Supporting Information

Water Harvesting Properties of a Zwitterionic Metal-Organic Framework

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Experimental Section

Materials. All reagents and solvents were commercially sourced and used without further purification. The Zincke salt, *N*,*N*'-bis(2,4-dinitrophenyl)-4,4'-bipyridinium dichloride, was synthesized as previously reported.[1] The ZW ligand, 1,1'-bis(3,5-dicarboxyphenyl)-4,4'-bipyridinium dichloride (H_4dcpb·2Cl) was synthesized as previously reported with some modifications (**Scheme S1**).[2]

Synthesis of (H_4dcpb·2Cl). Dimethyl-5-aminoisophthalate (2.4 g, 11.47 mmol) and *N*,*N*'-bis(2,4-dinitrophenyl)-4,4'-bipyridinium dichloride (3.0 g, 6.12 mmol) were dissolved in ethanol (40 mL) and stirred for 24 h at 110 °C. The product was filtered off and washed with cold ethanol to give 1,1'-bis(3,5-bis(methoxycarbonyl)phenyl)-4,4'-bipyridinium dichloride as a yellow powder. Yield: 0.546 g, 17.5%. For deprotection, 1,1'-bis(3,5-bis(methoxycarbonyl)phenyl)-4,4'-bipyridinium dichloride (3.0 g, 10.0 mmol) was dissolved in glacial acetic acid (50 mL) and 40% HBr (50 mL) and refluxed for 12 h at 118 °C. The final yellow product, (H_4dcpb·2Cl), was collected by vacuum filtration. Yield: 1.63 g, 54%. ^{1}H NMR (400 MHz, DMSO): δ = 13.92 (s, 4H), 9.80 (d, 4H), 9.16 (d, 4H), 8.79 (s, 2H), 8.72 (s, 4H) (**Figure S2**).

Synthesis of Ni-ZW-MOF. $[Ni(dcpb)(H_2O)_4\cdot 14H_2O]_n$ was synthesized as reported with some modifications.[3] $Ni(ClO_4)_2\cdot 6H_2O$ (36.6 mg, 0.10 mmol) and H_4dcpb·2Cl (6.0 mg, 0.01 mmol) were added to 2 mL dimethylformamide (DMF)/H_2O (1:1 v/v) in a glass vial and stirred for 10 min. Dicyandiamide (0.168 g, 2.0 mmol) was added with stirring. The resulting suspension was kept at 80 ºC for 3 days. A homogenous phase of SCXRD-quality green needle-like single crystals was

obtained, and several times exchanged with H_2O before vacuum filtration. The dried as-synthesized crystals were used for experiments. The bulk purity of the crystals was confirmed through PXRD (**Figure 2c**).

Powder X-ray Diffraction. PXRD data was collected at room temperature on a Bruker D2 Phaser diffractometer equipped with a Cu sealed tube (λ = 1.54178 Å). Powder samples were dispersed on low-background discs for analyses. The powder pattern module of CCDC's Mercury software package was used to calculate reference PXRD data from respective SCXRD data of the MOF.[4]

Single Crystal X-ray Diffraction. Single crystals of the Ni-ZW-MOF were selected for structural X-ray diffraction analysis and mounted on a MiTeGen loop using Paratone oil. Crystal data was collected on a Bruker Kappa Apex II X-ray diffractometer equipped with a Mo X-ray source (sealed tube, λ = 0.71073 Å), an APEX II CCD detector, and an Oxford Cryosystems Desktop Cooler low-temperature device. The APEX3 software suite was used for data collection, cell refinement, and reduction.[5] Absorption corrections were performed using SADABS.[6] Space group assignment was determined by surveying systematic absences, E-statistics, and the following structure refinement. Structure solution was performed with intrinsic phasing using SHELXT-2014/15 and refined by least-squares refinement against $|F|^2$, followed by difference Fourier synthesis using SHELXL-2018.[7,8] Notably, when published the first time, the crystal structure of Ni-ZW-MOF was reported in space group $P2_1/n$.[3] However, we show here that $C2/c$ is the correct space group. If not stated differently, all non-hydrogen atoms were refined with anisotropic displacement parameters. Aromatic hydrogen atoms were positioned with idealized geometry and

refined with fixed isotropic displacement parameters [$U_{eq}(H) = -1.2U_{eq}(C)$] using a riding model with $d_{C-H} = 0.95$ Å and O−H hydrogen atoms were located in the difference map, where the bond lengths were set to ideal values with $d_{O-H} = 0.84$ Å and were refined using a riding model. CCDC 2220643 contains supplementary crystallographic data for this paper. This data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk. Selected crystal data and refinement parameters are listed in **Tables S1-S7**.

