Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information for

A Family of three magnetic metal organic frameworks, their synthesis, structural, magnetic and vapour adsorption study

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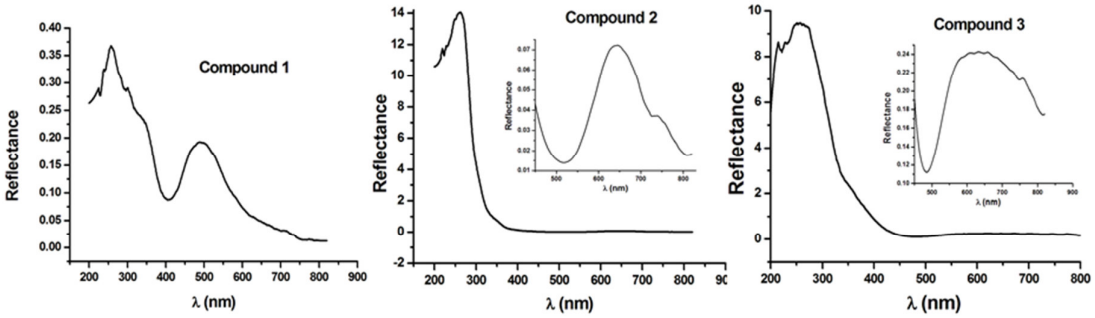

Fig. S1. Diffused Reflectance Spectra of compounds **1-3**.

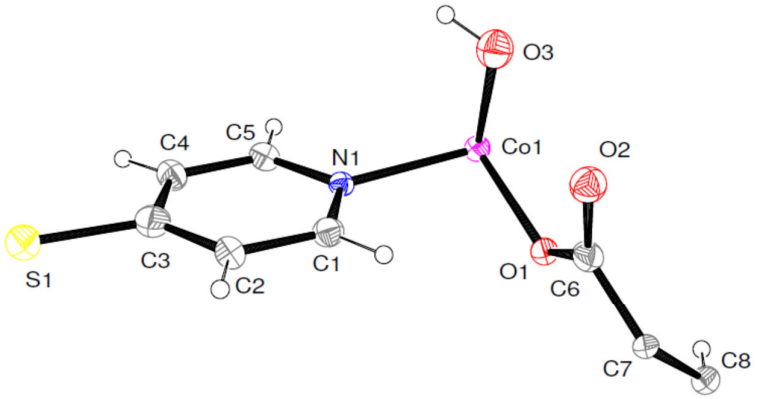

Fig. S2. Asymmetric unit of compound **1** (30% probability of ellipsoid). Colour code. Cobalt(magenta), Oxygen(red), Nitrogen(blue), Carbon(light grey), Sulphur(yellow).

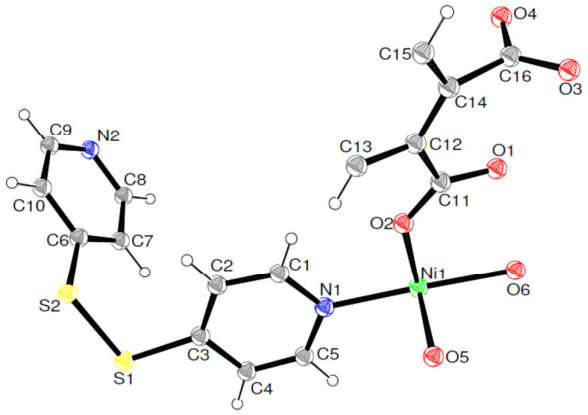

Fig. S3. Asymmetric unit of compound **2** (30% probability of ellipsoid) (solvent molecules are removed for clarity). Colour code. Nickel(green), Oxygen(red), Nitrogen(blue), Carbon(light grey), Sulphur(yellow).

