Electronic Supplementary Information for Dalton Transactions

Supporting Information For

Thermal spin-crossover in the $[M_3Zn_6Cl_6L_{12}]$ (M^{II} = Zn, Fe; L = 5,6-dimethoxy-1,2,3-benzotriazolate) system: structural, electrochemical, Mössbauer, and UV-Vis spectroscopic studies

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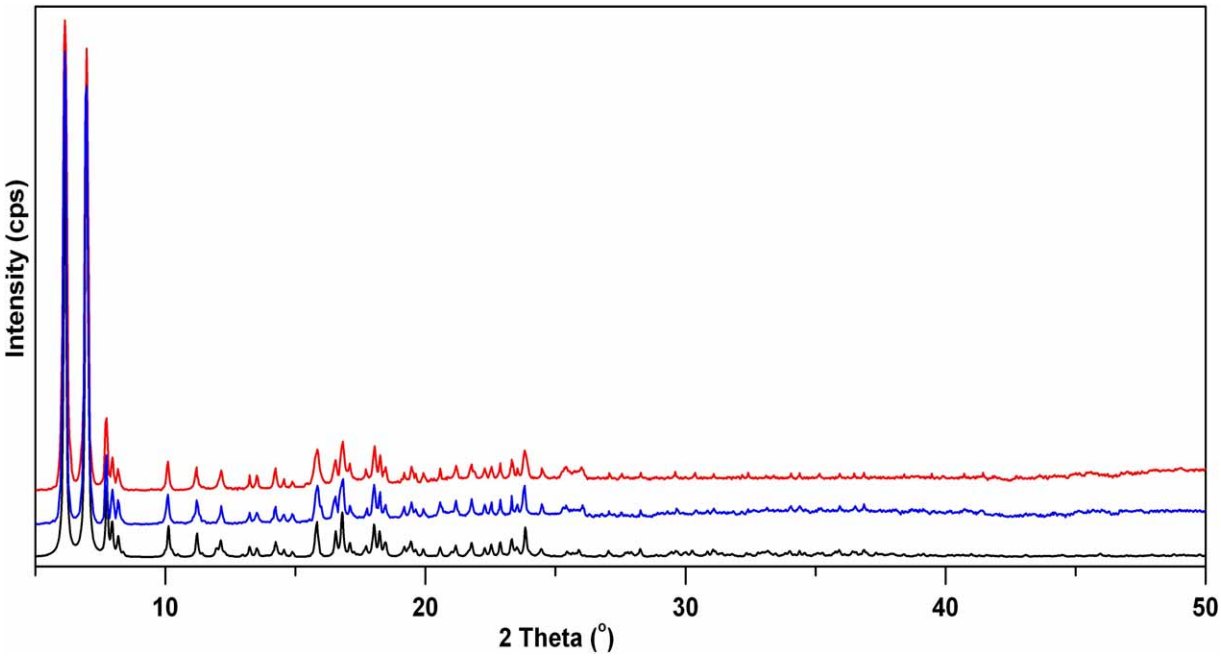


Fig. S1 Theoretical XRPD pattern (black) and experimental XRPD patterns of **1** synthesized by solvothermal method (blue) and vapour diffusion method (red).

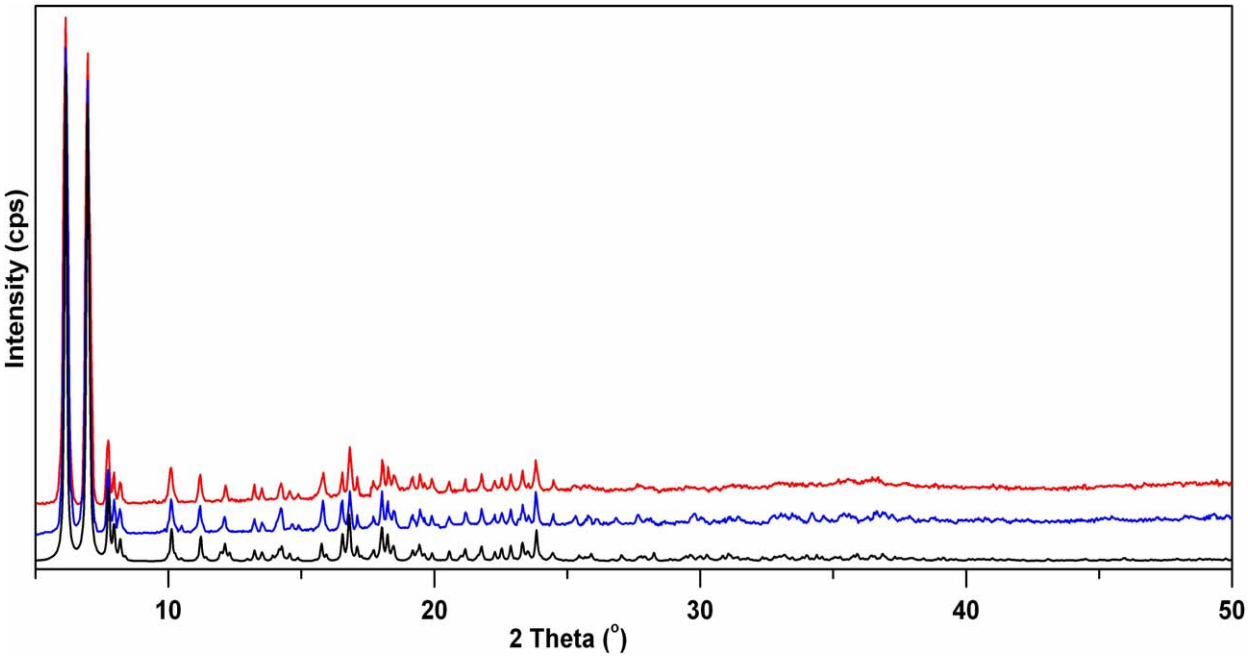


Fig. S2 Theoretical XRPD pattern (black) and experimental XRPD patterns of **2** synthesized by solvothermal method (blue) and vapour diffusion method (red).

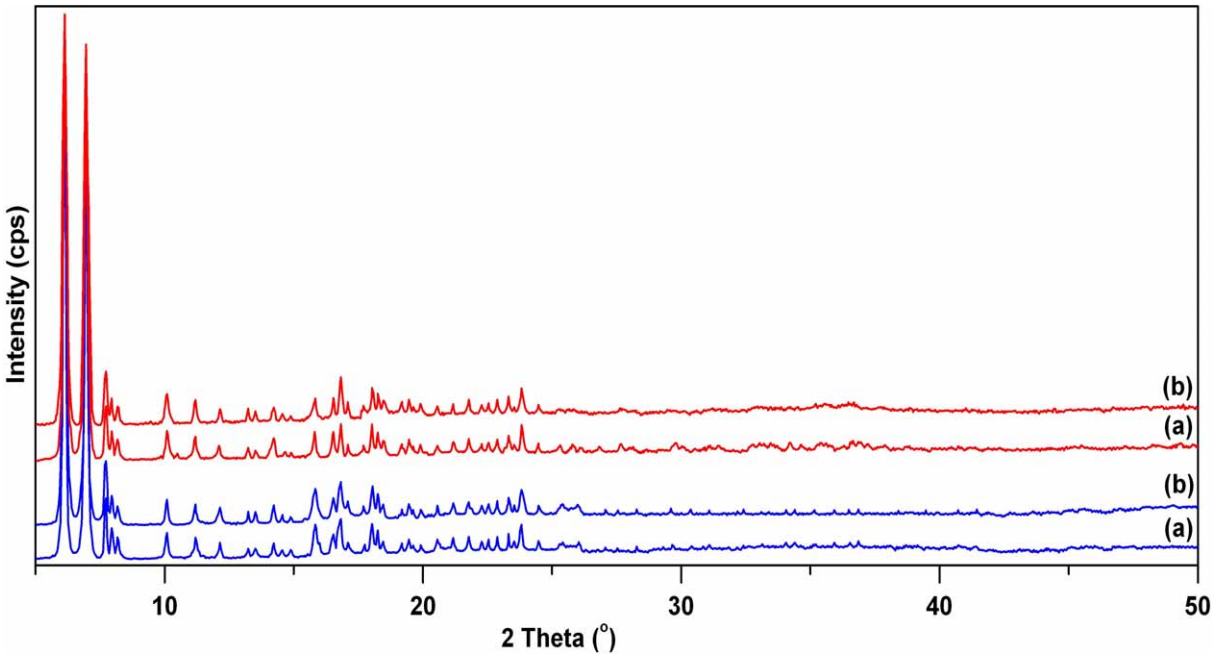


Fig. S3 Comparison among the experimental XRPD patterns of **1** (blue) and **2** (red) synthesized by (a) solvothermal method and (b) vapour diffusion method.

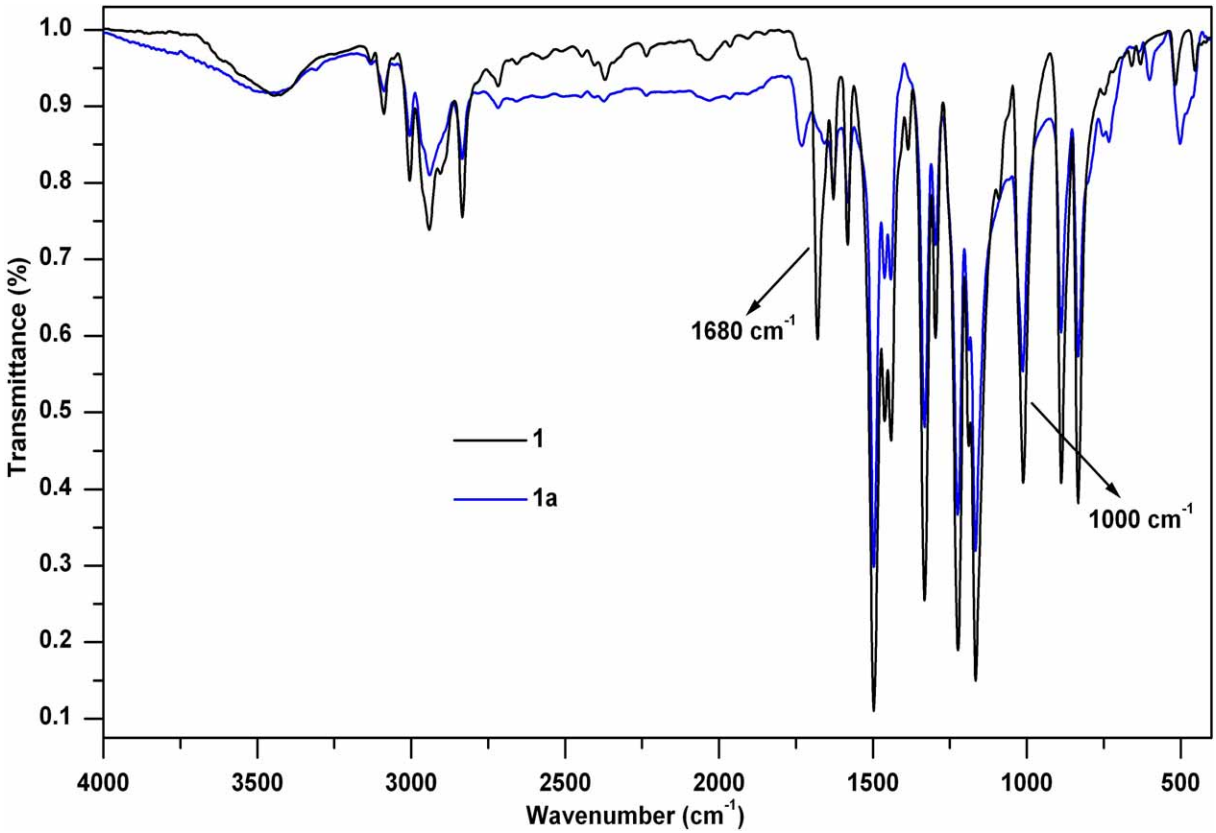


Fig. S4 FT-IR spectra of **1** (black) and **1a** (blue).

