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Supplementary Material

The elusive nitro-functionalised member of the IRMOF-9 family

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General Information

Table S 1 *Synthesis ratios, percentage compositions in the frameworks, experimental yields and framework formulations of the MOFs synthesized.*

MOF	*Ligand synthesis ratio (mol%)*[a]		*Ligand incorporation in MOF (mol%)*[a]		*Yield (%)*	*Framework Formulation*
	H_2bpdc	**H_2bpdcNO$_2$**	**Bpdc**	**bpdcNO$_2$**		
WUF-22(8)	6	94	8	92	9	$Zn_4O[(\mathbf{bpdc})_{0.24}(\mathbf{bpdcNO_2})_{2.79}]$
WUF-22(10)	9	91	10	90	18	$Zn_4O[(\mathbf{bpdc})_{0.3}(\mathbf{bpdcNO_2})_{2.70}]$
WUF-22(14)	13	87	14	86	34	$Zn_4O[(\mathbf{bpdc})_{0.42}(\mathbf{bpdcNO_2})_{2.58}]$

[a] As determined via ^{1}H NMR spectroscopy.

Optical Microscopy

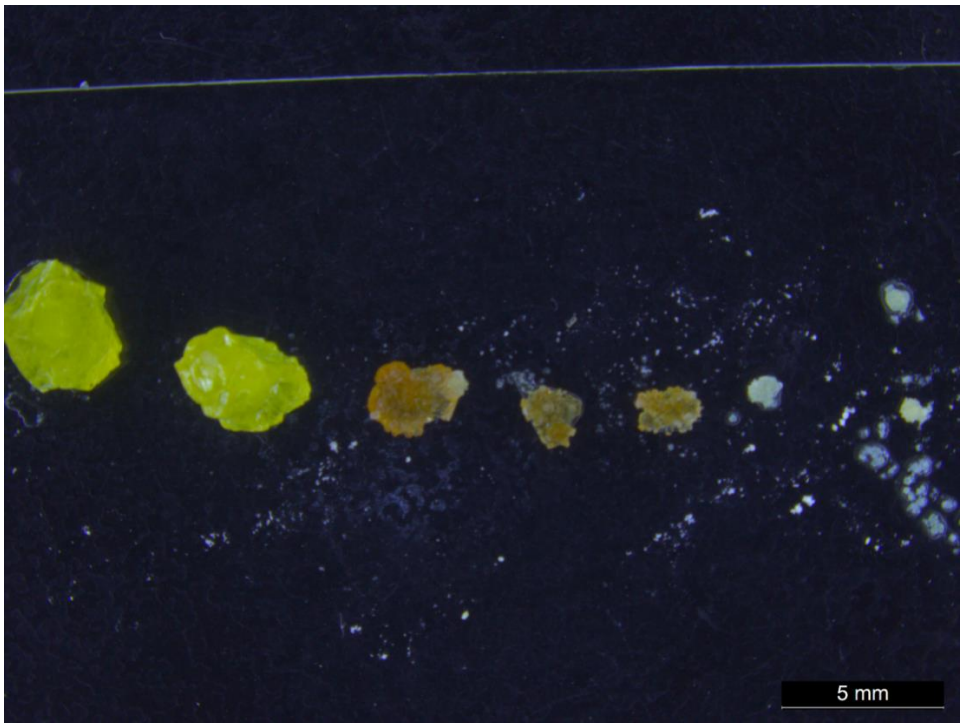

Figure S 1 *An image showing representative examples of the large yellow crystals and the large orange crystals [catena-(dimethylammonium tris(μ_2-formato)zinc(II)] that form in the reaction of WUF-21.*

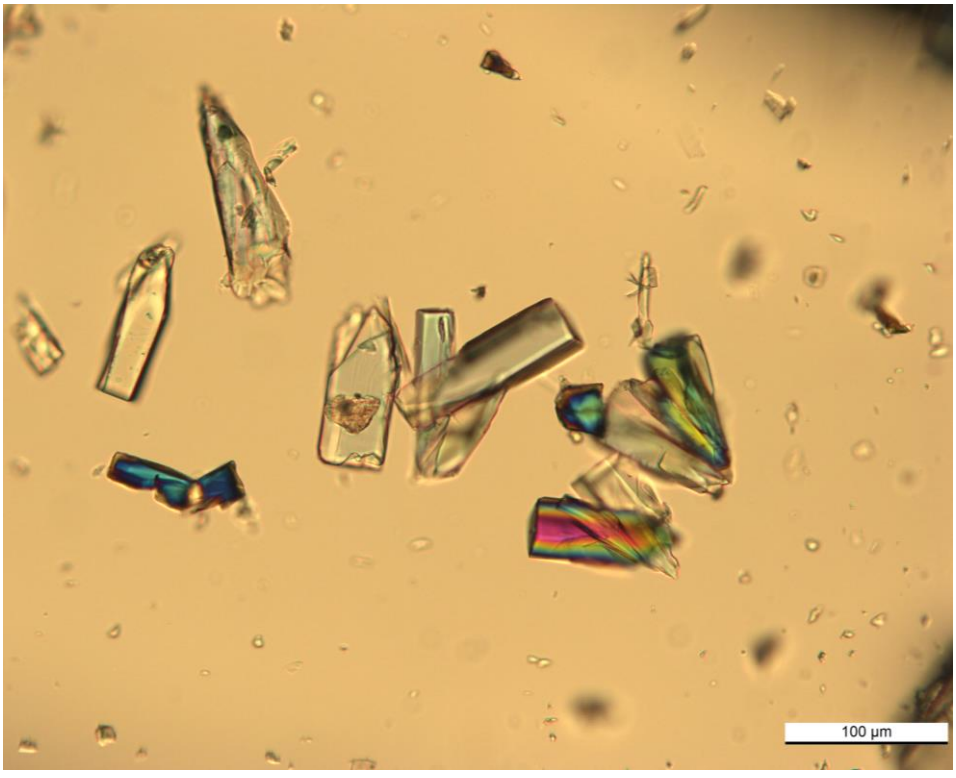

Figure S 2 *An image showing the morphology of a few crystals of WUF-21.*

Single Crystal X-ray Diffraction

Table S 2 *Crystal data and structure refinement for WUF-21.*

Identification code	WUF-21
Empirical formula	$C_{65}H_{50}N_7O_{30}Zn_5$
Formula weight	1735.97
Temperature/K	292.15
Crystal system	monoclinic
Space group	C2/c
a/Å	32.809(6)
b/Å	34.904(6)
c/Å	24.682(5)
α/°	90
β/°	117.928(8)
γ/°	90
Volume/Å^3	24973(8)
Z	8
ρ_{calc}g/cm^3	0.923
μ/mm^{-1}	1.527
F(000)	7032.0
Crystal size/mm^3	0.15 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	11.106 to 67.014
Index ranges	-23 ≤ h ≤ 23, -22 ≤ k ≤ 24, -17 ≤ l ≤ 17
Reflections collected	28673
Independent reflections	4717 [R_{int} = 0.1252, R_{sigma} = 0.1003]
Data/restraints/parameters	4717/1131/845
Goodness-of-fit on F^2	1.866
Final R indexes [I>=2σ (I)]	R_1 = 0.1864, wR_2 = 0.4542
Final R indexes [all data]	R_1 = 0.2452, wR_2 = 0.5017
Largest diff. peak/hole / e Å^{-3}	0.95/-0.76

Data were collected at room temperature using a rotating anode instrument with Cu radiation (1.54178) to a resolution of 1.40 Å. The data quality is mediocre, but the analysis has allowed the definitive assignment of the structure of this porous MOF.

A RIGU restraint was applied to all non-hydrogen atoms to allow for anisotropic refinement. All C-H groups are riding models with fixed Uiso at 1.2 or 1.5 times their carrier atoms. The hydrogen atoms of the μ_3-hydroxido groups [O1D(H111), O112(H112)] were implanted into the structure in approximate positions and allowed to ride on their carrier oxygen atoms.

All phenyl rings were fitted as hexagons and refined as free rotating groups. Planarity restraints were applied to rings C93, C94, C95, C99, C100, C101 and C93A, C94A, C95A, C99A C11A, C10A. The thermal parameters of C101 were set to match its partner atom in the disorder model (C11A) to achieve a reasonable ellipsoid shape. The disorder model includes these two phenyl rings together with their attached carboxylate groups (C92A C10A C11A C93A C94A C95A C99A O91A and C92 O91 C93 C94 C95 C99 C100 C101) and was modelled as two-component disorder using a free variable (~50:50). The position of C92 was fixed and part of a free rotating group with O91. The position of the carboxylate carbon C3 also required fixing to give reasonable bond lengths and angles.

Distance restraints (DFIX 1.5 with sigma of 0.02) were applied between phenyl ring carbons and attached nitro groups for C6-N7 and C35-N36. Nitro groups based on N7, N36, N66 and N96 were refined as freely rotating rigid groups with N-O bond distance restraints (SADI). Planarity restraints were applied to nitro groups together with their attached carbon of the phenyl ring. The nitro groups N96 O97 O98 and N96A O97A O98A were given fixed occupancy of 0.5 based on the approximately equal proportions of the disordered phenyl rings they are attached to.

The disordered nitro groups of N71 O71 O72 and N66 O67 O68 were modelled as a two-component disorder via a free variable (15:85, respectively) and the atomic positions and thermal parameters for N71 O71 O72 were fixed. The thermal parameters of N96A O97A O98A were also fixed. In order to achieve reasonable ellipsoid shapes, nitro groups N7 O8 O9 and N36 O37 O38 were constrained to have the same ADPs as N66 O67 O68, respectively.

DMF ligands were refined as freely rotating rigid groups with similarity restraints on all bond distances, thermal parameters, and with planarity restraints. The disordered parts of the DMF ligands sharing atom O1F (C2FA C4FA C5FA N3FA and C2FB C4FB C5FB N3FB) were modelled as a two-component disorder via a free variable (0.33:0.67, respectively). Terminal methyl group carbon C5FB was constrained to have identical ADPs as its partner atom in the disorder model (C5FA) to avoid being NPD.

The data have not been subject to the SQUEEZE routine in PLATON.

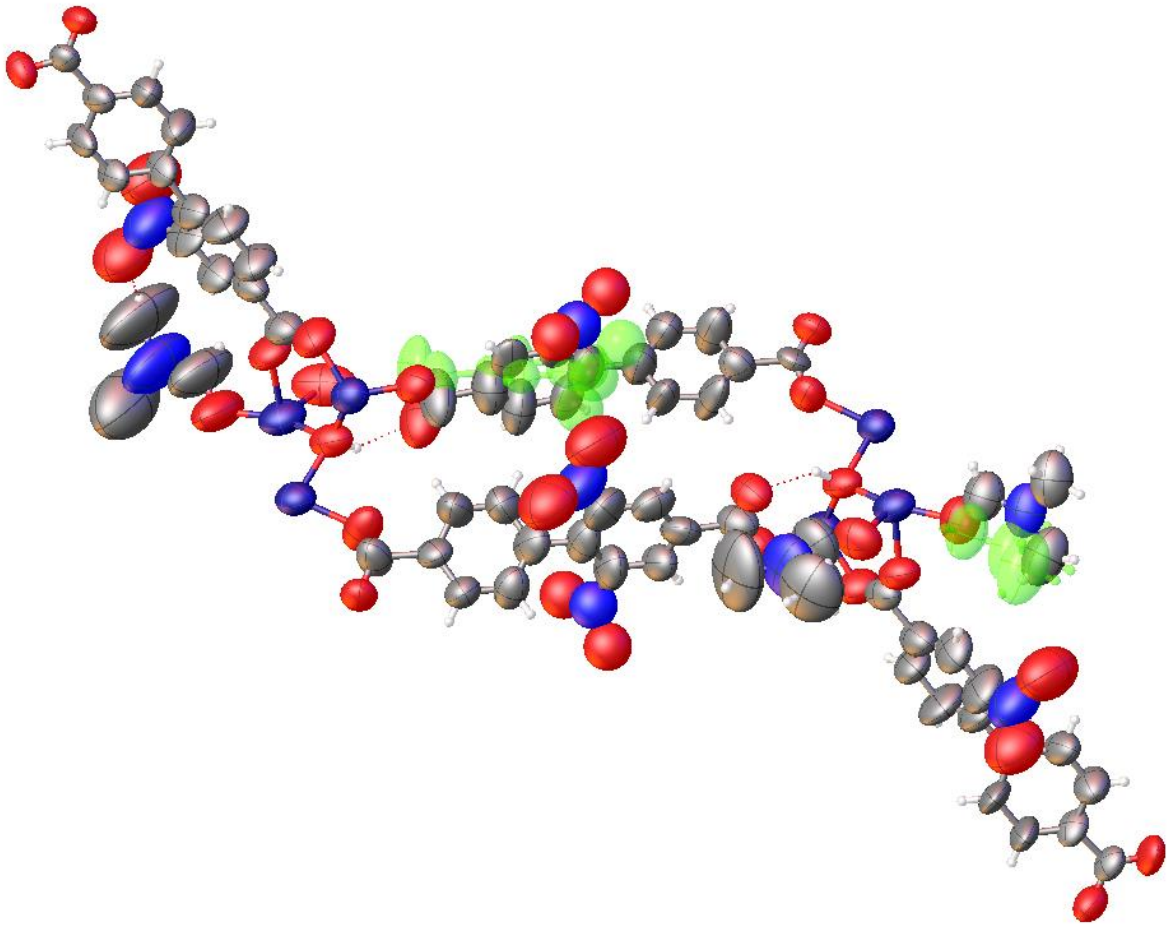

Figure S 3 *The asymmetric unit of WUF-21 with disordered groups shown in green.*

WUF-23

Table S 3 *Crystal data and structure refinement for WUF-23.*

Identification code	WUF-23
Empirical formula	$C_{129}H_{104}N_{12}O_{73}Zn_{12}$
Formula weight	3774.68
Temperature/K	173.15
Crystal system	triclinic
Space group	P-1
a/Å	17.212(3)
b/Å	22.812(5)
c/Å	32.761(7)
α/°	92.65(3)
β/°	90.42(3)
γ/°	102.29(3)
Volume/Å^3	12553(5)
Z	2
ρ_{calc}g/cm^3	0.999
μ/mm^{-1}	1.187
F(000)	3812.0
Crystal size/mm^3	0.1 × 0.1 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	1.244 to 41.63
Index ranges	-17 ≤ h ≤ 17, -22 ≤ k ≤ 22, -32 ≤ l ≤ 32
Reflections collected	138388
Independent reflections	25062 [R_{int} = 0.1050, R_{sigma} = 0.0556]
Data/restraints/parameters	25062/1017/1636
Goodness-of-fit on F^2	2.089
Final R indexes [I>=2σ (I)]	R_1 = 0.1757, wR_2 = 0.4740
Final R indexes [all data]	R_1 = 0.1876, wR_2 = 0.4827
Largest diff. peak/hole / e Å^{-3}	2.49/-1.13

Data were collected at the Australian Synchrotron on the MX2 beamline with wavelength 0.71073 Å radiation at 100 K. Two data sets were merged with data truncation at 1.00 Å.

A RIGU restraint was applied to all carbon atoms. All C-H groups are riding models with fixed Uiso at 1.2 times their carrier atoms. Methyl group C-H were refined with AFIX 33 to allow the refinement to converge. Hydrogen atoms attached to bound water molecules are riding models with fixed Uiso at 1.5 times their carrier atoms. In later cycles some of these were fixed (AFIX 1) to allow for convergence. The hydrogen atoms of the μ_3-hydroxido groups [O123(H123), O456(H456), O789(H789), O012(H012)] were implanted into the structure in approximate positions ~1 Å from the carrier oxygen atoms and SOF and Uij fixed (AFIX 1).

Every phenyl ring in this structure was fitted as a regular hexagon and refined as free rotating groups (AFIX 66). A SIMU restraint with sigma of 0.04 was applied to phenyl rings C113 – C117 & C142 - C147. Furthermore to control the displacement parameters of some atoms in these rings an EADP constraint was applied to atoms (C141 = C11), (C142 = C12), (C143 = C17).

