Electronic Supplementary Information

Structural Response to Desolvation in a Pyridyl-Phenanthrene Diarylethene-based Metal-Organic Framework

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Additional data related to potential energy surface calculations:

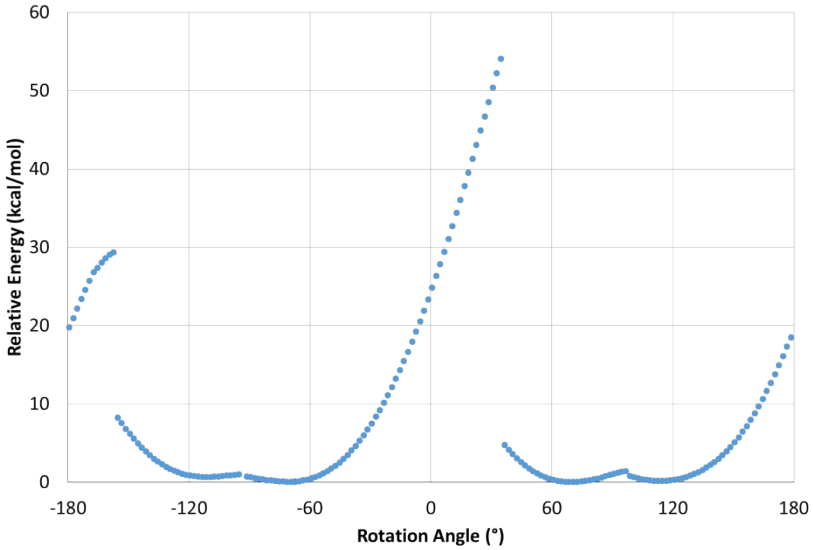
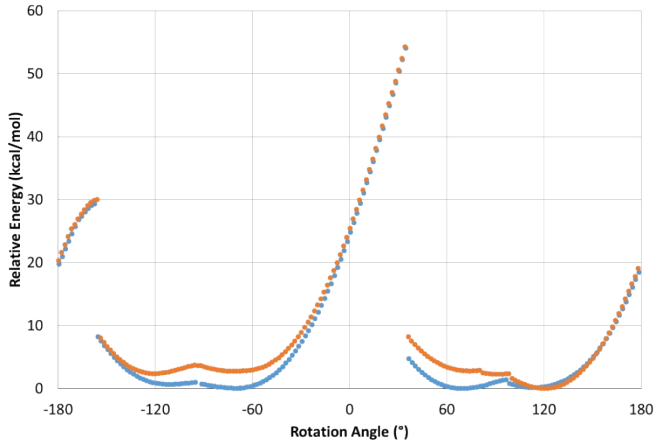
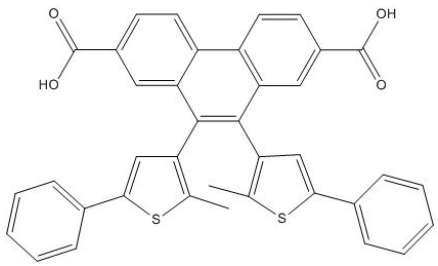


Figure S1: Full scale image of calculated potential energy surface for the dihedral rotation of one thiophene ring of **TPDPy**.





PhTPDC

Figure S2: Calculated potential energy surface for the dihedral rotation of one thiophene ring of **TPDPy** (blue dots) and **PhTPDC** (previous work, orange triangles).

Single crystal visible absorption spectroscopy:

Visible absorption spectroscopy on single crystal samples were measured using an inverted microscope (Olympus model IMT-2) coupled through a fiber optic cable to a spectrometer (Ocean Optics USB4000-UV-VIS). All experiments were performed using the tungsten lamp of the microscope with a 495 nm long pass filter to prevent cyclization by shorter wavelengths.

