Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Material

Solvent Influenced Coordination Variation of Flexible Ligands to Y(III) towards MOF Structural Diversities

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1. Synthesis of Yfum MOFs

Synthesis of Yfum_H_2O. $Y(NO_3)_3 \cdot 6H_2O$ (38.30 mg, 0.1 mmol) or $YCl_3 \cdot 6H2O$ (30.34 mg, 0.1 mmol) and H_2fum (11.61 mg, 0.1 mmol) were dissolved in solvent mixture (3.5 mL of DI water and 1.5 mL of DMF) in a scintillation vial. The reaction mixture was sealed and placed in a thermal oven at 80 °C for 48 hours, then cooled to room temperature by turning off the oven, after which colorless plate crystals were found on the bottom of the vial.

Synthesis of Yfum_NO_3. $Y(NO_3)_3 \cdot 6H_2O$ (38.30 mg, 0.1 mmol) and H_2fum (11.61 mg, 0.1 mmol) were dissolved in solvent (5 mL of DMF) prepared in a scintillation vial. The reaction mixture was sealed and placed in a thermal oven at 80 °C for 48 hours, then cooled to room temperature by turning off the oven, after which colorless plate crystals were found on the bottom of the vial.

Synthesis of Yfum_Cl. $YCl_3 \cdot 6H_2O$ (30.34 mg, 0.1 mmol) and H_2fum (11.61 mg, 0.1 mmol) were dissolved in solvent (5 mL of DMF) prepared in a scintillation vial. The reaction mixture was sealed and placed in a thermal oven at 80 °C for 48 hours, then cooled to room temperature by turning off the oven, after which colorless blunt rod crystals were found on the bottom of the vial.

2. Single crystal X-ray analysis of Y-fum MOFs

CCDC 2112101-2112103 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via https://www.ccdc.cam.ac.uk/ (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

All crystals were coated with paratone-N oil and the diffraction data measured at 100 K with synchrotron radiation on a Rayonix MX225HS detector at BL2D SMC with a silicon (111) double crystal monochromator (DCM) at the Pohang Accelerator Laboratory, Korea. The PAL BL2D-SMDC Program[1] was used for data collection and HKL3000sm for cell refinement, reduction[2]. Absorption correction was performed by using the HKL3000sm Scalepack program[3]. All crystal structures were solved using the SHELXT-2014/5 programs[4] by direct method and refined by full-matrix least-squares calculation using the SHELXL-2018/3 programs[5]. All the non-hydrogen atoms were refined anisotropically. All hydrogen atoms were added to their geometrically ideal positions. The detailed data of the three crystals are shown in Table S4.

3. Supplementary figures

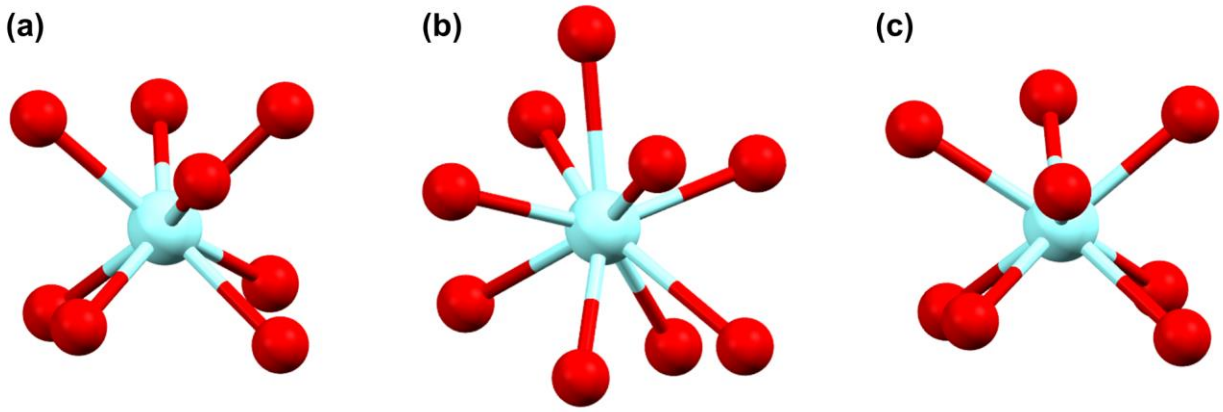

Figure S1. Comparison of the geometry around Y(III) in each Ymuco MOF structure. (a) Distorted square antiprism geometry of **1**. (b) Distorted mono-capped square antiprism geometry of **2**. (c) Distorted square antiprism geometry of **3**. Cyan: Y; red: O.

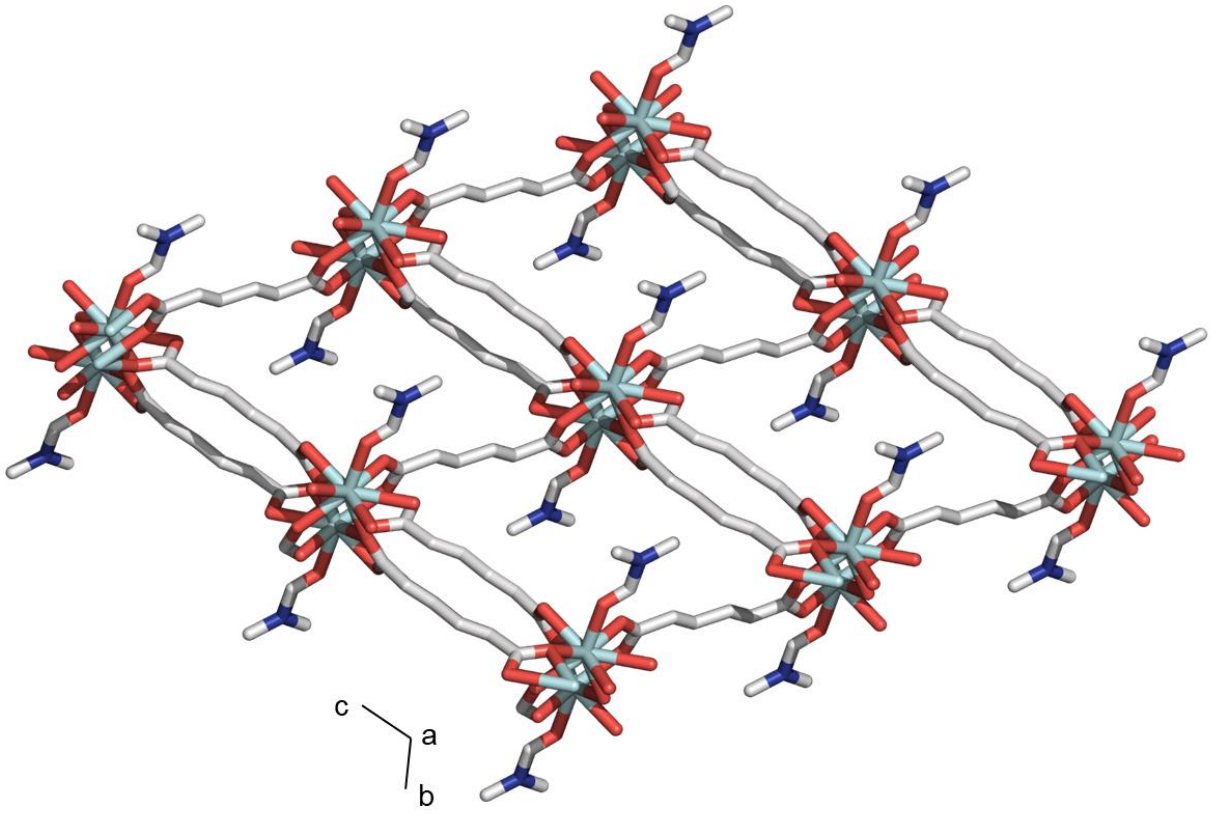

Figure S2. The *a*-axis view of **2**. 3D network structure with a diamond-shaped pore is occupied by DMF molecules coordinated to Y(III). Cyan: Y; red: O; gray: C. Disordered atoms and hydrogen atoms are omitted for clarity.

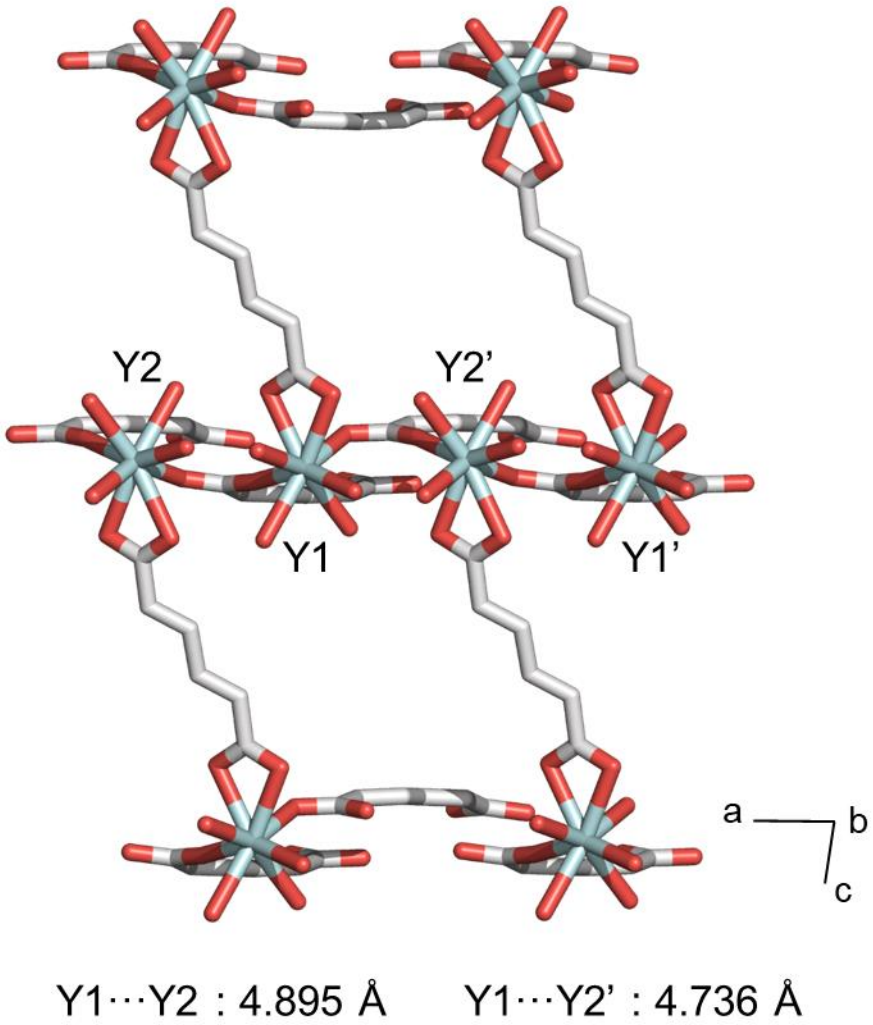

Figure S3. The *b*-axis view of **3**. 1D chain of Y(III) ions along *a*-axis with the distance between two Y ions ranges from 4.895 Å and 4.736 Å. Cyan: Y; red: O; gray: C. DMF molecules and hydrogen atoms are omitted for clarity.

