Supporting materials

Crown ether-like octanuclear molybdenum(V) clusters for cations-bound and gas adsorptions

Ru-Dan Dai, Zhen-Lang Xie, Cheng Liu, Dong Xin, Zhao-Hui Zhou*

Gulei Innovation Institute, Xiamen University, Zhangzhou, 363200; College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, 361005, China., Tel: + 86-592-2184531; Fax: + 86-592-2183047 zhzhou@xmu.edu.cn

Figure and Table Options

Fig. S1. Calculated and simulated PXRD patterns of **1** ~ **3**.

Fig. S2. TG-DTG curves of **1** ~ **3**.

Fig. S3. EPR curves of **1** ~ **3.**

Fig. S4. IR spectrum of compound **1**

Fig. S5. IR spectrum of compound **2.**

Fig. S6. IR spectrum of compound **3.**

Fig. S7. Solid-state UV-vis spectra of compounds **1** – **3**, respectively. Color codes: black for **1**, red for **2** and blue for **3.**

Fig. S8. (a) UV-vis absorption spectra of **1** in solution (balck curve) and solid-state (red curve); (b) Solution UV-vis spectra of **1** – **3**, respectively. Color codes: black for **1**, red for **2** and blue for **3.**

Fig. S9. N_2, CH_4 and H_2 adsorptions for **1** (a), **2** (b), and **3** (c) at different pressures at 298 K, respectively.

Table S1. Crystallographic data and structural refinements for complexes $Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 26H_2O$ (**1**), $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 7H_2O$ (**2**) and $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**) and $(Mo_8O_{26})_n\cdot 4n(3\text{-}H_2apz)$ (**4**), respectively.

Table S2. Selected bond distances (Å) in $Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 26H_2O$ (**1**).

Table S3. Selected bond angles (°) in $Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 26H_2O$ (**1**).

Table S4. Selected hydrogen bond distances (Å) and angles (°) in $Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 26H_2O$ (**1**).

Table S5. Selected bond distances (Å) in $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 7H_2O$ (**2**).

Table S6. Selected bond angles (°) in $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 7H_2O$ (**2**).

Table S7. Selected hydrogen bond distances (Å) and angles (°) in $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 7H_2O$ (**2**).

Table S8. Selected bond distances (Å) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**).

Table S9. Selected bond angles (°) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**).

Table S10. Selected hydrogen bond distances (Å) and angles (°) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4\ (3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**).

Table S11. Selected bond distances (Å) in $(Mo_8O_{26})_n\cdot 4n(3\text{-}H_2apz)$ (**4**).

Table S12. Selected bond angles (°) in $(Mo_8O_{26})_n\cdot 4n(3\text{-}H_2apz)$ (**4**)..

Table S13 Selected hydrogen bond distances (Å) and angles (°) in $(Mo_8O_{26})_n\cdot 4n(3\text{-}H_2apz)$ (**4**).

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

Table S15. Comparisons of CO_2 adsorption data for **1**, **2** and **3** with some typical MOFs at 1 bar, 298 K.

Table S16. Detail calibrated adsorption data of O_2, CH_4, H_2, N_2 and CO_2 for $Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 26H_2O$ (**1**) at 298 K.

Table S17. Detail calibrated adsorption data of O_2, CH_4, H_2, N_2 and CO_2 for $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 7H_2O$ (**2**) at 298 K.

Table S18. Detail calibrated adsorption data of O_2, CH_4, H_2, N_2 and CO_2 for $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**) at 298 K.

