Supplementary Information for

The Role of Temperature on Framework Dimensionality: Supramolecular Isomers of $Zn_3(RCOO)_8$ Based Metal Organic Frameworks.

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Section S1: Experimental Section

Materials: All the reagents and solvents were commercially available and used without further purification.

Synthesis of Zn-FDA compounds:-

Synthesis of $[Zn_{1.5}(FDA)_2(Me_2NH_2)]\cdot xG$ (1):- Single crystal of **1** was prepared by reacting $Zn(NO_3)_2.6H_2O$ (74.32 mg, 0.25 mmol), $FDAH_2$ (39mg, 0.25 mmol) in 3 mL of DMF by solvothermal technique, in a screw-capped glass vial. The vial was heated under autogenous pressure at 90°C for 2 days and then cooled to RT by 24 h period. Colourless crystals were obtained in ~ 50% yield. The compound looses solvent at RT and changes structure as we found from PXRD.

Synthesis of $[Zn_3(FDA)_4(Me_2NH_2)_2]\cdot xG$ (2):- Single crystal of **2** was prepared by reacting $Zn(NO_3)_2.6H_2O$ (99.16 mg, 0.33 mmol), $FDAH_2$ (52 mg, 0.33 mmol) in 4.5 mL of DMF at by the solvothermal technique, in a Teflon-lined autoclave . The autoclave was heated under autogenous pressure to 120 °C for 2 days and then cooled to RT by 24 h period. The pale yellow crystals were obtained in ~ 60% yield. The compound looses solvent at RT and changes structure as we found from PXRD.

Synthesis of $[Zn_{1.5}(FDA)_2(Me_2NH_2)]\cdot xG$ (3) :- Single crystal of **3** was prepared by reacting $ZnCl_2$ (68.14mg, 0.5mmol), $FDAH_2$ (78mg, 0.5 mmol) in 6 mL of DMF at by the solvothermal technique, in a Teflon-lined autoclave . The autoclave was heated under autogenous pressure to 160 °C for 3 days and then cooled to RT by 24 h period. Colourless crystals were obtained in ~ 15% yield with some impurities.

Measurements:- X-ray powder pattern were measured on Bruker D8 Advanced X-Ray diffractometer at room temperature using Cu Kα radiation (λ= 1.5406 Å) at a scan rate of 0.3 sec/step and step size of 0.01° in 2θ.

X-ray Structural Studies:- Single-crystal X-ray data of compounds **1-3** were collected at 150 K on a Bruker KAPPA APEX II CCD Duo diffractometer (operated at 1500 W power: 50 kV, 30 mA) using graphite-monochromated Mo KR radiation (λ = 0.71073 Å). Crystal was on nylon CryoLoops (Hampton Research) with Paraton-N (Hampton Research). The data integration and reduction were processed with SAINT[1] software. A multi-scan absorption correction was applied to the collected reflections. The structure was solved by the direct method using SHELXTL[2] and was refined on F^2 by full-matrix least-squares technique using the SHELXL-97[3] program package within the WINGX[4] programme. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were located in successive difference Fourier maps and they were treated as riding atoms using SHELXL default parameters. The structures were examined using the *Adsym* subroutine of PLATON[5] to assure that no additional symmetry could be applied to the models. Identification of the guest entities within the voids of the frameworks was not possible by modelling of electron densities due to the disorder contents of the large pores in the frameworks. The routine SQUEEZE was applied to the structures in order to remove diffuse electron density associated with badly disordered solvent molecules.

References:

(S1) *SAINT Plus*, (Version 7.03); Bruker AXS Inc.: Madison, WI, 2004.

(S2) G. M. Sheldrick, *SHELXTL*, *Reference Manual*: version 5.1: Bruker AXS; Madison, WI, 1997.

(S3) G. M. Sheldrick, *Acta Crystallogr. Sect. A* **2008**, 112 –122.

(S4) WINGX version 1.80.05 Louis Farrugia, University of Glasgow.

(S5) A. L. Spek, (2005) PLATON, *A Multipurpose Crystallographic Tool*, Utrecht University, Utrecht, The Netherlands.

(S6) Z. Chen, S. Xiang, H. D. Arman, J. U. Mondal, P. Li, D. Zhao and B. Chen *Inorg. Chem.*2011, **50**, 3442.

Section S2: Single crystal structural analysis.

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

Identification code	Compound **1**
Empirical formula	C14 H12 N O10 Zn1.5
Formula weight	452.30
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.3167(16) Å alpha = 95.596(4) deg. b = 9.8122(17) Å beta = 97.431(3) deg. c = 11.596(2) Å gamma = 97.238(3) deg.
Volume	1035.8(3) $Å^3$
Z, Calculated density	2, 1.450 Mg/m^3
Absorption coefficient	1.796 mm^{-1}
F(000)	456
Crystal size	0.20 x 0.10 x 0.10 mm
Theta range for data collection	1.78 to 27.48 deg.
Limiting indices	-12<=h<=12, -12<=k<=12, -15<=l<=15
Reflections collected / unique	18291 / 4734 [R(int) = 0.0174]
Completeness to theta = 27.48	99.9 %
Max. and min. transmission	0.8408 and 0.7152
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4734 / 0 / 241
Goodness-of-fit on F^2	0.477
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.1117
R indices (all data)	R1 = 0.0379, wR2 = 0.1171
Largest diff. peak and hole	1.366 and -0.844 $e.A^{-3}$

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

Identification code	Compound **2**
Empirical formula	C28 H24 N2 O20 Zn3
Formula weight	904.60
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 12.7693(10) Å alpha = 85.019(2) deg. b = 12.7842(9) Å beta = 65.8700(10) deg. c = 14.7758(11) Å gamma = 89.613(2) deg.
Volume	2191.9(3) $Å^3$
Z, Calculated density	2, 1.371 Mg/m^3
Absorption coefficient	1.698 mm^{-1}
F(000)	912
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	2.33 to 28.70 deg.
Limiting indices	-16<=h<=17, -17<=k<=17, -16<=l<=19
Reflections collected / unique	42640 / 11299 [R(int) = 0.0147]
Completeness to theta = 28.70	99.6 %
Max. and min. transmission	0.8486 and 0.7276
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11299 / 0 / 485
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0940
R indices (all data)	R1 = 0.0334, wR2 = 0.0958
Largest diff. peak and hole	1.942 and -0.955 $e.Å^{-3}$

Table S3. Crystal data and structure refinement for compound **3**.

Identification code	Compound **3**
Empirical formula	C14 H12 N O10 Zn1.5
Formula weight	452.30
Temperature	150(2) K
Wavelength	0.71069 Å
Crystal system, space group	monoclinic, P 21/c
Unit cell dimensions	a = 9.426(5) Å alpha = 90.000 deg. b = 15.424(5) Å beta = 92.474(5) deg. c = 17.359(5) Å gamma = 90.000 deg.
Volume	2521.4(17) A^3
Z, Calculated density	4, 1.191 Mg/m^3
Absorption coefficient	1.476 mm^{-1}
F(000)	912
Crystal size	0.30 x 0.20 x 0.20 mm
Theta range for data collection	2.53 to 28.64 deg.
Limiting indices	-12<=h<=9, -20<=k<=20, -23<=l<=23
Reflections collected / unique	25095 / 6457 [R(int) = 0.0303]
Completeness to theta = 28.64	99.5 %
Max. and min. transmission	0.7568 and 0.6658
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6457 / 0 / 243
Goodness-of-fit on F^2	1.525
Final R indices [I>2sigma(I)]	R1 = 0.1038, wR2 = 0.3378
R indices (all data)	R1 = 0.1152, wR2 = 0.3523
Largest diff. peak and hole	1.387 and -5.154 $e.Å^{-3}$

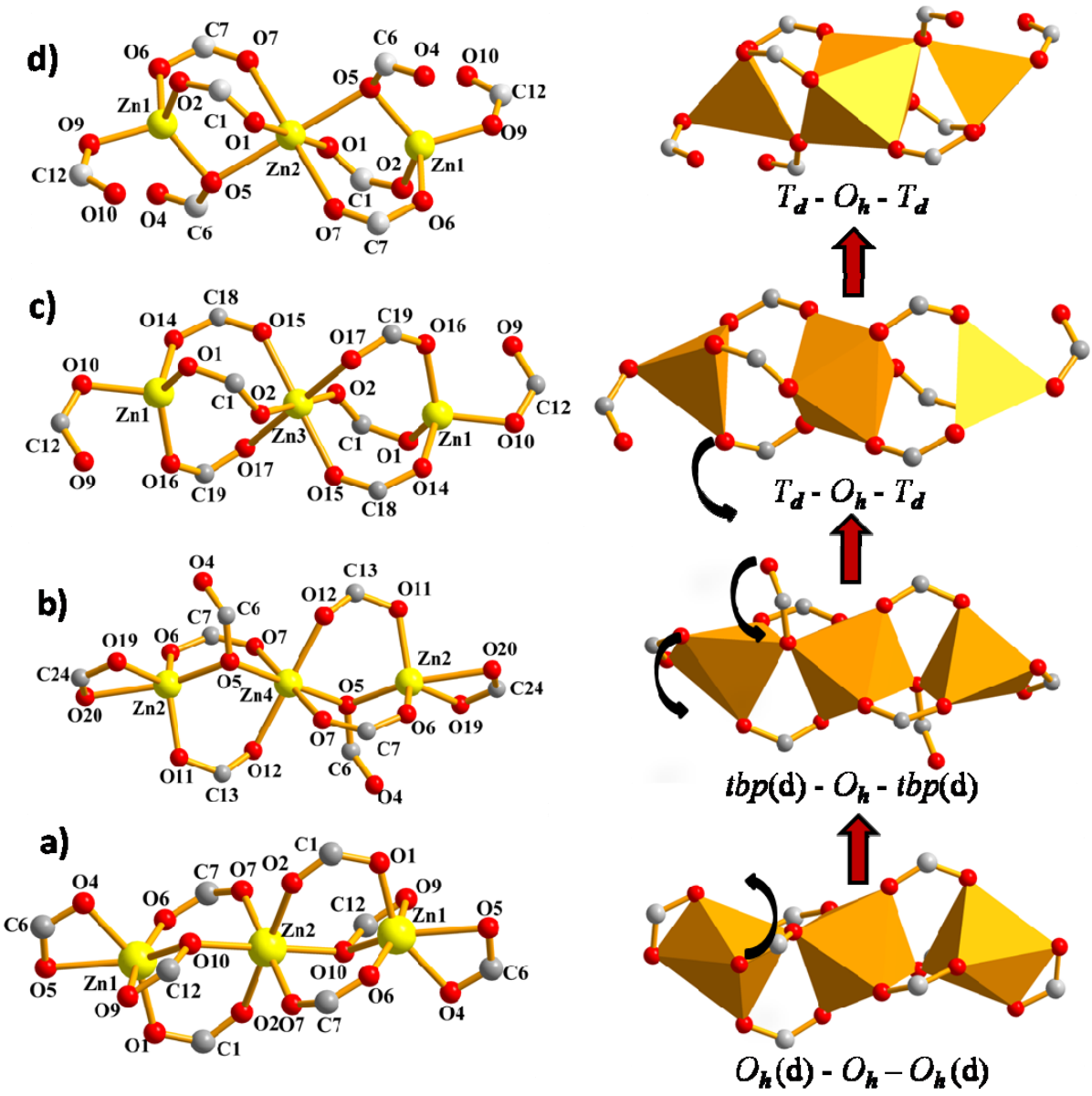

Figure S1: The change in coordination environment of $Zn_3(RCOO)_8$ trimeric units a) Compound **1**; b) and c) Compound **2**; d) Compound **3**. (Colour code; Carbon: gray, Oxygen: red, Zinc: yellow).