Thermogravimetric Analysis. TG data was recorded using a TGA Q50 from TA Instruments. All measurements were performed using platinum crucibles in a dynamic nitrogen atmosphere (50 mL/min) and a heating rate of 3 °C/min. The instrument was corrected for buoyancy and current effects and was calibrated using standard reference materials.

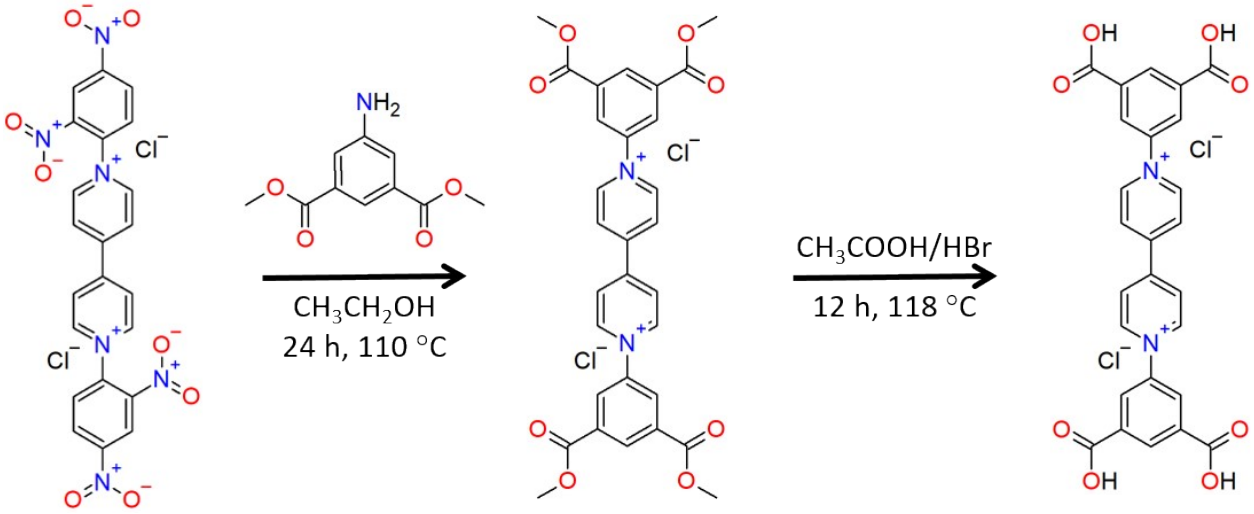
Ultraviolet-Visible Diffuse Reflectance Spectroscopy. DRS data was collected using an Agilent Cary 60 equipped with a Harrick video barrelino and an Agilent fiber optic coupler. The samples were examined as powders packed in a stainless-steel sample holder and taken in reference to baseline material of a HALON disc. Samples were diluted as needed using barium sulfate.

Proton Nuclear Magnetic Resonance Spectroscopy. ^{1}H-NMR data was obtained using an Avance DMX-400 from Bruker.

Gravimetric Water Adsorption/Desorption Studies. Water adsorption and desorption measurements were performed using a modified TG analyzer setup and platinum crucibles. The primary gas inlet was setup with dry nitrogen gas. The secondary gas inlet provided humidified nitrogen by passing the nitrogen through a gas washing bottle. The relative humidity was adjusted through the volume of water in the gas washing bottle. The gas flow was regulated using the internal mass flow controller. The relative humidity was monitored using a humidity sensor downstream of the TG chamber.

Water Sorption Isotherm. A water isotherm was measured using a modified TG analyzer setup and platinum crucibles. The primary gas inlet was set up with dry nitrogen gas. The secondary gas inlet provided humidified nitrogen by passing the nitrogen through a gas washing bottle. The relative humidity was adjusted through the volume of water in the gas washing bottle. The gas flow was regulated using the internal mass flow controller. The relative humidity was monitored using a humidity sensor downstream of the TG chamber. Data points were collected after 60 min of exposure to humidified nitrogen between 0-80% RH at 30 °C. Respective water uptakes were calculated from the mass increase of the sample at each data point.

Supplementary Schemes and Figures



Scheme S1. Two-step synthesis of tetratopic ZW ligand H_4dcpb·2Cl.