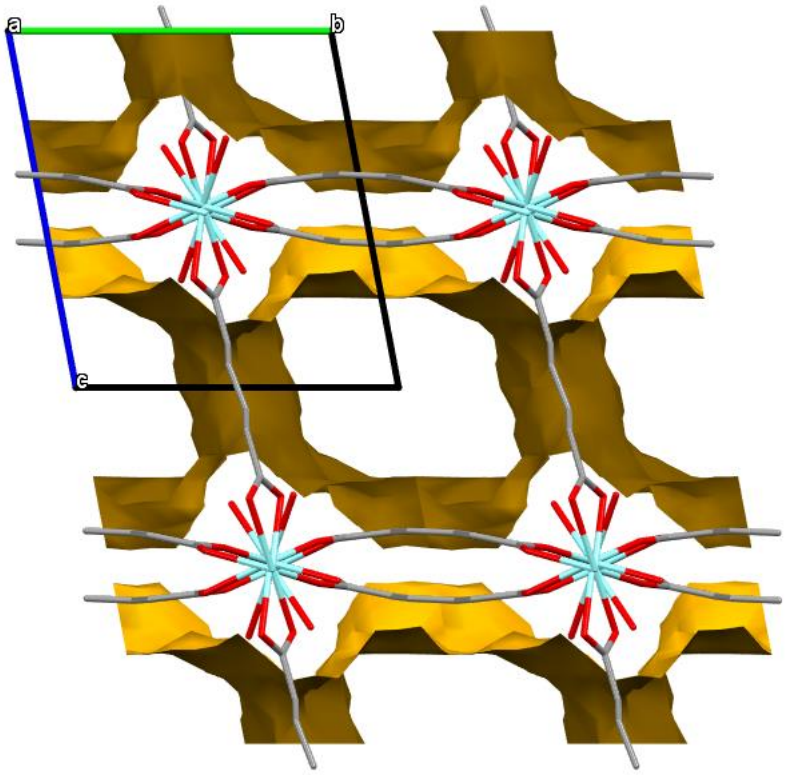

Figure S4. Void space of **3**: 49.9 % (506.65 Å^3).

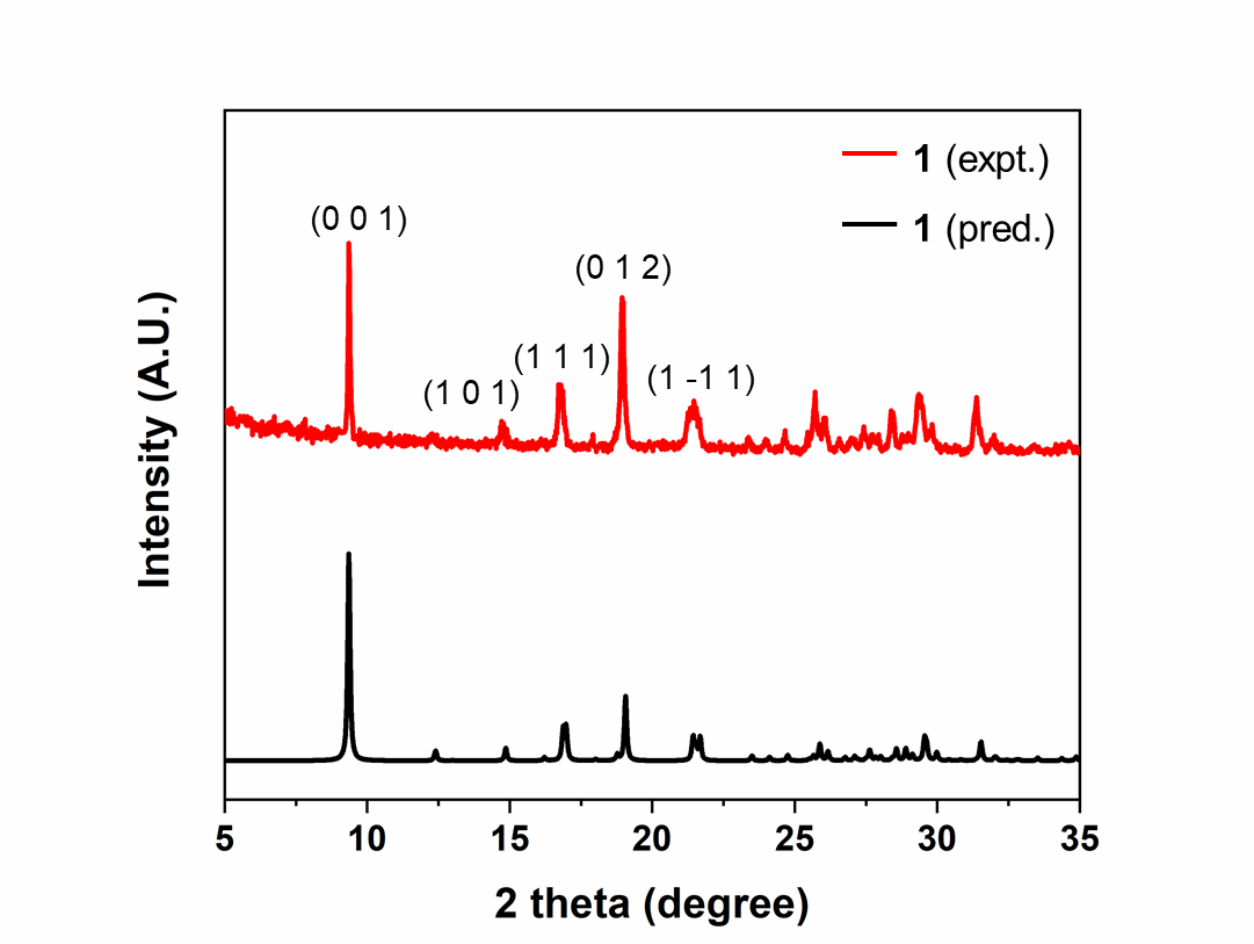

Figure S5. Comparison of the experimental (red) and predicted (black) PXRD patterns with **1**.

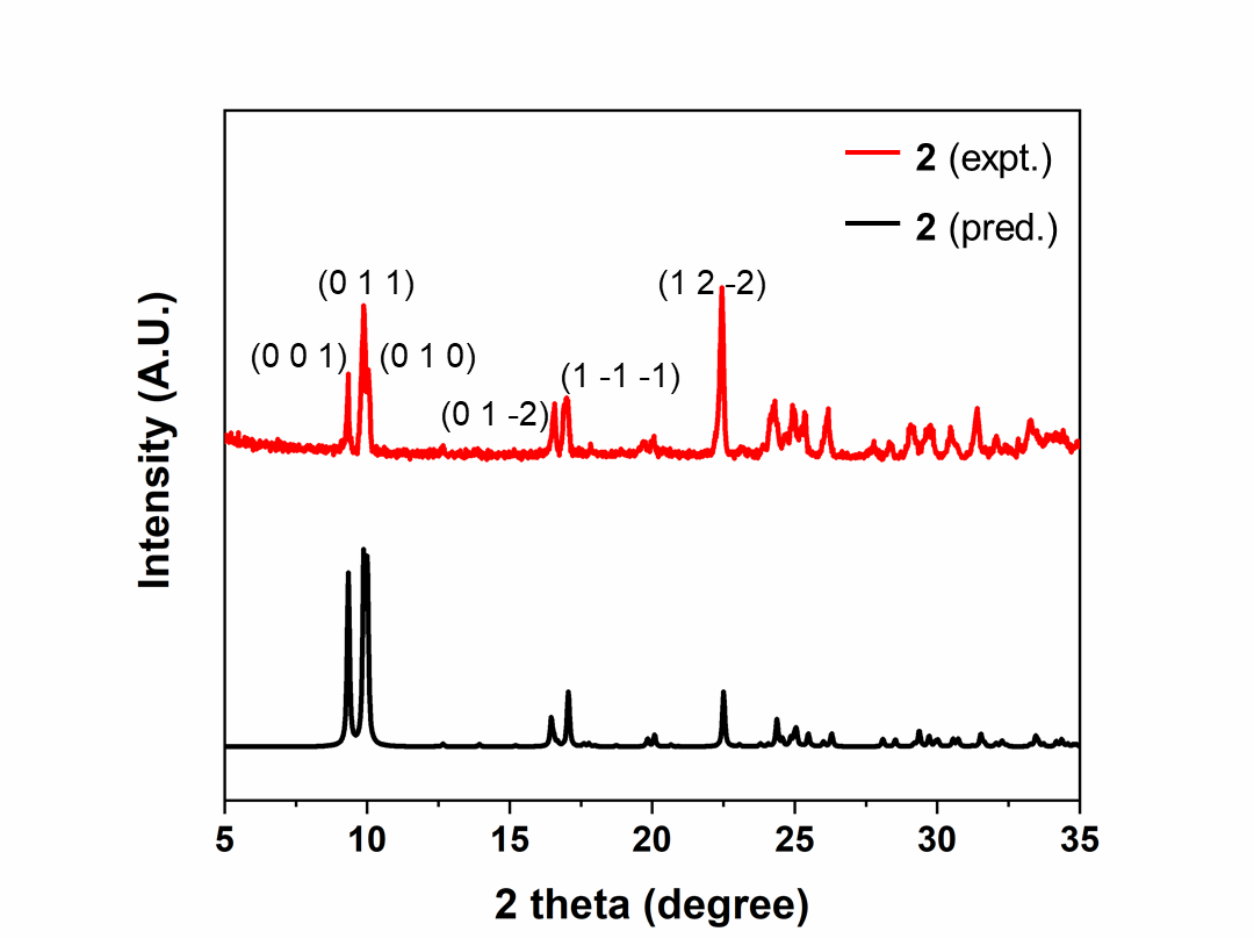

Figure S6. Comparison of the experimental (red) and predicted (black) PXRD patterns with **2**.