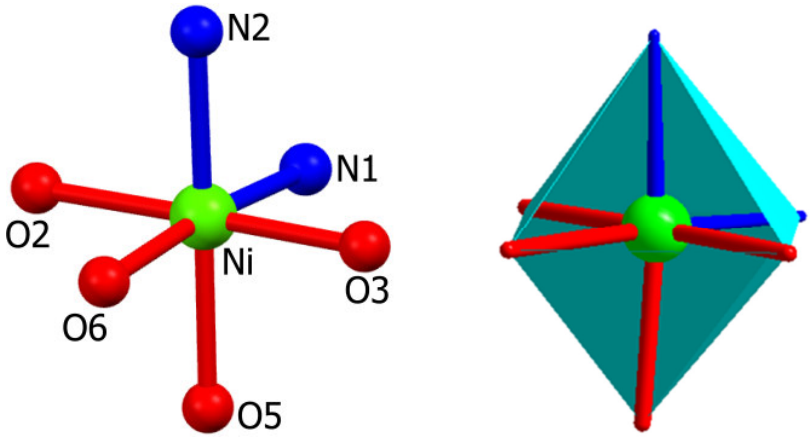

Fig. S4. Illustration of co-ordination environment around Ni(II) centre found in compound **2**. Colour code. Nickel(green), Oxygen(red), Nitrogen(blue).

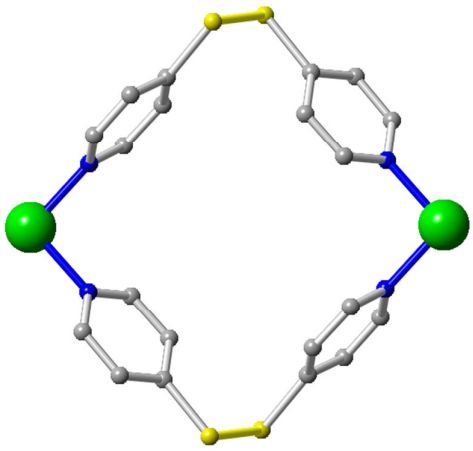

Fig. S5. Centro-symmetric dimer found in compound **2**. Colour code. Nickel(green), Nitrogen(blue),Carbon(light grey), Sulphur(yellow).

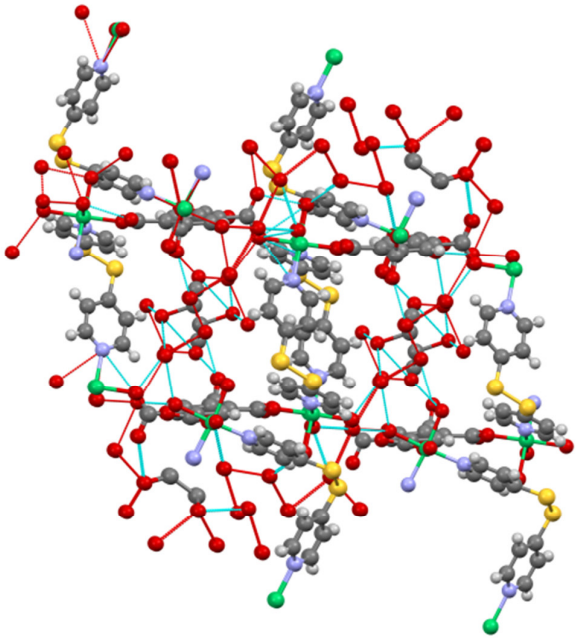

Fig. S6. Hydrogen bonding interactions in compound **2**.

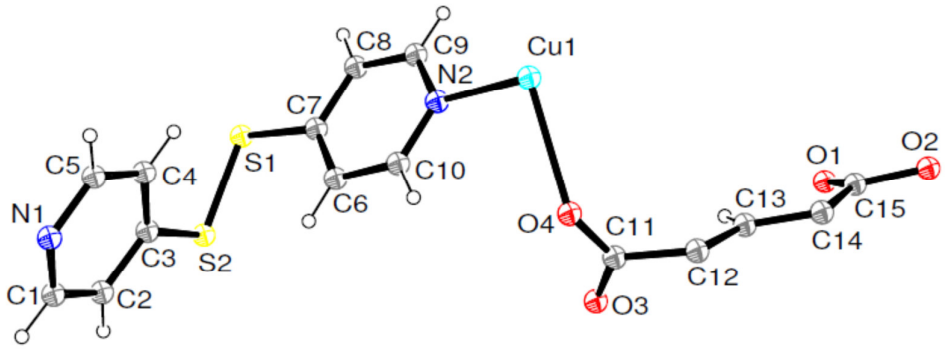

Fig. S7. Asymmetric unit of compound **3** (30% probability of ellipsoid). (solvent molecules are omitted for clarity). Colour code. Copper(cyan), Oxygen(red), Nitrogen(blue), Carbon(light grey), Sulphur(yellow).

