Electronic Supporting Information

Anion-directed assembly of a non-interpenetrated square-grid metal–organic framework with nanoscale porosity

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Experimental Section

Self-assembly of a non-interpenetrated square grid metal–organic framework $[Zn(DPNDI)_2(DMAc)_2.2ClO_4]_n$ (DPNDI = *N,N′*-di(4-pyridyl)-1,4,5,8-naphthalenediimide). A solution of $Zn(ClO_4)_2.6H_2O$ (48 mg, 0.13 mmol) and DPNDI (110 mg, 0.26 mmol) in 1:2 DMAc/MeCN mixture (40 mL) was allowed to stand at room temperature for 24 h. After that MeCN was evaporated under reduced pressure at 25 °C and small portions (5 mL each) of concentrated DMAc solutions were setup for crystallization. Upon slow Et_2O vapor diffusion into DMAc solutions, pale yellow crystals were obtained, which were used for crystallographic and thermogravimetric studies.

As-synthesized crystalline MOF was suspended in fresh Et_2O and washed (centrifugation) three times with Et_2O to exchange entrapped DMAc, MeCN, and H_2O solvents that have higher boiling points. Et_2O was easily removed under reduced pressure to obtain evacuated bulk materials as a microcrystalline off-white powder (37 mg, 11%). This material was analyzed by powder X-ray diffraction (Fig. S1).

Self-assembly of a 1D linear coordination polymer $[Zn(DPNDI)_2(DMAc)(NO_3)_2]_n$. A solution of $Zn(NO_3)_2.6H_2O$ (39 mg, 0.13 mmol) and DPNDI (110 mg, 0.26 mmol) in 2:1 DMAc/MeCN (40 mL) was allowed to stand at room temperature for 24 h. After that MeCN was evaporated under reduced pressure at 25 °C and small portions (5 mL each) of concentrated DMAc solutions were setup for crystallization. Upon slow Et_2O vapor diffusion into the DMAc solutions, yellowish white crystals were obtained (50 mg, 25%), which were used for crystallographic analysis.

Crystallographic data collection and refinement. Suitable single crystals of the square-grid MOF and 1D coordination polymer were mounted on a goniometer head of a Bruker SMART APEX II diffractometer using a nylon loop with a small amount of Paratone oil (Hampton Research). Crystals were cooled to 153 K in a cold stream of N_2 gas. After finding a crystal that indexed to give a satisfactory unit cell, a full low-temperature data set at 173 K was recorded using a sample-to-detector distance of 6 cm. Diffraction data of the compound was measured with Mo Kα (λ = 0.71073 Å) radiation. Reflections were found at $\theta = 20°$ ($\mathrm{Sin}\theta_{max}$/wavelength = 0.504 < 0.550 caused an A-level alert) for the square-grid MOF crystal and at ca. 28° for the 1D coordination polymer. The Bruker suite of programs on the APEX II was used to integrate the data and SADABS was used for absorption corrections.[S1,S2] Both structures were readily solved by direct methods and refined using the SHELXTL.[S3] The non-interpenetrated square-grid MOF crystal has very large pores (ca. 20 x 20 Å) containing disordered solvent molecules, which contributed to an A-level alert. SQUEEZE routine implemented on PLATON was used to remove electron densities corresponding to disordered solvent molecules. All atoms of the complex backbones (Zn(II), DPNDI ligands, Zn(II)-coordinated DMAc and NO_3^- ions, and ClO_4^- anions were fully accounted for. Crystallographic data has been deposited at the Cambridge Crystallographic Data Center with reference numbers CCDC 929885 and 929886. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif.

Powder X-ray crystal diffraction (PXRD) analysis. PXRD analysis of the square-grid MOF was conducted on Siemens D500 powder diffractometer using Ni-filtered unmonochromated Cu Kα radiation with a graphite diffracted beam monochromater. One degree divergence apertures and 0.15 degree

receiving aperture. Scanning was done between 5θ and 65 θ, at 0.02 steps, 0.5 °/min. Samples were dispersed on quartz zero-background holder. Data were processed using MDI Jade 6.5 software.

Thermogravimetric analysis (TGA). TGA of an air-dried ground sample of square-grid MOF was conduced on a Thermogravimetric Analyzer Instrument Q50 with a heating rate of 10 °C/min under an Ar-atmosphere. The initial 8% weight loss at 20–100 °C corresponds to loss of volatile solvents (Et_2O, MeCN), the next 17% loss at 100–200 °C corresponds to loss of H_2O (came from $Zn(ClO_4)_2.6H_2O$) and DMAc molecules. The MOF showed excellent thermal stability between 200 and 350 °C, indicating no network collapse upon solvent evaporation. A sharp 15% weight loss from 65 to 50% occurred at 350–400 °C. Over 45% weight was lost by 500 °C.

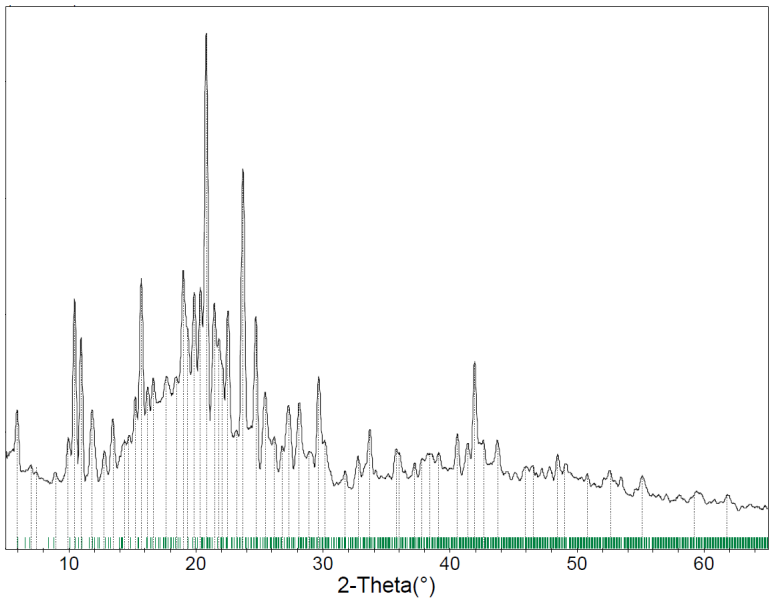

Fig. S1. The PXRD pattern of solvent exchanged and evacuated non-interpenetrated square grid MOF. Green bars represent simulated peaks obtained from single crystal analysis of the as-synthesized crystalline MOF.

References.

S1 *SMART and SAINT*, Bruker AXS Inc., Madison, WI, USA, 2007.65.

S2 *SADABS*, Bruker AXS Inc., Madison, WI, USA, 2001.

S3 G. M. Sheldrick, *Shelxs97* and *Shelxl97*, Programs for Crystallographic Solution and Refinement. *Acta Crystallogr.*, 2008, **A64**, 112.

