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Supplementary Information

'Eye' Of The Molecule — A Viewpoint

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Synthesis of MOF-711.

Zirconyl chloride octahydrate, $ZrOCl_2 \cdot 8H_2O$ (purity, 98 %), 1,4-dicarboxylic acid (H_2BDC), and N,N-dimethylformamide (DMF) (purity ≥ 99.9 %), were purchased form Sigma Aldrich Co. All chemicals obtained were used without further purification. Scintillation vials (20 mL) and polypropylene cabs with foil liner were purchased form Wheaton.

In a 20 mL scintillation vial, a mixture solution of $ZrOCl_2 \cdot 8H_2O$ (8.0 mg, 0.045 mmol) and H_2BDC (12.0 mg, 0.060 mmol) in DMF (1 mL) was prepared. The solution was sonicated for 1 min and formic acid (1 mL) was added to the solution. The vial was capped and placed in a preheated 90 °C oven. After 2 days, truncated octahedral shape single crystals, UiO-66, with size range from 50 to 100 μm were obtained on the wall of the vial. We also observed about 1% of rod-shaped crystals ($50 \times 20 \times 20\ \mu m^3$), MOF-711, in the batch. We tried multiple times to reproduce MOF-711. However, since then we only obtained UiO-66 from the synthesis condition. The crystallization condition of MOF-711 seems very narrow and sensitive to temperature. We believe that a subtle temperature difference can affect the formation of the crystals. It is recommended that several vials containing the solution be set together and placed in different locations in the oven. Also, the amount of formic acid might be critical to obtain crystals.

