Supporting materials

Constructions of octanuclear polyoxomolybdenum(V)-based porous materials with lithium additives

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Figure and Table Options

Table S2. Selected bond distances (Å) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 62.5H_2O$ (**1**).

Table S3. Selected bond angles (°) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 62.5H_2O$ (**1**).

Table S4. Selected hydrogen bond distances (Å) and angles (°) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 62.5H_2O$ (**1**).

Table S5. Selected bond distances (Å) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 2(Hdmtrz)\cdot 27H_2O$ (**2**).

Table S6. Selected bond angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 2(Hdmtrz)\cdot 27H_2O$ (**2**).

Table S7. Selected hydrogen bond distances (Å) and angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 2(Hdmtrz)\cdot 27H_2O$ (**2**).

Table S8. Selected bond distances (Å) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 20.5H_2O$ (**3**).

Table S9. Selected bond angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 20.5H_2O$ (**3**).

Table S10. Selected hydrogen bond distances (Å) and angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 20.5H_2O$ (**3**).

Table S11. Selected bond distances (Å) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 25H_2O$ (**4**).

Table S12. Selected bond angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 25H_2O$ (**4**).

Table S13. Selected hydrogen bond distances (Å) and angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 25H_2O$ (**4**).

Table S14. Bond valence calculations for **1** – **4** respectively.

Table S15. Comparisons of CO_2 adsorption data for 1 with some typical MOFs at 1 bar, 298 K.

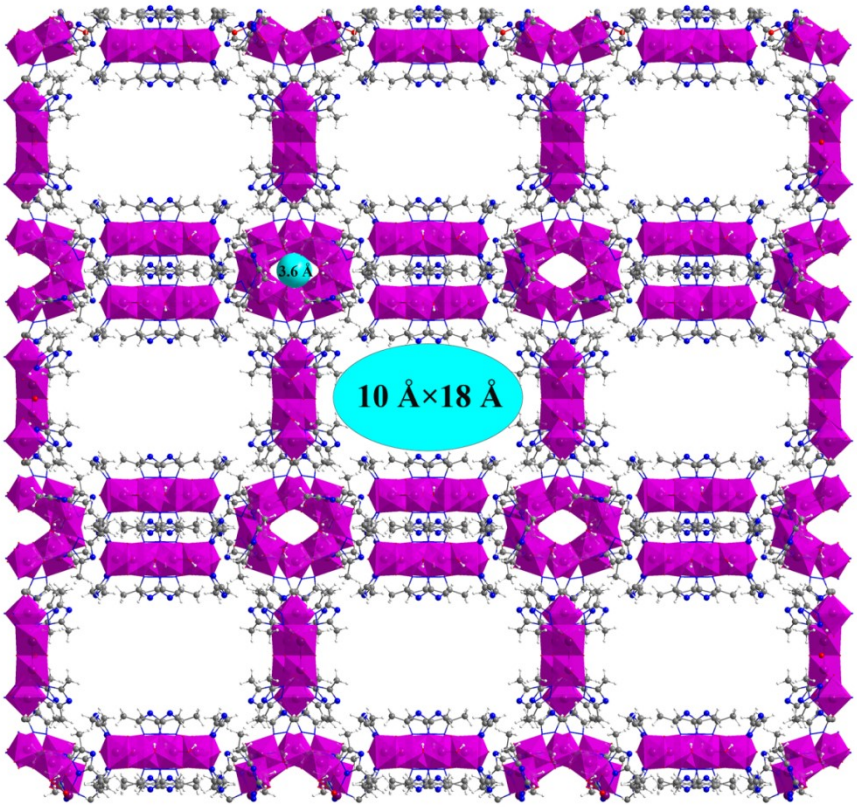

Fig. S1. Packing diagram of compound **1**.

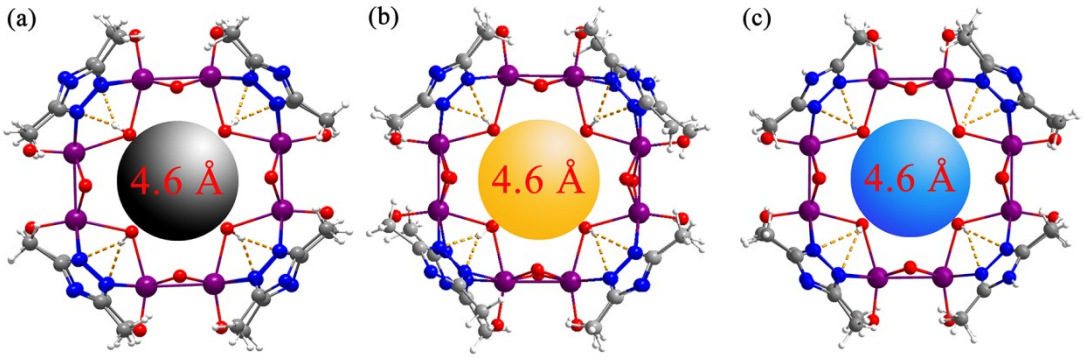

Fig. S2. Intrinsic voids within compounds **2** – **4**.

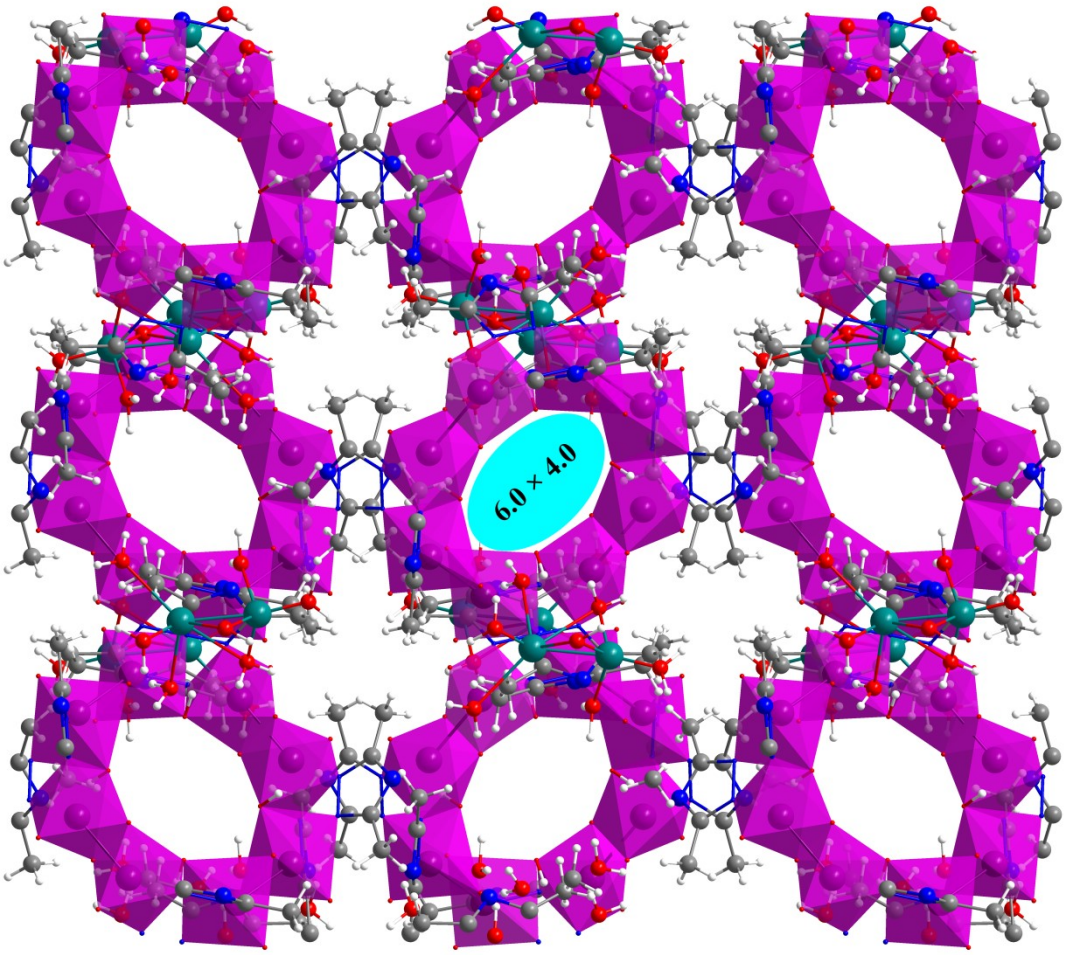

Fig. S3. The packing diagram of compound **4** along the *a*-axis.

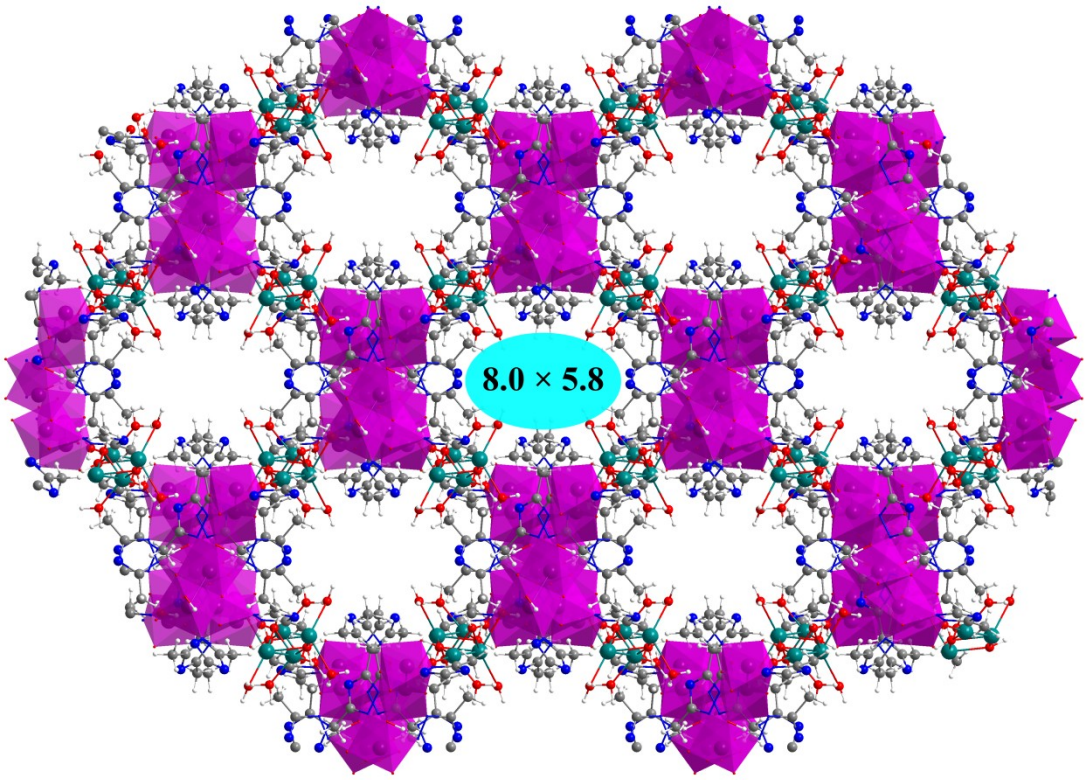

Fig. S4. The packing diagram of compound **4** along the *c*-axis.

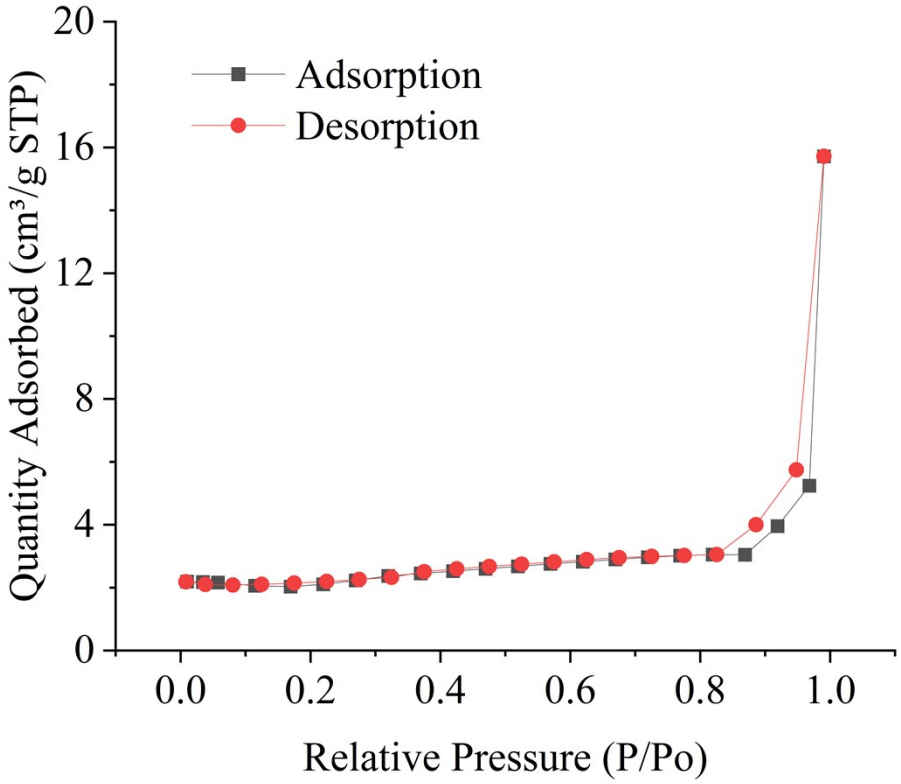

Fig. S5. N_2 adsorption-desorption isotherm of bulk sample **1** at 77 K.