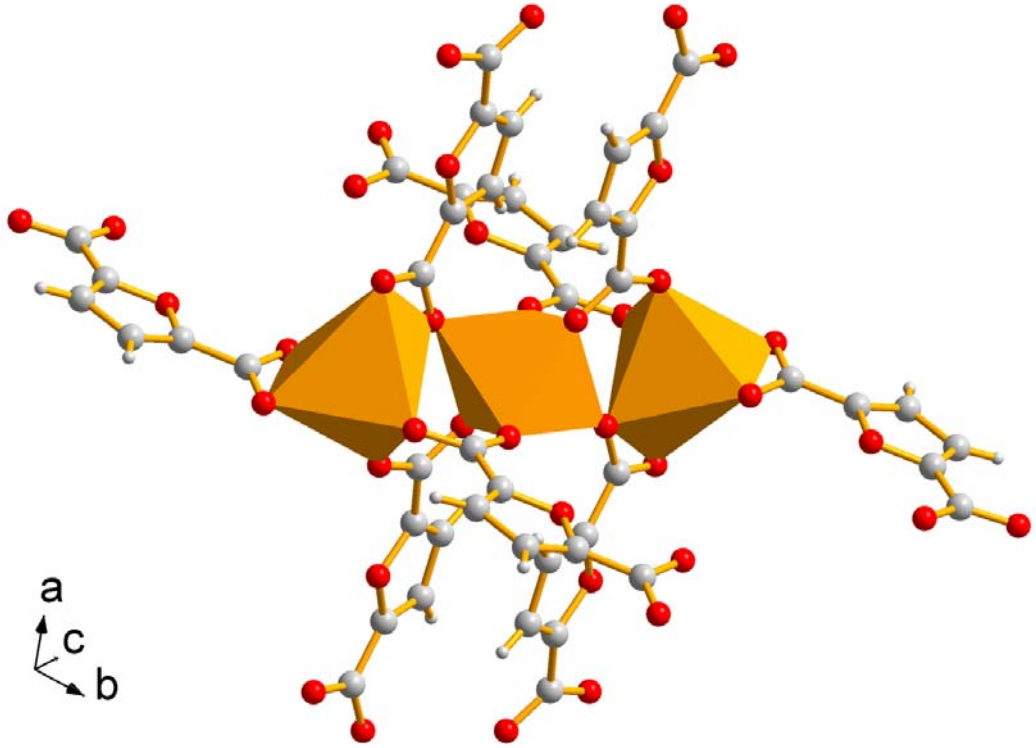

Figure S2: Eight connected $Zn_3(RCOO)_8$ node of compound **1**. [O_h (d) - O_h - O_h (d)] (Colour code; Carbon: gray, Oxygen: red, Zinc: yellow).

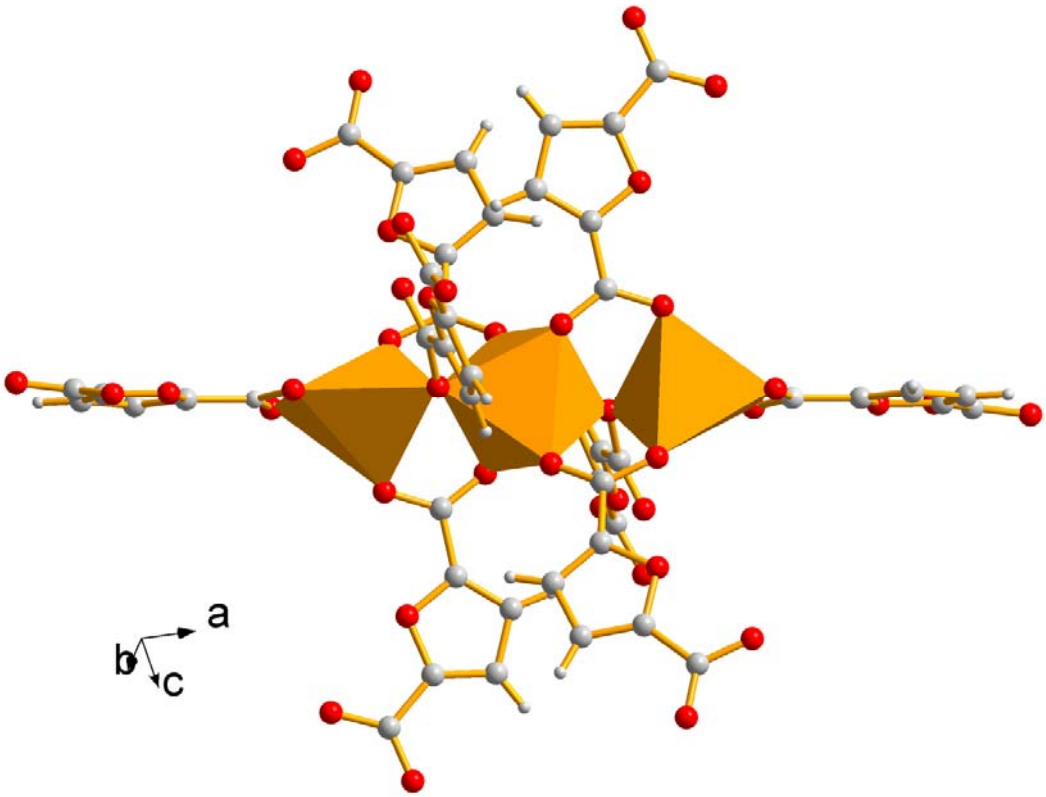

Figure S3: Eight connected $Zn_3(RCOO)_8$ node of compound **2**. [*tbp* (d) - O_h - *tbp* (d)] (Colour code; Carbon: gray, Oxygen: red, Zinc: yellow).

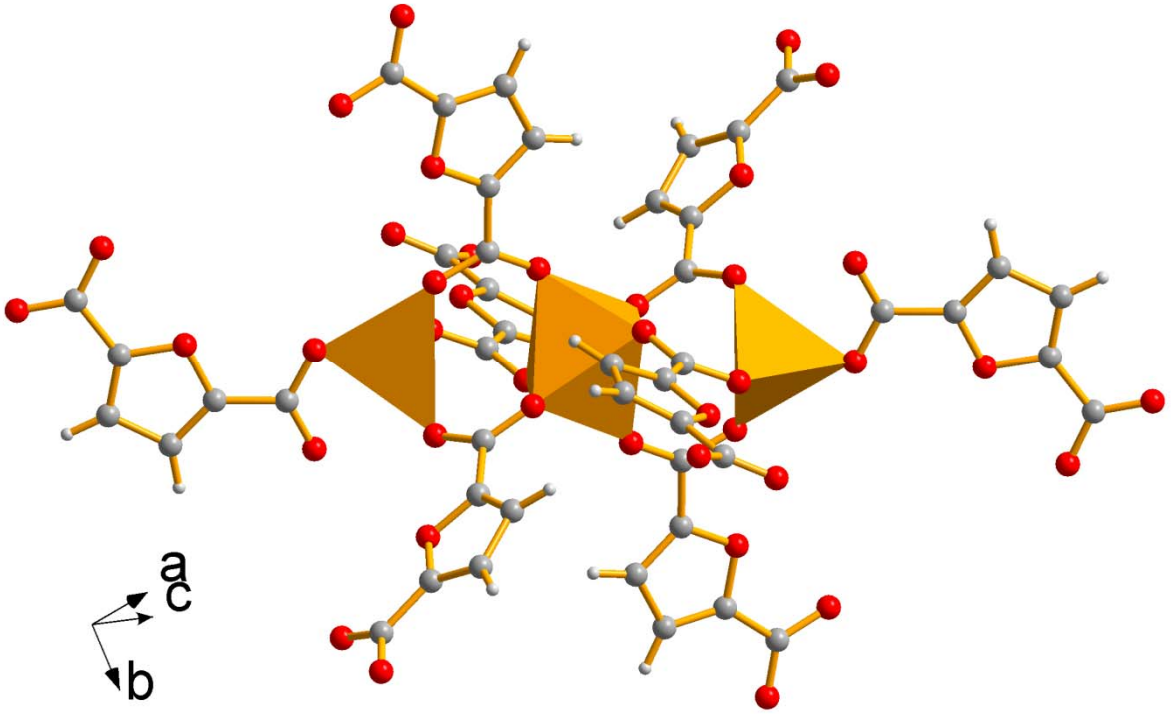

Figure S4: Eight connected $Zn_3(RCOO)_8$ node of compound **2**. [T_d - O_h - T_d] (Colour code; Carbon: gray, Oxygen: red, Zinc: yellow).

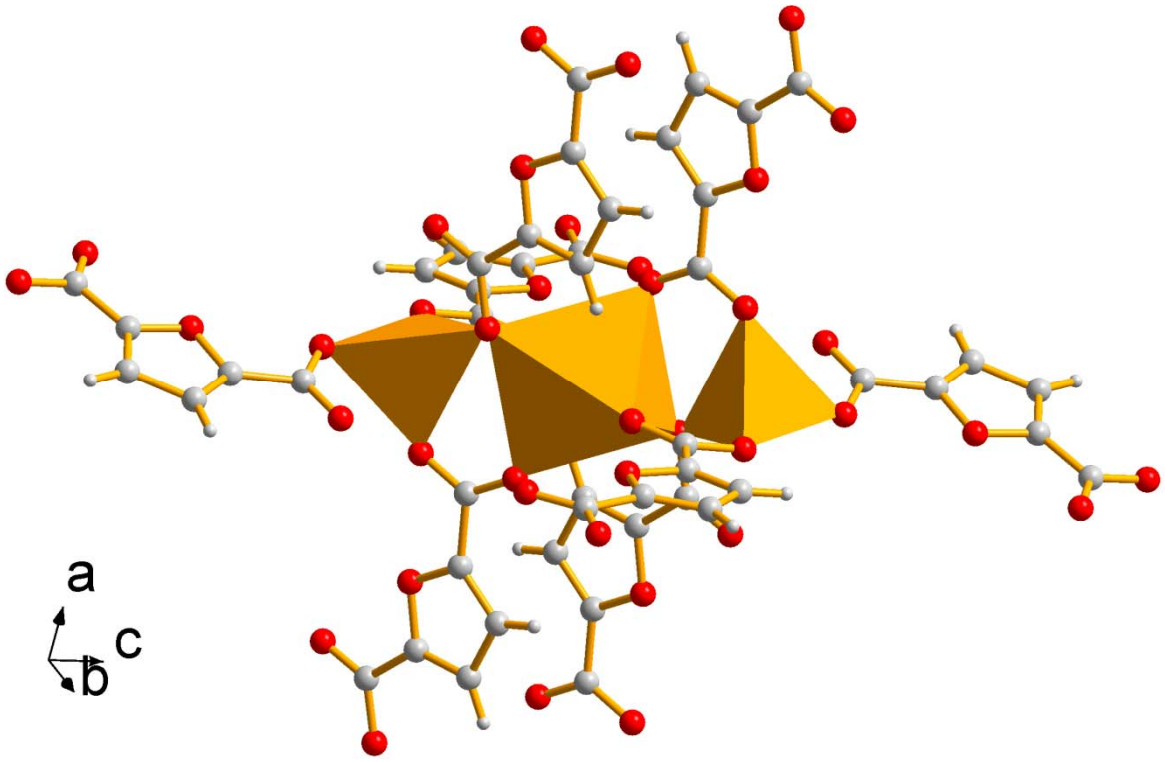

Figure S5: Eight connected $Zn_3(RCOO)_8$ node of compound **3**. [T_d - O_h - T_d] (Colour code; Carbon: gray, Oxygen: red, Zinc: yellow).

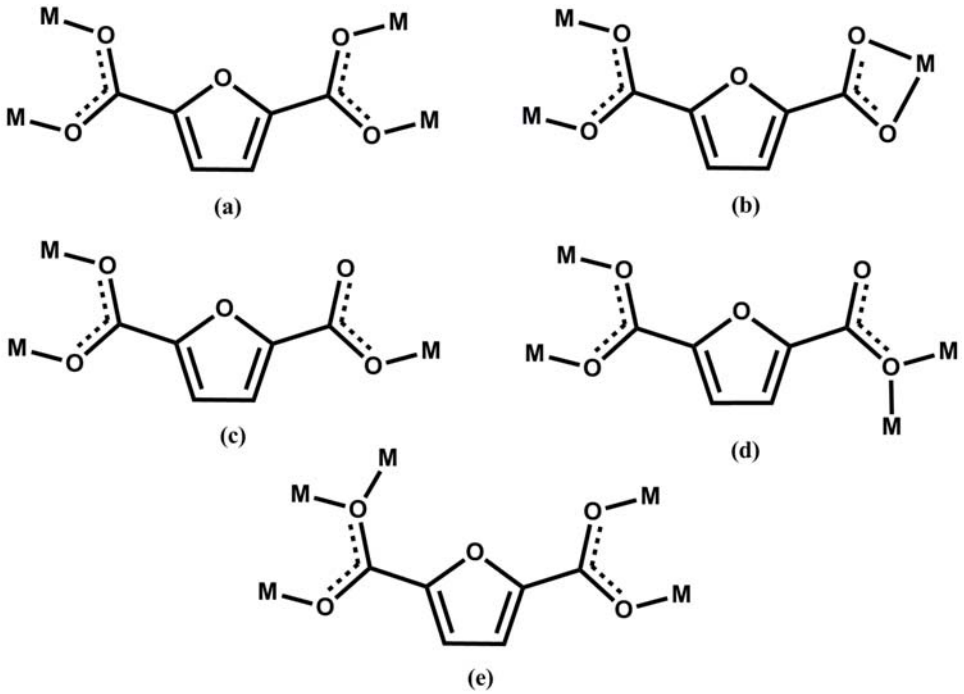

Figure S6: The different coordination modes of FDA^{2-} ligand.