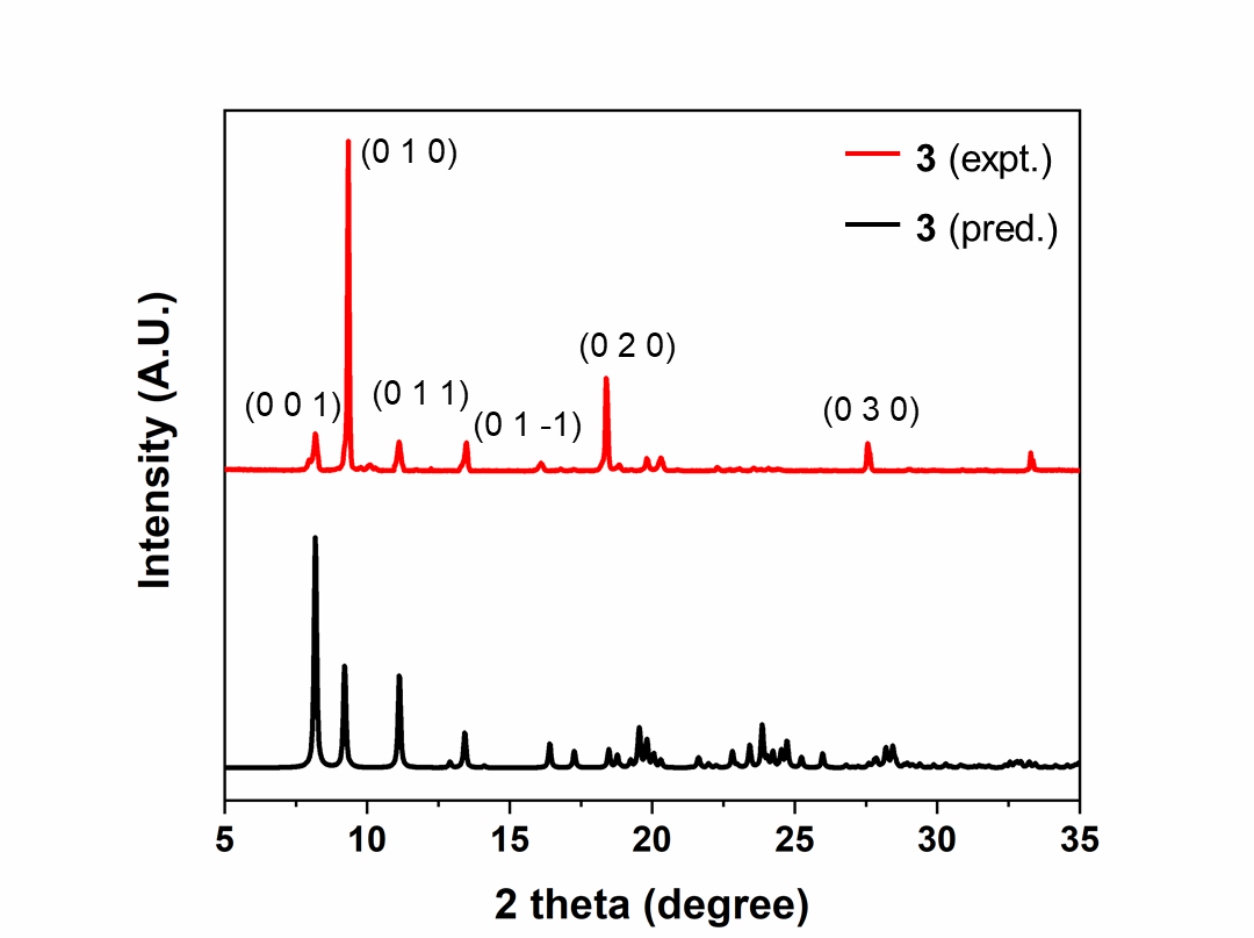

Figure S7. Comparison of the experimental (red) and predicted (black) PXRD patterns with **3**.

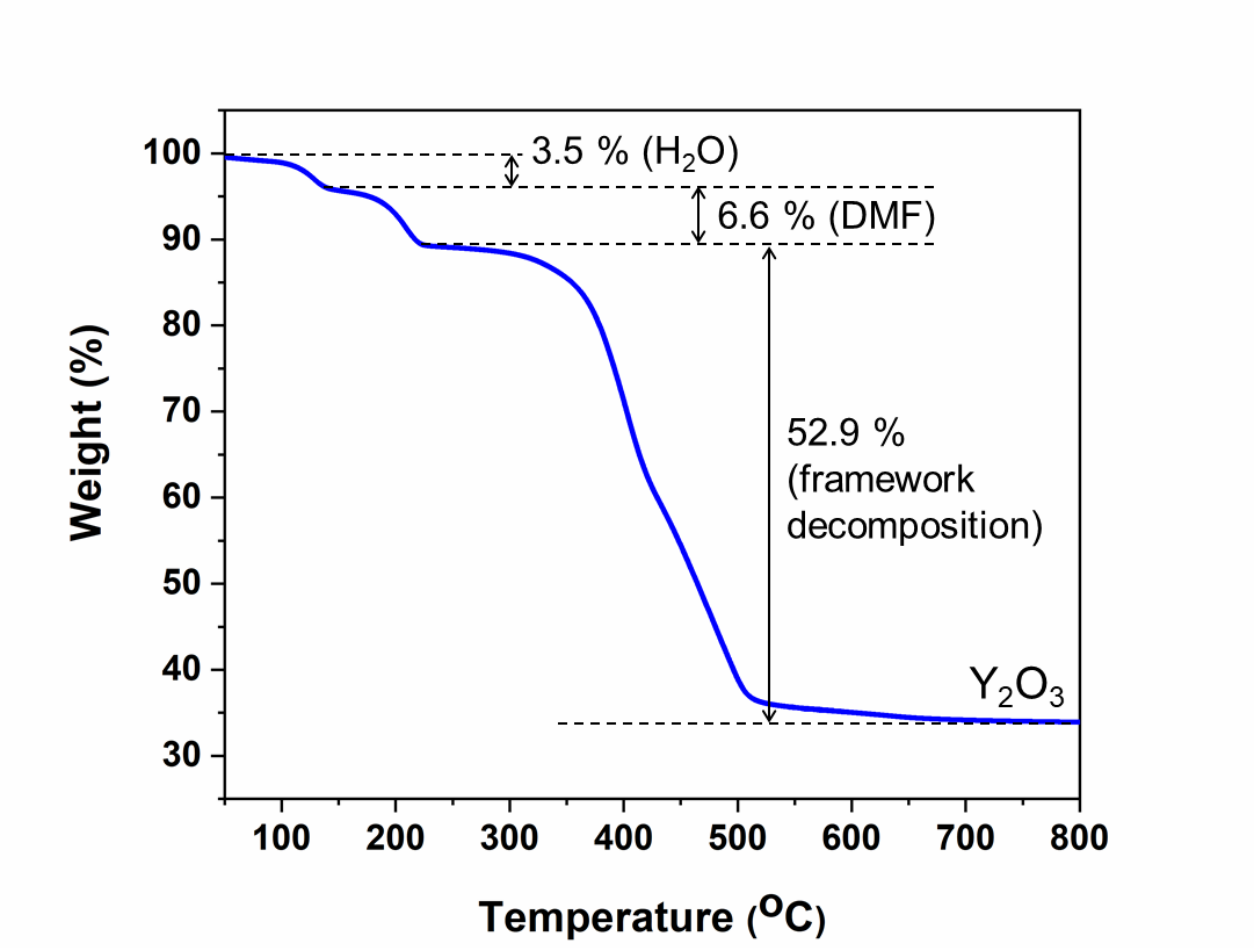

Figure S8. Thermogravimetric analysis of **1**.

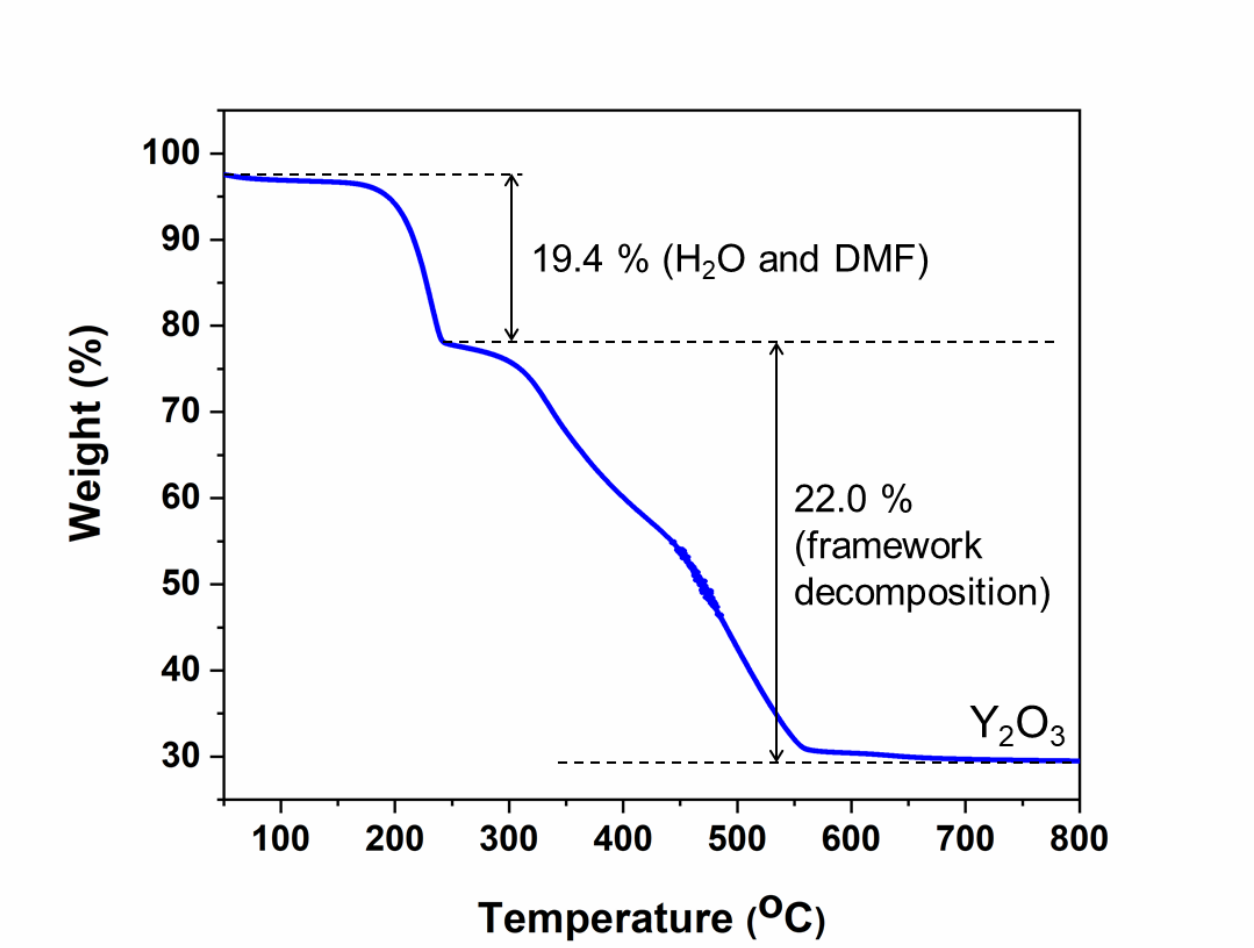

Figure S9. Thermogravimetric analysis of **2**.