Nitro groups were refined as freely rotating rigid groups about the nitrogen atom and alongside distance and planarity restraints between phenyl ring carbons and nitrogen atoms (DFIX 1.46 with sigma of 0.01; FLAT with sigma of 0.1 for N35, N77, N95, N125, N136, N145 & FLAT with sigma 0.04 for N15 and N27) and phenyl ring carbons and oxygen (DANG 2.3 with sigma 0.02). The thermal parameters of all nitro groups were fixed (10.3). The nitro groups based on N95 and N155 were assigned 0.5 occupancy. The nitro group based on N145 behaved poorly toward refinement and the atomic coordinates of N145 were fixed.

Distance restraints were applied to two carboxylate groups (DFIX 1.26 O9 C11 O10 C11 & DFIX 1.26 O109 C111 O110 C111) and one carbon-nitrogen bond length in a bound DMF molecule was restrained (DFIX 1.36 N34 C6BA & DFIX 1.45 N137 C108 N137 C8AA) and a similarity restraint was applied to another (SADI N4 C19 N4 C1A)

DMF molecules were treated with RIGU and FLAT (sigma of 0.1) for C2B-O1B-N3B-C4B-C5B and RIGU and SIMU (0.04 0.08) for O1D-C2D-N3D-C4D-C5D, O1M-C2M-N3M-C4M-C5M & O1C-C2C-N3C-C4C-C5C. DFIX restraints were placed on C=O (1.22 Å), C-N (1.36 Å) and N-Me (1.45 Å) bonds for C2B-O1B-N3B-C4B-C5B and O1C-C2C-N3C-C4C-C5C. O1D-C2D-N3D-C4D-C5D, O1M-C2M-N3M-C4M-C5M are free rotating groups (AFIX 6).

An ISOR restraint was applied to the four monodentate aqua ligands (O1W – O4W) at the ends of the SBU. It was necessary to apply EADP to O1T=C1T, O1T=O2T, C1R=O1R.

The data have not been subjected to the SQUEEZE routine within PLATON.

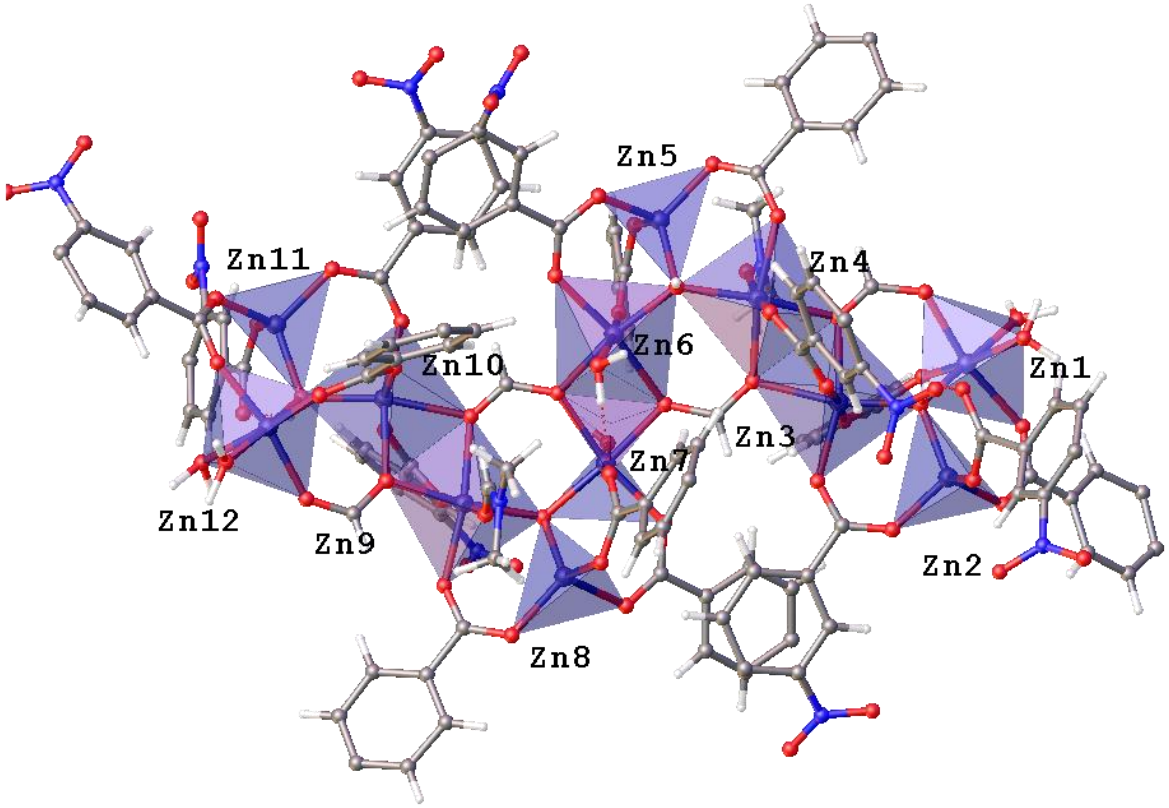

Figure S 4 *A view of the dodecazinc SBU in the structure of WUF-23. The coordination geometries of the zinc atoms are shown in polyhedral representation with Zn1, Zn3, Zn4, Zn6, Zn7, Zn9, Zn10 and Zn12 being octahedral in geometry and Zn2, Zn5, Zn8 and Zn11 being tetrahedral in geometry.*

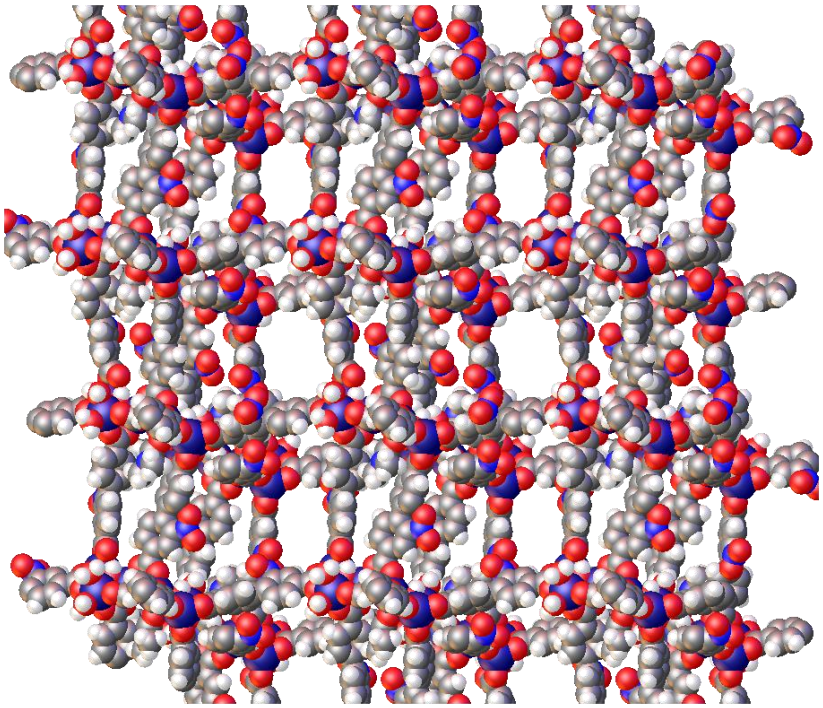

Figure S 5 *A view parallel to the 100 direction.*

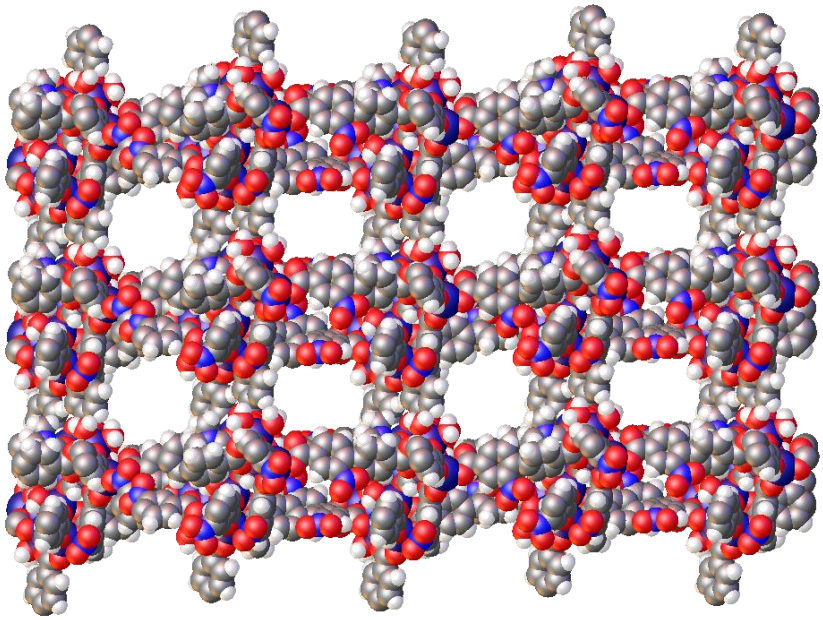

Figure S 6 *A view parallel to the 010 direction.*

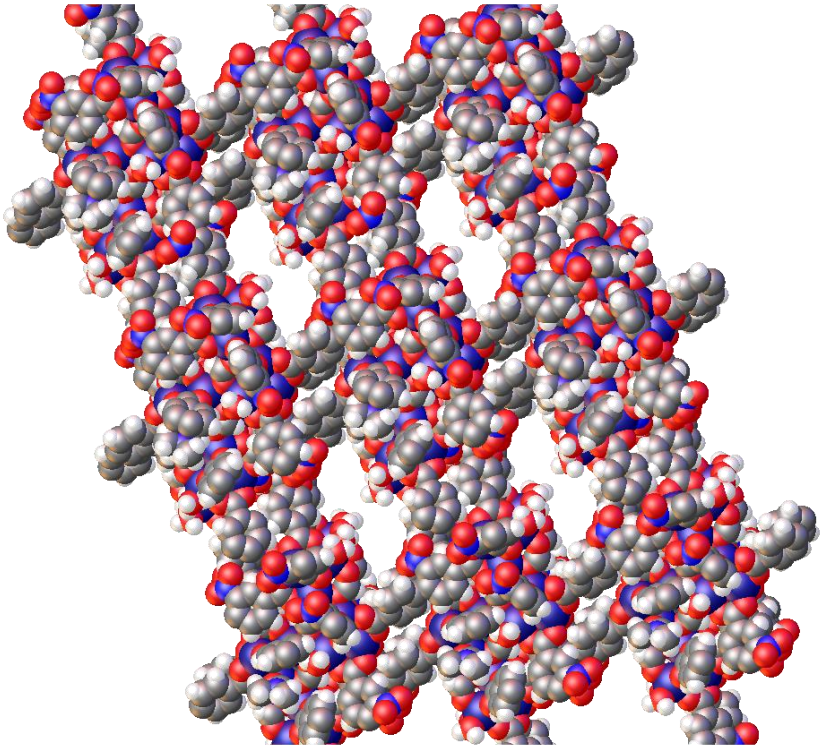

Figure S 7 *A view parallel to the 001 direction.*

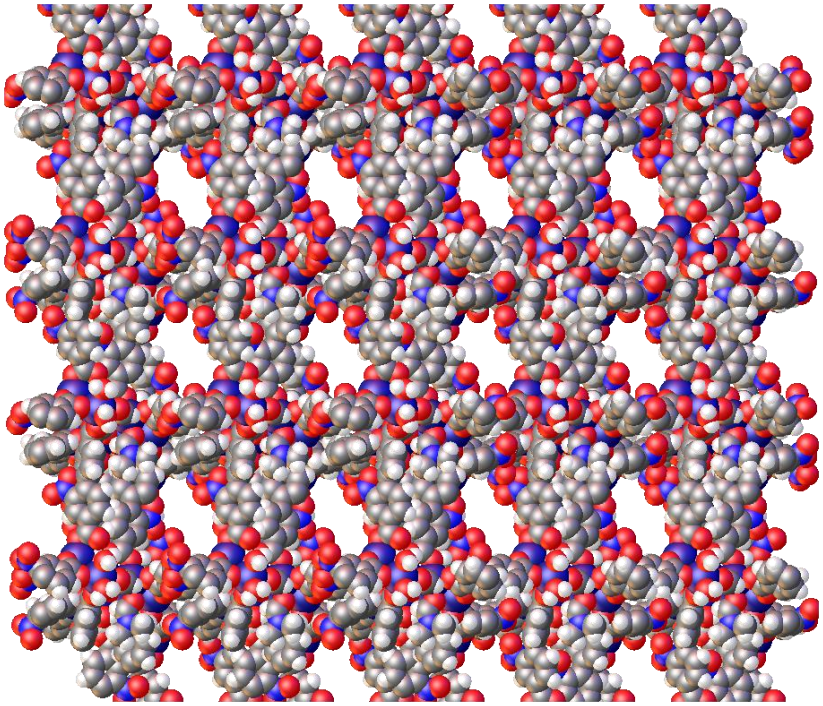

Figure S 8 *A view parallel to the 110 direction.*

WUF-22

Table S 4 *Crystal data and structure refinement forWUF-22.*

Identification code	WUF-22
Empirical formula	$C_{42}H_{22.67}N_3O_{19.83}Zn_4$
Formula weight	1148.10
Temperature/K	292.15
Crystal system	Monoclinic
Space group	C2/m
a/Å	24.3610(12)
b/Å	24.2585(10)
c/Å	17.2141(12)
α/°	90
β/°	91.458(6)
γ/°	90
Volume/Å^3	10169.6(10)
Z	4
ρ_{calc}g/cm^3	0.750
μ/mm^{-1}	1.396
F(000)	2297.0
Crystal size/mm^3	0.15 × 0.15 × 0.01
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	11.418 to 76.116
Index ranges	-19 ≤ h ≤ 19, -19 ≤ k ≤ 17, -11 ≤ l ≤ 13
Reflections collected	11546
Independent reflections	2659 [R_{int} = 0.1341, R_{sigma} = 0.1437]
Data/restraints/parameters	2659/522/263
Goodness-of-fit on F^2	1.878
Final R indexes [I>=2σ (I)]	R_1 = 0.1720, wR_2 = 0.4597
Final R indexes [all data]	R_1 = 0.2173, wR_2 = 0.4916
Largest diff. peak/hole / e Å^{-3}	1.06/-1.77

Data were collected at room temperature using a rotating anode instrument with Cu radiation (1.54178) to 0.9 Å and truncated to 1.25 Å resolution.

A RIGU restraint was applied to all non-hydrogen atoms. All C-H groups are riding models with fixed Uiso at 1.2 times their carrier atoms. A hydrogen atom (H1W) of the water molecule that occupies a special position (O1W; 0.0, 0.5, 1; occupancy 0.25) was included to complete the model (occupancy 0.5) and subject to a distance restraint (DFIX 0.95 with sigma of 0.02). O1W was itself given a fixed Uiso of 0.3 in the refinement. O2W refined to 0.29 occupancy and was set to 0.33 and the two hydrogens were fixed in position and occupancy and in site occupancy factors to match the oxygen. All oxygen atoms were subject to an ISOR restraint with standard uncertainties 0.05 0.1 and carbon atoms C11 C15 C14 C35 C13 C12 C29 C30 C31 C32 C33 C34 C4 C22 C5 C10 C9 C8 C7 C6 C28 C27 C26 C25 C24 C23 were also treated with ISOR with standard uncertainties 0.1 0.2. Each of the complete phenyl rings in this structure were fitted as hexagons and refined as free rotating groups.

A fixed occupancy of 0.5 was assigned to the nitrophenyl group lying across the mirror plane (C10 C9 C8 C7 C6 N90 O91 O92). The atomic positions and thermal parameters of the nitro group N90 O91 O92 of this ligand ring were fixed (10.2) as was the atomic positions and thermal parameters for the other nitro group in this structure N27 O29 O28.

The data have not been subjected to the SQUEEZE routine within PLATON.