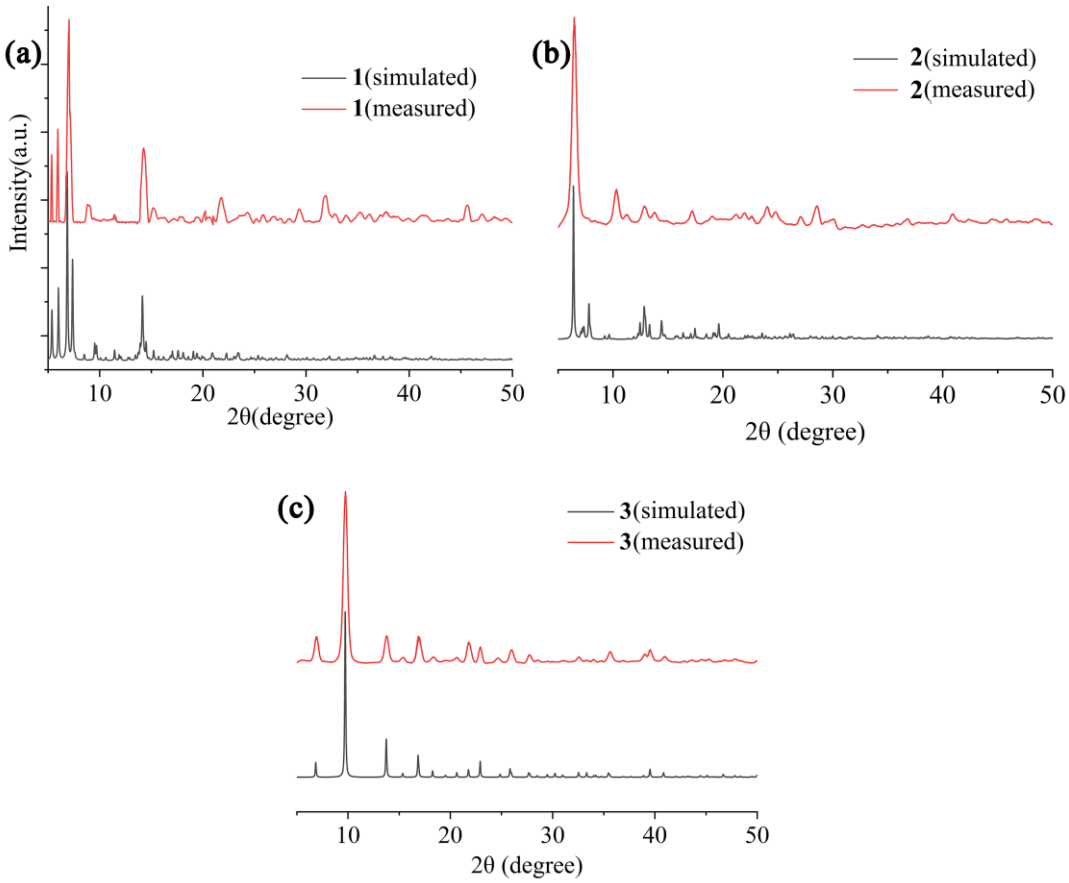


Fig. S1. Calculated and simulated PXRD patterns of **1** ~ **3**.

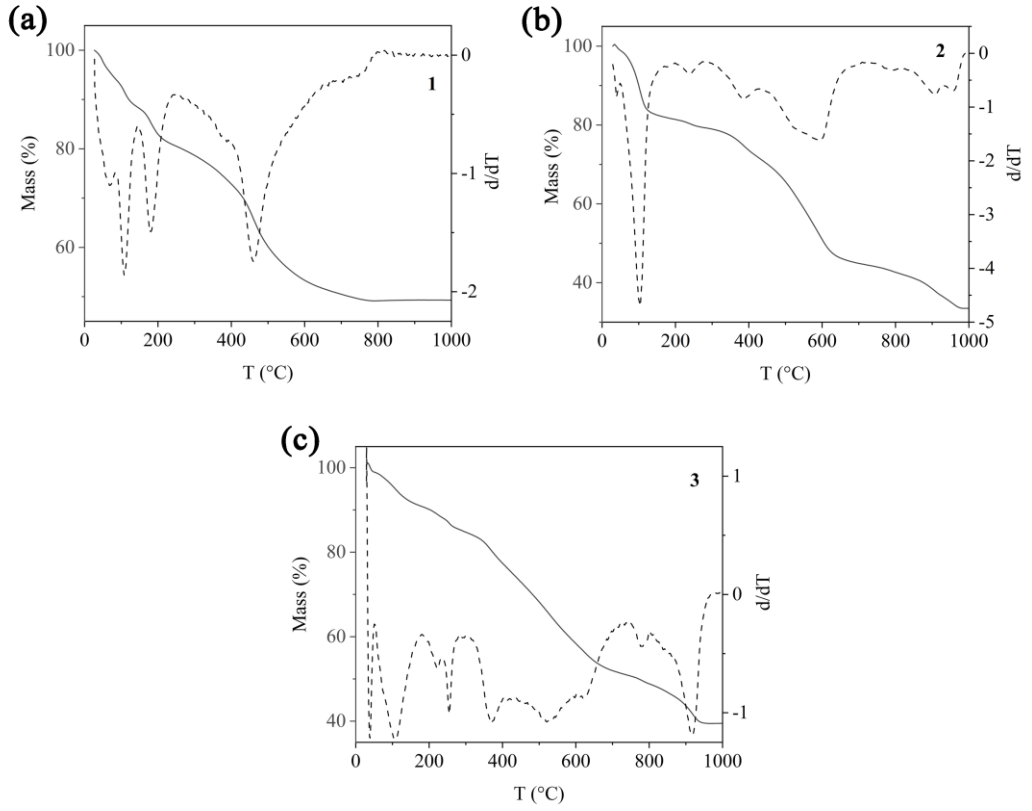


Fig. S2. TG-DTG curves of **1** ~ **3**.