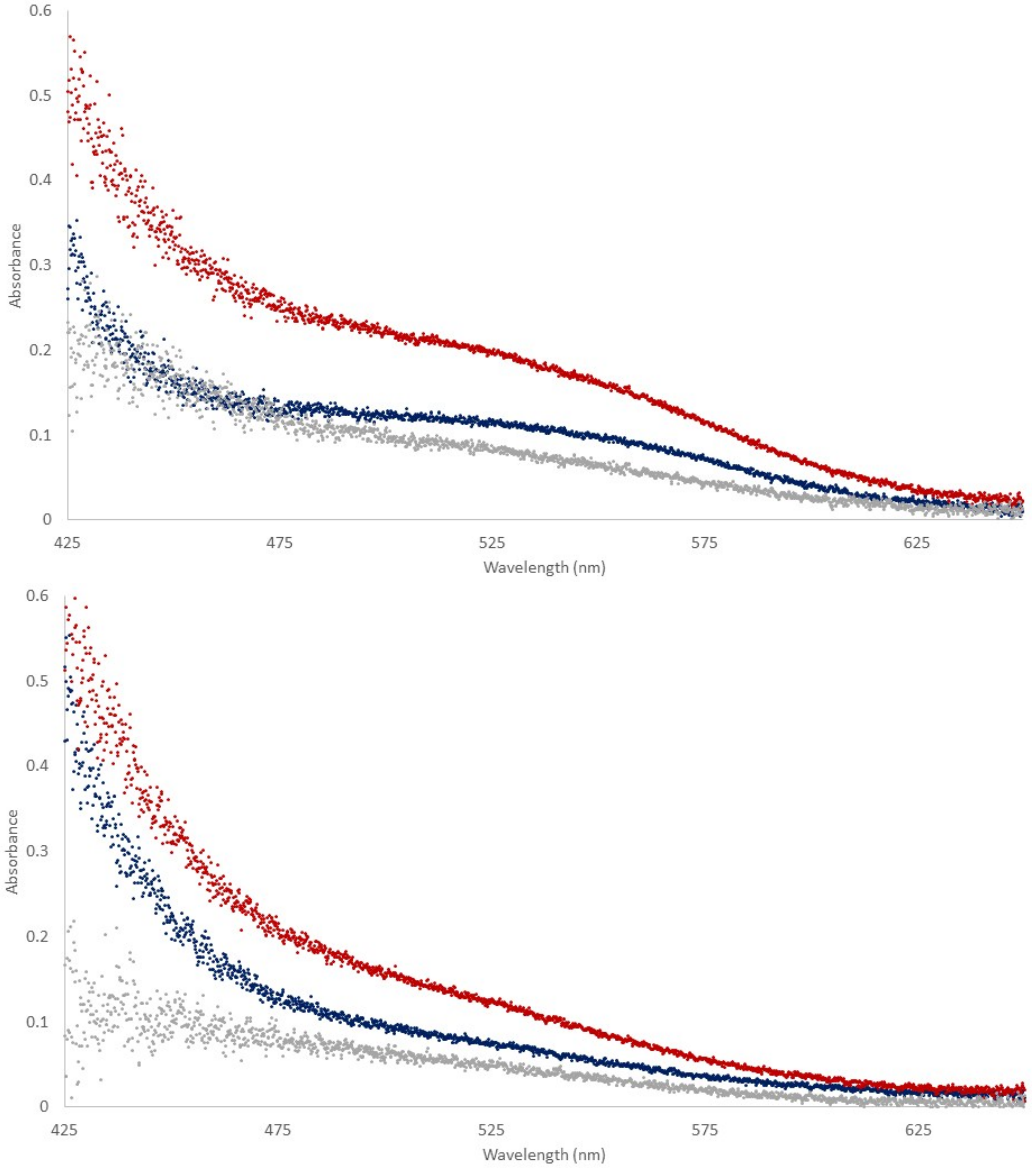


Figure S3: Visible light absorption spectra of UBMOF-3 (top) and UBMOF-3a (bottom). Prior to irradiation (blue), following (red), and difference (grey).

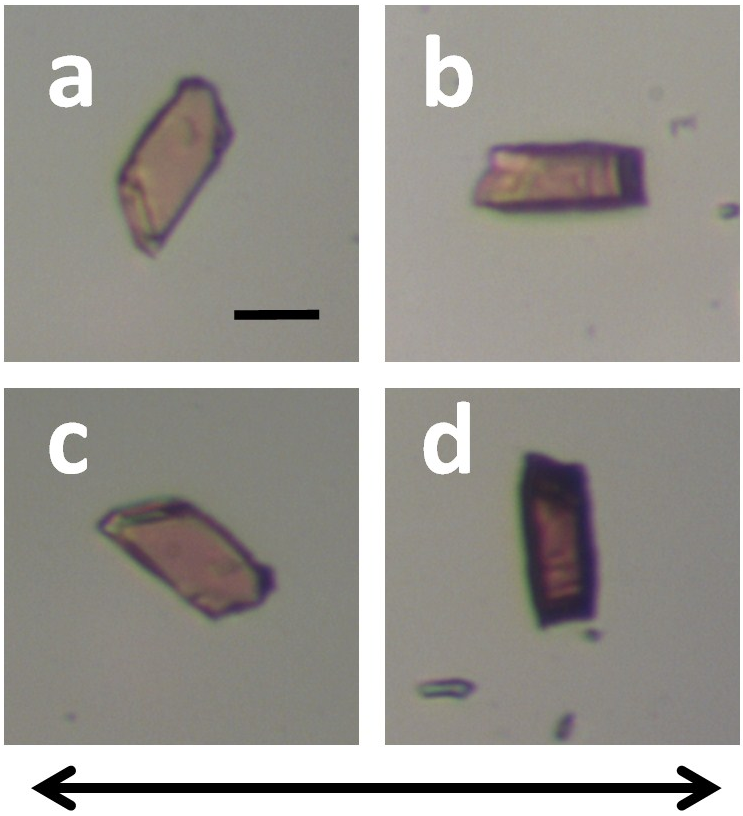


Figure S4: Images of a cut-block of a **UBMOF-3** crystal viewed normal to (100) (a,c) and perpendicular to (100) (b,d). These crystals grow as thin (100) plates. All images are recorded along vibration directions using linearly polarized light aligned with the horizon as denoted by the double arrow. Polarization for (d) is parallel to the a-axis. Scale bar in (a) is approximately 10 µm.

Table S1: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **UBMOF-3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Zn1	1844.8(2)	2079.3(8)	4655.0(4)	17.6(2)
Zn2	2500	2500	5000	17.6(2)
O1	1850.2(11)	3281(5)	3809(3)	30.2(8)
O2	2267.7(11)	3922(5)	4297(3)	30.2(8)
O3	2177.3(10)	977(5)	4697(3)	23.8(12)
O4	1979.7(15)	-198(6)	5456(5)	70(2)
O5	2647.2(11)	1926(5)	4086(3)	29.1(13)
O6	1903.8(12)	3270(6)	5554(3)	40.8(15)
O7	1679(4)	605(19)	3670(11)	152(7)
N1A	1487(2)	1326(17)	4595(10)	82(3)
C17A	1295(3)	1596(17)	3956(8)	82(3)
C16A	1032(3)	1173(19)	3909(8)	82(3)
C15A	960(3)	479(18)	4501(10)	82(3)
C14A	1151(3)	209(17)	5140(9)	82(3)
C13A	1415(3)	632(18)	5187(8)	82(3)

N2	1733(3)	-353(17)	2480(10)	93(5)
C1	2068.2(17)	3871(8)	3800(4)	30.2(8)
C2	2077.9(16)	4601(8)	3062(4)	32.7(19)
C3	1857.6(17)	4739(12)	2500(5)	53(2)
C4	1869.8(17)	5382(12)	1844(5)	53(2)
C5	2109.5(15)	5869(8)	1712(4)	28.0(18)
C6	2336.2(16)	5725(9)	2280(4)	31.7(19)
C7	2327.3(16)	5099(8)	2963(4)	27.4(18)
C8	2128.1(14)	6553(8)	1008(4)	24.2(16)
C9	2150.0(17)	-124(7)	5085(6)	42(2)
C10	2336.8(16)	-1364(7)	5040(5)	29.2(19)
C11	2484.1(16)	-1393(7)	4493(4)	26.7(18)
C12	2351.6(18)	-2476(7)	5540(5)	36(2)
C15	935(3)	1430(20)	4890(11)	85(3)
C16	982(3)	1965(19)	4230(9)	85(3)
C17	1243(4)	2180(17)	4145(8)	85(3)
N1	1457(3)	1857(18)	4721(11)	85(3)
C13	1410(3)	1317(19)	5382(9)	85(3)
C14	1149(4)	1102(19)	5466(8)	85(3)
C18	647(5)	1030(40)	5060(20)	167(8)
C19	601(6)	80(30)	5591(18)	167(8)
C20	348(8)	-30(30)	5747(15)	167(8)
C21	139(5)	800(40)	5370(20)	167(8)
C22	185(6)	1750(30)	4833(19)	167(8)
C23	438(8)	1860(30)	4676(16)	167(8)
C21A	150(4)	-280(30)	4789(16)	129(5)
C22A	198(5)	690(30)	4267(14)	129(5)
C23A	460(6)	970(20)	4206(13)	129(5)
C18A	672(4)	290(30)	4667(16)	129(5)
C19A	624(5)	-680(30)	5188(14)	129(5)
C20A	363(6)	-970(20)	5249(13)	129(5)
C24	1765(6)	560(40)	3070(20)	179(13)
C25	1459(6)	-930(40)	2403(19)	218(16)
C26	1788(8)	640(40)	1930(20)	270(20)