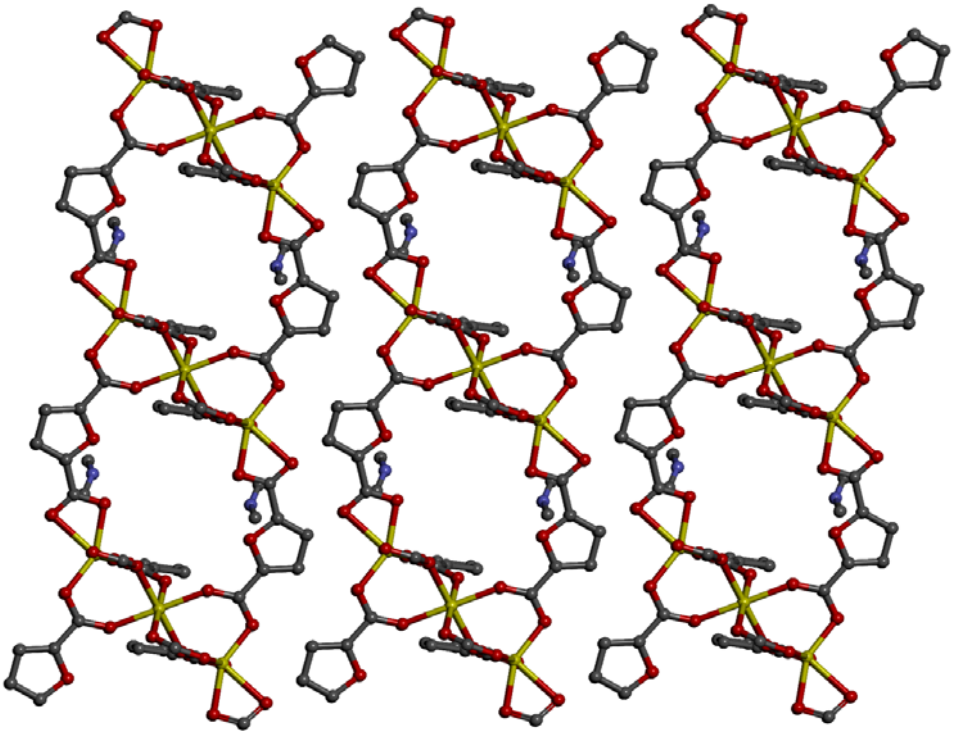

Figure S7: Compound **1** along *a* axis (Colour code; Carbon: gray, Nitrogen: blue, Oxygen: red, Zinc: yellow).

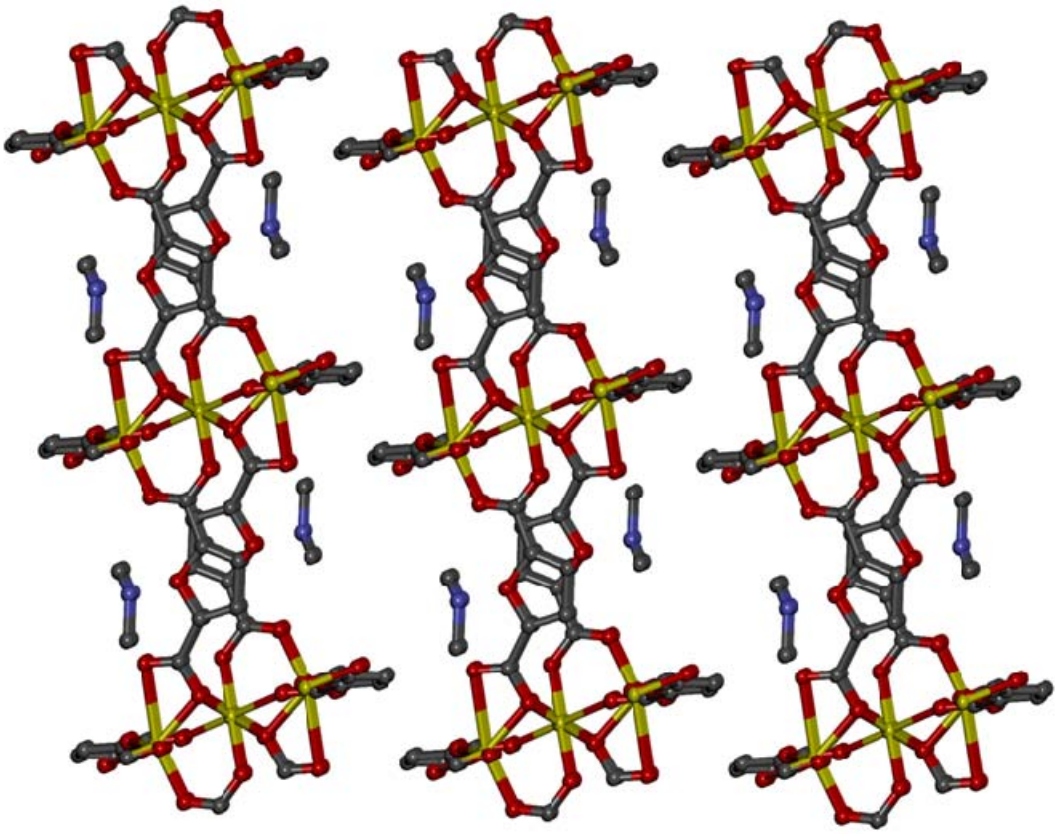

Figure S8: Compound **1** along *b* axis (Colour code; Carbon: gray, Nitrogen: blue, Oxygen: red, Zinc: yellow).

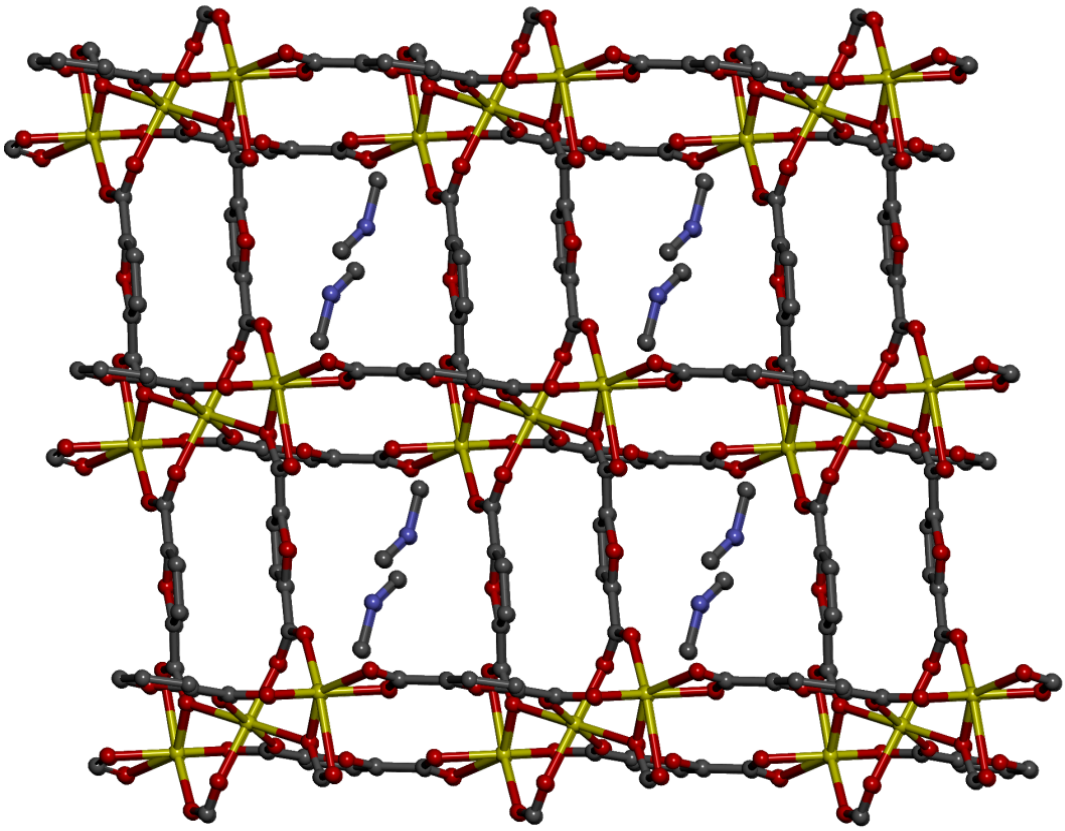

Figure S9: Compound **1** along *c* axis (Colour code; Carbon: gray, Nitrogen: blue, Oxygen: red, Zinc: yellow).

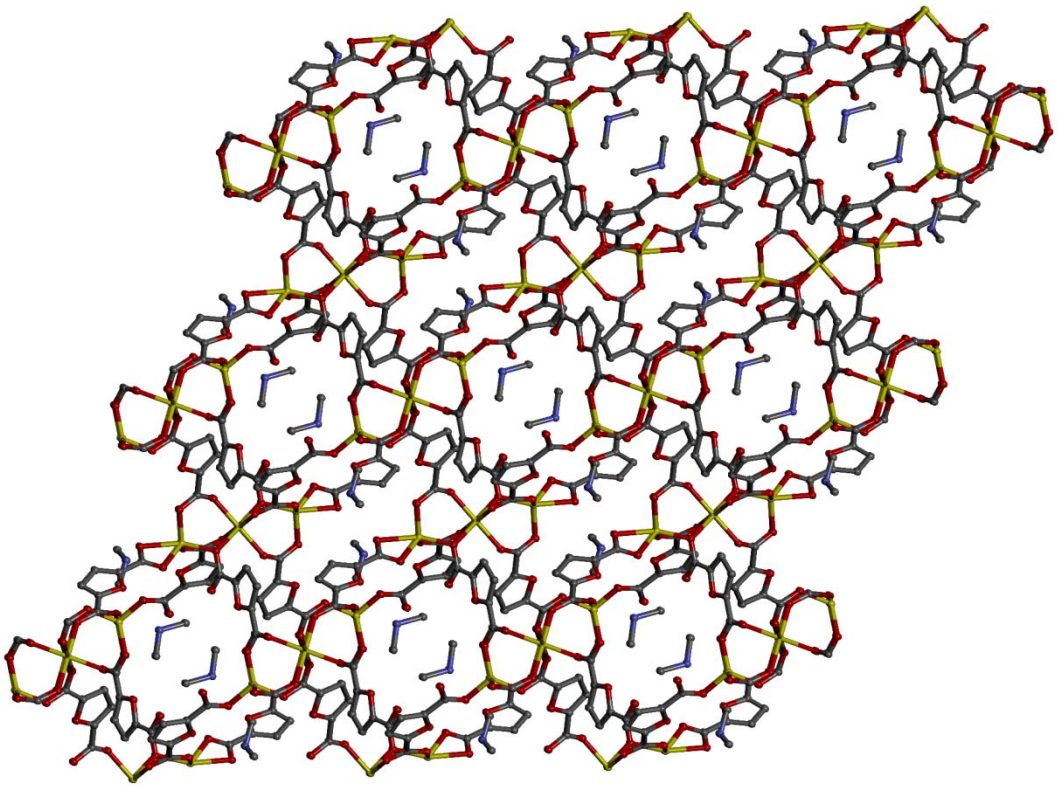

Figure S10: Perspective view of the 3D framework of compound **2** along *b* axis (Colour code; Carbon: grey, Nitrogen: blue, Oxygen: red, Zinc: yellow).