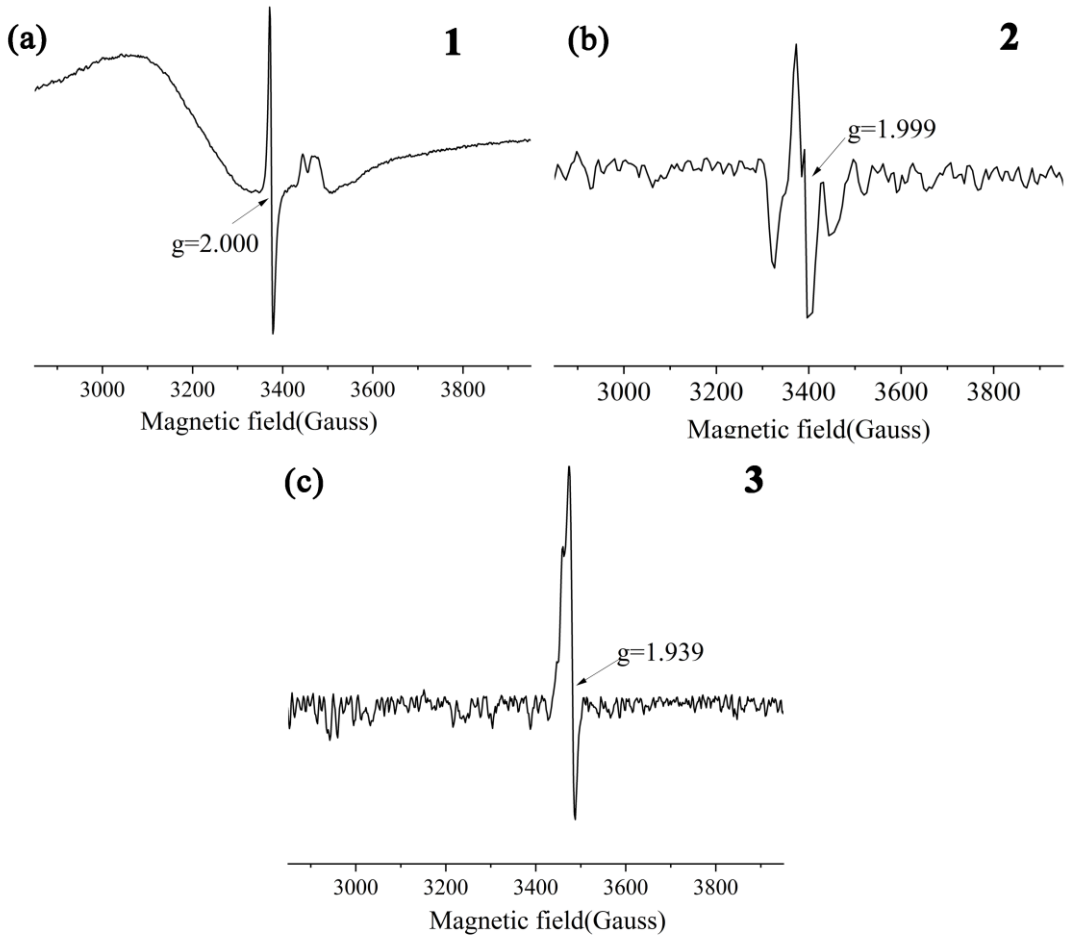


Fig. S3. EPR curves of **1** ~ **3**.

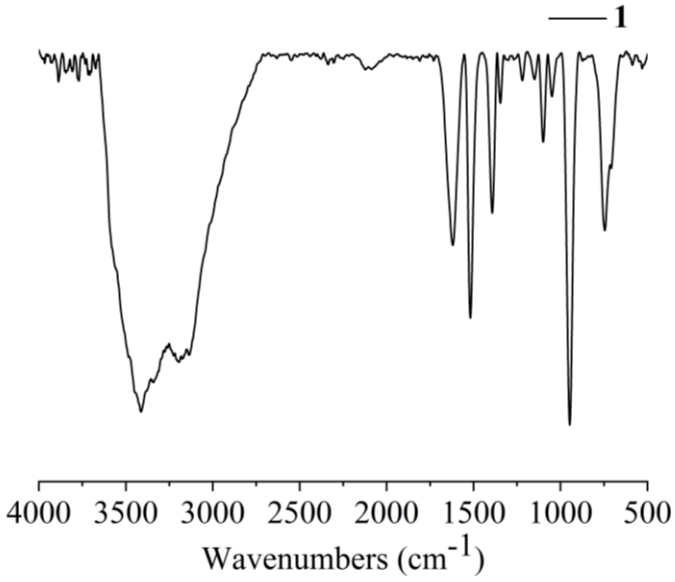


Fig. S4. IR spectrum of compound **1**.

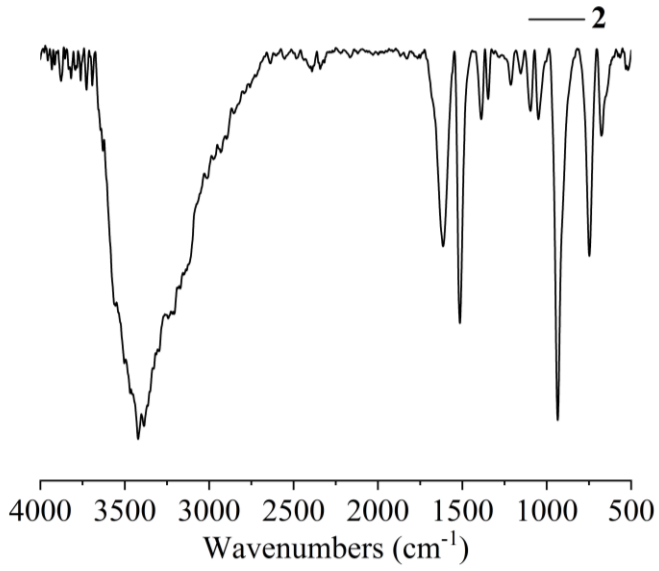


Fig. S5. IR spectrum of compound **2**.