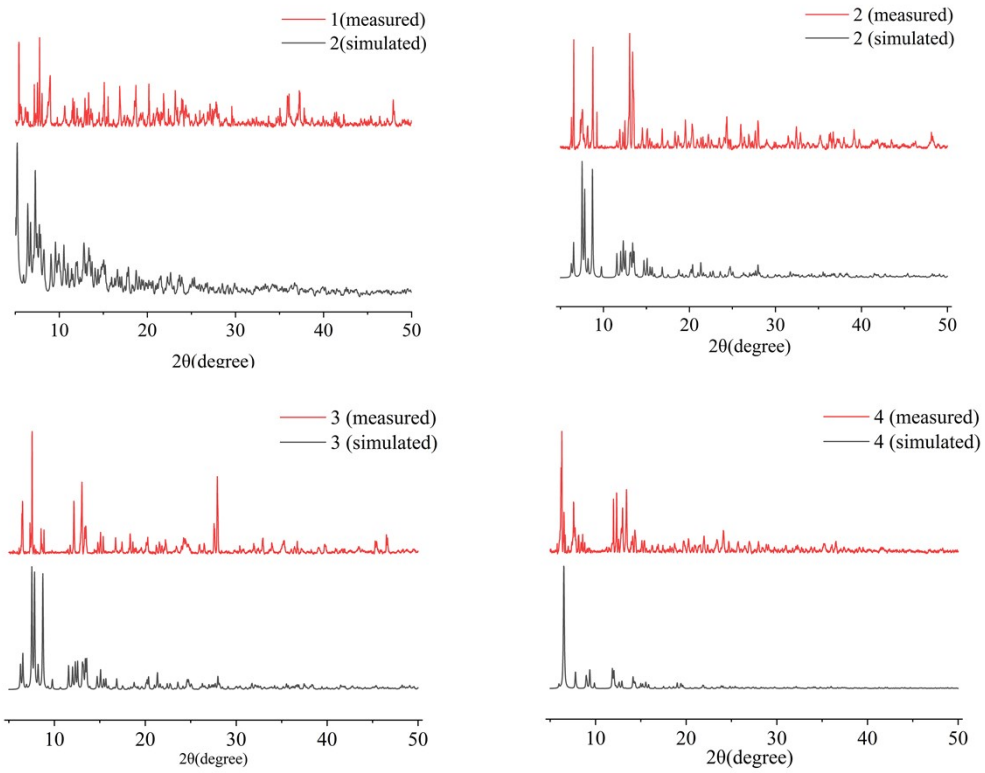

Fig. S6. Experimental and simulated PXRD patterns of **1** – **4**.

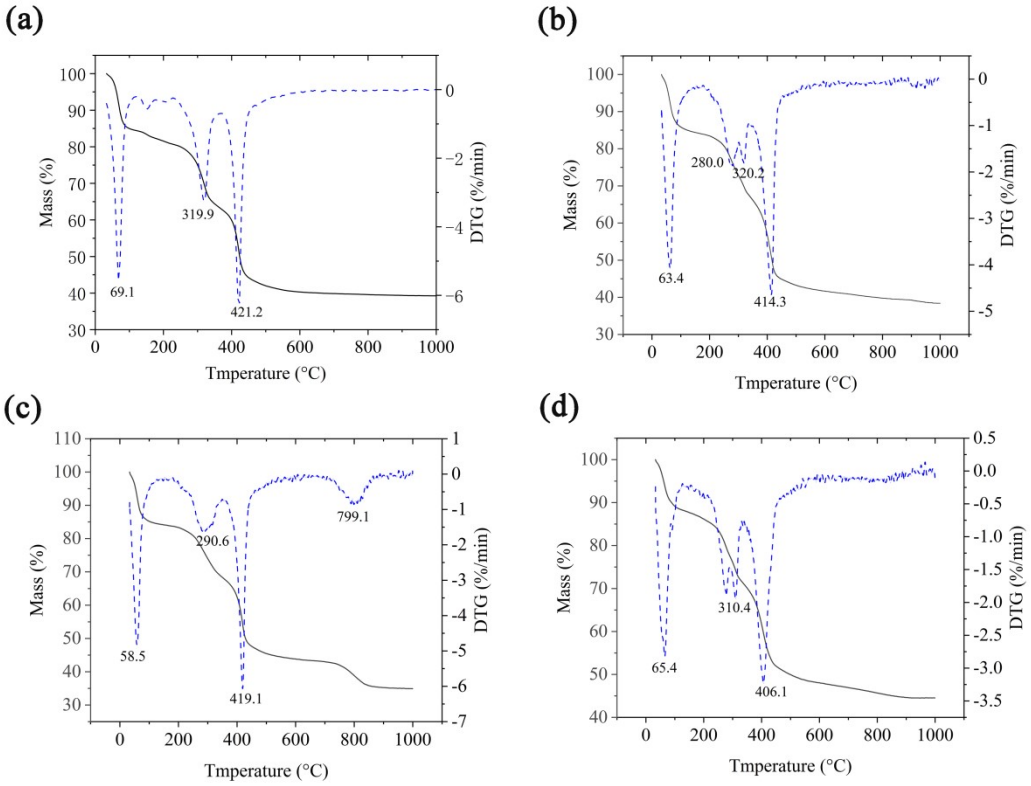

Fig. S7. TG-DTG curves of **1 – 4**.

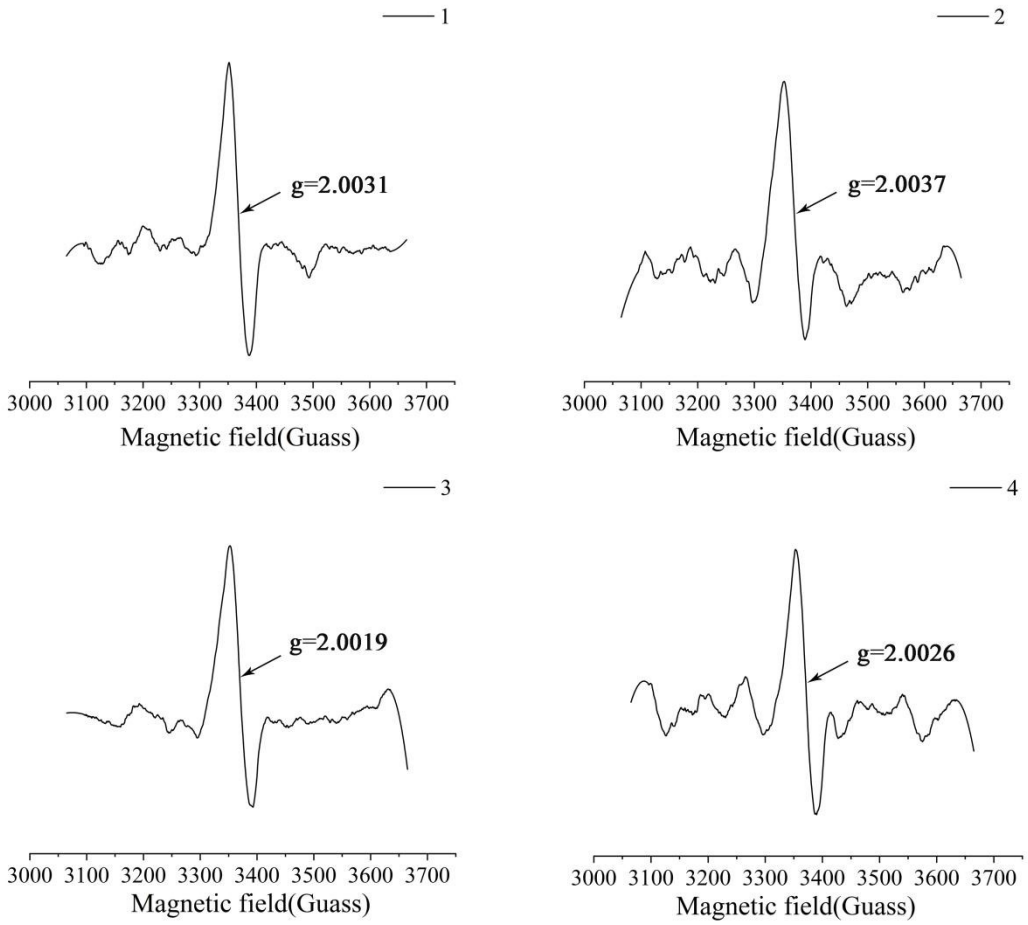

Fig. S8. EPR curves of **1 – 4**.

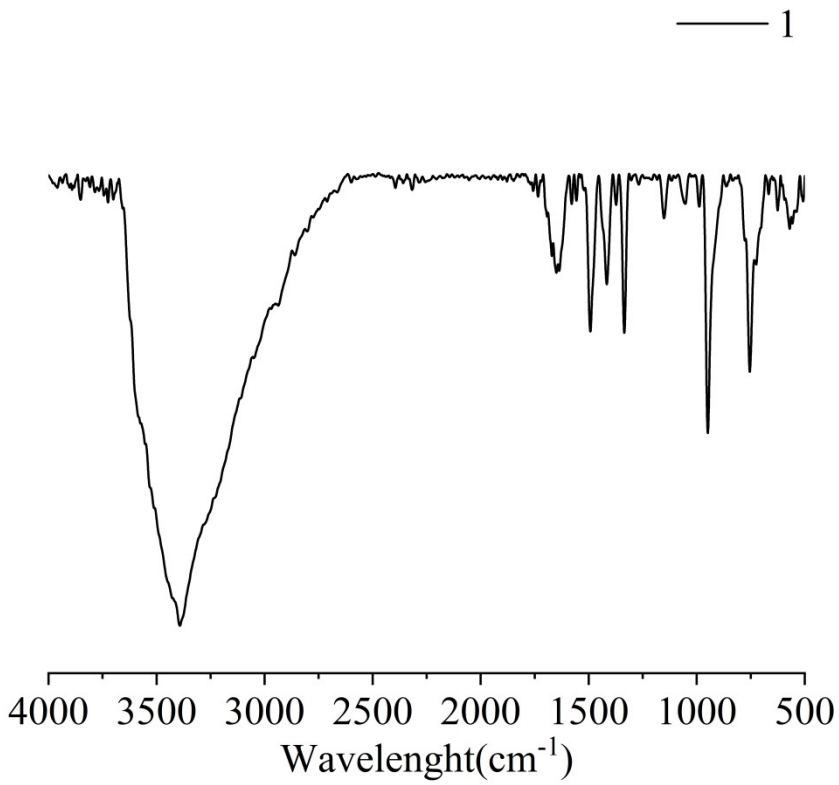

Fig. S9. IR spectrum of compound **1**.

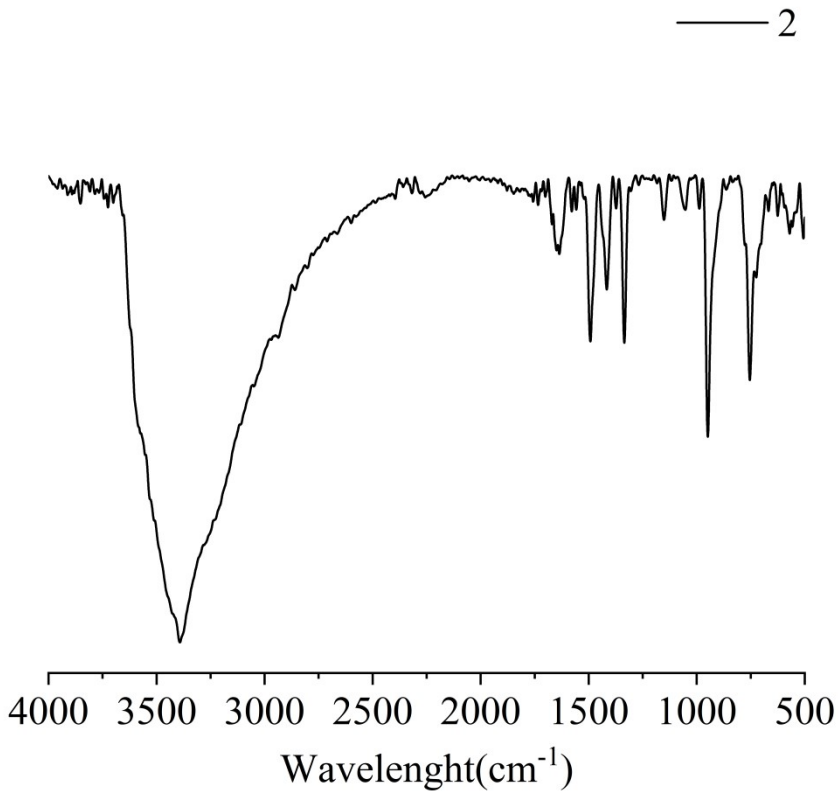

Fig. S10. IR spectrum of compound **2**.