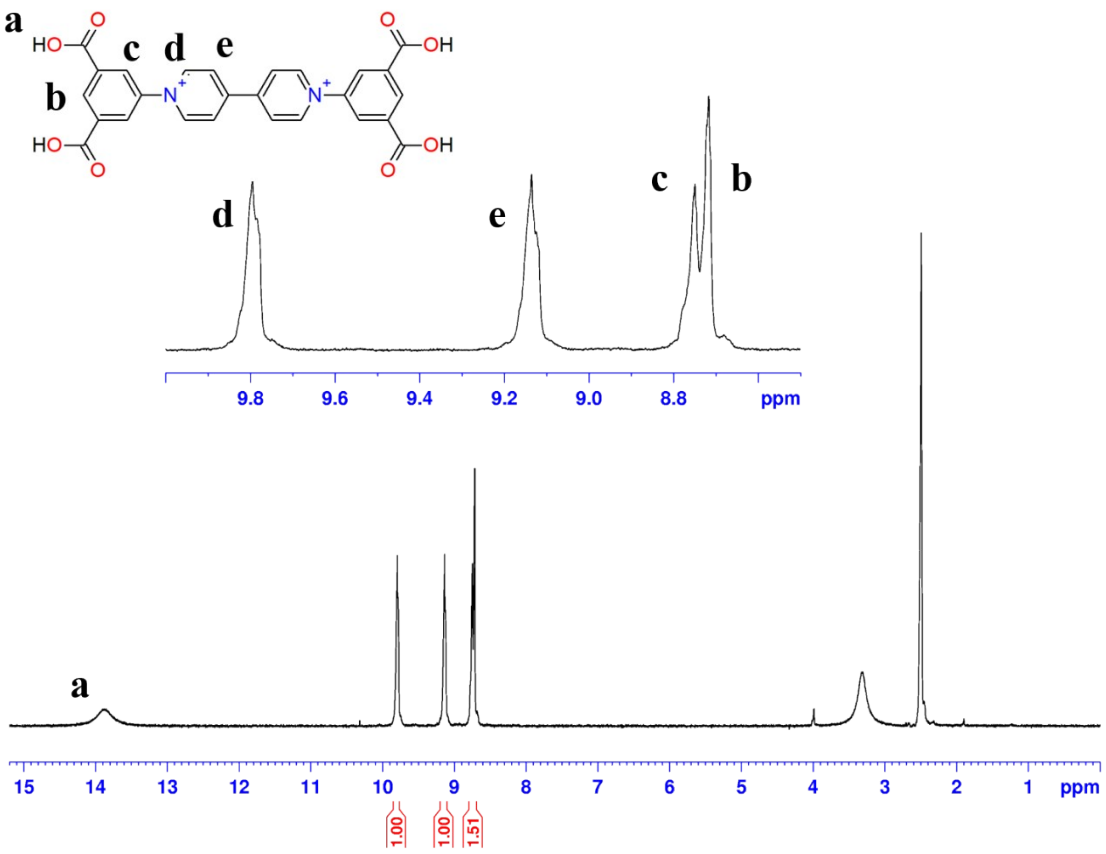


Figure S1. ^{1}H-NMR of 1,1'-bis(3,5-dicarboxyphenyl)-4,4'-bipyridinium dichloride (H_4dcpb·2Cl) in DMSO.

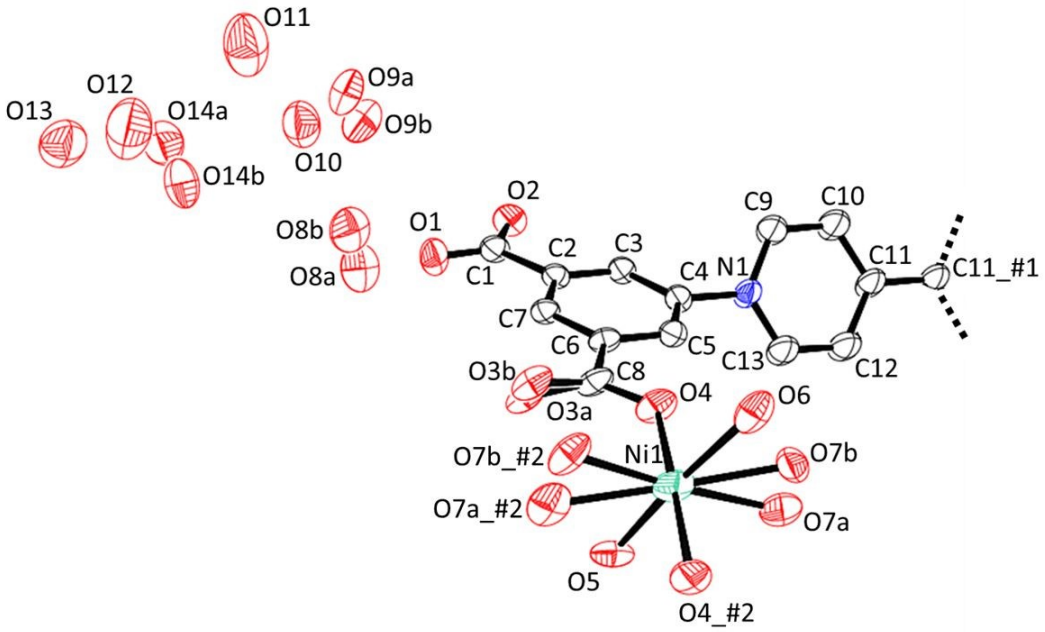


Figure S2. Crystal structure of Ni-ZW-MOF with view of the coordination sphere of the Ni(II) cation with displacement ellipsoids drawn at the 50% probability level. Selected atoms are labeled. Symmetry codes: #1 = -x+3/2, -y+3/2, -z+1; #2 = -x+1, y, -z+3/2

