Supplementary Information

Reversible Water Ad-/de-sorption Behavior of a 3D Polycatenation Network, [Zn(bpp)(BDC)]·1.5(H_2O), Constructed by 2D Undulated Layered MOF

Supporting Information

Table S1. Crystal data and structure refinement.

Identification code	ic18161	
Empirical formula	C21 H20 N2 O5 Zn	
Formula weight	445.76	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.9706(8) Å	α= 90°.
	b = 11.4874(5) Å	β= 119.0890(10)°.
	c = 19.5792(11) Å	γ = 90°.
Volume	4121.7(3) $Å^3$	
Z	8	
Density (calculated)	1.437 Mg/m^3	
Absorption coefficient	1.226 mm^{-1}	
F(000)	1840	
Crystal size	0.37 x 0.09 x 0.08 mm^3	
Theta range for data collection	2.38 to 27.54°.	
Index ranges	-27<=h<=25, -14<=k<=14, -21<=l<=25	
Reflections collected	22559	
Independent reflections	4747 [R(int) = 0.0660]	
Completeness to theta = 27.54°	99.5 %	
Max. and min. transmission	0.9072 and 0.6605	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4747 / 0 / 351	
Goodness-of-fit on F^2	1.573	
Final R indices [I>2sigma(I)]	R1 = 0.0684, wR2 = 0.2246	
R indices (all data)	R1 = 0.0892, wR2 = 0.2305	
Largest diff. peak and hole	1.383 and -0.826 e.$Å^{-3}$	

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

	x	y	z	U(eq)
Zn(1)	8696(1)	6272(1)	8069(1)	16(1)
N(1)	9356(2)	4880(4)	8223(2)	20(1)
N(2)	13014(2)	715(4)	8482(2)	19(1)
O(1)	9439(2)	7268(3)	8890(2)	22(1)
O(2)	8475(2)	8424(3)	8402(2)	25(1)
O(3)	7943(2)	6430(3)	6947(2)	23(1)
O(4)	8973(2)	7056(3)	7020(2)	27(1)
O(5)	7310(3)	9026(5)	8698(3)	45(1)
O(6)	10000	8878(7)	7500	91(4)
C(1)	9135(3)	3748(5)	8189(4)	34(1)
C(2)	9608(5)	2835(6)	8333(6)	69(3)
C(3)	10327(4)	3022(7)	8523(7)	90(4)
C(4)	10533(4)	4179(7)	8526(5)	51(2)
C(5)	10056(3)	5062(5)	8384(3)	28(1)
C(6)	11030(30)	1980(30)	9120(40)	430(40)
C(7)	10720(30)	1010(30)	8720(40)	470(30)
C(8)	11415(4)	178(6)	9215(4)	38(2)
C(9)	11987(3)	311(4)	8982(3)	26(1)
C(10)	12667(3)	767(5)	9484(3)	32(1)
C(11)	13171(3)	945(5)	9218(3)	26(1)
C(12)	12352(3)	268(5)	7995(3)	23(1)
C(13)	11841(3)	52(5)	8218(3)	27(1)
C(14)	9128(3)	8242(4)	8867(3)	19(1)
C(15)	9580(3)	9156(4)	9445(3)	16(1)
C(16)	10303(3)	8922(4)	10015(3)	17(1)
C(17)	9283(3)	10246(5)	9450(3)	21(1)
C(18)	8302(3)	6874(4)	6635(3)	19(1)
C(19)	7878(3)	7186(4)	5785(3)	16(1)
C(20)	7145(3)	7402(5)	5427(3)	22(1)
C(21)	8250(3)	7280(4)	5351(3)	19(1)

Table S3. Bond lengths [Å] and angles [°].