Bond lengths and angles of Zn(II) coordination spheres in the square-grid MOF and 1D polymer:

MOF: **Bond angles (°)**	
O1-Zn-O2	180
N1-Zn-N4	180
N2-Zn-N3	180
O1-Zn-N1	93.02
O1-Zn-N2	91.82
O1-Zn-N3	88.18
O1-Zn-N4	86.98
N1-Zn-N2	92.90
N2-Zn-N4	87.10
N3-Zn-N4	92.90
N1-Zn-N3	87.10
O2-Zn-N1	86.98
O2-Zn-N2	88.18
O2-Zn-N3	91.82
O2-Zn-N4	93.02
Bond Distances (Å)	
Zn-O1	2.112
Zn-O2	2.112
Zn-N1	2.159
Zn-N2	2.213
Zn-N3	2.213
Zn-N4	2.159

1D Coordination polymer: **Bond Angles (°)**	
N1-Zn-N2	151.99
N1-Zn-O1	110.14
N1-Zn-O2	91.17
N1-Zn-O3	94.09
N1-Zn-O4	80.52
N2-Zn-O1	110.14
N2-Zn-O2	90.32
N2-Zn-O3	90.76
N2-Zn-O4	80.33
O1-Zn-O2	79.26
O1-Zn-O3	87.46
O2-Zn-O3	166.71
O2-Zn-O4	139.64
O1-Zn-O4	140.67
O3-Zn-O4	53.49
Bond Distances (Å)	
Zn-N1	2.084
Zn-N2	2.097
Zn-O1	2.050
Zn-O2	2.141
Zn-O3	2.179
Zn-O4	2.563

Bond lengths and bond angles of square-grid MOF:

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for the square-grid MOF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(41)	1832(4)	157(2)	12180(3)	68(2)
O(41)	964(2)	26(1)	11000(2)	34(1)
Zn(1)	0	0	10000	26(1)
C(1)	1341(3)	498(2)	9566(3)	45(2)
C(2)	1727(3)	828(2)	9219(3)	50(2)
C(3)	1304(3)	1178(2)	8711(3)	33(1)
C(4)	530(3)	1194(2)	8562(3)	36(1)
C(5)	192(3)	856(2)	8942(3)	32(1)
C(6)	1781(3)	1391(2)	7598(3)	38(1)
C(7)	2198(3)	1740(2)	7233(3)	34(1)
C(8)	2483(3)	2187(2)	7625(3)	31(1)
C(9)	2383(3)	2303(2)	8369(3)	43(1)
C(10)	1972(3)	1954(2)	8752(3)	48(2)
C(11)	2669(4)	2733(2)	8745(3)	62(2)
C(12)	3034(3)	3076(2)	8376(3)	55(2)
C(13)	3122(3)	2975(2)	7643(3)	36(1)
C(14)	2859(3)	2527(2)	7261(3)	31(1)
C(15)	2961(3)	2410(2)	6518(3)	38(1)
C(16)	2714(3)	1964(2)	6158(3)	53(2)
C(17)	2323(4)	1630(2)	6512(3)	57(2)
C(18)	3338(3)	2771(2)	6116(3)	40(1)
C(19)	3472(3)	3352(2)	7241(3)	37(1)
C(20)	3869(3)	3592(2)	6097(3)	31(1)
C(21)	3411(3)	3885(2)	5525(3)	36(1)
C(22)	4642(3)	3652(2)	6302(3)	41(1)
C(23)	4930(3)	4031(2)	5939(3)	36(1)
C(24)	3761(3)	4249(2)	5192(3)	40(1)
N(1)	596(2)	506(1)	9436(2)	31(1)
N(2)	1684(2)	1527(1)	8325(2)	36(1)
N(3)	3533(2)	3226(1)	6488(2)	33(1)
N(4)	4499(2)	4340(1)	5405(2)	29(1)
O(1)	1516(2)	1004(1)	7291(2)	54(1)
O(2)	1863(3)	2027(1)	9385(2)	73(1)
O(3)	3693(2)	3751(1)	7534(2)	48(1)
O(4)	3465(2)	2692(1)	5492(2)	59(1)
C(41)	1178(4)	60(2)	11737(5)	57(2)
C(42)	658(8)	75(3)	12302(9)	177(6)
C(43)	2073(5)	179(3)	13022(4)	106(3)
C(44)	2435(6)	234(6)	11783(7)	218(8)
Cl(31)	1569(1)	4520(1)	4612(2)	137(1)
O(31)	1430(8)	4229(5)	5236(8)	389(9)
O(32)	1895(5)	4224(4)	4186(5)	256(6)
O(33)	918(4)	4711(3)	4150(7)	278(6)
O(34)	2086(3)	4877(2)	4983(4)	127(2)

Table 2. Bond lengths (Å) and angles (°) of the square-grid MOF.

N(41)-C(41)	1.258(8)
N(41)-C(43)	1.422(8)
N(41)-C(44)	1.480(11)
O(41)-C(41)	1.246(7)
O(41)-Zn(1)	2.112(3)
Zn(1)-O(41)#1	2.112(4)
Zn(1)-N(1)	2.159(3)
Zn(1)-N(1)#1	2.159(3)
Zn(1)-N(4)#2	2.213(4)
Zn(1)-N(4)#3	2.213(4)
C(1)-N(1)	1.320(6)
C(1)-C(2)	1.383(7)
C(1)-H(1)	0.9500
C(2)-C(3)	1.377(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.370(7)
C(3)-N(2)	1.451(6)
C(4)-C(5)	1.380(6)
C(4)-H(4)	0.9500
C(5)-N(1)	1.353(6)
C(5)-H(5)	0.9500
C(6)-O(1)	1.212(6)
C(6)-N(2)	1.388(6)
C(6)-C(7)	1.473(7)
C(7)-C(17)	1.382(7)
C(7)-C(8)	1.414(6)
C(8)-C(9)	1.406(6)
C(8)-C(14)	1.407(6)
C(9)-C(11)	1.365(7)
C(9)-C(10)	1.484(7)
C(10)-O(2)	1.201(6)
C(10)-N(2)	1.395(6)
C(11)-C(12)	1.403(7)
C(11)-H(11)	0.9500
C(12)-C(13)	1.370(7)
C(12)-H(12)	0.9500
C(13)-C(14)	1.402(6)
C(13)-C(19)	1.484(7)
C(14)-C(15)	1.407(6)
C(15)-C(16)	1.375(7)
C(15)-C(18)	1.485(7)
C(16)-C(17)	1.404(7)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-O(4)	1.203(5)
C(18)-N(3)	1.389(6)
C(19)-O(3)	1.214(6)
C(19)-N(3)	1.402(6)
C(20)-C(21)	1.365(7)

C(20)-C(22)	1.371(7)
C(20)-N(3)	1.439(6)
C(21)-C(24)	1.389(7)
C(21)-H(21)	0.9500
C(22)-C(23)	1.388(7)
C(22)-H(22)	0.9500
C(23)-N(4)	1.335(6)
C(23)-H(23)	0.9500
C(24)-N(4)	1.323(6)
C(24)-H(24)	0.9500
N(4)-Zn(1)#4	2.213(4)
C(41)-C(42)	1.561(12)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
Cl(31)-O(33)	1.342(7)
Cl(31)-O(32)	1.346(6)
Cl(31)-O(34)	1.381(5)
Cl(31)-O(31)	1.431(9)
C(41)-N(41)-C(43)	127.9(7)
C(41)-N(41)-C(44)	116.5(6)
C(43)-N(41)-C(44)	115.5(7)
C(41)-O(41)-Zn(1)	144.2(4)
O(41)-Zn(1)-O(41)#1	179.997(1)
O(41)-Zn(1)-N(1)	86.98(14)
O(41)#1-Zn(1)-N(1)	93.02(14)
O(41)-Zn(1)-N(1)#1	93.02(14)
O(41)#1-Zn(1)-N(1)#1	86.98(14)
N(1)-Zn(1)-N(1)#1	179.999(1)
O(41)-Zn(1)-N(4)#2	91.79(13)
O(41)#1-Zn(1)-N(4)#2	88.20(13)
N(1)-Zn(1)-N(4)#2	87.10(13)
N(1)#1-Zn(1)-N(4)#2	92.90(13)
O(41)-Zn(1)-N(4)#3	88.21(13)
O(41)#1-Zn(1)-N(4)#3	91.80(13)
N(1)-Zn(1)-N(4)#3	92.90(13)
N(1)#1-Zn(1)-N(4)#3	87.10(13)
N(4)#2-Zn(1)-N(4)#3	180.000(1)
N(1)-C(1)-C(2)	123.2(5)
N(1)-C(1)-H(1)	118.4
C(2)-C(1)-H(1)	118.4
C(3)-C(2)-C(1)	117.6(5)
C(3)-C(2)-H(2)	121.2
C(1)-C(2)-H(2)	121.2
C(4)-C(3)-C(2)	120.6(4)