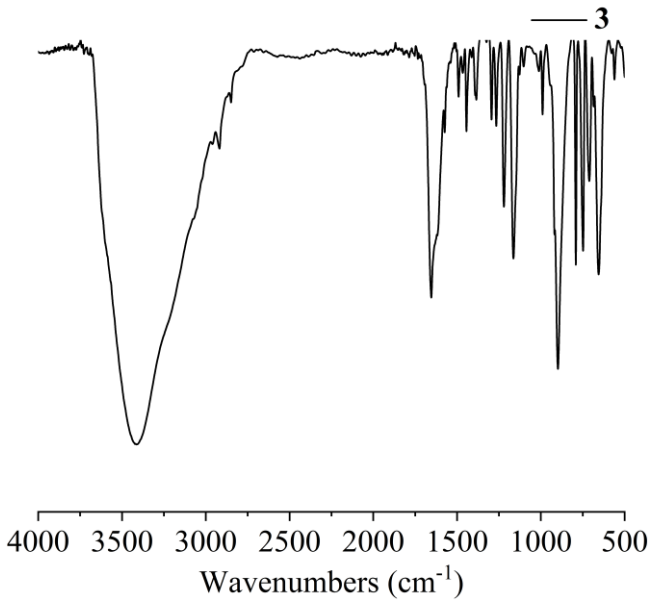
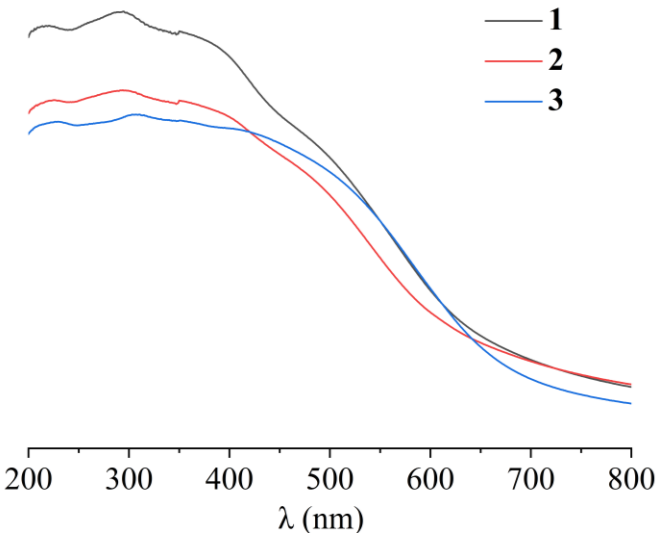


Fig. S6. IR spectrum of compound



3.

Fig. S7 Solid-state UV-vis spectra of compounds **1** – **3**, respectively. Color codes: black for **1**, red for **2** and blue for **3**.

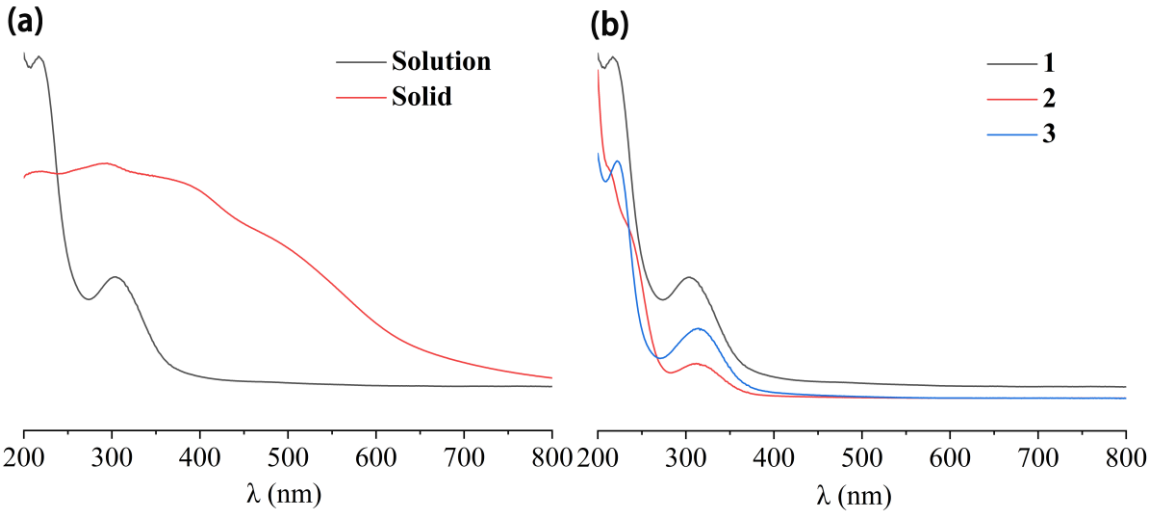


Fig. S8 (a) UV-vis absorption spectra of **1** in solution (balck curve) and solid-state (red curve); (b) Solution UV-vis spectra of **1** – **3**, respectively. Color codes: black for **1**, red for **2** and blue for **3.**