Table S2: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **UBMOF-3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn1	27.7(4)	17.7(4)	8.8(4)	1.3(2)	7.0(3)	-0.4(3)
Zn2	27.7(4)	17.7(4)	8.8(4)	1.3(2)	7.0(3)	-0.4(3)
O1	37(2)	36.8(19)	15.3(17)	14.2(15)	2.6(16)	4.5(16)
O2	37(2)	36.8(19)	15.3(17)	14.2(15)	2.6(16)	4.5(16)
O3	36(3)	12(2)	22(3)	0(2)	2(3)	1(2)
O4	86(5)	25(3)	125(7)	7(4)	79(5)	7(3)

O5	51(4)	28(3)	12(3)	0(2)	13(3)	0(2)
O6	55(4)	46(4)	29(3)	-8(3)	26(3)	5(3)
C1	37(2)	36.8(19)	15.3(17)	14.2(15)	2.6(16)	4.5(16)
C2	34(5)	40(5)	25(5)	14(4)	9(4)	7(4)
C3	20(3)	101(6)	32(4)	39(4)	-6(3)	-6(3)
C4	20(3)	101(6)	32(4)	39(4)	-6(3)	-6(3)
C5	25(4)	40(4)	20(4)	17(3)	5(4)	2(3)
C6	27(5)	51(5)	17(4)	11(4)	3(4)	-4(4)
C7	32(5)	33(4)	18(4)	6(3)	6(4)	0(3)
C8	13(4)	42(4)	14(4)	4(3)	-3(3)	5(3)
C9	42(5)	14(4)	79(7)	8(4)	39(5)	1(3)
C10	34(5)	14(3)	45(5)	-5(3)	22(4)	-5(3)
C11	48(5)	17(4)	16(4)	-4(3)	7(4)	-9(3)
C12	57(6)	18(4)	40(5)	-2(3)	30(5)	-4(3)

Table S3: Bond Lengths for **UBMOF-3**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Zn1	O1	1.937(5)		C3	C4	1.369(11)
Zn1	O3	1.980(5)		C4	C5	1.378(10)
Zn1	O6	1.977(6)		C5	C6	1.397(11)
Zn1	O7	2.307(19)		C5	C8	1.473(10)
Zn1	N1A	1.944(12)		C6	C7	1.404(10)
Zn1	N1	2.021(12)		C8	$O5^{4}$	1.248(9)
Zn2	$O2^{1}$	2.063(5)		C8	$O6^{5}$	1.281(9)
Zn2	O2	2.063(5)		C9	C10	1.525(10)
Zn2	$O3^{1}$	2.171(5)		C10	C11	1.382(10)
Zn2	O3	2.171(5)		C10	C12	1.390(11)
Zn2	$O5^{1}$	2.062(5)		C11	$C12^{6}$	1.368(11)
Zn2	O5	2.062(5)		C12	$C11^{6}$	1.368(11)
O1	C1	1.249(9)		C15	C16	1.3900
O2	C1	1.220(9)		C15	C14	1.3900
O3	C9	1.288(9)		C15	C18	1.61(2)
O4	C9	1.218(9)		C16	C17	1.3900
O5	$C8^{2}$	1.248(9)		C17	N1	1.3900
O6	$C8^{3}$	1.281(9)		N1	C13	1.3900
O7	C24	1.28(3)		C13	C14	1.3900
N1A	C17A	1.3900		C18	C19	1.3900
N1A	C13A	1.3900		C18	C23	1.3900
C17A	C16A	1.3900		C19	C20	1.3900
C16A	C15A	1.3900		C20	C21	1.3900
C15A	C14A	1.3900		C21	C22	1.3900
C15A	C18A	1.57(2)		C22	C23	1.3900
C14A	C13A	1.3900		C21A	$C21A^{7}$	1.94(4)
N2	C24	1.37(3)		C21A	C22A	1.3900

N2	C25	1.48(3)		C21A	C20A	1.3900
N2	C26	1.45(3)		C22A	C23A	1.3900
C1	C2	1.539(10)		C23A	C18A	1.3900
C2	C3	1.369(12)		C18A	C19A	1.3900
C2	C7	1.407(11)		C19A	C20A	1.3900

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

Table S4: Bond Angles for **UBMOF-3.**

Atom	Atom	Atom	Angle/˚		Atom	Atom	Atom	Angle/˚
O1	Zn1	O3	100.4(2)		O2	C1	C2	118.1(7)
O1	Zn1	O6	108.6(2)		C3	C2	C1	122.8(7)
O1	Zn1	O7	77.4(5)		C3	C2	C7	119.4(7)
O1	Zn1	N1A	110.0(6)		C7	C2	C1	117.7(7)
O1	Zn1	N1	106.9(6)		C2	C3	C4	122.1(8)
O3	Zn1	O7	83.3(5)		C3	C4	C5	120.9(8)
O3	Zn1	N1	141.9(5)		C4	C5	C6	117.4(7)
O6	Zn1	O3	106.8(2)		C4	C5	C8	122.0(7)
O6	Zn1	O7	166.6(5)		C6	C5	C8	120.6(7)
O6	Zn1	N1	89.2(5)		C5	C6	C7	122.6(7)
N1A	Zn1	O3	126.8(5)		C6	C7	C2	117.4(7)
N1A	Zn1	O6	103.4(5)		O5[4]	C8	O6[5]	126.4(7)
N1A	Zn1	O7	63.2(7)		O5[4]	C8	C5	118.7(7)
N1	Zn1	O7	77.5(7)		O6[5]	C8	C5	114.9(6)
O2	Zn2	O2[1]	180.0		O3	C9	C10	116.6(7)
O2	Zn2	O3	87.9(2)		O4	C9	O3	122.3(7)
O2	Zn2	O3[1]	92.1(2)		O4	C9	C10	121.1(7)
O2[1]	Zn2	O3	92.1(2)		C11	C10	C9	119.9(7)
O2[1]	Zn2	O3[1]	87.9(2)		C11	C10	C12	120.6(7)
O3	Zn2	O3[1]	180.0		C12	C10	C9	119.4(7)
O5	Zn2	O2[1]	94.8(2)		C12[6]	C11	C10	118.9(7)
O5[1]	Zn2	O2[1]	85.2(2)		C11[6]	C12	C10	120.5(7)
O5[1]	Zn2	O2	94.8(2)		C16	C15	C14	120.0
O5	Zn2	O2	85.2(2)		C16	C15	C18	125.8(19)
O5[1]	Zn2	O3[1]	90.2(2)		C14	C15	C18	114.0(19)
O5[1]	Zn2	O3	89.8(2)		C17	C16	C15	120.0
O5	Zn2	O3	90.2(2)		N1	C17	C16	120.0
O5	Zn2	O3[1]	89.8(2)		C17	N1	Zn1	123.6(10)
O5[1]	Zn2	O5	180.0		C17	N1	C13	120.0
C1	O1	Zn1	115.9(5)		C13	N1	Zn1	116.4(10)
C1	O2	Zn2	136.6(5)		N1	C13	C14	120.0
Zn1	O3	Zn2	105.1(2)		C13	C14	C15	120.0
C9	O3	Zn1	104.7(5)		C19	C18	C15	125(3)