C(4)-C(3)-N(2)	120.0(4)
C(2)-C(3)-N(2)	119.4(4)
C(3)-C(4)-C(5)	118.1(5)
C(3)-C(4)-H(4)	120.9
C(5)-C(4)-H(4)	120.9
N(1)-C(5)-C(4)	122.2(4)
N(1)-C(5)-H(5)	118.9
C(4)-C(5)-H(5)	118.9
O(1)-C(6)-N(2)	120.0(4)
O(1)-C(6)-C(7)	123.3(4)
N(2)-C(6)-C(7)	116.8(4)
C(17)-C(7)-C(8)	119.8(4)
C(17)-C(7)-C(6)	120.3(4)
C(8)-C(7)-C(6)	119.9(4)
C(9)-C(8)-C(14)	119.2(4)
C(9)-C(8)-C(7)	121.1(4)
C(14)-C(8)-C(7)	119.7(4)
C(11)-C(9)-C(8)	120.4(4)
C(11)-C(9)-C(10)	119.8(5)
C(8)-C(9)-C(10)	119.9(4)
O(2)-C(10)-N(2)	119.9(4)
O(2)-C(10)-C(9)	123.7(5)
N(2)-C(10)-C(9)	116.4(4)
C(9)-C(11)-C(12)	120.4(5)
C(9)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(13)-C(12)-C(11)	120.2(5)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	120.3(4)
C(12)-C(13)-C(19)	119.7(4)
C(14)-C(13)-C(19)	119.9(4)
C(13)-C(14)-C(15)	121.4(4)
C(13)-C(14)-C(8)	119.4(4)
C(15)-C(14)-C(8)	119.1(4)
C(16)-C(15)-C(14)	120.8(4)
C(16)-C(15)-C(18)	119.5(4)
C(14)-C(15)-C(18)	119.7(4)
C(15)-C(16)-C(17)	120.0(5)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
C(7)-C(17)-C(16)	120.5(5)
C(7)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
O(4)-C(18)-N(3)	119.7(4)
O(4)-C(18)-C(15)	123.7(5)
N(3)-C(18)-C(15)	116.7(4)
O(3)-C(19)-N(3)	120.6(4)
O(3)-C(19)-C(13)	122.9(5)
N(3)-C(19)-C(13)	116.4(4)
C(21)-C(20)-C(22)	120.0(4)

C(21)-C(20)-N(3)	119.6(4)
C(22)-C(20)-N(3)	120.5(4)
C(20)-C(21)-C(24)	117.3(5)
C(20)-C(21)-H(21)	121.3
C(24)-C(21)-H(21)	121.3
C(20)-C(22)-C(23)	117.8(5)
C(20)-C(22)-H(22)	121.1
C(23)-C(22)-H(22)	121.1
N(4)-C(23)-C(22)	123.9(4)
N(4)-C(23)-H(23)	118.1
C(22)-C(23)-H(23)	118.1
N(4)-C(24)-C(21)	124.8(5)
N(4)-C(24)-H(24)	117.6
C(21)-C(24)-H(24)	117.6
C(1)-N(1)-C(5)	118.3(4)
C(1)-N(1)-Zn(1)	123.0(3)
C(5)-N(1)-Zn(1)	118.6(3)
C(6)-N(2)-C(10)	125.9(4)
C(6)-N(2)-C(3)	117.5(4)
C(10)-N(2)-C(3)	116.4(4)
C(18)-N(3)-C(19)	125.5(4)
C(18)-N(3)-C(20)	118.1(4)
C(19)-N(3)-C(20)	116.4(4)
C(24)-N(4)-C(23)	116.0(4)
C(24)-N(4)-Zn(1)#4	123.0(3)
C(23)-N(4)-Zn(1)#4	120.8(3)
O(41)-C(41)-N(41)	128.6(6)
O(41)-C(41)-C(42)	126.4(8)
N(41)-C(41)-C(42)	104.4(8)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
N(41)-C(43)-H(43A)	109.5
N(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
N(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
N(41)-C(44)-H(44A)	109.5
N(41)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
N(41)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
O(33)-Cl(31)-O(32)	110.6(6)
O(33)-Cl(31)-O(34)	113.1(5)
O(32)-Cl(31)-O(34)	108.9(5)
O(33)-Cl(31)-O(31)	110.7(7)

O(32)-Cl(31)-O(31)	107.7(7)
O(34)-Cl(31)-O(31)	105.6(6)

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

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(41)	72(4)	71(4)	53(4)	-12(3)	6(3)	3(3)
O(41)	44(2)	30(2)	31(2)	-2(2)	17(2)	1(2)
Zn(1)	38(1)	14(1)	36(1)	1(1)	28(1)	0(1)
C(1)	39(4)	46(3)	61(4)	25(3)	32(3)	6(3)
C(2)	37(3)	56(4)	61(4)	25(3)	25(3)	1(3)
C(3)	46(4)	28(3)	33(3)	-3(2)	25(3)	-13(2)
C(4)	50(4)	29(3)	32(3)	5(2)	17(3)	-7(2)
C(5)	39(3)	24(3)	37(3)	2(2)	16(3)	-3(2)
C(6)	49(3)	31(3)	36(3)	-6(3)	18(3)	-14(3)
C(7)	53(3)	22(3)	34(3)	-1(2)	20(3)	-15(2)
C(8)	40(3)	32(3)	25(3)	1(2)	16(2)	-8(2)
C(9)	70(4)	32(3)	35(3)	-8(3)	26(3)	-25(3)
C(10)	71(4)	43(3)	38(4)	-2(3)	28(3)	-22(3)
C(11)	109(5)	54(4)	39(4)	-14(3)	47(4)	-45(4)
C(12)	96(5)	38(3)	44(4)	-17(3)	40(3)	-40(3)
C(13)	49(3)	30(3)	33(3)	-2(2)	15(3)	-14(2)
C(14)	34(3)	25(3)	38(3)	0(2)	17(2)	-9(2)
C(15)	59(3)	23(3)	41(3)	2(2)	29(3)	-13(2)
C(16)	98(5)	39(3)	40(3)	-8(3)	45(3)	-25(3)
C(17)	109(5)	29(3)	48(4)	-13(3)	44(4)	-28(3)
C(18)	59(4)	36(3)	35(3)	-1(3)	29(3)	-8(3)
C(19)	40(3)	30(3)	46(4)	3(3)	20(3)	-9(2)
C(20)	41(3)	20(3)	43(3)	-3(2)	29(3)	-8(2)
C(21)	34(3)	32(3)	47(3)	7(3)	17(3)	-11(2)
C(22)	52(4)	29(3)	47(3)	19(3)	20(3)	2(3)
C(23)	28(3)	26(3)	60(4)	-2(3)	21(3)	-2(2)
C(24)	49(4)	35(3)	38(3)	7(3)	18(3)	3(3)
N(1)	42(3)	24(2)	37(3)	2(2)	28(2)	-3(2)
N(2)	56(3)	28(2)	32(3)	-2(2)	25(2)	-18(2)
N(3)	45(3)	22(2)	36(3)	-2(2)	20(2)	-13(2)
N(4)	34(3)	26(2)	35(3)	0(2)	21(2)	-2(2)
O(1)	88(3)	40(2)	46(2)	-9(2)	37(2)	-33(2)
O(2)	129(4)	61(3)	49(3)	-22(2)	58(3)	-51(3)
O(3)	71(3)	31(2)	52(2)	-7(2)	33(2)	-24(2)
O(4)	104(3)	37(2)	55(3)	-10(2)	56(2)	-25(2)
C(41)	71(5)	36(3)	65(5)	9(3)	22(4)	14(3)
C(42)	239(14)	98(7)	263(16)	-45(8)	183(14)	-33(8)
C(43)	150(8)	94(6)	50(5)	-15(4)	-12(5)	24(5)