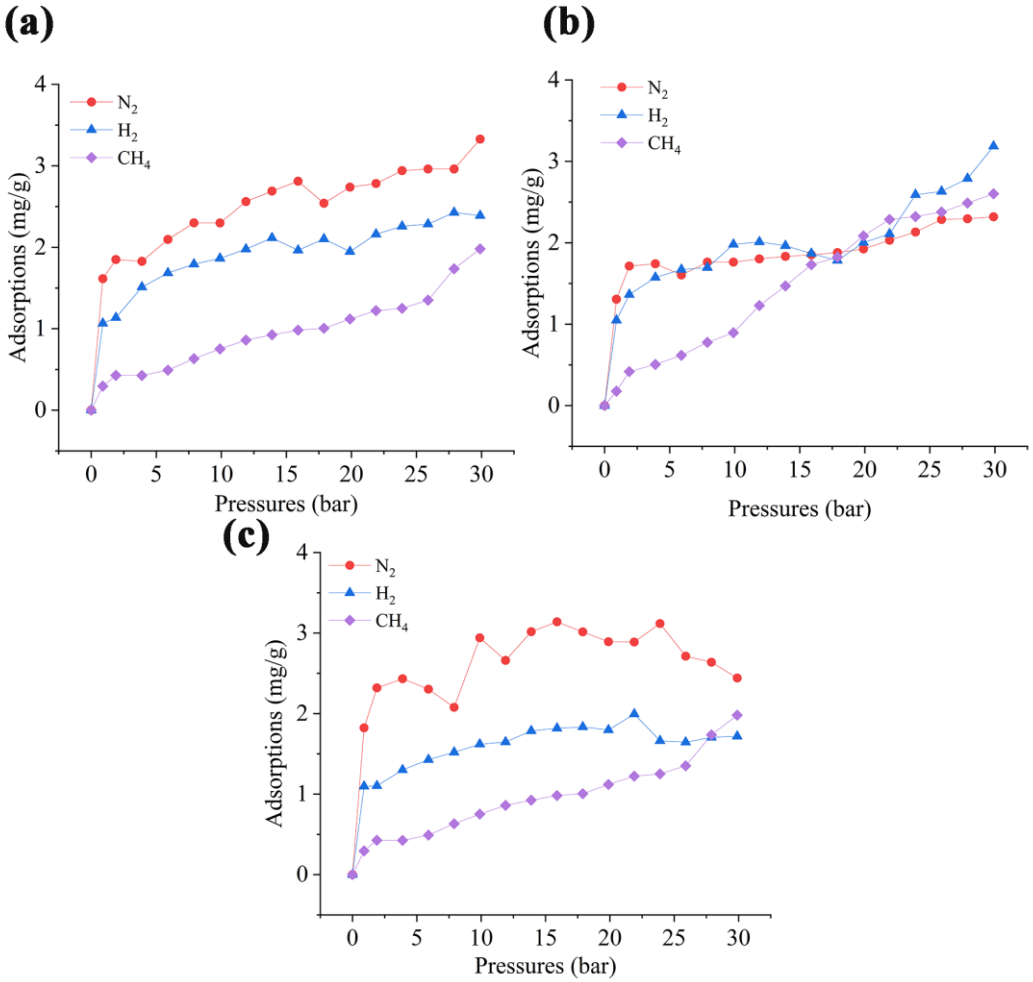


Fig. S9 N_2, CH_4 and H_2 adsorptions for **1** (a), **2** (b), and **3** (c) at different pressures at 298 K, respectively.

Table S1. Crystallographic data and structural refinements for complexes $Na_8[Mo_8O_8(\mu_2\text{-}OH)_8(\mu_2\text{-}O)_8(3\text{-}apz)_4]_2\cdot 26H_2O$ (**1**), $K_8[Mo_8O_8(\mu_2\text{-}OH)_8(\mu_2\text{-}O)_8(3\text{-}apz)_4]_2\cdot 7H_2O$ (**2**) and $(NH_4)_2[Mo_8O_8(\mu_2\text{-}O)_{12}(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**) and $(Mo_8O_{26})_n\cdot 4n(3\text{-}H_2apz)$ (**4**), respectively.

Identification codes	**1**	**2**	**3**	**4**
Empirical formula	$C_{24}H_{29}Mo_{16}N_{23}Na_2O_{49}$	$C_{24}H_{78}K_8Mo_{16}N_{24}O_{68}$	$C_{24}H_{36}Mo_8N_{26}O_{20}$	$C_{19}H_{24}Mo_8N_{12}O_{26}$
Formula weight	3004.72	3638.94	1748.29	1519.95
Temperature/K	100(1)	100(1)	100(1)	100(1)
Crystal system	tetragonal	monoclinic	tetragonal	triclinic
Space group	$P\,\text{-}42_1c$	$P\,2_1/n$	$I\,4/m$	$P\,\bar{1}$
a/Å	32.8779(2)	15.3641(1)	18.2472(7)	7.8832(6)
b/Å	32.8779(2)	24.4988(2)	18.2472(7)	10.3837(8)
c/Å	20.6940(2)	25.6724(2)	10.4717(12)	11.8466(8)
α/°	90	90	90	104.127(6)
β/°	90	96.397(1)	90	104.250(7)
γ/°	90	90	90	102.460(7)
Volume/Å^3	22369.3(3)	9603.0(1)	3486.7(5)	871.3(1)
Z	8	4	2	2
ρ_{calc}g/cm^3	1.784	2.517	1.665	2.839
μ/mm^{-1}	14.911	20.653	12.001	23.857
F(000)	11360	7032	1688.0	724.0
Crystal size/mm^3	0.15 × 0.10 × 0.10	0.15 × 0.15 × 0.10	0.20 × 0.10 × 0.10	0.15 × 0.11 × 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/°	5.046 to 127.99	5 to 136.494	6.85 to 127.954	8.11 to 127.99

Index ranges	$-38 \le h \le 26$, $-35 \le k \le 38$, $-17 \le l \le 24$	$-18 \le h \le 18$, $-29 \le k \le 27$, $-20 \le l \le 30$	$-21 \le h \le 12$, $-20 \le k \le 18$, $-11 \le l \le 12$	$-9 \le h \le 9$, $-12 \le k \le 12$, $-13 \le l \le 7$
Reflections collected	46232	62561	5042	7409
Independent reflections	18230 (R_{int} = 0.0526, R_σ = 0.0601)	17569 (R_{int} = 0.0263, R_σ = 0.0207)	1545 (R_{int} = 0.0332, R_σ = 0.0318)	2867 (R_{int} = 0.0567, R_σ = 0.0525)
Data/restraints/parameters	18230/114/1065	17549/66/1181	1545/2/109	2867/0/265
Goodness–of–fit on F^2	1.056	1.012	1.061	1.052
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0506, wR_2 = 0.1302	R_1 = 0.0441, wR_2 = 0.1150	R_1 = 0.0468, wR_2 = 0.1358	R_1 = 0.0449, wR_2 = 0.1170
Final R indexes [all data]	R_1 = 0.0594, wR_2 = 0.1356	R_1 = 0.0478, wR_2 = 0.1182	R_1 = 0.0535, wR_2 = 0.1406	R_1 = 0.0480, wR_2 = 0.1195
Largest diff. peak/hole/e·Å^{-3}	1.79/-0.98	3.17/-2.38	1.10/-0.55	1.54/-1.74

Table S2. Selected bond distances (Å) in $Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2 \cdot 26H_2O$ (**1**).