C9	O3	Zn2	123.8(6)		C19	C18	C23	120.0
C8[2]	O5	Zn2	134.0(5)		C23	C18	C15	114(3)
C8[3]	O6	Zn1	125.6(5)		C18	C19	C20	120.0
C24	O7	Zn1	125(2)		C21	C20	C19	120.0
C17A	N1A	Zn1	117.8(10)		C22	C21	C20	120.0
C17A	N1A	C13A	120.0		C21	C22	C23	120.0
C13A	N1A	Zn1	122.0(10)		C22	C23	C18	120.0
C16A	C17A	N1A	120.0		C22A	C21A	C21A[7]	112(3)
C17A	C16A	C15A	120.0		C22A	C21A	C20A	120.0
C16A	C15A	C14A	120.0		C20A	C21A	C21A[7]	118(3)
C16A	C15A	C18A	128.3(16)		C21A	C22A	C23A	120.0
C14A	C15A	C18A	109.5(16)		C18A	C23A	C22A	120.0
C13A	C14A	C15A	120.0		C23A	C18A	C15A	118(2)
C14A	C13A	N1A	120.0		C23A	C18A	C19A	120.0
C24	N2	C25	105(2)		C19A	C18A	C15A	121(2)
C24	N2	C26	98(2)		C20A	C19A	C18A	120.0
C26	N2	C25	119(2)		C19A	C20A	C21A	120.0
O1	C1	C2	114.0(7)		O7	C24	N2	135(3)
O2	C1	O1	127.9(7)					

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

Table S5: Torsion Angles for **UBMOF-3.**

A	B	C	D	Angle/˚		A	B	C	D	Angle/˚
Zn1	O1	C1	O2	-9.7(11)		C6	C5	C8	O5[1]	4.1(12)
Zn1	O1	C1	C2	170.0(5)		C6	C5	C8	O6[2]	-174.5(7)
Zn1	O3	C9	O4	-14.3(12)		C7	C2	C3	C4	-1.7(16)
Zn1	O3	C9	C10	163.7(7)		C8	C5	C6	C7	179.1(7)
Zn1	O7	C24	N2	166(2)		C9	C10	C11	C12[3]	-179.4(8)
Zn1	N1A	C17A	C16A	-175.1(11)		C9	C10	C12	C11[3]	179.4(8)
Zn1	N1A	C13A	C14A	174.9(12)		C11	C10	C12	C11[3]	1.1(14)
Zn1	N1	C13	C14	-178.6(11)		C12	C10	C11	C12[3]	-1.1(14)
Zn2	O2	C1	O1	50.0(13)		C15	C16	C17	N1	0.0
Zn2	O2	C1	C2	-129.7(6)		C15	C18	C19	C20	171(3)
Zn2	O3	C9	O4	105.7(10)		C15	C18	C23	C22	-172(2)
Zn2	O3	C9	C10	-76.3(9)		C16	C15	C14	C13	0.0
O1	C1	C2	C3	7.5(12)		C16	C15	C18	C19	157.0(16)
O1	C1	C2	C7	-170.3(7)		C16	C15	C18	C23	-31(2)
O2	C1	C2	C3	-172.8(9)		C16	C17	N1	Zn1	178.5(12)
O2	C1	C2	C7	9.4(11)		C16	C17	N1	C13	0.0
O3	C9	C10	C11	-13.1(12)		C17	N1	C13	C14	0.0
O3	C9	C10	C12	168.6(8)		N1	C13	C14	C15	0.0
O4	C9	C10	C11	165.0(9)		C14	C15	C16	C17	0.0

O4	C9	C10	C12	-13.3(14)		C14	C15	C18	C19	-19(3)
N1A	C17A	C16A	C15A	0.0		C14	C15	C18	C23	152.6(14)
C17A	N1A	C13A	C14A	0.0		C18	C15	C16	C17	-176(2)
C17A	C16A	C15A	C14A	0.0		C18	C15	C14	C13	176.5(18)
C17A	C16A	C15A	C18A	161.2(19)		C18	C19	C20	C21	0.0
C16A	C15A	C14A	C13A	0.0		C19	C18	C23	C22	0.0
C16A	C15A	C18A	C23A	-5(2)		C19	C20	C21	C22	0.0
C16A	C15A	C18A	C19A	165.9(13)		C20	C21	C22	C23	0.0
C15A	C14A	C13A	N1A	0.0		C21	C22	C23	C18	0.0
C15A	C18A	C19A	C20A	-171(2)		C23	C18	C19	C20	0.0
C14A	C15A	C18A	C23A	157.5(12)		C21A[4]	C21A	C22A	C23A	144(2)
C14A	C15A	C18A	C19A	-31.3(19)		C21A[4]	C21A	C20A	C19A	-142(2)
C13A	N1A	C17A	C16A	0.0		C21A	C22A	C23A	C18A	0.0
C1	C2	C3	C4	-179.5(10)		C22A	C21A	C20A	C19A	0.0
C1	C2	C7	C6	178.1(7)		C22A	C23A	C18A	C15A	171(2)
C2	C3	C4	C5	2.7(18)		C22A	C23A	C18A	C19A	0.0
C3	C2	C7	C6	0.2(12)		C23A	C18A	C19A	C20A	0.0
C3	C4	C5	C6	-2.1(15)		C18A	C15A	C14A	C13A	-164.4(16)
C3	C4	C5	C8	179.5(10)		C18A	C19A	C20A	C21A	0.0
C4	C5	C6	C7	0.6(13)		C20A	C21A	C22A	C23A	0.0
C4	C5	C8	O5[1]	-177.5(8)		C25	N2	C24	O7	33(5)
C4	C5	C8	O6[2]	3.9(12)		C26	N2	C24	O7	156(4)
C5	C6	C7	C2	0.3(12)						

