Supplementary Information

The synthesis and characterisation of coordination and hydrogen-bonded networks based on 4-(3,5-dimethyl-1*H*-pyrazol-4-yl)benzoic acid

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1 General Experimental

NMR Spectroscopy

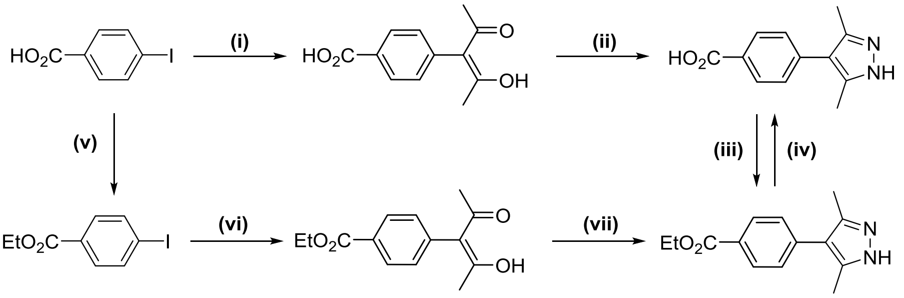
^{1}H NMR and ^{13}C NMR spectra obtained at the University of Wollongong were recorded on a Varian Mercury VX-300-MHz NMR spectrometer operating at 300 MHz for ^{1}H and 75.5 MHz for ^{13}C. ^{1}H NMR and ^{13}C NMR spectra recorded at the University of Bath were on a Bruker AV300 spectrometer operating at 300 MHz for ^{1}H and 75.5 MHz for ^{13}C. NMR spectra obtained at the University of Canterbury were recorded on a Varian INOVA instrument operating at 500 MHz for ^{1}H and 126 MHz for ^{13}C ^{1}H NMR spectra were referenced to the residual protio peaks at 7.26 ppm ($CDCl_3$) and 2.50 ppm (d_6-DMSO). ^{13}C NMR spectra were referenced to the solvent peaks at 77.0 ppm ($CDCl_3$) and 39.6 ppm (d_6-DMSO).

Mass Spectrometry

Mass spectra were recorded in negative ion mode using alcohol / water mixtures on a Waters Quattro Micro ESI mass spectrometer (Milford, Massachusetts, USA) and high–resolution ESI spectra were obtained using a Waters Xevo Quadrupole time-of-flight mass spectrometer at the University of Wollongong. Mass spectra were recorded in positive ion electrospray ionisation mode with a Bruker MaXiS 3G UHR-TOF instrument with samples dissolved in HPLC-grade methanol or acetonitrile at the University of Canterbury.

2 Synthesis of 4-(3,5-dimethyl-1*H*-pyrazol-4-yl)benzoic acid, H_2L

4-(3,5-Dimethyl-1*H*-pyrazol-4-yl)benzoic acid has been prepared previously by Elguero and co-workers.[1] We investigated two pathways for the synthesis of $\mathbf{H_2L}$ from 4-iodobenzoic acid as shown in Scheme S1 below.



Scheme S1. (i) CuI (5 mol%), L-proline (20 mol%), K_2CO_3, DMSO (ii) $H_2NNH_2{\cdot}H_2O$ (iii) EtOH, H_2SO_4 (vi) $NaOH_{(aq)}$, EtOH (vi) CuI (10 mol%), L-proline (20 mol%), K_2CO_3, DMSO (vii) $H_2NNH_2{\cdot}H_2O$.

Procedure (i) *4-(1-Acetyl-2-hydroxy-propenyl)benzoic acid*

The synthesis of this molecule has been reported in the literature.[2] The procedure below is what we used on a larger scale. Occasionally we found this to result in ≈ 50% conversion and the mixture could be carried through step (ii) and step (iii) and separation of ethyl 4-iodobenzoate and ethyl 4-(3,5 dimethyl-1*H*-pyrazol-4-yl)benzoate could be easily achieved by column chromatography on silica gel.

4-Iodobenzoic acid (4.96 g, 20 mmol), CuI (0.23 g, 5 mol %), L-proline (0.45 g, 20 mol%) and K_2CO_3 (11.10 g, 80 mmol) were placed under nitrogen. Dry DMSO (80 mL) was admitted by canula and the mixture stirred for 5 min before 2,4-pentanedione (6.2 mL, 60 mmol) was admitted by syringe and the mixture stirred at 90 °C under N_2 overnight. The cooled reaction mixture was then poured into 1 N HCl (300 mL) and further diluted with H_2O to bring the total volume to 500 mL. The aqueous solution was chilled in a refrigerator and the precipitated product collected by filtration and washed with H_2O (3 x 70 mL). The solid was taken up in EtOH (40 mL) and refluxed with decolourising carbon and filtered. Dilution with H_2O precipitated the product and it was collected by filtration, washed with H_2O and oven dried. Yield 3.05 g (69%). Found: C, 65.4; H, 5.54. $C_{12}H_{12}O_4$ requires C, 65.4; H, 5.50. A ratio of 5:1 ratio of enol:keto form was determined by ^1H NMR. δ_H (300 MHz; DMSO-d_6) (enol form) 2.09 (6 H, s) 7.40 (2 H, d, J = 8.19 Hz), 7.97 (2 H, d, J = 8.32 Hz); (keto form) 1.86 (6 H, s), 5.51 (1 H, s), 7.34 (2 H, d, J = 8.26 Hz), 7.74 (2 H, d, J = 8.47 Hz). Signals due to the two tautomeric forms are apparent in ^{13}C NMR spectra of this compound and no attempt was made to definitively assign signals to individual tautomers. A full list of signals observed in ^{13}C NMR spectra is given. δ_C (75.5 MHz, DMSO-d_6) 24.05, 30.18, 71.05, 114.38, 129.56, 129.69, 129.93, 130.20, 131.47, 137.96, 141.11, 167.17, 190.66, 202.96.

Procedure (ii) *4-(3,5-Dimethyl-1*H*-pyrazol-4-yl)benzoic acid*

In cases where (i) gave only a 50 % conversion and an ≈ 1:1 mixture of starting 4-iodobenzoic acid and 4-(1-acetyl-2-hydroxy-propenyl)benzoic acid product was obtained, the mixture was subjected to the procedure below.

Hydrazine hydrate (0.7 cm^3, 14 mmol) was added to 4-iodobenzoic acid and 4-(1-acetyl-2-hydroxy-propenyl)benzoic acid (4.38 g mixture) dissolved in ethanol (40 mL) and the mixture was refluxed for 3 h. The volume of the solution was reduced by rotary evaporation to approximately ⅓ and H_2O (100 mL) was added with stirring. The precipitate was filtered and washed with water and oven dried (4.33 g). This was used for the next step.

Procedure (iii) ***Ethyl (3,5-dimethyl-1*****H*****-pyrazol-4-yl)benzoate***

In cases where (i) gave a 50% conversion and an ≈ 1:1 mixture of starting 4-iodobenzoic acid and 4-(3,5-dimethyl-1*H*-pyrazol-4-yl)benzoic acid product was obtained from (ii) the mixture could be esterified and separation effected using the procedures below.

Concentrated H_2SO_4 (5 mL) was added drop wise to 4-iodobenzoic acid and 4-(3,5-dimethyl-1*H*-pyrazol-4-yl)benzoic acid (4.33 g mixture) in EtOH (40 mL) and the mixture refluxed overnight. The EtOH was removed by rotary evaporation and the syrupy mixture was taken up in chilled EtOAc (100 mL). A solution of 2 M Na_2CO_3 was added in portions with stirring until the pH of the aqueous phase = 7. The biphasic solution was transferred to separation funnel and the lower layer was run off and discarded. The organic phase was washed with H_2O, brine and dried over Na_2SO_4 and the solvent removed to provide ethyl 4-iodobenzoate and ethyl (3,5-dimethyl-1*H*-pyrazol-4-yl)benzoate (4.31 g mixture). The compounds were taken up in DCM and loaded onto a column of silica gel (4 × 10 cm, d × h) and eluted with DCM to release ethyl 4-iodobenzoate (2.20 g). The eluent was changed to EtOAc to release ethyl (3,5-dimethyl-1*H*-pyrazol-4-yl)benzoate (1.87 g) ($R_f = 0.50$).

Procedure (iv) ***4-(3,5-Dimethyl-1*****H*****-pyrazol-4-yl)benzoic acid, H_2L***

Procedure (a): LiOH (4.0 g, 170 mmol) dissolved in distilled water (20 mL) was added with stirring to ethyl-4-(3,5-dimethyl-1*H*-pyrazol-4-yl)-benzoate (0.80 g, 3.3 mmol) dissolved in THF (40 mL). The resulting slurry was refluxed for 72 h after which the mixture was reduced to approximately ⅓ the volume under reduced pressure. Distilled water (100 mL) was added and the solution filtered. The filtrate was adjusted to pH 3 by the addition of dilute aqueous HCl and the resulting white precipitate filtered and dried *in vacuo*. Yield 0.55 g (78%).