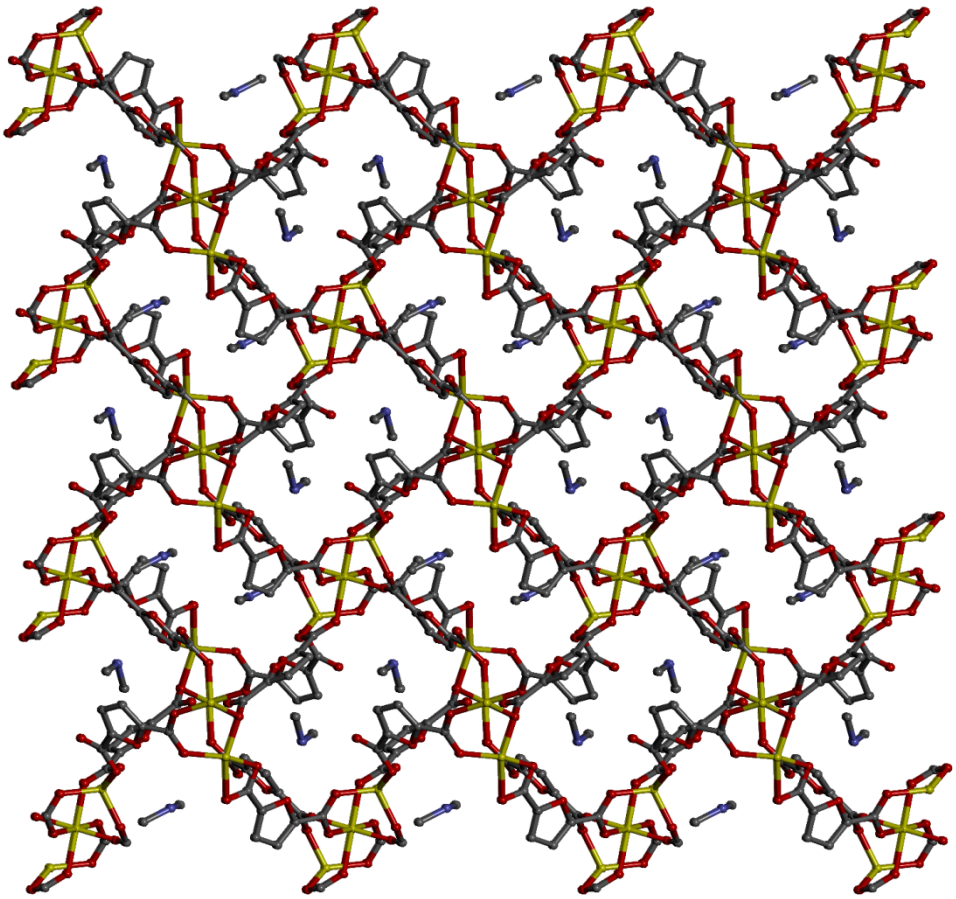

Figure S11: Perspective view of the 3D framework of compound **2** along *c* axis.
(Colour code; Carbon: grey, Nitrogen: blue, Oxygen: red, Zinc: yellow).

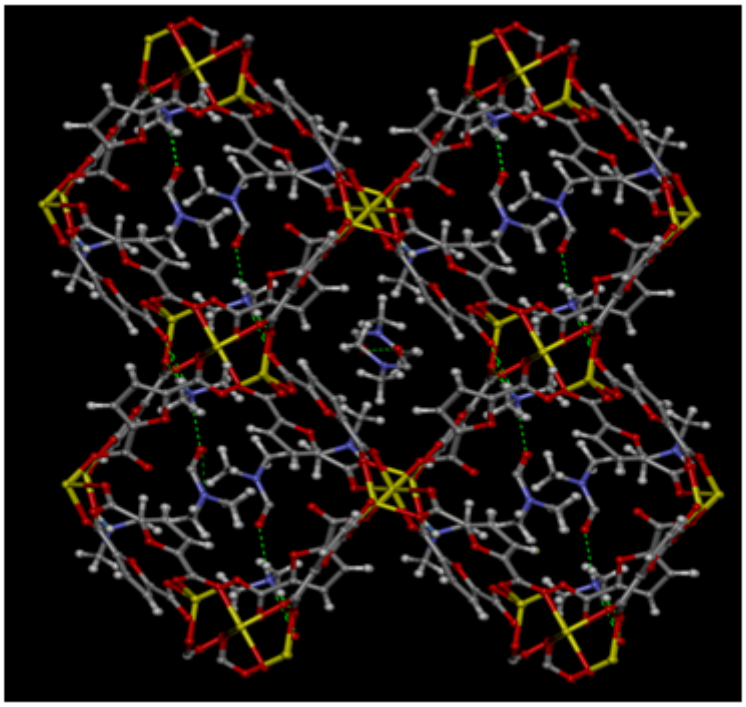

Figure S12: Perspective view of the 3D framework with hydrogen bonded DMF molecules of compound **2** along *a* axis (Colour code; Carbon: gray, Nitrogen: blue, Oxygen: red, Zinc: yellow).

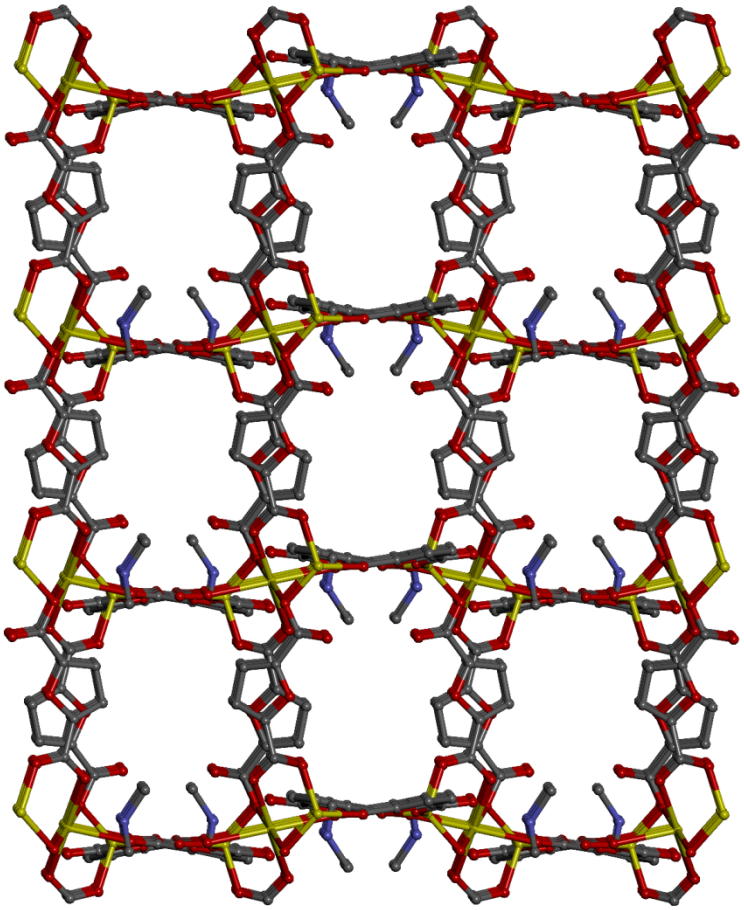

Figure S13: Perspective view of the 3D framework of compound **3** along *c* axis.
(Colour code; Carbon: grey, Nitrogen: blue, Oxygen: red, Zinc: yellow).

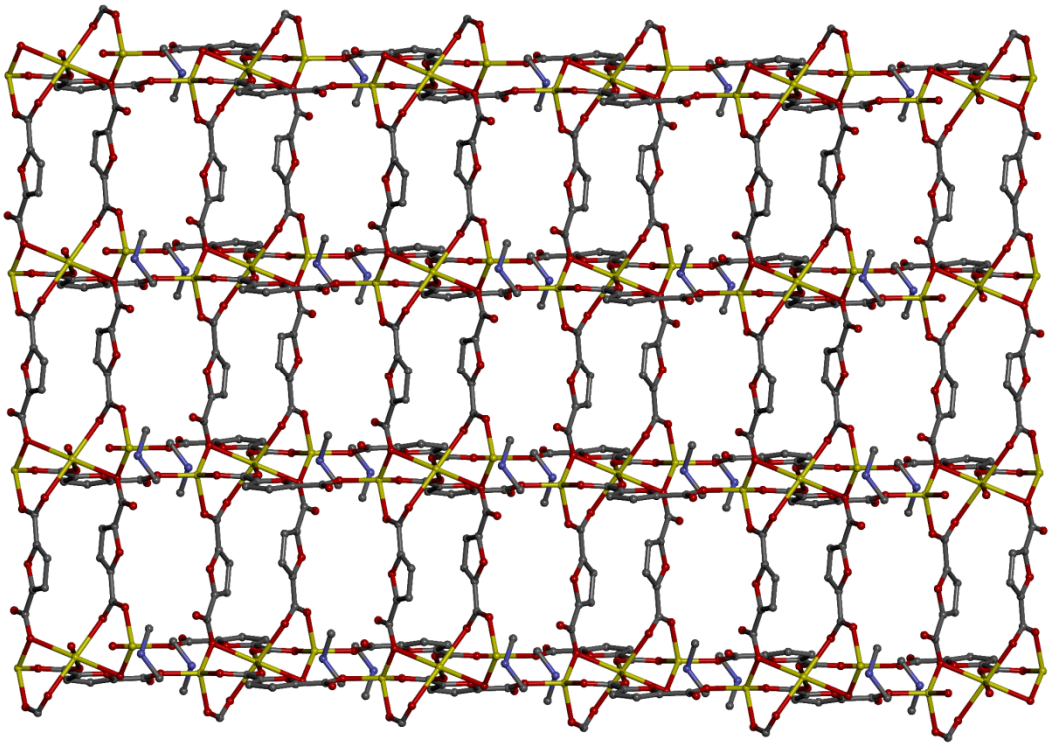

Figure S14: Perspective view of the 3D framework of compound **3** along *b* axis. (Colour code; Carbon: grey, Nitrogen: blue, Oxygen: red, Zinc: yellow).

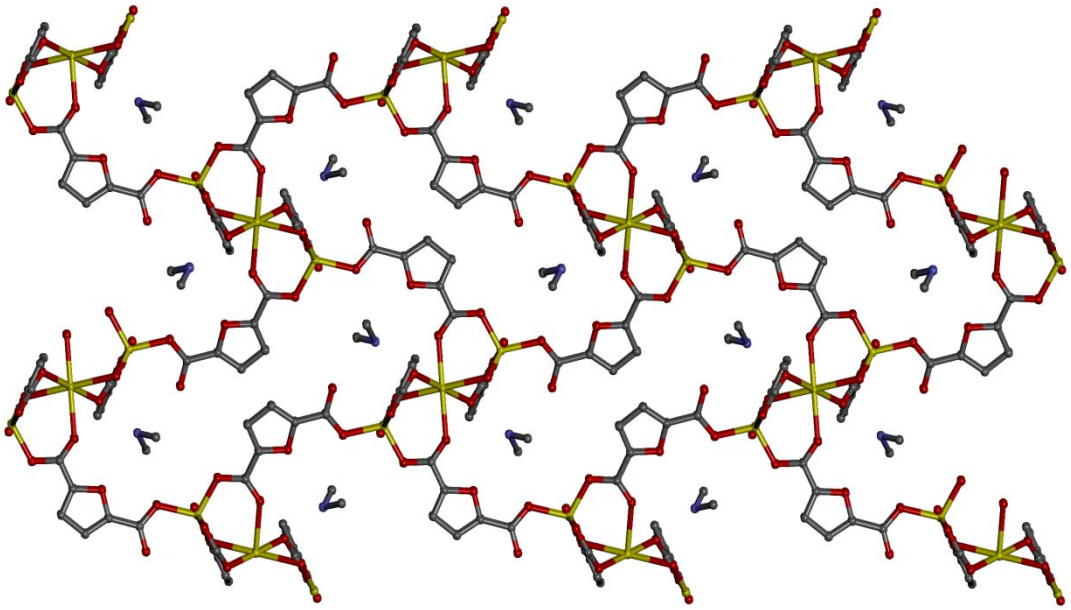

Figure S15: Perspective view of the 3D framework of compound **3** along *a* axis.
(Colour code; Carbon: grey, Nitrogen: blue, Oxygen: red, Zinc: yellow).

Section S3: TGA and PXRD analysis.

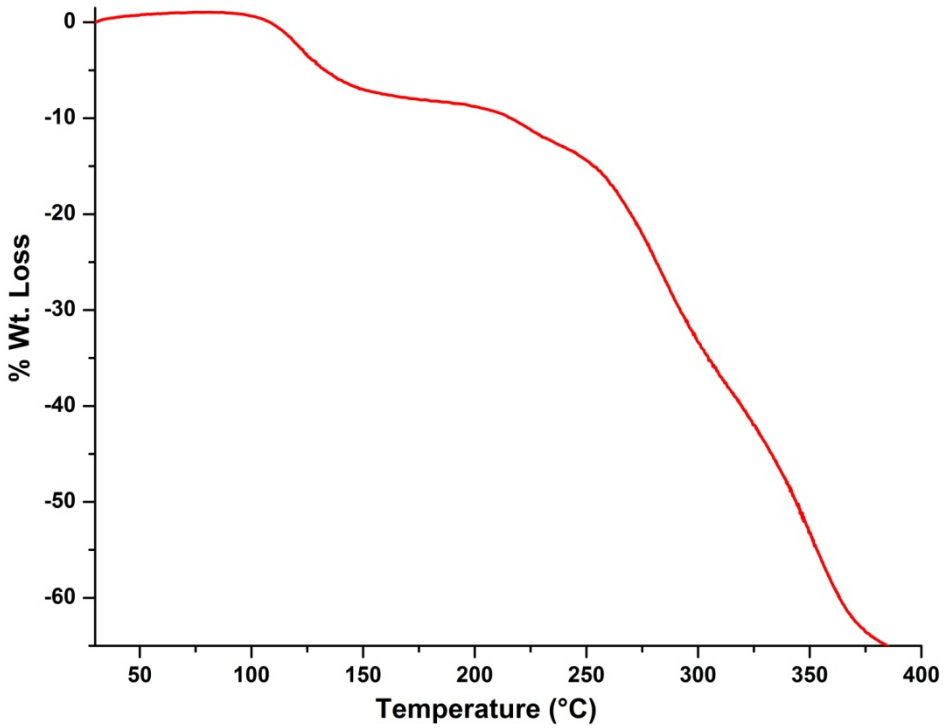

Figure S16: Thermogravimetric data for compound **1**.