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

Table S6: Hydrogen Atom Coordinates (Å×10[4]) and Isotropic Displacement Parameters (Å[2]×10[3]) for **UBMOF-3.**

Atom	*x*	*y*	*z*	U(eq)
H17A	1344	2070	3552	98
H16A	901	1357	3472	98
H14A	1102	-265	5545	98
H13A	1546	448	5624	98
H3	1691	4377	2566	63
H4	1711	5494	1475	63
H6	2503	6063	2201	38
H7	2484	5015	3343	33
H11	2472	-641	4147	32
H12	2247	-2450	5907	43
H16	836	2186	3836	102
H17	1275	2549	3694	102
H13	1557	1096	5775	102
H14	1117	733	5917	102

H24	1876	1346	3016	215
H25A	1459	-1661	2778	327
H25B	1398	-1341	1909	327
H25C	1337	-163	2473	327
H26A	1896	168	1623	407
H26B	1888	1453	2182	407
H26C	1620	972	1620	407

Table S7: Atomic Occupancy for **UBMOF-3.**

Atom	*Occupancy*		Atom	*Occupancy*		Atom	*Occupancy*
O7	0.750(12)		N1A	0.5		C17A	0.5
H17A	0.5		C16A	0.5		H16A	0.5
C15A	0.5		C14A	0.5		H14A	0.5
C13A	0.5		H13A	0.5		N2	0.750(12)
C15	0.5		C16	0.5		H16	0.5
C17	0.5		H17	0.5		N1	0.5
C13	0.5		H13	0.5		C14	0.5
H14	0.5		C18	0.5		C19	0.5
C20	0.5		C21	0.5		C22	0.5
C23	0.5		C21A	0.5		C22A	0.5
C23A	0.5		C18A	0.5		C19A	0.5
C20A	0.5		C24	0.750(12)		H24	0.750(12)
C25	0.750(12)		H25A	0.750(12)		H25B	0.750(12)
H25C	0.750(12)		C26	0.750(12)		H26A	0.750(12)
H26B	0.750(12)		H26C	0.750(12)			

Table S8: Solvent masks information for **UBMOF-3.**

Number	X	Y	Z	Volume	Electron count	Content
1	0.000	-0.030	-0.348	2074.0	731.4	DMF+H_2O
2	0.500	0.025	-0.118	2074.0	731.4	DMF+H_2O

Additional crystallographic information tables for **UBMOF-3a**

Table S9: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **UBMOF-3a**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Zn1	3285.2(2)	2896.6(6)	4991.2(3)	20.9(2)
Zn2	2500	2500	5000	14.5(2)
S1	4705(4)	6801(18)	2031(10)	258(7)
S1A	4731(5)	6948(18)	8043(11)	269(8)
O1	3300.7(11)	1899(4)	5913(2)	29.0(9)
O2	2785.1(10)	1182(4)	5628.1(19)	25.9(9)
O3	2882.0(9)	4075(3)	5115.3(18)	22.0(8)
O4	3074.4(14)	5096(4)	4130(2)	47.8(13)
O5	3265.8(10)	1770(4)	4132.1(19)	27.4(9)
O6	2699.6(11)	1854(4)	4033.3(19)	28.1(9)
N1	3716.3(15)	3936(6)	5002(3)	44.2(15)
C1	3031.8(15)	1279(6)	6052(3)	25.7(13)
C2	3020.5(14)	542(6)	6764(3)	26.4(13)
C3	2719.4(17)	27(6)	6989(3)	32.5(14)
C4	2708.4(16)	-649(7)	7661(3)	31.9(14)
C5	3310.1(17)	376(8)	7191(3)	43.9(18)
C6	3305.6(17)	-285(8)	7857(4)	45.1(18)
C7	2894.9(17)	5116(6)	4667(3)	32.9(15)
C8	2683.4(16)	6331(5)	4854(3)	26.8(13)
C9	2514.9(18)	6418(6)	5479(3)	34.4(16)
C10	2673.5(18)	7438(6)	4356(3)	32.0(15)
C11	2981.5(15)	1514(5)	3819(3)	23.9(12)
C12	2996.7(15)	801(6)	3098(3)	27.3(13)
C13	3855(3)	4382(12)	4396(4)	100(4)
C14	4103(3)	5325(15)	4383(6)	127(6)
C15	4224(3)	5915(13)	4991(5)	90(4)
C16	4120(3)	5311(16)	5623(5)	136(7)
C17	3854(3)	4430(13)	5603(5)	108(5)
C18	4467(3)	7025(13)	5013(5)	88(4)
C23	4576(3)	7692(11)	5672(6)	85(3)
C22	4795(3)	8821(13)	5672(7)	100(4)
C21	4901(3)	9404(12)	4998(6)	90(4)
C20	4800(3)	8729(12)	4369(7)	93(4)
C19	4581(3)	7632(13)	4364(7)	98(4)
C24	4898(5)	9430(20)	3721(11)	70(5)
C24A	4908(5)	9470(20)	6285(11)	73(5)
C25	4776(6)	8750(30)	2958(15)	108(8)
C25A	4779(7)	8900(30)	7014(16)	114(9)
C26	4929(7)	7490(30)	2814(13)	117(9)

C26A	4926(10)	7680(40)	7239(18)	194(19)
C27	4507(9)	9190(40)	2420(20)	194(17)
C27A	4507(12)	9290(50)	7520(30)	260(30)
C28	4412(4)	8218(18)	1880(10)	63(5)
C28A	4434(5)	8400(20)	8110(11)	76(5)

