

**Two-folded interpenetrated metal-organic framework constructed by zinc(II) and mixed ligands**

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**Materials and Measurements.** Reagents and solvents employed were commercially available. C, H and N analyses were carried out with a Perkin Elmer 240C elemental analyzer. Powder X-ray diffraction (PXRD) measurements were performed on a Bruker D8 Advance X-ray diffractometer using Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ), in which the X-ray tube was operated at 40 kV and 40 mA. The gas sorption isotherms were measured by Micromeritics ASAP 2020 M+C surface area analyzer.

**Gas Sorption Measurements**

In the gas sorption measurement, Ultra-high-purity grade, N<sub>2</sub> (>99.999%) were used throughout the adsorption experiments. All of the measured sorption isotherms have been repeated several times to confirm the reproducibility within experimental error. Adsorption measurements (up to 1 bar) were performed on Micromeritics ASAP 2020 M+C surface area analyzer. About 100 mg of samples **1** were activated at 80 °C for one night by using the “outgas” function of the surface area analyzer. Helium was used for the estimation of the dead volume, assuming that it is not adsorbed at any of the studied temperatures. To provide high accuracy and precision in determining P/P<sub>0</sub>, the saturation pressure P<sub>0</sub> was measured throughout the N<sub>2</sub> analyses by means of a dedicated saturation pressure transducer, which allowed us to monitor the vapor pressure for each data point.

Elemental analysis calcd. for C<sub>69</sub>H<sub>75</sub>N<sub>15</sub>O<sub>23</sub>Zn<sub>3</sub> (1): C, 49.37; H, 4.50; N, 12.52, Found: C, 49.34; H, 4.41; N, 12.58.

**Table S1** Bond lengths [Å] and angles [deg] for the title compound.

Zn1	-O7	2.499(5)	Zn3	-N4_f	2.017(3)
Zn1	-O8	2.023(6)	Zn2	-O9_h	2.335(9)
Zn1	-O12	1.953(3)	Zn3	-O3_b	1.977(4)
Zn1	-N1	2.024(4)	Zn3	-N11	2.070(5)
Zn1	-N7	2.042(3)	Zn3	-O6	2.025(4)
Zn2	-O13	1.983(4)	Zn3	-O5	2.455(4)
Zn2	-N6	2.012(4)	Zn2	-O10'_h	1.924(9)
Zn2	-N10_e	2.023(5)	Zn2	-O10_h	2.443(14)
O7 -Zn1 -O8	56.7(2)	O10_h -Zn2 -O10'_h	21.2(4)		
O7 -Zn1 -O12	137.74(14)	O9_h -Zn2 -O10_h	63.9(4)		
O7 -Zn1 -N1	101.06(16)	O10'_h -Zn2 -N10_e	109.1(3)		
O7 -Zn1 -N7	83.61(15)	O5 -Zn3 -O6	56.58(16)		
O8 -Zn1 -O12	102.50(19)	O5 -Zn3 -N11	144.45(15)		
O8 -Zn1 -N1	104.85(19)	O3_b -Zn3 -O5	89.17(14)		
O8 -Zn1 -N7	137.7(2)	O4_b -Zn3 -O5	128.49(14)		
O12 -Zn1 -N1	120.64(16)	O5 -Zn3 -N4_f	100.87(15)		
O12 -Zn1 -N7	97.67(13)	O6 -Zn3 -N11	89.07(18)		
N1 -Zn1 -N7	95.91(15)	O3_b -Zn3 -O6	118.43(14)		
O13 -Zn2 -N6	102.25(17)	O4_b -Zn3 -O6	168.11(14)		
O13 -Zn2 -N10_e	94.11(17)	O6 -Zn3 -N4_f	108.31(16)		
O9_h -Zn2 -O13	162.9(3)	O3_b -Zn3 -N11	101.39(17)		
O10_h -Zn2 -O13	102.5(4)	O4_b -Zn3 -N11	83.52(16)		
O10'_h -Zn2 -O13	113.4(3)	N4_f -Zn3 -N11	98.43(17)		
O3_b -Zn3 -O4_b	54.58(12)	O9_h -Zn2 -N10_e	96.8(3)		
N6 -Zn2 -N10_e	109.55(18)	O3_b -Zn3 -N4_f	129.02(17)		
O9_h -Zn2 -N6	86.4(3)	O4_b -Zn3 -N4_f	82.06(14)		
O10_h -Zn2 -N6	145.2(3)	O10'_h -Zn2 -N6	124.2(3)		
O10_h -Zn2 -N10_e	92.7(4)	O9_h -Zn2 -O10'_h	50.4(3)		

Symmetry transformations used to generate equivalent atoms:

b = [1455.00] = -1+x, y, z

e = [1556.00] = x, y, 1+z

f = [1564.00] = x, 1+y, -1+z

h = [1665.00] = 1+x, 1+y, z