C(44)	95(8)	440(20)	110(9)	3(11)	17(7)	-118(11)
Cl(31)	71(2)	123(2)	200(3)	-54(2)	9(2)	11(1)
O(31)	401(18)	343(18)	458(18)	75(12)	180(14)	-182(14)
O(32)	206(8)	274(10)	202(7)	-165(7)	-79(6)	156(7)
O(33)	89(5)	179(8)	463(15)	-124(8)	-90(7)	68(5)
O(34)	67(3)	138(5)	184(6)	-68(4)	48(4)	-34(3)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for the square-grid MOF.

	x	y	z	U(eq)
H(1)	1626	254	9916	54
H(2)	2264	814	9326	59
H(4)	236	1433	8208	43
H(5)	-343	868	8853	39
H(11)	2621	2801	9258	74
H(12)	3220	3378	8635	66
H(16)	2808	1882	5668	64
H(17)	2142	1326	6255	69
H(21)	2876	3842	5361	44
H(22)	4970	3440	6680	49
H(23)	5466	4073	6079	44
H(24)	3446	4447	4782	47
H(42A)	125	50	11988	266
H(42B)	738	387	12598	266
H(42C)	785	-204	12674	266
H(43A)	1635	132	13228	159
H(43B)	2304	503	13192	159
H(43C)	2448	-83	13227	159
H(44A)	2307	51	11281	327
H(44B)	2920	114	12128	327
H(44C)	2476	588	11678	327

Table 5. Torsional angles (°) in the square-grid MOF.

C(41)-O(41)-Zn(1)-O(41)#1	45(5)
C(41)-O(41)-Zn(1)-N(1)	136.1(5)
C(41)-O(41)-Zn(1)-N(1)#1	-43.9(5)
C(41)-O(41)-Zn(1)-N(4)#2	49.1(5)
C(41)-O(41)-Zn(1)-N(4)#3	-130.9(5)
N(1)-C(1)-C(2)-C(3)	-0.3(9)
C(1)-C(2)-C(3)-C(4)	0.1(8)
C(1)-C(2)-C(3)-N(2)	-179.2(5)
C(2)-C(3)-C(4)-C(5)	0.7(7)
N(2)-C(3)-C(4)-C(5)	180.0(4)
C(3)-C(4)-C(5)-N(1)	-1.4(7)
O(1)-C(6)-C(7)-C(17)	-1.7(8)
N(2)-C(6)-C(7)-C(17)	179.5(5)
O(1)-C(6)-C(7)-C(8)	179.3(5)
N(2)-C(6)-C(7)-C(8)	0.5(7)
C(17)-C(7)-C(8)-C(9)	-178.2(5)
C(6)-C(7)-C(8)-C(9)	0.8(7)
C(17)-C(7)-C(8)-C(14)	3.1(7)
C(6)-C(7)-C(8)-C(14)	-177.9(4)
C(14)-C(8)-C(9)-C(11)	-2.1(8)
C(7)-C(8)-C(9)-C(11)	179.2(6)
C(14)-C(8)-C(9)-C(10)	178.5(5)
C(7)-C(8)-C(9)-C(10)	-0.1(8)
C(11)-C(9)-C(10)-O(2)	0.8(9)
C(8)-C(9)-C(10)-O(2)	-179.9(6)
C(11)-C(9)-C(10)-N(2)	178.9(5)
C(8)-C(9)-C(10)-N(2)	-1.8(8)
C(8)-C(9)-C(11)-C(12)	3.1(9)
C(10)-C(9)-C(11)-C(12)	-177.6(6)
C(9)-C(11)-C(12)-C(13)	-1.6(10)
C(11)-C(12)-C(13)-C(14)	-0.9(9)
C(11)-C(12)-C(13)-C(19)	176.8(5)
C(12)-C(13)-C(14)-C(15)	-178.2(5)
C(19)-C(13)-C(14)-C(15)	4.2(7)
C(12)-C(13)-C(14)-C(8)	1.8(8)
C(19)-C(13)-C(14)-C(8)	-175.8(4)
C(9)-C(8)-C(14)-C(13)	-0.3(7)
C(7)-C(8)-C(14)-C(13)	178.3(4)
C(9)-C(8)-C(14)-C(15)	179.7(5)
C(7)-C(8)-C(14)-C(15)	-1.6(7)
C(13)-C(14)-C(15)-C(16)	178.6(5)
C(8)-C(14)-C(15)-C(16)	-1.4(8)
C(13)-C(14)-C(15)-C(18)	-1.7(7)
C(8)-C(14)-C(15)-C(18)	178.3(5)
C(14)-C(15)-C(16)-C(17)	3.0(9)
C(18)-C(15)-C(16)-C(17)	-176.7(5)
C(8)-C(7)-C(17)-C(16)	-1.6(9)
C(6)-C(7)-C(17)-C(16)	179.4(5)
C(15)-C(16)-C(17)-C(7)	-1.5(9)

C(16)-C(15)-C(18)-O(4)	-2.5(8)
C(14)-C(15)-C(18)-O(4)	177.8(5)
C(16)-C(15)-C(18)-N(3)	176.2(5)
C(14)-C(15)-C(18)-N(3)	-3.5(7)
C(12)-C(13)-C(19)-O(3)	0.5(8)
C(14)-C(13)-C(19)-O(3)	178.1(5)
C(12)-C(13)-C(19)-N(3)	-179.0(5)
C(14)-C(13)-C(19)-N(3)	-1.4(7)
C(22)-C(20)-C(21)-C(24)	-2.3(7)
N(3)-C(20)-C(21)-C(24)	177.0(4)
C(21)-C(20)-C(22)-C(23)	3.1(7)
N(3)-C(20)-C(22)-C(23)	-176.1(4)
C(20)-C(22)-C(23)-N(4)	0.1(7)
C(20)-C(21)-C(24)-N(4)	-2.0(7)
C(2)-C(1)-N(1)-C(5)	-0.4(8)
C(2)-C(1)-N(1)-Zn(1)	-178.7(4)
C(4)-C(5)-N(1)-C(1)	1.3(7)
C(4)-C(5)-N(1)-Zn(1)	179.6(3)
O(41)-Zn(1)-N(1)-C(1)	33.7(4)
O(41)#1-Zn(1)-N(1)-C(1)	-146.3(4)
N(1)#1-Zn(1)-N(1)-C(1)	104(32)
N(4)#2-Zn(1)-N(1)-C(1)	125.7(4)
N(4)#3-Zn(1)-N(1)-C(1)	-54.3(4)
O(41)-Zn(1)-N(1)-C(5)	-144.5(3)
O(41)#1-Zn(1)-N(1)-C(5)	35.5(3)
N(1)#1-Zn(1)-N(1)-C(5)	-74(32)
N(4)#2-Zn(1)-N(1)-C(5)	-52.6(3)
N(4)#3-Zn(1)-N(1)-C(5)	127.4(3)
O(1)-C(6)-N(2)-C(10)	178.5(5)
C(7)-C(6)-N(2)-C(10)	-2.6(7)
O(1)-C(6)-N(2)-C(3)	3.8(7)
C(7)-C(6)-N(2)-C(3)	-177.4(4)
O(2)-C(10)-N(2)-C(6)	-178.6(5)
C(9)-C(10)-N(2)-C(6)	3.2(8)
O(2)-C(10)-N(2)-C(3)	-3.8(8)
C(9)-C(10)-N(2)-C(3)	178.0(5)
C(4)-C(3)-N(2)-C(6)	-89.8(6)
C(2)-C(3)-N(2)-C(6)	89.5(6)
C(4)-C(3)-N(2)-C(10)	94.9(6)
C(2)-C(3)-N(2)-C(10)	-85.8(6)
O(4)-C(18)-N(3)-C(19)	-174.6(5)
C(15)-C(18)-N(3)-C(19)	6.6(7)
O(4)-C(18)-N(3)-C(20)	1.3(7)
C(15)-C(18)-N(3)-C(20)	-177.4(4)
O(3)-C(19)-N(3)-C(18)	176.2(5)
C(13)-C(19)-N(3)-C(18)	-4.2(7)
O(3)-C(19)-N(3)-C(20)	0.2(7)
C(13)-C(19)-N(3)-C(20)	179.7(4)
C(21)-C(20)-N(3)-C(18)	83.4(6)
C(22)-C(20)-N(3)-C(18)	-97.4(5)
C(21)-C(20)-N(3)-C(19)	-100.3(5)

