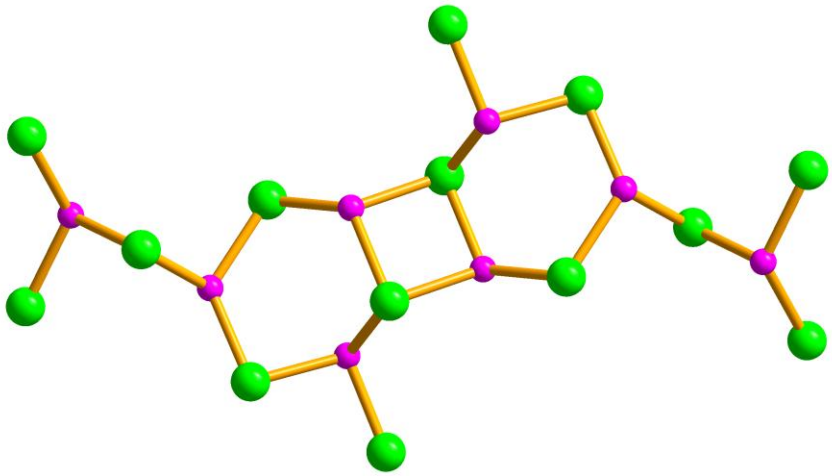

Fig. S2 The 14 Ni(II) ions of **2** in a crystallographic inversion center are bridged *via* eight μ^3-hydroxo oxygen atoms (shown in pink).

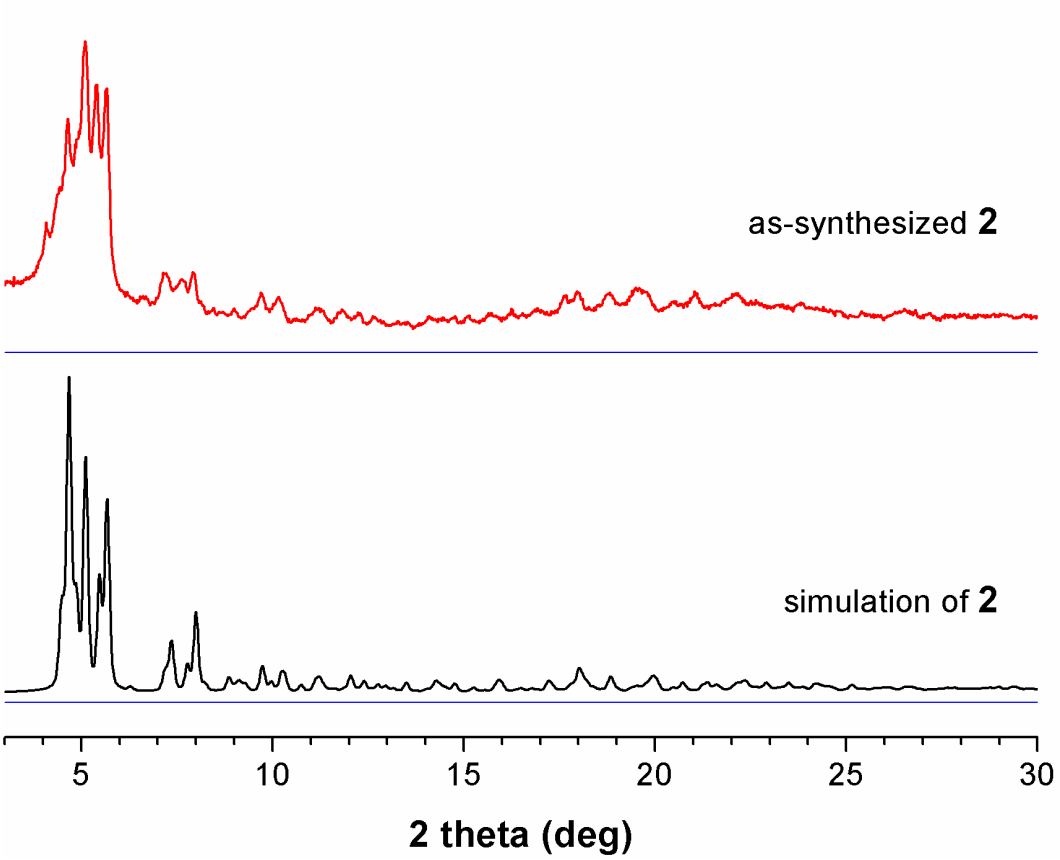

Fig. S3 PXRD patterns of **2**. (a) A simulated PXRD pattern from the single crystal structure of **2** and (b) a PXRD of the as-synthesized sample.