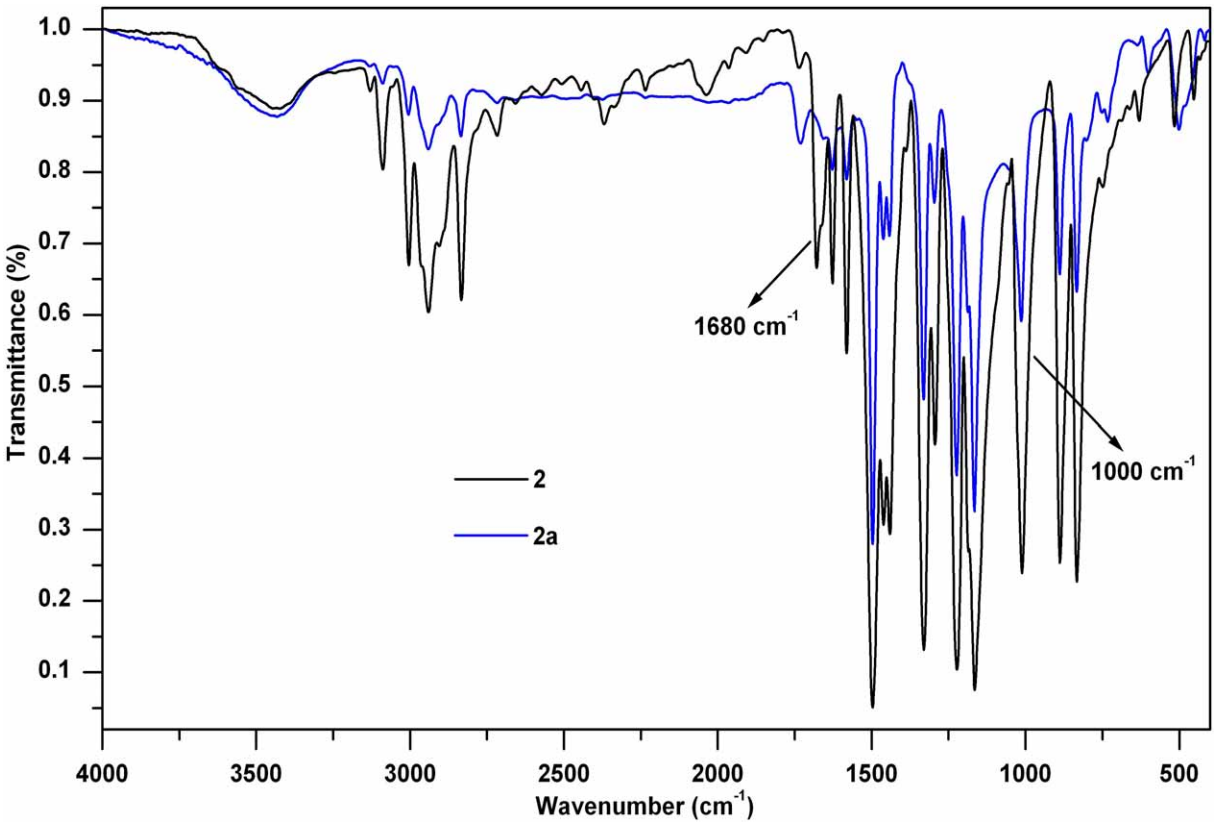


Fig. S5 FT-IR spectra of **2** (black) and **2a** (blue).

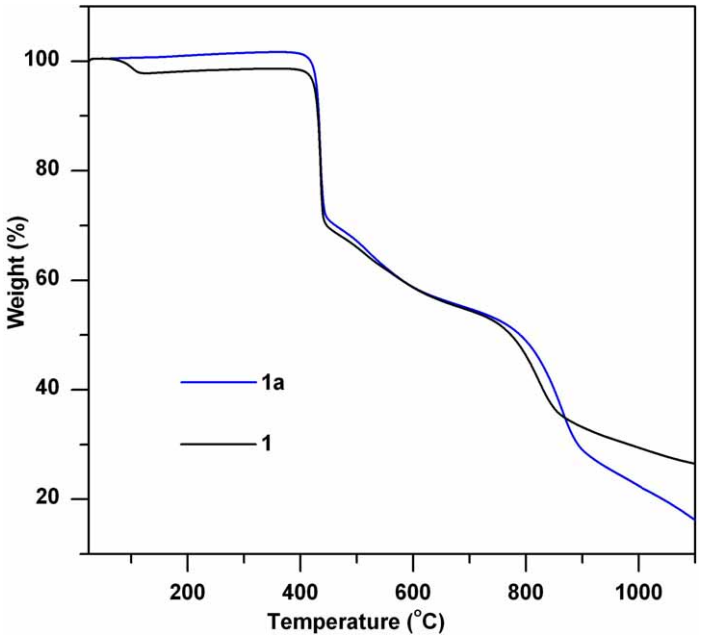


Fig. S6 TG analysis of **1** (black) and **1a** (blue) under N_2 atmosphere.

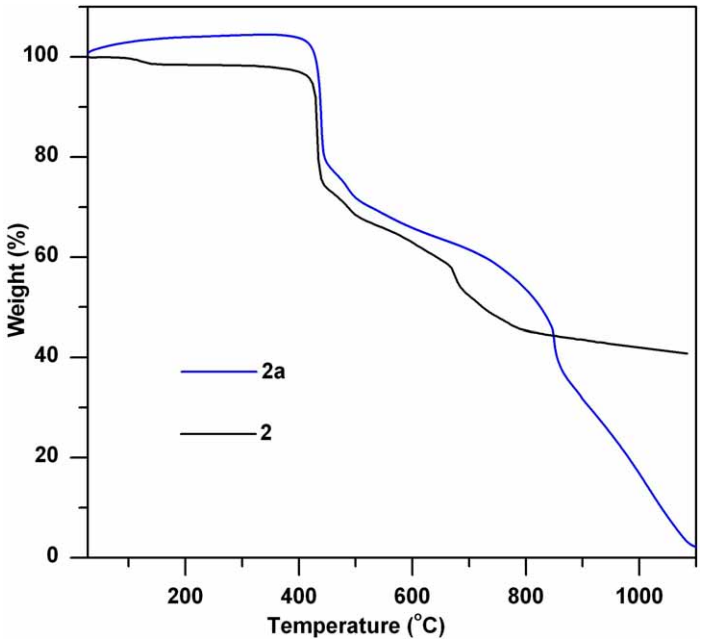


Fig. S7 TG analysis of **2** (black) and **2a** (blue) under N_2 atmosphere.

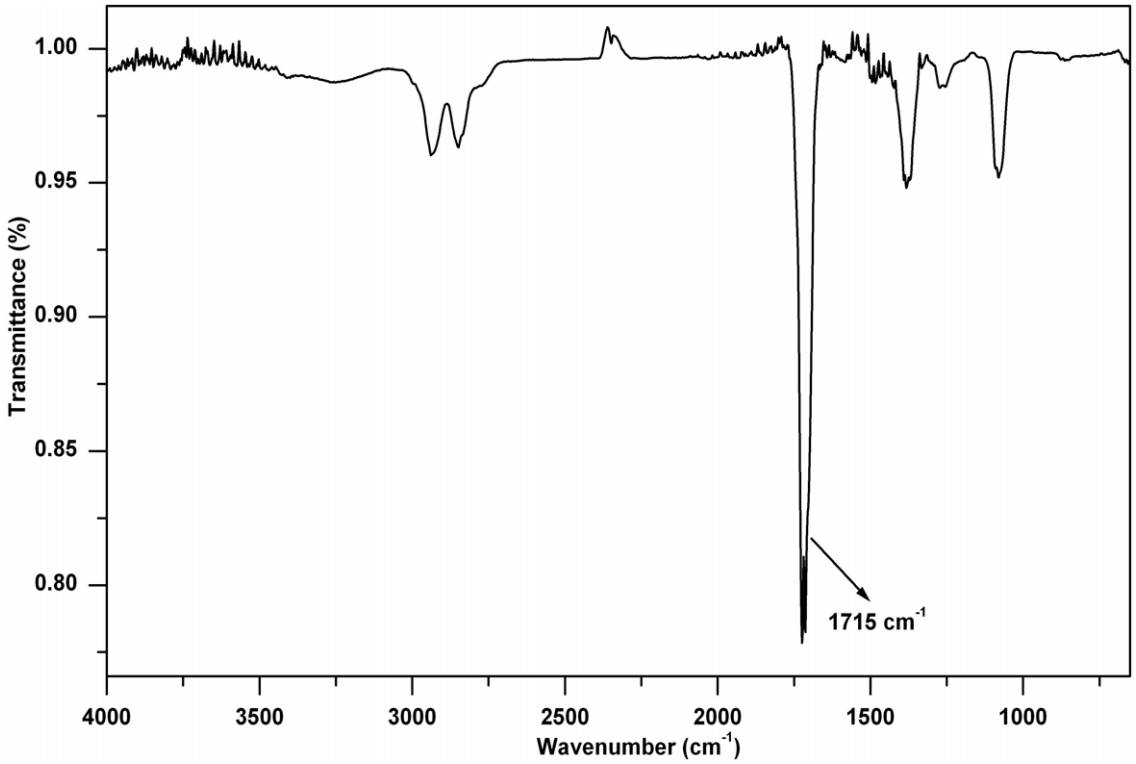


Fig. S8 FT-IR spectrum of the volatile molecules liberated from as-synthesized **1** at 130 ºC.