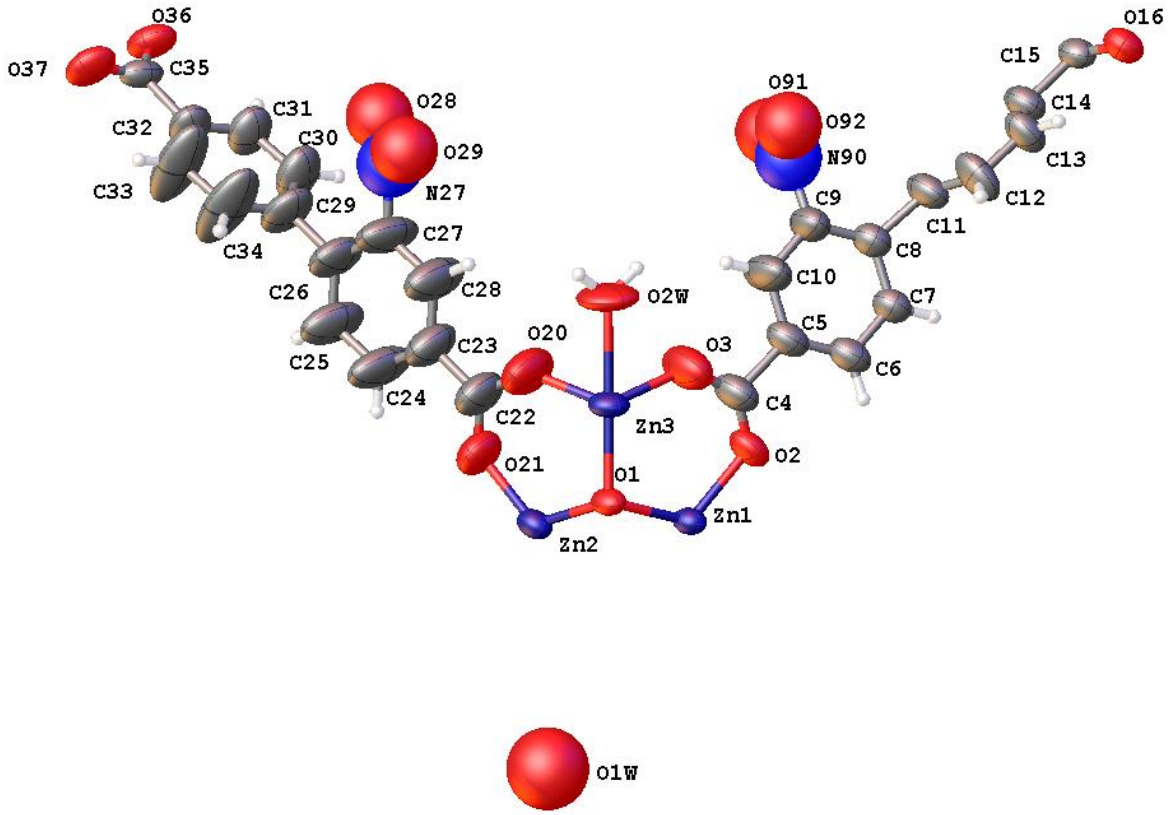

Figure S 9 *The contents of the asymmetric unit of WUF-22.*

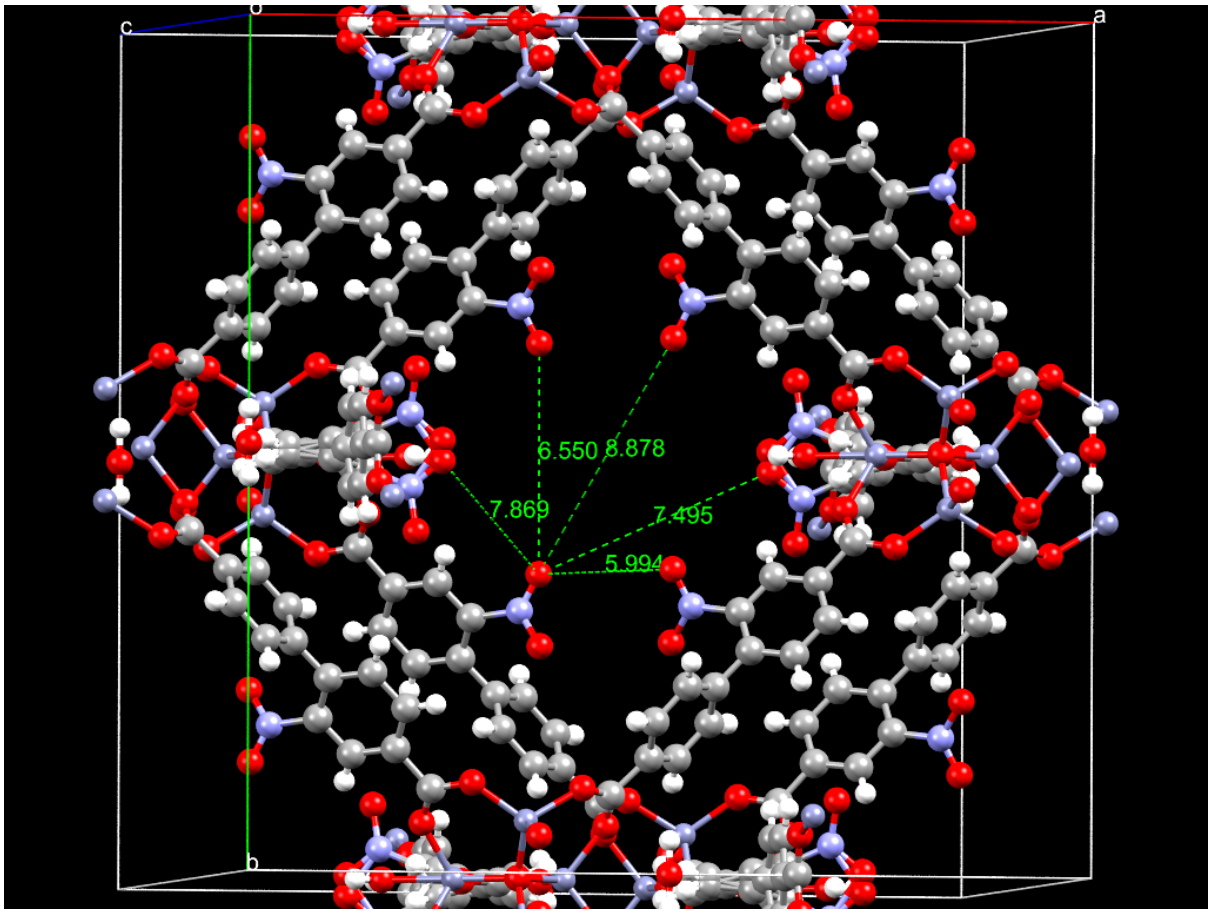

Figure S 10 *A view slightly offset from the c-axis of WUF-22 with five of the shortest atom-to-atom contact distances shown.*

Nuclear Magnetic Resonance Spectroscopy

The signal at 7.85 ppm in H_2bpdc was integrated against the signal at 7.73 ppm for H_2bpdcNO$_2$ in ^{1}H NMR spectra in d_6-DMSO solutions (Fig. S11).

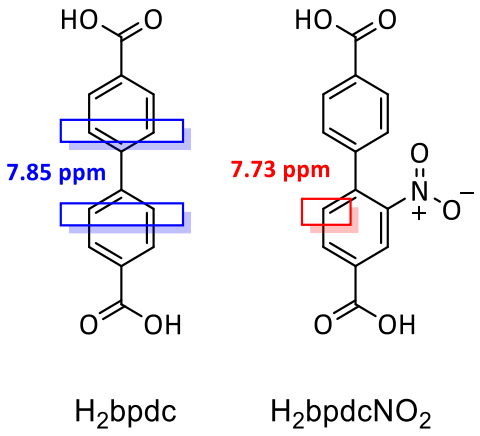

Figure S 11 *The structures of H_2bpdc and H_2bpdcNO$_2$ annotated with chemical shifts of the protons used to identify and quantify the ratios of these molecules in the starting mixtures and MOF samples.*

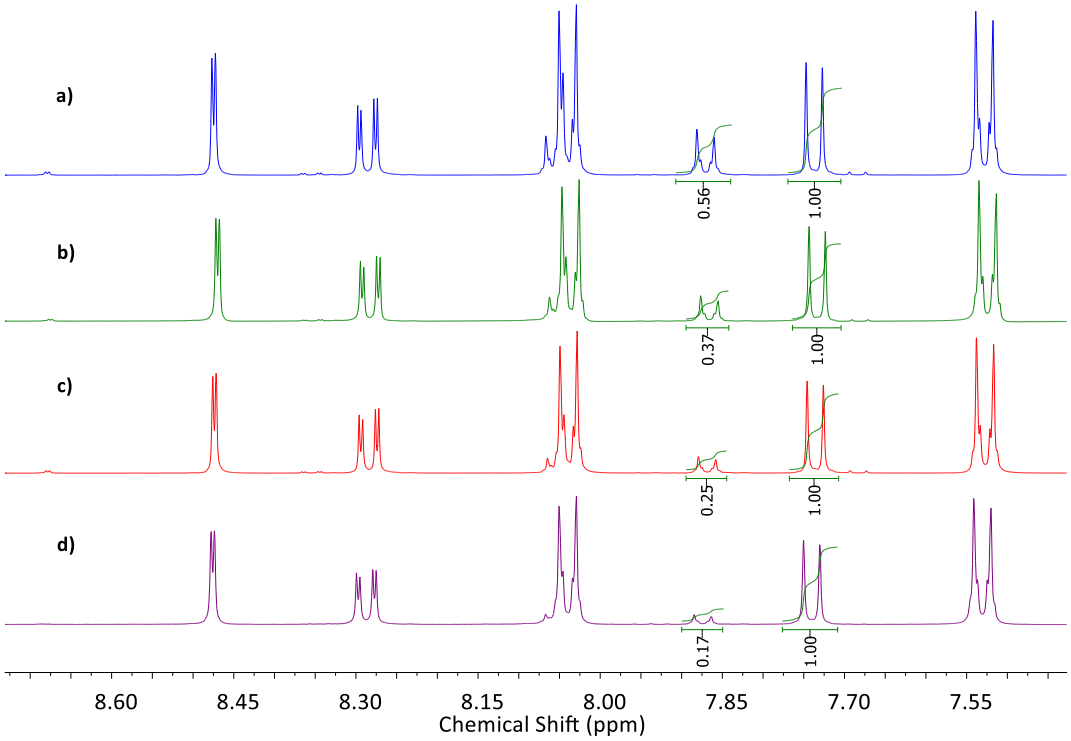

Figure S 12 *Stacked ^{1}H NMR spectra of ligand mixtures before MOF synthesis.* ***(a)*** *(blue) 12% H_2bpdc in H_2bpdcNO$_2$,* ***(b)*** *(green) 9% H_2bpdc in H_2bpdcNO$_2$,* ***(c)*** *(red) 6% H_2bpdc in H_2bpdcNO$_2$,* ***(d)*** *(purple) 4% H_2bpdc in H_2bpdcNO$_2$.*