Procedure (b): 1 M Aqueous NaOH (18 mL, 18 mmol) was added to ethyl 4-(3,5-dimethyl-1*H*-pyrazol-4-yl)benzoate (1.21 g, 4.95 mmol) dissolved in ethanol (18 mL) and the mixture stirred overnight at room temperature. The solvent was removed by rotary evaporation and the residue taken up in water (20 mL) and filtered. 1 M Aqueous HCl was added to the filtrate with stirring to precipitate the product as a white powder, which was collected by filtration and washed with water and oven dried (80 °C). Yield 0.98 g (90%).

Analytical data: M.pt. 278-281 °C (decomp); δ_H (300 MHz, d_6-DMSO): 2.22 (s, 6H), 7.40 (d, 2H, $J = 8.1$ Hz), 7.95 (d, 2H, $J = 8.1$ Hz); δ_C (125 MHz, d_6-DMSO): 12.3, 116.7, 128.4, 129.1, 130.2, 139.5, 167.9; υ_{max}(KBr) cm^{-1}: 3284 s sh, 2467 w br, 1942 w br, 1680 s, 1609 s, 1528 m, 1266 s, 1177 m, 1010 s, 865 m, 804 m. *m/z* (ESMS): Found 217.0974, $C_{12}H_{13}N_2O_2$ requires 217.0977 $[M+H^+]$.

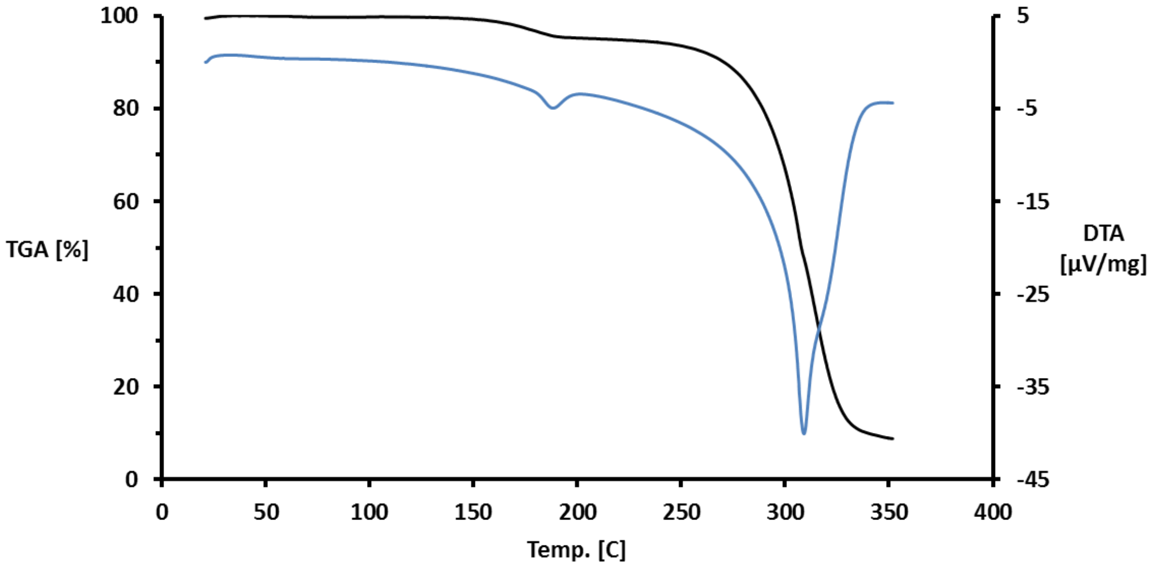


Figure S 1 TG—DTA traces for **H_2L**; The black curve represents the TGA; the blue curve represents the DTA.

Procedure (v) *Ethyl 4-iodobenzoate*

This step was accomplished by a Fisher esterification of 4-iodobenzoic acid in ethanol and sulfuric acid in 95 % yield and gave identical spectral characteristics to those reported.[3]

Procedure (vi) *Ethyl 4-(2-hydroxy-4-oxopent-2-en-3-yl)benzoate*

Under N_2, 2,4-pentanedione (5.0 mL, 49 mmol) was added to a stirred mixture of L-proline (0.38 g, 20 mol %), CuI (0.31 g, 1.6 mmol, 10 mol %), anhydrous K_2CO_3 (9 g, 65 mmol) and ethyl 4-iodobenzoate (4.52 g, 16 mmol) in anhydrous DMSO (25 mL). The resulting mixture was heated to 90 °C with vigorous stirring under N_2 for 8 h. The mixture was then poured into 10% HCl solution (250 mL) and extracted with ethyl acetate. The extract was washed with water, dried and evaporated under reduced pressure to give a dark brown residue. The residue was purified by flash chromatography on silica gel eluting with 5:1 CH_2Cl_2/hexanes. The title compound was isolated as pale yellow crystals following concentration of the solvent. Yield 1.7 g (44%). M.pt. 55-57 °C; δ_H (300 MHz, $CDCl_3$): 1.33 (t, 3H, *J* = 7.3 Hz), 1.86 (s, 6H), 4.33 (q, 2H, *J* = 7.3 Hz), 7.44 (d, 2H, *J* = 8.1 Hz), 7.98 (d, 2H, *J* = 8.1 Hz), 16.87 (s, 1H); δ_C (125 MHz, $CDCl_3$): 14.2, 24.0, 60.8, 114.3, 129.1, 129.5, 131.6, 141.5, 165.6, 190.6; υ_{max}(KBr) cm^{-1}: 2983 m sh, 1712 s, 1607 m br, 1284 s, 1176 m, 1110 s, 1024 m, 916 m. *m/z* (ESMS): Found 249.1121, $C_{14}H_{17}O_4$ requires 249.1127 $[M+H^+]$.

Procedure (vii) *Ethyl 4-(3,5-dimethyl-1*H*-pyrazol-4-yl)benzoate*

Hydrazine hydrate (310 µL, 6.4 mmol) in methanol (5 mL) was added drop wise to a solution of ethyl-4-(2,4-pentanedion-3-yl)-benzoic acid (1.30 g, 5.2 mmol) in methanol (40 mL). The resulting solution was refluxed for 8 h and allowed to cool to room temperature. The solvents were evaporated to give the product as a pale yellow solid. Yield 1.04 g (81%). M.pt. 79-84 °C; δ_H (500 MHz, $CDCl_3$): 1.32 (t, 3H, *J* = 7.1 Hz), 2.28 (s, 6H), 4.31 (q, 2H, *J* = 7.1 Hz), 7.34 (d, 2H, *J* = 8.3 Hz), 8.08 (d, 2H, *J* = 8.3 Hz); δ_c (125 MHz, $CDCl_3$): 11.9, 14.7, 61.3, 118.2, 128.7, 129.3, 130.2, 142.4, 166.9; υ_{max}(KBr) cm^{-1}: 2980 br, 1711 s, 1609 m, 1273 s, 1180 s sh, 1104 m, 1007 m, 865 m, 712 m. *m/z* (ESMS): Found 267.1103, $C_{14}H_{16}N_2O_2Na$ requires 267.1104 $[M+Na^+]$.

3 Powder X-ray Diffraction data

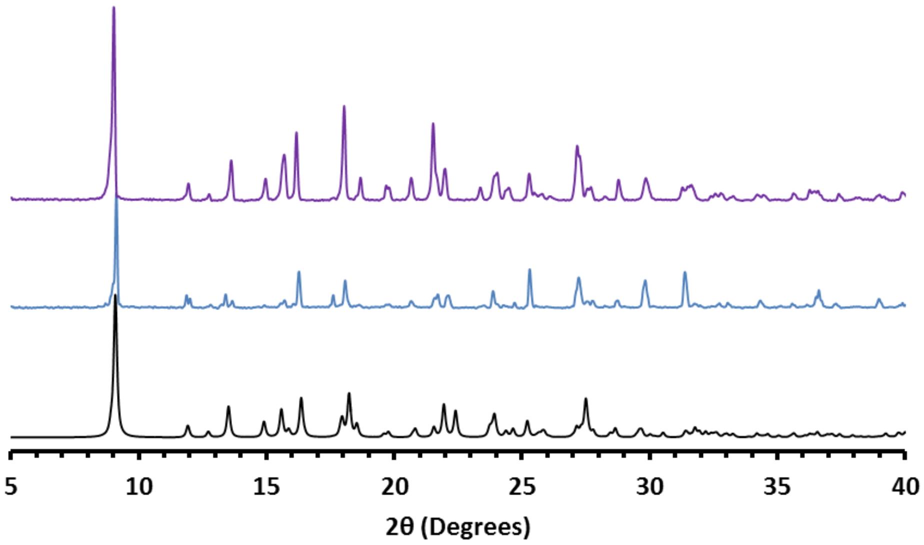


Figure S 2 Simulated pattern from the crystal structure of $[Co(H\mathbf{L})_2(OH_2)_4]\cdot 2DMF$ **1** (black); experimental pattern for $[Co(H\mathbf{L})_2(OH_2)_4]\cdot 2DMF$ **1** (blue); experimental pattern for $[Ni(H\mathbf{L})_2(OH_2)_4]\cdot 2DMF$ **2** (purple).