Atom–Atom	Distances/Å	Atom–Atom	Distances/Å
Mo01–Mo06	2.575(2)	Mo0E–O010	1.961(1)
Mo01–O00I	2.153(1)	Mo0E–O014	1.947(1)
Mo01–O00S	2.194(1)	Mo0E–O017	2.194(1)
Mo01–O00T	1.959(1)	Mo0E–O02D	1.663(1)
Mo01–O012	1.939(1)	Mo0E–N02J	2.184(2)
Mo01–N01V	2.170(1)	Mo0F–Mo0G	2.566(2)
Mo01–O026	1.710(1)	Mo0F–O00H	2.099(1)
Mo02–Mo03	2.577(2)	Mo0F–O00J	1.977(1)
Mo02–O00L	1.952(9)	Mo0F–O015	2.180(1)
Mo02–O00M	1.940(1)	Mo0F–O01E	1.929(1)
Mo02–O00N	2.184(9)	Mo0F–N01H	2.214(1)
Mo02–O00P	2.099(1)	Mo0F–O01N	1.729(1)
Mo02–O01M	1.708(1)	Mo0G–O00J	1.960(1)
Mo02–N023	2.165(1)	Mo0G–O016	2.190(1)
Mo03–O00L	1.939(1)	Mo0G–O018	2.148(1)
Mo03–O00M	1.949(9)	Mo0G–O01E	1.979(1)
Mo03–O00Q	2.101(1)	Mo0G–N01T	2.149(1)
Mo03–O011	2.186(1)	Mo0G–O020	1.697(1)
Mo03–O01G	1.683(1)	O00J–Na3	3.017(2)
Mo03–N01L	2.206(1)	O00K–Na21	2.941(2)
Mo04–Mo05	2.570(2)	O00N–Na1	2.458(2)
Mo04–O00N	2.151(1)	O00N–Na21	2.901(3)
Mo04–O00P	2.109(1)	O00R–Na21	2.812(3)
Mo04–O00R	1.978(9)	O00S–Na3	2.595(1)
Mo04–O01J	1.951(1)	O00V–Na3	2.407(2)
Mo04–O01Q	1.724(1)	O00W–Na1	2.382(2)
Mo04–N01Y	2.153(1)	O00W–Na21	2.851(3)
Mo05–O00O	2.145(1)	O011–Na1	2.424(2)
Mo05–O00R	1.991(1)	O011–Na21	2.971(3)
Mo05–O00W	2.146(1)	O015–Na3	2.435(1)
Mo05–N01C	2.154(1)	O016–Na3	2.398(2)
Mo05–O01J	1.952(1)	O017–Na1	2.416(2)
Mo05–O01R	1.690(1)	O017–Na21	2.971(3)
Mo06–O00T	1.976(9)	N01C–N01O	1.431(2)
Mo06–O00V	2.165(1)	N01C–C02Y	1.291(2)
Mo06–O00X	2.095(1)	N01H–N029	1.341(2)
Mo06–O012	1.949(1)	N01H–C039	1.301(2)
Mo06–N01U	2.170(1)	N01I–N01V	1.407(2)
Mo06–O028	1.675(1)	N01I–C03D	1.312(2)
Mo07–Mo0D	2.574(2)	N01L–N01P	1.392(2)
Mo07–O00I	2.074(1)	N01L–C02B	1.262(2)
Mo07–O00S	2.161(1)	N01O–C034	1.322(2)
Mo07–O00Z	1.964(1)	N01P–C02G	1.341(2)