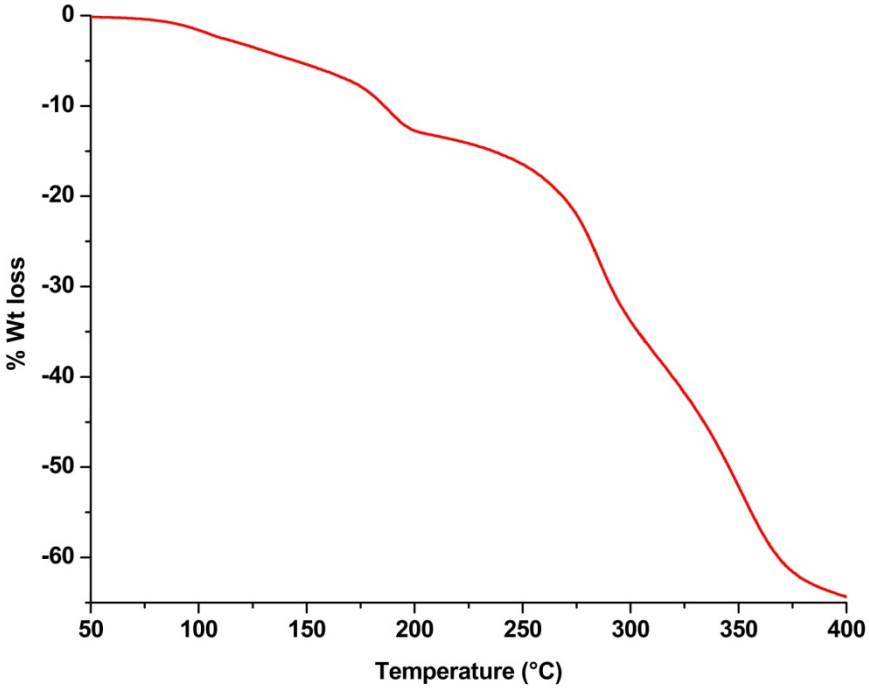

Figure S17: Thermogravimetric data for compound **2**.

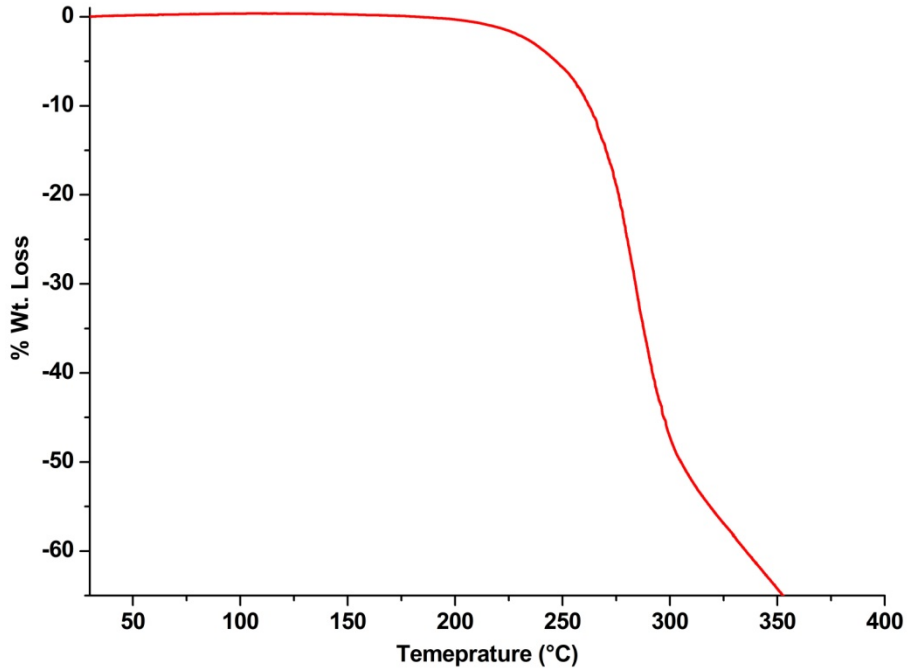

Figure S18: Thermogravimetric data for compound **3**.

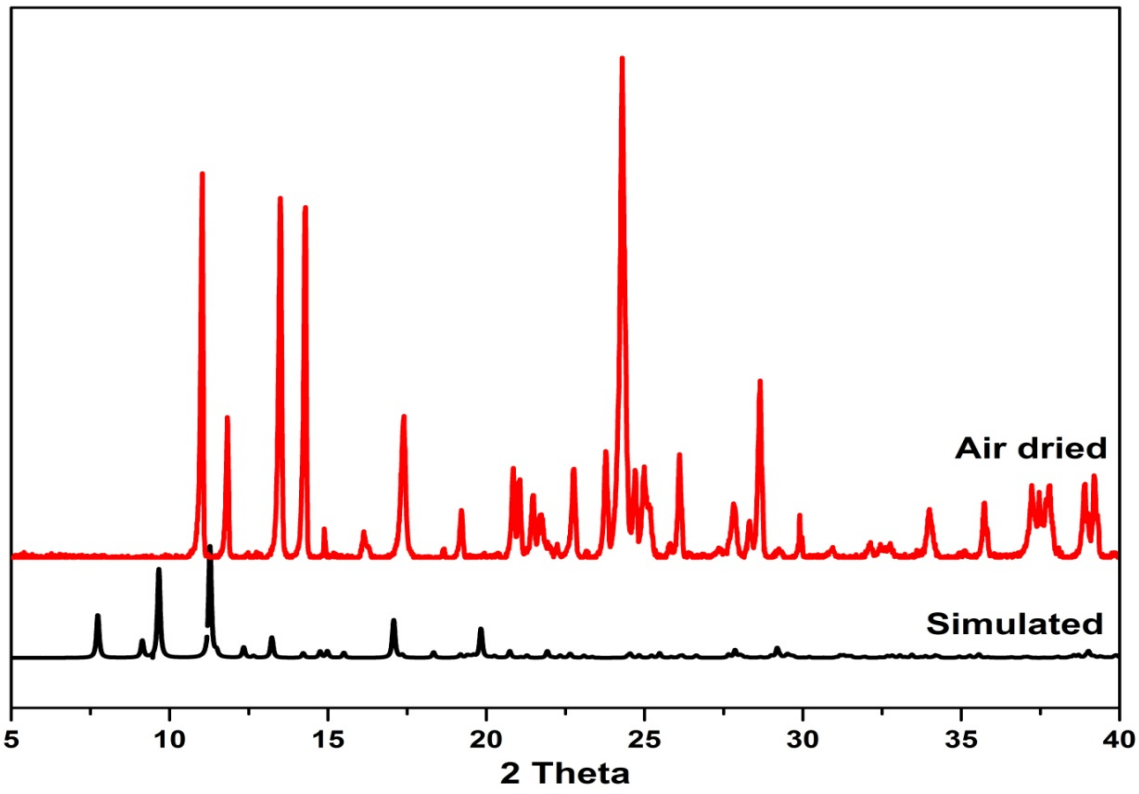

Figure S19: PXRD data for compound **1**.

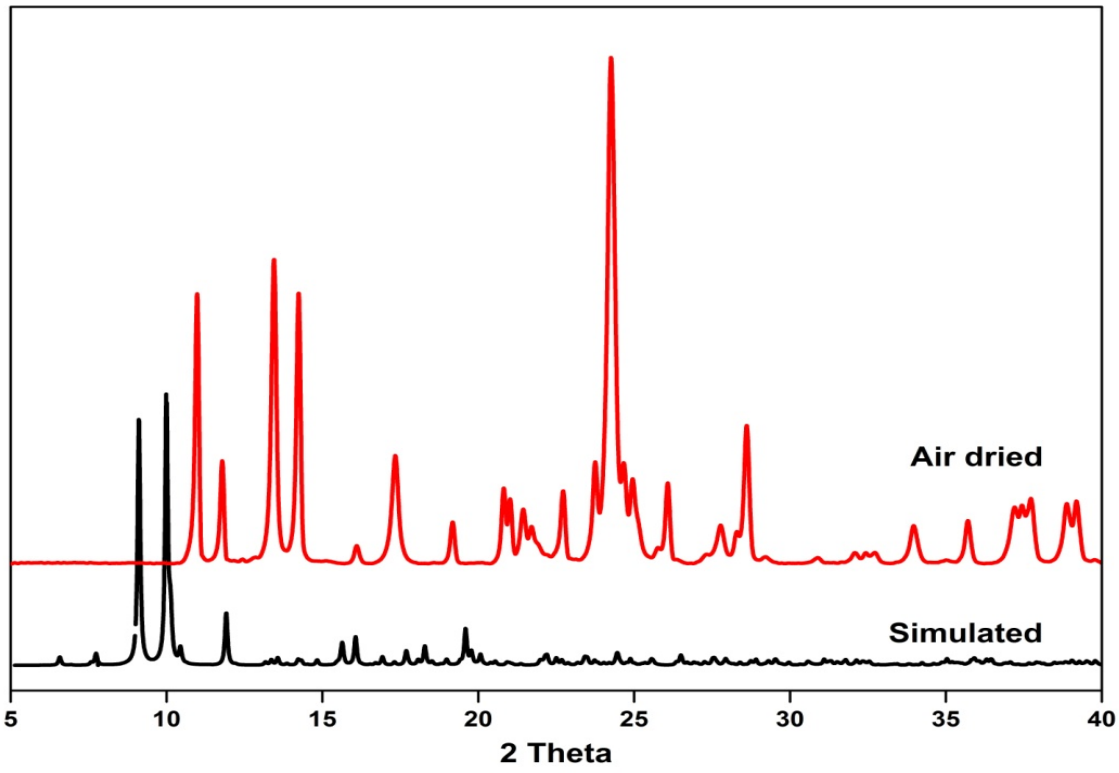

Figure S20: PXRD data for compound **2**.

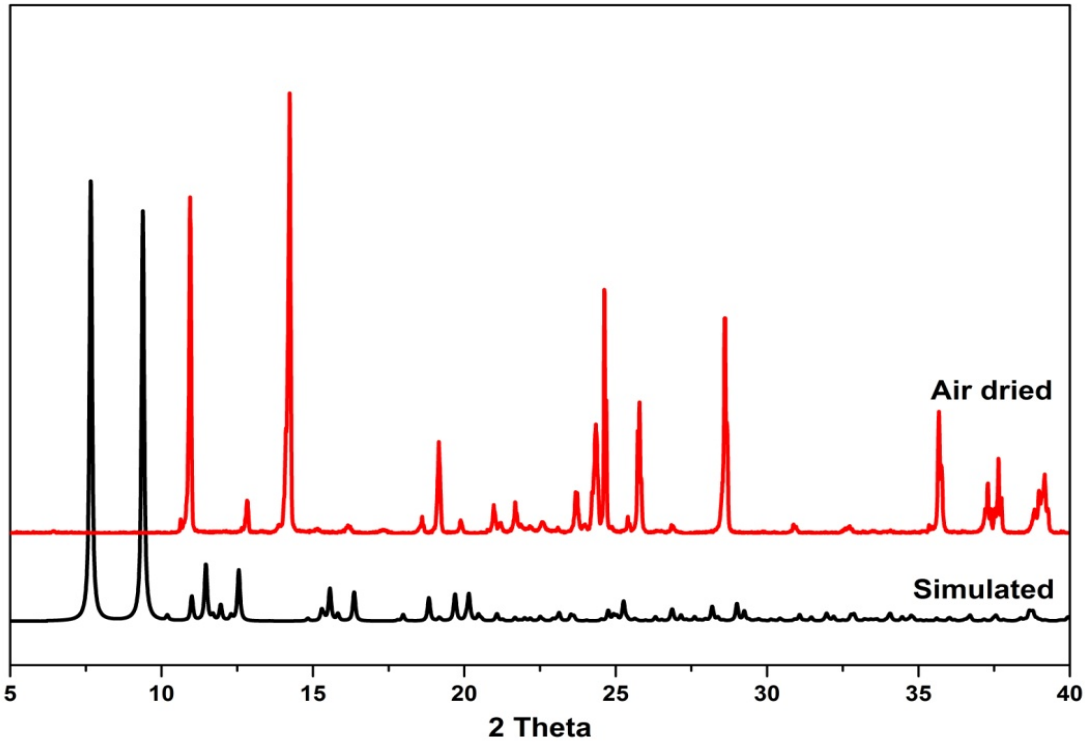

Figure S21: PXRD data for compound **3**.