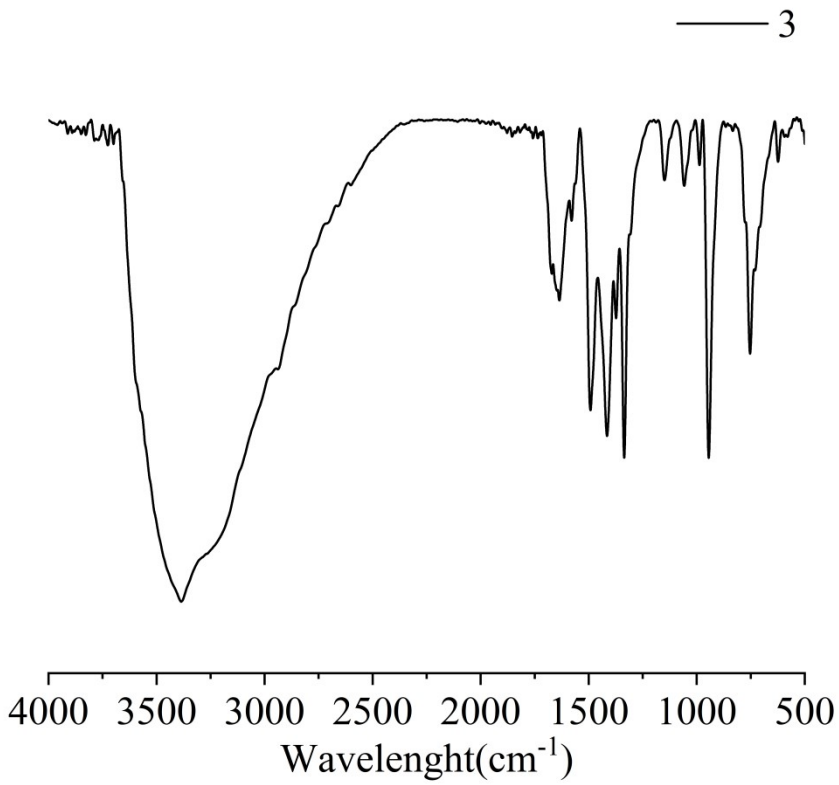

Fig. S11. IR spectrum of compound **3**.

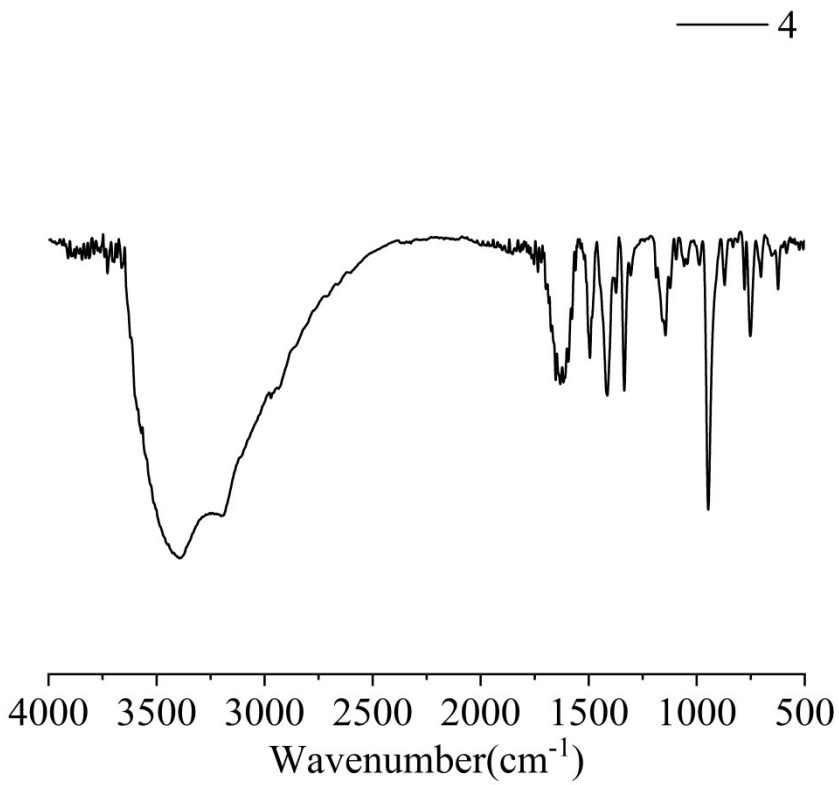

Fig. S12. IR spectrum of compound **4**.

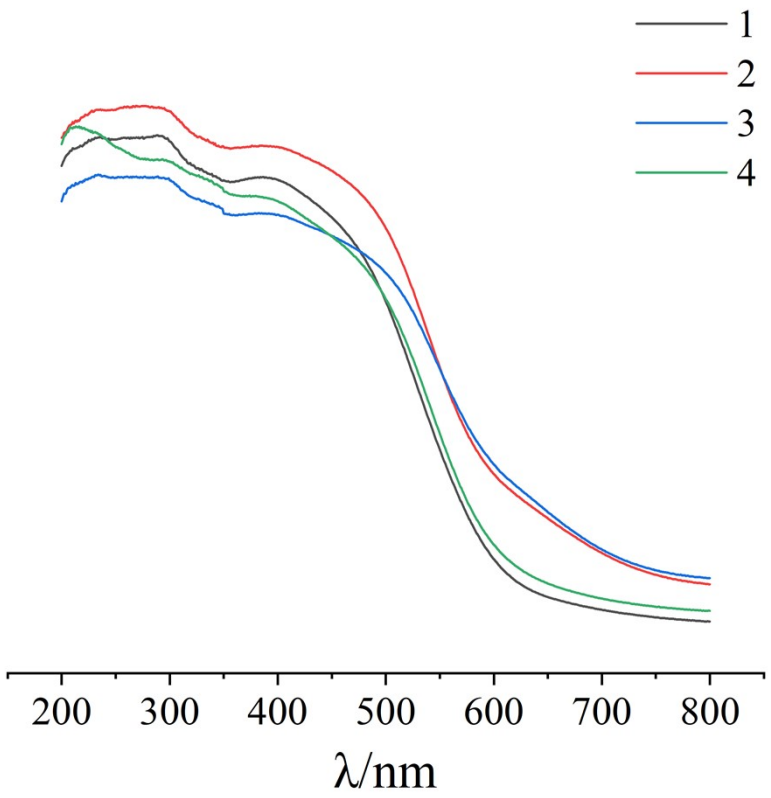

Fig. S13 Solid-state UV-vis spectra of compounds **1** – **4**, respectively. Color codes: black for **1**, red for **2**, blue for **3** and green for **4**.

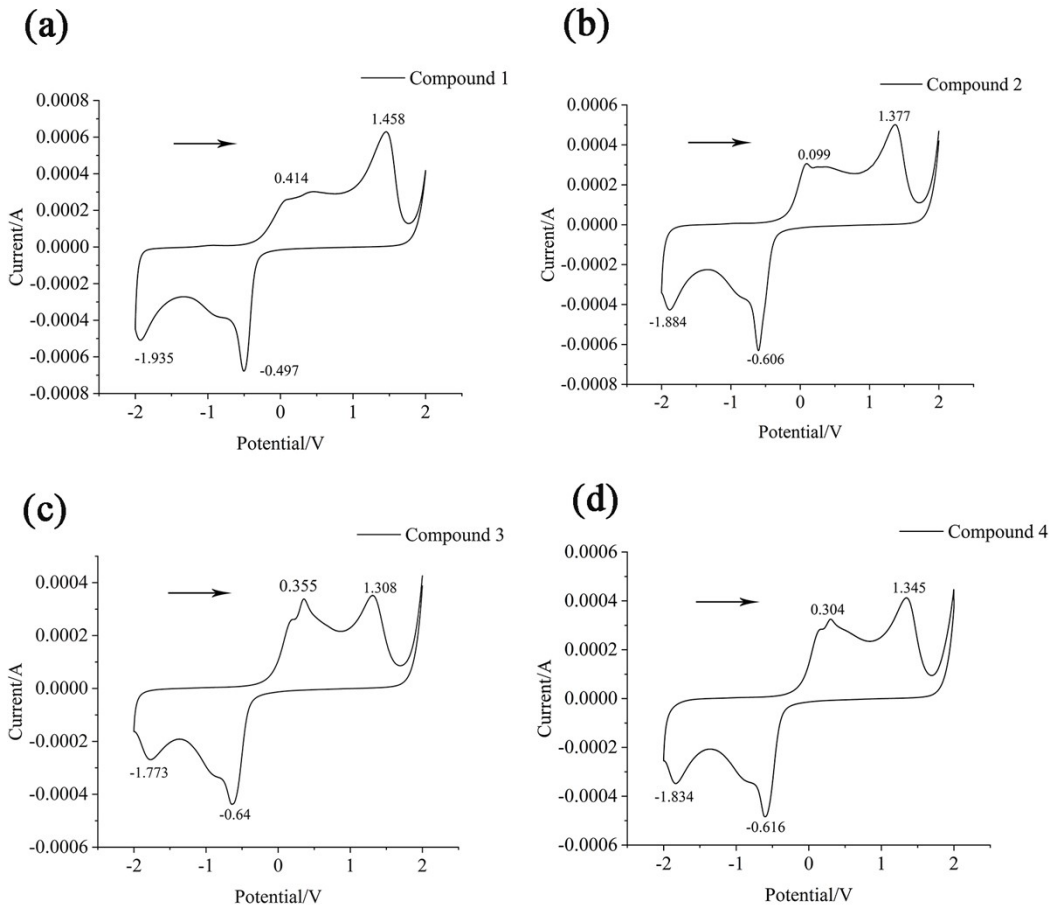

Fig. S14 Cyclic voltammograms for **1** – **4**.

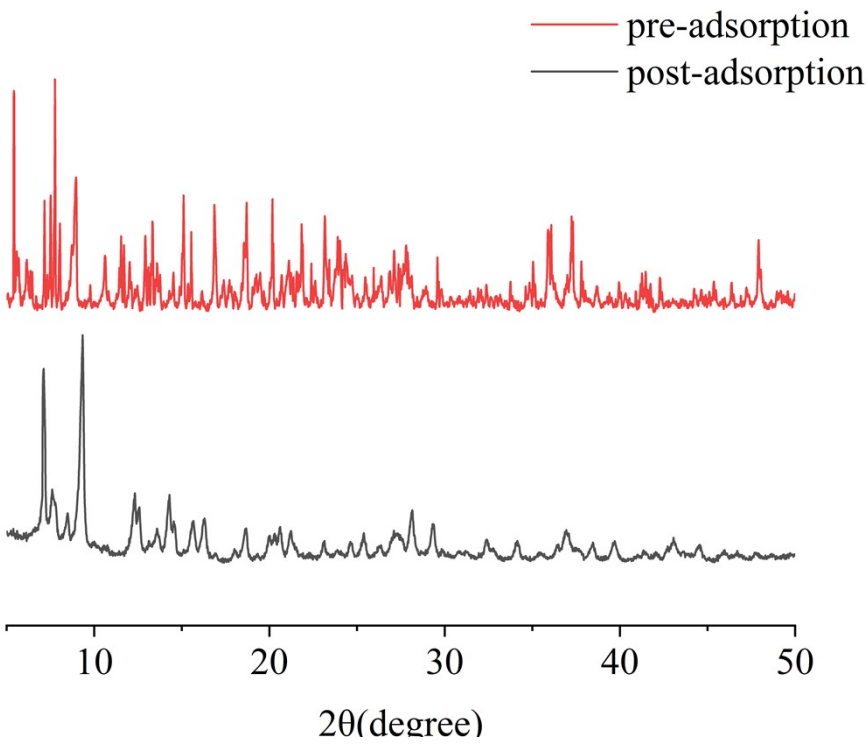

Fig. S15. Powder XRD comparison of crystal 1 pre- and post- adsorption.

Table S1. Crystallographic data and structural refinements for complexes $(NH_4)_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 62.5H_2O$ (**1**), $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 2(Hdmtrz)\cdot 27H_2O$ (**2**) and $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 20.5H_2O$ (**3**) and $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 25H_2O$ (**4**), respectively.