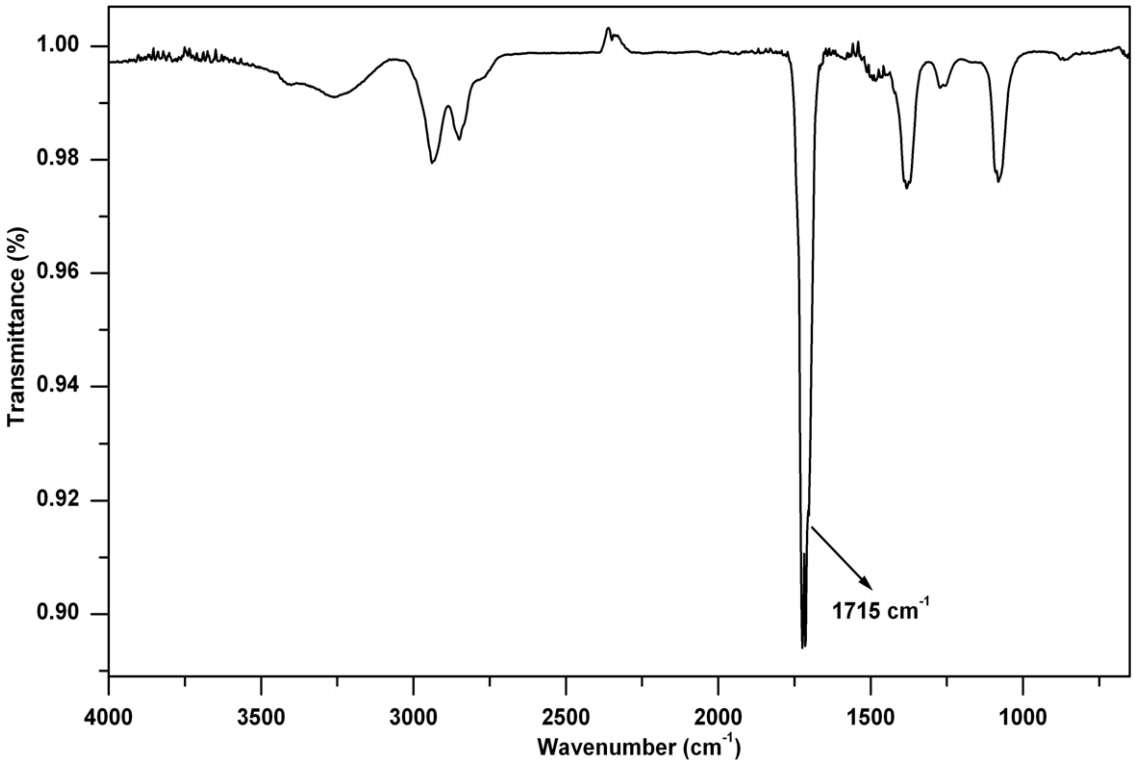
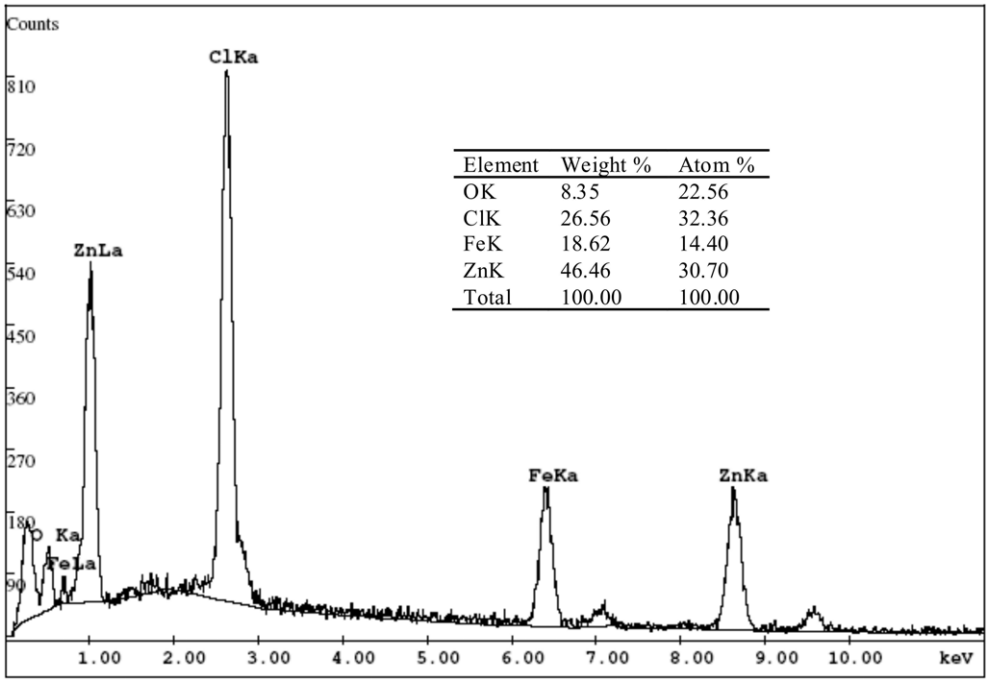


Fig. S9 FT-IR spectrum of the volatile molecules liberated from as-synthesized **2** at 130 ºC.



Element	Weight %	Atom %
OK	8.35	22.56
ClK	26.56	32.36
FeK	18.62	14.40
ZnK	46.46	30.70
Total	100.00	100.00

Fig. S10 EDX spectrum of **2**. Weight % and atom % of the elements (excluding carbon) are shown in the inset.

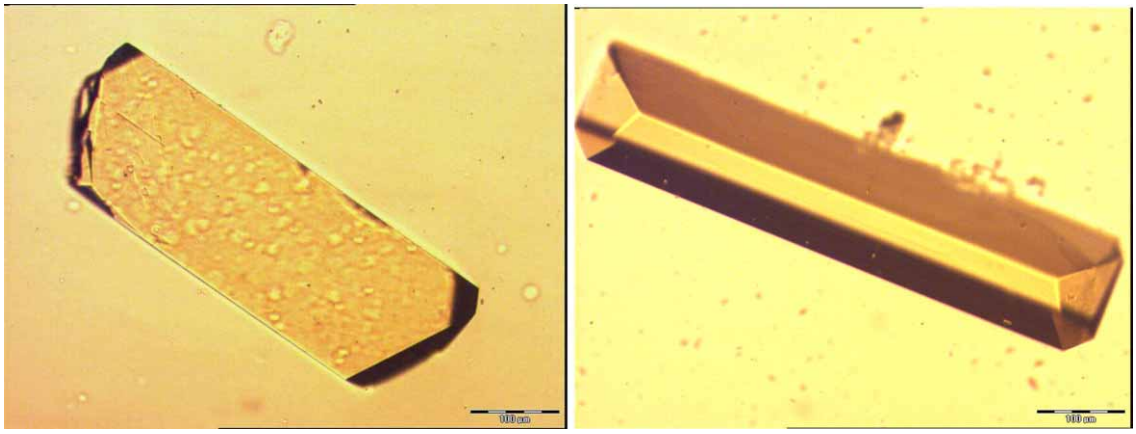


Fig. S11 Optical micrographs of the single crystals of **1**.

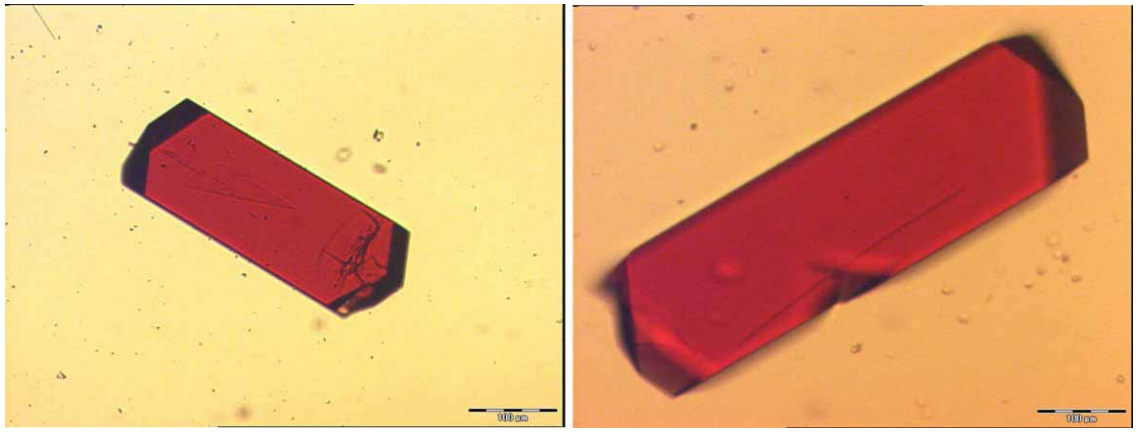


Fig. S12 Optical micrographs of the single crystals of **2**.

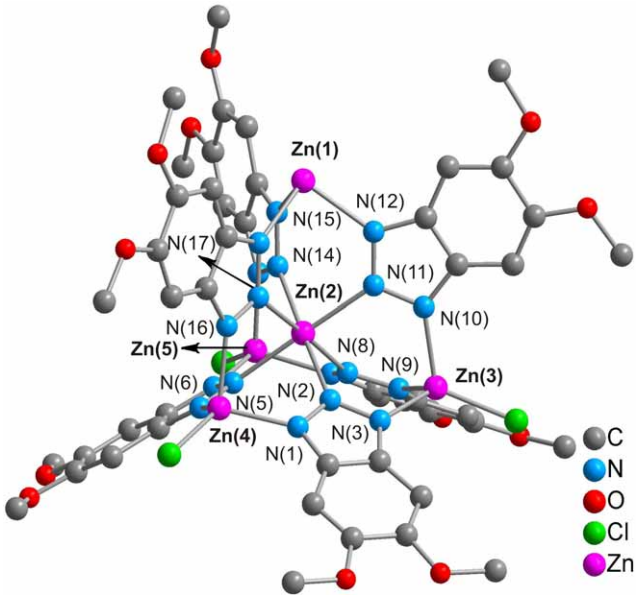


Fig. S13 Ball-and-stick representation of the asymmetric unit of **1**. Hydrogen atoms are omitted for clarity.

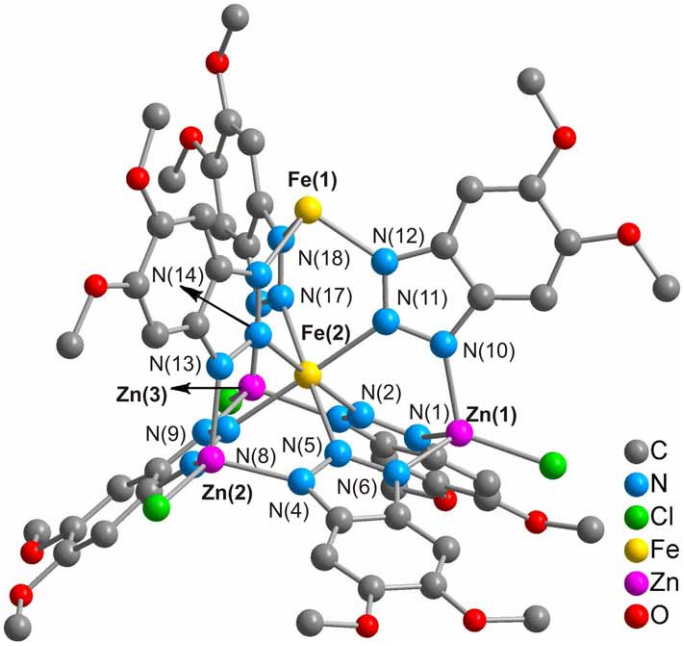


Fig. S14 Ball-and-stick representation of the asymmetric unit of **2**. Hydrogen atoms are omitted for clarity.

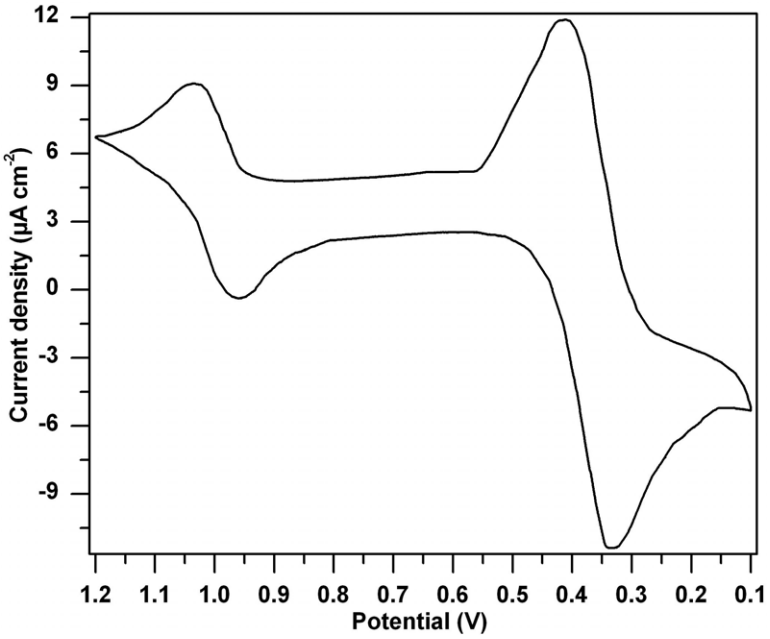


Fig. S15 Detailed cyclic voltammogram of **2** (redox couple of **2** and ferrocene are seen on the left and right side of the diagram, respectively.

Table S1 Operating parameters for the ICP-AES spectrometer.

Incident output power	1150 W
Nebulizer	PTFE, Mira Mist
Plasma gas flow rate	12 L min^{-1}
Auxiliary gas flow rate	0.5 L min^{-1}
Aerosol carrier gas flow	0.6 L min^{-1}

Table S1 (continued)

Solution uptake rate	1 mL min^{-1}
Signal integration time	10 s
Integration for determination	3
Wavelength	Fe = 259.93 nm, Zn = 213.85 nm

Table S2 Bond lengths (Å) for **1**.