C(22)-C(20)-N(3)-C(19)	78.9(5)
C(21)-C(24)-N(4)-C(23)	5.0(7)
C(21)-C(24)-N(4)-Zn(1)#4	-169.5(4)
C(22)-C(23)-N(4)-C(24)	-4.0(7)
C(22)-C(23)-N(4)-Zn(1)#4	170.6(4)
Zn(1)-O(41)-C(41)-N(41)	-165.4(4)
Zn(1)-O(41)-C(41)-C(42)	4.0(10)
C(43)-N(41)-C(41)-O(41)	-177.7(6)
C(44)-N(41)-C(41)-O(41)	-1.1(12)
C(43)-N(41)-C(41)-C(42)	11.1(9)
C(44)-N(41)-C(41)-C(42)	-172.3(9)

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

Bond Length and Bond angle table of 1D coordination polymer

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for the 1D coordination polymer. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	5240(1)	1802(1)	4311(1)	20(1)
N(1)	3495(2)	1277(1)	4904(1)	26(1)
O(1)	3902(2)	1891(1)	5269(1)	29(1)
O(2)	2668(2)	980(1)	5045(1)	36(1)
O(3)	3973(1)	972(1)	4384(1)	28(1)
N(4)	6621(2)	3087(1)	4410(1)	26(1)
O(4)	6519(1)	2457(1)	3992(1)	26(1)
O(5)	6018(2)	3197(1)	4908(1)	31(1)
O(6)	7305(2)	3562(1)	4308(1)	39(1)
C(1)	7036(2)	908(1)	5577(1)	22(1)
C(2)	7742(2)	650(1)	6368(1)	22(1)
C(3)	7709(2)	1018(1)	7132(1)	20(1)
C(4)	7013(2)	1641(1)	7089(1)	21(1)
C(5)	6340(2)	1861(1)	6266(1)	21(1)
C(6)	9208(2)	1204(1)	8485(1)	22(1)
C(7)	8132(2)	-13(1)	8190(1)	19(1)
C(8)	10685(2)	1338(1)	9898(1)	22(1)
C(9)	9871(2)	894(1)	9347(1)	19(1)
C(10)	9672(2)	148(1)	9593(1)	18(1)
C(11)	8832(2)	-314(1)	9044(1)	18(1)
C(12)	8662(2)	-1046(1)	9291(1)	22(1)
C(13)	4033(2)	2567(2)	2687(2)	34(1)
C(14)	3278(2)	2993(2)	2057(2)	36(1)
C(15)	2460(2)	3381(1)	2300(1)	23(1)
C(16)	2405(2)	3334(2)	3149(2)	38(1)
C(17)	3200(2)	2896(2)	3737(2)	39(1)
C(18)	867(2)	3484(1)	1005(1)	24(1)
C(19)	135(2)	3978(1)	322(1)	21(1)
C(20)	342(2)	4769(1)	334(1)	19(1)
C(21)	1220(2)	5110(1)	991(1)	20(1)
C(22)	1944(2)	4633(1)	1694(1)	21(1)
C(23)	1418(2)	5882(1)	985(1)	23(1)
N(11)	6334(2)	1496(1)	5519(1)	20(1)
N(12)	8362(1)	734(1)	7974(1)	19(1)
N(13)	4007(2)	2510(1)	3517(1)	23(1)
N(14)	1690(2)	3853(1)	1662(1)	22(1)
O(11)	9378(2)	1827(1)	8223(1)	33(1)
O(12)	7387(1)	-379(1)	7703(1)	25(1)
O(13)	777(2)	2797(1)	1012(1)	35(1)
O(14)	2731(1)	4880(1)	2264(1)	27(1)
C(41)	5228(2)	522(1)	2967(1)	22(1)
C(42)	5117(2)	-156(1)	3503(2)	26(1)
C(43)	4668(2)	-261(2)	1628(2)	36(1)

C(44)	5211(2)	1084(2)	1574(2)	35(1)
N(41)	5016(2)	451(1)	2101(1)	26(1)
O(41)	5533(1)	1153(1)	3328(1)	25(1)
C(45)	731(2)	6343(1)	325(2)	25(1)
C(46)	746(6)	9430(4)	7998(4)	171(4)
C(47)	1897(3)	9601(2)	8844(2)	44(1)
C(48)	1265(3)	8139(2)	8469(2)	47(1)
C(49)	-478(3)	8569(2)	7197(2)	46(1)
N(46)	761(4)	8823(2)	8024(3)	93(2)
O(46)	243(2)	9972(2)	7602(2)	65(1)

Table 7. Bond lengths [Å] and angles [°] for the 1D coordination polymer.

Zn(1)-O(41)	2.0496(16)
Zn(1)-N(11)	2.0839(17)
Zn(1)-N(13)	2.0973(18)
Zn(1)-O(4)	2.1409(17)
Zn(1)-O(3)	2.1791(17)
N(1)-O(2)	1.232(3)
N(1)-O(1)	1.263(3)
N(1)-O(3)	1.267(3)
N(4)-O(6)	1.237(3)
N(4)-O(5)	1.252(3)
N(4)-O(4)	1.279(3)
C(1)-N(11)	1.341(3)
C(1)-C(2)	1.388(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.386(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.387(3)
C(3)-N(12)	1.443(2)
C(4)-C(5)	1.391(3)
C(4)-H(4)	0.9500
C(5)-N(11)	1.349(3)
C(5)-H(5)	0.9500
C(6)-O(11)	1.213(3)
C(6)-N(12)	1.402(3)
C(6)-C(9)	1.487(3)
C(7)-O(12)	1.211(3)
C(7)-N(12)	1.408(3)
C(7)-C(11)	1.486(3)
C(8)-C(9)	1.378(3)
C(8)-C(12)#1	1.410(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.412(3)
C(10)-C(11)	1.413(3)
C(10)-C(10)#1	1.418(4)
C(11)-C(12)	1.380(3)
C(12)-C(8)#1	1.410(3)