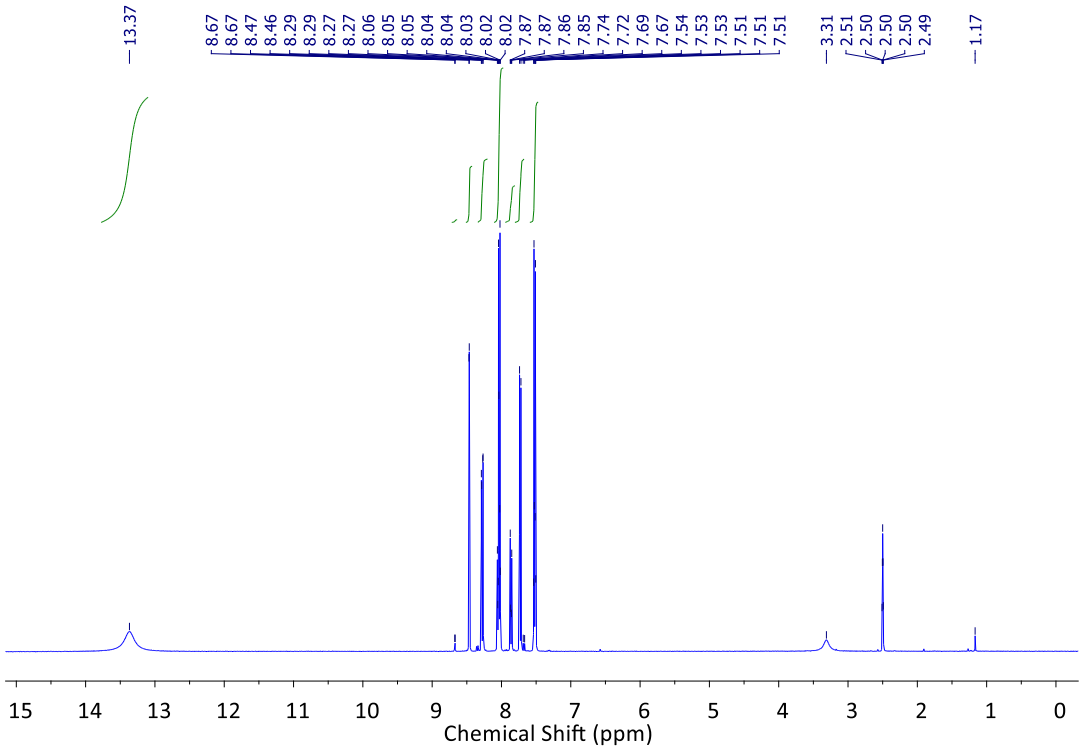

Figure S 13 *Full ^{1}H NMR spectrum of 12% H_2bpdc in H_2bpdcNO$_2$.*

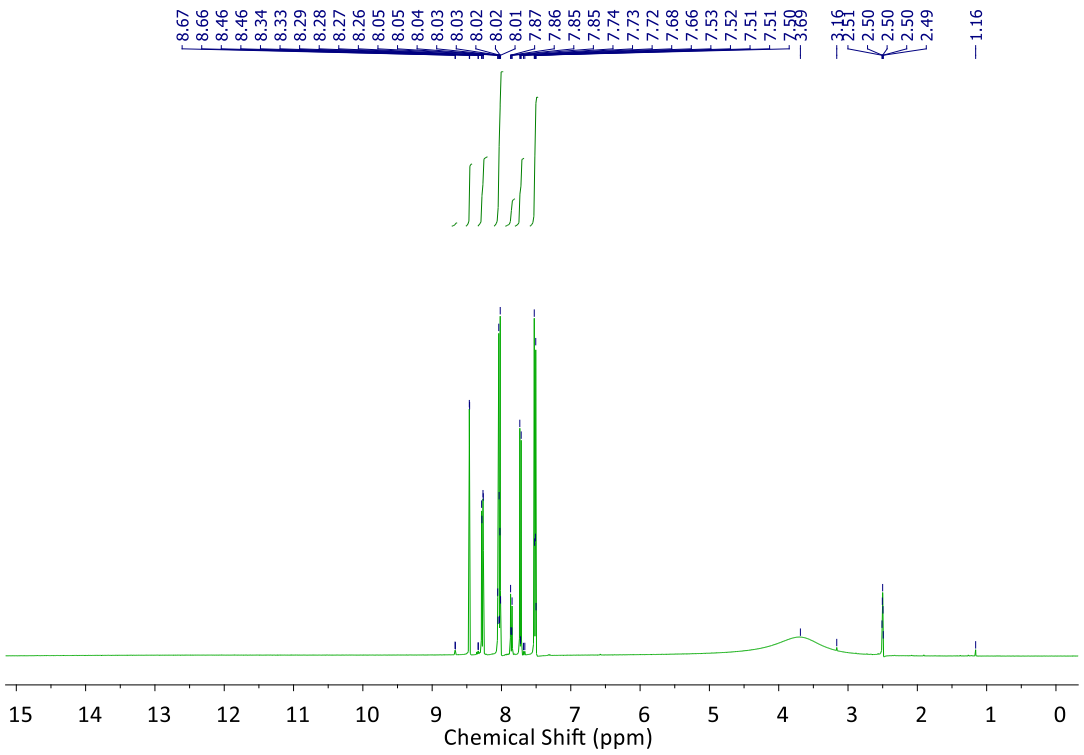

Figure S 14 *Full ^{1}H NMR spectrum of 9% H_2bpdc in H_2bpdcNO$_2$.*

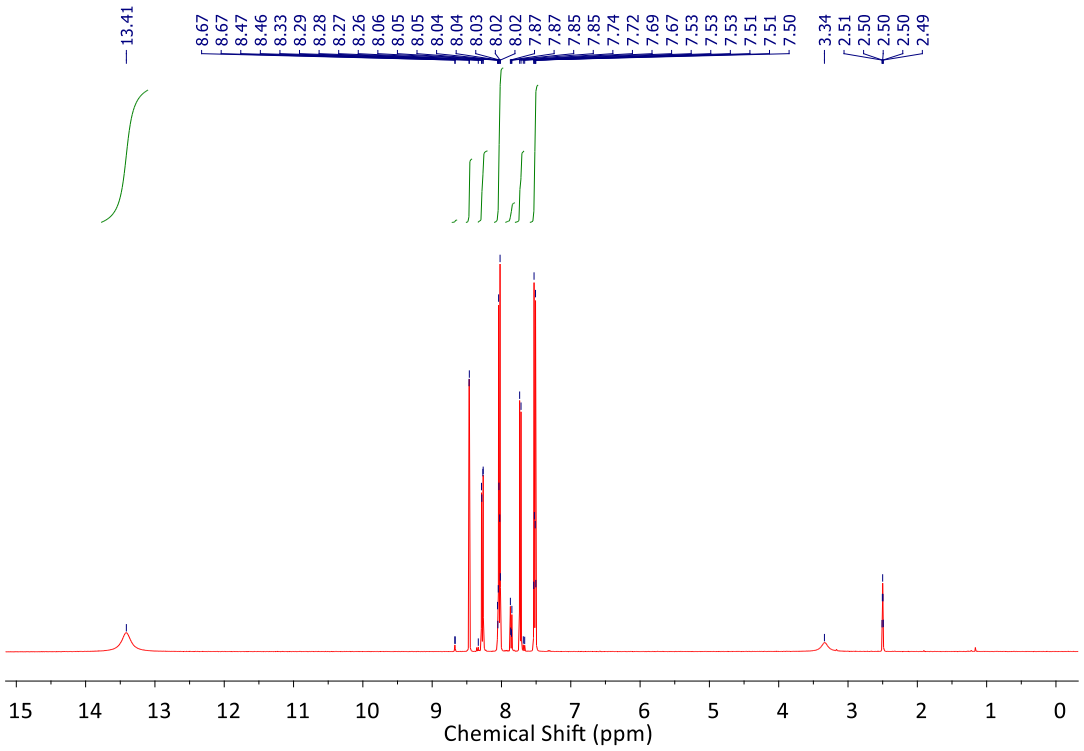

Figure S 15 *Full ^{1}H NMR spectrum of 8% H_2bpdc in H_2bpdcNO$_2$.*

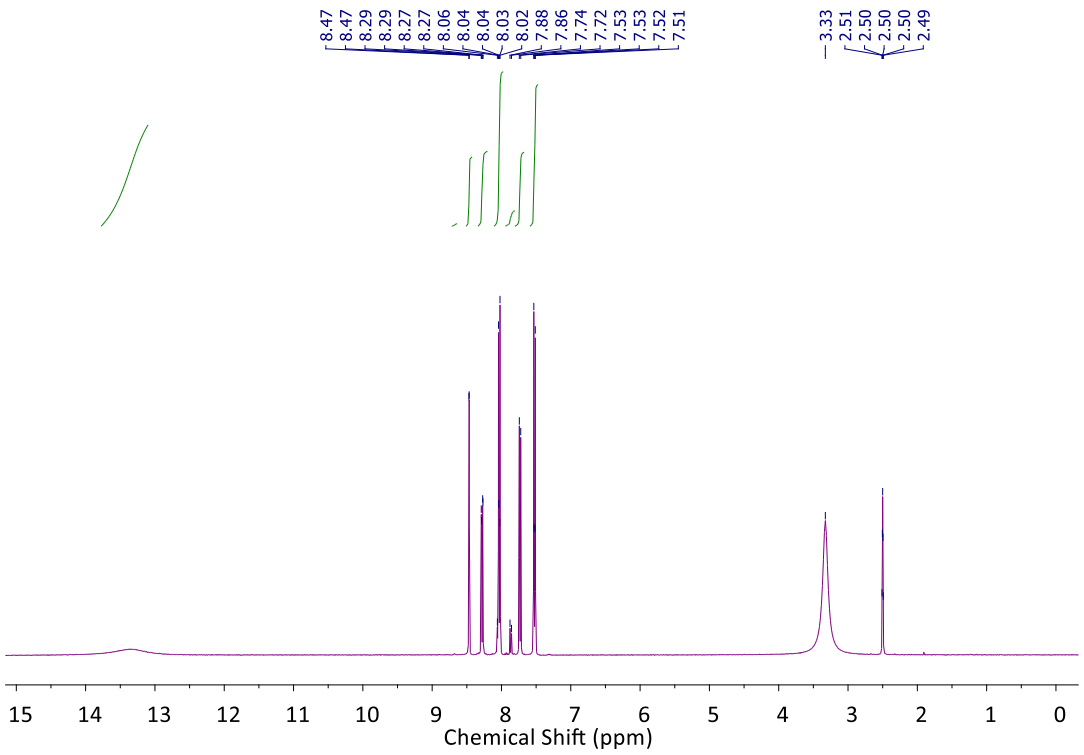

Figure S 16 *Full ^{1}H NMR spectrum of 4% H_2bpdc in H_2bpdcNO$_2$.*

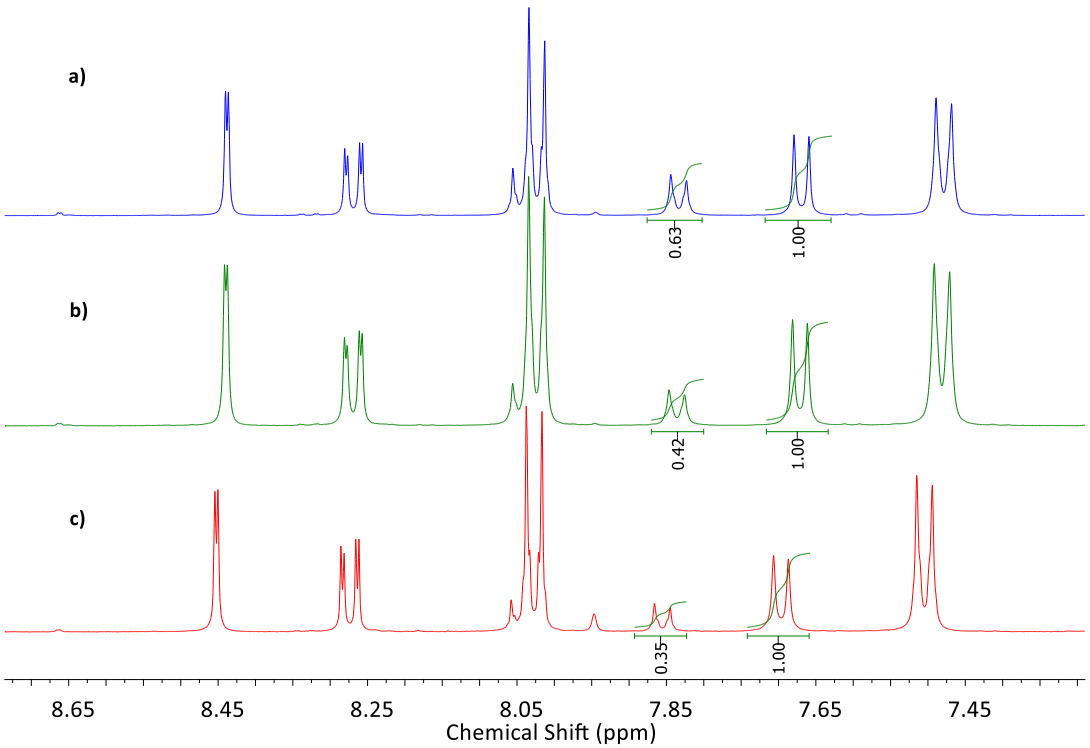

Figure S 17 *Stacked ^{1}H NMR spectra of MOFs after digestion in DCl/DMSO.* ***(a)*** *WUF-22(14) (blue),* ***(b)*** *WUF-22(10) (green),* ***(c)*** *WUF-22(8) (red).*