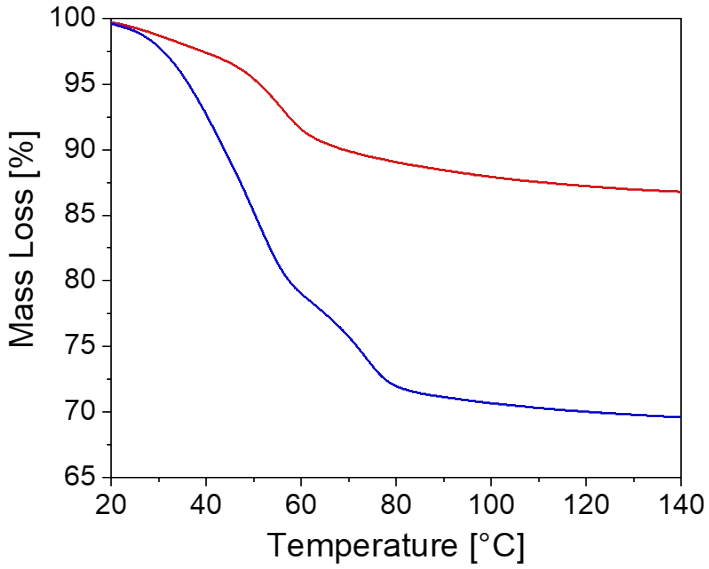


Figure S3. TGA curve of Ni-ZW-MOF (activated at 120 °C for 1 h under dynamic N_2 atmosphere) after exposure to a controlled 80% RH atmosphere for 2 h (red) and immersion in water for 2 h (blue).

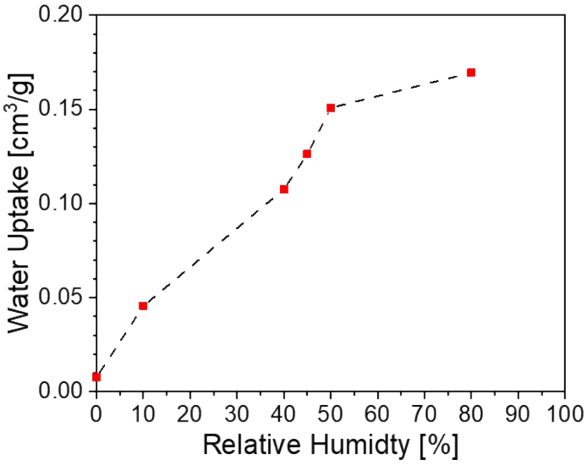


Figure S4. Water adsorption isotherm of Ni-ZW-MOF measured at 30 °C. Two steps are observed corresponding to coordination of water molecules to the Ni node followed by adsorption into the pores.

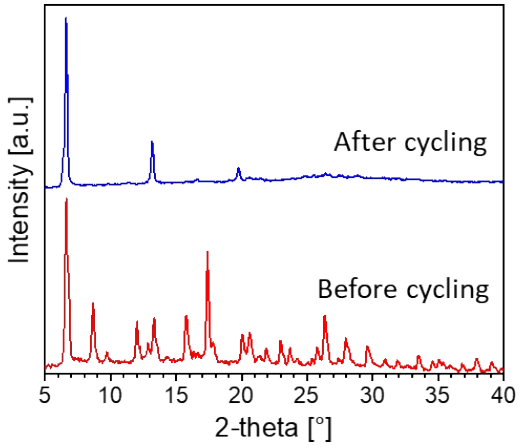


Figure S5. PXRD of Ni-ZW-MOF before (bottom, red) and after (top, blue) dynamic water adsorption-desorption cycling experiments (14 cycles; adsorption conditions: 30 °C and 45% RH; desorption conditions: 80 °C and 0% RH). The sample after cycling was resuspended in water to regain crystallinity.

Supplementary Tables

Table S1. Crystal Data and structure refinement for Ni-ZW-MOF.