Mo07–O019	1.697(1)	N01T–N02M	1.421(2)
Mo07–O01F	1.967(1)	N01T–C03M	1.342(2)
Mo07–N01I	2.195(1)	N01U–N025	1.404(2)
Mo08–Mo0A	2.575(2)	N01U–C03E	1.295(2)
Mo08–O00K	1.933(9)	N01V–C02I	1.284(2)
Mo08–O00U	2.122(1)	N01Y–N023	1.380(2)
Mo08–O013	1.914(1)	N01Y–C02K	1.321(2)
Mo08–O017	2.160(1)	N01Z–C02K	1.398(2)
Mo08–O01K	1.666(1)	N023–C02A	1.408(2)
Mo08–N024	2.180(1)	N024–N02J	1.379(2)
Mo09–Mo0C	2.566(2)	N024–C02T	1.334(2)
Mo09–O00V	2.202(1)	N025–C02X	1.354(2)
Mo09–O00X	2.131(1)	C027–C02B	1.384(3)
Mo09–O00Y	1.958(1)	C027–C02G	1.441(3)
Mo09–O01A	1.923(1)	N029–C03J	1.341(2)
Mo09–O01W	1.703(1)	C02A–C02F	1.387(2)
Mo09–N025	2.164(1)	C02F–C02K	1.362(2)
Mo0A–O00K	1.966(9)	C02G–N02H	1.357(2)
Mo0A–O00O	2.115(1)	C02I–C02Z	1.293(3)
Mo0A–O00W	2.179(1)	C02I–N13	1.481(4)
Mo0A–O013	1.954(1)	N02J–C03F	1.301(3)
Mo0A–N01O	2.180(1)	N02L–C02X	1.395(2)
Mo0A–O022	1.674(1)	N02M–C03Z	1.314(2)
Mo0B–Mo0E	2.562(2)	C02T–C03V	1.411(3)
Mo0B–O00Q	2.098(1)	C02T–N1	1.332(4)
Mo0B–O010	1.957(1)	C02X–C035	1.401(3)
Mo0B–O011	2.206(1)	C02Y–C032	1.411(2)
Mo0B–O014	1.995(1)	C02Y–N036	1.391(2)
Mo0B–N01P	2.157(1)	C02Z–C03D	1.291(3)
Mo0B–O01X	1.634(1)	N031–C03Z	1.461(3)
Mo0C–O00H	2.126(1)	C032–C034	1.421(3)
Mo0C–O00Y	1.946(1)	C035–C03E	1.461(3)
Mo0C–O015	2.184(1)	C039–C03G	1.372(3)
Mo0C–O01A	1.942(1)	N03C–C03J	1.431(3)
Mo0C–O021	1.707(1)	C03D–N11	1.342(4)
Mo0C–N029	2.174(1)	C03F–C03V	1.291(3)
Mo0D–O00Z	1.942(1)	C03F–N17	1.232(5)
Mo0D–O016	2.198(1)	C03G–C03J	1.371(3)
Mo0D–O018	2.126(1)	C03L–C03M	1.441(3)
Mo0D–O01F	1.976(1)	C03L–C03Z	1.331(3)
Mo0D–O02C	1.729(1)	Na3–O2	2.271(2)
Mo0D–N02M	2.198(2)	Na1–O2	2.401(2)
Mo0E–O00U	2.130(1)	O2–Na21	1.431(3)

Table S4. Selected hydrogen bond distances (Å) and angles (°) in $Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2 \cdot 26H_2O$ (**1**).

	D–H···A	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(°)
	O4–H4···O27	0.86	1.87	2.683(8)	157
	N11–H11A···O19	0.88	2.52	2.962(8)	111
	N11–H11B···O29	0.88	2.35	3.212(8)	168
Intra	O8–H8···O31	0.86	1.88	2.627(6)	145
Intra	O11–H11··N2	0.86	1.91	2.671(6)	146
	C02A–H02A···O43	0.95	2.33	3.248(2)	162
Intra	C02Z–H02Z···O46	0.95	2.54	3.269(9)	133
Intra	O15–H15··N7	0.85	1.91	2.479(6)	123
Intra	O15–H15··N19	0.85	1.88	2.461(6)	124

Symmetry codes: (a) x, -1 + y, z; (b) 1 – x, 1 – y, 1 – z.

Table S5 Selected bond distances (Å) in $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2 \cdot 7H_2O$ (**2**).

Atom–Atom	Distances/Å	Atom–Atom	Distances/Å
Mo1–Mo8	2.554(8)	Mo8–O39	2.178(5)
Mo1–K6	4.076(8)	Mo8–N8	2.179(6)
Mo1–K7	3.896(5)	Mo9–Mo10	2.564(8)
Mo1–O2	2.148(5)	Mo9–K7A	3.901(3)
Mo1–O5	1.960(4)	Mo9–O14	2.172(5)
Mo1–O13	1.942(5)	Mo9–O17	1.948(5)
Mo1–O27	1.701(5)	Mo9–O40	2.116(5)
Mo1–O49	2.112(5)	Mo9–O43	1.954(4)
Mo1–N10	2.165(6)	Mo9–O50	1.695(5)
Mo2–Mo3	2.561(8)	Mo9–N14	2.190(6)
Mo2–K3	4.111(4)	Mo10–K7A	4.109(4)
Mo2–O2	2.160(5)	Mo10–O6	2.107(5)
Mo2–O29	1.939(5)	Mo10–O9	2.201(4)
Mo2–O32	1.707(6)	Mo10–O17	1.948(5)
Mo2–O48	1.957(4)	Mo10–O24	1.702(5)
Mo2–O49	2.100(5)	Mo10–O43	1.963(5)
Mo2–N4	2.185(6)	Mo10–N5	2.187(6)
Mo3–K61	3.834(9)	Mo11–Mo12	2.561(7)
Mo3–O3	2.172(5)	Mo11–K51	4.115(4)
Mo3–O29	1.931(5)	Mo11–K61	3.909(8)
Mo3–O44	2.112(5)	Mo11–O4	1.963(5)
Mo3–O48	1.957(5)	Mo11–O6	2.127(4)
Mo3–O55	1.703(5)	Mo11–O9	2.166(5)
Mo3–N7	2.176(6)	Mo11–O12	1.953(4)
Mo4–Mo5	2.576(9)	Mo11–O25	1.698(5)
Mo4–O3	2.199(5)	Mo11–N2	2.165(6)
Mo2–O5	2.195(3)	Mo12–O4	1.950(4)
Mo4–O21	1.956(5)	Mo12–O8	2.153(5)
Mo4–O31	1.697(5)	Mo12–O12	1.945(5)
Mo4–O44	2.101(5)	Mo12–O1A	2.113(5)
Mo4–O47	1.952(5)	Mo12–O23	1.702(5)
Mo4–N12	2.188(6)	Mo12–N9	2.189(6)
Mo5–O19	2.112(5)	Mo13–Mo14	2.567(8)
Mo5–O21	1.959(5)	Mo13–O8	2.151(4)
Mo5–O41	2.198(5)	Mo13–O15	1.951(5)
Mo5–O47	1.973(5)	Mo13–O1A	2.119(5)
Mo5–O51	1.693(5)	Mo13–O42	1.955(5)
Mo5–N15	2.181(7)	Mo13–O52	1.693(5)
Mo6–Mo7	2.568(8)	Mo13–N3	2.190(6)
Mo6–O11	1.954(5)	Mo14–K32	3.976(3)
Mo6–O18	1.951(5)	Mo14–K8	4.128(2)
Mo6–O19	2.103(5)	Mo14–O15	1.954(5)
Mo6–O41	2.211(5)	Mo14–O16	2.103(5)
Mo6–O54	1.705(5)	Mo14–O42	1.960(4)