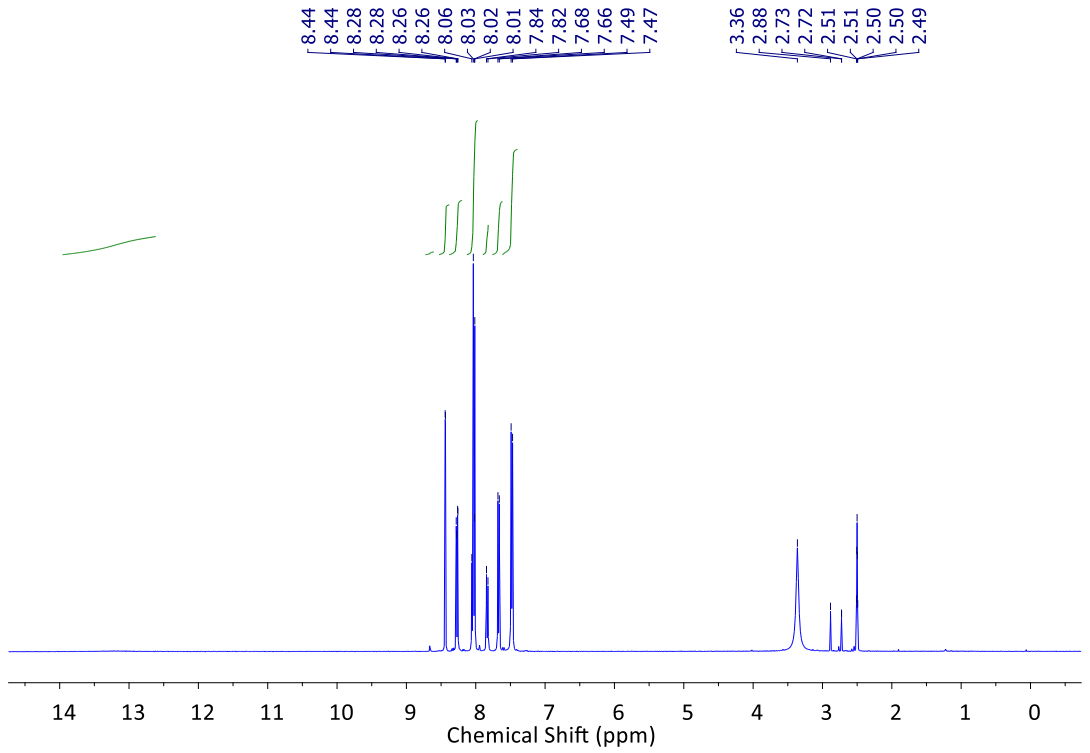

Figure S 18 *^{1}H NMR spectrum of WUF-22(14).*

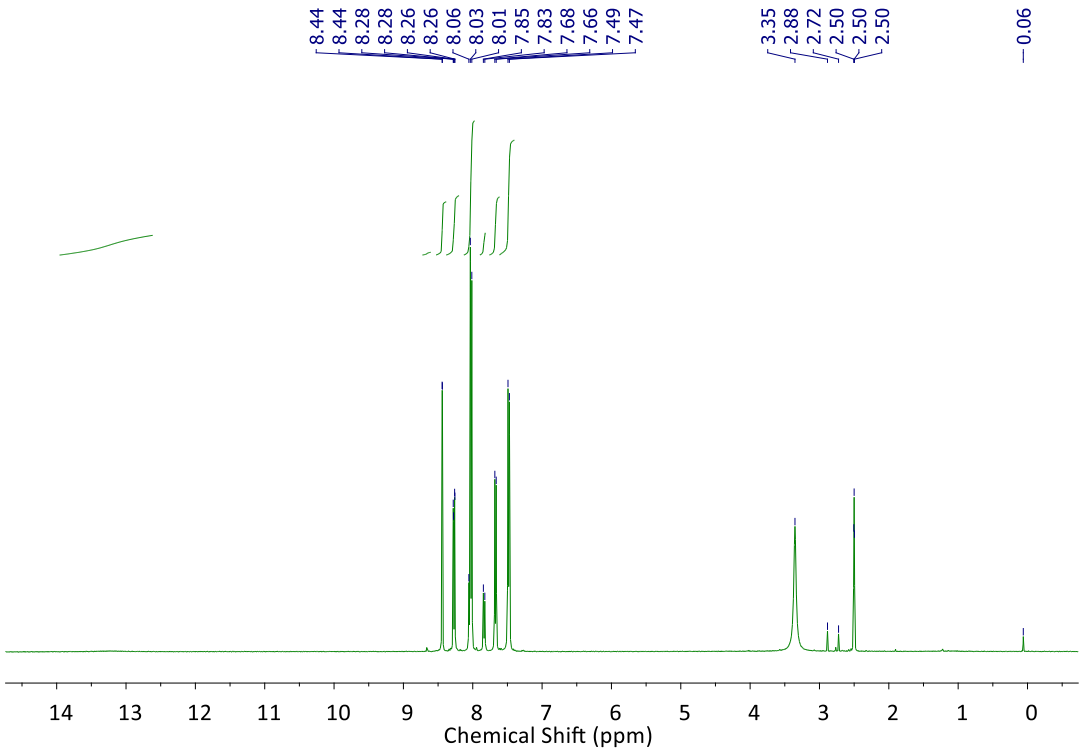

Figure S 19 *^{1}H NMR spectrum of WUF-22(10).*

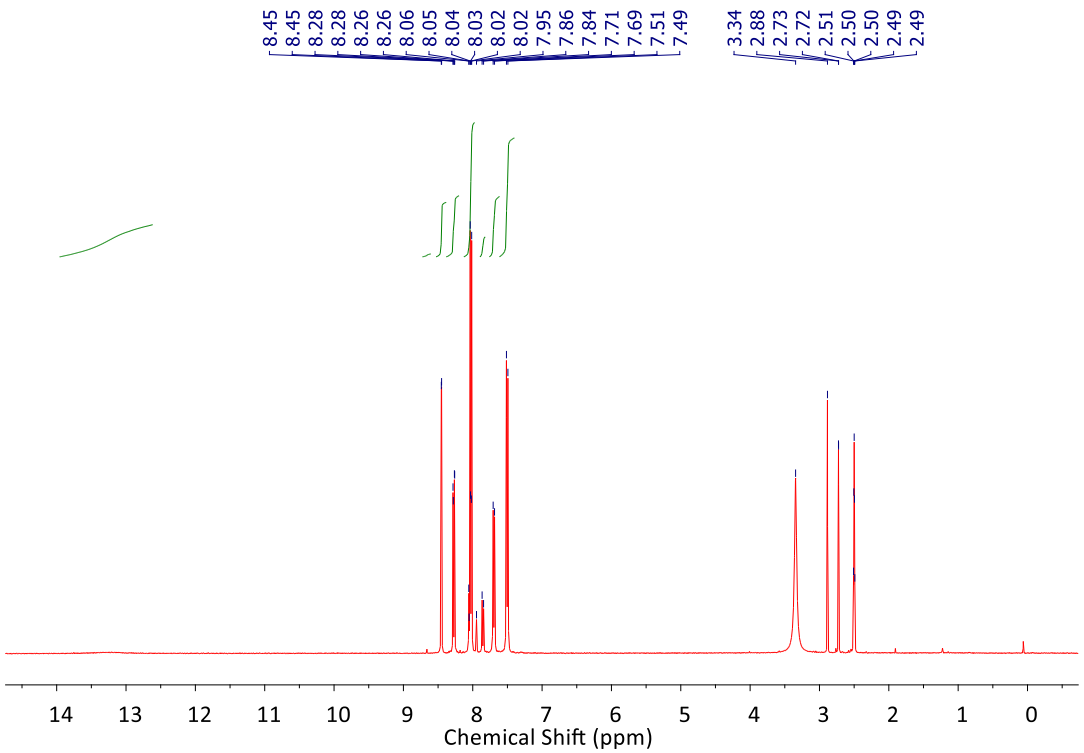

Figure S 20 *^{1}H NMR spectrum of WUF-22(8).*

Powder X-ray Diffraction

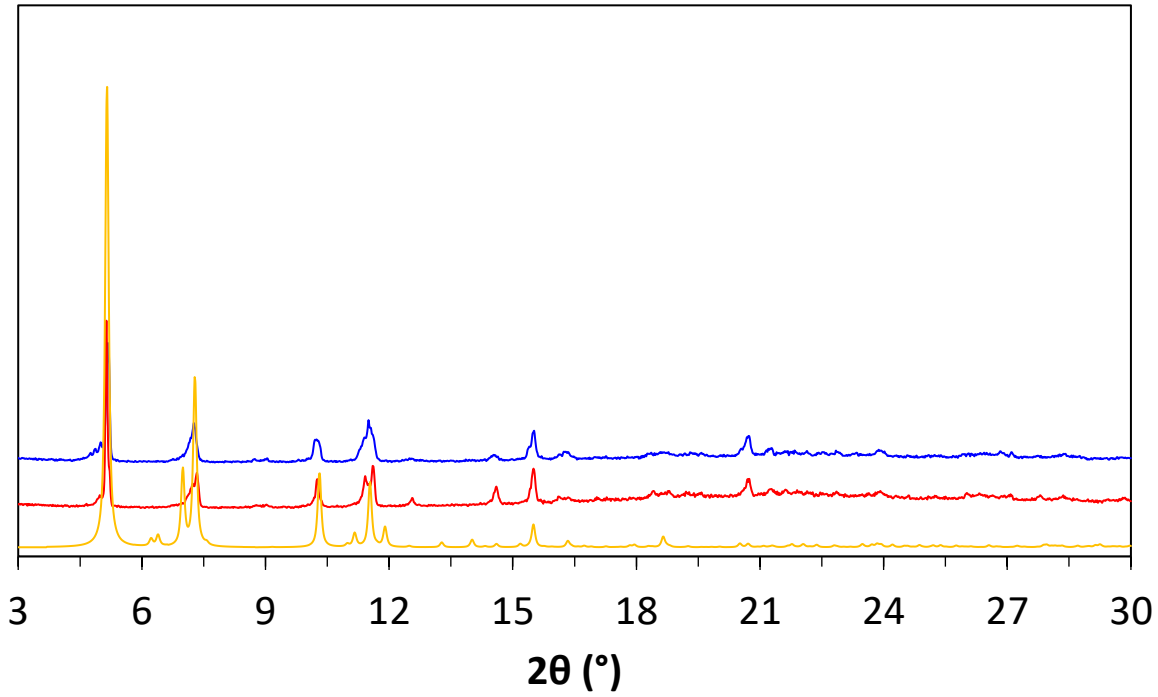

Figure S 21 *A stacked plot of PXRD patterns for 'as synthesised' MOFs in DMF; WUF-22(14) (blue) and WUF-22(8) (red) compared with calculated pattern for IRMOF-9 (yellow).*[1]

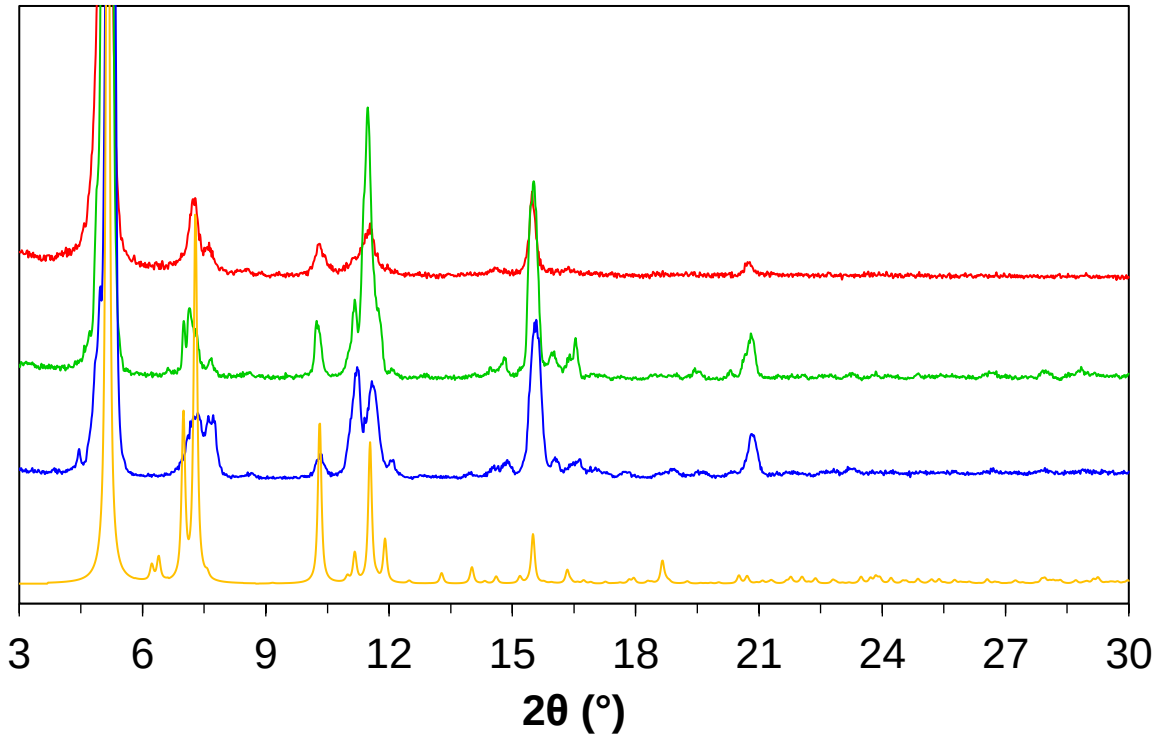

Figure S 22 *Stacked PXRD patterns for MOFs after solvent exchange to DCM and vacuum drying; WUF-22(8) (red), WUF-22(10) (green), WUF-22(14) (blue) and calculated pattern of IRMOF-9 from single crystal data[1] (yellow).*

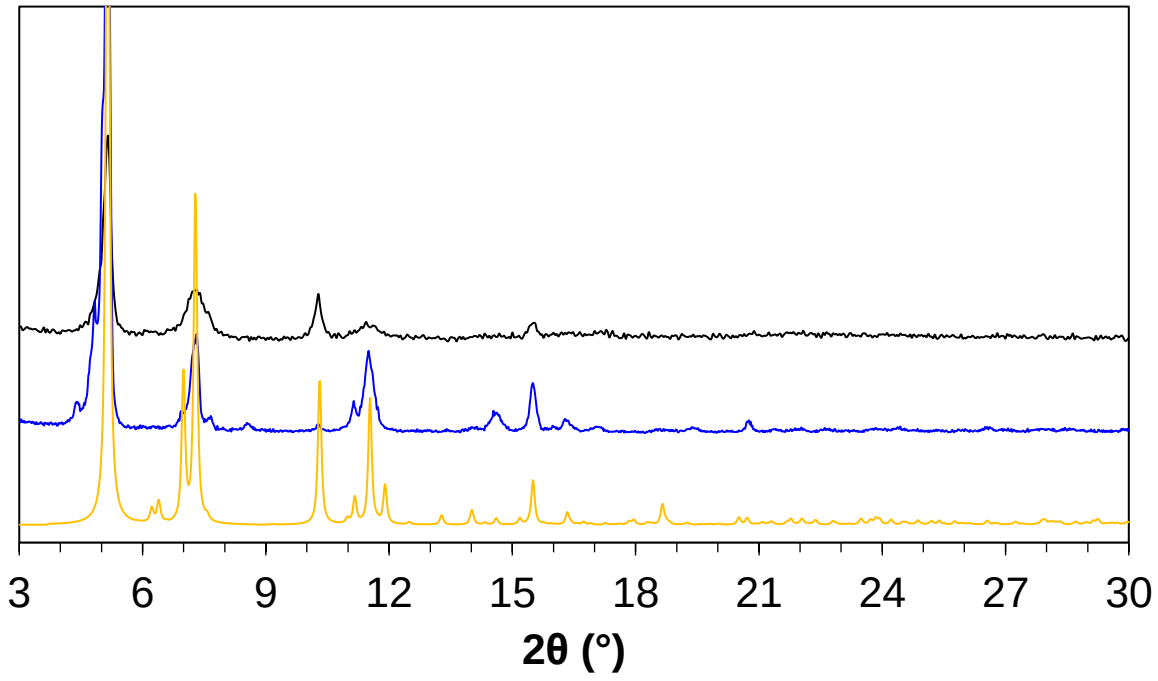

Figure S 23 *Stacked PXRD patterns for WUF-22(14) activated by different methods. Pattern after solvent exchange to acetone then heating at 60 °C for 6 h then 120 °C for 6 h under dynamic vacuum (0.04°step size, 3°/min) (black). Pattern after solvent exchange to cyclohexane and freeze drying then*

heating at 120 °C for 6 h under dynamic vacuum (blue). Calculated pattern of IRMOF-9 from single crystal data[1] (yellow).

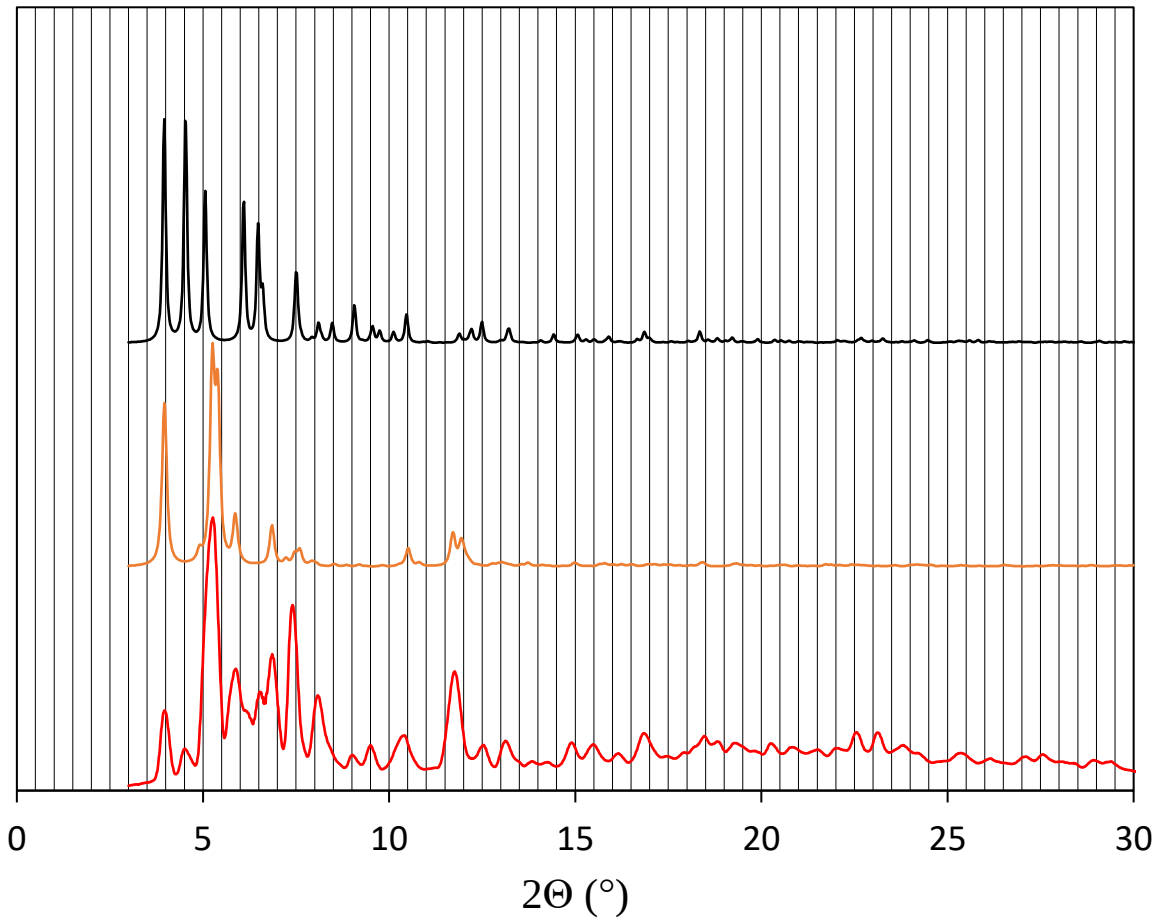

Figure S 24 *The calculated PXRD patterns of WUF-21 (black), WUF-23 (orange) and the experimental pattern obtained after 2 years (red).*

Thermogravimetric-Differential Scanning Calorimetry

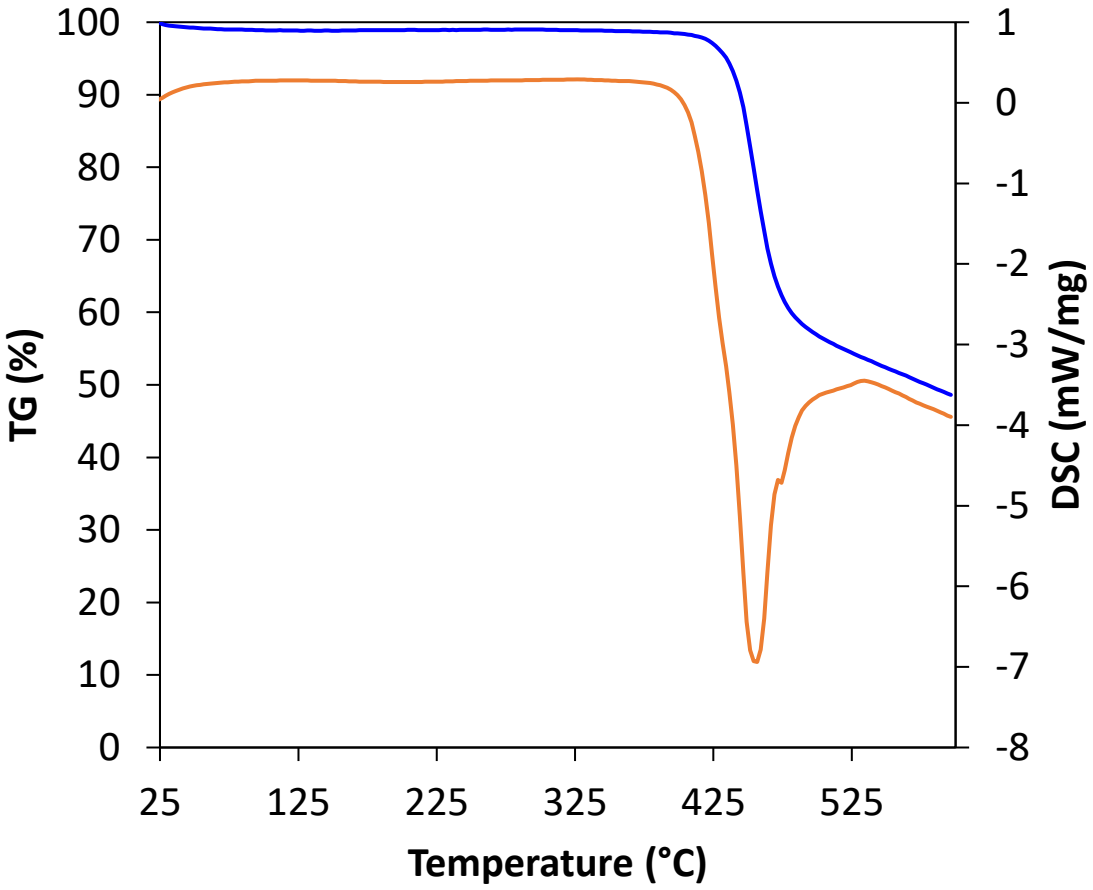

Figure S 25 *TG-DSC data for activated WUF-22(14) under a combined flow of N_2 (10 ml/min) and compressed air N_2/O_2, 80/20 (10 ml/min) from 25-600 °C. TG is the blue line and DSC the orange line.*

Geometric Surface Area Calculations

Models containing the atomic coordinates for the framework atoms for $[(Zn_4O)_4(bpdc\text{-}NO_2)_{11}(bpdc)_1]$ and $[(Zn_4O)_4(bpdc\text{-}NO_2)_{10}(bpdc)_2]$ were generated for geometric surface area calculations from the crystal structure by removing one of the disordered components, and one or two nitro groups were replaced by hydrogen atom(s) placed in calculated positions and models in P1 were generated. The fractional xyz coordinates for $[(Zn_4O)_4(bpdc\text{-}NO_2)_{11}(bpdc)_1]$ and $[(Zn_4O)_4(bpdc\text{-}NO_2)_{10}(bpdc)_2]$ are provided below. The geometric surface areas of $(Zn_4O)_4(bpdc\text{-}NO_2)_{11}(bpdc)_1$ and $(Zn_4O)_4(bpdc\text{-}NO_2)_{10}(bpdc)_2$ were calculated following the method of Duren et. al.[2] with a probe diameter set to 3.72 Å to match nitrogen.[3] The diameters of framework atoms were taken from the DREIDING force field and set to their van der Waals diameters by multiplying their Lennard-Jones well-depth diameters, σ, by $2^{1/6}$.