Identification code	Ni-ZW-MOF	
Empirical formula	$C_{26}H_{49.98}N_2NiO_{26}$	
Formula weight	865.37	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/c	
Unit cell dimensions	a = 27.238(3) Å	α = 90°
	b = 6.9170(6) Å	β = 97.872(4)°
	c = 21.7928(19) Å	γ = 90°
Volume	4067.2(7) Å^3	
Z	4	
Density (calculated)	1.413 Mg/m^3	
Absorption coefficient	0.569 mm^{-1}	
F(000)	1824	
Crystal size	0.150 x 0.100 x 0.020 mm^3	
Theta range for data collection	2.249 to 28.341°	
Index ranges	-36<=h<=32, -9<=k<=9, -23<=l<=29	
Reflections collected	22076	
Independent reflections	5061 [R(int) = 0.0919]	
Completeness to theta = 25.242°	99.8%	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5061 / 135 / 329	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R_1 = 0.1055, wR_2 = 0.2431	
R indices (all data)	R_1 = 0.1832, wR_2 = 0.2819	
Largest diff. peak and hole	0.956 and -0.749 e.Å^{-3}	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ni-ZW-MOF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4545(2)	6687(9)	3833(2)	33(1)
C(2)	4879(2)	7155(8)	4429(2)	26(1)
C(3)	5384(2)	7207(8)	4441(2)	28(1)
C(4)	5681(2)	7555(8)	4993(2)	27(1)
C(5)	5490(2)	7889(8)	5539(2)	27(1)
C(6)	4984(2)	7861(8)	5534(2)	27(1)
C(7)	4678(2)	7474(8)	4980(2)	26(1)
C(8)	4773(2)	8206(9)	6128(2)	34(1)
C(9)	6422(2)	8781(12)	4626(3)	47(1)
C(10)	6924(2)	8799(12)	4625(3)	51(1)
C(11)	7227(2)	7533(12)	5004(3)	45(1)
C(12)	7000(2)	6323(12)	5393(3)	52(1)
C(13)	6496(2)	6358(12)	5380(3)	48(1)
N(1)	6219(2)	7573(8)	5011(2)	37(1)
Ni(1)	5000	8650(2)	7500	40(1)
O(1)	4087(2)	6599(8)	3846(2)	49(1)
O(2)	4757(2)	6460(7)	3368(2)	39(1)
O(3A)	4313(5)	8430(70)	6141(13)	36(4)
O(3B)	4309(5)	7790(80)	6091(14)	35(5)
O(4)	5088(2)	8572(7)	6592(2)	41(1)
O(5)	4781(3)	5911(12)	7353(4)	40(2)
O(6)	5315(3)	11444(14)	7662(3)	42(2)
O(7A)	5762(3)	7919(17)	7678(4)	49(3)
O(7B)	5717(3)	9548(19)	7693(4)	44(3)
O(8A)	3664(4)	5025(17)	2806(4)	70(3)
O(8B)	3789(7)	3700(40)	2865(8)	67(4)
O(9A)	3647(6)	7800(30)	1881(8)	72(4)
O(9B)	3784(12)	7020(50)	2007(14)	81(5)
O(10)	3523(2)	4608(13)	1014(3)	87(2)
O(11)	2816(3)	9720(16)	1934(4)	114(3)
O(12)	2036(3)	7136(16)	1996(4)	126(3)
O(13)	1673(3)	4408(13)	1044(3)	101(2)
O(14A)	2514(9)	3020(30)	545(13)	84(5)
O(14B)	2625(3)	2683(14)	1058(5)	77(3)

Table S3. Bond lengths [Å] and angles [°] for Ni-ZW-MOF.

C(1)-O(2)	1.242(7)
C(1)-O(1)	1.252(7)
C(1)-C(2)	1.515(8)
C(2)-C(3)	1.374(8)
C(2)-C(7)	1.403(7)
C(3)-C(4)	1.376(7)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(7)
C(4)-N(1)	1.460(7)
C(5)-C(6)	1.377(8)
C(5)-H(5)	0.9500
C(6)-C(7)	1.397(7)
C(6)-C(8)	1.505(7)
C(7)-H(7)	0.9500
C(8)-O(4)	1.259(7)
C(8)-O(3A)	1.266(13)
C(8)-O(3B)	1.287(14)
C(9)-N(1)	1.354(8)
C(9)-C(10)	1.369(9)
C(9)-H(9)	0.9500
C(10)-C(11)	1.394(9)
C(10)-H(10)	0.9500
C(11)-C(12)	1.395(9)
C(11)-C(11)#1	1.488(13)
C(12)-C(13)	1.372(9)
C(12)-H(12)	0.9500
C(13)-N(1)	1.325(8)
C(13)-H(13)	0.9500
Ni(1)-O(5)	1.999(8)
Ni(1)-O(4)	2.026(4)
Ni(1)-O(4)#2	2.026(4)
Ni(1)-O(7B)	2.039(7)
Ni(1)-O(7B)#2	2.039(7)
Ni(1)-O(7A)#2	2.120(7)
Ni(1)-O(7A)	2.120(7)
Ni(1)-O(6)	2.125(10)
O(5)-H(5A)	0.8859
O(5)-H(5B)	0.8867
O(6)-H(6A)	0.9107