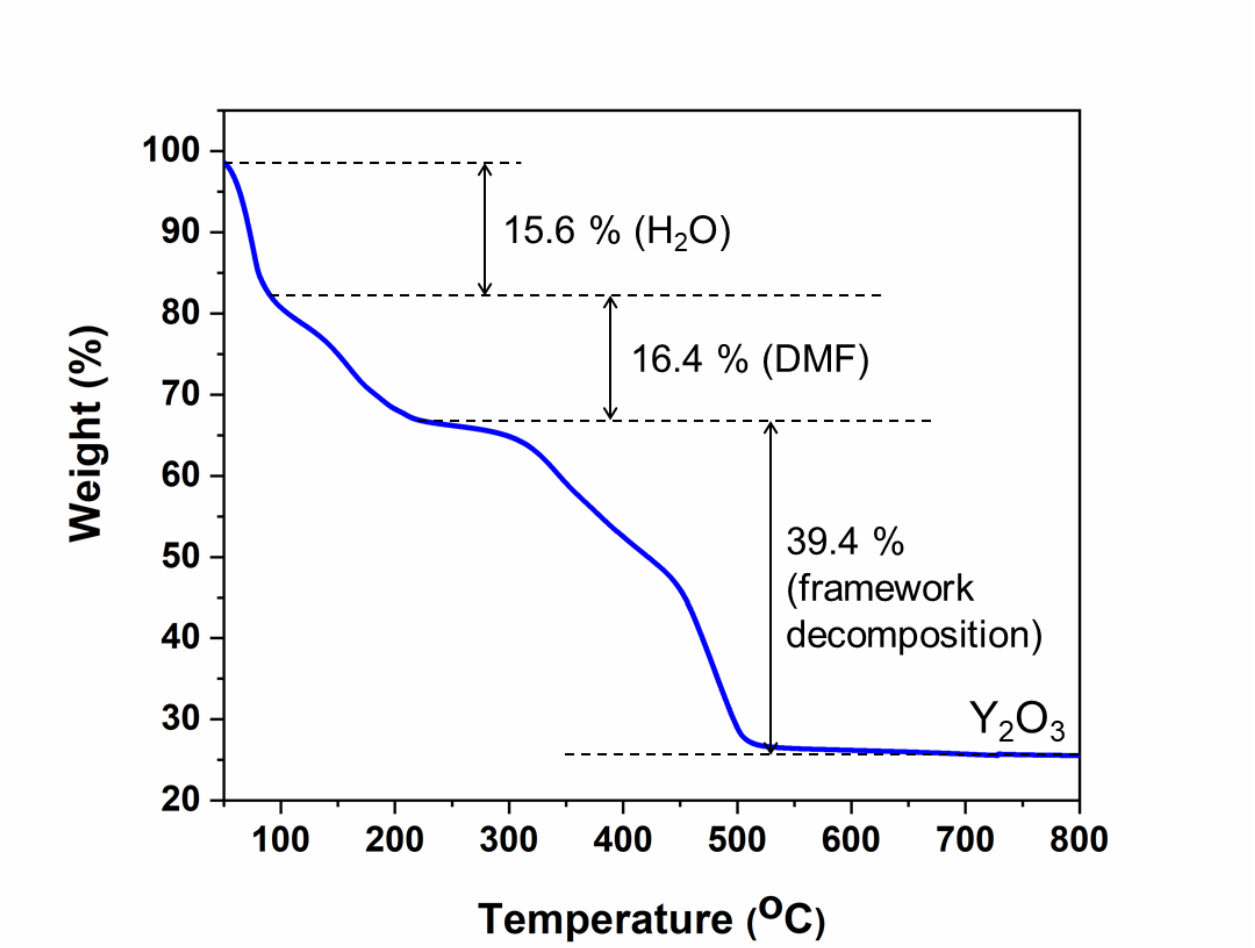

Figure S10. Thermogravimetric analysis of **3.**

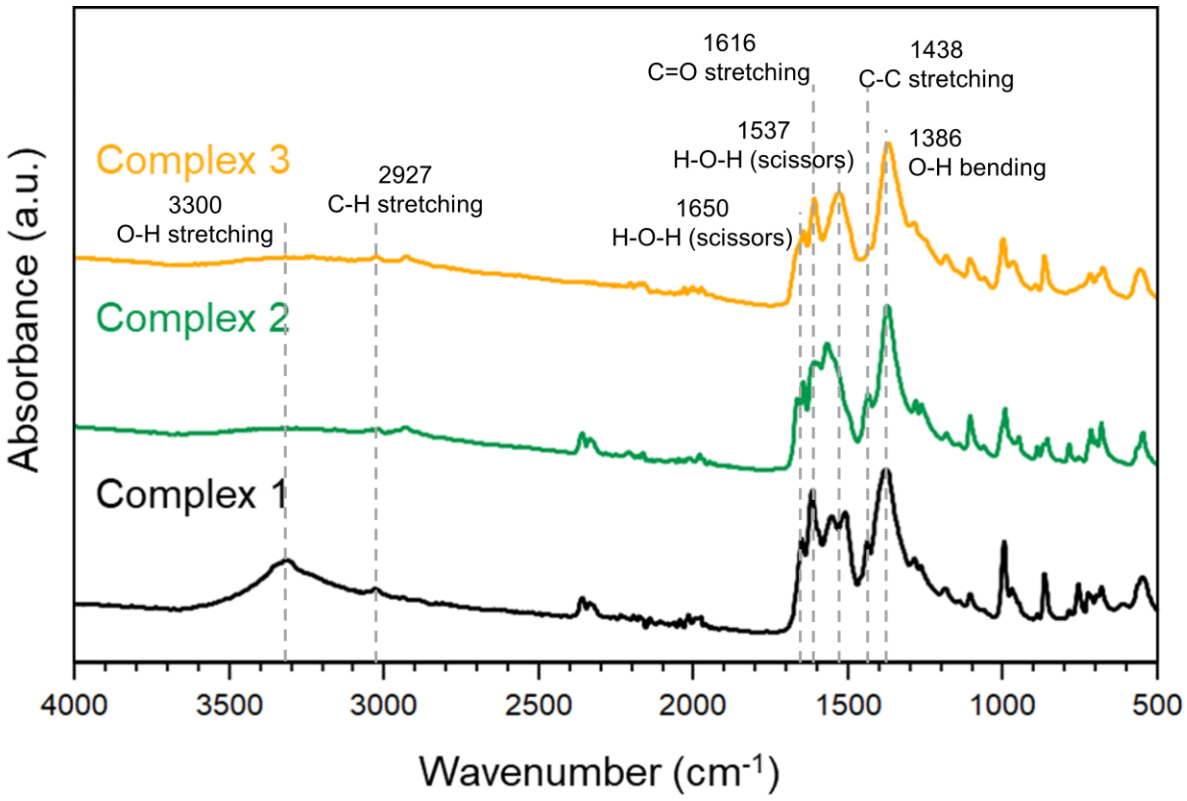

Figure S11. FT-IR spectra of the Ymuco MOFs. **1**(black), **2** (green) and **3** (yellow).

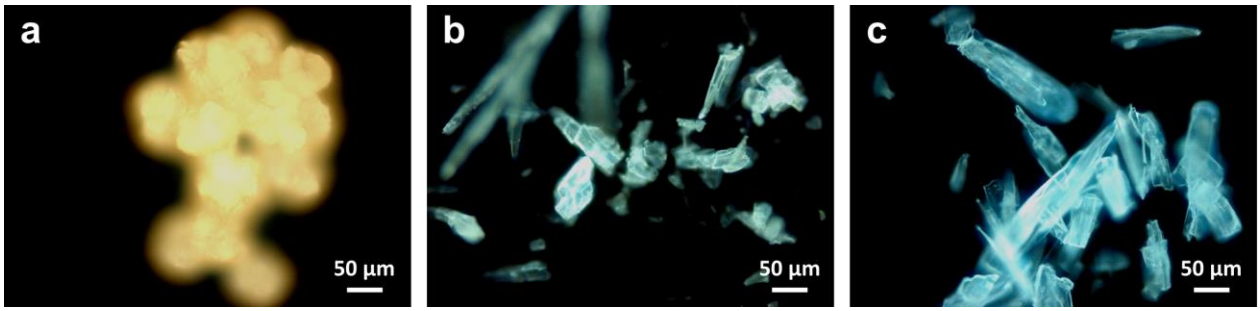

Figure S12. Photoluminescence microscopy images of the Ymuco MOFs. (a) **1**, (b) **2** and (c) **3**.

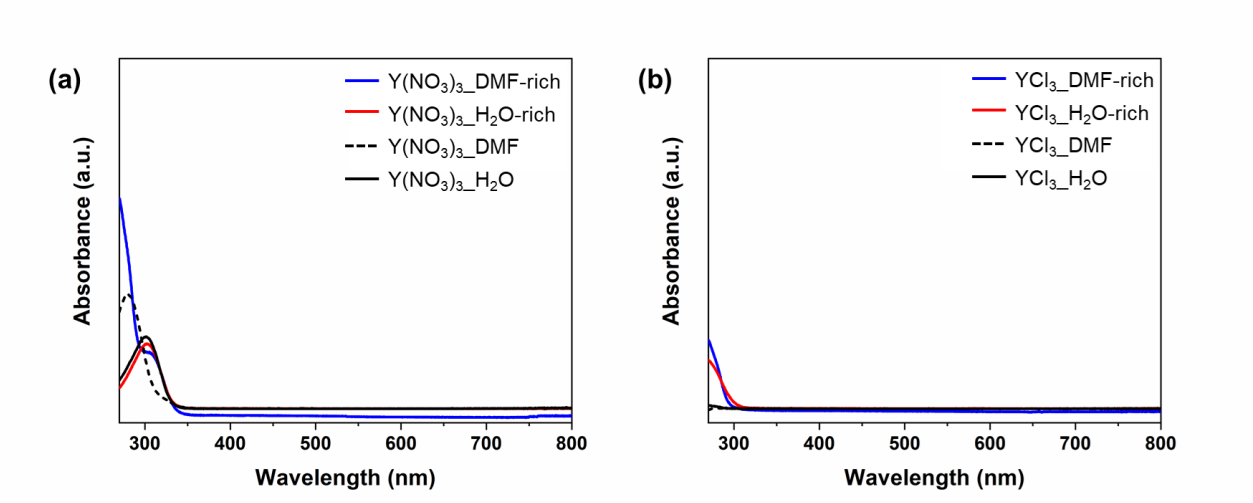

Figure S13. Solution UV-Vis spectra of yttrium precursors under different solvent environments. (a) $Y(NO_3)_3$ and (b) YCl_3.

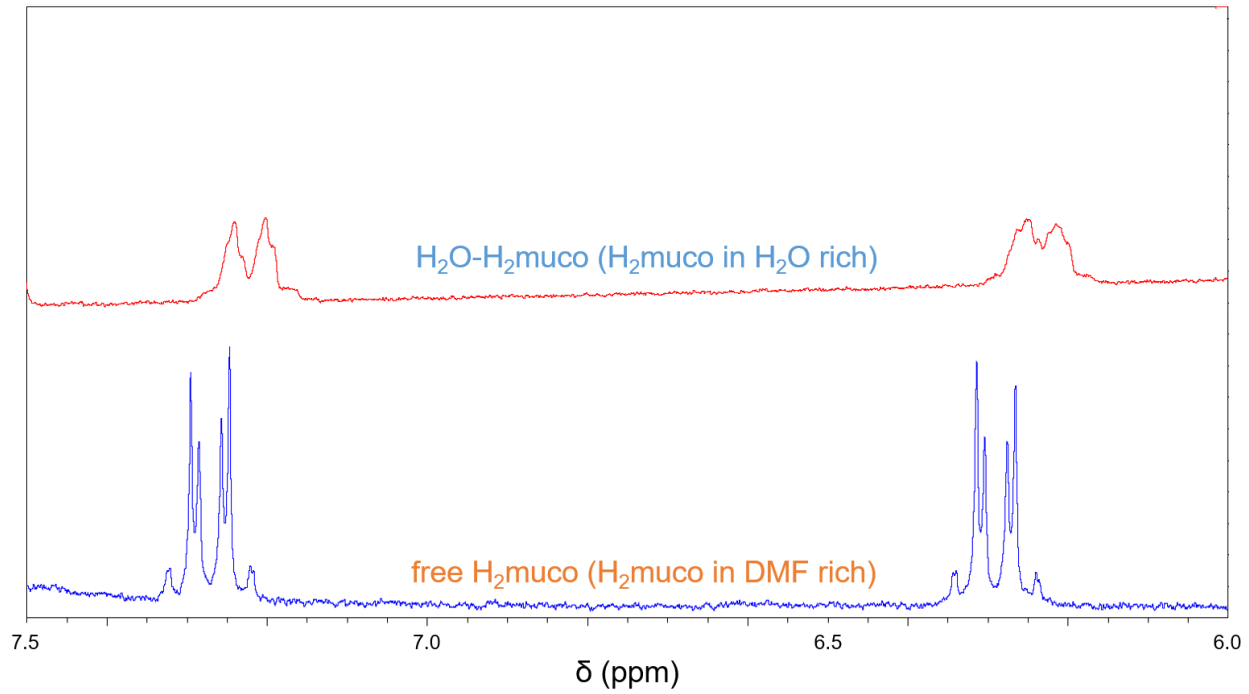

Figure S14. ^{1}H-NMR spectra of H_2muco dissolved in H_2O rich and DMF rich solvent environment. All ^{1}H-NMR spectra used dimethyl sulfoxide (DMSO-d6) as a reference solvent.