Identification codes	**1**	**2**	**3**	**4**
Empirical formula	$C_{32}H_{52}Mo_8N_{24}O_{20}$	$C_{40}H_{95}Li_4Mo_8N_{30}O_{34.5}$	$C_{40}H_{93}Li_4Mo_8N_{30}O_{35}$	$C_{32}H_{126}Li_4Mo_8N_{24}O_{57}$
Formula weight	1860.49	2343.73	2349.72	2554.84
Temperature/K	100(1)	100(1)	100(1)	100(1)
Crystal system	tetragonal	triclinic	triclinic	monoclinic
Space group	*C2/*m	$P\bar{1}$	$P\bar{1}$	*C2/c*
a/Å	29.8259(3)	13.3591(3)	13.3561(3)	23.6874(2)
b/Å	46.5268(6)	14.9668(4)	14.9592(4)	19.5226(2)
c/Å	24.3732(3)	15.2348(6)	27.3998(7)	23.3310(2)
α/°	90	90.435(3)	81.012(2)	90
β/°	94.152(1)	96.397(1)	89.971(2)	106.7668(9)
γ/°	90	107.431(2)	72.593(2)	90
Volume/Å^3	33734.0(7)	2577.61(5)	5153.3(2)	3486.7(5)
Z	10	1	2	4
ρ_{calc}g/cm^3	0.916	1.510	1.514	1.643
μ/mm^{-1}	6.223	8.386	8.395	8.567
F(000)	9080.0	1169.0	2342.0	5160.0
Crystal size/mm^3	0.15 × 0.15 × 0.10	0.15 × 0.10 × 0.1	0.20 × 0.10 × 0.10	0.10 × 0.10 × 0.10
Radiation (Å)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2θ range for data collection/°	5.216 to 130.178	6.272 to 133.17	6.276 to 133.834	6.514 to 151.994

Index ranges	$-39 \le h \le 29$, $-50 \le k \le 54$, $-28 \le l \le 20$	$-14 \le h \le 15$ $-17 \le k \le 17$, $-18 \le l \le 18$	$-10 \le h \le 15$, $-16 \le k \le 17$, $-32 \le l \le 30$	$-29 \le h \le 21$, $-19 \le k \le 24$, $-28 \le l \le 26$
Reflections collected	62493	17187	34844	19901
Independent reflections	28854 (R_{int} = 0.0471, R_σ = 0.0575)	9096 (R_{int} = 0.0341, R_σ = 0.0469)	17853 (R_{int} = 0.0262, R_σ = 0.0343)	10176 (R_{int} = 0.0238, R_σ = 0.0326)
Data/restraints/parameters	28854/0/969	9096/72/603	17853/4/1099	10176/31/463
Goodness–of–fit on F^2	1.025	1.058	1.045	1.042
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0597, wR_2 = 0.1441	R_1 = 0.0362 wR_2 = 0.09097	R_1 = 0.0314, wR_2 = 0.0848	R_1 = 0.0366, wR_2 = 0.1061
Final R indexes [all data]	R_1 = 0.0905, wR_2 = 0.1660	R_1 = 0.0416, wR_2 = 0.1013	R_1 = 0.0383, wR_2 = 0.0895	R_1 = 0.0424, wR_2 = 0.1117
Largest diff. peak/hole/e·Å^{-3}	0.75/-0.64	1.26/-1.11	1.04/-1.06	1.02/-0.68

Table S2. Selected bond distances (ÅÅ) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 62.5H_2O$ (**1**).

Atom–Atom	Lengths/Å	Atom–Atom	Lengths/Å
Mo1–Mo2	2.555(1)	Mo6–O13	1.967(5)
Mo1–O2	2.149(6)	Mo6–O14	1.960(5)
Mo1–O4	1.931(6)	Mo6–O15	1.681(5)
Mo1–O3	1.946(6)	Mo6–O16	2.206(4)
Mo1–O1	1.688(6)	Mo6–N23	2.183(6)
Mo1–N12[4]	2.204(7)	Mo6–N20	2.194(6)
Mo1–N3	2.228(8)	Mo7–Mo8	2.5503(8)
Mo2–O6	2.167(5)	Mo7–O18	1.946(5)
Mo2–O4	1.932(6)	Mo7–O17	1.949(5)
Mo2–O3	1.923(7)	Mo7–O19	1.708(5)
Mo2–O5	1.675(7)	Mo7–O16	2.157(5)
Mo2–N8	2.208(9)	Mo7–N24	2.223(6)
Mo2–N5	2.172(8)	Mo7–N21	2.183(7)
Mo3–O6	2.174(5)	Mo8–O11[1]	2.175(5)
Mo3–O8	1.938(6)	Mo8–O18	1.943(4)
Mo3–O9	1.936(7)	Mo8–O17	1.939(5)
Mo3–O7	1.686(6)	Mo8–O20	1.682(5)
Mo3–N9	2.198(9)	Mo8–N17[1]	2.210(5)
Mo3–N6	2.204(8)	Mo8–N14[1]	2.192(7)
Mo4–Mo3	2.546(1)	Mo9–Mo92	2.559(1)
Mo4–O2[4]	2.181(5)	Mo9–O23	2.208(5)
Mo4–O8	1.935(6)	Mo9–O22	1.943(5)
Mo4–O9	1.937(6)	Mo9–O222	1.950(6)
Mo4–O10	1.689(5)	Mo9–O21	1.642(5)
Mo4–N11	2.202(7)	Mo9–N30	2.217(6)
Mo4–N2[4]	2.212(9)	Mo9–N26	2.179(8)
Mo5–O11	2.165(4)	Mo10–Mo10[3]	2.551(1)
Mo5–O13	1.945(5)	Mo10–O24	1.929(6)
Mo5–O14	1.936(5)	Mo10–O23	2.163(5)
Mo5–O12	1.698(5)	Mo10–O26	1.931(7)
Mo5–N18	2.189(6)	Mo10–O25	1.690(6)
Mo5–N15	2.207(7)	Mo10–N29	2.183(7)
Mo6–Mo5	2.5542(8)	Mo10–N27	2.185(7)

Symmetry codes: [1] 3/2 – *x*, 1/2 – *y*, 2 – *z*; [2] 1 – *x*, *y*, 2 – *z*; [3] *x*,1 – *y*, - *y*; [4] 1 – *x*, *y*, 1 – *z*

Table S3. Selected bond angles (°) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(\text{-}dmtrz)_8]\cdot 62.5H_2O$ (**1**).

Atom–Atom	Angles/	Atom–Atom	Angles/
O13–Mo6–Mo5	48.9(1)	O25–Mo10–O26	107.1(3)
O13–Mo6–O16	89.1(2)	O25–Mo10–N29	89.0(3)
O13–Mo6–N23	165.6(2)	O25–Mo10–N27	87.8(3)
O13–Mo6–N20	84.7(2)	N29–Mo10–Mo103	134.1(2)
O14–Mo6–Mo5	48.6(2)	N29–Mo10–N27	90.5(3)
O14–Mo6–O13	93.4(2)	N27–Mo10–Mo103	134.8(2)
O14–Mo6–O16	88.6(2)	Mo10–O24–Mo103	82.8(3)
O14–Mo6–N23	86.1(2)	Mo10–O23–Mo9	118.4(2)
O14–Mo6–N20	165.1(2)	Mo9–O22–Mo92	82.2(2)
O15–Mo6–Mo5	97.74(2)	Mo103–O26–Mo10	82.7(4)
O15–Mo6–O13	105.7(2)	N29–N30–Mo9	121.3(5)
O15–Mo6–O14	106.4(2)	C38–N30–Mo9	130.6(5)
O15–Mo6–O16	157.9(2)	C38–N30–N29	108.0(6)
O15–Mo6–N23	88.2(2)	N27–N26–Mo9	122.3(6)
O15–Mo6–N20	88.4(2)	C34–N26–Mo9	133.0(6)
O16–Mo6–Mo5	104.3(1)	C34–N26–N27	104.6(8)
N23–Mo6–Mo5	134.2(1)	N30–N29–Mo10	123.6(5)
N23–Mo6–O16	76.5(2)	C39–N29–Mo10	132.1(6)
N23–Mo6–N20	92.1(2)	C39–N29–N30	104.3(7)
N20–Mo6–Mo5	133.22(2)	N26–N27–Mo10	123.1(6)
N20–Mo6–O16	76.5(2)	C35–N27–Mo10	131.1(7)
O18–Mo7–Mo8	48.9(1)	C35–N27–N26	105.8(7)
O18–Mo7–O17	93.2(2)	C39–N28–C38	103.8(7)
O18–Mo7–O16	87.72(2)	C34–N25–C35	103.0(9)
O18–Mo7–N24	86.0(2)	N29–C39–C40	123.1(9)
O18–Mo7–N21	164.7(2)	N28–C39–N29	112.5(7)
O17–Mo7–Mo8	48.82(2)	N28–C39–C40	124.4(8)
O17–Mo7–O16	89.3(2)	N30–C38–N28	111.5(7)
O17–Mo7–N24	166.9(2)	N30–C38–C37	124.8(7)
O17–Mo7–N21	84.8(2)	N28–C38–C37	123.7(8)
O19–Mo7–Mo8	98.12(2)	N26–C34–C33	121.3(1)
O19–Mo7–O18	106.8(2)	N25–C34–N26	112.7(8)
O19–Mo7–O17	107.0(2)	N25–C34–C33	126.0(1)
O19–Mo7–O16	157.12(2)	N27–C35–N25	113.8(1)
O19–Mo7–N24	85.8(2)	N27–C35–C36	126.0(1)
O19–Mo7–N21	88.2(3)	N25–C35–C36	120.2(1)
O16–Mo7–Mo8	104.72(1)	O24–Mo4–Mo3	105.4(1)
O16–Mo7–N24	77.5(2)	O24–Mo4–N11	75.3(2)
O16–Mo7–N21	77.1(2)	O24–Mo4–N24	76.4(3)
N24–Mo7–Mo8	134.1(2)	O8–Mo4–Mo3	48.9(2)
N21–Mo7–Mo8	133.2(2)	O8–Mo4–O24	89.1(2)

N21–Mo7–N24	92.4(2)	O8–Mo4–O9	93.2(3)
O11–Mo5–Mo6	104.41(1)	O8–Mo4–N11	86.3(3)
O11–Mo5–N18	76.2(2)	O8–Mo4–N24	165.4(3)
O11–Mo5–N15	76.9(2)	O9–Mo4–Mo3	48.9(2)
O13–Mo5–Mo6	49.6(2)	O9–Mo4–O24	88.7(2)
O13–Mo5–O11	89.1(2)	O9–Mo4–N11	164.0(2)
O13–Mo5–N18	165.2(2)	O9–Mo4–N24	86.3(3)
O13–Mo5–N15	85.5(2)	O10–Mo4–Mo3	96.4(2)
O14–Mo5–Mo6	49.4(1)	O10–Mo4–O24	158.2(3)
O14–Mo5–O11	88.3(2)	O10–Mo4–O8	105.7(3)
O14–Mo5–O13	94.9(2)	O10–Mo4–O9	106.0(3)
O14–Mo5–N18	85.7(2)	O10–Mo4–N11	89.4(3)
O14–Mo5–N15	165.2(2)	O10–Mo4–N24	88.4(3)
O12–Mo5–Mo6	98.2(2)	N11–Mo4–Mo3	134.8(2)
O12–Mo5–O11	157.3(2)	N11–Mo4–N24	90.2(3)
O12–Mo5–O13	106.3(2)	N24–Mo4–Mo3	134.5(2)
O12–Mo5–O14	106.5(2)	O2–Mo1–Mo2	103.7(1)
O12–Mo5–N18	87.6(2)	O2–Mo1–N124	75.5(2)
O12–Mo5–N15	87.6(2)	O2–Mo1–N3	77.6(3)
N18–Mo5–Mo6	134.7(2)	O4–Mo1–Mo2	48.6(2)
N18–Mo5–N15	90.2(2)	O4–Mo1–O2	89.1(2)
N15–Mo5–Mo6	134.6(2)	O4–Mo1–O3	93.3(3)
O111–Mo8–Mo7	103.9(1)	O4–Mo1–N124	86.4(2)
O111–Mo8–N171	75.7(2)	O4–Mo1–N3	166.6(3)
O111–Mo8–N141	76.8(2)	O3–Mo1–Mo2	48.3(2)
O18–Mo8–Mo7	49.1(2)	O3–Mo1–O2	89.2(2)
O18–Mo8–O111	88.6(2)	O3–Mo1–N124	164.7(3)
O18–Mo8–N171	164.4(2)	O3–Mo1–N3	87.7(3)
O18–Mo8–N141	85.3(2)	O1–Mo1–Mo2	98.8(2)
O17–Mo8–Mo7	49.2(1)	O1–Mo1–O2	157.4(2)
O17–Mo8–O111	87.2(1)	O1–Mo1–O4	106.8(3)
O17–Mo8–O18	93.6(2)	O1–Mo1–O3	105.5(3)
O17–Mo8–N171	85.1(2)	O1–Mo1–N124	89.2(3)
O17–Mo8–N141	164.0(2)	O1–Mo1–N3	85.8(3)
O20–Mo8–Mo7	97.52(2)	N124–Mo1–Mo2	134.8(2)
O20–Mo8–O111	158.6(2)	N124–Mo1–N3	89.2(3)
O20–Mo8–O18	106.0(2)	N3–Mo1–Mo2	135.5(2)
O20–Mo8–O17	107.0(2)	O6–Mo2–Mo1	104.3(2)
O20–Mo8–N171	89.2(2)	O6–Mo2–N8	76.1(3)
O20–Mo8–N141	88.6(3)	O6–Mo2–N5	76.8(3)
N171–Mo8–Mo7	133.8(2)	O4–Mo2–Mo1	48.6(2)