O(6)-H(6B)	0.9123
O(7A)-H(7AA)	0.8695
O(7A)-H(7AB)	0.8707
O(7B)-H(7BA)	0.8900
O(7B)-H(7BB)	0.8894
O(9B)-H(9BA)	0.8704
O(9B)-H(9BB)	0.8697
O(10)-H(10A)	0.8680
O(10)-H(10B)	0.8667
O(11)-H(11A)	0.8717
O(11)-H(11B)	0.8702
O(13)-H(13A)	0.8703
O(13)-H(13B)	0.8686
O(14B)-H(14A)	0.8701
O(14B)-H(14B)	0.8700

O(2)-C(1)-O(1)	126.0(5)
O(2)-C(1)-C(2)	115.8(5)
O(1)-C(1)-C(2)	118.2(5)
C(3)-C(2)-C(7)	119.1(5)
C(3)-C(2)-C(1)	120.3(5)
C(7)-C(2)-C(1)	120.6(5)
C(2)-C(3)-C(4)	119.3(5)
C(2)-C(3)-H(3)	120.4
C(4)-C(3)-H(3)	120.4
C(3)-C(4)-C(5)	122.4(5)
C(3)-C(4)-N(1)	119.5(5)
C(5)-C(4)-N(1)	118.1(5)
C(6)-C(5)-C(4)	119.1(5)
C(6)-C(5)-H(5)	120.5
C(4)-C(5)-H(5)	120.5
C(5)-C(6)-C(7)	119.2(5)
C(5)-C(6)-C(8)	119.4(5)
C(7)-C(6)-C(8)	121.4(5)
C(6)-C(7)-C(2)	120.9(5)
C(6)-C(7)-H(7)	119.5
C(2)-C(7)-H(7)	119.5
O(4)-C(8)-O(3A)	121.6(15)
O(4)-C(8)-O(3B)	130.6(15)
O(4)-C(8)-C(6)	115.1(5)

O(3A)-C(8)-C(6)	122.3(14)
O(3B)-C(8)-C(6)	113.4(17)
N(1)-C(9)-C(10)	120.0(6)
N(1)-C(9)-H(9)	120.0
C(10)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	120.3(6)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	117.5(6)
C(10)-C(11)-C(11)#1	121.6(7)
C(12)-C(11)-C(11)#1	121.0(7)
C(13)-C(12)-C(11)	120.2(6)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
N(1)-C(13)-C(12)	120.6(6)
N(1)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
C(13)-N(1)-C(9)	121.4(6)
C(13)-N(1)-C(4)	119.7(5)
C(9)-N(1)-C(4)	118.8(5)
O(5)-Ni(1)-O(4)	83.7(3)
O(5)-Ni(1)-O(4)#2	93.4(3)
O(4)-Ni(1)-O(4)#2	176.9(3)
O(4)-Ni(1)-O(7B)	88.4(3)
O(4)#2-Ni(1)-O(7B)	92.6(3)
O(5)-Ni(1)-O(7B)#2	89.9(5)
O(4)-Ni(1)-O(7B)#2	92.6(3)
O(4)#2-Ni(1)-O(7B)#2	88.4(3)
O(7B)-Ni(1)-O(7B)#2	144.5(8)
O(5)-Ni(1)-O(7A)#2	58.8(4)
O(4)-Ni(1)-O(7A)#2	93.3(2)
O(4)#2-Ni(1)-O(7A)#2	85.9(2)
O(5)-Ni(1)-O(7A)	93.8(4)
O(4)-Ni(1)-O(7A)	85.9(2)
O(4)#2-Ni(1)-O(7A)	93.3(2)
O(7A)#2-Ni(1)-O(7A)	152.4(7)
O(5)-Ni(1)-O(6)	173.6(4)
O(4)-Ni(1)-O(6)	95.0(3)
O(4)#2-Ni(1)-O(6)	87.8(3)
O(7A)#2-Ni(1)-O(6)	127.6(4)