C(12)-H(12)	0.9500
C(13)-N(13)	1.331(3)
C(13)-C(14)	1.383(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.371(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.371(3)
C(15)-N(14)	1.443(3)
C(16)-C(17)	1.387(3)
C(16)-H(16)	0.9500
C(17)-N(13)	1.339(3)
C(17)-H(17)	0.9500
C(18)-O(13)	1.213(3)
C(18)-N(14)	1.399(3)
C(18)-C(19)	1.484(3)
C(19)-C(45)#2	1.380(3)
C(19)-C(20)	1.415(3)
C(20)-C(21)	1.413(3)
C(20)-C(20)#2	1.414(4)
C(21)-C(23)	1.381(3)
C(21)-C(22)	1.480(3)
C(22)-O(14)	1.211(3)
C(22)-N(14)	1.406(3)
C(23)-C(45)	1.407(3)
C(23)-H(23)	0.9500
C(41)-O(41)	1.258(3)
C(41)-N(41)	1.330(3)
C(41)-C(42)	1.495(3)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-N(41)	1.462(3)
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-N(41)	1.455(3)
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(19)#2	1.380(3)
C(45)-H(45)	0.9500
C(46)-N(46)	1.069(7)
C(46)-O(46)	1.214(4)
C(46)-C(47)	1.690(9)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-N(46)	1.447(4)
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800

C(49)-N(46)	1.775(6)
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
O(41)-Zn(1)-N(11)	110.14(7)
O(41)-Zn(1)-N(13)	97.61(7)
N(11)-Zn(1)-N(13)	151.99(7)
O(41)-Zn(1)-O(4)	79.26(6)
N(11)-Zn(1)-O(4)	91.17(7)
N(13)-Zn(1)-O(4)	90.32(7)
O(41)-Zn(1)-O(3)	87.47(6)
N(11)-Zn(1)-O(3)	94.09(7)
N(13)-Zn(1)-O(3)	90.75(7)
O(4)-Zn(1)-O(3)	166.71(6)
O(2)-N(1)-O(1)	121.7(2)
O(2)-N(1)-O(3)	120.9(2)
O(1)-N(1)-O(3)	117.39(19)
N(1)-O(3)-Zn(1)	103.47(14)
O(6)-N(4)-O(5)	122.6(2)
O(6)-N(4)-O(4)	119.2(2)
O(5)-N(4)-O(4)	118.21(19)
N(4)-O(4)-Zn(1)	108.34(13)
N(11)-C(1)-C(2)	123.2(2)
N(11)-C(1)-H(1)	118.4
C(2)-C(1)-H(1)	118.4
C(1)-C(2)-C(3)	118.1(2)
C(1)-C(2)-H(2)	121.0
C(3)-C(2)-H(2)	121.0
C(2)-C(3)-C(4)	119.96(18)
C(2)-C(3)-N(12)	120.01(19)
C(4)-C(3)-N(12)	119.97(19)
C(3)-C(4)-C(5)	117.9(2)
C(3)-C(4)-H(4)	121.0
C(5)-C(4)-H(4)	121.0
N(11)-C(5)-C(4)	123.0(2)
N(11)-C(5)-H(5)	118.5
C(4)-C(5)-H(5)	118.5
O(11)-C(6)-N(12)	120.78(19)
O(11)-C(6)-C(9)	122.8(2)
N(12)-C(6)-C(9)	116.43(18)
O(12)-C(7)-N(12)	120.92(18)
O(12)-C(7)-C(11)	122.50(19)
N(12)-C(7)-C(11)	116.57(18)
C(9)-C(8)-C(12)#1	120.1(2)
C(9)-C(8)-H(8)	119.9
C(12)#1-C(8)-H(8)	119.9
C(8)-C(9)-C(10)	120.46(18)
C(8)-C(9)-C(6)	119.50(19)
C(10)-C(9)-C(6)	120.04(18)
C(9)-C(10)-C(11)	121.45(17)
C(9)-C(10)-C(10)#1	119.5(2)

C(11)-C(10)-C(10)#1	119.0(2)
C(12)-C(11)-C(10)	120.50(18)
C(12)-C(11)-C(7)	119.66(19)
C(10)-C(11)-C(7)	119.84(18)
C(11)-C(12)-C(8)#1	120.33(19)
C(11)-C(12)-H(12)	119.8
C(8)#1-C(12)-H(12)	119.8
N(13)-C(13)-C(14)	123.6(2)
N(13)-C(13)-H(13)	118.2
C(14)-C(13)-H(13)	118.2
C(15)-C(14)-C(13)	118.3(2)
C(15)-C(14)-H(14)	120.8
C(13)-C(14)-H(14)	120.8
C(16)-C(15)-C(14)	119.7(2)
C(16)-C(15)-N(14)	121.0(2)
C(14)-C(15)-N(14)	119.3(2)
C(15)-C(16)-C(17)	118.0(2)
C(15)-C(16)-H(16)	121.0
C(17)-C(16)-H(16)	121.0
N(13)-C(17)-C(16)	123.4(2)
N(13)-C(17)-H(17)	118.3
C(16)-C(17)-H(17)	118.3
O(13)-C(18)-N(14)	120.4(2)
O(13)-C(18)-C(19)	123.4(2)
N(14)-C(18)-C(19)	116.18(19)
C(45)#2-C(19)-C(20)	120.84(19)
C(45)#2-C(19)-C(18)	119.5(2)
C(20)-C(19)-C(18)	119.64(19)
C(21)-C(20)-C(19)	121.91(18)
C(21)-C(20)-C(20)#2	118.9(2)
C(19)-C(20)-C(20)#2	119.2(2)
C(23)-C(21)-C(20)	121.08(19)
C(23)-C(21)-C(22)	119.36(19)
C(20)-C(21)-C(22)	119.56(19)
O(14)-C(22)-N(14)	120.19(19)
O(14)-C(22)-C(21)	123.4(2)
N(14)-C(22)-C(21)	116.37(19)
C(21)-C(23)-C(45)	120.0(2)
C(21)-C(23)-H(23)	120.0
C(45)-C(23)-H(23)	120.0
C(1)-N(11)-C(5)	117.84(17)
C(1)-N(11)-Zn(1)	120.45(14)
C(5)-N(11)-Zn(1)	121.68(14)
C(6)-N(12)-C(7)	125.59(17)
C(6)-N(12)-C(3)	117.64(17)
C(7)-N(12)-C(3)	116.67(17)
C(13)-N(13)-C(17)	116.9(2)
C(13)-N(13)-Zn(1)	114.79(15)
C(17)-N(13)-Zn(1)	128.28(15)
C(18)-N(14)-C(22)	126.15(18)
C(18)-N(14)-C(15)	117.07(18)

C(22)-N(14)-C(15)	116.12(18)
O(41)-C(41)-N(41)	120.0(2)
O(41)-C(41)-C(42)	120.7(2)
N(41)-C(41)-C(42)	119.3(2)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
N(41)-C(43)-H(43A)	109.5
N(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
N(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
N(41)-C(44)-H(44A)	109.5
N(41)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
N(41)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(41)-N(41)-C(44)	120.4(2)
C(41)-N(41)-C(43)	123.7(2)
C(44)-N(41)-C(43)	115.8(2)
C(41)-O(41)-Zn(1)	137.97(15)
C(19)#2-C(45)-C(23)	120.0(2)
C(19)#2-C(45)-H(45)	120.0
C(23)-C(45)-H(45)	120.0
N(46)-C(46)-O(46)	143.7(10)
N(46)-C(46)-C(47)	98.4(5)
O(46)-C(46)-C(47)	118.0(7)
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
N(46)-C(48)-H(48A)	109.5
N(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
N(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
N(46)-C(49)-H(49A)	109.5
N(46)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
N(46)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(46)-N(46)-C(48)	148.3(7)