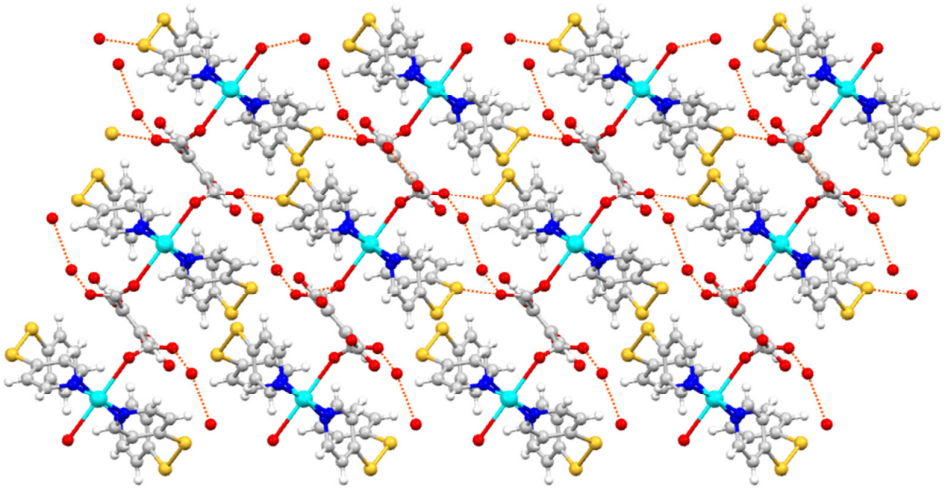

Fig. S8. Illustration of 3D networks found in **3** through H-bonding interaction between 2D layers through solvated water molecules. Colour code. Copper(cyan), Oxygen(red), Nitrogen(blue), Carbon(light grey), Sulphur(yellow).

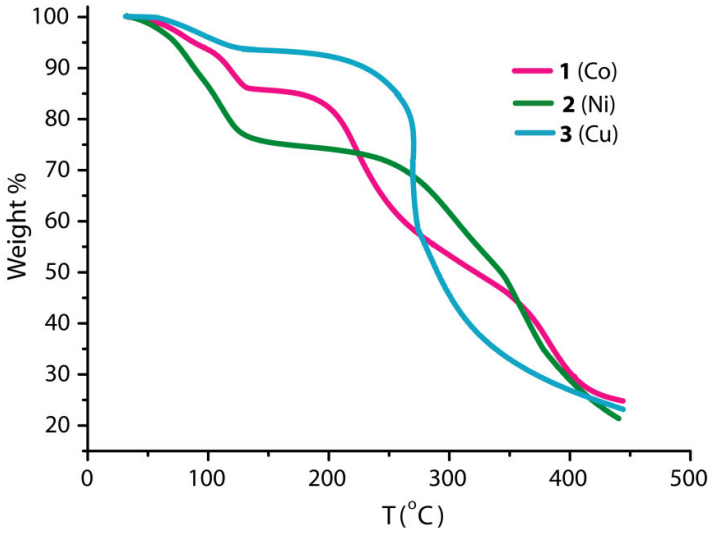

Fig. S9. TGA plot of compounds **1-3**.

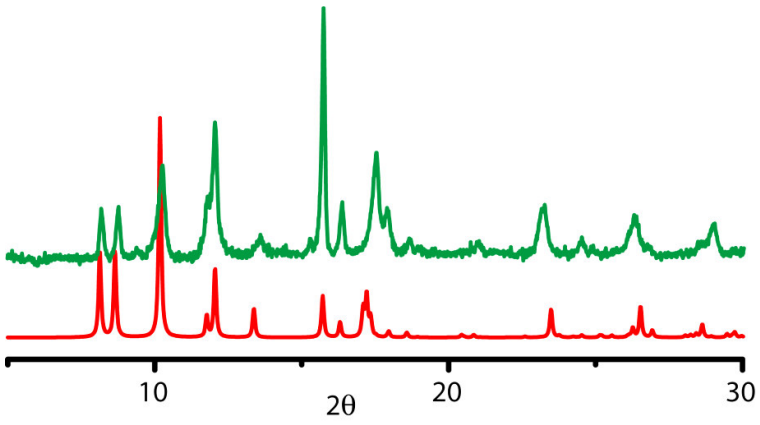

Fig. S10. PXRD patterns of compound **1**; Simulated (red), As-synthesized (green).