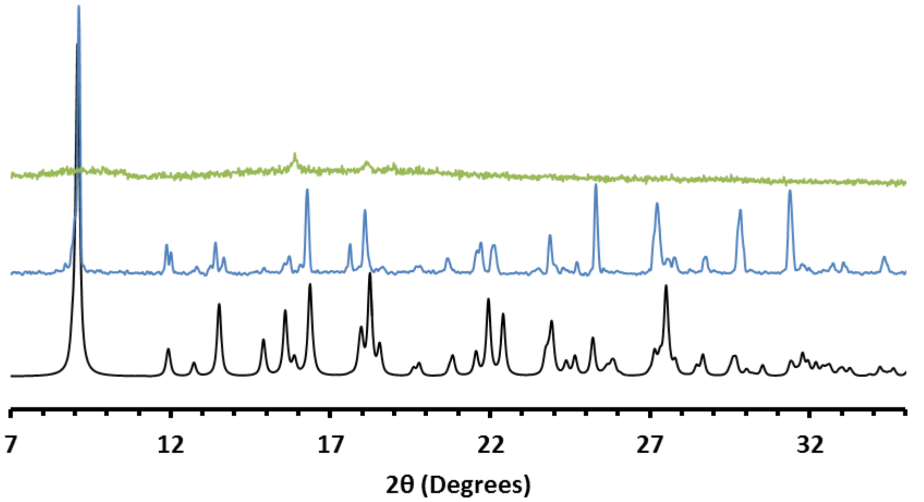


Figure S 3 Simulated pattern from the crystal structure of $[Co(H\mathbf{L})_2(OH_2)_4]\cdot 2DMF$ **1** (black); experimental pattern for $[Co(H\mathbf{L})_2(OH_2)_4]\cdot 2DMF$ **1** (blue); experimental pattern for thermally desolvated product 1-*desolv* (green).

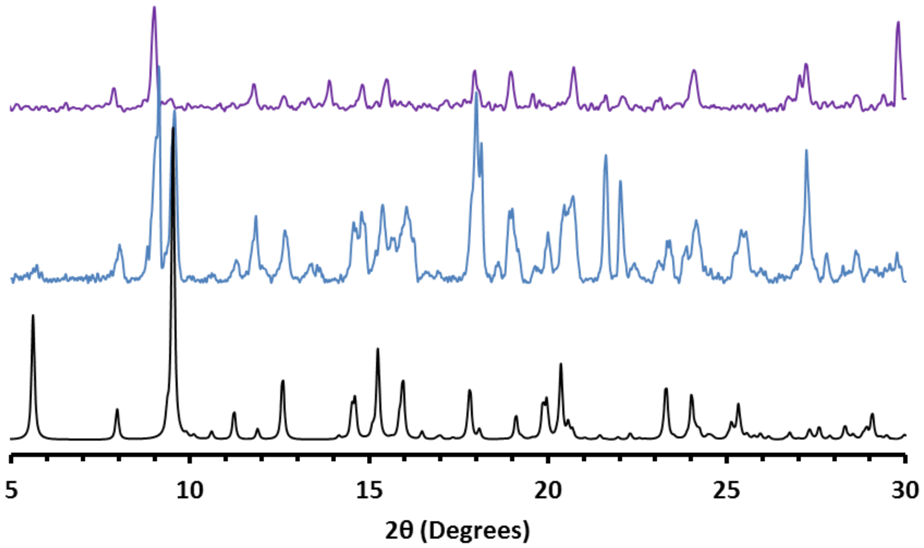


Figure S 4 Simulated pattern from the crystal structure of $[Zn(H\mathbf{L})_2]$ **3** (black); experimental pattern for $[Zn(H\mathbf{L})_2]$ **3** (blue); experimental pattern for the initially formed powder in the reaction (purple).

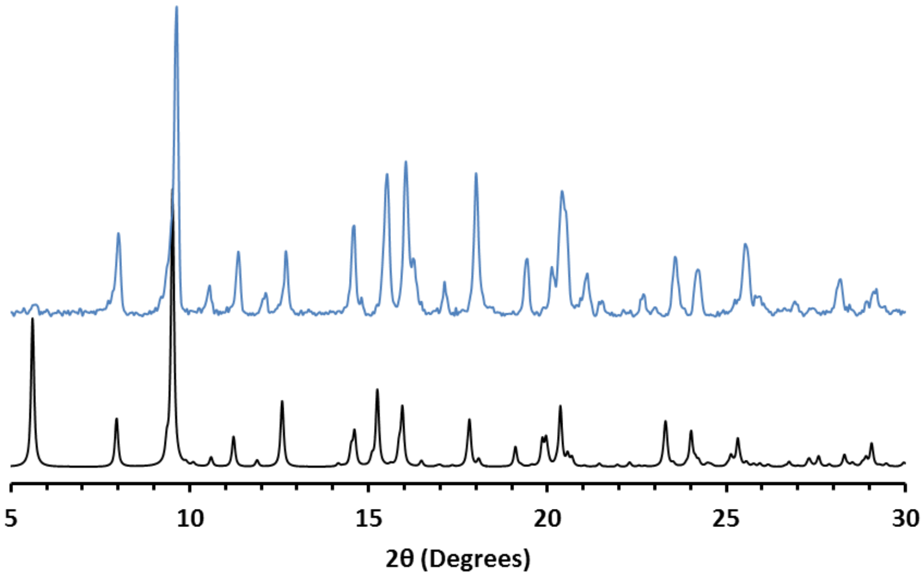


Figure S 5 Simulated pattern (black) and experimental pattern (blue) for $\{[Zn(H\mathbf{L})_2]\cdot 2CH_3OH\cdot H_2O\}$ **4**.

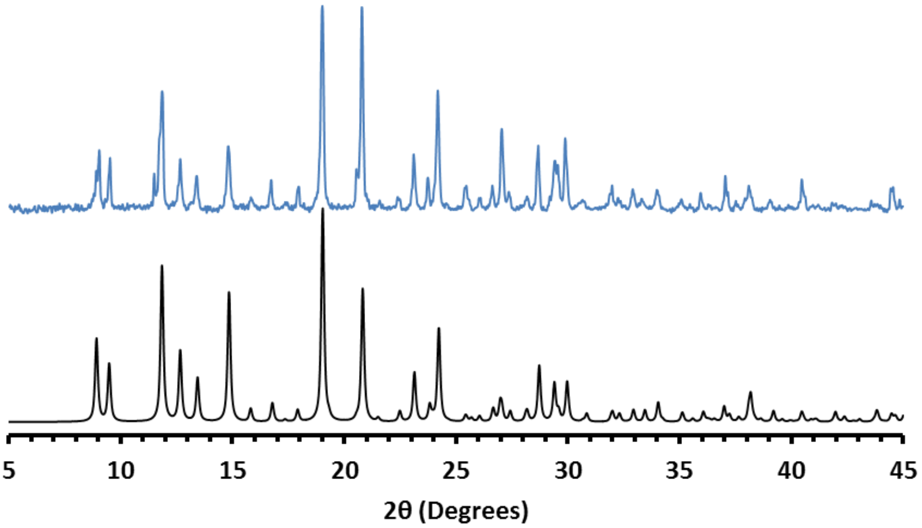


Figure S 6 Simulated pattern (black) and experimental pattern (blue) for [Co(H**L**)$_2$] **5**.

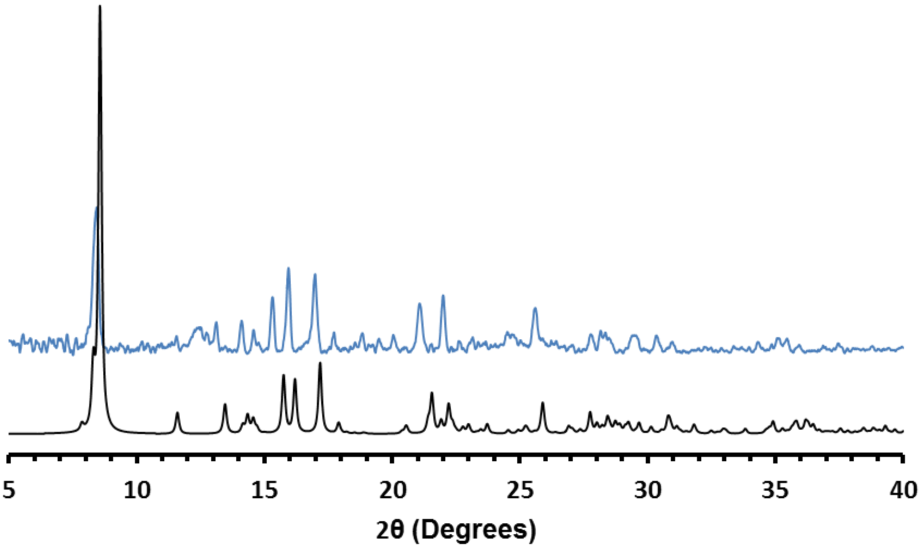


Figure S 7 Simulated pattern (black) and experimental pattern (blue) for {[Cd(**HL**)$_2$(MeOH)$_2$]·1.8MeOH} **6**.