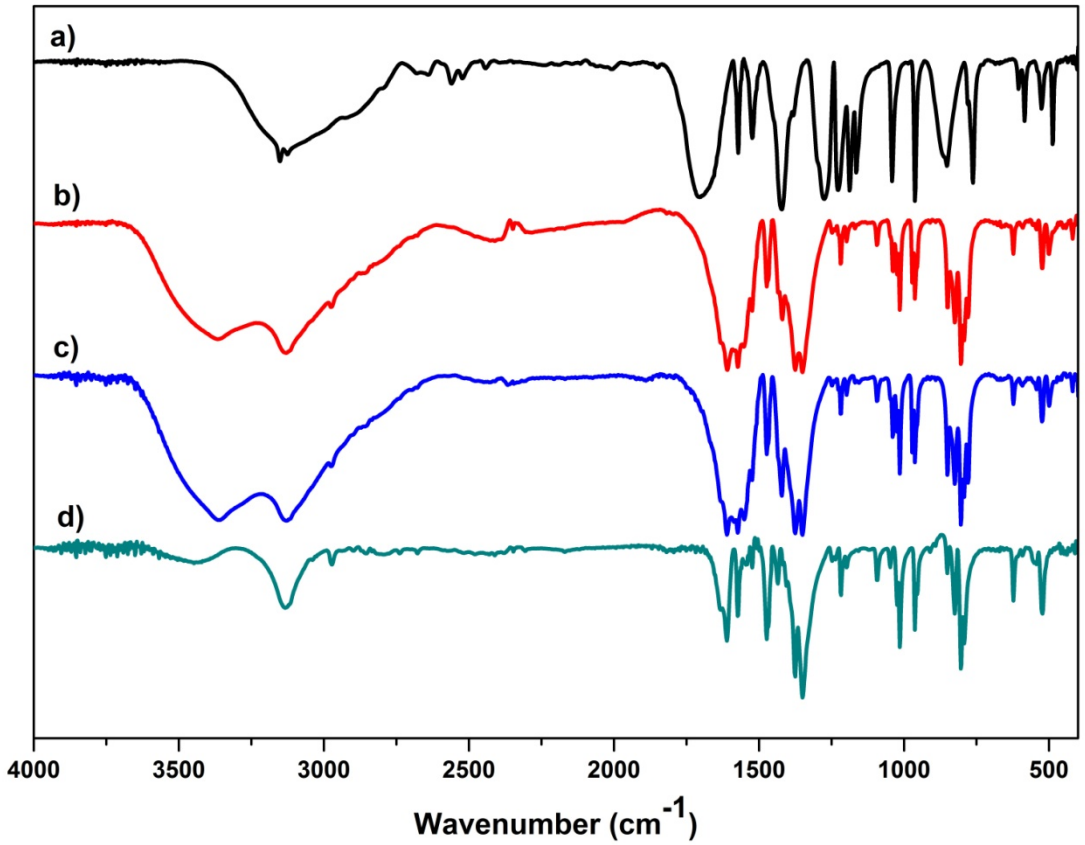

Figure S22: IR data for a) FDA ligand; b) compound **1**; c) compound **2**; d) compound **3**.

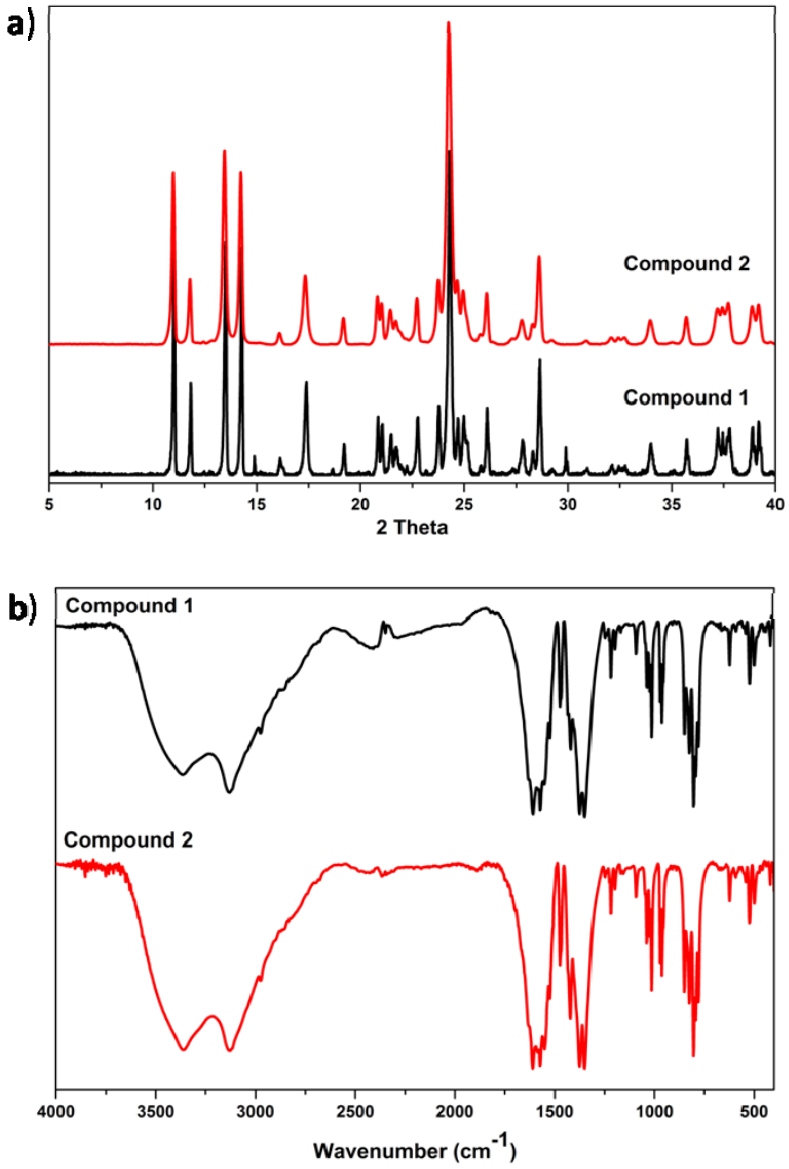

Figure S23: a) Comparison of PXRD data of compound **1** and compound **2**;
b) Comparison of IR data of compound **1** and compound **2.**

Section S4: Single crystal structural analysis data tables

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	4015(1)	2689(1)	2637(1)	30(1)
Zn(2)	5000	5000	5000	29(1)
C(1)	4108(2)	5459(2)	2305(2)	32(1)
C(2)	3901(3)	6590(2)	1563(2)	34(1)
C(3)	3787(4)	6638(3)	392(2)	50(1)
C(4)	3594(4)	8021(4)	210(3)	60(1)
C(5)	3608(3)	8714(3)	1270(3)	47(1)
C(6)	3579(4)	10185(3)	1677(5)	74(1)
C(7)	2044(2)	3351(2)	4319(2)	30(1)
C(8)	566(2)	3297(2)	4673(2)	29(1)
C(9)	111(2)	3468(2)	5734(2)	33(1)
C(10)	-1433(2)	3355(2)	5529(2)	33(1)
C(11)	-1821(2)	3131(2)	4349(2)	29(1)
C(12)	-3225(2)	2981(2)	3579(2)	31(1)
C(13)	314(11)	9836(12)	-2021(18)	355(13)
C(14)	2595(9)	11243(11)	-2046(10)	181(4)
O(1)	4112(2)	4286(2)	1740(2)	38(1)
O(2)	4237(2)	5742(2)	3392(1)	36(1)
O(3)	3804(2)	7861(2)	2126(2)	37(1)
O(4)	3898(3)	10568(3)	2745(4)	92(1)
O(5)	3295(4)	11013(3)	992(4)	110(2)
O(6)	2137(2)	2901(2)	3279(2)	39(1)
O(7)	3080(2)	3842(2)	5115(2)	34(1)
O(8)	-608(2)	3071(2)	3798(1)	30(1)
O(9)	-3321(2)	2606(3)	2528(2)	54(1)
O(10)	-4369(2)	3198(2)	4071(1)	31(1)
N(1)	1098(10)	10684(10)	-2210(20)	475(17)

Table S2. Selected bond lengths [Å] and angles [deg] for compound **1**.

Zn(1)-O(1)	1.9625(19)
Zn(1)-O(6)	2.0151(16)
Zn(1)-O(10)#1	2.0699(16)
Zn(1)-O(4)#2	2.087(3)
Zn(1)-O(5)#2	2.360(5)
Zn(1)-C(6)#2	2.558(4)
Zn(2)-O(7)	2.0217(16)
Zn(2)-O(7)#3	2.0218(16)
Zn(2)-O(2)#3	2.1366(17)
Zn(2)-O(2)	2.1366(17)
Zn(2)-O(10)#1	2.1643(15)
Zn(2)-O(10)#4	2.1643(16)
O(4)-Zn(1)#5	2.087(3)
O(5)-Zn(1)#5	2.360(5)
O(10)-Zn(1)#6	2.0699(16)
O(10)-Zn(2)#6	2.1643(15)
O(1)-Zn(1)-O(6)	98.74(8)
O(1)-Zn(1)-O(10)#1	106.23(7)
O(6)-Zn(1)-O(10)#1	104.71(7)
O(1)-Zn(1)-O(4)#2	151.61(13)
O(6)-Zn(1)-O(4)#2	95.68(10)
O(10)#1-Zn(1)-O(4)#2	93.47(10)
O(1)-Zn(1)-O(5)#2	95.54(9)
O(6)-Zn(1)-O(5)#2	103.90(10)
O(10)#1-Zn(1)-O(5)#2	140.58(10)
O(4)#2-Zn(1)-O(5)#2	57.12(13)
O(1)-Zn(1)-C(6)#2	123.12(13)
O(6)-Zn(1)-C(6)#2	103.15(9)
O(10)#1-Zn(1)-C(6)#2	117.46(12)
O(4)#2-Zn(1)-C(6)#2	28.90(15)
O(5)#2-Zn(1)-C(6)#2	28.35(14)
O(7)-Zn(2)-O(7)#3	180.000(1)
O(7)-Zn(2)-O(2)#3	85.01(7)
O(7)#3-Zn(2)-O(2)#3	94.99(7)
O(7)-Zn(2)-O(2)	94.99(7)
O(7)#3-Zn(2)-O(2)	85.01(7)
O(2)#3-Zn(2)-O(2)	180.0
O(7)-Zn(2)-O(10)#1	88.11(6)
O(7)#3-Zn(2)-O(10)#1	91.89(6)
O(2)#3-Zn(2)-O(10)#1	88.61(6)
O(2)-Zn(2)-O(10)#1	91.39(6)
O(7)-Zn(2)-O(10)#4	91.89(6)
O(7)#3-Zn(2)-O(10)#4	88.11(6)
O(2)#3-Zn(2)-O(10)#4	91.39(6)
O(2)-Zn(2)-O(10)#4	88.61(6)
O(10)#1-Zn(2)-O(10)#4	180.0
O(5)-C(6)-Zn(1)#5	66.8(3)
O(4)-C(6)-Zn(1)#5	54.10(19)
C(5)-C(6)-Zn(1)#5	168.4(3)
C(1)-O(1)-Zn(1)	116.68(15)
C(1)-O(2)-Zn(2)	142.27(16)
C(5)-O(3)-C(2)	106.15(19)

C(6)-O(4)-Zn(1)#5	97.0(3)
C(6)-O(5)-Zn(1)#5	84.9(3)
C(7)-O(6)-Zn(1)	125.23(14)
C(7)-O(7)-Zn(2)	129.35(15)
C(12)-O(10)-Zn(1)#6	99.92(13)
C(12)-O(10)-Zn(2)#6	133.53(14)
Zn(1)#6-O(10)-Zn(2)#6	103.80(7)

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z #2 x,y-1,z #3 -x+1,-y+1,-z+1
#4 -x,-y+1,-z+1 #5 x,y+1,z #6 x-1,y,z