O(7A)-Ni(1)-O(6)	79.8(4)
C(8)-O(4)-Ni(1)	129.1(4)
Ni(1)-O(5)-H(5A)	110.3
Ni(1)-O(5)-H(5B)	110.0
H(5A)-O(5)-H(5B)	103.6
Ni(1)-O(6)-H(6A)	111.5
Ni(1)-O(6)-H(6B)	112.1
H(6A)-O(6)-H(6B)	102.1
Ni(1)-O(7A)-H(7AA)	128.0
Ni(1)-O(7A)-H(7AB)	127.4
H(7AA)-O(7A)-H(7AB)	104.3
Ni(1)-O(7B)-H(7BA)	110.8
Ni(1)-O(7B)-H(7BB)	110.8
H(7BA)-O(7B)-H(7BB)	103.3
H(9BA)-O(9B)-H(9BB)	104.5
H(10A)-O(10)-H(10B)	104.9
H(11A)-O(11)-H(11B)	104.3
H(13A)-O(13)-H(13B)	104.6
H(14A)-O(14B)-H(14B)	104.4

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

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ni-ZW-MOF. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + \cdots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(3)	36(3)	21(2)	1(2)	1(2)	-7(2)
C(2)	33(2)	28(2)	19(2)	0(2)	4(2)	-6(2)
C(3)	31(2)	31(2)	21(2)	-2(2)	5(2)	-3(2)
C(4)	30(3)	31(2)	21(2)	-2(2)	5(2)	-5(2)
C(5)	33(2)	28(2)	20(2)	-2(2)	2(2)	-4(2)
C(6)	35(2)	29(2)	16(2)	2(2)	6(2)	4(2)
C(7)	30(2)	30(2)	19(2)	2(2)	6(2)	0(2)
C(8)	41(3)	44(3)	17(2)	6(2)	4(2)	10(3)
C(9)	32(3)	71(3)	37(3)	22(3)	7(2)	-5(3)
C(10)	33(3)	81(3)	40(3)	27(3)	7(2)	-3(3)
C(11)	30(3)	77(3)	29(3)	22(3)	4(2)	-1(3)
C(12)	35(3)	81(3)	40(3)	29(3)	5(2)	0(3)
C(13)	34(3)	74(3)	36(3)	23(3)	6(2)	0(3)

N(1)	27(2)	60(3)	24(2)	13(2)	3(2)	-2(2)
Ni(1)	61(1)	45(1)	14(1)	0	7(1)	0
O(1)	38(3)	85(4)	23(2)	4(2)	-1(2)	-19(3)
O(2)	50(3)	49(3)	19(2)	-6(2)	8(2)	-7(2)
O(3A)	42(6)	40(11)	27(5)	-1(8)	9(4)	25(5)
O(3B)	37(6)	47(12)	22(6)	5(8)	9(4)	23(6)
O(4)	53(3)	53(3)	18(2)	0(2)	7(2)	7(2)
O(5)	62(6)	33(4)	27(4)	8(3)	12(4)	0(4)
O(6)	45(5)	61(6)	20(4)	-7(4)	0(3)	10(5)
O(7A)	59(6)	69(8)	20(4)	9(4)	7(4)	-5(5)
O(7B)	45(6)	57(7)	28(5)	3(5)	1(4)	-24(5)
O(8A)	78(6)	69(7)	56(5)	-21(5)	-10(4)	-13(6)
O(8B)	68(9)	76(9)	56(7)	-34(8)	6(7)	-8(9)
O(9A)	50(8)	92(12)	67(8)	-2(7)	-12(5)	10(6)
O(9B)	67(11)	94(14)	78(10)	12(10)	-10(9)	10(9)
O(10)	70(4)	116(6)	75(5)	-1(4)	3(3)	-19(4)
O(11)	80(5)	190(10)	73(5)	-5(6)	10(4)	-24(6)
O(12)	78(5)	205(10)	94(6)	17(6)	6(4)	2(6)
O(13)	92(6)	138(7)	73(5)	19(5)	12(4)	11(5)
O(14A)	75(9)	81(9)	95(10)	-6(10)	12(9)	-4(8)
O(14B)	59(6)	87(6)	85(7)	-29(6)	10(5)	-17(5)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ni-ZW-MOF.

	x	y	z	U(eq)
H(3)	5527	7005	4072	33
H(5)	5705	8133	5912	33
H(7)	4329	7426	4975	32
H(9)	6216	9616	4357	56
H(10)	7067	9678	4365	61
H(12)	7196	5472	5668	62
H(13)	6343	5503	5638	57
H(5A)	5035	5178	7284	60
H(5B)	4690	5416	7695	60
H(6A)	5079	12349	7703	64
H(6B)	5450	11894	7328	64
H(7AA)	5993	8155	7449	74
H(7AB)	5908	7203	7978	74

H(7BA)	5741	10815	7632	66
H(7BB)	5828	9410	8094	66
H(9BA)	3543	6394	1790	122
H(9BB)	4049	6384	1951	122
H(10A)	3568	3753	735	131
H(10B)	3820	4939	1177	131
H(11A)	2503	9506	1956	172
H(11B)	2823	10897	1794	172
H(13A)	1674	3547	753	152
H(13B)	1883	3973	1348	152
H(14A)	2364	3361	1105	116
H(14B)	2826	3506	921	116

Table S6. Torsion angles [°] for Ni-ZW-MOF.