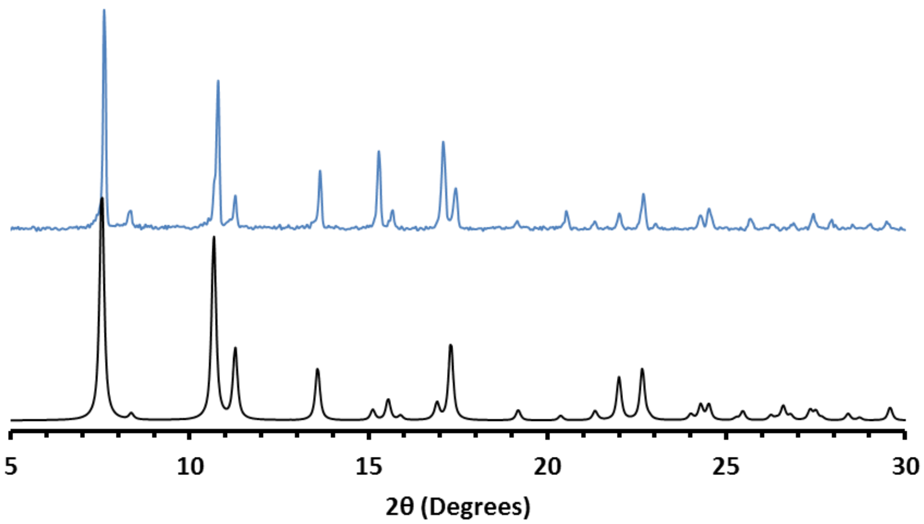


Figure S 8 Simulated pattern (black) and experimental pattern (blue) for {[Cu(**HL**)$_2$]·4MeOH·H$_2$O} 8.

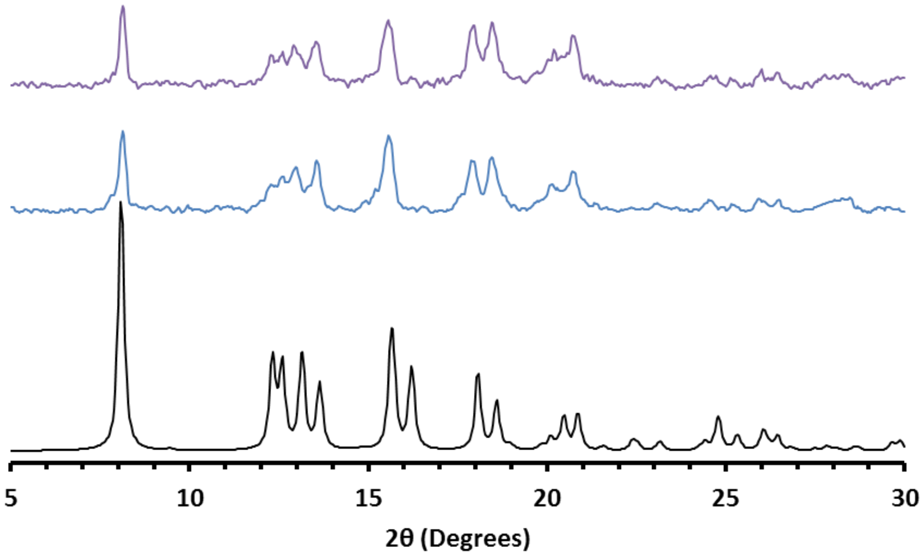


Figure S 9 Simulated pattern (black) and experimental pattern (blue) for TGA dried sample at 75 °C {[Cu(**HL**)$_2$]·1½H$_2$O} and experimental pattern (purple) for TGA dried sample at 100 °C [Cu(**HL**)$_2$] .

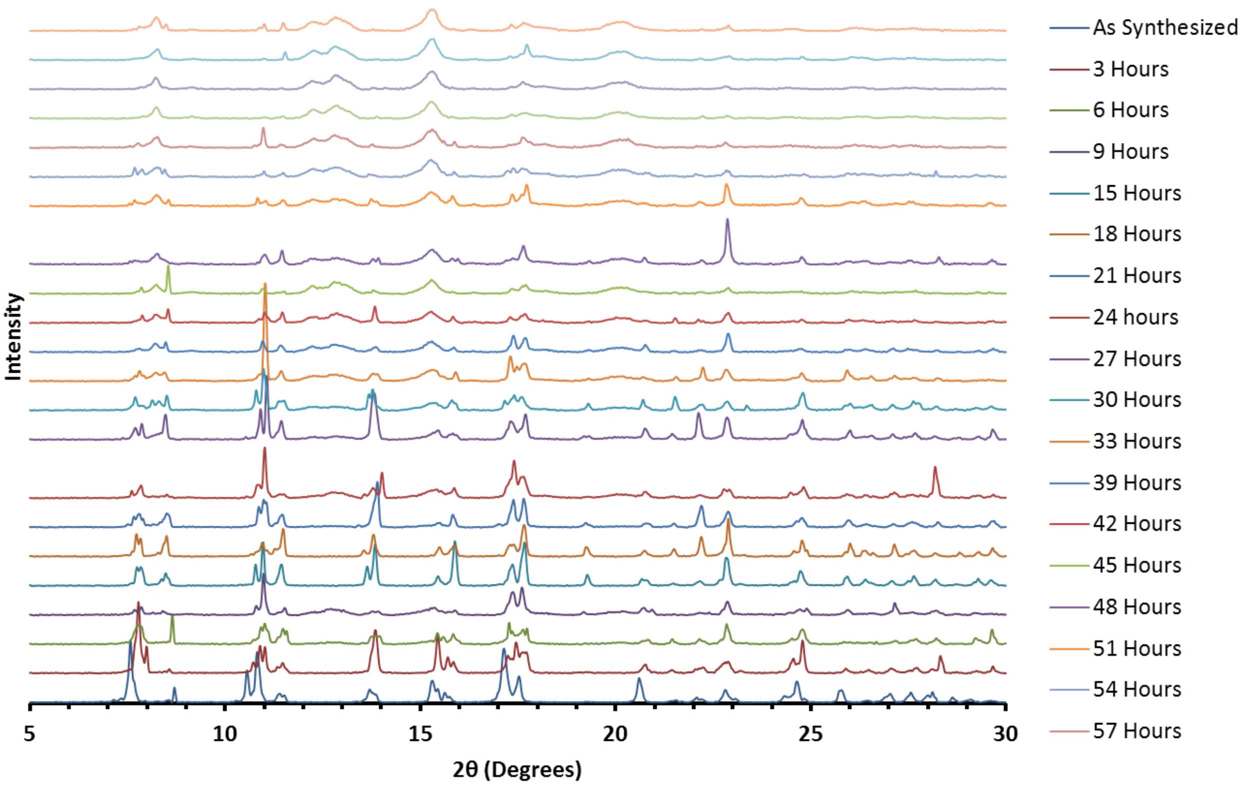


Figure S 10 Experimental PXRD patterns over the first 57 hours from removing **8** from solution.

4 TG-DTA data

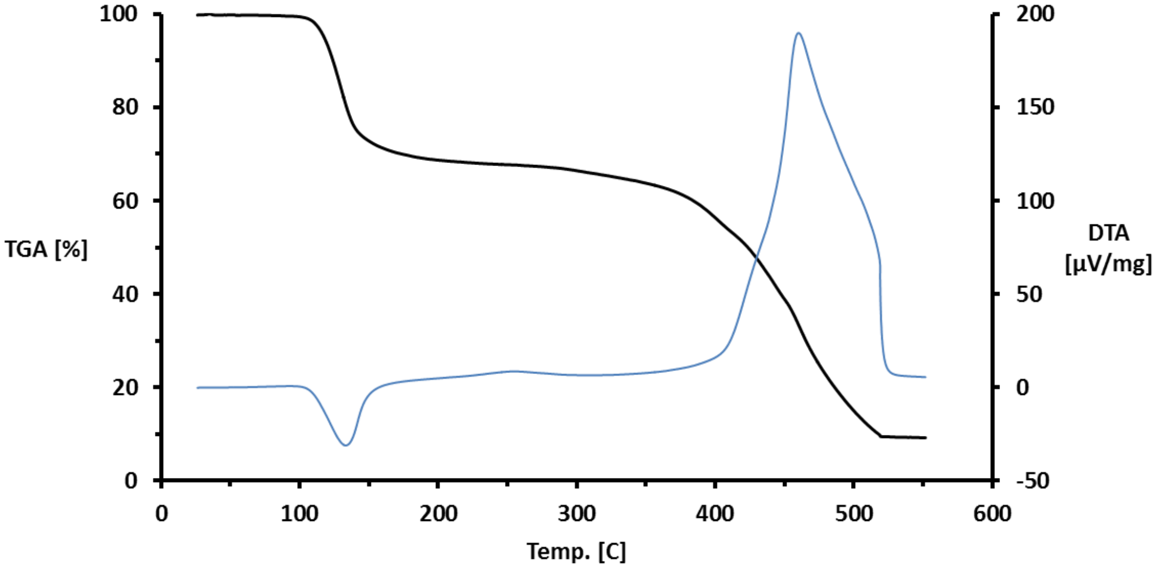


Figure S 11. TG—DTA traces for {[Co(**HL**)$_2$(OH$_2$)$_4$]·2 DMF} **1**;. The black curve represents the TGA; the blue curve represents the DTA.