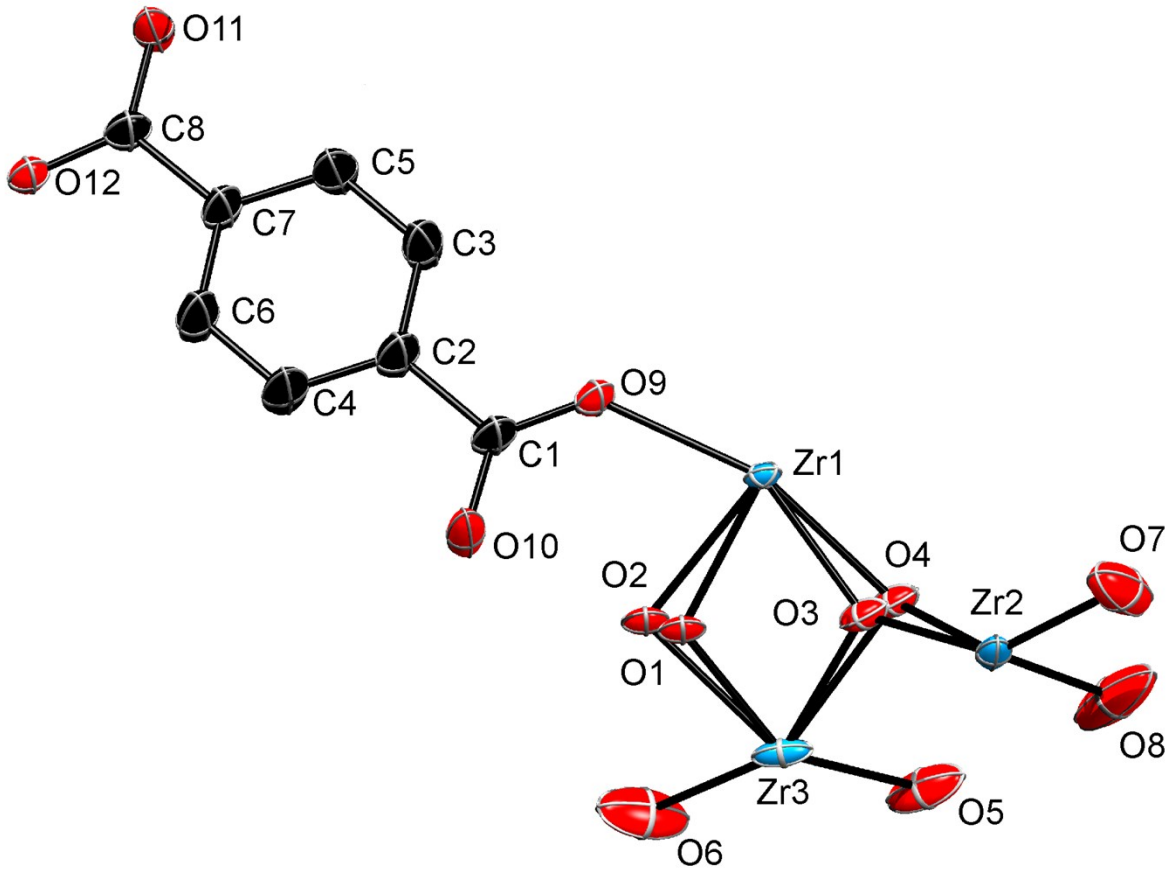

Figure S1. Asymmetric unit of MOF-711. The structure is refined anisotropically and presented in an ellipsoid model with 50 % of electron probability.

Table 1. Crystal data and structure refinement for MOF-711.

Identification code	MOF-711
Empirical formula	$C_{16}H_8O_{16}Zr_3$
Formula weight	729.88
Temperature/K	273.15
Crystal system	orthorhombic
Space group	*Pnnm*
a/Å	13.4687(15)
b/Å	14.8959(17)
c/Å	21.264(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4266.2(8)
Z	4
ρ_{calc}g/cm^3	1.136
μ/mm^{-1}	0.969
F(000)	1408.0
Crystal size/mm^3	0.050 × 0.04 × 0.05
Radiation	synchrotron (λ = 0.7749)
2Θ range for data collection/°	3.64 to 59.554
Index ranges	-17 ≤ h ≤ 16, -19 ≤ k ≤ 19, -26 ≤ l ≤ 27
Reflections collected	49328
Independent reflections	4839 [R_{int} = 0.0907, R_{sigma} = 0.0462]
Data/restraints/parameters	4839/0/178
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0442, wR_2 = 0.1284
Final R indexes [all data]	R_1 = 0.0565, wR_2 = 0.1387
Largest diff. peak/hole / e Å^{-3}	1.38/-0.87

Table 2. Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for MOF-711. Ueq is defined as 1/3 of the trace of the orthogonalised UIJ tensor.

Atom	x	y	z	U(eq)
Zr1	5000	5000	3849.8(2)	14.88(13)
Zr2	6133.6(4)	6327.4(3)	5000	24.92(15)
Zr3	6464.8(4)	3968.1(3)	5000	24.50(14)
O1	6125(5)	5117(5)	4506(3)	23.2(11)
O2	6525(6)	5183(6)	4364(4)	23.2(11)
O3	5138(5)	4008(4)	4508(3)	23.6(9)
O4	5193(5)	3643(4)	4363(3)	23.6(9)
O5	6522(4)	2517(3)	5000	55(2)
O6	8075(3)	4236(4)	5000	68.5(17)
O7	7755(4)	6454(4)	5000	69.6(17)
O8	5828(7)	7736(3)	5000	103(3)
O9	4163.3(19)	3996.4(16)	3317.2(11)	26.0(5)
O10	3414(3)	3138(2)	4050.0(13)	57.7(10)
O11	2054(2)	1452(2)	951.2(12)	49.2(9)
O12	1111.7(19)	761.6(16)	1680.1(11)	27.0(5)
C1	3612(3)	3360(3)	3491.5(17)	37.1(10)
C2	3167(4)	2791(3)	2978.0(18)	43.9(11)
C3	3416(4)	2957(4)	2362(2)	59.4(15)
C4	2512(4)	2116(3)	3122.6(19)	62.4(17)
C5	2979(4)	2469(4)	1884.8(19)	60.4(16)
C6	2075(4)	1623(3)	2639(2)	60.5(15)
C7	2297(3)	1803(3)	2023.0(18)	42.8(11)
C8	1783(3)	1300(3)	1508.2(17)	37(1)