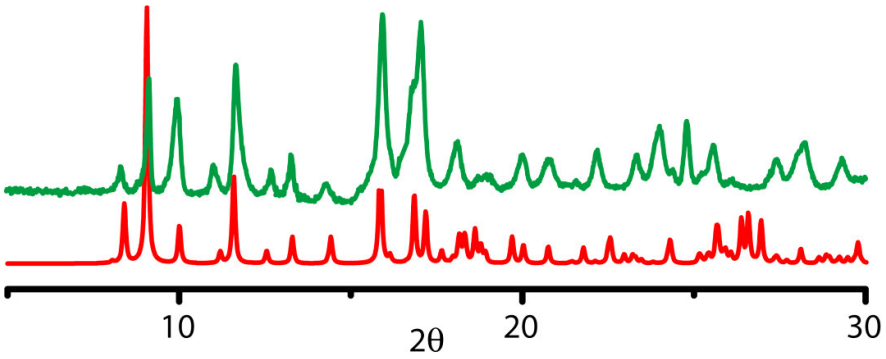

Fig. S11. PXRD patterns of compound **2**; Simulated (red), As-synthesized (green).

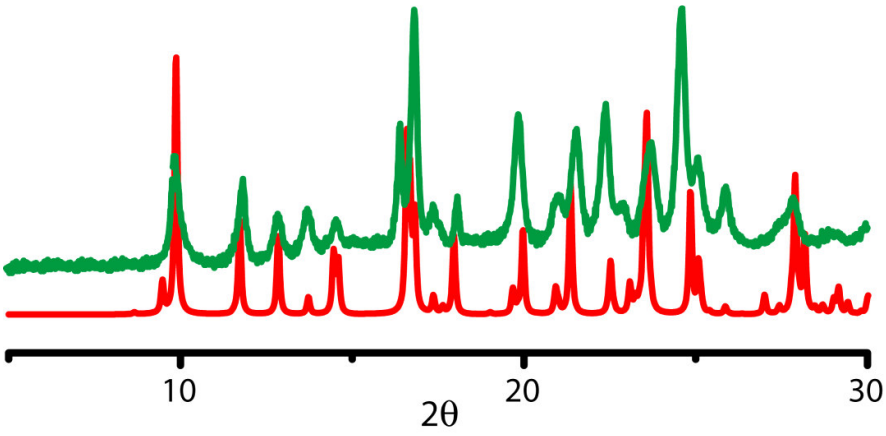

Fig. S12. PXRD patterns of compound **3**; Simulated (red), As-synthesized (green).

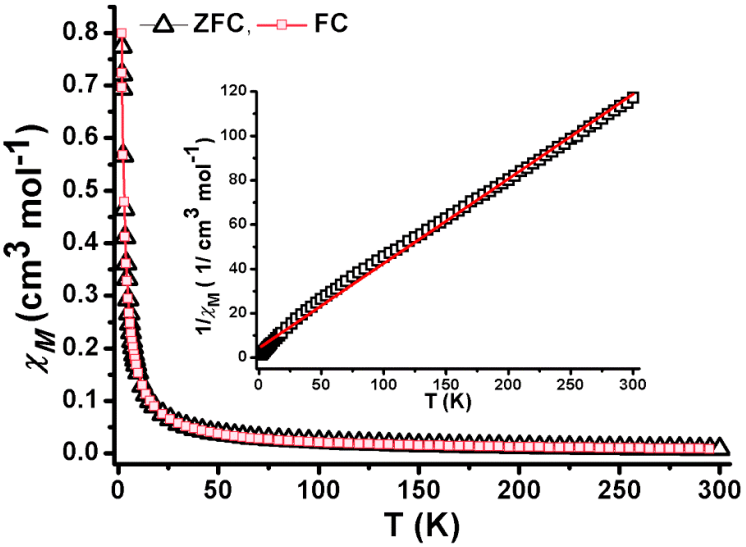

Fig. S13. Temperature dependence of the FC and ZFC susceptibility (χ_M) of **1** at 0.1 T. Inset shows temperature dependence of $1/\chi_M$. The red solid line represents the Curie-Weiss fitting to the curve.