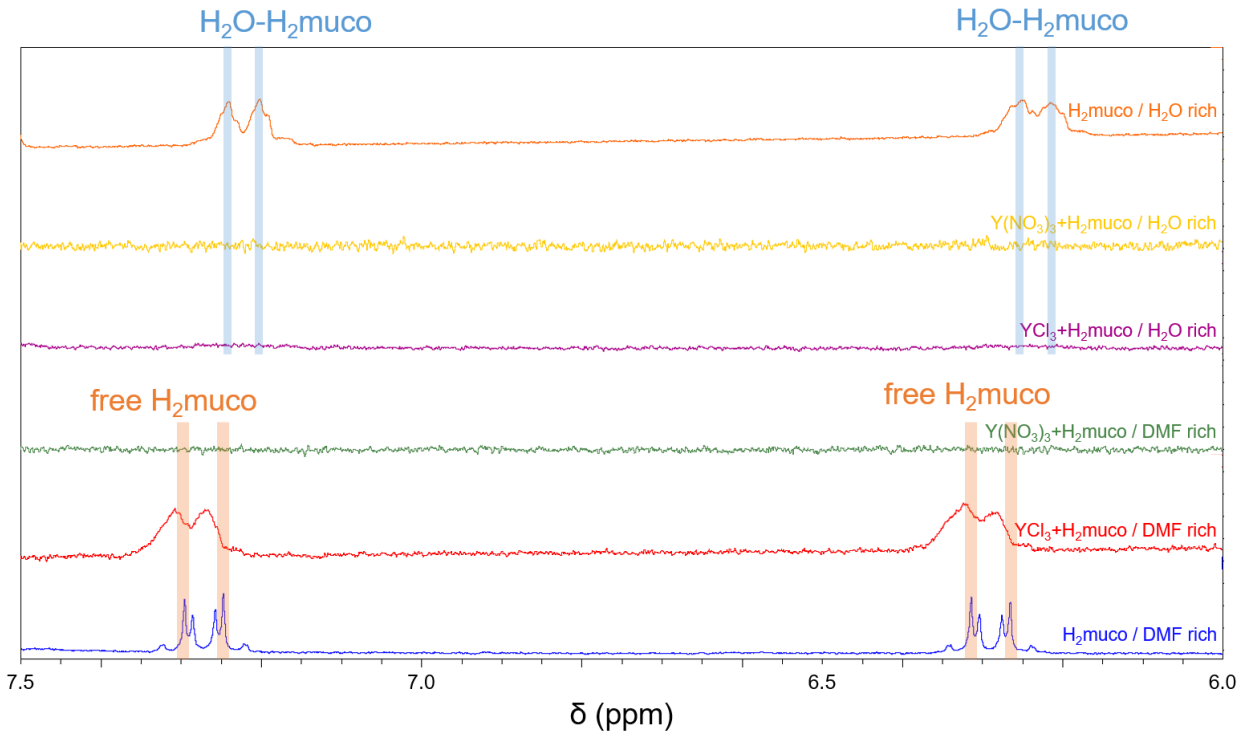

Figure S15. ^{1}H-NMR spectra of metal precursors and H_2muco just mixed in H_2O rich and DMF rich solvent environment. All ^{1}H-NMR spectra used dimethyl sulfoxide (DMSO-d6) as a reference solvent.

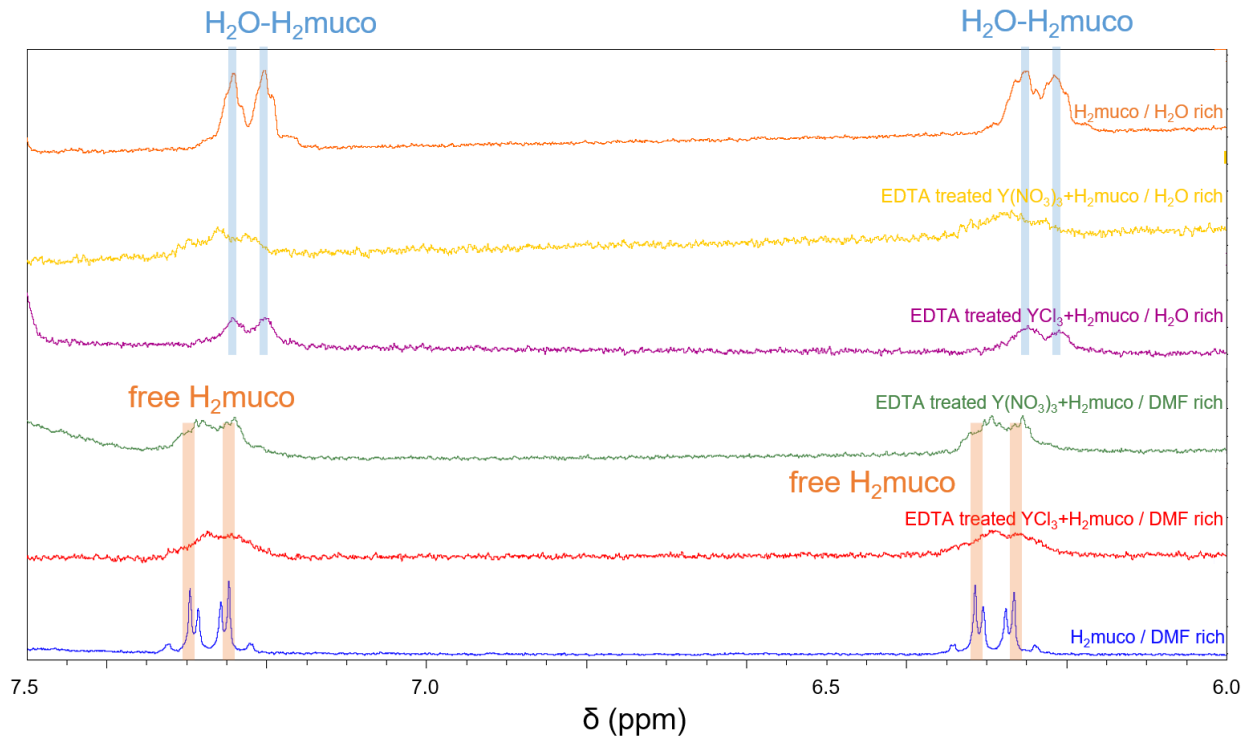

Figure S16. ^{1}H-NMR spectra after treatment of EDTA to the solutions (Y+H_2muco in H_2O rich or DMF rich solvent). All ^{1}H-NMR spectra used dimethyl sulfoxide (DMSO-d6) as a reference solvent.

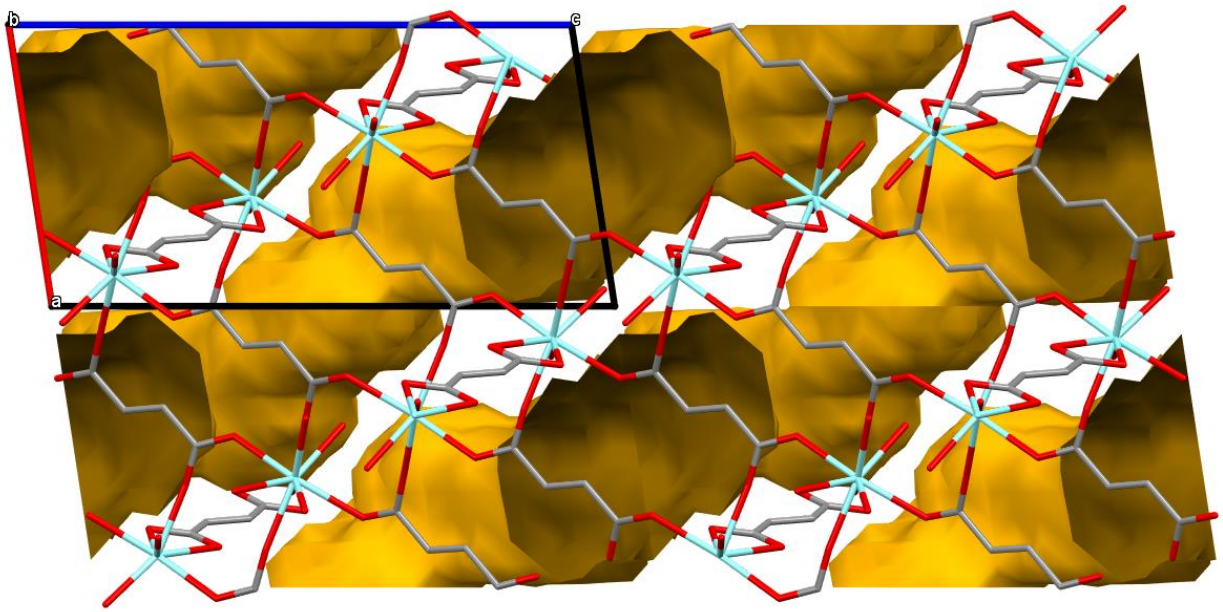

Figure S17. Void space of **Yfum_H_2O**: 32.3 % (445.61 Å^3).