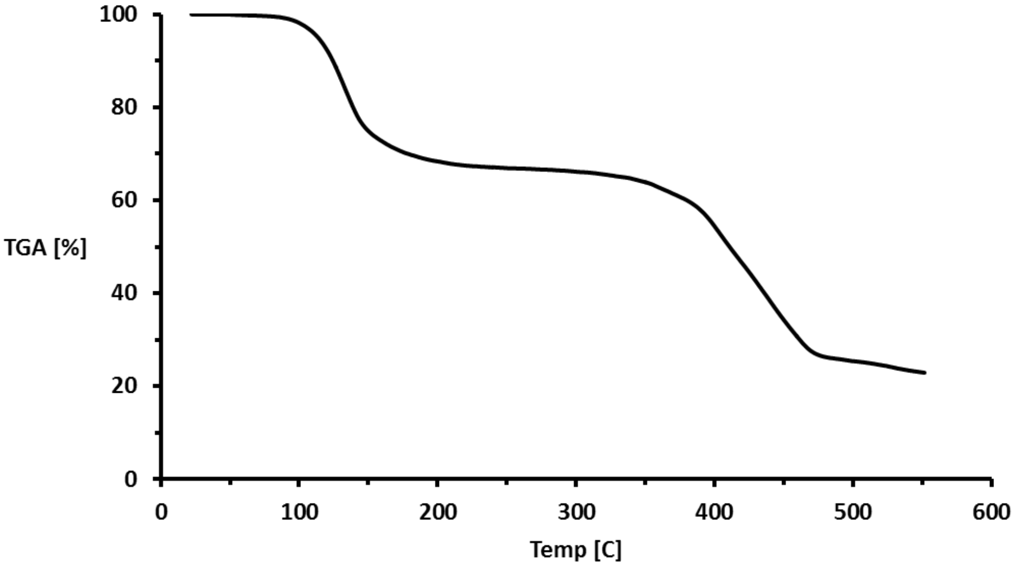


Figure S 12. TG trace for {[Ni(**HL**)$_2$(OH$_2$)$_4$]·2DMF} **2**.

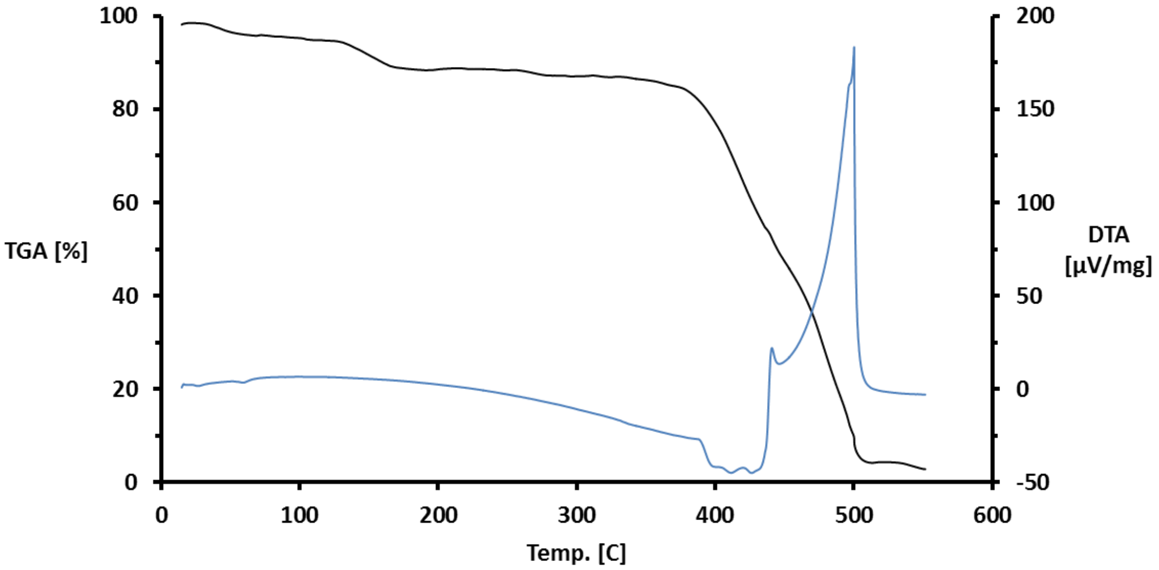


Figure S 13 TG-DTA of {[Zn(**HL**)$_2$]·2CH$_3$OH·H$_2$O}∞ **4**. The black curve represents the TGA; the blue curve represents the DTA.

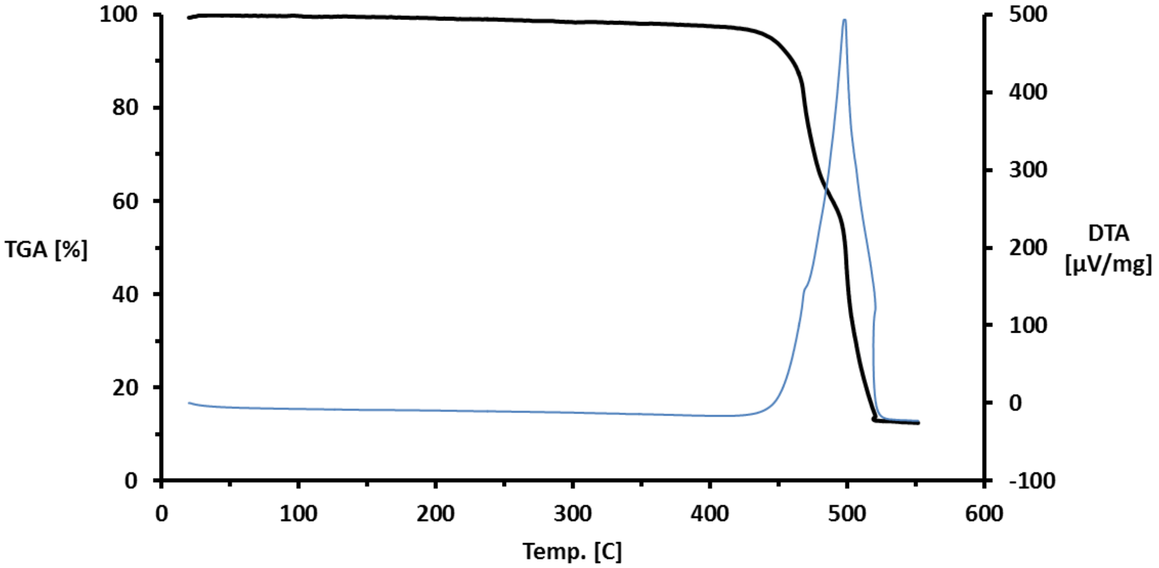


Figure S 14 The TG-DTA curves for [Co(**HL**)$_2$] **5**. The black curve represents the TGA; the blue curve represents the DTA.

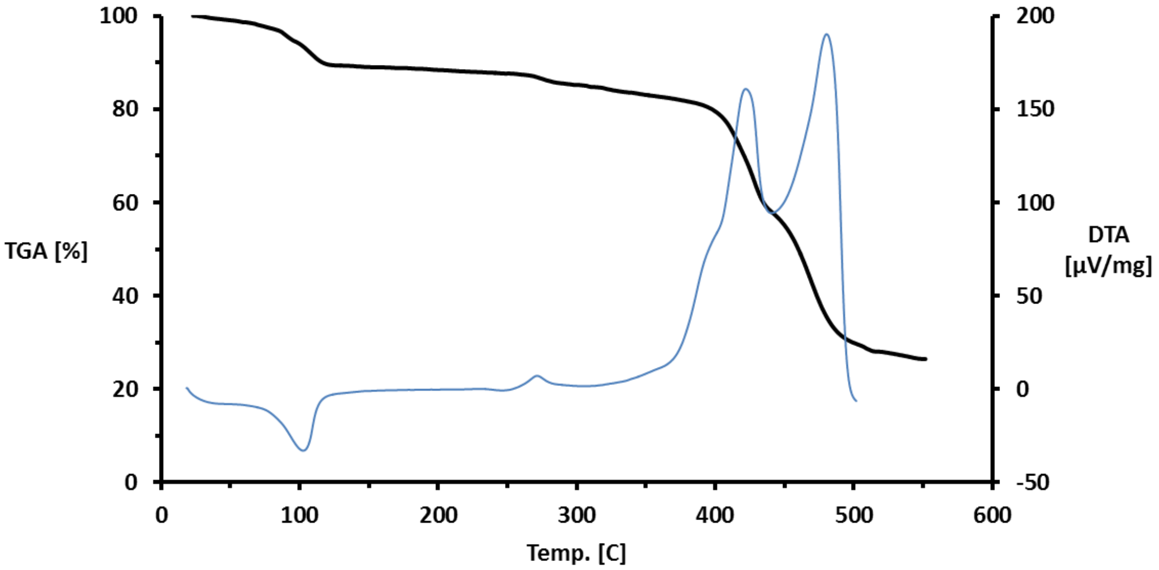


Figure S 15 The TG-DTA curves for [Cd(**HL**)$_2$(MeOH)$_2$] **6**-*dry*. The black curve represents the TGA; the blue curve represents the DTA.