O(2)-C(1)-C(2)-C(3)	-3.4(8)
O(1)-C(1)-C(2)-C(3)	178.0(6)
O(2)-C(1)-C(2)-C(7)	178.8(5)
O(1)-C(1)-C(2)-C(7)	0.2(9)
C(7)-C(2)-C(3)-C(4)	0.5(8)
C(1)-C(2)-C(3)-C(4)	-177.3(5)
C(2)-C(3)-C(4)-C(5)	-1.1(9)
C(2)-C(3)-C(4)-N(1)	178.7(5)
C(3)-C(4)-C(5)-C(6)	0.4(9)
N(1)-C(4)-C(5)-C(6)	-179.4(5)
C(4)-C(5)-C(6)-C(7)	0.8(8)
C(4)-C(5)-C(6)-C(8)	179.5(5)
C(5)-C(6)-C(7)-C(2)	-1.3(8)
C(8)-C(6)-C(7)-C(2)	-180.0(5)
C(3)-C(2)-C(7)-C(6)	0.6(8)
C(1)-C(2)-C(7)-C(6)	178.5(5)
C(5)-C(6)-C(8)-O(4)	2.5(8)
C(7)-C(6)-C(8)-O(4)	-178.8(5)
C(5)-C(6)-C(8)-O(3A)	171(3)
C(7)-C(6)-C(8)-O(3A)	-10(3)
C(5)-C(6)-C(8)-O(3B)	-168(2)
C(7)-C(6)-C(8)-O(3B)	11(2)
N(1)-C(9)-C(10)-C(11)	2.1(12)
C(9)-C(10)-C(11)-C(12)	-2.3(12)

C(9)-C(10)-C(11)-C(11)#1	177.7(9)
C(10)-C(11)-C(12)-C(13)	2.1(12)
C(11)#1-C(11)-C(12)-C(13)	-177.9(9)
C(11)-C(12)-C(13)-N(1)	-1.8(12)
C(12)-C(13)-N(1)-C(9)	1.5(11)
C(12)-C(13)-N(1)-C(4)	178.5(7)
C(10)-C(9)-N(1)-C(13)	-1.7(11)
C(10)-C(9)-N(1)-C(4)	-178.7(7)
C(3)-C(4)-N(1)-C(13)	-121.3(7)
C(5)-C(4)-N(1)-C(13)	58.5(8)
C(3)-C(4)-N(1)-C(9)	55.7(8)
C(5)-C(4)-N(1)-C(9)	-124.4(7)
O(3A)-C(8)-O(4)-Ni(1)	24(3)
O(3B)-C(8)-O(4)-Ni(1)	0(3)
C(6)-C(8)-O(4)-Ni(1)	-167.7(4)

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

Table S7. Hydrogen bonds for Ni-ZW-MOF [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(9)-H(9)···O(3A^a)#3	0.95	2.15	3.10(3)	171.6
C(9)-H(9)···O(3B^b)#3	0.95	2.42	3.34(4)	165.5
C(10)-H(10)···O(14A^b)#4	0.95	2.58	3.34(3)	137.9
C(10)-H(10)···O(14B^a)#4	0.95	2.47	3.382(12)	161.8
C(12)-H(12)···O(14A^b)#5	0.95	2.59	3.31(3)	132.7
C(12)-H(12)···O(14B^a)#5	0.95	2.56	3.464(12)	158.0
C(13)-H(13)···O(1)#6	0.95	2.26	3.206(8)	173.3
O(5^a)-H(5A^a)···O(2)#6	0.89	1.96	2.699(10)	139.7
O(5^a)-H(5B^a)···O(2)#7	0.89	1.95	2.762(9)	152.0
O(6^a)-H(6A^a)···O(2)#8	0.91	1.98	2.725(10)	138.6
O(6^a)-H(6B^a)···O(2)#3	0.91	1.92	2.655(10)	136.5
O(7B^b)-H(7BA^b)···O(9B^b)#3	0.89	2.06	2.77(3)	135.4
O(7B^b)-H(7BB^b)···O(3B^b)#2	0.89	2.18	2.93(4)	141.7

Symmetry transformations used to generate equivalent atoms:
#1 = -x+3/2, -y+3/2, -z+1; #2 = -x+1, y, -z+3/2; #3 = -x+1, -y+2, -z+1; #4 = -x+1, y+1, -z+1/2; #5 = x+1/2, -y+1/2, z+1/2; #6 = -x+1, -y+1, -z+1; #7 = x, -y+1, z+1/2; #8 = x, -y+2, z+1/2.

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