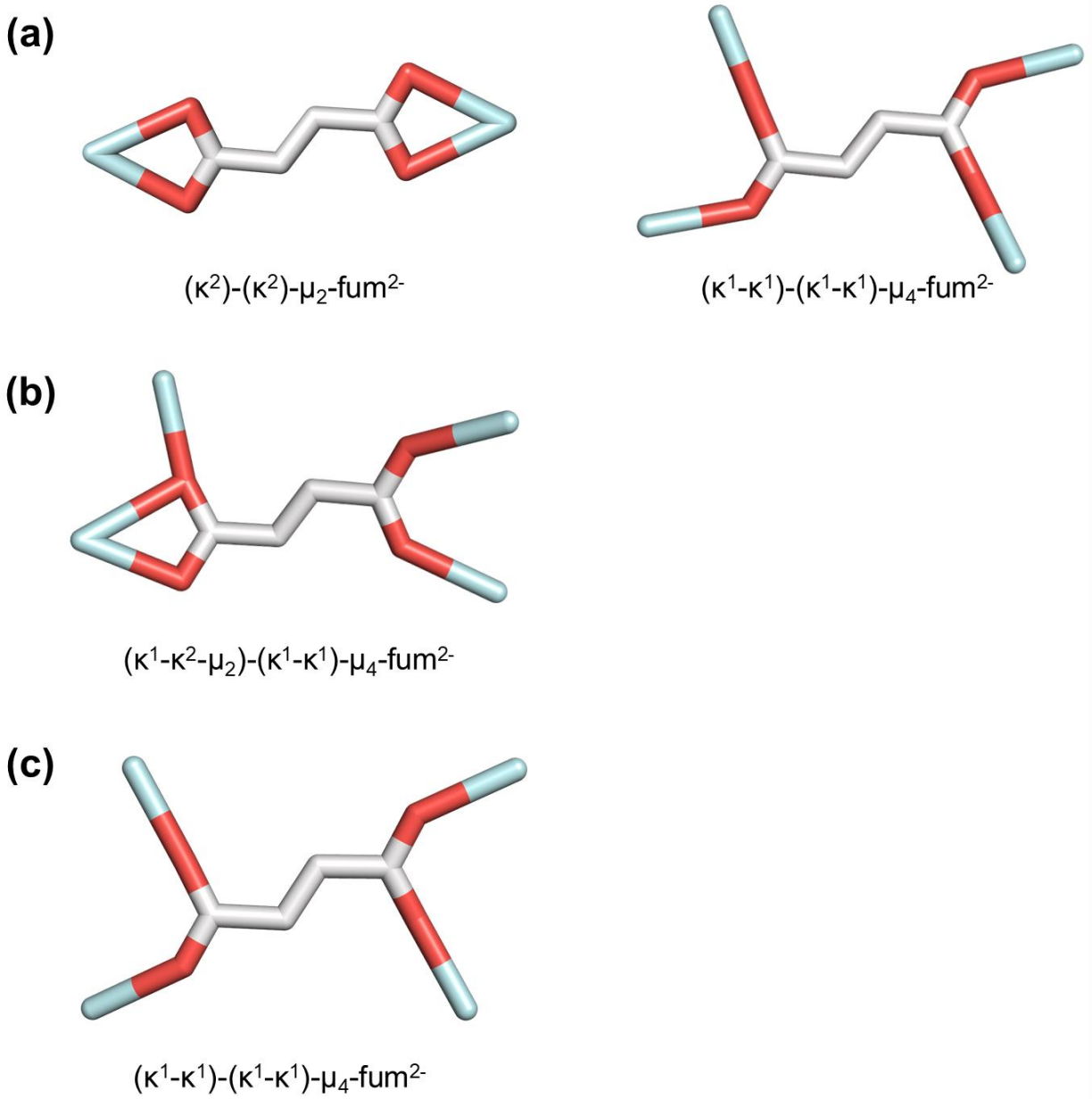

Figure S18. The coordination modes of H2fum in three different Yfum MOFs. (a) **Yfum_H_2O**. (b) **Yfum_NO_3**. (c) **Yfum_Cl**. Cyan: Y; red: O; gray: C. Hydrogen atoms are omitted for clarity.

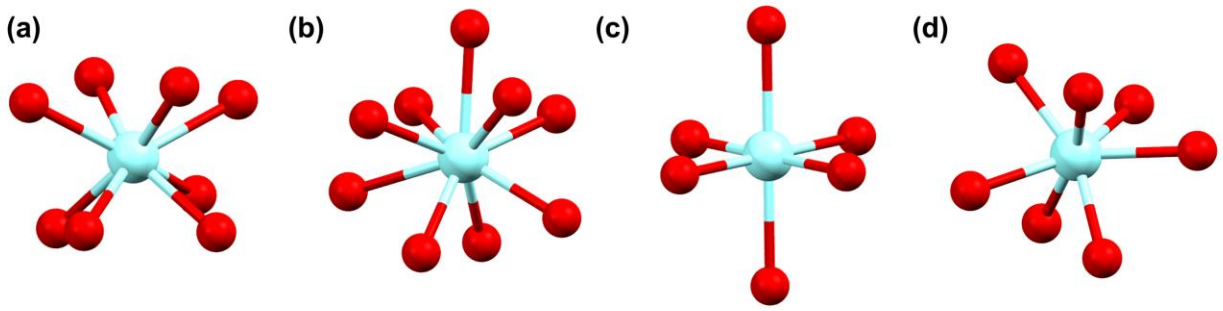

Figure S19. Comparison of the geometry around Y(III) in each Ymuco MOF structure. (a) Distorted square antiprism geometry of **Yfum_H_2O**. (b) Distorted mono-capped square antiprism geometry of **Yfum_NO_3**. (c) Elongated octahedral of **Yfum_Cl**. (d) Distorted capped trigonal prism geometry of **Yfum_Cl**. Cyan: Y; red: O.

4. Supplementary tables

Table S1. Selected bond lengths [Å] and angles [°] for **1**.

Y(1)-O(1A)	2.268(4)	O(1A)-Y(1)-O(1B)	81.16(15)
Y(1)-O(1B)	2.273(4)	O(1A)-Y(1)-O(2A)#1	74.76(14)
Y(1)-O(2A)#1	2.291(3)	O(1B)-Y(1)-O(2A)#1	85.73(13)
Y(1)-O(2B)#2	2.315(4)	O(1A)-Y(1)-O(2B)#2	149.52(12)
Y(1)-O(1SA)	2.353(4)	O(1B)-Y(1)-O(2B)#2	89.64(14)
Y(1)-O(3A)#3	2.385(4)	O(2A)#1-Y(1)-O(2B)#2	75.63(13)
Y(1)-O(4A)#4	2.395(4)	O(1A)-Y(1)-O(1SA)	69.09(13)
Y(1)-O(3A)#4	2.646(3)	O(1B)-Y(1)-O(1SA)	108.08(14)
Y(1)-C(6A)#4	2.895(5)	O(2A)#1-Y(1)-O(1SA)	138.26(15)
		O(2B)#2-Y(1)-O(1SA)	141.04(12)
		O(1A)-Y(1)-O(3A)#3	126.94(13)
		O(1B)-Y(1)-O(3A)#3	77.61(13)
		O(2A)#1-Y(1)-O(3A)#3	149.03(15)
		O(2B)#2-Y(1)-O(3A)#3	78.31(13)
		O(1SA)-Y(1)-O(3A)#3	72.38(14)
		O(1A)-Y(1)-O(4A)#4	93.89(14)
		O(1B)-Y(1)-O(4A)#4	166.28(12)
		O(2A)#1-Y(1)-O(4A)#4	80.61(12)
		O(2B)#2-Y(1)-O(4A)#4	88.26(14)
		O(1SA)-Y(1)-O(4A)#4	81.71(14)
		O(3A)#3-Y(1)-O(4A)#4	115.16(11)
		O(1A)-Y(1)-O(3A)#4	130.17(14)
		O(1B)-Y(1)-O(3A)#4	140.43(13)
		O(2A)#1-Y(1)-O(3A)#4	121.98(12)
		O(2B)#2-Y(1)-O(3A)#4	73.12(12)
		O(1SA)-Y(1)-O(3A)#4	71.30(13)
		O(3A)#3-Y(1)-O(3A)#4	64.31(14)
		O(4A)#4-Y(1)-O(3A)#4	51.15(11)

Symmetry transformations used to generate equivalent atoms:

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

#4 x,y+1,z-1 #5 -x,-y,-z+1 #6 x,y-1,z+1

Table S2. Selected bond lengths [Å] and angles [°] for **2**.

Y(1)-O(1A)	2.272(2)	O(1A)-Y(1)-O(1B)	79.63(9)
Y(1)-O(1B)	2.314(2)	O(1A)-Y(1)-O(1SA)	144.53(9)
Y(1)-O(1SA)	2.333(3)	O(1B)-Y(1)-O(1SA)	76.64(10)
Y(1)-O(2B)#1	2.343(3)	O(1A)-Y(1)-O(2B)#1	74.34(9)
Y(1)-O(2A)#1	2.378(2)	O(1B)-Y(1)-O(2B)#1	131.92(9)
Y(1)-O(4A)#2	2.407(2)	O(1SA)-Y(1)-O(2B)#1	140.67(9)
Y(1)-O(4A)#3	2.439(2)	O(1A)-Y(1)-O(2A)#1	123.67(9)
Y(1)-O(3A)#3	2.538(2)	O(1B)-Y(1)-O(2A)#1	81.83(8)
Y(1)-O(1A)#1	2.753(3)	O(1SA)-Y(1)-O(2A)#1	78.47(9)
Y(1)-C(6A)#3	2.857(3)	O(2B)#1-Y(1)-O(2A)#1	80.11(9)
Y(1)-C(1A)#1	2.930(3)	O(1A)-Y(1)-O(4A)#2	133.57(9)
Y(1)-Y(1)#1	4.0258(12)	O(1B)-Y(1)-O(4A)#2	146.57(9)
		O(1SA)-Y(1)-O(4A)#2	72.02(9)
		O(2B)#1-Y(1)-O(4A)#2	72.26(9)
		O(2A)#1-Y(1)-O(4A)#2	80.81(7)
		O(1A)-Y(1)-O(4A)#3	85.19(8)
		O(1B)-Y(1)-O(4A)#3	123.34(8)
		O(1SA)-Y(1)-O(4A)#3	86.22(9)
		O(2B)#1-Y(1)-O(4A)#3	94.11(9)
		O(2A)#1-Y(1)-O(4A)#3	146.64(7)
		O(4A)#2-Y(1)-O(4A)#3	66.25(8)
		O(1A)-Y(1)-O(3A)#3	72.98(9)
		O(1B)-Y(1)-O(3A)#3	71.05(8)
		O(1SA)-Y(1)-O(3A)#3	74.56(10)
		O(2B)#1-Y(1)-O(3A)#3	134.32(9)
		O(2A)#1-Y(1)-O(3A)#3	145.29(9)
		O(4A)#2-Y(1)-O(3A)#3	110.48(8)
		O(4A)#3-Y(1)-O(3A)#3	52.32(8)
		O(1A)-Y(1)-O(1A)#1	73.91(9)
		O(1B)-Y(1)-O(1A)#1	65.44(9)
		O(1SA)-Y(1)-O(1A)#1	117.94(9)
		O(2B)#1-Y(1)-O(1A)#1	68.80(9)
		O(2A)#1-Y(1)-O(1A)#1	50.05(8)
		O(4A)#2-Y(1)-O(1A)#1	120.64(7)

O(4A)#3-Y(1)-O(1A)#1	155.76(8)
O(3A)#3-Y(1)-O(1A)#1	128.83(8)

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+2,-y,-z+1 #5 x,y,z-1

Table S3. Bond lengths [Å] and angles [°] for **3**.