$(Zn_4O)_4(bpdc\text{-}NO_2)_{11}(bpdc)_1$:

Surface area: 1837.589801 ± 1.882591 [A^2]

Surface area: 2465.966331 ± 2.526355 [m^2/g]

Surface area: 1806.923561 ± 1.85117 [m^2/cm^3]

$(Zn_4O)_4(bpdc\text{-}NO_2)_{10}(bpdc)_2$:

Surface area: 1851.970565 ± 1.376748 [A^2]

Surface area: 2510.437193 ± 1.866250 [m^2/g]

Surface area: 1821.064334 ± 1.35377 [m^2/cm^3]

Unit cell parameters:

a = 24.36100; b = 24.25900; c = 17.21400 Å

α = 90.0000; β = 91.4600; γ = 90.0000°

Fractional Coordinates for $[(Zn_4O)_4(bpdcNO_2)_{10}(bpdc)_2]$				
Elmt	Label	x	y	Z
C	C1	0.132016	0.499979	0.545024
C	C2	0.368	0	0.454976
C	C2	0.368	1	0.454976
C	C3	0.867984	0.499979	0.454976
C	C4	0.631996	0	0.545024
C	C4	0.631996	1	0.545024
C	C5	0.135407	0.499979	0.452918
C	C6	0.635427	0	0.452918
C	C6	0.635427	1	0.452918
C	C7	0.36457	0	0.547082
C	C7	0.36457	1	0.547082
C	C8	0.864593	0.499979	0.547082
C	C9	0.090521	0.487984	0.403988
C	C10	0.4095	0.011995	0.596012
C	C11	0.590501	0.011995	0.403988
C	C12	0.909479	0.511975	0.596012
C	C13	0.905002	0.506987	0.675682
C	C14	0.40498	0.007008	0.675682
C	C15	0.094998	0.492972	0.324318
C	C16	0.595018	0.007008	0.324318
C	C17	0.35567	0.991014	0.707178
C	C18	0.855694	0.490993	0.707178
C	C19	0.144306	0.509007	0.292822
C	C20	0.644326	0.991014	0.292822
C	C21	0.189219	0.521003	0.340996
C	C22	0.689198	0.979018	0.340996
C	C23	0.810781	0.478997	0.659004
C	C24	0.3108	0.979018	0.659004
C	C25	0.684728	0.983388	0.421015
C	C26	0.31527	0.983388	0.578985
C	C27	0.184707	0.516592	0.421015
C	C28	0.815293	0.483408	0.578985
C	C29	0.852994	0.499979	0.79202
C	C30	0.35299	0	0.791986
C	C30	0.35299	1	0.791986
C	C31	0.147006	0.499979	0.20798
C	C32	0.647011	0	0.20801
C	C32	0.647011	1	0.20801

C	C33	0.147618	0.543881	0.168987
C	C34	0.852382	0.543881	0.831013
C	C35	0.147618	0.456078	0.168987
C	C36	0.647622	0.956099	0.16902
C	C37	0.647622	0.043901	0.16902
C	C38	0.35238	0.956099	0.830979
C	C39	0.35238	0.043901	0.830979
C	C40	0.852382	0.456078	0.831013
C	C41	0.854005	0.454306	0.91202
C	C42	0.854005	0.545694	0.91202
C	C43	0.646041	0.045715	0.08801
C	C44	0.35396	0.954285	0.911986
C	C45	0.145995	0.545694	0.08798
C	C46	0.145995	0.454306	0.08798
C	C47	0.35396	0.045715	0.911986
C	C48	0.646041	0.954285	0.08801
C	C49	0.644035	0	0.04501
C	C49	0.644035	1	0.04501
C	C50	0.35596	0	0.954988
C	C50	0.35596	1	0.954988
C	C51	0.855985	0.499979	0.954988
C	C52	0.144015	0.499979	0.04501
C	C53	0.145039	0.499979	0.955986
C	C54	0.854961	0.499979	0.044014
C	C55	0.35498	0	0.044014
C	C55	0.35498	1	0.044014
C	C56	0.645018	0	0.955986
C	C56	0.645018	1	0.955986
C	C57	0.743017	0.100993	0.762999
C	C58	0.243038	0.398986	0.762999
C	C59	0.743017	0.898965	0.762999
C	C60	0.756962	0.398986	0.237001
C	C61	0.243038	0.600973	0.762999
C	C62	0.756962	0.600973	0.237001
C	C63	0.25698	0.100993	0.237001
C	C64	0.25698	0.898965	0.237001
C	C65	0.788105	0.850695	0.757014
C	C66	0.788105	0.149305	0.757014
C	C67	0.288125	0.350674	0.757014
C	C68	0.2119	0.850695	0.242986
C	C69	0.288125	0.649285	0.757014
C	C70	0.2119	0.149305	0.242986
C	C71	0.711875	0.350674	0.242986
C	C72	0.711875	0.649285	0.242986
C	C73	0.78171	0.803166	0.800829

C	C74	0.718269	0.696772	0.199171
C	C75	0.21829	0.196793	0.199171
C	C76	0.281731	0.696772	0.800829
C	C77	0.281731	0.303186	0.800829
C	C78	0.718269	0.303186	0.199171
C	C79	0.21829	0.803166	0.199171
C	C80	0.78171	0.196793	0.800829
C	C81	0.17866	0.761985	0.200507
C	C82	0.82134	0.238015	0.799493
C	C83	0.678681	0.737994	0.200507
C	C84	0.678681	0.262006	0.200507
C	C85	0.82134	0.761985	0.799493
C	C86	0.17866	0.238015	0.200507
C	C87	0.321319	0.262006	0.799493
C	C88	0.321319	0.737994	0.799493
C	C89	0.632663	0.731687	0.246008
C	C90	0.867317	0.231708	0.753992
C	C91	0.367337	0.731687	0.753992
C	C92	0.367337	0.268313	0.753992
C	C93	0.632663	0.268313	0.246008
C	C94	0.13268	0.231708	0.246008
C	C95	0.867317	0.768292	0.753992
C	C96	0.13268	0.768292	0.246008
C	C97	0.626268	0.6842	0.289824
C	C98	0.12629	0.184179	0.289824
C	C99	0.873711	0.81578	0.710176
C	C100	0.873711	0.184179	0.710176
C	C101	0.12629	0.81578	0.289824
C	C102	0.626268	0.3158	0.289824
C	C103	0.373732	0.3158	0.710176
C	C104	0.373732	0.6842	0.710176
C	C105	0.334134	0.642978	0.71099
C	C106	0.16589	0.142998	0.28901
C	C107	0.665866	0.356981	0.28901
C	C108	0.665866	0.642978	0.28901
C	C109	0.834113	0.142998	0.71099
C	C110	0.16589	0.857002	0.28901
C	C111	0.834113	0.857002	0.71099
C	C112	0.334134	0.356981	0.71099
C	C113	0.906706	0.724886	0.753004
C	C114	0.593273	0.224906	0.246996
C	C115	0.09329	0.724886	0.246996
C	C116	0.09329	0.275114	0.246996
C	C117	0.593273	0.775094	0.246996
C	C118	0.406727	0.775094	0.753004

C	C119	0.406727	0.224906	0.753004
C	C120	0.906706	0.275114	0.753004
C	C121	0.40582	0.184509	0.695823
C	C122	0.40582	0.815491	0.695823
C	C123	0.9058	0.684488	0.695823
C	C124	0.9058	0.315512	0.695823
C	C125	0.59418	0.815491	0.304177
C	C126	0.59418	0.184509	0.304177
C	C127	0.0942	0.684488	0.304177
C	C128	0.0942	0.315512	0.304177
C	C129	0.05497	0.642895	0.302667
C	C130	0.05497	0.357105	0.302667
C	C131	0.445008	0.142916	0.697333
C	C132	0.445008	0.857084	0.697333
C	C133	0.945029	0.357105	0.697333
C	C134	0.945029	0.642895	0.697333
C	C135	0.554992	0.857084	0.302667
C	C136	0.554992	0.142916	0.302667
C	C137	0.01479	0.3583	0.243916
C	C138	0.985206	0.6417	0.756084
C	C139	0.485227	0.141679	0.756084
C	C140	0.985206	0.3583	0.756084
C	C141	0.514773	0.141679	0.243916
C	C142	0.01479	0.6417	0.243916
C	C143	0.485227	0.858279	0.756084
C	C144	0.514773	0.858279	0.243916
C	C145	0.986115	0.317903	0.813381
C	C146	0.01389	0.317903	0.186619
C	C147	0.513865	0.817882	0.186619
C	C148	0.986115	0.682097	0.813381
C	C149	0.486135	0.182077	0.813381
C	C150	0.513865	0.182077	0.186619
C	C151	0.01389	0.682097	0.186619
C	C152	0.486135	0.817882	0.813381
C	C153	0.946805	0.72369	0.811929
C	C154	0.946805	0.27631	0.811929
C	C155	0.446825	0.223711	0.811929
C	C156	0.446825	0.776289	0.811929
C	C157	0.0532	0.27631	0.188071
C	C158	0.0532	0.72369	0.188071
C	C159	0.553175	0.223711	0.188071
C	C160	0.553175	0.776289	0.188071
C	C161	0.032999	0.594501	0.743009
C	C162	0.466981	0.905478	0.256991
C	C163	0.533019	0.905478	0.743009

C	C164	0.032999	0.405499	0.743009
C	C165	0.533019	0.09448	0.743009
C	C166	0.466981	0.09448	0.256991
C	C167	0.967001	0.594501	0.256991
C	C168	0.967001	0.405499	0.256991
H	H1	0.557597	0.023084	0.42549
H	H2	0.057617	0.476895	0.42549
H	H3	0.4424	0.023084	0.57451
H	H4	0.942383	0.523105	0.57451
H	H5	0.564918	0.015417	0.291776
H	H6	0.935102	0.515396	0.708224
H	H7	0.064898	0.484604	0.291776
H	H8	0.43508	0.015417	0.708224
H	H9	0.785186	0.47537	0.546094
H	H10	0.28521	0.975391	0.546094
H	H11	0.214814	0.524589	0.453906
H	H12	0.714793	0.975391	0.453906
H	H13	0.649621	0.077085	0.19569
H	H14	0.35038	0.077085	0.804306
H	H15	0.850382	0.422895	0.804282
H	H16	0.850382	0.577105	0.804282
H	H17	0.149618	0.577105	0.195718
H	H18	0.35038	0.922915	0.804306
H	H19	0.649621	0.922915	0.19569
H	H20	0.149618	0.422895	0.195718
H	H21	0.646528	0.079682	0.06262
H	H22	0.853518	0.579702	0.937414
H	H23	0.35347	0.920318	0.93738
H	H24	0.35347	0.079682	0.93738
H	H25	0.146482	0.579702	0.062586
H	H26	0.146482	0.420298	0.062586
H	H27	0.646528	0.920318	0.06262
H	H28	0.853518	0.420298	0.937414
H	H29	0.24907	0.200998	0.168895
H	H30	0.749086	0.700977	0.168895
H	H31	0.250914	0.298982	0.831105
H	H32	0.24907	0.799002	0.168895
H	H33	0.749086	0.298982	0.168895
H	H34	0.750935	0.200998	0.831105
H	H35	0.250914	0.700977	0.831105
H	H36	0.750935	0.799002	0.831105
H	H37	0.817025	0.269797	0.828897
H	H38	0.18297	0.269797	0.171103
H	H39	0.317005	0.230183	0.828897
H	H40	0.682995	0.769776	0.171103

H	H41	0.682995	0.230183	0.171103
H	H42	0.18297	0.730203	0.171103
H	H43	0.817025	0.730203	0.828897
H	H44	0.317005	0.769776	0.828897
H	H45	0.590039	0.320788	0.324981
H	H46	0.338415	0.388804	0.681992
H	H47	0.838435	0.111216	0.681992
H	H48	0.838435	0.888784	0.681992
H	H49	0.16156	0.888784	0.318008
H	H50	0.661585	0.388804	0.318008
H	H51	0.16156	0.111216	0.318008
H	H52	0.338415	0.611196	0.681992
H	H53	0.661585	0.611196	0.318008
H	H54	0.1211	0.314687	0.343577
H	H55	0.378921	0.185292	0.656423
H	H56	0.1211	0.685271	0.343577
H	H57	0.878901	0.685271	0.656423
H	H58	0.378921	0.814667	0.656423
H	H59	0.878901	0.314687	0.656423
H	H60	0.621079	0.814667	0.343577
H	H61	0.621079	0.185292	0.343577
H	H62	0.05558	0.384187	0.34102
H	H63	0.94442	0.384187	0.65898
H	H64	0.4444	0.884167	0.65898
H	H65	0.5556	0.115792	0.34102
H	H66	0.4444	0.115792	0.65898
H	H67	0.5556	0.884167	0.34102
H	H68	0.05558	0.615771	0.34102
H	H69	0.94442	0.615771	0.65898
H	H70	0.487089	0.818665	0.147219
H	H71	0.012932	0.681273	0.852781
H	H72	0.487089	0.181294	0.147219
H	H73	0.012932	0.318686	0.852781
H	H74	0.512911	0.818665	0.852781
H	H75	0.987068	0.318686	0.147219
H	H76	0.512911	0.181294	0.852781
H	H77	0.987068	0.681273	0.147219
H	H78	0.05246	0.24931	0.149776
H	H79	0.552485	0.749289	0.149776
H	H80	0.447515	0.749289	0.850224
H	H81	0.447515	0.250711	0.850224
H	H82	0.947535	0.75069	0.850224
H	H83	0.947535	0.24931	0.850224
H	H84	0.552485	0.250711	0.149776
H	H85	0.05246	0.75069	0.149776

H	H86	0.409961	0.679171	0.675019
N	N1	0.922013	0.821963	0.657004
N	N2	0.922013	0.177996	0.657004
N	N3	0.577966	0.677975	0.342996
N	N4	0.07799	0.821963	0.342996
N	N5	0.422034	0.321984	0.657004
N	N6	0.07799	0.177996	0.342996
N	N7	0.26201	0.957006	0.693987
N	N8	0.761988	0.456985	0.693987
N	N9	0.238012	0.542974	0.306013
N	N10	0.737992	0.957006	0.306013
O	O1	0.858795	0.499979	0.2524
O	O2	0.641226	0	0.7476
O	O2	0.641226	1	0.7476
O	O3	0.141205	0.499979	0.7476
O	O4	0.35877	0	0.2524
O	O4	0.35877	1	0.2524
O	O5	0.412295	0.999959	0.43208
O	O6	0.587705	0.999959	0.56792
O	O7	0.912274	0.499979	0.43208
O	O8	0.087726	0.499979	0.56792
O	O9	0.180317	0.499979	0.573905
O	O10	0.819683	0.499979	0.426095
O	O11	0.680297	0	0.573905
O	O11	0.680297	1	0.573905
O	O12	0.3197	0	0.426095
O	O12	0.3197	1	0.426095
O	O13	0.856292	0.544087	0.076905
O	O14	0.143708	0.455872	0.923095
O	O15	0.35627	0.955893	0.076905
O	O16	0.143708	0.544087	0.923095
O	O17	0.643728	0.955893	0.923095
O	O18	0.856292	0.455872	0.076905
O	O19	0.643728	0.044107	0.923095
O	O20	0.35627	0.044107	0.076905
O	O21	0.25057	0.935364	0.286802
O	O22	0.750593	0.435385	0.286802
O	O23	0.750593	0.564574	0.286802
O	O24	0.25057	0.064595	0.286802
O	O25	0.749428	0.064595	0.713198
O	O26	0.749428	0.935364	0.713198
O	O27	0.249407	0.564574	0.713198
O	O28	0.249407	0.435385	0.713198
O	O29	0.703017	0.109114	0.800713
O	O30	0.203037	0.609094	0.800713