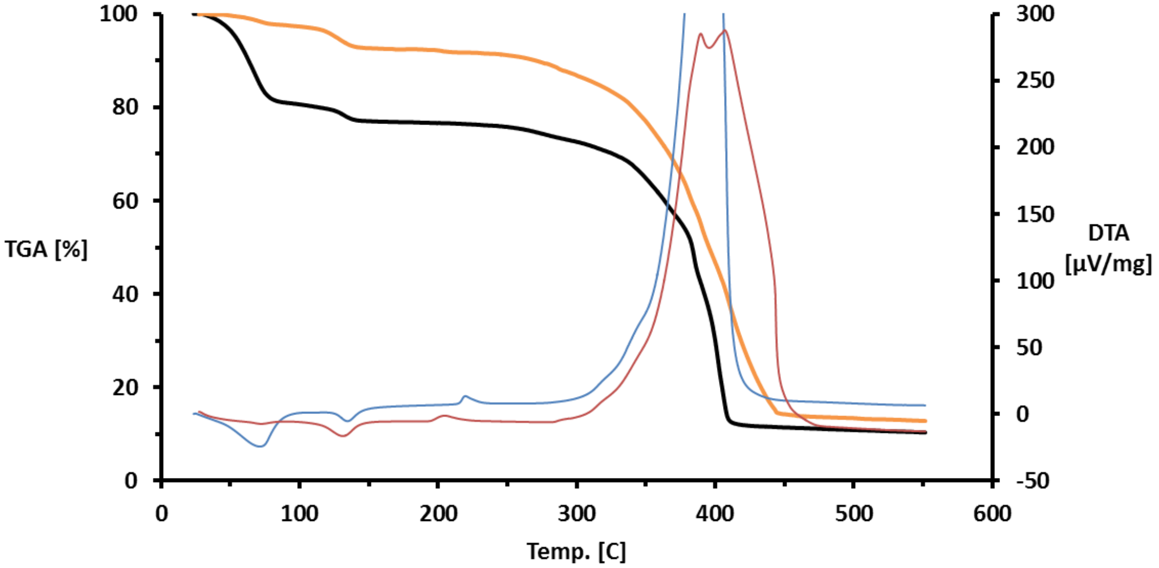


Figure S 16 The TG-DTA curves for {[Cu(**HL**)$_2$]·4MeOH·H_2O}∞ **8** (TG, black; DTA, blue) and after 1 day air drying {[Cu(**HL**)$_2$]·1.5H_2O}∞ (TG, orange; DTA red).

5 Infrared Spectroscopy

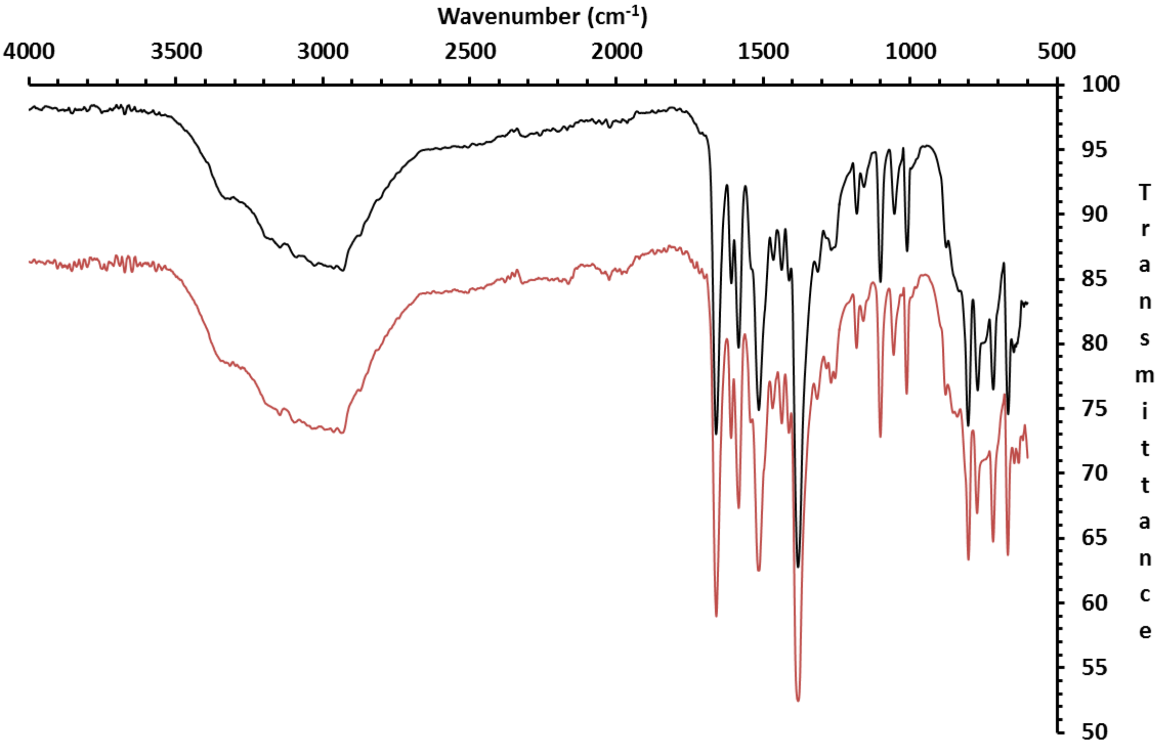


Figure S 17 Infrared spectra of {[Co(**HL**)$_2$(OH$_2$)$_4$]·2 DMF} **1** (black) and {[Ni(**HL**)$_2$(OH$_2$)$_4$]·2 DMF} **2** (red)

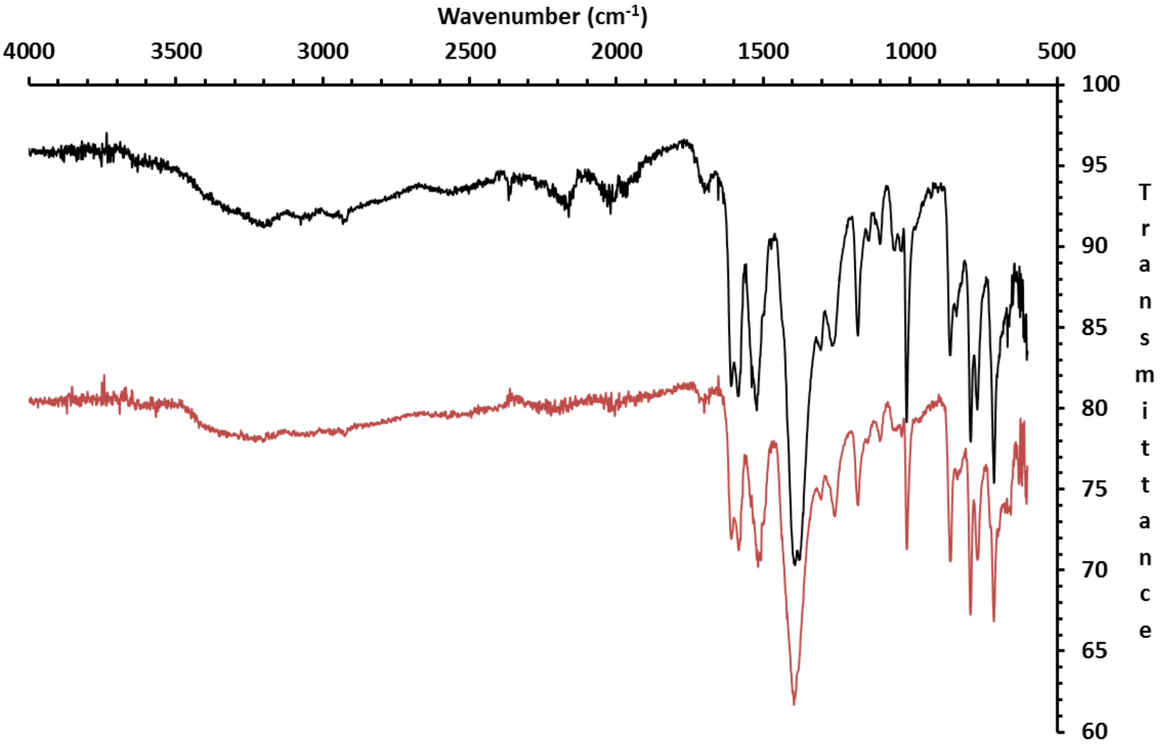


Figure S 18 Infrared spectra of {[Co(**HL**)$_2$(OH$_2$)$_4$]·2 DMF} **1** after thermal treatment (black) and {[Ni(**HL**)$_2$(OH$_2$)$_4$]·2 DMF} **2** after thermal treatment (red)