Zn(1)-N(12)#1	2.139(5)	N(10)-N(11)	1.351(8)	C(1)-C(6)	1.380(10)
Zn(1)-N(12)	2.139(5)	N(10)-C(25)	1.365(9)	C(1)-C(2)	1.435(10)
Zn(1)-N(18)	2.139(6)	N(11)-N(12)	1.335(7)	C(2)-C(3)	1.359(11)
Zn(1)-N(18)#1	2.139(6)	N(12)-C(30)	1.364(9)	C(3)-C(4)	1.436(12)
Zn(1)-N(15)#1	2.150(6)	N(13)-N(14)	1.343(8)	C(4)-C(5)	1.345(11)
Zn(1)-N(15)	2.150(6)	N(13)-C(38)	1.352(9)	C(5)-C(6)	1.403(11)
Zn(2)-N(14)	2.157(6)	N(14)-N(15)	1.345(7)	C(9)-C(14)	1.379(11)
Zn(2)-N(11)	2.160(5)	N(15)-C(33)	1.349(10)	C(9)-C(10)	1.431(11)
Zn(2)-N(2)	2.172(6)	N(16)-N(17)	1.339(8)	C(10)-C(11)	1.377(13)
Zn(2)-N(17)	2.177(5)	N(16)-C(41)	1.371(8)	C(11)-C(12)	1.428(15)
Zn(2)-N(5)	2.197(6)	N(17)-N(18)	1.345(7)	C(12)-C(13)	1.362(13)
Zn(2)-N(8)	2.232(6)	N(18)-C(46)	1.357(9)	C(13)-C(14)	1.421(11)
Zn(3)-N(10)	2.004(5)	O(1)-C(4)	1.362(10)	C(17)-C(22)	1.358(11)
Zn(3)-N(9)	2.005(6)	O(1)-C(7)	1.430(12)	C(17)-C(18)	1.417(11)
Zn(3)-N(3)	2.011(6)	O(2)-C(3)	1.363(9)	C(18)-C(19)	1.349(13)
Zn(3)-Cl(3)	2.154(2)	O(2)-C(8)	1.420(10)	C(19)-C(20)	1.414(14)
Zn(4)-N(16)	2.002(5)	O(3)-C(11)	1.338(11)	C(20)-C(21)	1.368(12)
Zn(4)-N(1)	2.006(6)	O(3)-C(15)	1.414(16)	C(21)-C(22)	1.420(11)
Zn(4)-N(4)	2.014(6)	O(4)-C(12)	1.348(11)	C(25)-C(30)	1.380(10)
Zn(4)-Cl(1)	2.169(2)	O(4)-C(16)	1.425(15)	C(25)-C(26)	1.401(11)
Zn(5)-N(7)	1.997(6)	O(5)-C(19)	1.366(11)	C(26)-C(27)	1.347(12)
Zn(5)-N(13)	2.004(6)	O(5)-C(23)	1.407(17)	C(27)-C(28)	1.434(12)
Zn(5)-N(6)	2.012(6)	O(6)-C(20)	1.371(10)	C(28)-C(29)	1.364(11)
Zn(5)-Cl(2)	2.169(2)	O(6)-C(24)	1.380(12)	C(29)-C(30)	1.406(10)
N(1)-N(2)	1.339(8)	O(7)-C(28)	1.363(10)	C(33)-C(38)	1.392(10)
N(1)-C(6)	1.356(9)	O(7)-C(31)	1.472(12)	C(33)-C(34)	1.408(11)
N(2)-N(3)	1.334(8)	O(8)-C(27)	1.352(10)	C(34)-C(35)	1.367(13)
N(3)-C(1)	1.348(9)	O(8)-C(32)	1.450(13)	C(35)-C(36)	1.462(13)
N(4)-N(5)	1.328(8)	O(9)-C(35)	1.341(11)	C(36)-C(37)	1.341(13)
N(4)-C(9)	1.340(9)	O(9)-C(39)	1.486(14)	C(37)-C(38)	1.404(12)
N(5)-N(6)	1.332(8)	O(10)-C(36)	1.371(12)	C(41)-C(46)	1.381(10)
N(6)-C(14)	1.343(9)	O(10)-C(40)	1.472(15)	C(41)-C(42)	1.402(10)
N(7)-N(8)	1.333(8)	O(11)-C(43)	1.351(9)	C(42)-C(43)	1.355(10)
N(7)-C(22)	1.375(9)	O(11)-C(47)	1.426(11)	C(43)-C(44)	1.439(11)
N(8)-N(9)	1.339(8)	O(12)-C(44)	1.381(9)	C(44)-C(45)	1.345(11)
N(9)-C(17)	1.356(9)	O(12)-C(48)	1.459(13)	C(45)-C(46)	1.407(10)

Symmetry operator used to create equivalent atoms is #1: -x, -y, -z.

Table S3 Bond angles (°) for **1**.

N(12)#1-Zn(1)-N(12)	180	N(7)-Zn(5)-Cl(2)	117.94(19)
N(12)#1-Zn(1)-N(18)	88.2(2)	N(13)-Zn(5)-Cl(2)	119.53(19)
N(12)-Zn(1)-N(18)	91.8(2)	N(6)-Zn(5)-Cl(2)	115.77(18)
N(12)#1-Zn(1)-N(18)#1	91.8(2)	N(2)-N(1)-C(6)	107.9(6)
N(12)-Zn(1)-N(18)#1	88.2(2)	N(2)-N(1)-Zn(4)	120.1(5)
N(18)-Zn(1)-N(18)#1	180	C(6)-N(1)-Zn(4)	131.9(5)
N(12)#1-Zn(1)-N(15)#1	91.4(2)	N(3)-N(2)-N(1)	109.6(5)
N(12)-Zn(1)-N(15)#1	88.6(2)	N(3)-N(2)-Zn(2)	126.8(4)
N(18)-Zn(1)-N(15)#1	88.0(2)	N(1)-N(2)-Zn(2)	123.5(4)
N(18)#1-Zn(1)-N(15)#1	92.0(2)	N(2)-N(3)-C(1)	107.8(5)
N(12)#1-Zn(1)-N(15)	88.6(2)	N(2)-N(3)-Zn(3)	117.0(4)
N(12)-Zn(1)-N(15)	91.4(2)	C(1)-N(3)-Zn(3)	135.2(5)
N(18)-Zn(1)-N(15)	92.0(2)	N(5)-N(4)-C(9)	106.8(6)
N(18)#1-Zn(1)-N(15)	88.0(2)	N(5)-N(4)-Zn(4)	119.2(4)
N(15)#1-Zn(1)-N(15)	180	C(9)-N(4)-Zn(4)	134.0(5)
N(14)-Zn(2)-N(11)	90.1(2)	N(4)-N(5)-N(6)	110.7(5)
N(14)-Zn(2)-N(2)	179.0(2)	N(4)-N(5)-Zn(2)	124.0(4)
N(11)-Zn(2)-N(2)	89.3(2)	N(6)-N(5)-Zn(2)	124.9(4)
N(14)-Zn(2)-N(17)	91.2(2)	N(5)-N(6)-C(14)	107.4(6)
N(11)-Zn(2)-N(17)	90.8(2)	N(5)-N(6)-Zn(5)	118.4(4)
N(2)-Zn(2)-N(17)	89.5(2)	C(14)-N(6)-Zn(5)	134.2(5)
N(14)-Zn(2)-N(5)	90.5(2)	N(8)-N(7)-C(22)	106.8(6)
N(11)-Zn(2)-N(5)	178.5(2)	N(8)-N(7)-Zn(5)	116.8(4)
N(2)-Zn(2)-N(5)	90.1(2)	C(22)-N(7)-Zn(5)	136.4(5)
N(17)-Zn(2)-N(5)	90.6(2)	N(7)-N(8)-N(9)	109.9(5)
N(14)-Zn(2)-N(8)	90.1(2)	N(7)-N(8)-Zn(2)	125.4(4)
N(11)-Zn(2)-N(8)	91.1(2)	N(9)-N(8)-Zn(2)	123.4(4)
N(2)-Zn(2)-N(8)	89.1(2)	N(8)-N(9)-C(17)	108.0(6)
N(17)-Zn(2)-N(8)	177.7(2)	N(8)-N(9)-Zn(3)	118.9(4)
N(5)-Zn(2)-N(8)	87.5(2)	C(17)-N(9)-Zn(3)	133.0(5)
N(10)-Zn(3)-N(9)	97.8(2)	N(11)-N(10)-C(25)	106.5(5)
N(10)-Zn(3)-N(3)	98.5(2)	N(11)-N(10)-Zn(3)	119.7(4)
N(9)-Zn(3)-N(3)	102.6(2)	C(25)-N(10)-Zn(3)	133.7(5)
N(10)-Zn(3)-Cl(3)	119.57(18)	N(12)-N(11)-N(10)	110.9(5)
N(9)-Zn(3)-Cl(3)	115.45(18)	N(12)-N(11)-Zn(2)	125.1(4)
N(3)-Zn(3)-Cl(3)	119.22(19)	N(10)-N(11)-Zn(2)	123.9(4)
N(16)-Zn(4)-N(1)	97.7(2)	N(11)-N(12)-C(30)	107.0(5)
N(16)-Zn(4)-N(4)	98.8(2)	N(11)-N(12)-Zn(1)	124.0(4)
N(1)-Zn(4)-N(4)	101.1(2)	C(30)-N(12)-Zn(1)	129.0(4)
N(16)-Zn(4)-Cl(1)	118.59(18)	N(14)-N(13)-C(38)	107.5(5)
N(1)-Zn(4)-Cl(1)	117.80(19)	N(14)-N(13)-Zn(5)	118.6(4)
N(4)-Zn(4)-Cl(1)	118.90(18)	C(38)-N(13)-Zn(5)	133.9(5)
N(7)-Zn(5)-N(13)	98.8(2)	N(13)-N(14)-N(15)	110.5(5)
N(7)-Zn(5)-N(6)	103.2(2)	N(13)-N(14)-Zn(2)	125.2(4)
N(13)-Zn(5)-N(6)	98.2(2)	N(15)-N(14)-Zn(2)	124.3(4)

Table S3 (continued)