Table 3. Bond Lengths for MOF-711.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zr1	**O12**[1]	2.190(2)	**Zr2**	**O10**[6]	2.255(3)
Zr1	**O12**[2]	2.190(2)	**Zr2**	**O10**[3]	2.255(3)
Zr1	**O9**	2.188(2)	**Zr2**	**O7**	2.192(5)
Zr1	**O9**[3]	2.188(2)	**Zr2**	**O8**	2.138(5)
Zr1	**O4**[3]	2.312(6)	**Zr2**	**O4**[6]	2.243(7)
Zr1	**O4**	2.312(6)	**Zr2**	**O4**[3]	2.243(7)
Zr1	**O3**[3]	2.044(6)	**Zr2**	**O3**[3]	2.068(7)
Zr1	**O3**	2.044(6)	**Zr2**	**O3**[6]	2.068(7)
Zr1	**O2**[3]	2.343(8)	**Zr2**	**O2**	2.239(8)
Zr1	**O2**	2.343(8)	**Zr2**	**O2**[5]	2.239(8)
Zr1	**O1**[3]	2.067(7)	**Zr2**	**O1**[5]	2.087(7)
Zr1	**O1**	2.067(7)	**Zr2**	**O1**	2.087(7)
Zr3	**O11**[1]	2.261(3)	**O12**	**C8**	1.262(5)
Zr3	**O11**[4]	2.261(3)	**O9**	**C1**	1.260(5)
Zr3	**O6**	2.205(5)	**O11**	**C8**	1.260(5)
Zr3	**O5**	2.163(4)	**O10**	**C1**	1.261(5)
Zr3	**O4**[5]	2.236(7)	**C7**	**C8**	1.497(5)
Zr3	**O4**	2.236(7)	**C7**	**C6**	1.371(6)
Zr3	**O3**	2.072(7)	**C7**	**C5**	1.384(6)
Zr3	**O3**[5]	2.072(7)	**C2**	**C1**	1.507(5)
Zr3	**O2**	2.260(8)	**C2**	**C4**	1.372(6)
Zr3	**O2**[5]	2.260(8)	**C2**	**C3**	1.375(6)
Zr3	**O1**	2.060(7)	**C4**	**C6**	1.393(6)
Zr3	**O1**[5]	2.060(7)	**C5**	**C3**	1.380(6)

[1]1/2+X,1/2-Y,1/2-Z; [2]1/2-X,1/2+Y,1/2-Z; [3]1-X,1-Y,+Z; [4]1/2+X,1/2-Y,1/2+Z; [5]+X,+Y,1-Z; [6]1-X,1-Y,1-Z.