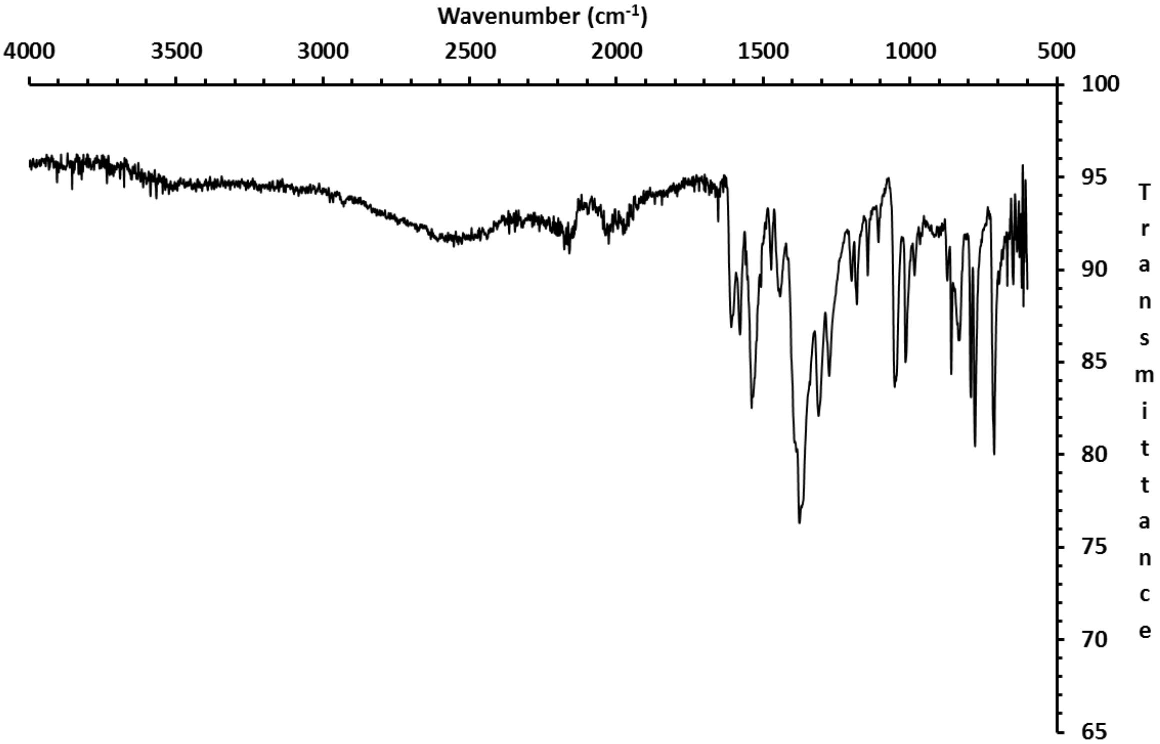


Figure S 19 IR spectrum of {[Zn(**HL**)$_2$]·Xsolv} **3.**

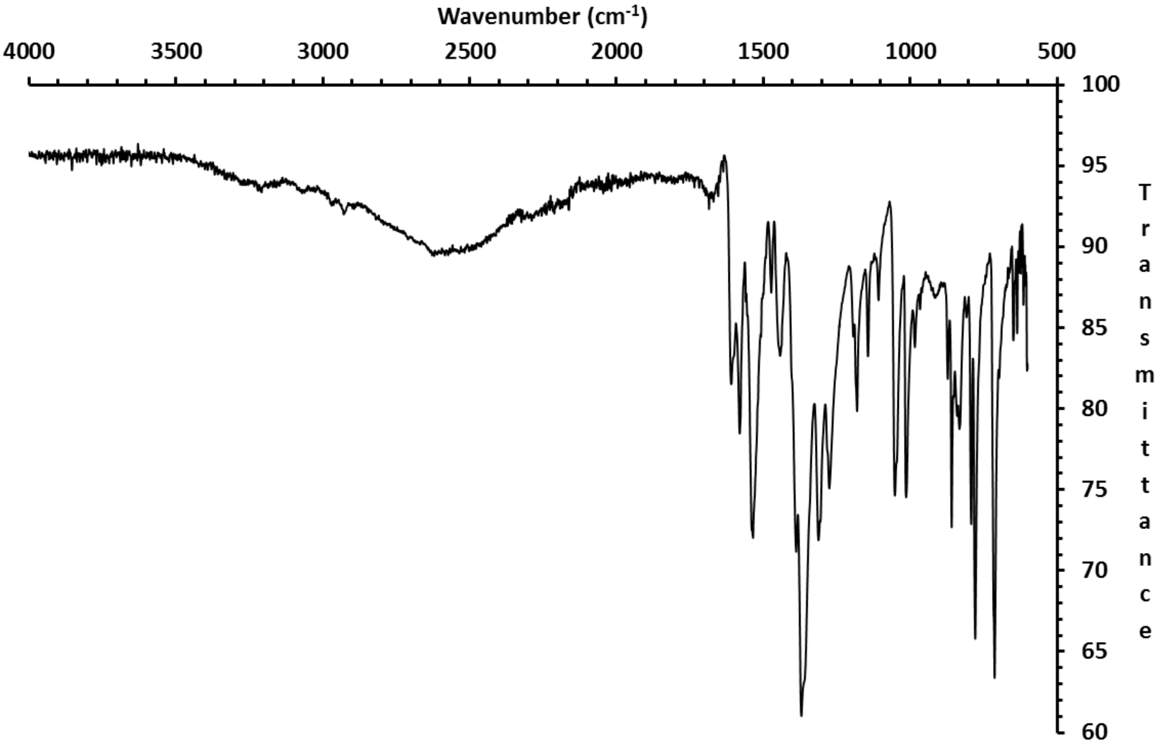


Figure S 20 IR spectrum of [Co(**HL**)$_2$] **5.**

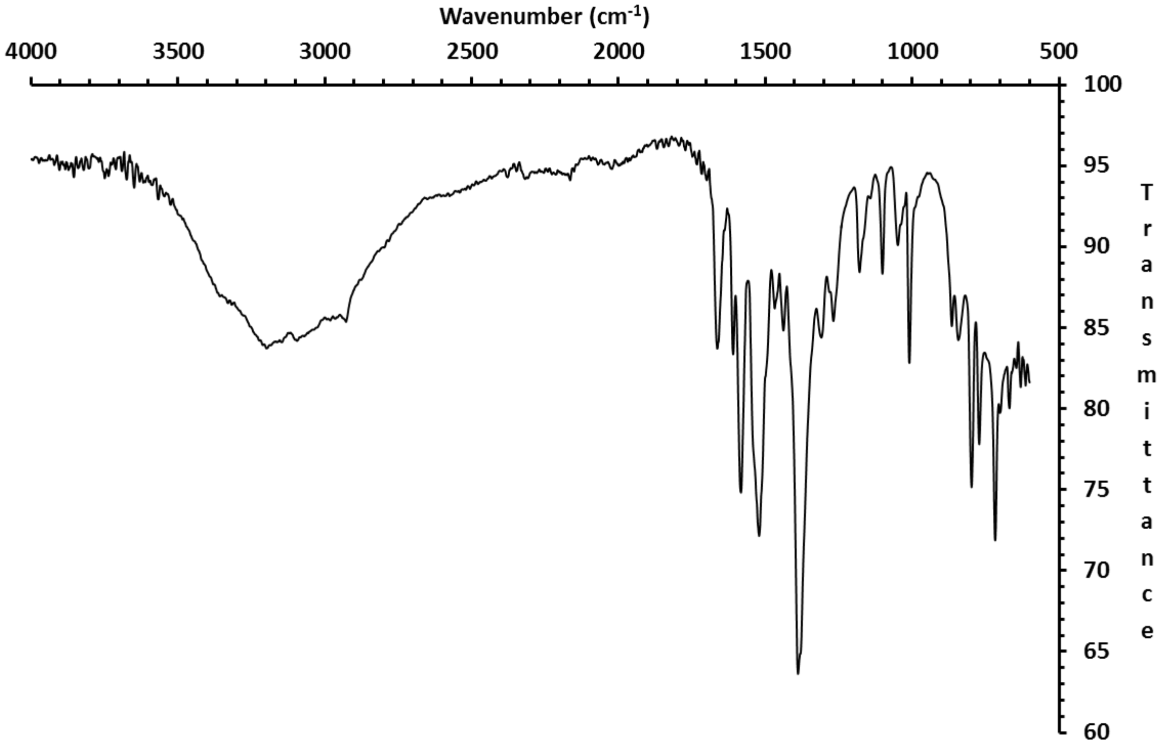


Figure S 21 IR spectrum of {[Cd(**HL**)$_2$(MeOH)$_2$]·1.8 MeOH} **6.**

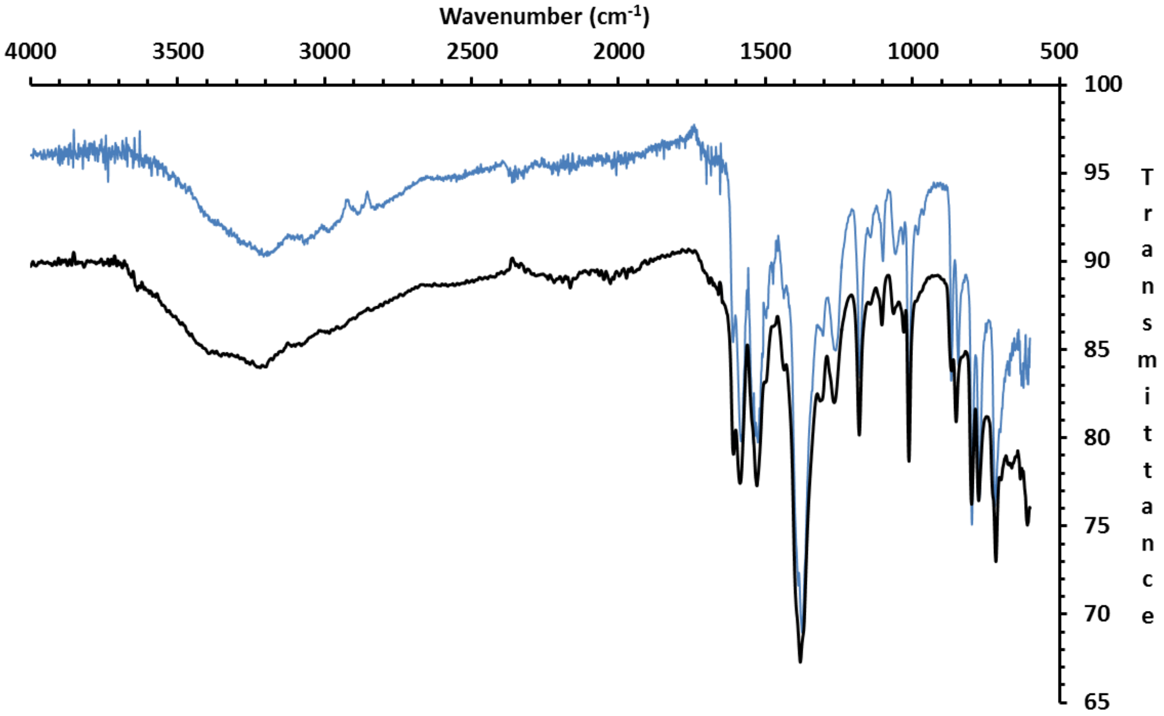


Figure S 22 IR Spectrum of {[Cu(**HL**)$_2$]·1½ H$_2$O}. TGA drying (blue); air drying (black).

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[1] C. Foces-Foces, C. Cativiela, M. M. Zurbano, I. Sobrados, N. Jagerovic, J. J. Elguero, *J. Chem. Crystallography* 1996, **26**, 579.

[2] Y. Jiang, N. Wu, H. Wu, M. He, *Synlett* 2005, **18**, 2731.

[3] AIST: Integrated Spectral Database System of Organic Compounds.

Identification code	$H_2\mathbf{L}$	$H_2\mathbf{L}\cdot HNO_3$	1	4	5	6	7	8	8-*dry*
Empirical formula	$C_{12}H_{12}N_2O_2$	$C_{12}H_{13}N_3O_5$	$C_{30}H_{44}CoN_6O_{10}$	$C_{50}H_{53}N_8O_{10.5}Zn_2$	$C_{24}H_{22}CoN_4O_4$	$C_{14.8}H_{22.2}Cd_{0.5}N_2O_{4.8}$	$C_{24}H_{26}Cu_2N_4O_{10}S$	$C_{28}H_{38}CuN_4O_9$	$C_{51}H_{43}Cu_4N_{10}O_8$
Formula weight	216.24	279.25	707.64	1064.74	489.39	361.15	689.63	638.16	1178.11
Temperature/K	123(2)	123(2)	150(2)	100.0(1)	120(2)	150(2)	100(2)	120.0(1)	100(2)
Crystal system	triclinic	triclinic	monoclinic	orthorhombic	tetragonal	monoclinic	monoclinic	tetragonal	monoclinic
Space group	P-1	P-1	$P2_1/c$	Fdd2	I-42d	C2/c	C2/m	$I4_1/a$	I2/a
a/Å	9.6538(5)	7.4272(4)	7.6150(3)	22.3458(7)	14.85742(19)	15.2670(4)	32.685(7)	23.5927(4)	18.658(4)
b/Å	10.4193(6)	8.9566(6)	19.8070(7)	29.7691(11)	14.85742(19)	21.2820(4)	29.520(6)	23.5927(4)	13.470(3)
c/Å	21.9388(14)	10.4607(6)	11.4480(5)	33.3734(11)	39.7127(9)	12.6080(4)	9.7350(19)	11.7356(3)	18.736(4)
α/°	91.284(4)	72.810(4)	90.00	90	90.00	90.00	90.00	90	90.00
β/°	101.971(4)	70.221(4)	102.902(2)	90	90.00	119.841(2)	103.71(3)	90	92.11(3)
γ/°	102.808(4)	78.066(4)	90.00	90	90.00	90.00	90.00	90	90.00
Volume/$Å^3$	2099.6(2)	621.14(6)	1683.11(12)	22200.5(13)	8766.3(2)	3553.34(16)	9125(3)	6532.2(3)	4705.6(16)
Z	8	2	2	16	16	8	8	8	4
$\rho_{calc}g/cm^3$	1.368	1.493	1.396	1.274	1.483	1.350	1.004	1.298	1.663
μ/mm^{-1}	0.095	0.118	0.573	1.563	6.476	0.668	1.016	1.401	1.852
F(000)	912.0	292.0	746.0	8848.0	4048.0	1499.0	2816.0	2680.0	2396.0