Zn(1)-O(1)	1.971(3)	Zn(1)-O(3)	1.995(3)
Zn(1)-N(1)	2.039(4)	Zn(1)-N(2)#1	2.058(4)
N(1)-C(5)	1.360(7)	N(1)-C(1)	1.370(7)
N(2)-C(11)	1.340(6)	N(2)-C(12)	1.345(6)
N(2)-Zn(1)#2	2.058(4)	O(1)-C(14)	1.284(6)
O(2)-C(14)	1.239(6)	O(3)-C(18)	1.285(6)
O(4)-C(18)	1.250(6)	C(1)-C(2)	1.375(9)
C(2)-C(3)	1.383(10)	C(3)-C(4)	1.396(11)
C(3)-C(6)	1.81(5)	C(4)-C(5)	1.355(9)
C(6)-C(7)	1.34(7)	C(7)-C(8)	1.62(5)
C(8)-C(9)	1.483(8)	C(9)-C(10)	1.382(9)
C(9)-C(13)	1.406(8)	C(10)-C(11)	1.400(8)
C(12)-C(13)	1.363(8)	C(14)-C(15)	1.497(7)
C(15)-C(17)	1.400(7)	C(15)-C(16)	1.405(7)
C(16)-C(17)#3	1.371(7)	C(17)-C(16)#3	1.371(7)
C(18)-C(19)	1.499(6)	C(19)-C(20)	1.367(7)
C(19)-C(21)	1.410(7)	C(20)-C(21)#4	1.383(7)
C(21)-C(20)#4	1.383(7)		
O(1)-Zn(1)-O(3)	137.25(14)	O(1)-Zn(1)-N(1)	97.14(16)
O(3)-Zn(1)-N(1)	110.59(16)	O(1)-Zn(1)-N(2)#1	106.54(16)
O(3)-Zn(1)-N(2)#1	97.52(15)	N(1)-Zn(1)-N(2)#1	104.41(17)
C(5)-N(1)-C(1)	117.3(5)	C(5)-N(1)-Zn(1)	119.4(4)
C(1)-N(1)-Zn(1)	123.3(4)	C(11)-N(2)-C(12)	117.8(5)
C(11)-N(2)-Zn(1)#2	120.5(4)	C(12)-N(2)-Zn(1)#2	121.0(3)
C(14)-O(1)-Zn(1)	106.9(3)	C(18)-O(3)-Zn(1)	103.1(3)
N(1)-C(1)-C(2)	121.5(6)	C(1)-C(2)-C(3)	121.3(7)
C(2)-C(3)-C(4)	116.3(6)	C(2)-C(3)-C(6)	120.6(17)
C(4)-C(3)-C(6)	118.2(18)	C(5)-C(4)-C(3)	121.1(6)
C(4)-C(5)-N(1)	122.5(6)	C(7)-C(6)-C(3)	99(6)
C(6)-C(7)-C(8)	96(5)	C(9)-C(8)-C(7)	113(2)
C(10)-C(9)-C(13)	116.9(5)	C(10)-C(9)-C(8)	122.0(6)
C(13)-C(9)-C(8)	120.9(6)	C(9)-C(10)-C(11)	119.7(5)
N(2)-C(11)-C(10)	122.4(5)	N(2)-C(12)-C(13)	122.9(5)
C(12)-C(13)-C(9)	120.2(5)	O(2)-C(14)-O(1)	122.3(4)
O(2)-C(14)-C(15)	120.2(5)	O(1)-C(14)-C(15)	117.4(4)
C(17)-C(15)-C(16)	118.5(4)	C(17)-C(15)-C(14)	120.9(4)

C(16)-C(15)-C(14)	120.6(4)	C(17)#3-C(16)-C(15)	120.7(5)
C(16)#3-C(17)-C(15)	120.7(5)	O(4)-C(18)-O(3)	121.9(4)
O(4)-C(18)-C(19)	121.0(4)	O(3)-C(18)-C(19)	117.1(4)
C(20)-C(19)-C(21)	119.4(5)	C(20)-C(19)-C(18)	121.6(5)
C(21)-C(19)-C(18)	119.0(4)	C(19)-C(20)-C(21)#4	122.3(5)
C(20)#4-C(21)-C(19)	118.2(5)		

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,y+1/2,z #2 x+1/2,y-1/2,z #3 -x+2,-y+2,-z+2 #4 -x+3/2,-y+3/2,-z+1

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	15(1)	17(1)	13(1)	-2(1)	4(1)	0(1)
N(1)	19(2)	16(2)	26(2)	2(2)	11(2)	1(2)
N(2)	24(2)	18(2)	19(2)	-3(2)	14(2)	-1(2)
O(1)	22(2)	18(2)	22(2)	-6(1)	6(2)	-1(1)
O(2)	21(2)	21(2)	20(2)	-5(1)	0(2)	-4(2)
O(3)	29(2)	26(2)	15(2)	1(1)	12(2)	-4(2)
O(4)	22(2)	27(2)	20(2)	1(2)	2(2)	-4(2)
O(5)	42(3)	38(3)	66(3)	17(2)	35(3)	12(2)
O(6)	40(5)	33(5)	167(11)	0	25(6)	0
C(1)	30(3)	21(3)	63(4)	10(3)	31(3)	4(2)
C(2)	71(6)	20(4)	152(9)	29(4)	83(6)	15(4)
C(3)	54(5)	46(5)	199(11)	72(6)	86(7)	39(4)
C(4)	27(4)	52(4)	84(5)	37(4)	34(4)	15(3)
C(5)	16(3)	31(3)	31(3)	12(2)	7(2)	2(2)
C(6)	530(70)	160(30)	830(130)	60(50)	510(90)	120(40)
C(7)	650(70)	190(30)	400(60)	-10(40)	130(50)	110(40)
C(8)	47(4)	34(4)	48(4)	29(3)	35(3)	24(3)
C(9)	37(3)	13(3)	39(3)	7(2)	27(3)	9(2)
C(10)	51(4)	32(3)	25(3)	8(2)	29(3)	17(3)
C(11)	27(3)	28(3)	19(2)	1(2)	8(2)	1(2)
C(12)	21(3)	26(3)	20(3)	-10(2)	9(2)	-6(2)
C(13)	28(3)	25(3)	32(3)	-5(2)	18(3)	-2(3)
C(14)	20(3)	21(3)	13(2)	-4(2)	5(2)	-5(2)
C(15)	16(2)	15(2)	16(2)	0(2)	8(2)	-2(2)
C(16)	16(3)	17(3)	19(2)	3(2)	9(2)	5(2)
C(17)	17(3)	25(3)	21(2)	1(2)	9(2)	0(2)
C(18)	22(3)	16(3)	17(2)	-4(2)	9(2)	-1(2)
C(19)	15(2)	13(2)	13(2)	1(2)	1(2)	-3(2)
C(20)	25(3)	20(3)	26(3)	-4(2)	17(3)	-5(2)
C(21)	17(3)	19(3)	18(2)	4(2)	5(2)	2(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3)