N(14)-N(15)-C(33)	106.7(6)	O(4)-C(12)-C(13)	123.5(10)
N(14)-N(15)-Zn(1)	124.4(4)	O(4)-C(12)-C(11)	113.5(9)
C(33)-N(15)-Zn(1)	128.9(5)	C(13)-C(12)-C(11)	123.0(9)
N(17)-N(16)-C(41)	107.8(5)	C(12)-C(13)-C(14)	115.5(9)
N(17)-N(16)-Zn(4)	118.0(4)	N(6)-C(14)-C(9)	106.9(6)
C(41)-N(16)-Zn(4)	134.2(5)	N(6)-C(14)-C(13)	131.1(8)
N(16)-N(17)-N(18)	109.9(5)	C(9)-C(14)-C(13)	122.0(7)
N(16)-N(17)-Zn(2)	125.6(4)	N(9)-C(17)-C(22)	107.4(7)
N(18)-N(17)-Zn(2)	124.5(4)	N(9)-C(17)-C(18)	130.4(8)
N(17)-N(18)-C(46)	107.5(5)	C(22)-C(17)-C(18)	122.2(7)
N(17)-N(18)-Zn(1)	124.0(4)	C(19)-C(18)-C(17)	116.6(9)
C(46)-N(18)-Zn(1)	128.5(4)	C(18)-C(19)-O(5)	125.3(10)
C(4)-O(1)-C(7)	115.2(7)	C(18)-C(19)-C(20)	121.2(8)
C(3)-O(2)-C(8)	117.4(7)	O(5)-C(19)-C(20)	113.5(9)
C(11)-O(3)-C(15)	116.9(10)	C(21)-C(20)-O(6)	122.9(10)
C(12)-O(4)-C(16)	115.9(9)	C(21)-C(20)-C(19)	123.2(8)
C(19)-O(5)-C(23)	116.1(9)	O(6)-C(20)-C(19)	113.9(8)
C(20)-O(6)-C(24)	117.4(8)	C(20)-C(21)-C(22)	115.0(8)
C(28)-O(7)-C(31)	115.7(7)	C(17)-C(22)-N(7)	108.0(7)
C(27)-O(8)-C(32)	115.0(8)	C(17)-C(22)-C(21)	121.8(7)
C(35)-O(9)-C(39)	114.8(8)	N(7)-C(22)-C(21)	130.1(8)
C(36)-O(10)-C(40)	114.0(9)	N(10)-C(25)-C(30)	107.8(6)
C(43)-O(11)-C(47)	116.7(7)	N(10)-C(25)-C(26)	129.6(7)
C(44)-O(12)-C(48)	114.2(7)	C(30)-C(25)-C(26)	122.5(7)
N(3)-C(1)-C(6)	107.9(6)	C(27)-C(26)-C(25)	115.9(8)
N(3)-C(1)-C(2)	131.3(7)	C(26)-C(27)-O(8)	124.5(8)
C(6)-C(1)-C(2)	120.8(7)	C(26)-C(27)-C(28)	122.2(8)
C(3)-C(2)-C(1)	115.8(7)	O(8)-C(27)-C(28)	113.2(8)
C(2)-C(3)-O(2)	123.8(7)	O(7)-C(28)-C(29)	123.9(8)
C(2)-C(3)-C(4)	122.4(7)	O(7)-C(28)-C(27)	114.3(7)
O(2)-C(3)-C(4)	113.7(7)	C(29)-C(28)-C(27)	121.7(8)
C(5)-C(4)-O(1)	125.5(8)	C(28)-C(29)-C(30)	115.9(7)
C(5)-C(4)-C(3)	121.5(8)	N(12)-C(30)-C(25)	107.7(6)
O(1)-C(4)-C(3)	112.9(7)	N(12)-C(30)-C(29)	130.7(7)
C(4)-C(5)-C(6)	116.9(7)	C(25)-C(30)-C(29)	121.6(7)
N(1)-C(6)-C(1)	106.8(6)	N(15)-C(33)-C(38)	108.3(6)
N(1)-C(6)-C(5)	130.7(7)	N(15)-C(33)-C(34)	130.6(7)
C(1)-C(6)-C(5)	122.5(7)	C(38)-C(33)-C(34)	121.2(7)
N(4)-C(9)-C(14)	108.2(7)	C(35)-C(34)-C(33)	117.2(8)
N(4)-C(9)-C(10)	129.3(8)	O(9)-C(35)-C(34)	125.8(9)
C(14)-C(9)-C(10)	122.5(7)	O(9)-C(35)-C(36)	113.8(9)
C(11)-C(10)-C(9)	114.8(9)	C(34)-C(35)-C(36)	120.3(8)
O(3)-C(11)-C(10)	123.3(10)	C(37)-C(36)-O(10)	125.7(9)
O(3)-C(11)-C(12)	114.5(9)	C(37)-C(36)-C(35)	122.3(9)
C(10)-C(11)-C(12)	122.1(9)	O(10)-C(36)-C(35)	112.1(9)

Table S3 (continued)

C(36)-C(37)-C(38)	116.7(8)	O(11)-C(43)-C(44)	113.3(7)
N(13)-C(38)-C(33)	107.0(7)	C(42)-C(43)-C(44)	121.3(7)
N(13)-C(38)-C(37)	130.8(7)	C(45)-C(44)-O(12)	125.0(7)
C(33)-C(38)-C(37)	122.2(7)	C(45)-C(44)-C(43)	122.1(7)
N(16)-C(41)-C(46)	106.7(6)	O(12)-C(44)-C(43)	112.9(7)
N(16)-C(41)-C(42)	131.0(6)	C(44)-C(45)-C(46)	116.8(7)
C(46)-C(41)-C(42)	122.3(6)	N(18)-C(46)-C(41)	108.1(6)
C(43)-C(42)-C(41)	116.4(7)	N(18)-C(46)-C(45)	130.9(7)
O(11)-C(43)-C(42)	125.4(7)	C(41)-C(46)-C(45)	121.0(7)

Symmetry operator used to create equivalent atoms is #1: -x, -y, -z.

Table S4 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Zn(1)	0	0	0	32(1)
Zn(2)	-1326(1)	476(1)	842(1)	34(1)
Zn(3)	-751(1)	959(1)	2371(1)	40(1)
Zn(4)	-2181(1)	2267(1)	173(1)	38(1)
Zn(5)	-2318(1)	-1342(1)	805(1)	44(1)
Cl(1)	-2701(1)	3376(2)	-220(1)	58(1)
Cl(2)	-2953(1)	-2424(2)	764(1)	68(1)
Cl(3)	-417(1)	1209(2)	3307(1)	77(1)
N(1)	-1763(3)	2359(4)	1030(3)	39(1)
N(2)	-1449(2)	1685(4)	1298(2)	36(1)
N(3)	-1230(3)	1882(4)	1869(2)	38(1)
N(4)	-2618(3)	1125(4)	187(3)	40(1)
N(5)	-2317(3)	461(4)	469(3)	39(1)
N(6)	-2679(3)	-235(4)	434(3)	39(1)
N(7)	-1889(3)	-969(4)	1614(3)	42(1)
N(8)	-1569(3)	-234(4)	1636(3)	39(1)
N(9)	-1303(3)	-75(4)	2203(3)	40(1)
N(10)	-148(3)	665(4)	1817(2)	40(1)
N(11)	-357(2)	485(4)	1233(2)	36(1)
N(12)	113(2)	325(4)	935(2)	37(1)
N(13)	-1580(3)	-1416(4)	380(3)	41(1)
N(14)	-1196(2)	-734(4)	404(3)	37(1)
N(15)	-728(2)	-899(4)	98(3)	37(1)
N(16)	-1445(2)	1876(4)	-185(2)	38(1)
N(17)	-1124(2)	1197(4)	65(2)	34(1)
N(18)	-647(3)	1029(4)	-229(2)	38(1)
O(1)	-2137(4)	5143(4)	1931(3)	78(2)
O(2)	-1532(3)	4601(4)	2904(3)	64(2)
O(3)	-4721(4)	1118(6)	-911(6)	164(6)

Table S4 (continued)

Atom	x	y	z	U(eq)
O(4)	-4802(4)	-443(6)	-614(5)	141(4)
O(5)	-1352(4)	-1892(6)	3980(3)	102(3)
O(6)	-2010(4)	-2937(4)	3303(3)	82(2)
O(7)	2322(3)	393(8)	1770(3)	123(4)
O(8)	2009(3)	756(9)	2776(3)	152(5)
O(9)	-436(5)	-3541(5)	-1012(5)	131(4)
O(10)	-1397(5)	-4142(5)	-676(5)	147(5)
O(11)	-1019(3)	3544(5)	-1925(3)	95(3)
O(12)	-145(4)	2522(5)	-2015(4)	107(3)
C(1)	-1406(3)	2697(5)	1968(3)	39(2)
C(2)	-1306(3)	3224(5)	2498(3)	45(2)
C(3)	-1566(4)	4023(5)	2443(4)	51(2)
C(4)	-1917(4)	4326(6)	1889(4)	54(2)
C(5)	-2000(4)	3835(5)	1390(3)	49(2)
C(6)	-1740(3)	3005(5)	1439(3)	38(2)
C(7)	-2459(6)	5496(7)	1382(5)	95(4)
C(8)	-1167(5)	4371(6)	3460(4)	65(2)
C(9)	-3186(3)	842(5)	-40(3)	47(2)
C(10)	-3686(4)	1295(7)	-395(5)	79(3)
C(11)	-4213(5)	811(7)	-564(6)	97(4)
C(12)	-4248(4)	-80(8)	-410(6)	95(4)
C(13)	-3772(4)	-510(6)	-71(5)	64(2)
C(14)	-3227(3)	-17(5)	111(3)	44(2)
C(15)	-4693(8)	1977(11)	-1119(11)	243(15)
C(16)	-4874(6)	-1319(9)	-446(10)	168(9)
C(17)	-1455(4)	-729(5)	2554(3)	45(2)
C(18)	-1275(4)	-885(6)	3178(4)	57(2)
C(19)	-1478(5)	-1626(7)	3395(4)	68(3)
C(20)	-1850(5)	-2212(6)	3015(4)	64(3)
C(21)	-2030(4)	-2073(5)	2412(4)	53(2)
C(22)	-1819(3)	-1287(5)	2191(3)	44(2)
C(23)	-981(8)	-1335(12)	4380(6)	146(7)
C(24)	-2290(5)	-3600(7)	2951(5)	77(3)
C(25)	483(3)	618(6)	1887(3)	48(2)
C(26)	923(4)	730(8)	2406(4)	78(3)
C(27)	1520(4)	663(9)	2331(4)	87(4)
C(28)	1698(4)	448(9)	1762(4)	88(4)
C(29)	1269(3)	312(7)	1261(4)	61(3)
C(30)	646(3)	399(5)	1338(3)	44(2)
C(31)	2520(5)	151(15)	1197(5)	175(10)
C(32)	1849(6)	900(15)	3370(5)	180(10)
C(33)	-818(4)	-1705(5)	-126(3)	46(2)
C(34)	-474(4)	-2190(6)	-488(4)	65(3)
C(35)	-698(6)	-2988(7)	-669(5)	91(4)

Table S4 (continued)

Atom	x	y	z	U(eq)
C(36)	-1252(6)	-3327(7)	-462(6)	97(4)
C(37)	-1569(5)	-2872(6)	-104(5)	76(3)
C(38)	-1353(3)	-2036(5)	52(4)	47(2)
C(39)	109(11)	-3193(10)	-1255(11)	222(13)
C(40)	-1929(10)	-4532(10)	-448(10)	214(13)
C(41)	-1169(3)	2151(5)	-658(3)	38(2)
C(42)	-1317(4)	2835(6)	-1064(4)	53(2)
C(43)	-955(4)	2925(6)	-1497(4)	60(2)
C(44)	-449(4)	2344(7)	-1535(4)	64(3)
C(45)	-296(4)	1707(6)	-1133(4)	55(2)
C(46)	-672(3)	1609(5)	-684(3)	41(2)
C(47)	-1511(7)	4147(10)	-1916(6)	142(7)
C(48)	347(8)	1913(11)	-2087(8)	171(9)

Table S5 Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	29(1)	35(1)	32(1)	-1(1)	6(1)	3(1)
Zn(2)	29(1)	36(1)	36(1)	2(1)	6(1)	4(1)
Zn(3)	40(1)	46(1)	34(1)	3(1)	9(1)	9(1)
Zn(4)	35(1)	40(1)	39(1)	6(1)	7(1)	8(1)
Zn(5)	37(1)	39(1)	57(1)	2(1)	14(1)	-2(1)
Cl(1)	62(1)	55(1)	57(1)	18(1)	8(1)	20(1)
Cl(2)	52(1)	47(1)	104(2)	8(1)	10(1)	-12(1)
Cl(3)	104(2)	85(2)	39(1)	-6(1)	1(1)	-3(2)
N(1)	38(3)	40(4)	39(3)	2(3)	8(2)	3(3)
N(2)	35(3)	38(4)	35(3)	7(3)	5(2)	9(3)
N(3)	38(3)	37(4)	38(3)	-1(3)	6(2)	7(3)
N(4)	34(3)	43(4)	43(3)	4(3)	5(3)	4(3)
N(5)	34(3)	41(4)	43(3)	6(3)	9(2)	5(3)
N(6)	32(3)	39(4)	48(3)	3(3)	10(3)	-3(3)
N(7)	41(3)	38(4)	50(4)	7(3)	14(3)	4(3)
N(8)	38(3)	38(4)	41(3)	4(3)	6(3)	3(3)
N(9)	38(3)	44(4)	38(3)	7(3)	10(3)	6(3)
N(10)	34(3)	56(4)	30(3)	2(3)	4(2)	8(3)
N(11)	34(3)	39(4)	36(3)	1(3)	4(2)	3(2)
N(12)	29(3)	46(4)	37(3)	-3(3)	8(2)	4(2)
N(13)	38(3)	38(4)	51(4)	-3(3)	13(3)	-5(3)
N(14)	34(3)	36(4)	41(3)	0(3)	9(2)	-1(2)
N(15)	35(3)	36(4)	43(3)	-2(3)	11(2)	1(3)
N(16)	34(3)	41(4)	38(3)	2(3)	5(2)	9(3)
N(17)	33(3)	34(3)	34(3)	1(2)	6(2)	5(2)
N(18)	36(3)	40(4)	40(3)	6(3)	14(2)	5(3)
O(1)	113(6)	43(4)	70(4)	-9(3)	-15(4)	31(4)