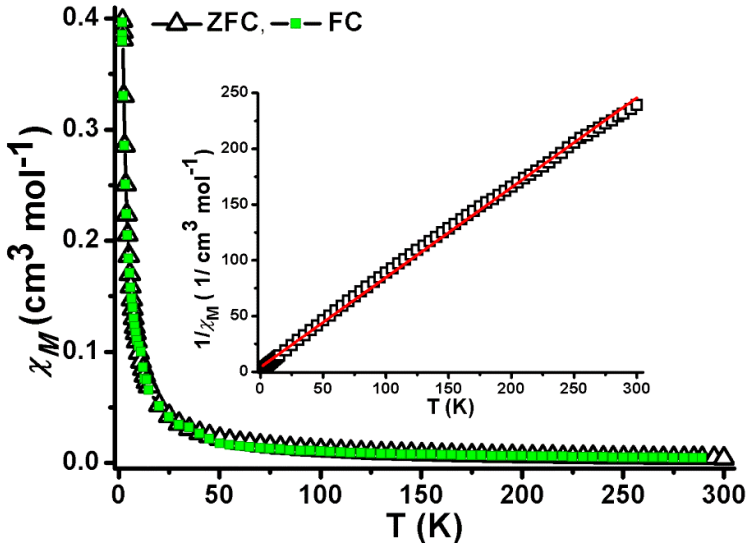

Fig. S14. Temperature dependence of the FC and ZFC susceptibility (χ_M) of **2** at 0.01 T. Inset shows temperature dependence of $1/\chi_M$. The red solid line represents the Curie-Weiss fitting to the curve.

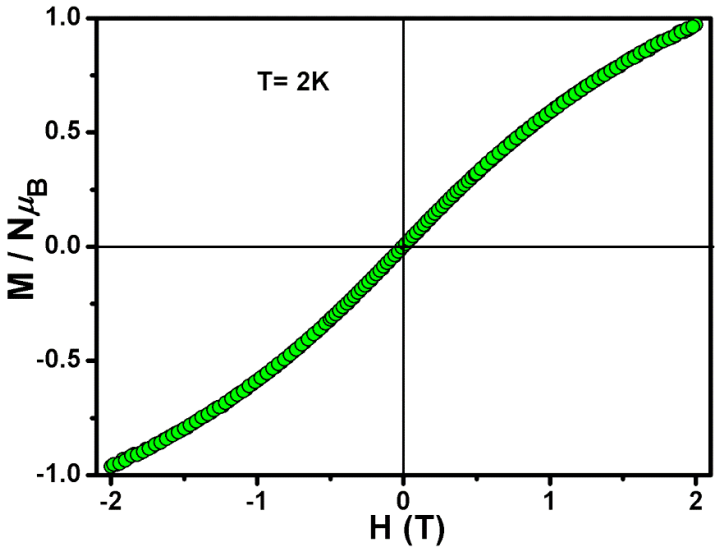

Fig. S15. M/Nμ_B vs H curve for **2** recorded at 2 K.

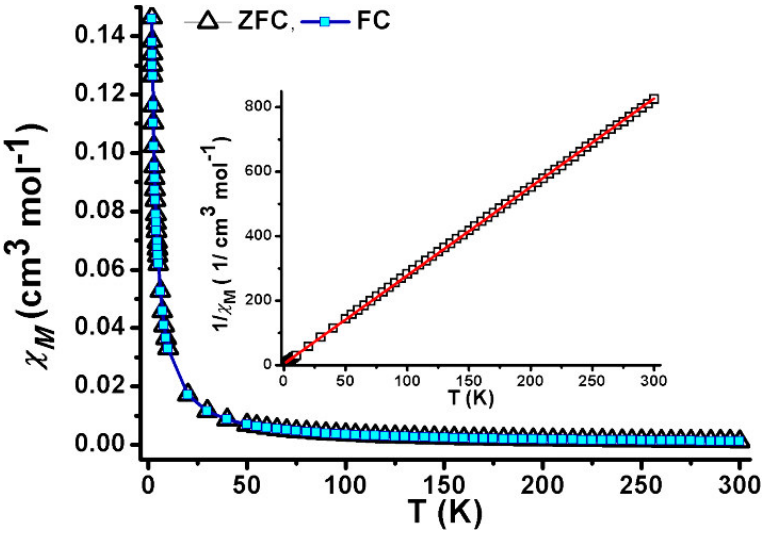

Fig. S16. Temperature dependence of the FC and ZFC susceptibility (χ_M) of **3** at 0.01 T. Inset shows temperature dependence of $1/\chi_M$. The red solid line represents the Curie-Weiss fitting to the curve.