	x	y	z	U(eq)
H(5B)	7740(30)	8760(50)	8740(30)	25(16)
H(5A)	7260(30)	9820(60)	8570(40)	33(17)
H(6OA)	9470(100)	7400(200)	7420(140)	290(140)
H(1)	8560(30)	3840(50)	8080(30)	34(18)
H(2)	9290(60)	2060(100)	8150(60)	160(40)
H(4)	10980(50)	4500(100)	8440(60)	110(40)
H(5)	10100(50)	6080(90)	8110(60)	120(30)
H(6B)	10721(10)	1891(19)	8412(10)	-321(4)
H(6A)	10994(11)	2220(20)	9018(11)	-246(4)
H(7B)	11115(10)	1415(19)	9256(11)	-330(4)
H(7A)	10731(10)	996(19)	8763(11)	-263(4)
H(8B)	11650(30)	10(40)	9710(30)	6(12)
H(8A)	11170(40)	-580(80)	8880(50)	70(30)
H(10)	12770(40)	1210(50)	10060(40)	50(20)
H(11)	13760(40)	1530(60)	9750(40)	60(20)
H(12)	12320(30)	180(50)	7550(30)	26(16)
H(13)	11480(30)	-290(60)	7920(40)	41(19)
H(16)	10500(40)	8150(80)	10090(50)	80(30)
H(17)	8700(30)	10470(40)	9020(30)	18(13)
H(20)	6970(30)	7520(50)	5610(30)	5(15)
H(21)	8760(30)	7160(40)	5600(30)	3(11)

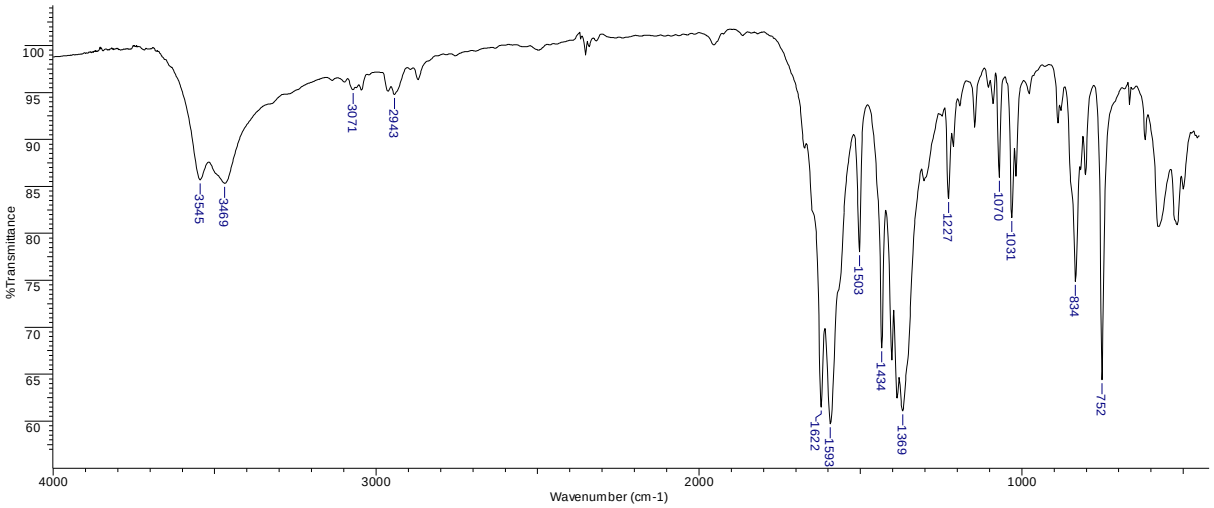

Figure S1 IR spectrum of compound **1**