C(46)-N(46)-C(49)	102.8(6)
C(48)-N(46)-C(49)	108.5(3)

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

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for the 1D coordination polymer. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	22(1)	21(1)	14(1)	5(1)	1(1)	4(1)
N(1)	25(1)	33(1)	19(1)	6(1)	5(1)	4(1)
O(1)	34(1)	32(1)	20(1)	3(1)	6(1)	4(1)
O(2)	27(1)	50(1)	35(1)	5(1)	12(1)	-3(1)
O(3)	29(1)	34(1)	22(1)	1(1)	9(1)	2(1)
N(4)	31(1)	26(1)	17(1)	5(1)	2(1)	-1(1)
O(4)	32(1)	25(1)	21(1)	0(1)	6(1)	-1(1)
O(5)	39(1)	31(1)	23(1)	0(1)	10(1)	3(1)
O(6)	47(1)	36(1)	32(1)	2(1)	10(1)	-17(1)
C(1)	23(1)	26(1)	15(1)	2(1)	5(1)	2(1)
C(2)	20(1)	27(1)	18(1)	4(1)	4(1)	6(1)
C(3)	18(1)	23(1)	14(1)	6(1)	0(1)	0(1)
C(4)	24(1)	21(1)	15(1)	2(1)	2(1)	0(1)
C(5)	23(1)	19(1)	18(1)	3(1)	2(1)	3(1)
C(6)	23(1)	24(1)	17(1)	4(1)	1(1)	0(1)
C(7)	19(1)	22(1)	15(1)	3(1)	3(1)	3(1)
C(8)	26(1)	20(1)	19(1)	4(1)	1(1)	0(1)
C(9)	20(1)	21(1)	15(1)	4(1)	2(1)	2(1)
C(10)	18(1)	20(1)	14(1)	3(1)	2(1)	2(1)
C(11)	18(1)	22(1)	14(1)	2(1)	1(1)	3(1)
C(12)	23(1)	22(1)	17(1)	1(1)	0(1)	-1(1)
C(13)	39(1)	40(1)	23(1)	9(1)	11(1)	21(1)
C(14)	46(2)	43(2)	18(1)	9(1)	10(1)	22(1)
C(15)	24(1)	22(1)	19(1)	6(1)	2(1)	6(1)
C(16)	43(2)	48(2)	27(1)	14(1)	16(1)	26(1)
C(17)	50(2)	48(2)	21(1)	12(1)	14(1)	24(1)
C(18)	28(1)	22(1)	20(1)	4(1)	3(1)	6(1)
C(19)	23(1)	20(1)	20(1)	3(1)	4(1)	5(1)
C(20)	19(1)	21(1)	18(1)	3(1)	5(1)	5(1)
C(21)	19(1)	22(1)	18(1)	4(1)	4(1)	5(1)
C(22)	20(1)	24(1)	20(1)	5(1)	5(1)	4(1)
C(23)	22(1)	24(1)	21(1)	1(1)	3(1)	1(1)
N(11)	21(1)	21(1)	15(1)	5(1)	2(1)	1(1)
N(12)	19(1)	22(1)	13(1)	4(1)	0(1)	2(1)
N(13)	26(1)	23(1)	16(1)	4(1)	3(1)	6(1)
N(14)	24(1)	22(1)	18(1)	5(1)	2(1)	6(1)
O(11)	35(1)	29(1)	25(1)	12(1)	-6(1)	-7(1)
O(12)	23(1)	26(1)	20(1)	3(1)	-3(1)	-1(1)

O(13)	44(1)	20(1)	32(1)	5(1)	-4(1)	5(1)
O(14)	22(1)	30(1)	24(1)	6(1)	-1(1)	0(1)
C(41)	17(1)	24(1)	23(1)	2(1)	4(1)	2(1)
C(42)	27(1)	24(1)	26(1)	4(1)	6(1)	0(1)
C(43)	37(1)	41(2)	29(1)	-9(1)	5(1)	-4(1)
C(44)	47(2)	37(1)	26(1)	7(1)	16(1)	6(1)
N(41)	26(1)	30(1)	22(1)	1(1)	6(1)	2(1)
O(41)	30(1)	22(1)	25(1)	-1(1)	10(1)	1(1)
C(45)	28(1)	20(1)	24(1)	2(1)	4(1)	2(1)
C(46)	254(8)	159(6)	188(6)	145(5)	205(7)	175(6)
C(47)	40(2)	59(2)	35(1)	11(1)	12(1)	16(1)
C(48)	57(2)	31(1)	48(2)	-2(1)	8(1)	11(1)
C(49)	53(2)	44(2)	42(2)	-4(1)	16(1)	13(1)
N(46)	139(4)	50(2)	137(4)	48(2)	117(3)	54(2)
O(46)	72(2)	72(2)	70(2)	45(1)	51(1)	50(1)

Table 9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for the 1D coordination polymer

	x	y	z	U(eq)
H(1)	7051	655	5052	26
H(2)	8233	234	6385	26
H(4)	6997	1909	7604	25
H(5)	5863	2288	6230	25
H(8)	10806	1842	9731	27
H(12)	8102	-1354	8914	26
H(13)	4601	2299	2518	41
H(14)	3326	3017	1471	43
H(16)	1840	3595	3328	46
H(17)	3171	2867	4327	47
H(23)	2019	6101	1427	28
H(42A)	5448	-43	4127	39
H(42B)	5508	-589	3336	39
H(42C)	4324	-282	3396	39
H(43A)	5320	-509	1519	55
H(43B)	4111	-154	1066	55
H(43C)	4341	-597	1981	55
H(44A)	4507	1356	1320	53
H(44B)	5499	892	1101	53
H(44C)	5759	1432	1946	53
H(45)	862	6874	325	30
H(47A)	1852	9310	9359	67
H(47B)	1941	10144	8984	67
H(47C)	2566	9447	8680	67
H(48A)	2081	8197	8661	70
H(48B)	1065	7706	8066	70

H(48C)	992	8050	8981	70
H(49A)	-1043	8394	7473	69
H(49B)	-310	8161	6834	69
H(49C)	-763	9013	6828	69

Table 10. Torsion angles [°] for the 1D coordination polymer.