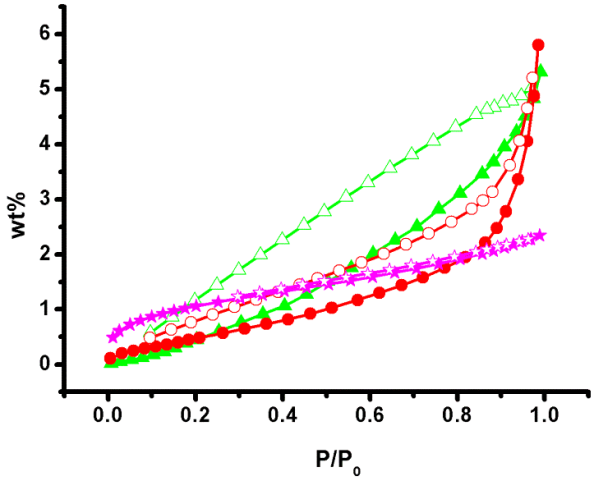

Fig. S17. N_2 adsorption isotherms of compounds **1**-**3** at 77 K. **1**(green), **2**(red), **3**(magenta).

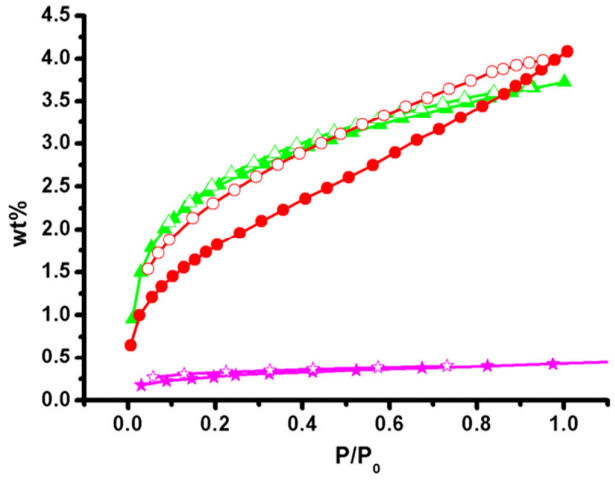

Fig. S18. CO_2 adsorption isotherms of compounds **1**-**3** at 195 K. **1**(red), **2**(green), **3**(magenta).

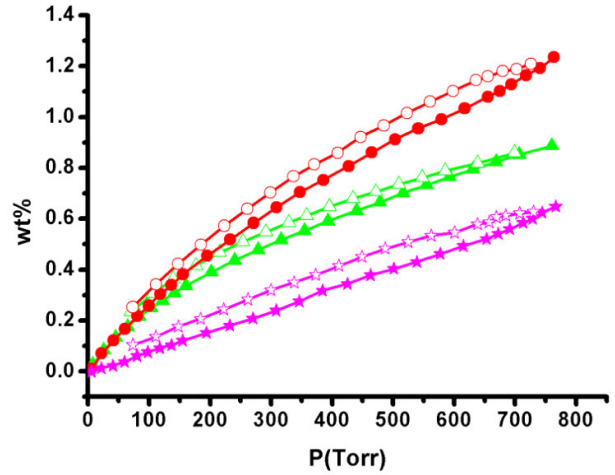

Fig. S19. CO_2 adsorption isotherms of compounds **1**-**3** at 298 K. **1**(magenta), **2**(green), **3**(red).

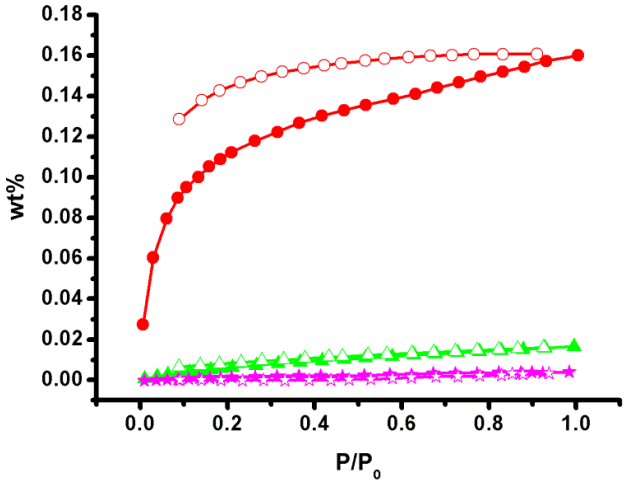

Fig. S20. H_2 sorption isotherms of compounds **1**-**3** at 77 K. **1**(magenta), **2**(green), **3**(red).