Y(1)-O(1A)	2.234(3)	O(1A)-Y(1)-O(4A)#1	152.64(12)
Y(1)-O(4A)#1	2.254(3)	O(1A)-Y(1)-O(2A)#2	104.88(11)
Y(1)-O(2A)#2	2.355(3)	O(4A)#1-Y(1)-O(2A)#2	81.29(11)
Y(1)-O(3A)#3	2.357(3)	O(1A)-Y(1)-O(3A)#3	81.70(11)
Y(1)-O(2W)	2.396(3)	O(4A)#1-Y(1)-O(3A)#3	109.67(11)
Y(1)-O(1W)	2.410(3)	O(2A)#2-Y(1)-O(3A)#3	143.00(12)
Y(1)-O(1B)	2.437(3)	O(1A)-Y(1)-O(2W)	84.24(12)
Y(1)-O(2B)	2.457(3)	O(4A)#1-Y(1)-O(2W)	76.10(11)
Y(1)-C(1B)	2.800(4)	O(2A)#2-Y(1)-O(2W)	143.36(12)
		O(3A)#3-Y(1)-O(2W)	72.75(12)
		O(1A)-Y(1)-O(1W)	71.52(12)
		O(4A)#1-Y(1)-O(1W)	84.83(12)
		O(2A)#2-Y(1)-O(1W)	75.17(11)
		O(3A)#3-Y(1)-O(1W)	139.21(11)
		O(2W)-Y(1)-O(1W)	74.41(12)
		O(1A)-Y(1)-O(1B)	129.69(11)
		O(4A)#1-Y(1)-O(1B)	77.66(11)
		O(2A)#2-Y(1)-O(1B)	73.53(11)
		O(3A)#3-Y(1)-O(1B)	74.63(11)
		O(2W)-Y(1)-O(1B)	127.52(11)
		O(1W)-Y(1)-O(1B)	146.01(11)
		O(1A)-Y(1)-O(2B)	77.57(11)
		O(4A)#1-Y(1)-O(2B)	128.96(11)
		O(2A)#2-Y(1)-O(2B)	71.92(11)
		O(3A)#3-Y(1)-O(2B)	74.23(11)
		O(2W)-Y(1)-O(2B)	144.15(12)
		O(1W)-Y(1)-O(2B)	126.42(11)
		O(1B)-Y(1)-O(2B)	53.63(10)

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1,-y+1,-z #5 x,y+1,z

Table S4. Crystal Data and Structure Refinements for **Yfum_H_2O**, **Yfum_NO_3**, and **Yfum_Cl**.

Compound	**Yfum_H_2O**	**Yfum_NO_3**	**Yfum_Cl**
Empirical formula	$C_{18}H_{29}N_2O_{18.5}Y_2$	$C_{10}H_{16}N_3O_9Y_1$	$C_{34}H_{58}N_6O_{26}Y_4$
Formula weight	747.25	411.17	1322.50
Temperature/K	100(2)	100(2)	100(2)
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	*P*-1	$P2_1/c$	*P*-1
***a*/Å**	8.5200(17)	12.470(3)	9.5730(19)
***b*/Å**	10.069(2)	10.334(2)	14.857(3)
***c*/Å**	16.751(3)	13.219(3)	19.601(4)
***α*/°**	81.28(3)	90	99.49(3)
***β*/°**	79.95(3)	111.93(3)	95.46(3)
***γ*/°**	79.63(3)	90	101.53(3)
Volume/Å^3	1381.1(5)	1580.2(6)	2670.4(10)
Z	2	4	2
ρ_{calc}**g/cm^3**	1.797	1.728	1.645
***μ*/mm^{-1}**	0.878	0.926	1.045
F(000)	754	832	1336
Crystal size/mm^3	0.098 × 0.018 × 0.003	0.054 × 0.025 × 0.021	0.035 × 0.007 × 0.006
Radiation	synchrotron (λ = 0.750 Å)	synchrotron (λ = 0.800 Å)	synchrotron (λ = 0.800 Å)
***θ* range for data collection/°**	1.313 to 29.585	1.982 to 33.536	1.603 to 32.178
Index ranges	$-11 \le h \le 11$ $-13 \le k \le 13$ $-22 \le l \le 21$	$-17 \le h \le 17$ $-14 \le k \le 14$ $-17 \le l \le 17$	$-11 \le h \le 11$ $-18 \le k \le 18$ $-24 \le l \le 24$
Reflections collected	10423	6616	15358
Independent reflections	5825 [R(int) = 0.0398]	3678 [R(int) = 0.0289]	8689 [R(int) = 0.0387]
Data/restraints /parameters	5825 / 0 / 374	3678 / 0 / 213	8689 / 0 / 651
Goodness-of-fit on F^2	1.115	1.089	1.173
***R*$_1$, *wR*$_2$ [I > 2σ(I)]**	R_1 = 0.0699 wR_2 = 0.2312	R_1 = 0.0570 wR_2 = 0.1544	R_1 = 0.1002 wR_2 = 0.3066
***R*$_1$, *wR*$_2$ [all data]**	R_1 = 0.0789 wR_2 = 0.2438	R_1 = 0.0621 wR_2 = 0.1583	R_1 = 0.1413 wR_2 = 0.3316
Largest diff. peak /hole / e Å^{-3}	2.317/−1.310	1.424/−2.006	0.319/−0.225

Table S5. Selected bond lengths [Å] and angles [°] for **Yfum_H_2O**.

Y(1)-O(4B)#1	2.246(4)	O(4B)#1-Y(1)-O(1B)	150.75(12)
Y(1)-O(1B)	2.252(4)	O(4B)#1-Y(1)-O(2C)#1	101.57(13)
Y(1)-O(2C)#1	2.295(3)	O(1B)-Y(1)-O(2C)#1	82.54(13)
Y(1)-O(2B)#2	2.320(3)	O(4B)#1-Y(1)-O(2B)#2	81.72(13)
Y(1)-O(2)	2.418(4)	O(1B)-Y(1)-O(2B)#2	103.69(13)
Y(1)-O(1)	2.442(3)	O(2C)#1-Y(1)-O(2B)#2	161.31(12)
Y(1)-O(1A)	2.443(3)	O(4B)#1-Y(1)-O(2)	137.23(13)
Y(1)-O(2A)	2.494(3)	O(1B)-Y(1)-O(2)	71.23(13)
Y(1)-C(1A)	2.816(4)	O(2C)#1-Y(1)-O(2)	88.66(13)
Y(2)-O(1C)	2.258(4)	O(2B)#2-Y(1)-O(2)	77.04(12)
Y(2)-O(4C)#1	2.280(4)	O(4B)#1-Y(1)-O(1)	72.94(13)
Y(2)-O(3B)	2.298(3)	O(1B)-Y(1)-O(1)	135.46(13)
Y(2)-O(3C)#3	2.309(3)	O(2C)#1-Y(1)-O(1)	77.16(12)
Y(2)-O(3)	2.376(4)	O(2B)#2-Y(1)-O(1)	86.42(12)
Y(2)-O(4)	2.412(3)	O(2)-Y(1)-O(1)	69.10(13)
Y(2)-O(4A)#4	2.453(3)	O(4B)#1-Y(1)-O(1A)	80.22(13)
Y(2)-O(3A)#4	2.492(3)	O(1B)-Y(1)-O(1A)	73.90(12)
Y(2)-C(4A)#4	2.816(4)	O(2C)#1-Y(1)-O(1A)	124.40(12)
		O(2B)#2-Y(1)-O(1A)	74.25(11)
		O(2)-Y(1)-O(1A)	127.25(12)
		O(1)-Y(1)-O(1A)	148.90(12)
		O(4B)#1-Y(1)-O(2A)	72.64(13)
		O(1B)-Y(1)-O(2A)	80.93(13)
		O(2C)#1-Y(1)-O(2A)	74.11(12)
		O(2B)#2-Y(1)-O(2A)	123.98(11)
		O(2)-Y(1)-O(2A)	148.98(12)
		O(1)-Y(1)-O(2A)	128.89(12)
		O(1A)-Y(1)-O(2A)	53.13(11)
		O(1C)-Y(2)-O(4C)#1	146.55(12)
		O(1C)-Y(2)-O(3B)	99.85(13)
		O(4C)#1-Y(2)-O(3B)	83.39(12)
		O(1C)-Y(2)-O(3C)#3	82.06(13)
		O(4C)#1-Y(2)-O(3C)#3	106.90(12)

O(3B)-Y(2)-O(3C)#3	158.51(12)
O(1C)-Y(2)-O(3)	140.48(13)
O(4C)#1-Y(2)-O(3)	72.59(13)
O(3B)-Y(2)-O(3)	87.36(13)
O(3C)#3-Y(2)-O(3)	78.22(13)
O(1C)-Y(2)-O(4)	73.76(14)
O(4C)#1-Y(2)-O(4)	138.07(13)
O(3B)-Y(2)-O(4)	75.72(12)
O(3C)#3-Y(2)-O(4)	84.43(11)
O(3)-Y(2)-O(4)	70.53(13)
O(1C)-Y(2)-O(4A)#4	78.00(13)
O(4C)#1-Y(2)-O(4A)#4	73.64(12)
O(3B)-Y(2)-O(4A)#4	126.37(12)
O(3C)#3-Y(2)-O(4A)#4	75.07(11)
O(3)-Y(2)-O(4A)#4	127.88(12)
O(4)-Y(2)-O(4A)#4	147.03(12)
O(1C)-Y(2)-O(3A)#4	71.03(13)
O(4C)#1-Y(2)-O(3A)#4	77.82(13)
O(3B)-Y(2)-O(3A)#4	75.31(12)
O(3C)#3-Y(2)-O(3A)#4	124.76(11)
O(3)-Y(2)-O(3A)#4	147.18(13)
O(4)-Y(2)-O(3A)#4	128.99(12)
O(4A)#4-Y(2)-O(3A)#4	53.00(11)

Symmetry transformations used to generate equivalent atoms:

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

#4 x+1,y-1,z #5 x-1,y+1,z #6 x+1,y,z

Table S6. Selected bond lengths [Å] and angles [°] for **Yfum_NO$_3$**.

Y(1)-O(1A)	2.290(2)	O(1A)-Y(1)-O(3A)#1	78.36(8)
Y(1)-O(3A)#1	2.312(2)	O(1A)-Y(1)-O(4A)#2	74.11(8)
Y(1)-O(4A)#2	2.329(2)	O(3A)#1-Y(1)-O(4A)#2	134.97(8)
Y(1)-O(1SB)	2.346(2)	O(1A)-Y(1)-O(1SB)	144.29(8)
Y(1)-O(2A)#3	2.383(2)	O(3A)#1-Y(1)-O(1SB)	77.16(8)
Y(1)-O(1SA)	2.395(3)	O(4A)#2-Y(1)-O(1SB)	140.57(8)
Y(1)-O(2B)	2.422(2)	O(1A)-Y(1)-O(2A)#3	124.74(7)
Y(1)-O(1B)	2.527(3)	O(3A)#1-Y(1)-O(2A)#3	78.50(8)
Y(1)-O(1A)#3	2.641(2)	O(4A)#2-Y(1)-O(2A)#3	88.74(8)
Y(1)-C(1A)#3	2.877(3)	O(1SB)-Y(1)-O(2A)#3	74.71(7)
Y(1)-Y(1)#3	3.9614(13)	O(1A)-Y(1)-O(1SA)	74.11(7)
		O(3A)#1-Y(1)-O(1SA)	76.20(8)
		O(4A)#2-Y(1)-O(1SA)	127.16(8)
		O(1SB)-Y(1)-O(1SA)	75.07(7)
		O(2A)#3-Y(1)-O(1SA)	144.06(7)
		O(1A)-Y(1)-O(2B)	99.54(8)
		O(3A)#1-Y(1)-O(2B)	145.04(9)
		O(4A)#2-Y(1)-O(2B)	75.22(9)
		O(1SB)-Y(1)-O(2B)	86.28(8)
		O(2A)#3-Y(1)-O(2B)	126.62(8)
		O(1SA)-Y(1)-O(2B)	69.82(8)
		O(1A)-Y(1)-O(1B)	137.90(8)
		O(3A)#1-Y(1)-O(1B)	143.42(7)
		O(4A)#2-Y(1)-O(1B)	69.29(8)
		O(1SB)-Y(1)-O(1B)	71.89(8)
		O(2A)#3-Y(1)-O(1B)	74.97(8)
		O(1SA)-Y(1)-O(1B)	113.02(8)
		O(2B)-Y(1)-O(1B)	51.68(8)
		O(1A)-Y(1)-O(1A)#3	73.33(8)
		O(3A)#1-Y(1)-O(1A)#3	68.31(8)
		O(4A)#2-Y(1)-O(1A)#3	70.01(8)
		O(1SB)-Y(1)-O(1A)#3	119.77(7)
		O(2A)#3-Y(1)-O(1A)#3	51.52(7)
		O(1SA)-Y(1)-O(1A)#3	135.59(7)

O(2B)-Y(1)-O(1A)#3	145.15(8)
O(1B)-Y(1)-O(1A)#3	111.39(7)

Symmetry transformations used to generate equivalent atoms:

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

#4 x,-y+3/2,z-1/2 #5 -x+1,y-1/2,-z+1/2

Table S7. Selected bond lengths [Å] and angles [°] for **Yfum_Cl**.