Table S10: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **UBMOF-3a**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn1	37.4(4)	15.9(3)	9.4(3)	-0.2(2)	1.9(3)	-7.2(3)
Zn2	33.9(5)	6.6(4)	3.0(4)	0.5(3)	1.8(3)	-0.8(3)
O1	39(3)	35(2)	13.6(19)	4.0(16)	-1.1(17)	-1.6(19)
O2	47(3)	22(2)	9.2(17)	4.9(14)	-0.3(18)	-3.3(17)
O3	42(2)	9.3(17)	14.1(18)	-0.5(13)	1.3(16)	-4.1(16)
O4	90(4)	25(2)	30(2)	4.2(18)	25(3)	8(2)
O5	39(2)	32(2)	11.3(18)	-7.2(16)	4.5(17)	-1.0(19)
O6	46(3)	29(2)	9.3(18)	-1.3(15)	5.1(17)	-2.0(19)
N1	54(4)	46(3)	33(3)	4(3)	0(3)	-24(3)
C1	39(4)	25(3)	13(3)	3(2)	2(3)	-3(3)
C2	31(3)	31(3)	16(3)	10(2)	-5(2)	-4(3)
C3	47(4)	36(3)	15(3)	4(2)	3(3)	-2(3)
C4	38(4)	43(4)	14(3)	9(2)	6(2)	-5(3)
C5	34(4)	74(5)	24(3)	25(3)	1(3)	-11(3)
C6	33(4)	71(5)	31(4)	26(3)	-4(3)	-5(3)
C7	55(4)	19(3)	25(3)	5(2)	7(3)	-7(3)
C8	48(4)	7(2)	25(3)	2(2)	11(3)	-6(2)
C9	81(5)	10(3)	12(3)	-2.3(19)	-6(3)	-7(3)
C10	64(4)	17(3)	15(3)	-3(2)	11(3)	-8(3)
C11	35(4)	19(3)	18(3)	-3(2)	2(2)	-7(2)
C12	38(3)	29(3)	16(3)	-7(2)	4(2)	0(3)
C13	132(9)	138(10)	30(4)	-7(5)	13(5)	-107(8)
C14	164(12)	168(13)	53(6)	-30(7)	48(7)	-123(11)
C15	101(8)	109(9)	61(6)	-20(6)	23(6)	-66(7)
C16	158(11)	211(16)	40(5)	-10(7)	7(6)	-141(12)
C17	140(10)	152(11)	33(5)	0(6)	-9(5)	-114(9)
C18	95(8)	116(9)	52(6)	-2(5)	11(5)	-64(7)
C23	90(8)	83(7)	82(7)	6(6)	-10(6)	-45(6)
C22	89(8)	93(9)	119(10)	-3(7)	-11(7)	-47(7)
C21	102(8)	92(8)	77(7)	4(6)	-9(6)	-59(7)
C20	82(7)	93(8)	104(9)	12(7)	-2(6)	-47(6)
C19	108(9)	101(9)	84(8)	-6(7)	-5(7)	-53(7)

Table S11: Bond Lengths for **UBMOF-3a.**						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
Zn1	Zn2	3.1455(7)		C9	C10[5]	1.381(9)
Zn1	O1	1.954(4)		C10	C9[5]	1.380(9)
Zn1	O3	1.989(4)		C11	C12	1.500(7)
Zn1	O5	1.924(4)		C12	C4[6]	1.391(8)
Zn1	N1	1.990(5)		C12	C6[6]	1.408(9)
Zn2	Zn1[1]	3.1456(7)		C13	C14	1.347(12)
Zn2	O2	2.050(4)		C14	C15	1.336(13)
Zn2	O2[1]	2.051(4)		C15	C16	1.374(14)
Zn2	O3[1]	2.165(4)		C15	C18	1.452(13)
Zn2	O3	2.165(4)		C16	C17	1.363(12)
Zn2	O6	2.062(4)		C18	C23	1.433(14)
Zn2	O6[1]	2.062(4)		C18	C19	1.416(14)
S1	C26[2]	1.62(3)		C23	C22	1.401(13)
S1	C26	1.81(2)		C22	C21	1.435(16)
S1	C28	1.823(18)		C22	C24A	1.36(2)
S1A	C26A[3]	1.63(4)		C21	C21[7]	1.403(19)
S1A	C26A	1.83(2)		C21	C20	1.381(15)
S1A	C28A	1.850(18)		C20	C19	1.377(14)
O1	C1	1.259(7)		C20	C24	1.44(2)
O2	C1	1.242(7)		C24	C24A[7]	1.32(3)
O3	C7	1.308(7)		C24	C25	1.62(3)
O4	C7	1.232(7)		C24A	C24[7]	1.32(3)
O5	C11	1.280(7)		C24A	C25A	1.55(3)
O6	C11	1.241(7)		C25	C26	1.39(2)
N1	C13	1.329(9)		C25	C27	1.50(4)
N1	C17	1.312(10)		C25A	C26A	1.38(3)
C1	C2	1.494(7)		C25A	C27A	1.50(4)
C2	C3	1.370(8)		C26	S1[2]	1.62(3)
C2	C5	1.387(8)		C26	C26[2]	1.30(5)
C3	C4	1.402(8)		C26A	S1A[3]	1.63(4)
C4	C12[4]	1.391(8)		C26A	C26A[3]	1.12(8)
C5	C6	1.385(8)		C27	C27A[8]	1.49(6)
C6	C12[4]	1.408(9)		C27	C28	1.42(3)
C7	C8	1.496(8)		C27A	C27[9]	1.49(6)
C8	C9	1.347(8)		C27A	C28A	1.42(3)
C8	C10	1.415(8)				

[1]1/2-X,1/2-Y,1-Z; [2]1-X,+Y,1/2-Z; [3]1-X,+Y,3/2-Z; [4]+X,-Y,1/2+Z; [5]1/2-X,3/2-Y,1-Z; [6]+X,-Y,-1/2+Z; [7]1-X,2-Y,1-Z; [8]+X,2-Y,-1/2+Z; [9]+X,2-Y,1/2+Z

Table S12: Bond Angles for **UBMOF-3a.**								
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**