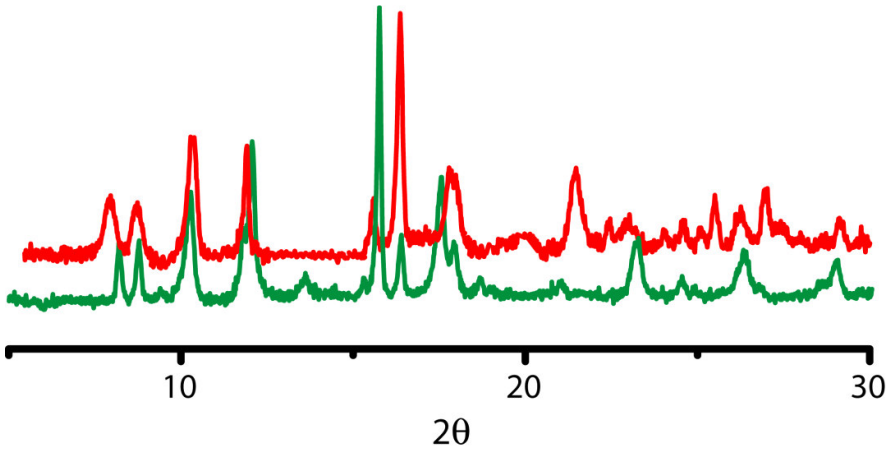

Fig. S21. PXRD pattern of water adsorbed sample of compound **1**; As-synthesized (green), H_2O adsorbed (red).

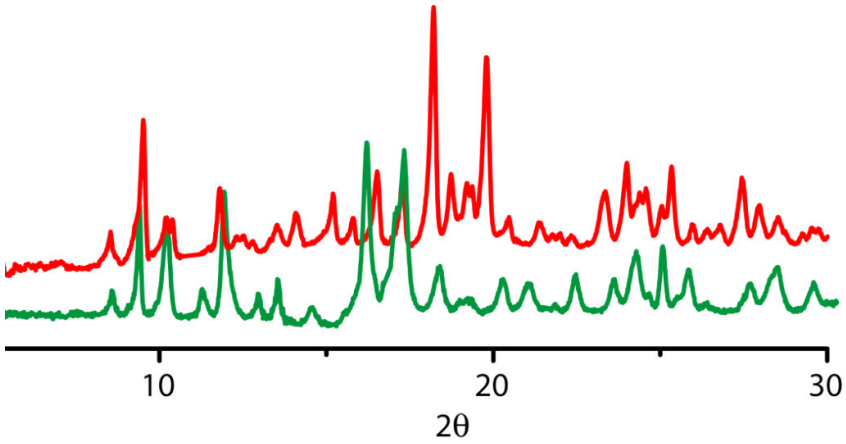

Fig. S22. PXRD pattern of water adsorbed sample of compound **2**; As-synthesized (green), H_2O adsorbed (red).

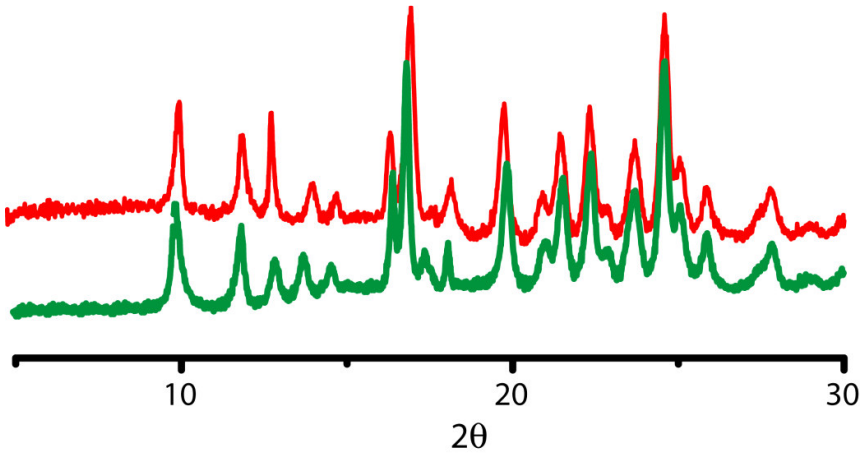

Fig. S23. PXRD pattern of water adsorbed sample of compound **3**; As-synthesized (green), H_2O adsorbed (red).