Table S5 (continued)

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(2)	81(4)	51(4)	56(3)	-17(3)	-5(3)	16(3)
O(3)	83(6)	86(7)	280(14)	45(8)	-111(7)	-12(5)
O(4)	62(5)	83(7)	247(12)	24(7)	-73(6)	-24(4)
O(5)	142(7)	111(7)	54(4)	30(4)	21(4)	-29(6)
O(6)	124(6)	54(4)	81(5)	14(4)	58(4)	-6(4)
O(7)	27(3)	281(13)	59(4)	-44(6)	-1(3)	10(5)
O(8)	42(4)	357(17)	49(4)	-66(7)	-14(3)	11(6)
O(9)	173(9)	64(5)	191(9)	-62(6)	136(8)	-42(5)
O(10)	187(10)	70(6)	218(11)	-87(7)	138(9)	-75(6)
O(11)	85(5)	113(6)	99(5)	74(5)	58(4)	58(4)
O(12)	111(6)	118(7)	114(6)	79(5)	84(5)	68(5)
C(1)	37(4)	42(5)	38(4)	0(3)	9(3)	6(3)
C(2)	39(4)	52(5)	46(4)	-3(4)	5(3)	1(3)
C(3)	56(5)	41(5)	53(5)	-10(4)	5(4)	4(4)
C(4)	61(5)	42(5)	58(5)	-1(4)	3(4)	9(4)
C(5)	58(5)	42(5)	44(4)	1(4)	-2(4)	7(4)
C(6)	41(4)	36(4)	38(4)	2(3)	6(3)	2(3)
C(7)	134(10)	48(7)	95(8)	10(6)	-10(7)	38(7)
C(8)	88(7)	58(6)	47(5)	-12(4)	-1(4)	6(5)
C(9)	35(4)	52(5)	52(4)	2(4)	0(3)	0(3)
C(10)	50(5)	53(6)	120(9)	15(6)	-32(5)	0(4)
C(11)	54(6)	65(8)	152(11)	18(7)	-48(6)	-4(5)
C(12)	46(5)	70(8)	153(11)	9(7)	-36(6)	-14(5)
C(13)	43(5)	51(6)	94(7)	6(5)	0(4)	-3(4)
C(14)	34(4)	42(5)	55(4)	3(4)	6(3)	1(3)
C(15)	138(14)	99(13)	420(40)	118(18)	-177(19)	-28(10)
C(16)	78(9)	82(11)	310(20)	38(13)	-60(12)	-37(8)
C(17)	48(4)	46(5)	45(4)	8(4)	19(3)	5(4)
C(18)	61(5)	66(6)	46(5)	14(4)	16(4)	-1(4)
C(19)	89(7)	67(7)	51(5)	13(5)	23(5)	-3(5)
C(20)	83(6)	52(6)	68(6)	16(5)	48(5)	11(5)
C(21)	58(5)	48(5)	59(5)	0(4)	29(4)	0(4)
C(22)	43(4)	40(5)	53(4)	9(4)	23(3)	9(3)
C(23)	176(15)	199(19)	60(8)	47(10)	8(9)	-49(14)
C(24)	98(8)	50(6)	97(8)	9(6)	54(7)	4(6)
C(25)	32(4)	75(6)	37(4)	-1(4)	4(3)	3(4)
C(26)	35(4)	157(11)	39(4)	-24(5)	-1(3)	9(5)
C(27)	44(5)	170(12)	43(5)	-29(6)	-3(4)	3(6)
C(28)	29(4)	182(13)	49(5)	-18(6)	-1(4)	4(6)
C(29)	32(4)	110(8)	41(4)	-12(5)	3(3)	2(4)
C(30)	29(3)	66(6)	36(4)	-4(4)	4(3)	7(3)
C(31)	32(5)	420(30)	76(8)	-45(13)	12(5)	24(10)
C(32)	73(8)	400(30)	54(7)	-74(12)	-26(6)	33(13)
C(33)	52(4)	35(5)	54(4)	-6(4)	18(4)	0(3)

Table S5 (continued)

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(34)	72(6)	44(5)	89(7)	-18(5)	45(5)	-11(4)
C(35)	117(9)	61(7)	116(9)	-41(6)	81(8)	-26(6)
C(36)	121(10)	52(7)	136(10)	-37(7)	74(8)	-36(6)
C(37)	85(7)	45(6)	113(8)	-30(5)	60(6)	-30(5)
C(38)	46(4)	43(5)	56(5)	-8(4)	18(4)	-4(3)
C(39)	310(30)	93(11)	340(30)	-106(14)	290(20)	-82(14)
C(40)	260(20)	97(12)	340(30)	-134(16)	220(20)	-124(14)
C(41)	34(3)	48(5)	35(4)	7(3)	9(3)	2(3)
C(42)	42(4)	62(6)	59(5)	20(4)	19(4)	18(4)
C(43)	57(5)	66(6)	63(5)	35(5)	22(4)	23(4)
C(44)	60(5)	81(7)	61(5)	26(5)	37(4)	27(5)
C(45)	53(5)	57(6)	59(5)	24(4)	25(4)	22(4)
C(46)	39(4)	44(5)	41(4)	9(3)	12(3)	7(3)
C(47)	143(12)	171(15)	134(11)	114(11)	90(10)	120(11)
C(48)	185(15)	174(15)	201(16)	124(13)	173(14)	117(13)

Table S6 Bond lengths (Å) for **2**.

Fe(1)-N(18)	2.005(8)	N(2)-N(3)	1.346(12)	O(3)-C(11)	1.353(16)
Fe(1)-N(18)#1	2.005(8)	N(3)-C(6)	1.372(13)	O(3)-C(15)	1.43(2)
Fe(1)-N(15)#1	2.020(8)	N(4)-C(9)	1.336(15)	O(4)-C(12)	1.357(16)
Fe(1)-N(15)	2.020(8)	N(4)-N(5)	1.365(13)	O(4)-C(16)	1.46(2)
Fe(1)-N(12)	2.026(9)	N(5)-N(6)	1.307(12)	O(5)-C(20)	1.371(15)
Fe(1)-N(12)#1	2.026(9)	N(6)-C(14)	1.357(14)	O(5)-C(24)	1.419(17)
Fe(2)-N(11)	2.125(9)	N(7)-N(8)	1.329(13)	O(6)-C(19)	1.360(15)
Fe(2)-N(17)	2.143(9)	N(7)-C(17)	1.346(15)	O(6)-C(23)	1.443(19)
Fe(2)-N(14)	2.165(9)	N(8)-N(9)	1.334(13)	O(7)-C(28)	1.373(15)
Fe(2)-N(8)	2.182(9)	N(9)-C(22)	1.348(14)	O(7)-C(32)	1.443(18)
Fe(2)-N(5)	2.201(9)	N(10)-N(11)	1.346(12)	O(8)-C(27)	1.363(16)
Fe(2)-N(2)	2.219(8)	N(10)-C(25)	1.356(14)	O(8)-C(31)	1.44(2)
Zn(1)-N(1)	2.019(10)	N(11)-N(12)	1.338(12)	O(9)-C(35)	1.346(14)
Zn(1)-N(6)	2.032(9)	N(12)-C(30)	1.385(14)	O(9)-C(39)	1.455(17)
Zn(1)-N(10)	2.040(9)	N(13)-N(14)	1.348(12)	O(10)-C(36)	1.355(14)
Zn(1)-Cl(1)	2.134(4)	N(13)-C(33)	1.357(13)	O(10)-C(40)	1.436(17)
Zn(2)-N(13)	1.992(9)	N(14)-N(15)	1.321(11)	O(11)-C(43)	1.362(16)
Zn(2)-N(4)	2.014(10)	N(15)-C(38)	1.369(13)	O(11)-C(47)	1.427(17)
Zn(2)-N(7)	2.061(10)	N(16)-N(17)	1.350(12)	O(12)-C(44)	1.351(15)
Zn(2)-Cl(2)	2.148(4)	N(16)-C(41)	1.376(14)	O(12)-C(48)	1.428(17)
Zn(3)-N(3)	1.990(9)	N(17)-N(18)	1.339(11)	C(1)-C(6)	1.362(16)
Zn(3)-N(16)	2.010(9)	N(18)-C(46)	1.375(14)	C(1)-C(2)	1.394(16)
Zn(3)-N(9)	2.018(9)	O(1)-C(3)	1.366(14)	C(2)-C(3)	1.351(17)
Zn(3)-Cl(3)	2.165(4)	O(1)-C(7)	1.417(17)	C(3)-C(4)	1.445(17)
N(1)-N(2)	1.342(12)	O(2)-C(4)	1.370(13)	C(4)-C(5)	1.345(16)
N(1)-C(1)	1.384(14)	O(2)-C(8)	1.418(15)	C(5)-C(6)	1.404(16)

Table S6 (continued)

C(9)-C(10)	1.358(17)	C(20)-C(21)	1.363(17)	C(34)-C(35)	1.350(16)
C(9)-C(14)	1.393(17)	C(21)-C(22)	1.381(16)	C(35)-C(36)	1.447(17)
C(10)-C(11)	1.394(19)	C(25)-C(30)	1.365(15)	C(36)-C(37)	1.346(16)
C(11)-C(12)	1.44(2)	C(25)-C(26)	1.375(17)	C(37)-C(38)	1.389(15)
C(12)-C(13)	1.345(18)	C(26)-C(27)	1.348(18)	C(41)-C(46)	1.378(15)
C(13)-C(14)	1.373(17)	C(27)-C(28)	1.443(19)	C(41)-C(42)	1.383(17)
C(17)-C(22)	1.385(16)	C(28)-C(29)	1.374(17)	C(42)-C(43)	1.367(18)
C(17)-C(18)	1.406(17)	C(29)-C(30)	1.388(16)	C(43)-C(44)	1.416(17)
C(18)-C(19)	1.328(19)	C(33)-C(38)	1.379(15)	C(44)-C(45)	1.365(17)
C(19)-C(20)	1.438(18)	C(33)-C(34)	1.415(16)	C(45)-C(46)	1.404(16)

Symmetry operator used to create equivalent atoms is #1: -x+1, -y, -z.

Table S7 Bond angles (°) for **2**.