O1	Zn1	Zn2	86.85(13)		O4	C7	C8	122.4(5)
O1	Zn1	O3	101.31(16)		C9	C8	C7	122.7(5)
O1	Zn1	N1	103.6(2)		C9	C8	C10	119.8(5)
O3	Zn1	Zn2	42.92(10)		C10	C8	C7	117.5(5)
O3	Zn1	N1	113.7(2)		C8	C9	C10[5]	121.4(5)
O5	Zn1	Zn2	85.06(12)		C9[5]	C10	C8	118.7(5)
O5	Zn1	O1	115.38(17)		O5	C11	C12	115.7(5)
O5	Zn1	O3	114.01(16)		O6	C11	O5	126.8(5)
O5	Zn1	N1	108.4(2)		O6	C11	C12	117.4(5)
N1	Zn1	Zn2	156.45(19)		C4[6]	C12	C6[6]	119.5(5)
Zn1	Zn2	Zn1[1]	180.0		C4[6]	C12	C11	120.7(5)
O2[1]	Zn2	Zn1	117.08(11)		C6[6]	C12	C11	119.8(5)
O2	Zn2	Zn1[1]	117.08(11)		N1	C13	C14	123.7(8)
O2[1]	Zn2	Zn1[1]	62.92(11)		C15	C14	C13	121.8(9)
O2	Zn2	Zn1	62.92(11)		C14	C15	C16	114.5(9)
O2	Zn2	O2[1]	180.0(2)		C14	C15	C18	124.7(9)
O2[1]	Zn2	O3	89.33(14)		C16	C15	C18	120.5(9)
O2[1]	Zn2	O3[1]	90.67(14)		C17	C16	C15	119.6(9)
O2	Zn2	O3[1]	89.33(14)		N1	C17	C16	124.1(8)
O2	Zn2	O3	90.67(14)		C23	C18	C15	123.3(9)
O2[1]	Zn2	O6[1]	94.34(15)		C19	C18	C15	121.0(9)
O2	Zn2	O6	94.34(15)		C19	C18	C23	115.3(9)
O2	Zn2	O6[1]	85.66(15)		C22	C23	C18	122.0(11)
O2[1]	Zn2	O6	85.66(15)		C23	C22	C21	120.4(11)
O3[1]	Zn2	Zn1	141.28(10)		C24A	C22	C23	123.8(14)
O3	Zn2	Zn1[1]	141.28(10)		C24A	C22	C21	115.7(12)
O3	Zn2	Zn1	38.72(10)		C21[7]	C21	C22	119.9(13)
O3[1]	Zn2	Zn1[1]	38.72(10)		C20	C21	C22	116.7(9)
O3	Zn2	O3[1]	180.00(14)		C20	C21	C21[7]	123.4(13)
O6	Zn2	Zn1	68.32(12)		C21	C20	C24	112.8(11)
O6[1]	Zn2	Zn1[1]	68.33(12)		C19	C20	C21	123.1(11)
O6[1]	Zn2	Zn1	111.67(12)		C19	C20	C24	123.2(13)
O6	Zn2	Zn1[1]	111.68(12)		C20	C19	C18	122.2(11)
O6[1]	Zn2	O3	89.03(15)		C20	C24	C25	116.1(17)
O6	Zn2	O3	90.97(15)		C24A[7]	C24	C20	124.3(18)
O6	Zn2	O3[1]	89.03(15)		C24A[7]	C24	C25	119.5(19)
O6[1]	Zn2	O3[1]	90.97(15)		C22	C24A	C25A	116.4(19)
O6	Zn2	O6[1]	180.0		C24[7]	C24A	C22	123.5(19)
C26[2]	S1	C26	44.1(18)		C24[7]	C24A	C25A	120(2)
C26[2]	S1	C28	106.2(15)		C26	C25	C24	114(2)
C26	S1	C28	98.1(14)		C26	C25	C27	116(3)
C26A[3]	S1A	C26A	37(3)		C27	C25	C24	130(2)
C26A[3]	S1A	C28A	103.2(17)		C26A	C25A	C24A	115(2)
C26A	S1A	C28A	92.3(16)		C26A	C25A	C27A	110(3)
C1	O1	Zn1	113.9(4)		C27A	C25A	C24A	135(2)
C1	O2	Zn2	136.3(4)		S1[2]	C26	S1	114.1(18)

Zn1	O3	Zn2	98.36(14)		C25	C26	S1[2]	136(2)
C7	O3	Zn1	109.3(4)		C25	C26	S1	106(2)
C7	O3	Zn2	121.7(4)		C26[2]	C26	S1	60.3(18)
C11	O5	Zn1	119.8(4)		C26[2]	C26	S1[2]	76(2)
C11	O6	Zn2	136.3(4)		C26[2]	C26	C25	111.7(18)
C13	N1	Zn1	122.2(5)		S1A[3]	C26A	S1A	117(2)
C17	N1	Zn1	122.4(5)		C25A	C26A	S1A	113(3)
C17	N1	C13	114.5(7)		C25A	C26A	S1A[3]	129(3)
O1	C1	C2	116.8(5)		C26A[3]	C26A	S1A[3]	81(3)
O2	C1	O1	124.8(5)		C26A[3]	C26A	S1A	62(3)
O2	C1	C2	118.3(5)		C26A[3]	C26A	C25A	118(2)
C3	C2	C1	119.0(5)		C27A[8]	C27	C25	102(3)
C3	C2	C5	120.4(5)		C28	C27	C25	116(3)
C5	C2	C1	120.6(5)		C28	C27	C27A[8]	138(4)
C2	C3	C4	118.9(6)		C27[9]	C27A	C25A	100(3)
C12[4]	C4	C3	121.1(6)		C28A	C27A	C25A	119(3)
C6	C5	C2	121.8(6)		C28A	C27A	C27[9]	134(5)
C5	C6	C12[4]	118.3(6)		C27	C28	S1	104(2)
O3	C7	C8	115.9(5)		C27A	C28A	S1A	106(2)
O4	C7	O3	121.6(6)					

[1]1/2-X,1/2-Y,1-Z; [2]1-X,+Y,1/2-Z; [3]1-X,+Y,3/2-Z; [4]+X,-Y,1/2+Z; [5]1/2-X,3/2-Y,1-Z; [6]+X,-Y,-1/2+Z; [7]1-X,2-Y,1-Z; [8]+X,2-Y,-1/2+Z; [9]+X,2-Y,1/2+Z

Table S13: Torsion Angles for **UBMOF-3a.**

A	B	C	D	Angle/˚		A	B	C	D	Angle/˚
Zn1	O1	C1	O2	6.3(7)		C22	C24A	C25A	C26A	75(3)
Zn1	O1	C1	C2	-177.5(4)		C22	C24A	C25A	C27A	-98(5)
Zn1	O3	C7	O4	19.2(8)		C21	C22	C24A	C24[4]	0(3)
Zn1	O3	C7	C8	-159.9(4)		C21	C22	C24A	C25A	176.6(17)
Zn1	O5	C11	O6	-4.6(8)		C21[4]	C21	C20	C19	-174.0(16)
Zn1	O5	C11	C12	171.5(4)		C21[4]	C21	C20	C24	-4(2)
Zn1	N1	C13	C14	165.2(12)		C21	C20	C19	C18	-6(2)
Zn1	N1	C17	C16	-170.1(12)		C21	C20	C24	C24A[4]	6(3)
Zn2	O2	C1	O1	-49.6(9)		C21	C20	C24	C25	-177.4(16)
Zn2	O2	C1	C2	134.2(5)		C20	C24	C25	C26	-68(3)
Zn2	O3	C7	O4	-94.2(7)		C20	C24	C25	C27	106(3)
Zn2	O3	C7	C8	86.7(6)		C19	C18	C23	C22	-3.4(19)
Zn2	O6	C11	O5	-17.7(9)		C19	C20	C24	C24A[4]	176.0(18)
Zn2	O6	C11	C12	166.3(4)		C19	C20	C24	C25	-8(2)
O1	C1	C2	C3	170.4(6)		C24	C20	C19	C18	-174.8(14)