N141–Mo8–Mo7	134.1(2)	O4–Mo2–O6	88.4(2)
N141–Mo8–N171	91.6(2)	O4–Mo2–N8	85.9(3)
Mo5–O11–Mo81	119.3(2)	O4–Mo2–N5	165.0(3)
Mo5–O13–Mo6	81.5(2)	O3–Mo2–Mo1	49.1(2)
Mo5–O14–Mo6	81.9(2)	O3–Mo2–O6	90.1(2)
Mo8–O18–Mo7	81.92(2)	O3–Mo2–O4	94.0(2)
Mo8–O17–Mo7	82.0(2)	O3–Mo2–N8	166.3(3)
Mo7–O16–Mo6	118.1(2)	O3–Mo2–N5	84.0(3)
N23–N24–Mo7	120.2(5)	O5–Mo2–Mo1	98.7(2)
C27–N24–Mo7	131.7(5)	O5–Mo2–O6	157.1(3)
C27–N24–N23	107.9(6)	O5–Mo2–O4	106.6(3)
N18–N17–Mo81	121.8(4)	O5–Mo2–O3	105.5(3)
C22–N17–Mo81	131.7(5)	O5–Mo2–N8	87.6(3)
C22–N17–N18	106.5(6)	O5–Mo2–N5	88.1(3)
N24–N23–Mo6	123.5(5)	N8–Mo2–Mo1	134.0(2)
C26–N23–Mo6	133.6(5)	N5–Mo2–Mo1	132.8(2)
C26–N23–N24	102.9(6)	N5–Mo2–N8	92.6(3)
N15–N14–Mo81	122.3(5)	O6–Mo3–Mo4	105.4(2)
C18–N14–Mo81	132.9(6)	O6–Mo3–N9	76.9(2)
C18–N14–N15	104.8(7)	O6–Mo3–N6	76.7(3)
N17–N18–Mo5	122.8(4)	O8–Mo3–Mo4	48.8(2)
C23–N18–Mo5	131.5(5)	O8–Mo3–O6	87.9(2)
C23–N18–N17	105.6(6)	O8–Mo3–N9	85.4(3)
C22–N16–C23	104.5(6)	O8–Mo3–N6	164.6(3)
N21–N20–Mo6	122.4(5)	O9–Mo3–Mo4	48.9(2)
C30–N20–Mo6	130.6(5)	O9–Mo3–O6	89.9(2)
C30–N20–N21	106.7(6)	O9–Mo3–O8	93.1(3)
N14–N15–Mo5	122.8(5)	O9–Mo3–N9	166.7(2)
C19–N15–Mo5	131.0(6)	O9–Mo3–N6	85.3(3)
C19–N15–N14	106.2(7)	O7–Mo3–Mo4	97.4(3)
C26–N22–C27	103.5(6)	O7–Mo3–O6	157.2(3)
N20–N21–Mo7	122.1(5)	O7–Mo3–O8	107.4(3)
C31–N21–Mo7	131.4(6)	O7–Mo3–O9	105.6(3)
C31–N21–N20	106.2(7)	O7–Mo3–N9	87.4(3)
C30–N19–C31	106.2(7)	O7–Mo3–N6	87.8(3)
C19–N13–C18	104.9(9)	N9–Mo3–Mo4	133.4(2)
N23–C26–C25	120.6(7)	N9–Mo3–N6	92.6(3)
N22–C26–N23	113.6(6)	N6–Mo3–Mo4	133.7(3)
N22–C26–C25	125.7(7)	Mo1–O2–Mo44	120.1(2)
N18–C23–N16	111.6(6)	Mo2–O6–Mo3	118.6(3)
N18–C23–C24	124.7(8)	Mo1–O4–Mo2	82.8(2)
N16–C23–C24	123.7(7)	Mo4–O8–Mo3	82.2(3)
N17–C22–N16	111.9(7)	Mo3–O9–Mo4	82.2(3)
N17–C22–C21	123.6(7)	Mo2–O3–Mo1	82.6(3)

N16–C22–C21	124.4(7)	N12–N11–Mo4	122.8(5)
N24–C27–N22	112.0(7)	C14–N11–Mo4	130.4(6)
N24–C27–C28	125.0(7)	C14–N11–N12	106.7(7)
N22–C27–C28	123.0(7)	C14–N10–C15	103.7(7)
N14–C18–N13	112.6(9)	N11–N12–Mo14	123.4(5)
N14–C18–C17	122.8(1)	C15–N12–Mo14	129.1(6)
N13–C18–C17	124.6(1)	C15–N12–N11	107.3(7)
N20–C30–N19	110.3(8)	N3–N2–Mo44	123.3(6)
N20–C30–C29	124.2(7)	C2–N2–Mo44	129.8(9)
N19–C30–C29	125.5(8)	C2–N2–N3	106.9(1)
N21–C31–N19	110.6(7)	N2–N3–Mo1	121.2(6)
N21–C31–C32	125.9(9)	C3–N3–Mo1	131.7(1)
N19–C31–C32	123.4(8)	C3–N3–N2	107.1(1)
N15–C19–C20	124.0(1)	N8–N9–Mo3	121.1(7)
N13–C19–N15	111.6(8)	C11–N9–Mo3	131.7(7)
N13–C19–C20	124.4(1)	C11–N9–N8	106.8(9)
O23–Mo9–Mo92	105.3(1)	N9–N8–Mo2	122.7(7)
O23–Mo9–N30	76.9(2)	C10–N8–Mo2	133.2(7)
O22–Mo9–Mo92	49.0(2)	C10–N8–N9	103.7(8)
O222–Mo9–Mo92	48.8(2)	C10–N7–C11	106.3(10)
O222–Mo9–O23	89.6(2)	N6–N5–Mo2	123.1(6)
O22–Mo9–O23	88.7(2)	C6–N5–Mo2	132.0(7)
O22–Mo9–O222	93.5(3)	C6–N5–N6	104.8(8)
O222–Mo9–N30	87.2(2)	N5–N6–Mo3	121.4(6)
O22–Mo9–N30	165.6(2)	C7–N6–Mo3	129.2(8)
O222–Mo9–N26	166.3(2)	C7–N6–N5	109.0(9)
O22–Mo9–N26	86.3(2)	C2–N1–C3	102.7(1)
O21–Mo9–Mo92	95.8(2)	C6–N4–C7	105.0(1)
O21–Mo9–O23	158.9(2)	N11–C14–N10	112.1(8)
O21–Mo9–O222	104.9(3)	N11–C14–C13	126.3(9)
O21–Mo9–O22	105.3(2)	N10–C14–C13	121.5(8)
O21–Mo9–N30	88.4(2)	N10–C15–C16	125.4(9)
O21–Mo9–N26	88.3(3)	N12–C15–N10	110.2(8)
N30–Mo9–Mo92	135.42(2)	N12–C15–C16	124.4(9)
N26–Mo9–Mo92	134.72(2)	N8–C10–C9	121.5(1)
N26–Mo9–O23	76.7(2)	N7–C10–N8	111.9(9)
N26–Mo9–N30	89.6(2)	N7–C10–C9	126.6(1)
O24–Mo10–Mo103	48.6(2)	N2–C2–N1	111.7(1)
O24–Mo10–O23	87.5(3)	N2–C2–C1	126.5(1)
O24–Mo10–O26	92.9(3)	N1–C2–C1	121.8(1)
O24–Mo10–N29	164.6(3)	N9–C11–N7	111.2(1)
O24–Mo10–N27	86.6(3)	N9–C11–C12	124.2(1)
O23–Mo10–Mo103	103.1(1)	N7–C11–C12	124.6(1)

O23–Mo10–N29	77.1(2)	N3–C3–N1	111.7(1)
O23–Mo10–N27	76.3(3)	N3–C3–C4	125.2(1)
O26–Mo10–Mo103	48.6(2)	N1–C3–C4	123.0(1)
O26–Mo10–O23	88.2(3)	N6–C7–N4	110.3(11)
O26–Mo10–N29	85.8(3)	N6–C7–C8	125.6(1)
O26–Mo10–N27	164.5(3)	N4–C7–C8	123.2(1)
O25–Mo10–Mo103	98.2(2)	N5–C6–C5	123.4(1)
O25–Mo10–O24	106.1(3)	N4–C6–N5	110.8(1)
O25–Mo10–O23	158.7(2)	N4–C6–C5	125.6(1)

Table S4. Selected hydrogen bond distances (Å) and angles (°) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 62.5H_2O$ (**1**).

	D–H···A	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(°)
Intra	O2–H2···N2	0.88	1.86	2.716(8)	157
Intra	O2–H2···N3	0.88	1.96	2.743(8)	147
Intra	O6–H6···N5	0.88	1.91	2.695(8)	148
Intra	O6–H6···N6	0.88	1.91	2.717(6)	145
Intra	O11–H11···N14	0.88	1.86	2.713(6)	146
Intra	O11–H11···N15	0.88	1.91	2.718(2)	162
Intra	O16–H16···N20	0.88	2.09	2.725(9)	126
Intra	O16–H16···N21	0.88	2.14	2.706(6)	122
Intra	O23–H23···N29	0.85	1.88	2.709(6)	146
Intra	O23–H23···N30	0.85	1.86	2.752(6)	156

Table S5 Selected bond distances (Å) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 2(Hdmtrz)\cdot 27H_2O$ (**2**).

Atom-Atom	**Lengths/Å**	**Atom-Atom**	**Lengths/Å**
Mo01–Mo03	2.556(4)	Mo02–N5	2.200(3)
Mo01–O1	1.946(3)	Mo03–O1	1.947(3)
Mo01–O4	1.701(3)	Mo03–O3	2.181(3)
Mo01–O5	1.949(3)	Mo03–O5	1.937(3)
Mo01–O7[1]	2.189(3)	Mo03–O11	1.696(3)
Mo01–N1[1]	2.203(3)	Mo03–N2	2.196(3)
Mo01–N6	2.193(3)	Mo03–N8	2.212(3)
Mo02–Mo04	2.554(5)	Mo04–O2	1.942(3)
Mo02–O2	1.945(3)	Mo04–O3	2.172(3)
Mo02–O6	1.943(3)	Mo04–O6	1.944(3)
Mo02–O7	2.182(3)	Mo04–O9	1.702(3)
Mo02–O10	1.702(3)	Mo04–N4	2.209(3)
Mo02–N16[1]	2.192(3)	Mo04–N3	2.204(3)

Symmetry codes:[1] $1-x, 1-y, 1-z$

Table S6. Selected bond angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 2(Hdmtrz)\cdot 27H_2O$ (**2**).

Atom-Atom	Angles/°	Atom-Atom	Angles/°
O1–Mo01–Mo03	49.0(7)	Mo04–O3–Mo03	119.5(1)
O1–Mo01–O5	93.5(1)	Mo03–O5–Mo01	82.2(1)
O1–Mo01–O7[1]	86.9(1)	Mo02–O6–Mo04	82.1(1)
O1–Mo01–N1[1]	83.9(1)	Mo02–O7–Mo011	118.6(1)
O1–Mo01–N6	161.8(1)	N5–N1–Mo01[1]	122.5(2)
O4–Mo01–Mo03	98.6(1)	C010–N1–Mo01[1]	129.4(3)
O4–Mo01–O1	106.9(1)	C010–N1–N5	106.0(3)
O4–Mo01–O5	106.2(1)	N4–N2–Mo03	122.8(2)
O4–Mo01–O7[1]	158.0(1)	C00Z–N2–Mo03	131.2(3)
O4–Mo01–N1[1]	87.8(1)	C00Z–N2–N4	106.0(3)
O4–Mo01–N6	90.5(1)	N6–N16–Mo02[1]	123.1(2)
O5–Mo01–Mo03	48.6(8)	C016–N16–Mo02[1]	129.8(3)
O5–Mo01–O7[1]	89.4(1)	C016–N16–N6	106.4(3)
O5–Mo01–N1[1]	165.8(1)	N2–N4–Mo04	122.8(2)
O5–Mo01–N6	85.9(1)	C015–N4–Mo04	131.1(3)
O7[1]–Mo01–Mo03	103.3(7)	C015–N4–N2	106.1(3)
O7[1]–Mo01–N11	76.4(1)	N1–N5–Mo02	122.4(2)
O7[1]–Mo01–N6	74.9(1)	C014–N5–Mo02	131.5(3)
N1[1]–Mo01–Mo03	132.5(9)	C014–N5–N1	106.1(3)
N6–Mo01–Mo03	134.5(9)	N16–N6–Mo01	122.4(3)
N6–Mo01–N1[1]	92.1(1)	C018–N6–Mo01	131.7(3)
O2–Mo02–Mo04	48.87(8)	C018–N6–N16	105.9(3)
O2–Mo02–O7	88.3(1)	N8–N3–Mo04	123.0(3)
O2–Mo02–N16[1]	83.5(1)	C011–N3–Mo04	130.8(3)
O2–Mo02–N5	163.3(1)	C011–N3–N8	106.0(3)
O6–Mo02–Mo04	48.9(8)	N3–N8–Mo03	122.4(2)
O6–Mo02–O2	92.9(1)	C013–N8–Mo03	130.5(3)
O6–Mo02–O7	88.8(1)	C013–N8–N3	106.6(3)
O6–Mo02–N16[1]	164.4(1)	C014–N10–C010	103.3(3)
O6–Mo02–N5	86.1(1)	C00Z–N11–C015	103.2(4)
O7–Mo02–Mo04	105.3(8)	C016–N12–C018	103.8(4)
O7–Mo02–N16[1]	75.9(1)	C011–N13–C013	104.5(4)
O7–Mo02–N5	75.0(1)	N2–C00Z–N11	112.1(4)
O10–Mo02–Mo04	97.7(1)	N2–C00Z–C019	124.2(4)
O10–Mo02–O2	107.0(1)	N11–C00Z–C019	123.7(4)
O10–Mo02–O6	106.9(1)	N1–C010–N10	112.2(4)
O10–Mo02–O7	156.9(1)	N1–C010–C017	124.8(4)
O10–Mo02–N16[1]	88.5(1)	N10–C010–C017	123.0(4)
O10–Mo02–N5	89.0(1)	N3–C011–N13	111.6(4)
N16[1]–Mo02–Mo04	131.9(9)	N3–C011–C01F	124.6(4)
N16[1]–Mo02–N5	92.8(1)	N13–C011–C01F	123.8(4)
N5–Mo02–Mo04	134.6(1)	N8–C013–N13	111.3(4)