N(11)-Fe(2)-N(17)	88.1(3)	N(6)-Zn(1)-N(10)	100.3(4)
N(11)-Fe(2)-N(14)	88.7(3)	N(1)-Zn(1)-Cl(1)	115.9(3)
N(17)-Fe(2)-N(14)	87.6(3)	N(6)-Zn(1)-Cl(1)	121.5(3)
N(11)-Fe(2)-N(8)	178.8(4)	N(10)-Zn(1)-Cl(1)	117.7(3)
N(17)-Fe(2)-N(8)	90.7(4)	N(13)-Zn(2)-N(4)	101.0(4)
N(14)-Fe(2)-N(8)	91.3(3)	N(13)-Zn(2)-N(7)	98.4(4)
N(11)-Fe(2)-N(5)	90.6(4)	N(4)-Zn(2)-N(7)	98.3(4)
N(17)-Fe(2)-N(5)	178.7(4)	N(13)-Zn(2)-Cl(2)	122.5(3)
N(14)-Fe(2)-N(5)	92.6(3)	N(4)-Zn(2)-Cl(2)	120.3(3)
N(8)-Fe(2)-N(5)	90.6(4)	N(7)-Zn(2)-Cl(2)	111.7(3)
N(11)-Fe(2)-N(2)	91.8(3)	N(3)-Zn(3)-N(16)	99.6(4)
N(17)-Fe(2)-N(2)	91.3(3)	N(3)-Zn(3)-N(9)	100.6(4)
N(14)-Fe(2)-N(2)	178.8(4)	N(16)-Zn(3)-N(9)	100.8(4)
N(8)-Fe(2)-N(2)	88.2(3)	N(3)-Zn(3)-Cl(3)	115.9(3)
N(5)-Fe(2)-N(2)	88.5(3)	N(16)-Zn(3)-Cl(3)	116.6(3)
N(18)-Fe(1)-N(18)#1	180	N(9)-Zn(3)-Cl(3)	120.1(3)
N(18)-Fe(1)-N(15)#1	86.4(3)	N(2)-N(1)-C(1)	106.0(9)
N(18)#1-Fe(1)-N(15)#1	93.6(3)	N(2)-N(1)-Zn(1)	118.7(7)
N(18)-Fe(1)-N(15)	93.6(3)	C(1)-N(1)-Zn(1)	135.2(8)
N(18)#1-Fe(1)-N(15)	86.4(3)	N(1)-N(2)-N(3)	111.1(8)
N(15)#1-Fe(1)-N(15)	180	N(1)-N(2)-Fe(2)	123.5(7)
N(18)-Fe(1)-N(12)	93.1(3)	N(3)-N(2)-Fe(2)	124.8(7)
N(18)#1-Fe(1)-N(12)	86.9(3)	N(2)-N(3)-C(6)	106.7(9)
N(15)#1-Fe(1)-N(12)	86.4(3)	N(2)-N(3)-Zn(3)	117.3(6)
N(15)-Fe(1)-N(12)	93.6(3)	C(6)-N(3)-Zn(3)	135.7(8)
N(18)-Fe(1)-N(12)#1	86.9(3)	C(9)-N(4)-N(5)	106.4(9)
N(18)#1-Fe(1)-N(12)#1	93.1(3)	C(9)-N(4)-Zn(2)	134.0(8)
N(15)#1-Fe(1)-N(12)#1	93.6(3)	N(5)-N(4)-Zn(2)	119.4(7)
N(15)-Fe(1)-N(12)#1	86.4(3)	N(6)-N(5)-N(4)	110.8(9)
N(12)-Fe(1)-N(12)#1	180	N(6)-N(5)-Fe(2)	126.7(7)
N(1)-Zn(1)-N(6)	98.8(4)	N(4)-N(5)-Fe(2)	122.5(7)
N(1)-Zn(1)-N(10)	98.5(4)	N(5)-N(6)-C(14)	107.9(9)

Table S7 (continued)

N(5)-N(6)-Zn(1)	116.7(7)	C(27)-O(8)-C(31)	115.8(12)
C(14)-N(6)-Zn(1)	135.0(8)	C(35)-O(9)-C(39)	115.5(10)
N(8)-N(7)-C(17)	107.4(9)	C(36)-O(10)-C(40)	116.1(10)
N(8)-N(7)-Zn(2)	119.6(7)	C(43)-O(11)-C(47)	116.0(11)
C(17)-N(7)-Zn(2)	133.0(8)	C(44)-O(12)-C(48)	116.0(11)
N(7)-N(8)-N(9)	110.1(8)	C(6)-C(1)-N(1)	108.3(9)
N(7)-N(8)-Fe(2)	123.0(7)	C(6)-C(1)-C(2)	122.9(11)
N(9)-N(8)-Fe(2)	126.9(7)	N(1)-C(1)-C(2)	128.8(11)
N(8)-N(9)-C(22)	108.0(9)	C(3)-C(2)-C(1)	116.1(12)
N(8)-N(9)-Zn(3)	115.9(7)	C(2)-C(3)-O(1)	125.3(12)
C(22)-N(9)-Zn(3)	136.0(8)	C(2)-C(3)-C(4)	121.5(11)
N(11)-N(10)-C(25)	107.7(8)	O(1)-C(3)-C(4)	113.3(10)
N(11)-N(10)-Zn(1)	119.2(7)	C(5)-C(4)-O(2)	125.7(11)
C(25)-N(10)-Zn(1)	133.0(8)	C(5)-C(4)-C(3)	121.3(11)
N(12)-N(11)-N(10)	110.4(8)	O(2)-C(4)-C(3)	113.0(10)
N(12)-N(11)-Fe(2)	125.0(7)	C(4)-C(5)-C(6)	116.8(11)
N(10)-N(11)-Fe(2)	124.5(6)	C(1)-C(6)-N(3)	107.8(10)
N(11)-N(12)-C(30)	106.2(8)	C(1)-C(6)-C(5)	121.4(10)
N(11)-N(12)-Fe(1)	124.4(7)	N(3)-C(6)-C(5)	130.7(11)
C(30)-N(12)-Fe(1)	129.4(7)	N(4)-C(9)-C(10)	129.6(12)
N(14)-N(13)-C(33)	106.8(8)	N(4)-C(9)-C(14)	108.1(10)
N(14)-N(13)-Zn(2)	119.6(7)	C(10)-C(9)-C(14)	122.3(12)
C(33)-N(13)-Zn(2)	133.6(8)	C(9)-C(10)-C(11)	116.8(13)
N(15)-N(14)-N(13)	110.4(8)	O(3)-C(11)-C(10)	125.4(14)
N(15)-N(14)-Fe(2)	125.8(7)	O(3)-C(11)-C(12)	114.2(12)
N(13)-N(14)-Fe(2)	123.8(7)	C(10)-C(11)-C(12)	120.4(13)
N(14)-N(15)-C(38)	108.0(8)	O(4)-C(12)-C(13)	126.6(13)
N(14)-N(15)-Fe(1)	123.5(6)	O(4)-C(12)-C(11)	112.6(12)
C(38)-N(15)-Fe(1)	128.5(7)	C(13)-C(12)-C(11)	120.8(13)
N(17)-N(16)-C(41)	107.2(8)	C(12)-C(13)-C(14)	118.2(13)
N(17)-N(16)-Zn(3)	119.6(7)	N(6)-C(14)-C(9)	106.8(11)
C(41)-N(16)-Zn(3)	133.2(7)	N(6)-C(14)-C(13)	131.7(12)
N(18)-N(17)-N(16)	111.0(8)	C(9)-C(14)-C(13)	121.4(12)
N(18)-N(17)-Fe(2)	125.4(7)	N(7)-C(17)-C(22)	107.9(10)
N(16)-N(17)-Fe(2)	123.6(6)	N(7)-C(17)-C(18)	130.3(11)
N(17)-N(18)-C(46)	106.3(8)	C(22)-C(17)-C(18)	121.8(11)
N(17)-N(18)-Fe(1)	124.0(7)	C(19)-C(18)-C(17)	116.5(12)
C(46)-N(18)-Fe(1)	129.7(7)	C(18)-C(19)-O(6)	124.6(13)
C(3)-O(1)-C(7)	114.9(10)	C(18)-C(19)-C(20)	121.8(12)
C(4)-O(2)-C(8)	116.3(10)	O(6)-C(19)-C(20)	113.6(12)
C(11)-O(3)-C(15)	117.2(12)	C(21)-C(20)-O(5)	124.8(11)
C(12)-O(4)-C(16)	115.5(12)	C(21)-C(20)-C(19)	122.0(12)
C(20)-O(5)-C(24)	114.9(10)	O(5)-C(20)-C(19)	113.1(11)
C(19)-O(6)-C(23)	115.0(12)	C(20)-C(21)-C(22)	115.9(11)
C(28)-O(7)-C(32)	117.2(11)	N(9)-C(22)-C(17)	106.6(10)

Table S7 (continued)

N(9)-C(22)-C(21)	131.4(11)	C(34)-C(35)-C(36)	121.6(11)
C(17)-C(22)-C(21)	122.0(11)	C(37)-C(36)-O(10)	125.3(11)
N(10)-C(25)-C(30)	107.5(10)	C(37)-C(36)-C(35)	121.0(11)
N(10)-C(25)-C(26)	130.0(11)	O(10)-C(36)-C(35)	113.7(10)
C(30)-C(25)-C(26)	122.5(10)	C(36)-C(37)-C(38)	118.2(11)
C(27)-C(26)-C(25)	118.0(12)	N(15)-C(38)-C(33)	106.6(9)
C(26)-C(27)-O(8)	126.0(13)	N(15)-C(38)-C(37)	132.8(10)
C(26)-C(27)-C(28)	120.0(13)	C(33)-C(38)-C(37)	120.6(10)
O(8)-C(27)-C(28)	114.0(12)	N(16)-C(41)-C(46)	106.8(10)
C(29)-C(28)-O(7)	124.4(12)	N(16)-C(41)-C(42)	129.2(10)
C(29)-C(28)-C(27)	121.3(12)	C(46)-C(41)-C(42)	124.0(11)
O(7)-C(28)-C(27)	114.3(12)	C(43)-C(42)-C(41)	115.1(11)
C(28)-C(29)-C(30)	116.5(11)	O(11)-C(43)-C(42)	123.3(12)
C(25)-C(30)-N(12)	108.1(9)	O(11)-C(43)-C(44)	114.1(12)
C(25)-C(30)-C(29)	121.6(11)	C(42)-C(43)-C(44)	122.7(12)
N(12)-C(30)-C(29)	130.3(11)	O(12)-C(44)-C(45)	125.1(11)
N(13)-C(33)-C(38)	108.1(9)	O(12)-C(44)-C(43)	114.0(12)
N(13)-C(33)-C(34)	129.3(10)	C(45)-C(44)-C(43)	120.8(12)
C(38)-C(33)-C(34)	122.6(10)	C(44)-C(45)-C(46)	117.3(11)
C(35)-C(34)-C(33)	116.0(11)	N(18)-C(46)-C(41)	108.7(9)
O(9)-C(35)-C(34)	125.4(11)	N(18)-C(46)-C(45)	131.4(10)
O(9)-C(35)-C(36)	113.0(10)	C(41)-C(46)-C(45)	119.9(11)

Symmetry operator used to create equivalent atoms is #1: -x+1, -y, -z.

Table S8 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Fe(2)	3783(1)	427(1)	707(1)	23(1)
Fe(1)	5000	0	0	25(1)
Zn(1)	3712(1)	-1373(1)	1438(1)	42(1)
Zn(2)	4464(1)	2188(1)	1501(1)	44(1)
Zn(3)	2044(1)	861(1)	-150(1)	36(1)
Cl(1)	3648(3)	-2502(3)	1835(2)	90(1)
Cl(2)	4743(2)	3328(3)	1940(2)	77(1)
Cl(3)	985(2)	1072(3)	-702(1)	62(1)
N(1)	2790(5)	-1000(6)	901(3)	34(2)
N(2)	2792(5)	-285(6)	645(4)	34(2)
N(3)	2136(5)	-127(6)	304(4)	33(2)
N(4)	4352(5)	1085(6)	1824(4)	41(2)
N(5)	4081(5)	394(6)	1528(4)	38(2)
N(6)	4008(5)	-247(6)	1799(4)	34(2)
N(7)	3446(5)	2258(6)	969(4)	38(2)

Table S8 (continued)