Crystal size/mm^3	0.19 × 0.19 × 0.1	0.28 × 0.14 × 0.06	0.15 × 0.13 × 0.05	0.31 × 0.25 × 0.24	0.13 × 0.08 × 0.01	0.3 × 0.25 × 0.25	0.08 × 0.06 × 0.01	0.19 × 0.09 × 0.06	0.1 × 0.03 × 0.03
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)	Cu Kα (λ = 1.5418)	MoKα (λ = 0.71073)	Synchrotron (λ = 0.71083)	CuKα (λ = 1.54184)	Synchrotron (λ = 0.71080)
2Θ range for data collection/°	1.9 to 56.3	5.58 to 56.86	7.18 to 55.08	5.61 to 147.578	6.36 to 131	7.66 to 54.9	2.56 to 44.96	8.416 to 139.84	4.36 to 51.98
Index ranges	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -29 ≤ l ≤ 29	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -13 ≤ l ≤ 13	-9 ≤ h ≤ 9, -25 ≤ k ≤ 25, -14 ≤ l ≤ 14	-25 ≤ h ≤ 27, -33 ≤ k ≤ 37, -41 ≤ l ≤ 37	-12 ≤ h ≤ 17, -17 ≤ k ≤ 17, -43 ≤ l ≤ 46	-19 ≤ h ≤ 19, -27 ≤ k ≤ 27, -16 ≤ l ≤ 16	-35 ≤ h ≤ 34, -30 ≤ k ≤ 30, -10 ≤ l ≤ 10	-27 ≤ h ≤ 27, -23 ≤ k ≤ 28, -14 ≤ l ≤ 9	-23 ≤ h ≤ 23, -16 ≤ k ≤ 16, -23 ≤ l ≤ 23
Reflections collected	27642	14759	24010	17046	13939	29301	42241	9018	30696
Independent reflections	10151 [R_{int} = 0.0671, R_{sigma} = 0.1106]	3077 [R_{int} = 0.0735, R_{sigma} = 0.0961]	3862 [R_{int} = 0.0823, R_{sigma} = 0.0697]	8656 [R_{int} = 0.0357, R_{sigma} = 0.0441]	3736 [R_{int} = 0.0302, R_{sigma} = 0.0269]	4032 [R_{int} = 0.0541, R_{sigma} = 0.0263]	5882 [R_{int} = 0.1489, R_{sigma} = 0.0873]	3092 [R_{int} = 0.0241, R_{sigma} = 0.0168]	4578 [R_{int} = 0.1242, R_{sigma} = 0.0670]
Data/restraints/parameters	10151/8/609	3077/3/193	3862/5/238	8656/1/688	3736/2/310	4032/12/244	5882/19/389	3092/9/223	4578/25/211
Goodness-of-fit on F^2	0.937	0.876	1.064	1.039	1.044	1.101	1.011	1.090	2.520
Final R indexes [I>=2σ (I)]	R_1 = 0.0540, wR_2 = 0.1007	R_1 = 0.0484, wR_2 = 0.1070	R_1 = 0.0528, wR_2 = 0.1084	R_1 = 0.0763, wR_2 = 0.2192	R_1 = 0.0418, wR_2 = 0.1172	R_1 = 0.0342, wR_2 = 0.0893	R_1 = 0.1023, wR_2 = 0.2701	R_1 = 0.0601, wR_2 = 0.1820	R_1 = 0.2556, wR_2 = 0.5936
Final R indexes [all data]	R_1 = 0.1326, wR_2 = 0.1305	R_1 = 0.1029, wR_2 = 0.1213	R_1 = 0.0929, wR_2 = 0.1252	R_1 = 0.0824, wR_2 = 0.2287	R_1 = 0.0487, wR_2 = 0.1230	R_1 = 0.0404, wR_2 = 0.0929	R_1 = 0.1337, wR_2 = 0.2914	R_1 = 0.0613, wR_2 = 0.1831	R_1 = 0.3323, wR_2 = 0.6441
Largest diff. peak/hole / e $Å^{-3}$	0.28/-0.33	0.41/-0.27	0.62/-0.66	1.57/-1.11	0.55/-0.45	0.82/-0.55	2.43/-0.99	0.87/-0.66	3.72/-2.04
Flack parameter				0.01(2)					
CCDC Number	1040598	1040599	1040600	1040601	1040602	1040603	1040604	1040605	1040606