O1	C1	C2	C5	-9.9(9)		C24[4]	C24A	C25A	C26A	-108(3)
O2	C1	C2	C3	-13.1(8)		C24[4]	C24A	C25A	C27A	78(5)
O2	C1	C2	C5	166.7(6)		C24	C25	C26	S1	170.6(16)
O3	C7	C8	C9	6.3(9)		C24	C25	C26	S1[5]	-34(4)
O3	C7	C8	C10	-175.8(6)		C24	C25	C26	C26[5]	-126(3)
O4	C7	C8	C9	-172.8(6)		C24	C25	C27	C27A[6]	30(5)
O4	C7	C8	C10	5.1(10)		C24	C25	C27	C28	-167(2)
O5	C11	C12	C4[1]	-170.7(5)		C24A	C22	C21	C21[4]	-2(2)
O5	C11	C12	C6[1]	9.1(8)		C24A	C22	C21	C20	177.5(14)
O6	C11	C12	C4[1]	5.8(8)		C24A[4]	C24	C25	C26	109(3)
O6	C11	C12	C6[1]	-174.4(6)		C24A[4]	C24	C25	C27	-77(4)
N1	C13	C14	C15	-2(3)		C24A	C25A	C26A	S1A[7]	16(5)
C1	C2	C3	C4	-179.3(6)		C24A	C25A	C26A	S1A	-173(2)
C1	C2	C5	C6	179.1(7)		C24A	C25A	C26A	C26A[7]	117(5)
C2	C3	C4	C12[2]	0.0(10)		C24A	C25A	C27A	C27[8]	-33(6)
C2	C5	C6	C12[2]	0.3(12)		C24A	C25A	C27A	C28A	172(3)
C3	C2	C5	C6	-1.1(11)		C25	C27	C28	S1	-5(4)
C5	C2	C3	C4	1.0(10)		C25A	C27A	C28A	S1A	1(5)
C7	C8	C9	C10[3]	178.8(6)		C26[5]	S1	C26	S1[5]	-55(2)
C7	C8	C10	C9[3]	-178.9(6)		C26[5]	S1	C26	C25	106.4(18)
C9	C8	C10	C9[3]	-1.0(10)		C26	S1	C28	C27	2(2)
C10	C8	C9	C10[3]	1.0(11)		C26[5]	S1	C28	C27	-42(3)
C13	N1	C17	C16	-1(2)		C26	C25	C27	C27A[6]	-156(3)
C13	C14	C15	C16	11(2)		C26	C25	C27	C28	7(5)
C13	C14	C15	C18	-174.1(14)		C26A[7]	S1A	C26A	S1A[7]	62(3)
C14	C15	C16	C17	-16(2)		C26A[7]	S1A	C26A	C25A	-110(3)
C14	C15	C18	C23	176.0(15)		C26A	S1A	C28A	C27A	0(3)
C14	C15	C18	C19	4(2)		C26A[7]	S1A	C28A	C27A	36(3)
C15	C16	C17	N1	11(3)		C26A	C25A	C27A	C27[8]	154(3)
C15	C18	C23	C22	-175.7(13)		C26A	C25A	C27A	C28A	-2(6)
C15	C18	C19	C20	176.8(13)		C27	C25	C26	S1	-4(4)
C16	C15	C18	C23	-10(2)		C27	C25	C26	S1[5]	151(3)
C16	C15	C18	C19	178.5(14)		C27	C25	C26	C26[5]	59(4)
C17	N1	C13	C14	-3.9(19)		C27[8]	C27A	C28A	S1A	-144(5)
C18	C15	C16	C17	169.5(14)		C27A	C25A	C26A	S1A	2(5)
C18	C23	C22	C21	4(2)		C27A	C25A	C26A	S1A[7]	-169(4)
C18	C23	C22	C24A	-179.1(15)		C27A	C25A	C26A	C26A[7]	-68(6)
C23	C18	C19	C20	4(2)		C27A[6]	C27	C28	S1	149(5)
C23	C22	C21	C21[4]	175.2(15)		C28	S1	C26	S1[5]	-160.3(18)
C23	C22	C21	C20	-5(2)		C28	S1	C26	C25	1(2)
C23	C22	C24A	C24[4]	-176.9(17)		C28	S1	C26	C26[5]	-105.0(16)
C23	C22	C24A	C25A	0(3)		C28A	S1A	C26A	S1A[7]	171(3)

C22	C21	C20	C19	7(2)		C28A	S1A	C26A	C25A	-1(3)
C22	C21	C20	C24	176.2(14)		C28A	S1A	C26A	C26A[7]	109(2)

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

Table S14: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **UBMOF-3a**.

Atom	*x*	*y*	*z*	U(eq)
H3	2521	127	6694	39
H4	2501	-1010	7820	38
H5	3517	726	7022	53
H6	3506	-388	8145	54
H9	2526	5675	5814	41
H10	2794	7395	3917	38
H13	3775	4014	3945	120
H14	4194	5579	3930	153
H16	4234	5505	6072	164
H17	3761	4157	6052	130
H23	4498	7360	6123	102
H19	4504	7272	3910	118

Table S15 Atomic Occupancy for UBMOF-3a.

Atom	*Occupancy*		Atom	*Occupancy*		Atom	*Occupancy*
S1	0.5		S1A	0.5		C24	0.5
C24A	0.5		C25	0.5		C25A	0.5
C26	0.5		C26A	0.5		C27	0.5
C27A	0.5		C28	0.5		C28A	0.5

Table S16: Solvent masks information for **UBMOF-3a.**

Number	X	Y	Z	Volume	Electron count	Content
1	0.000	-0.226	-0.580	1319.6	249.2	DMF+H_2O
2	0.500	0.880	-0.441	1319.6	249.2	DMF+H_2O