O1–Mo03–Mo01	48.9(8)	N8–C013–C01G	124.1(4)
O1–Mo03–O3	89.8(1)	N13–C013–C01G	124.6(4)
O1–Mo03–N2	166.2(1)	N5–C014–N10	112.4(4)
O1–Mo03–N8	85.5(12)	N5–C014–C01H	124.5(4)
O3–Mo03–Mo01	104.3(7)	N10–C014–C01H	123.0(4)
O3–Mo03–N2	76.4(1)	N4–C015–N11	112.6(4)
O3–Mo03–N8	75.9(1)	N4–C015–C01L	124.1(4)
O5–Mo03–Mo01	49.1(8)	N11–C015–C01L	123.3(4)
O5–Mo03–O1	93.9(1)	N16–C016–N12	112.0(4)
O5–Mo03–O3	87.8(1)	N16–C016–C01A	124.2(4)
O5–Mo03–N2	86.4(1)	N12–C016–C01A	123.8(4)
O5–Mo03–N8	163.6(1)	N6–C018–N12	111.8(4)
O11–Mo03–Mo01	98.6(9)	N6–C018–C01E	123.5(4)
O11–Mo03–O1	105.6(1)	N12–C018–C01E	124.6(4)
O11–Mo03–O3	157.1(1)	Li21–O16–Li1W	129.0(5)
O11–Mo03–O5	107.5(1)	O15–Li1W–O16	79.7(4)
O11–Mo03–N2	87.3(1)	O15–Li1W–O17	136.9(5)
O11–Mo03–N8	88.3(1)	O15–Li1W–O22	82.1(4)
N2–Mo03–Mo01	134.9(9)	O15–Li1W–O23	93.7(7)
N2–Mo03–N8	90.4(1)	O15–Li1W–O20	74.7(3)
N8–Mo03–Mo01	134.1(9)	O16–Li1W–O20	136.1(3)
O2–Mo04–Mo02	48.9(8)	O17–Li1W–O16	141.0(4)
O2–Mo04–O3	90.4(1)	O17–Li1W–O20	77.5(3)
O2–Mo04–O6	93.0(1)	O8–Li21–O13	96.6(5)
O2–Mo04–N4	166.5(1)	O8–Li21–O18	98.2(4)
O2–Mo04–N3	85.1(1)	O12–Li21–O8	123.3(5)
O3–Mo04–Mo02	105.1(8)	O12–Li21–O13	106.2(5)
O3–Mo04–N4	76.1(1)	O12–Li21–O18	105.7(5)
O3–Mo04–N3	75.7(1)	O13–Li21–O18	128.8(5)
O6–Mo04–Mo02	48.9(8)	O16–Li21–O8	124.5(5)
O6–Mo04–O3	86.4(1)	O16–Li21–O12	99.2(5)
O6–Mo04–N4	86.9(1)	O19–Li21–O8	112.3(6)
O6–Mo04–N3	162.1(1)	O19–Li21–O12	110.1(5)
O9–Mo04–Mo02	97.1(1)	O19–Li21–O16	78.6(5)
O9–Mo04–O2	105.6(1)	C01D–N9–N15	109.2(4)
O9–Mo04–O3	157.7(1)	C01D–N14–C01C	103.0(4)
O9–Mo04–O6	107.6(1)	C01C–N15–N9	103.6(4)
O9–Mo04–N4	87.2(1)	N14–C01C–C01P	122.5(4)
O9–Mo04–N3	90.0(1)	N15–C01C–N14	113.9(4)
N4–Mo04–Mo02	134.9(9)	N15–C01C–C01P	123.5(5)
N3–Mo04–Mo02	133.8(9)	N9–C01D–N14	110.3(4)
N3–Mo04–N4	90.8(1)	N9–C01D–C01Y	123.5(5)
Mo01–O1–Mo03	82.1(1)	N14–C01D–C01Y	126.2(5)
Mo04–O2–Mo02	82.2(1)		

Symmetry codes: [1]1 – *x*, 1 – *y*, 1 – *z*

Table S7. Selected hydrogen bond distances (Å) and angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 2(Hdmtrz)\cdot 27H_2O$ (**2**).

	D–H···A	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(°)
Intra	O1–H1···O7	0.95	1.78	2.673(7)	155
Intra	O1A–H1A···O47	0.85	1.88	2.702(6)	161
Intra	O2–H2···N4	0.95	2.05	2.696(7)	124
Intra	O2–H2···N10	0.95	2.00	2.642(7)	123
Intra	O3–H3···N7	0.95	1.87	2.663(8)	140
Intra	O3–H3···N12	0.95	1.89	2.695(9)	141
Intra	O6–H6···O48	1.00	1.77	2.713(7)	156
Intra	O14–H14···O6	0.95	1.82	2.648(7)	144
	N23–H23B···O24	0.88	2.60	3.258(12)	132

Table S8. Selected bond distances (Å) and angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 20.5H_2O$ (**3**).

Atom – Atom	Lengths/Å	Atom – Atom	Lengths/Å
Mo1 – Mo8	2.555(3)	Mo5 – Mo4	2.5577(3)
Mo1 – O9	2.162(2)	Mo5 – O11	2.195(2)
Mo1 – O19	1.950(2)	Mo5 – O15	1.933(2)
Mo1 – O20	1.939(2)	Mo5 – O16	1.949(2)
Mo1 – O1	1.698(2)	Mo5 – O5	1.692(2)
Mo1 – N1	2.215(3)	Mo5 – N16	2.194(3)
Mo1 – N4	2.200(3)	Mo5 – N13	2.209(3)
Mo2 – Mo3	2.5582(3)	Mo6 – Mo7	2.5599(3)
Mo2 – O9	2.160(2)	Mo6 – O11	2.177(2)
Mo2 – O13	1.940(2)	Mo6 – O18	1.941(2)
Mo2 – O14	1.945(2)	Mo6 – O17	1.943(2)
Mo2 – O2	1.692(2)	Mo6 – O6	1.692(2)
Mo2 – N5	2.198(3)	Mo6 – N17	2.209(3)
Mo2 – N2	2.198(3)	Mo6 – N14	2.208(3)
Mo3 – O13	1.943(2)	Mo7 – O18	1.947(2)
Mo3 – O10	2.188(2)	Mo7 – O12	2.158(2)
Mo3 – O14	1.938(2)	Mo7 – O17	1.937(2)
Mo3 – O3	1.701(2)	Mo7 – O7	1.703(2)
Mo3 – N7	2.196(3)	Mo7 – N19	2.203(3)
Mo3 – N10	2.205(3)	Mo7 – N22	2.182(3)
Mo4 – O15	1.948(2)	Mo8 – O12	2.177(2)
Mo4 – O10	2.185(2)	Mo8 – O19	1.950(2)
Mo4 – O16	1.947(2)	Mo8 – O20	1.951(2)
Mo4 – O4	1.695(2)	Mo8 – O8	1.693(2)
Mo4 – N8	2.184(3)	Mo8 – N23	2.191(3)
Mo4 – N11	2.201(3)	Mo8 – N20	2.203(3)

Table S9. Selected bond angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 20.5H_2O$ (**3**)

Atom – Atom	Angles/	Atom – Atom	Angles/
O11 – Mo6 – Mo7	103.8(6)	Mo6 – O18 – Mo7	82.33(8)
O11 – Mo6 – N17	76.3(9)	Mo7 – O12 – Mo8	119.7(1)
O11 – Mo6 – N14	75.8(9)	Mo5 – O15 – Mo4	82.45(8)
O18 – Mo6 – Mo7	48.9(6)	Mo4 – O10 – Mo3	118.93(9)
O18 – Mo6 – O11	88.6(9)	Mo7 – O17 – Mo6	82.6(8)
O18 – Mo6 – O17	93.3(9)	Mo4 – O16 – Mo5	82.1(8)
O18 – Mo6 – N17	87.0(9)	Mo8 – O19 – Mo1	81.8(8)
O18 – Mo6 – N14	164.4(1)	Mo1 – O20 – Mo8	82.1(8)
O17 – Mo6 – Mo7	48.6(7)	Mo3 – O14 – Mo2	82.4(8)
O17 – Mo6 – O11	88.1(8)	Li1 – O3W – Li2	97.0(3)
O17 – Mo6 – N17	164.4(9)	Li1 – O4W – Li2	80.4(3)
O17 – Mo6 – N14	85.2(1)	N7 – N8 – Mo4	123.6(2)
O6 – Mo6 – Mo7	98.3(8)	C11 – N8 – Mo4	129.7(2)
O6 – Mo6 – O11	157.8(1)	C11 – N8 – N7	106.0(3)
O6 – Mo6 – O18	106.9(1)	N17 – N16 – Mo5	123.6(2)
O6 – Mo6 – O17	106.2(1)	C20 – N16 – Mo5	130.4(2)
O6 – Mo6 – N17	88.5(1)	C20 – N16 – N17	105.9(3)
O6 – Mo6 – N14	88.4(1)	N20 – N19 – Mo7	122.8(2)
N17 – Mo6 – Mo7	135.6(7)	C8 – N19 – Mo7	129.5(2)
N14 – Mo6 – Mo7	133.4(7)	C8 – N19 – N20	105.9(3)
N14 – Mo6 – N17	90.3(1)	N10 – N11 – Mo4	122.2(2)
O9 – Mo1 – Mo8	106.2(6)	C2 – N11 – Mo4	131.7(2)
O9 – Mo1 – N1	76.1(9)	C2 – N11 – N10	106.1(3)
O9 – Mo1 – N4	75.0(9)	N22 – N23 – Mo8	122.9(2)
O19 – Mo1 – Mo8	49.1(7)	C14 – N23 – Mo8	129.1(2)
O19 – Mo1 – O9	86.8(8)	C14 – N23 – N22	107.3(3)
O19 – Mo1 – N1	86.8(1)	N2 – N1 – Mo1	122.7(2)
O19 – Mo1 – N4	161.7(9)	C26 – N1 – Mo1	131.7(2)
O20 – Mo1 – Mo8	49.1(6)	C26 – N1 – N2	105.5(3)
O20 – Mo1 – O9	91.6(9)	N8 – N7 – Mo3	122.2(2)
O20 – Mo1 – O19	93.4(9)	C12 – N7 – Mo3	131.5(2)
O20 – Mo1 – N1	167.7(9)	C12 – N7 – N8	106.3(3)
O20 – Mo1 – N4	84.7(9)	N19 – N20 – Mo8	122.1(2)
O1 – Mo1 – Mo8	96.8(8)	C5 – N20 – Mo8	131.4(2)
O1 – Mo1 – O9	156.8(1)	C5 – N20 – N19	106.3(3)
O1 – Mo1 – O19	107.1(1)	N11 – N10 – Mo3	122.4(2)
O1 – Mo1 – O20	105.6(1)	C3 – N10 – Mo3	128.8(2)
O1 – Mo1 – N1	86.1(1)	C3 – N10 – N11	106.1(2)
O1 – Mo1 – N4	90.9(1)	N4 – N5 – Mo2	123.2(2)