Table S3. Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **1**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zn(1)	20(1)	36(1)	29(1)	-9(1)	2(1)	4(1)
Zn(2)	16(1)	38(1)	28(1)	-10(1)	3(1)	2(1)
C(1)	24(1)	41(1)	29(1)	-6(1)	5(1)	6(1)
C(2)	34(1)	36(1)	30(1)	-7(1)	9(1)	5(1)
C(3)	68(2)	51(2)	34(1)	-3(1)	16(1)	20(1)
C(4)	84(2)	58(2)	48(2)	14(1)	29(2)	25(2)
C(5)	45(1)	39(1)	60(2)	1(1)	20(1)	8(1)
C(6)	43(2)	39(2)	143(4)	-7(2)	43(2)	3(1)
C(7)	19(1)	33(1)	37(1)	-5(1)	5(1)	5(1)
C(8)	17(1)	34(1)	35(1)	-5(1)	3(1)	5(1)
C(9)	22(1)	40(1)	36(1)	-2(1)	2(1)	6(1)
C(10)	22(1)	41(1)	35(1)	-2(1)	7(1)	6(1)
C(11)	18(1)	33(1)	35(1)	-6(1)	8(1)	4(1)
C(12)	20(1)	38(1)	32(1)	-6(1)	5(1)	6(1)
C(13)	117(7)	189(10)	700(30)	-226(16)	154(13)	-76(7)
C(14)	80(5)	219(10)	245(11)	18(9)	33(6)	17(5)
O(1)	43(1)	42(1)	31(1)	-6(1)	7(1)	11(1)
O(2)	28(1)	51(1)	26(1)	-6(1)	3(1)	9(1)
O(3)	34(1)	38(1)	38(1)	-11(1)	7(1)	5(1)
O(4)	49(1)	49(1)	162(3)	-49(2)	-6(2)	12(1)
O(5)	128(3)	57(2)	180(4)	49(2)	97(3)	41(2)
O(6)	20(1)	50(1)	41(1)	-15(1)	6(1)	3(1)
O(7)	18(1)	46(1)	36(1)	-6(1)	4(1)	3(1)
O(8)	16(1)	39(1)	34(1)	-7(1)	6(1)	3(1)
O(9)	31(1)	94(2)	33(1)	-14(1)	6(1)	13(1)
O(10)	16(1)	40(1)	34(1)	-10(1)	4(1)	3(1)
N(1)	108(6)	163(8)	1250(50)	302(17)	227(15)	69(6)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for compound **1**.

	x	y	z	U(eq)
H(8)	3827	5914	-178	60
H(7)	3480	8377	-506	71
H(9)	700	3629	6458	40
H(12)	-2057	3421	6091	39
H(13A)	-603	9811	-2513	533
H(13B)	175	9980	-1215	533
H(13C)	684	8975	-2167	533
H(14A)	2741	11977	-2527	272
H(14B)	3164	10532	-2259	272
H(14C)	2897	11598	-1238	272
H(1A)	697	11423	-1955	570
H(1B)	888	10620	-2999	570

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	2651(2)	3800(2)	690(1)	24(1)
C(2)	1993(2)	3319(2)	1711(1)	24(1)
C(3)	1820(2)	3620(2)	2618(2)	30(1)
C(4)	1066(2)	2845(2)	3331(2)	30(1)
C(5)	835(2)	2129(2)	2810(1)	22(1)
C(6)	60(2)	1185(1)	3105(1)	20(1)
C(7)	-1143(2)	-1532(1)	4158(1)	22(1)
C(8)	-942(2)	-2501(2)	3639(2)	26(1)
C(9)	-90(2)	-3197(2)	3427(2)	38(1)
C(10)	-288(2)	-3906(2)	2814(2)	40(1)
C(11)	-1245(2)	-3594(2)	2703(2)	29(1)
C(12)	1834(2)	3975(2)	-2108(2)	28(1)
C(13)	-2327(2)	712(2)	6320(1)	22(1)
C(14)	-2630(2)	1262(2)	7226(1)	23(1)
C(15)	-2212(2)	1211(2)	7936(2)	32(1)
C(16)	-2823(2)	1951(2)	8614(2)	34(1)
C(17)	-3568(2)	2400(2)	8260(2)	25(1)
C(18)	5545(2)	3195(2)	-1359(1)	24(1)
C(19)	4512(2)	6059(1)	-1741(1)	20(1)
C(20)	4738(2)	7045(2)	-2399(1)	24(1)
C(21)	5650(2)	7731(2)	-2822(2)	38(1)
C(22)	5350(2)	8501(2)	-3422(2)	42(1)
C(23)	4278(2)	8242(2)	-3304(2)	29(1)
C(24)	-3498(2)	1266(2)	3722(2)	36(1)
C(25)	560(3)	6919(2)	-1211(3)	53(1)
C(26)	1231(3)	6288(2)	89(2)	48(1)
C(27)	-5269(5)	2555(4)	5804(4)	105(2)
C(28)	-5953(4)	1200(4)	7193(4)	85(1)
N(1)	1544(2)	6698(1)	-953(2)	31(1)
N(2)	-5829(5)	1566(4)	6189(4)	135(2)
O(1)	2573(1)	3334(1)	-5(1)	33(1)
O(2)	3204(1)	4640(1)	571(1)	26(1)
O(3)	1400(1)	2397(1)	1811(1)	23(1)
O(4)	-26(1)	664(1)	2483(1)	32(1)
O(5)	-545(1)	1018(1)	4065(1)	20(1)
O(6)	-2007(1)	-1008(1)	4196(1)	27(1)
O(7)	-431(1)	-1324(1)	4496(1)	26(1)
O(8)	-1668(1)	-2728(1)	3205(1)	25(1)
O(9)	1418(2)	4703(2)	-1599(2)	46(1)
O(10)	2732(1)	3490(1)	-2158(1)	31(1)
O(11)	-2839(1)	968(1)	5760(1)	28(1)
O(12)	-1586(1)	30(1)	6171(1)	25(1)
O(13)	-3467(1)	1990(1)	7411(1)	25(1)
O(14)	4943(1)	3391(1)	-1852(1)	31(1)
O(15)	5462(1)	3577(1)	-588(1)	27(1)
O(16)	3623(1)	5538(1)	-1641(1)	25(1)

O(17)	5197(1)	5824(1)	-1362(1)	24(1)
O(18)	3886(1)	7347(1)	-2692(1)	24(1)
O(19)	-2515(2)	1619(2)	3462(1)	44(1)
O(20)	-3862(2)	476(2)	4326(2)	73(1)
Zn(1)	3438(1)	4027(1)	-1328(1)	20(1)
Zn(2)	-2152(1)	487(1)	4410(1)	19(1)
Zn(3)	5000	5000	0	16(1)
Zn(4)	0	0	5000	16(1)

Table S6. Selected bond lengths [Å] and angles [deg] for compound **2**.

O(1)-Zn(1)	1.9415(15)
O(2)-Zn(3)	2.1326(13)
O(5)-Zn(2)	2.0081(13)
O(5)-Zn(4)	2.1322(12)
O(6)-Zn(2)	1.9600(14)
O(7)-Zn(4)	2.0711(13)
O(10)-Zn(1)	1.9624(14)
O(11)-Zn(2)	1.9755(14)
O(12)-Zn(4)	2.0593(13)
O(14)-Zn(1)	1.9560(14)
O(15)-Zn(3)	2.0619(14)
O(16)-Zn(1)	1.9398(14)
O(17)-Zn(3)	2.1080(13)
O(19)-Zn(2)	2.1072(17)
O(20)-Zn(2)	2.238(2)
Zn(3)-O(15)#5	2.0619(14)
Zn(3)-O(17)#5	2.1080(13)
Zn(3)-O(2)#5	2.1326(13)
Zn(4)-O(12)#6	2.0593(13)
Zn(4)-O(7)#6	2.0711(13)
Zn(4)-O(5)#6	2.1322(12)

O(19)-C(24)-Zn(2)	57.59(12)
O(20)-C(24)-Zn(2)	63.66(14)
C(23)#4-C(24)-Zn(2)	178.26(18)
C(1)-O(1)-Zn(1)	114.00(13)
C(1)-O(2)-Zn(3)	132.17(13)
C(6)-O(5)-Zn(2)	112.74(11)
C(6)-O(5)-Zn(4)	122.27(11)
Zn(2)-O(5)-Zn(4)	103.22(6)
C(7)-O(6)-Zn(2)	123.35(12)
C(7)-O(7)-Zn(4)	134.79(13)
C(11)-O(8)-C(8)	106.17(15)
C(12)-O(10)-Zn(1)	113.37(13)
C(13)-O(11)-Zn(2)	116.10(12)
C(13)-O(12)-Zn(4)	128.45(12)
C(17)-O(13)-C(14)	106.04(15)
C(18)-O(14)-Zn(1)	124.42(13)
C(18)-O(15)-Zn(3)	135.94(13)
C(19)-O(16)-Zn(1)	123.47(12)
C(19)-O(17)-Zn(3)	132.82(12)
C(23)-O(18)-C(20)	106.34(15)
C(24)-O(19)-Zn(2)	92.90(15)
C(24)-O(20)-Zn(2)	86.53(17)
O(16)-Zn(1)-O(1)	124.50(7)
O(16)-Zn(1)-O(14)	109.57(6)
O(1)-Zn(1)-O(14)	107.06(7)
O(16)-Zn(1)-O(10)	106.96(6)
O(1)-Zn(1)-O(10)	104.75(7)
O(14)-Zn(1)-O(10)	101.59(6)
O(6)-Zn(2)-O(11)	121.78(6)
O(6)-Zn(2)-O(5)	105.01(6)

O(11)-Zn(2)-O(5)	96.51(6)
O(6)-Zn(2)-O(19)	123.07(7)
O(11)-Zn(2)-O(19)	106.88(7)
O(5)-Zn(2)-O(19)	96.31(6)
O(6)-Zn(2)-O(20)	90.19(8)
O(11)-Zn(2)-O(20)	91.24(9)
O(5)-Zn(2)-O(20)	155.62(7)
O(19)-Zn(2)-O(20)	59.31(7)
O(6)-Zn(2)-C(24)	108.96(7)
O(11)-Zn(2)-C(24)	99.85(7)
O(5)-Zn(2)-C(24)	125.80(7)
O(19)-Zn(2)-C(24)	29.50(8)
O(20)-Zn(2)-C(24)	29.82(8)
O(15)-Zn(3)-O(15)#5	180.0
O(15)-Zn(3)-O(17)#5	85.31(6)
O(15)#5-Zn(3)-O(17)#5	94.69(6)
O(15)-Zn(3)-O(17)	94.69(6)
O(15)#5-Zn(3)-O(17)	85.31(6)
O(17)#5-Zn(3)-O(17)	180.00(8)
O(15)-Zn(3)-O(2)#5	86.04(6)
O(15)#5-Zn(3)-O(2)#5	93.96(6)
O(17)#5-Zn(3)-O(2)#5	98.27(5)
O(17)-Zn(3)-O(2)#5	81.73(5)
O(15)-Zn(3)-O(2)	93.96(6)
O(15)#5-Zn(3)-O(2)	86.04(6)
O(17)#5-Zn(3)-O(2)	81.73(5)
O(17)-Zn(3)-O(2)	98.27(5)
O(2)#5-Zn(3)-O(2)	180.00(8)
O(12)#6-Zn(4)-O(12)	180.0
O(12)#6-Zn(4)-O(7)	86.72(6)
O(12)-Zn(4)-O(7)	93.28(6)
O(12)#6-Zn(4)-O(7)#6	93.28(6)
O(12)-Zn(4)-O(7)#6	86.72(6)
O(7)-Zn(4)-O(7)#6	180.00(4)
O(12)#6-Zn(4)-O(5)#6	91.40(5)
O(12)-Zn(4)-O(5)#6	88.60(5)
O(7)-Zn(4)-O(5)#6	88.09(5)
O(7)#6-Zn(4)-O(5)#6	91.91(5)
O(12)#6-Zn(4)-O(5)	88.60(5)
O(12)-Zn(4)-O(5)	91.40(5)
O(7)-Zn(4)-O(5)	91.91(5)
O(7)#6-Zn(4)-O(5)	88.09(5)
O(5)#6-Zn(4)-O(5)	180.00(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z #2 x-1,y,z+1 #3 x+1,y,z-1
#4 -x,-y+1,-z #5 -x+1,-y+1,-z #6 -x,-y,-z+1