Table 4. Bond Angles for MOF-711.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O12^{1}	Zr1	O12^{2}	118.10(12)	O10^{6}	Zr2	O10^{3}	127.21(14)
O12^{1}	Zr1	O4	140.6(2)	O7	Zr2	O10^{3}	72.58(11)
O12^{1}	Zr1	O4^{3}	73.33(18)	O7	Zr2	O10^{6}	72.58(11)
O12^{2}	Zr1	O4	73.33(18)	O7	Zr2	O4^{6}	142.41(18)
O12^{2}	Zr1	O4^{3}	140.6(2)	O7	Zr2	O4^{3}	142.41(18)
O12^{2}	Zr1	O2^{3}	141.2(2)	O7	Zr2	O2^{5}	80.3(3)
O12^{2}	Zr1	O2	72.6(2)	O7	Zr2	O2	80.3(3)
O12^{1}	Zr1	O2^{3}	72.6(2)	O8	Zr2	O10^{3}	72.87(13)
O12^{1}	Zr1	O2	141.2(2)	O8	Zr2	O10^{6}	72.87(13)
O9	Zr1	O12^{1}	74.67(10)	O8	Zr2	O7	96.2(3)
O9	Zr1	O12^{2}	74.46(10)	O8	Zr2	O4^{6}	80.1(3)
O9^{3}	Zr1	O12^{2}	74.67(10)	O8	Zr2	O4^{3}	80.1(3)
O9^{3}	Zr1	O12^{1}	74.46(10)	O8	Zr2	O2	142.4(2)
O9^{3}	Zr1	O9	117.66(12)	O8	Zr2	O2^{5}	142.4(2)
O9^{3}	Zr1	O4	141.60(19)	O4^{3}	Zr2	O10^{6}	138.5(2)
O9^{3}	Zr1	O4^{3}	72.86(19)	O4^{3}	Zr2	O10^{3}	70.6(2)
O9	Zr1	O4^{3}	141.60(19)	O4^{6}	Zr2	O10^{3}	138.5(2)
O9	Zr1	O4	72.86(19)	O4^{6}	Zr2	O10^{6}	70.6(2)
O9^{3}	Zr1	O2^{3}	140.6(2)	O4^{3}	Zr2	O4^{6}	74.3(4)
O9	Zr1	O2	140.6(2)	O3^{6}	Zr2	O7	147.75(19)
O9	Zr1	O2^{3}	73.2(2)	O3^{3}	Zr2	O7	147.75(19)
O9^{3}	Zr1	O2	73.2(2)	O3^{3}	Zr2	O8	94.5(3)
O4^{3}	Zr1	O4	123.6(3)	O3^{6}	Zr2	O8	94.5(3)
O4^{3}	Zr1	O2	77.1(3)	O3^{6}	Zr2	O1	92.4(3)
O4	Zr1	O2	77.4(3)	O3^{6}	Zr2	O1^{5}	62.1(3)
O4^{3}	Zr1	O2^{3}	77.4(3)	O3^{3}	Zr2	O1	62.1(3)
O4	Zr1	O2^{3}	77.1(3)	O3^{3}	Zr2	O1^{5}	92.4(3)
O3	Zr1	O9	84.7(2)	O2^{5}	Zr2	O10^{6}	70.4(2)
O3^{3}	Zr1	O9	143.3(2)	O2^{5}	Zr2	O10^{3}	138.3(2)
O3^{3}	Zr1	O3	93.5(4)	O2	Zr2	O10^{6}	138.3(2)
O3	Zr1	O1	62.1(3)	O2	Zr2	O10^{3}	70.4(2)
O3^{3}	Zr1	O1	62.8(3)	O2	Zr2	O4^{6}	124.5(3)
O2	Zr1	O2^{3}	124.3(4)	O2^{5}	Zr2	O4^{3}	124.5(3)
O1	Zr1	O9	141.7(2)	O2	Zr2	O4^{3}	80.7(3)
O1^{3}	Zr1	O9	85.1(2)	O2^{5}	Zr2	O4^{6}	80.7(3)
O11^{4}	Zr3	O11^{2}	126.92(14)	O2^{5}	Zr2	O2	74.3(4)
O6	Zr3	O11^{4}	72.83(11)	O1	Zr2	O7	94.6(3)
O6	Zr3	O11^{2}	72.83(11)	O1^{5}	Zr2	O7	94.6(3)
O6	Zr3	O4	142.41(18)	O1^{5}	Zr2	O8	147.9(2)
O6	Zr3	O4^{5}	142.41(18)	O1	Zr2	O8	147.9(2)