N1 – Mo1 – Mo8	134.7(7)	C6 – N5 – Mo2	130.7(2)
N4 – Mo1 – Mo8	133.7(7)	C6 – N5 – N4	105.9(3)
N4 – Mo1 – N1	91.2(10)	N16 – N17 – Mo6	122.25(2)
O11 – Mo5 – Mo4	104.8(6)	C1 – N17 – Mo6	131.4(2)
O11 – Mo5 – N13	75.9(9)	C1 – N17 – N16	106.4(2)
O15 – Mo5 – Mo4	49.02(6)	C17 – N30 – C18	103.5(3)
O15 – Mo5 – O11	89.4(8)	N1 – N2 – Mo2	122.4(2)
O15 – Mo5 – O16	93.1(9)	C13 – N2 – Mo2	130.8(2)
O15 – Mo5 – N16	165.2(9)	C13 – N2 – N1	106.7(3)
O15 – Mo5 – N13	85.2(9)	N13 – N14 – Mo6	123.1(2)
O16 – Mo5 – Mo4	48.9(7)	C7 – N14 – Mo6	129.9(2)
O16 – Mo5 – O11	87.1(8)	C7 – N14 – N13	106.4(3)
O16 – Mo5 – N16	86.8(9)	N5 – N4 – Mo1	122.3(2)
O16 – Mo5 – N13	162.9(1)	C4 – N4 – Mo1	131.1(2)
O5 – Mo5 – Mo4	97.2(8)	C4 – N4 – N5	106.6(2)
O5 – Mo5 – O11	157.9(9)	C22 – N24 – C14	105.3(3)
O5 – Mo5 – O15	106.1(1)	N23 – N22 – Mo7	122.9(2)
O5 – Mo5 – O16	107.1(1)	N23 – N22 – C22	105.6(3)
O5 – Mo5 – N16	87.9(1)	C22 – N22 – Mo7	131.5(2)
O5 – Mo5 – N13	89.6(1)	N14 – N13 – Mo5	122.6(2)
N16 – Mo5 – Mo4	135.1(7)	C9 – N13 – Mo5	130.7(2)
N16 – Mo5 – O11	75.9(9)	C9 – N13 – N14	106.1(2)
N16 – Mo5 – N13	90.5(1)	C20 – N18 – C1	103.8(3)
N13 – Mo5 – Mo4	133.9(7)	C7 – N15 – C9	104.0(3)
O9 – Mo2 – Mo3	105.0(6)	C6 – N6 – C4	103.7(3)
O9 – Mo2 – N5	75.1(9)	C3 – N12 – C2	103.8(3)
O9 – Mo2 – N2	76.9(9)	C12 – N9 – C11	104.6(3)
O13 – Mo2 – Mo3	48.8(6)	C26 – N3 – C13	103.9(3)
O13 – Mo2 – O9	87.5(8)	C5 – N21 – C8	104.0(3)
O13 – Mo2 – O14	93.3(9)	C10 – N25 – N26	110.1(3)
O13 – Mo2 – N5	162.6(9)	C10 – N27 – C15	103.9(3)
O13 – Mo2 – N2	86.3(9)	C18 – N29 – N28	102.6(3)
O14 – Mo2 – Mo3	48.7(6)	C15 – N26 – N25	102.6(3)
O14 – Mo2 – O9	91.0(8)	C17 – N28 – N29	110.0(3)
O14 – Mo2 – N5	86.5(9)	N17 – C1 – N18	112.0(3)
O14 – Mo2 – N2	167.9(1)	N17 – C1 – C23	124.2(3)
O2 – Mo2 – Mo3	98.4(8)	N18 – C1 – C23	123.7(3)
O2 – Mo2 – O9	156.5(9)	N11 – C2 – N12	112.1(3)
O2 – Mo2 – O13	107.6(1)	N11 – C2 – C21	124.5(3)
O2 – Mo2 – O14	105.5(1)	N12 – C2 – C21	123.3(3)
O2 – Mo2 – N5	89.1(1)	N10 – C3 – N12	111.9(3)
O2 – Mo2 – N2	86.1(1)	N10 – C3 – C24	125.0(3)

N5 – Mo2 – Mo3	134.9(7)	N12 – C3 – C24	123.2(3)
N5 – Mo2 – N2	90.3(1)	N4 – C4 – N6	111.9(3)
N2 – Mo2 – Mo3	134.3(7)	N4 – C4 – C31	124.6(3)
O18 – Mo7 – Mo6	48.7(6)	N6 – C4 – C31	123.4(3)
O18 – Mo7 – O12	90.8(9)	N20 – C5 – N21	112.0(3)
O18 – Mo7 – N19	167.3(1)	N20 – C5 – C30	123.8(3)
O18 – Mo7 – N22	85.9(9)	N21 – C5 – C30	124.1(3)
O12 – Mo7 – Mo6	104.2(6)	N5 – C6 – N6	111.9(3)
O12 – Mo7 – N19	76.6(9)	N5 – C6 – C32	124.0(3)
O12 – Mo7 – N22	74.2(9)	N6 – C6 – C32	124.1(3)
O17 – Mo7 – Mo6	48.8(6)	N14 – C7 – N15	111.6(3)
O17 – Mo7 – O18	93.3(9)	N14 – C7 – C37	124.7(3)
O17 – Mo7 – O12	86.5(9)	N15 – C7 – C37	123.7(3)
O17 – Mo7 – N19	84.4(1)	N19 – C8 – C19	124.2(3)
O17 – Mo7 – N22	160.6(1)	N21 – C8 – N19	111.8(3)
O7 – Mo7 – Mo6	98.2(8)	N21 – C8 – C19	124.0(3)
O7 – Mo7 – O18	105.3(1)	N13 – C9 – N15	112.0(3)
O7 – Mo7 – O12	157.5(1)	N13 – C9 – C34	125.1(3)
O7 – Mo7 – O17	107.6(1)	N15 – C9 – C34	122.9(3)
O7 – Mo7 – N19	87.2(1)	N25 – C10 – N27	109.7(3)
O7 – Mo7 – N22	91.1(1)	N25 – C10 – C35	122.5(3)
N19 – Mo7 – Mo6	132.5(7)	N27 – C10 – C35	127.8(3)
N22 – Mo7 – Mo6	134.7(7)	N8 – C11 – N9	111.9(3)
N22 – Mo7 – N19	92.0(1)	N8 – C11 – C27	124.3(3)
O15 – Mo4 – Mo5	48.5(6)	N9 – C11 – C27	123.8(3)
O15 – Mo4 – O10	88.2(8)	N7 – C12 – C28	124.0(3)
O15 – Mo4 – N8	83.8(9)	N9 – C12 – N7	111.2(3)
O15 – Mo4 – N11	162.4(9)	N9 – C12 – C28	124.7(3)
O10 – Mo4 – Mo5	105.9(6)	N2 – C13 – N3	111.5(3)
O10 – Mo4 – N11	74.3(9)	N2 – C13 – C25	124.8(3)
O16 – Mo4 – Mo5	49.0(6)	N3 – C13 – C25	123.6(3)
O16 – Mo4 – O15	92.7(9)	N23 – C14 – N24	111.1(3)
O16 – Mo4 – O10	90.1(9)	N23 – C14 – C33	124.4(3)
O16 – Mo4 – N8	165.7(1)	N24 – C14 – C33	124.5(3)
O16 – Mo4 – N11	85.9(1)	N27 – C15 – C39	123.5(3)
O4 – Mo4 – Mo5	97.5(8)	N26 – C15 – N27	113.8(3)
O4 – Mo4 – O15	107.6(10)	N26 – C15 – C39	122.7(3)
O4 – Mo4 – O10	156.4(9)	N30 – C17 – C38	126.2(3)
O4 – Mo4 – O16	105.9(1)	N28 – C17 – N30	109.8(3)
O4 – Mo4 – N8	88.3(1)	N28 – C17 – C38	124.0(3)
O4 – Mo4 – N11	89.5(1)	N30 – C18 – C29	122.9(3)
N8 – Mo4 – Mo5	131.5(7)	N29 – C18 – N30	114.1(3)

N8 – Mo4 – O10	75.9(9)	N29 – C18 – C29	122.9(3)
N8 – Mo4 – N11	93.1(1)	N16 – C20 – N18	111.9(3)
N11 – Mo4 – Mo5	134.7(7)	N16 – C20 – C36	124.2(3)
O13 – Mo3 – Mo2	48.7(6)	N18 – C20 – C36	124.0(3)
O13 – Mo3 – O10	88.4(8)	N24 – C22 – N22	110.7(3)
O13 – Mo3 – N7	85.6(9)	N24 – C22 – C16	126.4(3)
O13 – Mo3 – N10	164.4(10)	N22 – C22 – C16	123.0(3)
O10 – Mo3 – Mo2	102.7(6)	N1 – C26 – N3	112.3(3)
O10 – Mo3 – N7	74.7(9)	N1 – C26 – C40	123.9(3)
O10 – Mo3 – N10	76.1(9)	N3 – C26 – C40	123.8(3)
O14 – Mo3 – Mo2	48.9(6)	O10W – Li3 – O8W	120.3(3)
O14 – Mo3 – O13	93.4(9)	O9W – Li3 – O10W	122.8(3)
O14 – Mo3 – O10	86.8(8)	O9W – Li3 – O8W	97.7(3)
O14 – Mo3 – N7	161.5(1)	O7W – Li3 – O10W	101.8(3)
O14 – Mo3 – N10	83.9(9)	O7W – Li3 – O9W	107.4(3)
O3 – Mo3 – Mo2	98.9(8)	O7W – Li3 – O8W	105.3(3)
O3 – Mo3 – O13	106.6(1)	O14W – Li4 – O12W	103.0(3)
O3 – Mo3 – O10	158.3(9)	O11W – Li4 – O14W	121.6(3)
O3 – Mo3 – O14	107.2(1)	O11W – Li4 – O12W	110.3(3)
O3 – Mo3 – N7	90.6(1)	O13W – Li4 – O14W	105.1(3)
O3 – Mo3 – N10	88.7(1)	O13W – Li4 – O12W	108.2(3)
N7 – Mo3 – Mo2	134.2(7)	O13W – Li4 – O11W	108.0(3)
N7 – Mo3 – N10	92.0(1)	O3W – Li1 – Li2	42.4(2)
N10 – Mo3 – Mo2	132.5(7)	O4W – Li1 – O3W	97.0(3)
O12 – Mo8 – Mo1	105.4(6)	O4W – Li1 – Li2	60.3(2)
O12 – Mo8 – N23	74.9(9)	O2W – Li1 – O3W	112.5(3)
O12 – Mo8 – N20	75.3(9)	O2W – Li1 – O4W	116.7(3)
O19 – Mo8 – Mo1	49.1(6)	O2W – Li1 – Li2	146.2(3)
O19 – Mo8 – O12	88.35(9)	O1W – Li1 – O3W	107.3(3)
O19 – Mo8 – O20	93.0(9)	O1W – Li1 – O4W	116.3(3)
O19 – Mo8 – N23	163.05(10)	O1W – Li1 – O2W	106.5(3)
O19 – Mo8 – N20	86.1(1)	O1W – Li1 – Li2	103.6(3)
O20 – Mo8 – Mo1	48.7(6)	O3W – Li2 – O4W	75.8(2)
O20 – Mo8 – O12	89.0(8)	O3W – Li2 – Li1	40.58(2)
O20 – Mo8 – N23	83.9(9)	O6W – Li2 – O3W	98.4(3)
O20 – Mo8 – N20	164.3(9)	O6W – Li2 – O4W	129.7(3)
O8 – Mo8 – Mo1	97.7(8)	O6W – Li2 – O5W	91.7(3)
O8 – Mo8 – O12	156.8(1)	O6W – Li2 – Li1	132.0(3)
O8 – Mo8 – O19	106.9(1)	O4W – Li2 – Li1	39.28(2)
O8 – Mo8 – O20	106.9(1)	O5W – Li2 – O3W	154.9(4)
O8 – Mo8 – N23	89.8(1)	O5W – Li2 – O4W	80.0(3)
O8 – Mo8 – N20	88.2(1)	O5W – Li2 – Li1	118.0(3)

N23 – Mo8 – Mo1	132.3(7)	O02G – Li2 – O3W	94.8(3)
N23 – Mo8 – N20	92.3(1)	O02G – Li2 – O6W	126.4(4)
N20 – Mo8 – Mo1	134.6(8)	O02G – Li2 – O4W	103.9(3)
Mo2 – O9 – Mo1	120.4(1)	O02G – Li2 – O5W	97.6(3)
Mo6 – O11 – Mo5	119.3(10)	O02G – Li2 – Li1	88.4(3)
Mo2 – O13 – Mo3	82.4(8)		

Table S10. Selected hydrogen bond distances (Å) and angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 20.5H_2O$ (**3**).

	D–H···A	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(°)
Intra	O12–H12···N19	0.95	2.005	2.703(2)	164
Intra	O12–H12···N20	0.95	1.910	2.677(2)	136
Intra	O9–H9···N4	0.95	1.758	2.656(2)	156
Intra	O9–H9···N5	0.95	1.798	2.656(2)	160
Intra	O10–H10···N11	0.95	1.802	2.647(2)	146
Intra	O10–H10···N10	0.95	1.823	2.708(2)	163
Intra	O11–H11···N13	0.95	1.910	2.708(2)	140
Intra	O11–H11···N14	0.95	1.892	2.695(2)	154
	O02G–	0.93	1.888	2.738(2)	151
	H02b···O14	0.87	2.175	3.026(2)	166
	O5w–	0.87	1.868	2.701(2)	158
	H5wa···O11				
	O6w–				
	H6wa···O16				
	O3w–	0.87	1.928	2.791 (2)	172
	H3wb···O8w				
	O4w–H4b···O20	0.87	1.912	2.781 (2)	178
	O2w–	0.87	1.962	2.797 (2)	159
	H2wa···O7w	0.87	1.846	2.698(2)	175
	O9w–	0.87	1.956	2.799(2)	163
	H9wa···O18				
	O9w–				
	H9wb···O6w				

Table S11. Selected bond distances (Å) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 25H_2O$ (**4**).