Table S7. Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	19(1)	28(1)	24(1)	4(1)	-10(1)	0(1)
C(2)	21(1)	26(1)	24(1)	2(1)	-11(1)	-4(1)
C(3)	35(1)	32(1)	26(1)	0(1)	-14(1)	-8(1)
C(4)	35(1)	34(1)	21(1)	-1(1)	-12(1)	-6(1)
C(5)	21(1)	27(1)	17(1)	2(1)	-8(1)	0(1)
C(6)	19(1)	24(1)	19(1)	0(1)	-8(1)	2(1)
C(7)	30(1)	21(1)	20(1)	-2(1)	-14(1)	-2(1)
C(8)	35(1)	23(1)	30(1)	-6(1)	-22(1)	-1(1)
C(9)	46(1)	33(1)	54(1)	-18(1)	-37(1)	9(1)
C(10)	46(1)	33(1)	58(2)	-24(1)	-35(1)	12(1)
C(11)	35(1)	25(1)	35(1)	-12(1)	-21(1)	2(1)
C(12)	31(1)	29(1)	30(1)	-10(1)	-16(1)	-3(1)
C(13)	18(1)	24(1)	20(1)	-4(1)	-5(1)	3(1)
C(14)	20(1)	26(1)	24(1)	-7(1)	-8(1)	9(1)
C(15)	31(1)	38(1)	34(1)	-14(1)	-18(1)	16(1)
C(16)	36(1)	41(1)	34(1)	-19(1)	-22(1)	15(1)
C(17)	28(1)	26(1)	25(1)	-9(1)	-12(1)	7(1)
C(18)	25(1)	21(1)	24(1)	-6(1)	-8(1)	5(1)
C(19)	20(1)	20(1)	20(1)	-1(1)	-9(1)	3(1)
C(20)	22(1)	26(1)	27(1)	3(1)	-15(1)	2(1)
C(21)	28(1)	36(1)	53(1)	18(1)	-24(1)	-6(1)
C(22)	34(1)	38(1)	53(1)	22(1)	-23(1)	-6(1)
C(23)	30(1)	31(1)	30(1)	6(1)	-16(1)	3(1)
C(24)	44(1)	38(1)	35(1)	-4(1)	-26(1)	15(1)
C(25)	46(1)	46(2)	82(2)	-11(1)	-42(2)	10(1)
C(26)	51(2)	45(1)	41(1)	-7(1)	-13(1)	7(1)
C(27)	99(4)	78(3)	88(3)	-6(2)	11(3)	11(3)
C(28)	85(3)	72(3)	100(3)	-6(2)	-40(3)	9(2)
N(1)	27(1)	27(1)	41(1)	-10(1)	-15(1)	6(1)
N(2)	149(5)	113(4)	120(4)	-22(3)	-31(4)	-16(4)
O(1)	38(1)	36(1)	23(1)	2(1)	-11(1)	-11(1)
O(2)	20(1)	26(1)	30(1)	4(1)	-10(1)	-2(1)
O(3)	24(1)	27(1)	18(1)	1(1)	-8(1)	-4(1)
O(4)	40(1)	34(1)	21(1)	-4(1)	-12(1)	-8(1)
O(5)	17(1)	25(1)	18(1)	1(1)	-9(1)	1(1)
O(6)	28(1)	26(1)	33(1)	-8(1)	-18(1)	1(1)
O(7)	36(1)	23(1)	29(1)	-7(1)	-22(1)	2(1)
O(8)	33(1)	23(1)	29(1)	-9(1)	-20(1)	2(1)
O(9)	36(1)	50(1)	60(1)	-36(1)	-23(1)	4(1)
O(10)	36(1)	32(1)	33(1)	-11(1)	-22(1)	2(1)
O(11)	25(1)	38(1)	22(1)	-8(1)	-10(1)	12(1)
O(12)	23(1)	27(1)	21(1)	-5(1)	-5(1)	9(1)
O(13)	26(1)	27(1)	24(1)	-10(1)	-11(1)	12(1)
O(14)	32(1)	35(1)	30(1)	-13(1)	-15(1)	15(1)
O(15)	37(1)	21(1)	26(1)	-7(1)	-14(1)	7(1)
O(16)	24(1)	20(1)	36(1)	1(1)	-16(1)	0(1)

O(17)	24(1)	26(1)	24(1)	5(1)	-14(1)	0(1)
O(18)	22(1)	28(1)	27(1)	3(1)	-15(1)	3(1)
O(19)	31(1)	69(1)	37(1)	2(1)	-20(1)	14(1)
O(20)	90(2)	59(1)	95(2)	40(1)	-73(2)	-15(1)
Zn(1)	22(1)	19(1)	20(1)	-4(1)	-10(1)	1(1)
Zn(2)	18(1)	23(1)	19(1)	-1(1)	-10(1)	2(1)
Zn(3)	18(1)	15(1)	17(1)	-2(1)	-9(1)	2(1)
Zn(4)	16(1)	18(1)	16(1)	-5(1)	-9(1)	3(1)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for compound **2**.

	x	y	z	U(eq)
H(3)	2132	4215	2747	36
H(4)	786	2833	4021	36
H(9)	503	-3211	3639	45
H(10)	156	-4472	2544	48
H(15)	-1639	779	7972	38
H(16)	-2733	2098	9184	41
H(21)	6332	7703	-2736	45
H(22)	5804	9071	-3818	50
H(31A)	108	6285	-1097	79
H(31B)	835	7180	-1900	79
H(31C)	96	7436	-804	79
H(32A)	874	6827	519	71
H(32B)	1909	6071	174	71
H(32C)	705	5697	255	71
H(34A)	-5831	3086	5905	157
H(34B)	-4803	2546	5104	157
H(34C)	-4791	2706	6140	157
H(33A)	-5233	1292	7241	128
H(33B)	-6184	470	7331	128
H(33C)	-6525	1599	7667	128
H(1A)	1984	6228	-1353	37
H(1B)	1971	7294	-1078	37
H(2A)	-5437	1087	5775	162
H(2B)	-6533	1593	6188	162

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **3**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	7855(5)	72(4)	1056(3)	32(1)
C(2)	9387(5)	-154(4)	1008(3)	32(1)
C(3)	10047(5)	-862(4)	729(3)	37(1)
C(4)	11527(5)	-683(4)	808(3)	38(1)
C(5)	11657(5)	108(3)	1134(3)	32(1)
C(6)	12900(5)	663(4)	1362(3)	34(1)
C(7)	5648(5)	2229(3)	288(3)	33(1)
C(8)	5864(6)	1918(3)	4930(3)	34(1)
C(9)	6148(11)	1129(4)	5234(4)	57(2)
C(10)	6247(9)	561(4)	4593(3)	58(2)
C(11)	6052(6)	1038(3)	3959(3)	35(1)
C(12)	5956(6)	799(4)	3132(3)	35(1)
C(13)	6547(9)	-1904(5)	2037(5)	70(2)
C(14)	4065(8)	-1512(4)	2299(4)	55(2)
N(1)	5271(8)	-1397(5)	1807(4)	64(2)
O(1)	6985(4)	-437(3)	770(2)	45(1)
O(2)	7589(4)	771(3)	1390(2)	47(1)
O(3)	10361(3)	449(2)	1260(2)	34(1)
O(4)	12718(5)	1367(3)	1657(4)	60(1)
O(5)	14118(3)	327(2)	1224(2)	30(1)
O(6)	5613(5)	2258(2)	1033(2)	40(1)
O(7)	5550(4)	1566(2)	-106(2)	35(1)
O(8)	5783(4)	1881(2)	4150(2)	31(1)
O(9)	5711(4)	1424(3)	2666(2)	38(1)
O(10)	6096(6)	26(3)	2953(3)	54(1)
Zn(1)	5634(1)	1145(1)	1574(1)	28(1)
Zn(2)	5000	0	0	116(1)

Table S10. Bond lengths [Å] and angles [deg] for compound **3**.

O(1)-Zn(2)	2.351(4)
O(2)-Zn(1)	1.970(4)
O(5)-Zn(1)#3	1.981(3)
O(5)-Zn(2)#3	2.369(3)
O(6)-Zn(1)	1.956(4)
O(7)-Zn(2)	2.479(4)
O(9)-Zn(1)	1.942(3)
Zn(1)-O(5)#4	1.981(3)
Zn(2)-O(1)#5	2.351(4)
Zn(2)-O(5)#4	2.369(3)
Zn(2)-O(5)#6	2.369(3)
Zn(2)-O(7)#5	2.479(4)

C(1)-O(1)-Zn(2)	123.3(4)
C(1)-O(2)-Zn(1)	122.3(4)
C(5)-O(3)-C(2)	106.3(4)
C(6)-O(5)-Zn(1)#3	108.8(3)
C(6)-O(5)-Zn(2)#3	126.9(3)
Zn(1)#3-O(5)-Zn(2)#3	97.71(13)
C(7)-O(6)-Zn(1)	116.7(3)
C(7)-O(7)-Zn(2)	141.2(3)
C(8)-O(8)-C(11)	106.3(4)
C(12)-O(9)-Zn(1)	116.8(3)
O(9)-Zn(1)-O(6)	105.86(16)
O(9)-Zn(1)-O(2)	103.13(17)
O(6)-Zn(1)-O(2)	99.71(19)
O(9)-Zn(1)-O(5)#4	115.89(15)
O(6)-Zn(1)-O(5)#4	114.79(16)
O(2)-Zn(1)-O(5)#4	115.53(18)
O(1)#5-Zn(2)-O(1)	180.0(3)
O(1)#5-Zn(2)-O(5)#4	98.49(14)
O(1)-Zn(2)-O(5)#4	81.51(14)
O(1)#5-Zn(2)-O(5)#6	81.51(14)
O(1)-Zn(2)-O(5)#6	98.49(14)
O(5)#4-Zn(2)-O(5)#6	180.00(15)
O(1)#5-Zn(2)-O(7)	80.93(14)
O(1)-Zn(2)-O(7)	99.07(14)
O(5)#4-Zn(2)-O(7)	86.65(12)
O(5)#6-Zn(2)-O(7)	93.35(12)
O(1)#5-Zn(2)-O(7)#5	99.07(14)
O(1)-Zn(2)-O(7)#5	80.93(14)
O(5)#4-Zn(2)-O(7)#5	93.35(12)
O(5)#6-Zn(2)-O(7)#5	86.65(12)
O(7)-Zn(2)-O(7)#5	180.0

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z-1/2 #2 x,-y+1/2,z+1/2
#3 x+1,y,z #4 x-1,y,z #5 -x+1,-y,-z
#6 -x+2,-y,-z

Table S11. Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **3**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	16(2)	52(3)	29(2)	7(2)	2(2)	1(2)
C(2)	15(2)	58(3)	24(2)	-1(2)	1(2)	-1(2)
C(3)	25(2)	50(3)	37(3)	-5(2)	-2(2)	-4(2)
C(4)	22(2)	55(3)	37(3)	-9(2)	0(2)	6(2)
C(5)	18(2)	49(3)	29(2)	-4(2)	3(2)	-3(2)
C(6)	20(2)	49(3)	33(2)	-6(2)	5(2)	-1(2)
C(7)	32(2)	42(2)	24(2)	1(2)	5(2)	0(2)
C(8)	38(3)	44(3)	19(2)	2(2)	1(2)	-3(2)
C(9)	98(6)	47(3)	27(3)	2(2)	5(3)	9(3)
C(10)	102(6)	37(3)	34(3)	5(2)	4(3)	15(3)
C(11)	37(3)	37(2)	29(2)	2(2)	1(2)	0(2)
C(12)	34(3)	46(3)	26(2)	-5(2)	2(2)	-1(2)
C(13)	66(5)	60(4)	85(6)	16(4)	-5(4)	2(4)
C(14)	68(5)	45(3)	52(4)	5(3)	0(3)	0(3)
N(1)	62(4)	69(4)	60(4)	10(3)	-4(3)	3(3)
O(1)	16(2)	70(3)	49(2)	3(2)	-5(2)	1(2)
O(2)	21(2)	76(3)	44(2)	-2(2)	4(2)	7(2)
O(3)	16(2)	51(2)	34(2)	-8(2)	1(1)	2(1)
O(4)	28(2)	67(3)	86(4)	-32(3)	4(2)	-6(2)
O(5)	19(2)	46(2)	26(2)	-2(1)	2(1)	-4(1)
O(6)	52(2)	47(2)	22(2)	0(1)	2(2)	1(2)
O(7)	36(2)	40(2)	29(2)	0(1)	2(1)	-4(2)
O(8)	32(2)	37(2)	23(2)	1(1)	2(1)	1(1)
O(9)	49(2)	45(2)	20(2)	-2(1)	-1(2)	0(2)
O(10)	81(3)	39(2)	42(2)	-8(2)	7(2)	-3(2)
Zn(1)	21(1)	39(1)	22(1)	-6(1)	0(1)	0(1)
Zn(2)	107(2)	138(2)	102(2)	-11(1)	9(1)	1(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for compound **3**.

	x	y	z	U(eq)
H(3)	9621	-1361	529	45
H(4)	12262	-1042	663	46
H(9)	6255	986	5754	69
H(10)	6417	-33	4614	69
H(13A)	7328	-1722	1738	105
H(13B)	6365	-2509	1947	105
H(13C)	6780	-1812	2574	105
H(14A)	3345	-1850	2031	83
H(14B)	3684	-955	2426	83
H(14C)	4374	-1806	2764	83
H(1A)	5506	-832	1804	76
H(1B)	4997	-1545	1321	76