O	O31	0.203037	0.390906	0.800713
O	O32	0.29698	0.109114	0.199287
O	O33	0.796963	0.609094	0.199287
O	O34	0.703017	0.890886	0.800713
O	O35	0.29698	0.890886	0.199287
O	O36	0.796963	0.390906	0.199287
O	O37	0.440013	0.279979	0.615978
O	O38	0.559987	0.71998	0.384022
O	O39	0.05997	0.779999	0.384022
O	O40	0.05997	0.220001	0.384022
O	O41	0.940034	0.220001	0.615978
O	O42	0.940034	0.779999	0.615978
O	O43	0.944025	0.135001	0.652995
O	O44	0.944025	0.864999	0.652995
O	O45	0.05597	0.135001	0.347005
O	O46	0.05597	0.864999	0.347005
O	O47	0.555995	0.634981	0.347005
O	O48	0.444005	0.364978	0.652995
O	O49	0.470276	0.061915	0.30319
O	O50	0.470276	0.938085	0.30319
O	O51	0.970296	0.438105	0.30319
O	O52	0.029704	0.438105	0.69681
O	O53	0.529724	0.938085	0.69681
O	O54	0.529724	0.061915	0.69681
O	O55	0.029704	0.561895	0.69681
O	O56	0.970296	0.561895	0.30319
O	O57	0.571925	0.103096	0.797226
O	O58	0.928096	0.603075	0.202774
O	O59	0.428075	0.896863	0.202774
O	O60	0.071904	0.396884	0.797226
O	O61	0.428075	0.103096	0.202774
O	O62	0.571925	0.896863	0.797226
O	O63	0.928096	0.396884	0.202774
O	O64	0.071904	0.603075	0.797226
O	O65	0.242008	0.594996	0.283989
O	O66	0.741987	0.904984	0.283989
O	O67	0.757992	0.405004	0.716011
O	O68	0.25801	0.904984	0.716011
O	O69	0.275017	0.511975	0.297994
O	O70	0.724983	0.487984	0.702006
O	O71	0.774997	0.988005	0.297994
O	O72	0.225	0.988005	0.702006
Zn	Zn1	0.576734	0.999959	0.681295
Zn	Zn2	0.423266	0.999959	0.318705
Zn	Zn3	0.923287	0.499979	0.318705

Zn	Zn4	0.076713	0.499979	0.681295
Zn	Zn5	0.3586	0.065419	0.187781
Zn	Zn6	0.3586	0.934581	0.187781
Zn	Zn7	0.858576	0.434602	0.187781
Zn	Zn8	0.141424	0.565398	0.812219
Zn	Zn9	0.641404	0.934581	0.812219
Zn	Zn10	0.641404	0.065419	0.812219
Zn	Zn11	0.141424	0.434602	0.812219
Zn	Zn12	0.858576	0.565398	0.187781
Zn	Zn13	0.29286	0	0.317078
Zn	Zn13	0.29286	1	0.317078
Zn	Zn14	0.792885	0.499979	0.317078
Zn	Zn15	0.207115	0.499979	0.682922
Zn	Zn16	0.707135	0	0.682922
Zn	Zn16	0.707135	1	0.682922

Fractional Coordinates for $[(Zn_4O)_4(bpdcNO_2)_{11}(bpdc)_1]$				
Elmt	Label	x	y	z
C	C1	0.132016	0.499979	0.545024
C	C2	0.867984	0.499979	0.454976
C	C3	0.368004	0	0.454976
C	C3	0.368004	1	0.454976
C	C4	0.631996	0	0.545024
C	C4	0.631996	1	0.545024
C	C5	0.635427	0	0.452918
C	C5	0.635427	1	0.452918
C	C6	0.135407	0.499979	0.452918
C	C7	0.364573	0	0.547082
C	C7	0.364573	1	0.547082
C	C8	0.864593	0.499979	0.547082
C	C9	0.409499	0.011995	0.596012
C	C10	0.909479	0.511975	0.596012
C	C11	0.590501	0.011995	0.403988
C	C12	0.090521	0.487984	0.403988
C	C13	0.595018	0.007008	0.324318
C	C14	0.404982	0.007008	0.675682
C	C15	0.094998	0.492972	0.324318
C	C16	0.905002	0.506987	0.675682
C	C17	0.144306	0.509007	0.292822
C	C18	0.355674	0.991014	0.707178
C	C19	0.644326	0.991014	0.292822
C	C20	0.855694	0.490993	0.707178
C	C21	0.810781	0.478997	0.659004
C	C22	0.689198	0.979018	0.340996

C	C23	0.310802	0.979018	0.659004
C	C24	0.189219	0.521003	0.340996
C	C25	0.684728	0.983388	0.421015
C	C26	0.184707	0.516592	0.421015
C	C27	0.815293	0.483408	0.578985
C	C28	0.315272	0.983388	0.578985
C	C29	0.147006	0.499979	0.20798
C	C30	0.647011	0	0.20801
C	C30	0.647011	1	0.20801
C	C31	0.352989	0	0.79199
C	C31	0.352989	1	0.79199
C	C32	0.852994	0.499979	0.79202
C	C33	0.852382	0.543881	0.831013
C	C34	0.147618	0.543881	0.168987
C	C35	0.147618	0.456078	0.168987
C	C36	0.647622	0.043901	0.16902
C	C37	0.352378	0.043901	0.83098
C	C38	0.352378	0.956099	0.83098
C	C39	0.647622	0.956099	0.16902
C	C40	0.852382	0.456078	0.831013
C	C41	0.646041	0.045715	0.08801
C	C42	0.145995	0.454306	0.08798
C	C43	0.646041	0.954285	0.08801
C	C44	0.353959	0.045715	0.91199
C	C45	0.353959	0.954285	0.91199
C	C46	0.854005	0.454306	0.91202
C	C47	0.145995	0.545694	0.08798
C	C48	0.854005	0.545694	0.91202
C	C49	0.855985	0.499979	0.95499
C	C50	0.355965	0	0.95499
C	C50	0.355965	1	0.95499
C	C51	0.644035	0	0.04501
C	C51	0.644035	1	0.04501
C	C52	0.144015	0.499979	0.04501
C	C53	0.645018	0	0.955986
C	C53	0.645018	1	0.955986
C	C54	0.145039	0.499979	0.955986
C	C55	0.354982	0	0.044014
C	C55	0.354982	1	0.044014
C	C56	0.854961	0.499979	0.044014
C	C57	0.256983	0.100993	0.237001
C	C58	0.243038	0.600973	0.762999
C	C59	0.743017	0.100993	0.762999
C	C60	0.756962	0.600973	0.237001
C	C61	0.243038	0.398986	0.762999

C	C62	0.756962	0.398986	0.237001
C	C63	0.256983	0.898965	0.237001
C	C64	0.743017	0.898965	0.762999
C	C65	0.711875	0.350674	0.242986
C	C66	0.211895	0.850695	0.242986
C	C67	0.711875	0.649285	0.242986
C	C68	0.211895	0.149305	0.242986
C	C69	0.288125	0.350674	0.757014
C	C70	0.788105	0.149305	0.757014
C	C71	0.788105	0.850695	0.757014
C	C72	0.288125	0.649285	0.757014
C	C73	0.78171	0.803166	0.800829
C	C74	0.78171	0.196793	0.800829
C	C75	0.281731	0.303186	0.800829
C	C76	0.281731	0.696772	0.800829
C	C77	0.21829	0.196793	0.199171
C	C78	0.718269	0.696772	0.199171
C	C79	0.718269	0.303186	0.199171
C	C80	0.21829	0.803166	0.199171
C	C81	0.678681	0.737994	0.200507
C	C82	0.321319	0.737994	0.799493
C	C83	0.82134	0.761985	0.799493
C	C84	0.82134	0.238015	0.799493
C	C85	0.321319	0.262006	0.799493
C	C86	0.17866	0.238015	0.200507
C	C87	0.678681	0.262006	0.200507
C	C88	0.17866	0.761985	0.200507
C	C89	0.132683	0.768292	0.246008
C	C90	0.367337	0.268313	0.753992
C	C91	0.132683	0.231708	0.246008
C	C92	0.367337	0.731687	0.753992
C	C93	0.867317	0.768292	0.753992
C	C94	0.867317	0.231708	0.753992
C	C95	0.632663	0.731687	0.246008
C	C96	0.632663	0.268313	0.246008
C	C97	0.626268	0.3158	0.289824
C	C98	0.126289	0.81578	0.289824
C	C99	0.873711	0.184179	0.710176
C	C100	0.126289	0.184179	0.289824
C	C101	0.373732	0.3158	0.710176
C	C102	0.626268	0.6842	0.289824
C	C103	0.873711	0.81578	0.710176
C	C104	0.373732	0.6842	0.710176
C	C105	0.834113	0.142998	0.71099
C	C106	0.834113	0.857002	0.71099

C	C107	0.665866	0.356981	0.28901
C	C108	0.334134	0.356981	0.71099
C	C109	0.665866	0.642978	0.28901
C	C110	0.165887	0.142998	0.28901
C	C111	0.334134	0.642978	0.71099
C	C112	0.165887	0.857002	0.28901
C	C113	0.593273	0.224906	0.246996
C	C114	0.406727	0.775094	0.753004
C	C115	0.593273	0.775094	0.246996
C	C116	0.093294	0.275114	0.246996
C	C117	0.093294	0.724886	0.246996
C	C118	0.906706	0.275114	0.753004
C	C119	0.906706	0.724886	0.753004
C	C120	0.406727	0.224906	0.753004
C	C121	0.9058	0.684488	0.695823
C	C122	0.0942	0.684488	0.304177
C	C123	0.0942	0.315512	0.304177
C	C124	0.59418	0.184509	0.304177
C	C125	0.59418	0.815491	0.304177
C	C126	0.40582	0.815491	0.695823
C	C127	0.40582	0.184509	0.695823
C	C128	0.9058	0.315512	0.695823
C	C129	0.445008	0.142916	0.697333
C	C130	0.054971	0.357105	0.302667
C	C131	0.554992	0.857084	0.302667
C	C132	0.445008	0.857084	0.697333
C	C133	0.554992	0.142916	0.302667
C	C134	0.054971	0.642895	0.302667
C	C135	0.945029	0.642895	0.697333
C	C136	0.945029	0.357105	0.697333
C	C137	0.485227	0.858279	0.756084
C	C138	0.985206	0.6417	0.756084
C	C139	0.485227	0.141679	0.756084
C	C140	0.985206	0.3583	0.756084
C	C141	0.514773	0.858279	0.243916
C	C142	0.014794	0.3583	0.243916
C	C143	0.014794	0.6417	0.243916
C	C144	0.514773	0.141679	0.243916
C	C145	0.986115	0.682097	0.813381
C	C146	0.513865	0.182077	0.186619
C	C147	0.486135	0.817882	0.813381
C	C148	0.013885	0.682097	0.186619
C	C149	0.513865	0.817882	0.186619
C	C150	0.013885	0.317903	0.186619
C	C151	0.986115	0.317903	0.813381

C	C152	0.486135	0.182077	0.813381
C	C153	0.553175	0.776289	0.188071
C	C154	0.053195	0.27631	0.188071
C	C155	0.553175	0.223711	0.188071
C	C156	0.446825	0.776289	0.811929
C	C157	0.946805	0.27631	0.811929
C	C158	0.446825	0.223711	0.811929
C	C159	0.946805	0.72369	0.811929
C	C160	0.053195	0.72369	0.188071
C	C161	0.967001	0.594501	0.256991
C	C162	0.466981	0.09448	0.256991
C	C163	0.533019	0.09448	0.743009
C	C164	0.032999	0.594501	0.743009
C	C165	0.533019	0.905478	0.743009
C	C166	0.032999	0.405499	0.743009
C	C167	0.466981	0.905478	0.256991
C	C168	0.967001	0.405499	0.256991
H	H1	0.942383	0.523105	0.57451
H	H2	0.057617	0.476895	0.42549
H	H3	0.442403	0.023084	0.57451
H	H4	0.557597	0.023084	0.42549
H	H5	0.064898	0.484604	0.291776
H	H6	0.435082	0.015417	0.708224
H	H7	0.935102	0.515396	0.708224
H	H8	0.564918	0.015417	0.291776
H	H9	0.285207	0.975391	0.546094
H	H10	0.214814	0.524589	0.453906
H	H11	0.785186	0.47537	0.546094
H	H12	0.714793	0.975391	0.453906
H	H13	0.350379	0.922915	0.80431
H	H14	0.350379	0.077085	0.80431
H	H15	0.149618	0.422895	0.195718
H	H16	0.149618	0.577105	0.195718
H	H17	0.850382	0.577105	0.804282
H	H18	0.649621	0.077085	0.19569
H	H19	0.850382	0.422895	0.804282
H	H20	0.649621	0.922915	0.19569
H	H21	0.646528	0.079682	0.06262
H	H22	0.353472	0.079682	0.93738
H	H23	0.146482	0.579702	0.062586
H	H24	0.146482	0.420298	0.062586
H	H25	0.353472	0.920318	0.93738
H	H26	0.853518	0.579702	0.937414
H	H27	0.853518	0.420298	0.937414
H	H28	0.646528	0.920318	0.06262

H	H29	0.250914	0.700977	0.831105
H	H30	0.750935	0.799002	0.831105
H	H31	0.750935	0.200998	0.831105
H	H32	0.749086	0.298982	0.168895
H	H33	0.249065	0.200998	0.168895
H	H34	0.749086	0.700977	0.168895
H	H35	0.250914	0.298982	0.831105
H	H36	0.249065	0.799002	0.168895
H	H37	0.317005	0.769776	0.828897
H	H38	0.182975	0.730203	0.171103
H	H39	0.682995	0.230183	0.171103
H	H40	0.817025	0.269797	0.828897
H	H41	0.317005	0.230183	0.828897
H	H42	0.817025	0.730203	0.828897
H	H43	0.682995	0.769776	0.171103
H	H44	0.182975	0.269797	0.171103
H	H45	0.590039	0.320788	0.324981
H	H46	0.838435	0.111216	0.681992
H	H47	0.661585	0.611196	0.318008
H	H48	0.838435	0.888784	0.681992
H	H49	0.161565	0.888784	0.318008
H	H50	0.661585	0.388804	0.318008
H	H51	0.338415	0.611196	0.681992
H	H52	0.161565	0.111216	0.318008
H	H53	0.338415	0.388804	0.681992
H	H54	0.621079	0.185292	0.343577
H	H55	0.878901	0.314687	0.656423
H	H56	0.878901	0.685271	0.656423
H	H57	0.121099	0.314687	0.343577
H	H58	0.621079	0.814667	0.343577
H	H59	0.121099	0.685271	0.343577
H	H60	0.378921	0.185292	0.656423
H	H61	0.378921	0.814667	0.656423
H	H62	0.94442	0.384187	0.65898
H	H63	0.4444	0.115792	0.65898
H	H64	0.5556	0.884167	0.34102
H	H65	0.05558	0.384187	0.34102
H	H66	0.94442	0.615771	0.65898
H	H67	0.4444	0.884167	0.65898
H	H68	0.5556	0.115792	0.34102
H	H69	0.05558	0.615771	0.34102
H	H70	0.512911	0.818665	0.852781
H	H71	0.487089	0.181294	0.147219
H	H72	0.987068	0.681273	0.147219
H	H73	0.512911	0.181294	0.852781