Table S1. Selected bond lengths (Å) and bond angles (deg) of compounds **1**-**3.**

1		**2**		**3**	
Co1-O1	2.029(3)	Ni1-N1	2.09(1)	Cu1-N2	2.002(3)
Co1-N1	2.139(3)	Ni1-O3	2.076(8)	Cu1-O4	2.542(4)
Co1-O3	2.160(5)	Ni1-N2	2.09(1)	Cu1-N1	2.020(3)
O1-Co1-N1	92.4(1)	O2-Ni1-O6	89.8(4)	N2-Cu1-O4	93.3(1)
O1-Co1-O3	88.9(2)	O2-Ni1-O5	87.1(4)	N2-Cu1-N2	91.7(1)
O1-Co1-N1	88.4(1)	O2-Ni1-N1	89.4(4)	N2-Cu1-N1	88.7(1)
O1-Co1-O3	90.3(2)	O2-Ni1-O3	178.4(4)	N2-Cu1-N1	171.2(1)
O1-Co1-O1	178.8(1)	O2-Ni1-N2	92.0(4)	N2-Cu1-O4	84.6(1)
N1-Co1-O3	87.3(2)	O6-Ni1-O5	87.0(4)	O4-Cu1-N1	86.6(1)
N1-Co1-N1	96.2(1)	O6-Ni1-N1	177.4(4)	O4-Cu1-N1	95.5(1)
N1-Co1-O3	175.7(2)	O6-Ni1-O3	89.8(4)	O4-Cu1-O4	177.0(1)
O3-Co1-O3	89.4(2)	O6-Ni1-N2	87.5(4)	N1-Cu1-N1	92.2(1)
		O5-Ni1-N1	90.5(4)		
		O5-Ni1-O3	91.8(4)		
		O5-Ni1-N2	174.5(4)		
		N1-Ni1-O3	91.0(4)		
		N1-Ni1-N2	95.0(5)		
		O3-Ni1-N2	89.1(4)		

Table S2. H-bonding table of compounds **1**-**3**.

	D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	<D-H-A(°)
1	O(2) ···O(2A)[a]	-	-	2.975(6)	-
	O(2) ···O(3)[b]	-	-	2.586(7)	-
	C(1)-H(1)···O(2)[c]	0.93	2.690	3.531(7)	150.9(3)
2	O(1) ···O(6)	-	-	2.63(1)	-
	O(3) ···O(5)	-	-	3.00(1)	-
	O(3) ···O(6)	-	-	2.97(1)	-
	O(3) ···O(11)	-	-	2.84(2)	-
	O(4) ···O(5)	-	-	2.66(1)	-
	O(4) ···O(7)	-	-	2.62(2)	-
	O(5) ···O(10)	-	-	2.77(2)	-
	O(6) ···O(8)	-	-	2.82(1)	-
	O(6) ···O(9)	-	-	2.88(2)	-
	O(7) ···O(7A)	-	-	2.02(3)	-
	O(7) ···O(9)	-	-	2.92(3)	-
	O(8) ···O(9)	-	-	2.96(3)	-
	O(9) ···O(13)	-	-	2.81(4)	-
	O(10) ···O(11)	-	-	2.78(2)	-
	O(10) ···O(13)	-	-	2.86(3)	-
	O(11) ···O(12)	-	-	2.75(3)	-
	O(12) ···O(13)	-	-	2.70(5)	-
3	O(5) ···O(5A)	-	-	2.726(4)	-
	O(3) ···O(5)	-	-	2.671(5)	-
	O(3) ···S(2)	-	-	3.014(3)	-
	C(2)-H(2)···O(1)[d]	0.93	2.44	3.285(5)	151
	C(4)-H(4)···S(1)	0.93	2.73	3.200(3)	112
	C(6)-H(6)···S(2)	0.93	2.73	3.212(3)	113
	C(6)-H(6)···O(1)	0.93	2.45	3.241(6)	143
	C(8)-H(8)···O(5)[e]	0.93	2.48	3.374(5)	161
	C(9)-H(9)···O(3)[f]	0.93	2.57	3.331(5)	139
	C(9)-H(9)···O(4)[g]	0.93	2.47	2.978(5)	115
	C(13)-H(13)···O(1)	0.93	2.34	2.698(6)	103

Symmetry: [a] x, -y+1/4, -z+1/4; [b]-x+3/4, -y+3/4, +z; [c] x, -y+1/4, -z+1/4; [d]-x, 1-y, 1-z; [e]1-x, y, 1/2-z; [f]1+x, 1+y, z; [g]-x, 1+y, 1/2-z.