Atom–Atom	Lengths/Å	Atom–Atom	Lengths/Å
Mo01–Mo04	2.545(4)	Mo02–N00K	2.199(3)
Mo01–O005	1.946(3)	Mo03–O18	2.140(3)
Mo01–O18	2.165(3)	Mo03–O009	1.938(3)
Mo01–O008	1.949(3)	Mo03–O00A	1.934(3)
Mo01–O00D	1.686(3)	Mo03–O00E	1.707(3)
Mo01–N00F	2.199(3)	Mo03–N00G	2.193(3)
Mo01–N00L	2.186(3)	Mo03–N00P	2.168(4)
Mo02–Mo03	2.550(4)	Mo04–O005	1.942(3)
Mo02–O0061	2.163(3)	Mo04–O006	2.148(3)
Mo02–O009	1.949(3)	Mo04–O008	1.941(3)
Mo02–O00A	1.941(3)	Mo04–O00B	1.703(3)
Mo02–O00C	1.701(3)	Mo04–N00I1	2.189(4)
Mo02–N00J	2.208(3)	Mo04–N00M1	2.205(4)

Symmetry codes: [1]1/2 – *x*, 3/2 – *y* , 1 – *z*; [2]1 – *x*, 2 – *y*, 1 – *z*

Table S12. Selected bond angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 25H_2O$ (**4**).

Atom–Atom	Angles/°	Atom–Atom	Angles/°
O005–Mo01–Mo04	49.0(9)	Mo04–O005–Mo01	81.7(1)
O005–Mo01–O18	89.0(1)	Mo04–O006–Mo02[1]	119.9(1)
O005–Mo01–O008	93.5(2)	Mo03–O18–Mo01	120.8(1)
O005–Mo01–N00F	164.3(1)	Mo04–O008–Mo01	81.7(1)
O005–Mo01–N00L	84.9(1)	Mo03–O009–Mo02	82.0(1)
O18–Mo01–Mo04	105.7(7)	Mo03–O00A–Mo02	82.3(1)
O18–Mo01–N00F	75.4(1)	N00G–N00F–Mo01	122.2(2)
O18–Mo01–N00L	76.1(1)	C00R–N00F–Mo01	131.4(3)
O008–Mo01–Mo04	49.0(8)	C00R–N00F–N00G	106.4(3)
O008–Mo01–O18	89.7(1)	N00F–N00G–Mo03	122.9(3)
O008–Mo01–N00F	86.3(1)	C00W–N00G–Mo03	131.1(3)
O008–Mo01–N00L	165.7(1)	C00W–N00G–N00F	105.4(3)
O00D–Mo01–Mo04	97.0(1)	C00W–N00H–C00R	103.8(4)
O00D–Mo01–O005	105.56(1)	N00J–N00I–Mo04[1]	123.5(3)
O00D–Mo01–O18	157.2(1)	C00U–N00I–Mo04[1]	130.7(3)
O00D–Mo01–O008	106.4(1)	C00U–N00I–N00J	105.3(3)
O00D–Mo01–N00F	89.4(1)	N00I–N00J–Mo02	121.4(3)
O00D–Mo01–N00L	87.6(1)	C00Y–N00J–Mo02	130.8(3)
N00F–Mo01–Mo04	134.8(9)	C00Y–N00J–N00I	107.4(3)
N00L–Mo01–Mo04	133.4(1)	N00M–N00K–Mo02	122.3(3)
N00L–Mo01–N00F	91.3(1)	C014–N00K–Mo02	131.3(3)
O006[1]–Mo02–Mo03	104.5(7)	C014–N00K–N00M	106.1(4)
O006[1]–Mo02–N00J	75.8(1)	N00P–N00L–Mo01	121.1(2)
O006[1]–Mo02–N00K	75.4(1)	C00Z–N00L–Mo01	132.6(3)
O009–Mo02–Mo03	48.8(8)	C00Z–N00L–N00P	106.2(3)

O009–Mo02–O006[1]	89.5(1)	N00K–N00M–Mo04[1]	122.2(3)
O009–Mo02–N00J	165.3(1)	C012–N00M–Mo04[1]	131.2(3)
O009–Mo02–N00K	84.3(1)	C012–N00M–N00K	106.0(4)
O00A–Mo02–Mo03	48.7(8)	C00U–N00N–C00Y	104.5(4)
O00A–Mo02–O006[1]	88.2(1)	N00L–N00P–Mo03	123.7(2)
O00A–Mo02–O009	93.3(1)	C018–N00P–Mo03	131.7(3)
O00A–Mo02–N00J	84.7(1)	C018–N00P–N00L	104.6(4)
O00A–Mo02–N00K	163.5(1)	C014–N00Q–C012	103.0(4)
O00C–Mo02–Mo03	98.7(1)	N00F–C00R–N00H	111.7(4)
O00C–Mo02–O006[1]	156.7(1)	N00F–C00R–C00V	124.4(4)
O00C–Mo02–O009	106.5(1)	N00H–C00R–C00V	123.9(4)
O00C–Mo02–O00A	107.1(1)	C018–N00T–C00Z	104.1(4)
O00C–Mo02–N00J	87.9(1)	N00I–C00U–C010	124.0(4)
O00C–Mo02–N00K	89.1(1)	N00N–C00U–N00I	111.6(4)
N00J–Mo02–Mo03	133.0(9)	N00N–C00U–C010	124.4(4)
N00K–Mo02–Mo03	132.8(1)	N00G–C00W–C011	123.3(4)
N00K–Mo02–N00J	93.3(1)	N00H–C00W–N00G	112.7(4)
O18–Mo03–Mo02	104.0(7)	N00H–C00W–C011	123.9(4)
O18–Mo03–N00G	76.3(1)	N00J–C00Y–N00N	111.2(4)
O18–Mo03–N00P	75.5(1)	N00J–C00Y–C015	125.2(4)
O009–Mo03–Mo02	49.2(8)	N00N–C00Y–C015	123.6(4)
O009–Mo03–O18	88.0(1)	N00L–C00Z–N00T	112.2(4)
O009–Mo03–N00G	85.4(1)	N00L–C00Z–C016	123.0(4)
O009–Mo03–N00P	163.5(1)	N00T–C00Z–C016	124.8(4)
O00A–Mo03–Mo02	48.9(8)	N00M–C012–N00Q	112.3(4)
O00A–Mo03–O18	88.8(1)	N00M–C012–C01A	123.3(5)
O00A–Mo03–O009	93.8(1)	N00Q–C012–C01A	124.4(5)
O00A–Mo03–N00G	165.2(1)	N00K–C014–N00Q	112.7(4)
O00A–Mo03–N00P	86.3(1)	N00K–C014–C013	124.8(5)
O00E–Mo03–Mo02	98.2(1)	N00Q–C014–C013	122.5(5)
O00E–Mo03–O18	157.6(1)	N00P–C018–C01B	123.0(5)
O00E–Mo03–O009	106.8(1)	N00T–C018–N00P	112.9(5)
O00E–Mo03–O00A	106.2(1)	N00T–C018–C01B	124.1(5)
O00E–Mo03–N00G	88.0(1)	Li1P–O1L–Li36[2]	160.6(1)
O00E–Mo03–N00P	88.8(1)	O017–Li1P–Li1P[2]	104.7(1)
N00G–Mo03–Mo02	134.2(1)	O017–Li1P–O14	122.9(7)
N00P–Mo03–Mo02	135.0(1)	O1L[2]–Li1P–O017	113.3(9)
N00P–Mo03–N00G	90.1(1)	O1L–Li1P–O017	85.1(8)
O005–Mo04–Mo01	49.1(9)	O1L–Li1P–O1L2	85.9(8)
O005–Mo04–O006	90.2(1)	O1L[2]–Li1P–Li1P[2]	35.7(5)
O005–Mo04–N00I[1]	166.0(1)	O1L–Li1P–Li1P2	50.2(6)
O005–Mo04–N00M[1]	84.6(1)	O1L[2]–Li1P–O14	117.9(8)
O006–Mo04–Mo01	106.4(7)	O1L–Li1P–O14	75.1(9)
O006–Mo04–N00I[1]	75.8(1)	O1L[2]–Li1P–Li36	52.2(9)
O006–Mo04–N00M[1]	75.8(1)	O1L–Li1P–Li36	137.2(1)
O008–Mo04–Mo01	49.2(8)	O14–Li1P–Li1P2	102.1(9)
O008–Mo04–O005	93.9(1)	Li36–Li1P–O017	102.1(9)
O008–Mo04–O006	89.2(1)	Li36–Li1P–Li1P2	87.5(1)

O008–Mo04–N00I[1]	85.5(1)	Li36–Li1P–O14	128.7(1)
O008–Mo04–N00M[1]	165.0(1)	O1L[2]–Li36–Li1P	58.8(8)
O00B–Mo04–Mo01	97.5(1)	O1L[2]–Li36–O5	122.8(1)
O00B–Mo04–O005	105.9(1)	O37–Li36–O1L[2]	113.5(1)
O00B–Mo04–O006	156.0(1)	O37–Li36–Li1P	167.8(1)
O00B–Mo04–O008	106.7(1)	O37–Li36–O5	98.8(5)
O00B–Mo04–N00I[1]	87.5(1)	O37–Li36–O9	116.2(1)
O00B–Mo04–N00M[1]	87.9(1)	O5–Li36–Li1P	79.9(1)
N00I1–Mo04–Mo01	134.1(1)	O9–Li36–O1L[2]	101.7(1)
N00I1–Mo04–N00M[1]	92.3(1)	O9–Li36–Li1P	75.7(1)
N00M1–Mo04–Mo01	133.2(1)	O9–Li36–O5	104.4(1)

Symmetry codes: [1]1/2 – *x*, 3/2 – *y*,1 – *z*; [2]1 – *x*, 2 – *y*, 1 – *z*

Table S13. Selected hydrogen bond distances (Å) and angles (°) in $Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 25H_2O$ (**4**).

	D–H···A	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(°)
Intra	O18–H18···N00L	0.95	2.03	2.046(8)	141
Intra	O18–H18···N00P	0.95	2.03	2.641(7)	120
	O17–H01v···O009	0.87	1.898	2.739(8)	161
	O5–H5A···N00Q	1.031	2.089	3.046(7)	165

Table S14. Bond valence calculations for **1** – **4**, respectively.

Complexes	Atoms	N	$\sum S_{ij}$	Δ
$(NH_4)_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 62.5H_2O$ (**1**)	Mo1	**+5**	**5.029**	**0.029**
	Mo2	**+5**	**5.203**	**0.203**
	Mo3	**+5**	**5.061**	**0.061**
	Mo4	**+5**	**5.024**	**0.024**
	Mo5	**+5**	**5.013**	**0.013**
	Mo6	**+5**	**4.970**	**-0.031**
	Mo7	**+5**	**4.931**	**-0.069**
	Mo8	**+5**	**5.056**	**0.056**
	Mo9	**+5**	**5.204**	**0.204**
	Mo10	**+5**	**5.147**	**0.147**
		+5	**5.064**	**0.064**
$Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 2(Hdmtrz)_2\cdot 27H_2O$ (**2**)	Mo1	**+5**	**5.334**	**0.334**
	Mo2	**+5**	**4.975**	**-0.226**
	Mo3	**+5**	**4.949**	**-0.051**
	Mo4	**+5**	**4.965**	**-0.035**
		+5	**5.056_{av}**	**0.056_{av}**
$Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 20.5H_2O$ (**3**)	Mo1	**+5**	**4.965**	**-0.236**
	Mo2	**+5**	**5.036**	**0.036**
	Mo3	**+5**	**4.963**	**-0.037**
	Mo4	**+5**	**4.989**	**-0.011**
	Mo5	**+5**	**4.990**	**-0.010**
	Mo6	**+5**	**4.981**	**-0.019**
	Mo7	**+5**	**5.006**	**0.006**
	Mo8	**+5**	**4.978**	**-0.021**
		+5	**4.988_{av}**	**-0.002_{av}**
$Li_4[Mo_8O_8(\mu_2\text{-}OH)_4(\mu_2\text{-}O)_8(dmtrz)_8]\cdot 25H_2O$ (**4**)	Mo1	**+5**	**4.963**	**-0.037**
	Mo2	**+5**	**5.087**	**0.087**
	Mo3	**+5**	**5.053**	**0.053**
	Mo4	**+5**	**5.010**	**0.010**
		+5	**5.028_{av}**	**0.028_{av}**

Table S15. Comparisons of CO_2 adsorption data for **1** with some typical MOFs at 1 bar, 298 K.

Adsorbents	Common name	Amounts ($mmol \cdot g^{-1}$)
1	—	0.003
Al(OH)(bpydc)[1]	MOF-253	1.409
Zn(nbIm)(nIm)[2]	ZIF-78	2.068
Zn(IDC)[3]	IMOF-3	1.955
[Cu(tba)2][4]	—	1.830
[Mg(TCPBDA)][5]	—	1.495
Fe_2(DOBDC)[6]	—	2.027

List of abbreviations: H_2bpydc = 2,2′-bipyridine-5,5′-dicarboxylic acid; nbIm = 5-nitrobenzimidazole, nIm = 2-nitroimidazole; IDC = 2-methylimidazolate-4-amide-5-imidate; tba = 4-(1H-1,2,4-triazol-1-yl) benzoate; $TCPBDA_2$ = N,N,N',N' -tetrakis(4--carboxyphenyl)-b iphenyl-4'4-diamine; DOBDC = 2,5-dioxido--1,4-benzenedicarboxylate

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