H	H74	0.987068	0.318686	0.147219
H	H75	0.487089	0.818665	0.147219
H	H76	0.012932	0.681273	0.852781
H	H77	0.012932	0.318686	0.852781
H	H78	0.947535	0.24931	0.850224
H	H79	0.552485	0.749289	0.149776
H	H80	0.052465	0.24931	0.149776
H	H81	0.447515	0.749289	0.850224
H	H82	0.947535	0.75069	0.850224
H	H83	0.552485	0.250711	0.149776
H	H84	0.052465	0.75069	0.149776
H	H85	0.447515	0.250711	0.850224
N	N1	0.922013	0.177996	0.657004
N	N2	0.577966	0.677975	0.342996
N	N3	0.077987	0.821963	0.342996
N	N4	0.077987	0.177996	0.342996
N	N5	0.422034	0.321984	0.657004
N	N6	0.422034	0.677975	0.657004
N	N7	0.922013	0.821963	0.657004
N	N8	0.737992	0.957006	0.306013
N	N9	0.238012	0.542974	0.306013
N	N10	0.761988	0.456985	0.693987
N	N11	0.262008	0.957006	0.693987
O	O1	0.641226	0	0.7476
O	O1	0.641226	1	0.7476
O	O2	0.141205	0.499979	0.7476
O	O3	0.858795	0.499979	0.2524
O	O4	0.358774	0	0.2524
O	O4	0.358774	1	0.2524
O	O5	0.087726	0.499979	0.56792
O	O6	0.587705	0.999959	0.56792
O	O7	0.412295	0.999959	0.43208
O	O8	0.912274	0.499979	0.43208
O	O9	0.319703	0	0.426095
O	O9	0.319703	1	0.426095
O	O10	0.680297	0	0.573905
O	O10	0.680297	1	0.573905
O	O11	0.819683	0.499979	0.426095
O	O12	0.180317	0.499979	0.573905
O	O13	0.856292	0.544087	0.076905
O	O14	0.143708	0.455872	0.923095
O	O15	0.856292	0.455872	0.076905
O	O16	0.356272	0.955893	0.076905
O	O17	0.643728	0.044107	0.923095
O	O18	0.143708	0.544087	0.923095

O	O19	0.356272	0.044107	0.076905
O	O20	0.643728	0.955893	0.923095
O	O21	0.749428	0.935364	0.713198
O	O22	0.750593	0.564574	0.286802
O	O23	0.750593	0.435385	0.286802
O	O24	0.749428	0.064595	0.713198
O	O25	0.250572	0.064595	0.286802
O	O26	0.250572	0.935364	0.286802
O	O27	0.249407	0.435385	0.713198
O	O28	0.249407	0.564574	0.713198
O	O29	0.296983	0.109114	0.199287
O	O30	0.796963	0.609094	0.199287
O	O31	0.203037	0.390906	0.800713
O	O32	0.796963	0.390906	0.199287
O	O33	0.296983	0.890886	0.199287
O	O34	0.203037	0.609094	0.800713
O	O35	0.703017	0.890886	0.800713
O	O36	0.703017	0.109114	0.800713
O	O37	0.440013	0.279979	0.615978
O	O38	0.059966	0.779999	0.384022
O	O39	0.440013	0.71998	0.615978
O	O40	0.940034	0.220001	0.615978
O	O41	0.559987	0.71998	0.384022
O	O42	0.059966	0.220001	0.384022
O	O43	0.940034	0.779999	0.615978
O	O44	0.055975	0.135001	0.347005
O	O45	0.555995	0.634981	0.347005
O	O46	0.944025	0.135001	0.652995
O	O47	0.944025	0.864999	0.652995
O	O48	0.444005	0.364978	0.652995
O	O49	0.055975	0.864999	0.347005
O	O50	0.444005	0.634981	0.652995
O	O51	0.470276	0.938085	0.30319
O	O52	0.970296	0.438105	0.30319
O	O53	0.029704	0.438105	0.69681
O	O54	0.529724	0.061915	0.69681
O	O55	0.029704	0.561895	0.69681
O	O56	0.970296	0.561895	0.30319
O	O57	0.470276	0.061915	0.30319
O	O58	0.529724	0.938085	0.69681
O	O59	0.571925	0.896863	0.797226
O	O60	0.071904	0.396884	0.797226
O	O61	0.428075	0.896863	0.202774
O	O62	0.928096	0.396884	0.202774
O	O63	0.928096	0.603075	0.202774

O	O64	0.428075	0.103096	0.202774
O	O65	0.071904	0.603075	0.797226
O	O66	0.571925	0.103096	0.797226
O	O67	0.242008	0.594996	0.283989
O	O68	0.741987	0.904984	0.283989
O	O69	0.757992	0.405004	0.716011
O	O70	0.258013	0.904984	0.716011
O	O71	0.275017	0.511975	0.297994
O	O72	0.774997	0.988005	0.297994
O	O73	0.225003	0.988005	0.702006
O	O74	0.724983	0.487984	0.702006
Zn	Zn1	0.423266	0.999959	0.318705
Zn	Zn2	0.076713	0.499979	0.681295
Zn	Zn3	0.576734	0.999959	0.681295
Zn	Zn4	0.923287	0.499979	0.318705
Zn	Zn5	0.858576	0.565398	0.187781
Zn	Zn6	0.358596	0.934581	0.187781
Zn	Zn7	0.141424	0.565398	0.812219
Zn	Zn8	0.141424	0.434602	0.812219
Zn	Zn9	0.858576	0.434602	0.187781
Zn	Zn10	0.641404	0.065419	0.812219
Zn	Zn11	0.641404	0.934581	0.812219
Zn	Zn12	0.358596	0.065419	0.187781
Zn	Zn13	0.292865	0	0.317078
Zn	Zn13	0.292865	1	0.317078
Zn	Zn14	0.792885	0.499979	0.317078
Zn	Zn15	0.707135	0	0.682922
Zn	Zn15	0.707135	1	0.682922
Zn	Zn16	0.207115	0.499979	0.682922

Gas Adsorption Analyses

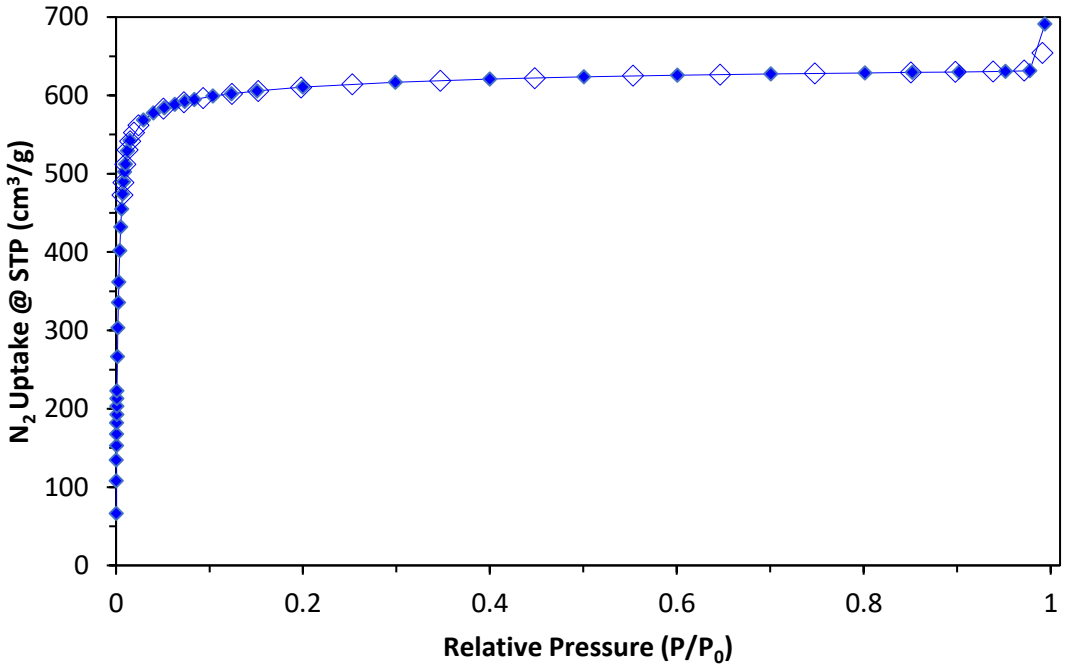

Figure S 26 *N_2 adsorption-desorption isotherm at 77 K for WUF-22(14). Solid markers indicate adsorption, open markers desorption. Line provided on the adsorption branch to guide the eye.*

BET Summary for WUF-22(14)		
Slope	1.393	
Intercept	1.81E-03	
Correlation coefficient, r	0.999939	
C, constant	769.702	
Surface Area	2496.763 m²/g	
Relative Pressure	**Volume @ STP**	**1 / [W((Po/P) - 1)]**
0.00801782	489.6347	0.013208
0.00901379	502.2272	0.014491
0.01003230	512.2514	0.015829
0.01211100	529.5111	0.018525
0.01504960	542.5539	0.022533
0.02921110	568.6903	0.042335
0.03995230	577.6148	0.057646

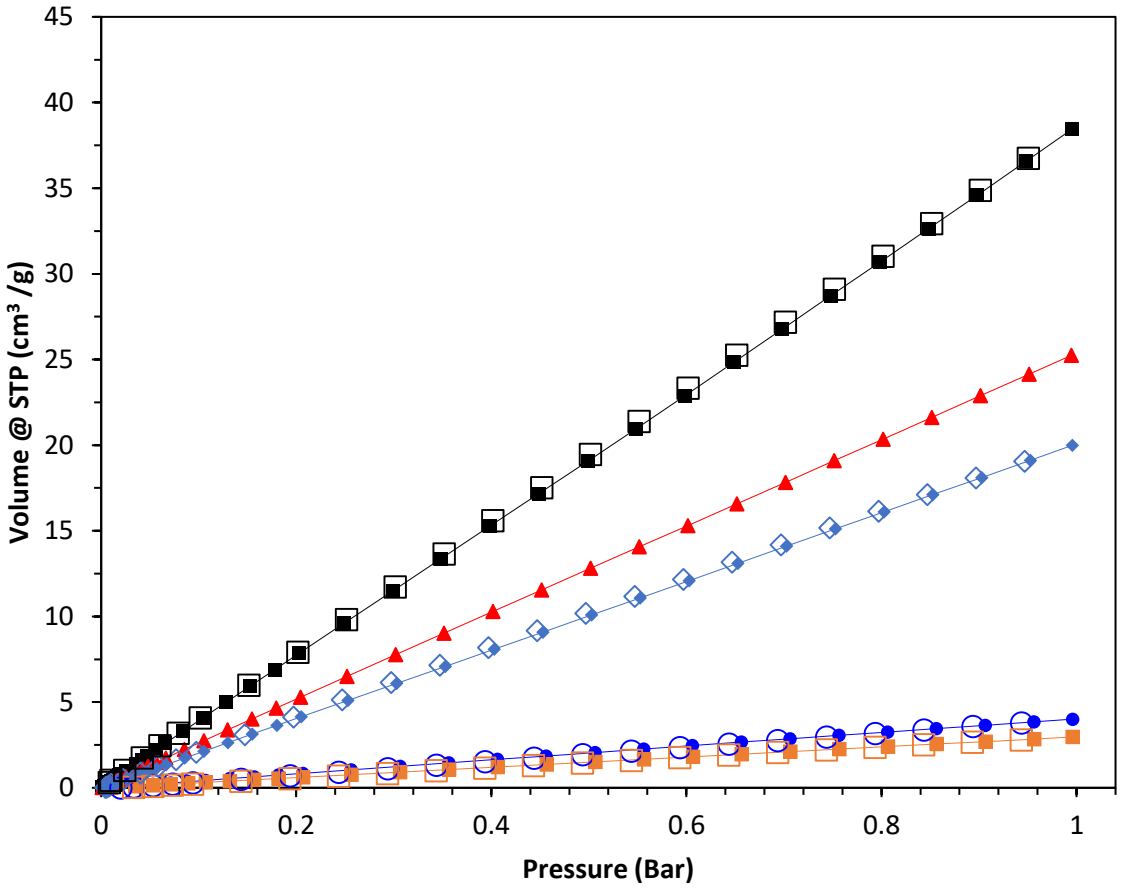

Figure S 27 Combined CO_2 and N_2 adsorption-desorption isotherms for WUF-22(14). CO_2 @ 273 K (black squares), CO_2 @ 288 K (red triangles), CO_2 @ 298 K (blue diamonds). For N_2 @ 273 K (blue circles), N_2 @ 298 K (orange squares). Solid markers indicate adsorption, open markers desorption. Lines provided on the adsorption legs to guide the eye.

Heat of Adsorption Calculation

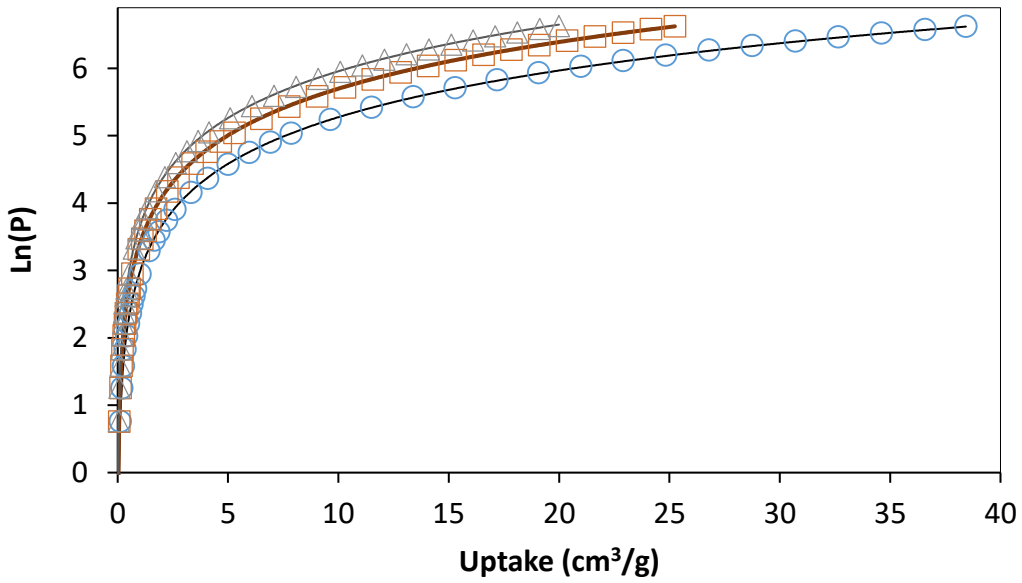

Figure S 28 *Virial fitting plot of the CO_2 adsorption data at 273 (circles), 288 (squares), and 298 K (triangles) for WUF-22(14). The line is the virial fitting of the data.*

Model	Virial fitting		
Equation	ln(x)+1/T*(a0+a1*x+a2*x^2+ a3*x^3+a4*x^4+a5*x^5+a6*x^6)+(b0+b1*x+b2*x^2+b3*x^3)		
Plot	273K	288K	298K
a0*	-2216.44224 Â± 40.11943	-2216.44224 Â± 40.11943	-2216.44224 Â± 40.11943
a1*	-0.01717 Â± 0.14826	-0.01717 Â± 0.14826	-0.01717 Â± 0.14826
a2*	0 Â± 0	0 Â± 0	0 Â± 0
a3*	0 Â± 0	0 Â± 0	0 Â± 0
a4*	0 Â± 0	0 Â± 0	0 Â± 0
a5*	0 Â± 0	0 Â± 0	0 Â± 0
a6*	0 Â± 0	0 Â± 0	0 Â± 0
b0*	11.09236 Â± 0.13936	11.09236 Â± 0.13936	11.09236 Â± 0.13936
b1*	0 Â± 0	0 Â± 0	0 Â± 0
b2*	0 Â± 0	0 Â± 0	0 Â± 0
b3*	0 Â± 0	0 Â± 0	0 Â± 0
T	273 Â± 0	288 Â± 0	298 Â± 0
Reduced Chi-Square*	0.002823		
R-Square (COD)	0.999696	0.999381	0.998577
R-Square (COD)*	0.999218		
Adj. R-Square*	0.999204		

Selectivity Calculations

Selectivity factors were calculated by the equation given below from their single-component isotherms based on a hypothetical mixture of CO_2 at 0.16 bar and N_2 at 0.77 bar:

$$S = \frac{q_1/q_2}{p_1/p_2}$$

Where *S* is the selectivity factor, q_i is the quantity adsorbed of component *i*, and p_i is the partial pressure of component *i.*

298 K

CO_2 data: *p* 0.16, *q* 3.1375

N_2 data: *p* 0.77, *q* 2.2591

S: 6.7

273 K

CO_2 data: *p* 0.16, *q* 5.9488

N_2 data: *p* 0.77, *q* 3.0585

S: 9.4

References

[1] M. Eddaoudi, J. Kim, N. Rosi, D. Vodak, J. Wachter, M. O'Keeffe, et al. *Science*. **2002**, *295*, 469.
[2] T. Düren, F. Millange, G. Férey, K. S. Walton, R. Q. Snurr. *J Phys Chem C*. **2007**, *111*, 15350.
[3] Y. S. Bae, O. K. Farha, J. T. Hupp, R. Q. Snurr. **2009**, *19*, 2131.