Atom	x	y	z	U(eq)
N(8)	3182(5)	1599(6)	670(4)	38(2)
N(9)	2522(5)	1774(6)	353(3)	35(2)
N(10)	4357(5)	-1391(6)	1014(4)	37(2)
N(11)	4362(4)	-715(6)	726(3)	30(2)
N(12)	4805(5)	-852(6)	471(3)	32(2)
N(13)	4989(5)	1802(6)	1057(4)	37(2)
N(14)	4740(5)	1131(6)	751(3)	33(2)
N(15)	5165(4)	968(5)	494(3)	28(2)
N(16)	2832(5)	583(6)	-417(3)	34(2)
N(17)	3503(5)	429(6)	-93(3)	31(2)
N(18)	3955(4)	270(5)	-339(3)	28(2)
O(1)	772(4)	-2966(5)	592(4)	59(3)
O(2)	10(4)	-1958(5)	-68(4)	52(2)
O(3)	4993(8)	1228(7)	3633(4)	90(4)
O(4)	4523(7)	-262(7)	3608(4)	82(4)
O(5)	1216(5)	4432(6)	251(4)	66(3)
O(6)	2292(6)	4977(7)	960(5)	96(4)
O(7)	6234(7)	-3438(6)	554(5)	89(4)
O(8)	5680(8)	-4042(7)	1173(6)	109(5)
O(9)	7145(5)	3453(6)	1248(4)	77(4)
O(10)	7353(5)	2520(7)	593(4)	82(4)
O(11)	2039(5)	622(9)	-2242(3)	95(4)
O(12)	3319(5)	325(9)	-2172(3)	83(4)
C(1)	2100(6)	-1323(7)	700(5)	35(3)
C(2)	1827(6)	-2078(8)	816(5)	42(3)
C(3)	1134(6)	-2253(8)	545(5)	46(3)
C(4)	697(6)	-1672(8)	168(5)	38(3)
C(5)	972(6)	-945(7)	63(5)	37(3)
C(6)	1697(6)	-777(7)	341(4)	32(3)
C(7)	1207(8)	-3610(10)	898(8)	96(7)
C(8)	-449(7)	-1426(10)	-448(5)	62(4)
C(9)	4440(6)	853(8)	2293(4)	39(3)
C(10)	4713(8)	1300(9)	2727(5)	56(4)
C(11)	4751(9)	883(10)	3168(5)	64(4)
C(12)	4489(8)	27(9)	3151(5)	57(4)
C(13)	4237(7)	-399(9)	2714(5)	50(3)
C(14)	4229(6)	8(8)	2285(5)	40(3)
C(15)	5235(15)	2089(12)	3675(7)	126(9)
C(16)	4178(13)	-1077(12)	3608(7)	104(7)
C(17)	2943(6)	2873(7)	839(5)	39(3)
C(18)	2956(7)	3695(8)	1034(5)	52(4)
C(19)	2374(8)	4167(9)	823(6)	63(4)
C(20)	1756(6)	3846(8)	426(5)	48(3)
C(21)	1746(6)	3054(7)	231(5)	39(3)

Table S8 (continued)

Atom	x	y	z	U(eq)
C(22)	2355(6)	2569(7)	450(4)	34(3)
C(23)	2898(12)	5313(13)	1364(11)	187(16)
C(24)	632(8)	4176(10)	-180(7)	84(6)
C(25)	4799(6)	-1987(7)	935(4)	35(3)
C(26)	4962(8)	-2789(9)	1133(6)	60(4)
C(27)	5452(9)	-3243(9)	1010(6)	66(4)
C(28)	5752(8)	-2908(9)	654(6)	60(4)
C(29)	5566(7)	-2117(8)	446(5)	46(3)
C(30)	5084(6)	-1659(7)	602(4)	34(3)
C(31)	5392(17)	-4402(15)	1529(12)	192(17)
C(32)	6605(13)	-3112(12)	237(10)	140(11)
C(33)	5594(6)	2070(7)	983(4)	35(3)
C(34)	6063(7)	2744(8)	1217(5)	47(3)
C(35)	6632(7)	2858(8)	1069(5)	51(4)
C(36)	6757(7)	2314(9)	698(5)	51(4)
C(37)	6301(6)	1677(8)	482(5)	40(3)
C(38)	5713(6)	1548(7)	631(4)	31(3)
C(39)	7078(9)	3979(13)	1650(8)	112(8)
C(40)	7470(10)	2046(14)	197(9)	132(10)
C(41)	2857(6)	531(8)	-893(4)	40(3)
C(42)	2307(7)	627(9)	-1351(5)	54(4)
C(43)	2507(7)	544(11)	-1762(5)	64(4)
C(44)	3224(7)	370(10)	-1725(5)	57(4)
C(45)	3749(6)	246(9)	-1269(5)	46(3)
C(46)	3557(6)	342(7)	-841(4)	34(3)
C(47)	1304(8)	758(17)	-2299(6)	120(9)
C(48)	4042(9)	209(17)	-2152(6)	119(9)

Table S9 Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(2)	19(1)	25(1)	23(1)	-4(1)	7(1)	-2(1)
Fe(1)	22(1)	28(1)	24(1)	-4(1)	7(1)	-3(1)
Zn(1)	40(1)	43(1)	45(1)	-6(1)	16(1)	-7(1)
Zn(2)	45(1)	43(1)	49(1)	-9(1)	23(1)	-6(1)
Zn(3)	28(1)	38(1)	40(1)	-3(1)	10(1)	-2(1)
Cl(1)	109(3)	74(3)	93(3)	30(3)	42(3)	-6(3)
Cl(2)	64(2)	69(3)	84(3)	-39(2)	10(2)	-14(2)
Cl(3)	34(2)	81(3)	58(2)	9(2)	0(2)	8(2)
N(1)	34(5)	40(6)	31(6)	0(5)	14(4)	-6(4)
N(2)	33(5)	34(6)	35(6)	-4(5)	11(5)	-12(4)
N(3)	26(5)	33(5)	40(6)	1(4)	11(5)	0(4)
N(4)	41(6)	45(6)	37(6)	-12(5)	12(5)	-5(5)

Table S9 (continued)

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(5)	35(5)	44(6)	33(6)	-7(5)	11(5)	-4(5)
N(6)	33(5)	35(6)	38(6)	2(5)	16(5)	-7(4)
N(7)	34(5)	35(6)	45(6)	-14(5)	12(5)	-7(5)
N(8)	34(5)	34(6)	46(6)	-3(5)	16(5)	4(4)
N(9)	29(5)	34(6)	33(6)	-4(5)	2(4)	-1(4)
N(10)	46(6)	30(5)	38(6)	4(5)	17(5)	-1(5)
N(11)	25(5)	37(5)	29(5)	-6(4)	10(4)	-1(4)
N(12)	26(5)	32(5)	35(6)	-3(4)	7(4)	-5(4)
N(13)	30(5)	44(6)	36(6)	-8(5)	11(5)	-1(4)
N(14)	32(5)	31(5)	33(6)	-6(4)	6(4)	-10(4)
N(15)	27(5)	34(5)	25(5)	-5(4)	12(4)	-3(4)
N(16)	25(5)	41(6)	33(6)	-1(5)	5(4)	-4(4)
N(17)	27(5)	39(5)	27(5)	-5(4)	9(4)	1(4)
N(18)	26(5)	30(5)	25(5)	-7(4)	4(4)	-3(4)
O(1)	38(5)	37(5)	90(8)	16(5)	6(5)	-12(4)
O(2)	25(4)	50(5)	72(7)	11(5)	7(4)	-7(4)
O(3)	165(12)	65(7)	31(6)	-14(5)	21(7)	-24(7)
O(4)	148(11)	67(7)	40(6)	-7(5)	43(7)	-18(7)
O(5)	41(5)	53(6)	85(8)	-22(5)	-1(5)	13(4)
O(6)	70(7)	51(6)	123(11)	-41(7)	-22(7)	15(5)
O(7)	119(10)	51(6)	137(11)	34(7)	94(9)	40(6)
O(8)	154(12)	63(7)	161(13)	58(8)	118(11)	62(8)
O(9)	61(6)	77(7)	114(9)	-61(7)	55(6)	-45(6)
O(10)	68(7)	94(8)	110(9)	-68(7)	66(7)	-59(6)
O(11)	54(6)	198(14)	21(5)	10(7)	-1(5)	47(8)
O(12)	50(6)	167(12)	30(5)	6(6)	13(5)	31(7)
C(1)	30(6)	33(6)	45(8)	-1(6)	16(6)	-8(5)
C(2)	31(6)	39(7)	52(8)	8(6)	10(6)	-2(6)
C(3)	36(7)	42(8)	58(9)	1(7)	13(7)	-4(6)
C(4)	23(6)	44(7)	44(8)	0(6)	9(6)	-4(5)
C(5)	33(6)	37(7)	42(8)	-4(6)	14(6)	-3(5)
C(6)	34(6)	32(6)	34(7)	-7(5)	18(6)	-8(5)
C(7)	57(10)	51(10)	142(18)	38(11)	-12(10)	-21(8)
C(8)	40(8)	73(10)	60(10)	15(8)	3(7)	0(7)
C(9)	46(7)	48(8)	23(7)	-16(6)	13(6)	-8(6)
C(10)	70(9)	46(8)	54(10)	-6(7)	25(8)	-12(7)
C(11)	93(12)	63(10)	34(9)	-10(8)	22(8)	-3(9)
C(12)	81(10)	58(9)	36(9)	-6(7)	26(8)	-6(8)
C(13)	54(8)	60(9)	37(8)	-1(7)	17(7)	4(7)
C(14)	39(7)	47(8)	32(8)	-9(6)	10(6)	0(6)
C(15)	230(30)	88(15)	48(11)	-30(10)	36(14)	-61(16)
C(16)	180(20)	93(14)	55(11)	12(10)	58(13)	-23(14)
C(17)	37(7)	37(7)	45(8)	-8(6)	16(6)	0(6)
C(18)	35(7)	50(8)	59(9)	-26(7)	1(6)	-3(6)

Table S9 (continued)

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(19)	55(9)	50(9)	72(11)	-36(8)	6(8)	4(7)
C(20)	35(7)	45(8)	53(9)	-7(7)	0(6)	3(6)
C(21)	38(7)	36(7)	40(8)	3(6)	9(6)	-5(6)
C(22)	29(6)	33(7)	40(7)	-8(6)	13(6)	-3(5)
C(23)	111(17)	92(16)	240(30)	-116(19)	-92(18)	38(13)
C(24)	59(10)	62(10)	98(14)	-14(10)	-16(9)	23(8)
C(25)	34(6)	32(7)	43(7)	4(6)	18(6)	7(5)
C(26)	67(9)	49(8)	83(11)	11(8)	52(9)	8(7)
C(27)	87(11)	37(8)	90(12)	9(8)	53(10)	17(8)
C(28)	62(9)	51(9)	83(11)	8(8)	46(9)	14(7)
C(29)	52(8)	38(7)	46(8)	10(6)	16(7)	8(6)
C(30)	34(6)	30(6)	39(7)	-5(5)	13(6)	3(5)
C(31)	300(40)	116(18)	280(40)	140(20)	240(30)	130(20)
C(32)	190(20)	75(13)	240(30)	56(16)	180(20)	65(14)
C(33)	28(6)	40(7)	34(7)	-8(6)	7(5)	-11(5)
C(34)	55(8)	41(7)	52(8)	-19(6)	26(7)	-15(6)
C(35)	42(7)	55(8)	65(9)	-30(7)	27(7)	-25(7)
C(36)	38(7)	62(9)	57(9)	-26(7)	21(7)	-14(7)
C(37)	38(7)	42(7)	41(8)	-16(6)	16(6)	-10(6)
C(38)	27(6)	28(6)	40(7)	-4(5)	12(5)	-7(5)
C(39)	81(12)	125(16)	151(19)	-110(15)	68(13)	-69(12)
C(40)	104(15)	160(20)	190(20)	-121(18)	125(17)	-88(14)
C(41)	32(6)	54(8)	32(7)	-5(6)	11(6)	3(6)
C(42)	38(7)	86(11)	30(7)	0(7)	3(6)	19(7)
C(43)	35(7)	115(13)	37(8)	1(8)	6(6)	20(8)
C(44)	39(7)	96(11)	36(8)	8(8)	10(6)	11(7)
C(45)	30(6)	67(9)	35(8)	-5(7)	4(6)	-3(6)
C(46)	34(6)	39(7)	30(7)	-6(5)	14(6)	-8(5)
C(47)	45(10)	240(30)	46(10)	-13(14)	-15(8)	55(13)
C(48)	62(11)	250(30)	47(10)	26(14)	25(9)	50(14)