O6	**Zr3**	**O2**[5]	79.6(3)	**O1**	**Zr2**	**O1**[5]	60.5(4)
O6	**Zr3**	**O2**	79.6(3)	**C8**	**O12**	**Zr1**[7]	132.0(2)
O5	**Zr3**	**O11**[4]	73.21(10)	**C1**	**O9**	**Zr1**	131.7(2)
O5	**Zr3**	**O11**[2]	73.21(10)	**C8**	**O11**	**Zr3**[8]	133.6(2)
O5	**Zr3**	**O6**	98.4(2)	**C1**	**O10**	**Zr2**[6]	133.9(2)
O5	**Zr3**	**O4**[5]	79.1(2)	**C6**	**C7**	**C8**	120.0(4)
O5	**Zr3**	**O4**	79.1(2)	**C6**	**C7**	**C5**	119.2(4)
O5	**Zr3**	**O2**[5]	143.0(2)	**C5**	**C7**	**C8**	120.7(3)
O5	**Zr3**	**O2**	143.0(2)	**O12**	**C8**	**C7**	116.0(3)
O4[5]	**Zr3**	**O11**[2]	138.64(19)	**O11**	**C8**	**O12**	126.4(3)
O4	**Zr3**	**O11**[2]	70.6(2)	**O11**	**C8**	**C7**	117.6(3)
O4[5]	**Zr3**	**O11**[4]	70.6(2)	**C4**	**C2**	**C1**	120.4(4)
O4	**Zr3**	**O11**[4]	138.64(19)	**C4**	**C2**	**C3**	120.2(4)
O4	**Zr3**	**O4**[5]	74.5(3)	**C3**	**C2**	**C1**	119.5(4)
O4[5]	**Zr3**	**O2**	124.3(3)	**O9**	**C1**	**O10**	126.8(3)
O4[5]	**Zr3**	**O2**[5]	80.7(3)	**O9**	**C1**	**C2**	116.4(3)
O4	**Zr3**	**O2**[5]	124.3(3)	**O10**	**C1**	**C2**	116.8(3)
O4	**Zr3**	**O2**	80.7(3)	**C2**	**C4**	**C6**	119.5(4)
O3[5]	**Zr3**	**O6**	147.49(18)	**C7**	**C6**	**C4**	120.7(4)
O3	**Zr3**	**O6**	147.49(18)	**C3**	**C5**	**C7**	120.3(4)
O3[5]	**Zr3**	**O5**	93.4(2)	**C2**	**C3**	**C5**	120.1(4)
O3	**Zr3**	**O5**	93.4(2)	**Zr3**	**O4**	**Zr1**	100.5(3)
O2[5]	**Zr3**	**O11**[2]	138.1(2)	**Zr3**	**O4**	**Zr2**[6]	103.9(3)
O2	**Zr3**	**O11**[4]	138.1(2)	**Zr2**[6]	**O4**	**Zr1**	100.3(3)
O2	**Zr3**	**O11**[2]	71.0(2)	**Zr1**	**O3**	**Zr3**	116.4(3)
O2[5]	**Zr3**	**O11**[4]	71.0(2)	**Zr1**	**O3**	**Zr2**[6]	116.5(3)
O2	**Zr3**	**O2**[5]	73.5(4)	**Zr2**[6]	**O3**	**Zr3**	116.9(3)
O1[5]	**Zr3**	**O6**	93.9(3)	**Zr3**	**O2**	**Zr1**	98.9(3)
O1	**Zr3**	**O6**	93.9(3)	**Zr2**	**O2**	**Zr1**	99.4(3)
O1	**Zr3**	**O5**	146.96(19)	**Zr2**	**O2**	**Zr3**	103.9(3)
O1[5]	**Zr3**	**O5**	146.96(19)	**Zr1**	**O1**	**Zr2**	114.6(3)
O1	**Zr3**	**O3**	61.7(3)	**Zr3**	**O1**	**Zr1**	115.9(3)
O1[5]	**Zr3**	**O3**	92.4(3)	**Zr3**	**O1**	**Zr2**	117.4(3)
O1[5]	**Zr3**	**O1**	61.3(4)				

[1]1/2-X,1/2+Y,1/2-Z; [2]1/2+X,1/2-Y,1/2-Z; [3]1-X,1-Y,+Z; [4]1/2+X,1/2-Y,1/2+Z; [5]+X,+Y,1-Z; [6]1-X,1-Y,1-Z; [7]1/2-X,-1/2+Y,1/2-Z; [8]-1/2+X,1/2-Y,-1/2+Z.