Y(1)-O(1A)	2.226(8)	Y(6)-O(2C)#5	2.260(6)
Y(1)-O(1A)#1	2.226(8)	Y(6)-O(2C)#4	2.260(6)
Y(1)-O(3B)#2	2.271(6)	Y(6)-O(4W)#6	2.577(5)
Y(1)-O(3B)#3	2.271(6)	Y(6)-O(4W)	2.577(5)
Y(1)-O(1W)	2.608(4)		
Y(1)-O(1W)#1	2.608(4)		
Y(2)-O(1B)#2	2.225(7)		
Y(2)-O(1B)	2.225(7)		
Y(2)-O(3A)#2	2.270(6)		
Y(2)-O(3A)	2.270(6)		
Y(2)-O(2W)	2.583(4)		
Y(2)-O(2W)#2	2.583(4)		
Y(3)-O(4A)	2.222(8)		
Y(3)-O(1C)	2.253(7)		
Y(3)-O(2B)	2.267(7)		
Y(3)-O(3D)#3	2.282(6)		
Y(3)-O(1SB)	2.301(10)		
Y(3)-O(1SA)	2.345(12)		
Y(3)-O(1SC)	2.386(12)		
Y(4)-O(4B)	2.252(7)		
Y(4)-O(1D)	2.253(7)		
Y(4)-O(2A)#4	2.285(6)		
Y(4)-O(3C)	2.292(6)		
Y(4)-O(1SE)	2.320(10)		
Y(4)-O(1SF)	2.328(11)		
Y(4)-O(1SD)	2.350(9)		
Y(5)-O(4C)	2.218(7)		
Y(5)-O(4C)#5	2.218(7)		
Y(5)-O(2D)#5	2.246(7)		
Y(5)-O(2D)	2.246(7)		
Y(5)-O(3W)	2.583(5)		
Y(5)-O(3W)#5	2.583(5)		
Y(6)-O(4D)#6	2.210(7)		
Y(6)-O(4D)	2.210(7)		

O(1A)-Y(1)-O(1A)#1	180.0(3)	O(4A)-Y(3)-O(1SB)	121.7(4)
O(1A)-Y(1)-O(3B)#2	88.3(2)	O(1C)-Y(3)-O(1SB)	76.8(3)
O(1A)#1-Y(1)-O(3B)#2	91.7(2)	O(2B)-Y(3)-O(1SB)	113.5(4)
O(1A)-Y(1)-O(3B)#3	91.7(2)	O(3D)#3-Y(3)-O(1SB)	78.0(3)
O(1A)#1-Y(1)-O(3B)#3	88.3(2)	O(4A)-Y(3)-O(1SA)	70.9(5)
O(3B)#2-Y(1)-O(3B)#3	180.0	O(1C)-Y(3)-O(1SA)	129.0(4)
O(1A)-Y(1)-O(1W)	86.6(3)	O(2B)-Y(3)-O(1SA)	77.5(4)
O(1A)#1-Y(1)-O(1W)	93.4(3)	O(3D)#3-Y(3)-O(1SA)	114.7(4)
O(3B)#2-Y(1)-O(1W)	88.8(2)	O(1SB)-Y(3)-O(1SA)	69.8(4)
O(3B)#3-Y(1)-O(1W)	91.2(2)	O(4A)-Y(3)-O(1SC)	78.3(4)
O(1A)-Y(1)-O(1W)#1	93.4(3)	O(1C)-Y(3)-O(1SC)	80.8(3)
O(1A)#1-Y(1)-O(1W)#1	86.6(3)	O(2B)-Y(3)-O(1SC)	81.9(4)
O(3B)#2-Y(1)-O(1W)#1	91.2(2)	O(3D)#3-Y(3)-O(1SC)	84.5(3)
O(3B)#3-Y(1)-O(1W)#1	88.8(2)	O(1SB)-Y(3)-O(1SC)	150.3(3)
O(1W)-Y(1)-O(1W)#1	180.00(12)	O(1SA)-Y(3)-O(1SC)	139.8(4)
O(1B)#2-Y(2)-O(1B)	180.0	O(4B)-Y(4)-O(1D)	156.8(3)
O(1B)#2-Y(2)-O(3A)#2	94.6(2)	O(4B)-Y(4)-O(2A)#4	93.8(2)
O(1B)-Y(2)-O(3A)#2	85.4(2)	O(1D)-Y(4)-O(2A)#4	82.9(2)
O(1B)#2-Y(2)-O(3A)	85.4(2)	O(4B)-Y(4)-O(3C)	84.2(2)
O(1B)-Y(2)-O(3A)	94.6(2)	O(1D)-Y(4)-O(3C)	93.3(2)
O(3A)#2-Y(2)-O(3A)	180.0	O(2A)#4-Y(4)-O(3C)	165.4(3)
O(1B)#2-Y(2)-O(2W)	91.3(3)	O(4B)-Y(4)-O(1SE)	126.2(3)
O(1B)-Y(2)-O(2W)	88.7(3)	O(1D)-Y(4)-O(1SE)	75.0(4)
O(3A)#2-Y(2)-O(2W)	87.3(2)	O(2A)#4-Y(4)-O(1SE)	115.6(3)
O(3A)-Y(2)-O(2W)	92.7(2)	O(3C)-Y(4)-O(1SE)	76.6(3)
O(1B)#2-Y(2)-O(2W)#2	88.7(3)	O(4B)-Y(4)-O(1SF)	76.2(3)
O(1B)-Y(2)-O(2W)#2	91.3(3)	O(1D)-Y(4)-O(1SF)	80.6(3)
O(3A)#2-Y(2)-O(2W)#2	92.7(2)	O(2A)#4-Y(4)-O(1SF)	83.1(3)
O(3A)-Y(2)-O(2W)#2	87.3(2)	O(3C)-Y(4)-O(1SF)	82.4(3)
O(2W)-Y(2)-O(2W)#2	180.0	O(1SE)-Y(4)-O(1SF)	146.5(3)
O(4A)-Y(3)-O(1C)	158.9(4)	O(4B)-Y(4)-O(1SD)	75.0(3)
O(4A)-Y(3)-O(2B)	97.6(3)	O(1D)-Y(4)-O(1SD)	125.8(3)
O(1C)-Y(3)-O(2B)	82.1(2)	O(2A)#4-Y(4)-O(1SD)	77.0(3)
O(4A)-Y(3)-O(3D)#3	81.4(3)	O(3C)-Y(4)-O(1SD)	116.1(3)
O(1C)-Y(3)-O(3D)#3	93.8(2)	O(1SE)-Y(4)-O(1SD)	69.9(3)
O(2B)-Y(3)-O(3D)#3	166.2(4)	O(1SF)-Y(4)-O(1SD)	143.6(3)

O(4C)-Y(5)-O(4C)#5	180.0	O(4D)#6-Y(6)-O(4D)	180.0(3)
O(4C)-Y(5)-O(2D)#5	88.8(3)	O(4D)#6-Y(6)-O(2C)#5	93.5(2)
O(4C)#5-Y(5)-O(2D)#5	91.2(3)	O(4D)-Y(6)-O(2C)#5	86.5(2)
O(4C)-Y(5)-O(2D)	91.2(3)	O(4D)#6-Y(6)-O(2C)#4	86.5(2)
O(4C)#5-Y(5)-O(2D)	88.8(3)	O(4D)-Y(6)-O(2C)#4	93.5(2)
O(2D)#5-Y(5)-O(2D)	180.0	O(2C)#5-Y(6)-O(2C)#4	180.0(3)
O(4C)-Y(5)-O(3W)	90.3(3)	O(4D)#6-Y(6)-O(4W)#6	88.0(3)
O(4C)#5-Y(5)-O(3W)	89.7(3)	O(4D)-Y(6)-O(4W)#6	92.0(3)
O(2D)#5-Y(5)-O(3W)	94.3(3)	O(2C)#5-Y(6)-O(4W)#6	87.4(3)
O(2D)-Y(5)-O(3W)	85.7(3)	O(2C)#4-Y(6)-O(4W)#6	92.6(3)
O(4C)-Y(5)-O(3W)#5	89.7(3)	O(4D)#6-Y(6)-O(4W)	92.0(3)
O(4C)#5-Y(5)-O(3W)#5	90.3(3)	O(4D)-Y(6)-O(4W)	88.0(3)
O(2D)#5-Y(5)-O(3W)#5	85.7(3)	O(2C)#5-Y(6)-O(4W)	92.6(3)
O(2D)-Y(5)-O(3W)#5	94.3(3)	O(2C)#4-Y(6)-O(4W)	87.4(3)
O(3W)-Y(5)-O(3W)#5	180.0(3)	O(4W)#6-Y(6)-O(4W)	180.0

Symmetry transformations used to generate equivalent atoms:

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

#4 x-1,y-1,z #5 -x,-y+1,-z #6 -x-1,-y,-z

5. References

(1) Shin, J. W.; Eom, K.; Moon, D. BL2D-SMC, the Supramolecular Crystallography Beamline at the Pohang Light Source II, Korea. J. Synchrotron Radiat. 2016, 23, 369–373.

(2) Otwinowski, Z.; Minor, W. Processing of X-Ray Diffraction Data Collected in Oscillation Mode. Methods Enzymol. 1997, 276, 307–326.

(3) Otwinowski, Z.; Borek, D.; Majewski, W.; Minor, W. Multiparametric Scaling of Diffraction Intensities. Acta Crystallogr. Sect. A Found. Crystallogr. 2003, 59, 228–234.

(4) Sheldrick, G. M. SHELXT - Integrated Space-Group and Crystal-Structure Determination. Acta Crystallogr. Sect. A Found. Crystallogr. 2015, 71, 3–8.

(5) Sheldrick, G. M. Crystal Structure Refinement with SHELXL. Acta Crystallogr. Sect. C Struct. Chem. 2015, 71, 3–8.