O(2)-N(1)-O(3)-Zn(1)	174.61(17)
O(1)-N(1)-O(3)-Zn(1)	-5.6(2)
O(41)-Zn(1)-O(3)-N(1)	-171.88(13)
N(11)-Zn(1)-O(3)-N(1)	78.10(13)
N(13)-Zn(1)-O(3)-N(1)	-74.29(13)
O(4)-Zn(1)-O(3)-N(1)	-168.9(2)
O(6)-N(4)-O(4)-Zn(1)	-178.64(16)
O(5)-N(4)-O(4)-Zn(1)	1.3(2)
O(41)-Zn(1)-O(4)-N(4)	171.99(14)
N(11)-Zn(1)-O(4)-N(4)	-77.72(14)
N(13)-Zn(1)-O(4)-N(4)	74.30(14)
O(3)-Zn(1)-O(4)-N(4)	168.9(2)
N(11)-C(1)-C(2)-C(3)	0.5(3)
C(1)-C(2)-C(3)-C(4)	-2.2(3)
C(1)-C(2)-C(3)-N(12)	175.12(19)
C(2)-C(3)-C(4)-C(5)	1.9(3)
N(12)-C(3)-C(4)-C(5)	-175.46(19)
C(3)-C(4)-C(5)-N(11)	0.2(3)
C(12)#1-C(8)-C(9)-C(10)	0.8(3)
C(12)#1-C(8)-C(9)-C(6)	-178.6(2)
O(11)-C(6)-C(9)-C(8)	3.0(4)
N(12)-C(6)-C(9)-C(8)	-177.4(2)
O(11)-C(6)-C(9)-C(10)	-176.4(2)
N(12)-C(6)-C(9)-C(10)	3.2(3)
C(8)-C(9)-C(10)-C(11)	179.1(2)
C(6)-C(9)-C(10)-C(11)	-1.5(3)
C(8)-C(9)-C(10)-C(10)#1	-0.8(4)
C(6)-C(9)-C(10)-C(10)#1	178.6(2)
C(9)-C(10)-C(11)-C(12)	179.1(2)
C(10)#1-C(10)-C(11)-C(12)	-0.9(4)
C(9)-C(10)-C(11)-C(7)	-0.3(3)
C(10)#1-C(10)-C(11)-C(7)	179.6(2)
O(12)-C(7)-C(11)-C(12)	2.0(3)
N(12)-C(7)-C(11)-C(12)	-179.14(19)
O(12)-C(7)-C(11)-C(10)	-178.5(2)
N(12)-C(7)-C(11)-C(10)	0.3(3)
C(10)-C(11)-C(12)-C(8)#1	0.9(3)
C(7)-C(11)-C(12)-C(8)#1	-179.6(2)
N(13)-C(13)-C(14)-C(15)	0.1(5)
C(13)-C(14)-C(15)-C(16)	-0.3(4)
C(13)-C(14)-C(15)-N(14)	177.6(2)
C(14)-C(15)-C(16)-C(17)	0.6(4)

N(14)-C(15)-C(16)-C(17)	-177.2(3)
C(15)-C(16)-C(17)-N(13)	-0.7(5)
O(13)-C(18)-C(19)-C(45)#2	3.0(4)
N(14)-C(18)-C(19)-C(45)#2	-176.9(2)
O(13)-C(18)-C(19)-C(20)	-176.1(2)
N(14)-C(18)-C(19)-C(20)	3.9(3)
C(45)#2-C(19)-C(20)-C(21)	179.7(2)
C(18)-C(19)-C(20)-C(21)	-1.1(3)
C(45)#2-C(19)-C(20)-C(20)#2	-0.9(4)
C(18)-C(19)-C(20)-C(20)#2	178.3(2)
C(19)-C(20)-C(21)-C(23)	179.1(2)
C(20)#2-C(20)-C(21)-C(23)	-0.3(4)
C(19)-C(20)-C(21)-C(22)	-0.5(3)
C(20)#2-C(20)-C(21)-C(22)	-179.9(2)
C(23)-C(21)-C(22)-O(14)	-1.8(3)
C(20)-C(21)-C(22)-O(14)	177.8(2)
C(23)-C(21)-C(22)-N(14)	179.6(2)
C(20)-C(21)-C(22)-N(14)	-0.8(3)
C(20)-C(21)-C(23)-C(45)	1.0(3)
C(22)-C(21)-C(23)-C(45)	-179.5(2)
C(2)-C(1)-N(11)-C(5)	1.6(3)
C(2)-C(1)-N(11)-Zn(1)	-176.46(17)
C(4)-C(5)-N(11)-C(1)	-1.9(3)
C(4)-C(5)-N(11)-Zn(1)	176.07(16)
O(41)-Zn(1)-N(11)-C(1)	-4.76(18)
N(13)-Zn(1)-N(11)-C(1)	-176.62(16)
O(4)-Zn(1)-N(11)-C(1)	-83.75(17)
O(3)-Zn(1)-N(11)-C(1)	84.03(17)
O(41)-Zn(1)-N(11)-C(5)	177.28(16)
N(13)-Zn(1)-N(11)-C(5)	5.4(3)
O(4)-Zn(1)-N(11)-C(5)	98.30(17)
O(3)-Zn(1)-N(11)-C(5)	-93.92(17)
O(11)-C(6)-N(12)-C(7)	176.3(2)
C(9)-C(6)-N(12)-C(7)	-3.4(3)
O(11)-C(6)-N(12)-C(3)	0.0(3)
C(9)-C(6)-N(12)-C(3)	-179.62(18)
O(12)-C(7)-N(12)-C(6)	-179.5(2)
C(11)-C(7)-N(12)-C(6)	1.7(3)
O(12)-C(7)-N(12)-C(3)	-3.2(3)
C(11)-C(7)-N(12)-C(3)	177.93(18)
C(2)-C(3)-N(12)-C(6)	116.7(2)
C(4)-C(3)-N(12)-C(6)	-65.9(3)
C(2)-C(3)-N(12)-C(7)	-59.8(3)
C(4)-C(3)-N(12)-C(7)	117.5(2)
C(14)-C(13)-N(13)-C(17)	-0.2(4)
C(14)-C(13)-N(13)-Zn(1)	178.7(2)
C(16)-C(17)-N(13)-C(13)	0.5(4)
C(16)-C(17)-N(13)-Zn(1)	-178.2(2)
O(41)-Zn(1)-N(13)-C(13)	-23.1(2)
N(11)-Zn(1)-N(13)-C(13)	149.22(19)
O(4)-Zn(1)-N(13)-C(13)	56.14(19)

O(3)-Zn(1)-N(13)-C(13)	-110.61(19)
O(41)-Zn(1)-N(13)-C(17)	155.7(2)
N(11)-Zn(1)-N(13)-C(17)	-32.0(3)
O(4)-Zn(1)-N(13)-C(17)	-125.1(2)
O(3)-Zn(1)-N(13)-C(17)	68.2(2)
O(13)-C(18)-N(14)-C(22)	174.4(2)
C(19)-C(18)-N(14)-C(22)	-5.6(3)
O(13)-C(18)-N(14)-C(15)	4.1(3)
C(19)-C(18)-N(14)-C(15)	-175.91(19)
O(14)-C(22)-N(14)-C(18)	-174.5(2)
C(21)-C(22)-N(14)-C(18)	4.1(3)
O(14)-C(22)-N(14)-C(15)	-4.1(3)
C(21)-C(22)-N(14)-C(15)	174.49(18)
C(16)-C(15)-N(14)-C(18)	-108.4(3)
C(14)-C(15)-N(14)-C(18)	73.8(3)
C(16)-C(15)-N(14)-C(22)	80.3(3)
C(14)-C(15)-N(14)-C(22)	-97.5(3)
O(41)-C(41)-N(41)-C(44)	4.4(3)
C(42)-C(41)-N(41)-C(44)	-174.6(2)
O(41)-C(41)-N(41)-C(43)	179.4(2)
C(42)-C(41)-N(41)-C(43)	0.4(3)
N(41)-C(41)-O(41)-Zn(1)	139.75(19)
C(42)-C(41)-O(41)-Zn(1)	-41.3(3)
N(11)-Zn(1)-O(41)-C(41)	87.2(2)
N(13)-Zn(1)-O(41)-C(41)	-96.7(2)
O(4)-Zn(1)-O(41)-C(41)	174.4(2)
O(3)-Zn(1)-O(41)-C(41)	-6.3(2)
C(21)-C(23)-C(45)-C(19)#2	-0.7(3)
O(46)-C(46)-N(46)-C(48)	-175.5(5)
C(47)-C(46)-N(46)-C(48)	5.6(8)
O(46)-C(46)-N(46)-C(49)	-4.7(7)
C(47)-C(46)-N(46)-C(49)	176.4(2)

Symmetry transformations used to generate equivalent atoms:
#1 –x+2,-y,-z+2 #2 –x,-y+1,-z