Mo6–N16	2.153(6)	Mo14–O45	2.157(4)
Mo7–O1	2.091(5)	Mo14–N13	2.185(6)
Mo7–O11	1.967(5)	Mo15–Mo16	2.558(7)
Mo7–O18	1.952(5)	Mo15–K8	3.744(9)
Mo7–O28	1.703(5)	Mo15–K8A	3.927(4)
Mo7–O39	2.180(4)	Mo15–O7	1.956(4)
Mo7–N11	2.186(6)	Mo15–O16	2.101(5)
Mo8–O1	2.111(4)	Mo15–O20	1.700(5)
Mo8–O5	1.956(5)	Mo15–O45	2.185(5)
Mo8–O13	1.945(4)	Mo15–O46	1.940(5)
Mo16–O46	1.949(5)	Mo15–N1	2.176(6)
Mo16–O53	1.688(5)	Mo16–O7	1.961(5)
Mo16–N6	2.151(6)	Mo16–O14	2.189(5)
Mo16–O46	1.949(5)	Mo16–O40	2.100(5)

Table S6. Selected bond angles (°) in $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-apz})_4]_2 \cdot 7H_2O$ (**2**).

Atom–Atom	**Angle/°**	Atom–Atom	**Angle/°**
Mo8–Mo1–K6	73.09(3)	O50–Mo9–K7A	30.2(2)
Mo8–Mo1–K7	130.86(8)	O50–Mo9–O14	160.8(2)
K7–Mo1–K6	64.98(1)	O50–Mo9–O17	104.6(2)
O2–Mo1–Mo8	99.94(2)	O50–Mo9–O40	93.9(2)
O2–Mo1–K6	170.86(3)	O50–Mo9–O43	104.9(2)
O2–Mo1–K7	123.84(6)	O50–Mo9–N14	90.0(2)
O2–Mo1–N10	75.5(2)	N14–Mo9–Mo10	138.32(6)
O5–Mo1–Mo8	49.20(4)	N14–Mo9–K7A	120.20(8)
O5–Mo1–K6	92.73(4)	Mo9–Mo10–K7A	66.96(6)
O5–Mo1–K7	107.45(5)	O6–Mo10–Mo9	136.50(3)
O5–Mo1–O2	86.79(7)	O6–Mo10–K7A	106.61(4)
O5–Mo1–O49	87.25(8)	O6–Mo10–O9	71.29(6)
O5–Mo1–N10	162.1(2)	O6–Mo10–N5	82.2(2)
O13–Mo1–Mo8	48.95(3)	O9–Mo10–Mo9	97.21(2)
O13–Mo1–K6	82.97(4)	O9–Mo10–K7A	155.48(3)
O13–Mo1–K7	140.98(7)	O17–Mo10–Mo9	48.81(4)
O13–Mo1–O2	87.97(9)	O17–Mo10–K7A	95.70(6)
O13–Mo1–O5	95.16(9)	O17–Mo10–O6	157.03(8)
O13–Mo1–O49	159.54(9)	O17–Mo10–O9	86.17(8)
O13–Mo1–N10	87.1(2)	O17–Mo10–O43	95.03(9)
O27–Mo1–Mo8	100.57(8)	O17–Mo10–N5	88.4(2)
O27–Mo1–K6	28.14(8)	O24–Mo10–Mo9	99.70(8)
O27–Mo1–K7	37.9(2)	O24–Mo10–K7A	37.70(8)
O27–Mo1–O2	159.5(2)	O24–Mo10–O6	95.8(2)
O27–Mo1–O5	106.7(2)	O24–Mo10–O9	163.1(2)
O27–Mo1–O13	105.6(2)	O24–Mo10–O17	105.3(2)
O27–Mo1–O49	93.0(2)	O24–Mo10–O43	105.1(2)
O27–Mo1–N10	89.6(2)	O24–Mo10–N5	91.2(2)
O49–Mo1–Mo8	136.42(2)	O43–Mo10–Mo9	48.94(3)
O49–Mo1–K6	117.26(3)	O43–Mo10–K7A	69.65(4)
O49–Mo1–K7	55.62(6)	O43–Mo10–O6	87.83(8)
O49–Mo1–O2	71.85(8)	O43–Mo10–O9	85.83(8)
O49–Mo1–N10	84.6(2)	O43–Mo10–N5	161.8(2)
N10–Mo1–Mo8	136.08(7)	N5–Mo10–Mo9	137.24(5)
N10–Mo1–K6	105.17(6)	N5–Mo10–K7A	127.90(5)
N10–Mo1–K7	80.86(7)	N5–Mo10–O9	76.52(9)
Mo3–Mo2–K3	112.32(6)	Mo12–Mo11–K51	140.75(6)
O2–Mo2–Mo3	97.50(2)	Mo12–Mo11–K61	77.30(3)
O2–Mo2–K3	146.64(3)	K61–Mo11–K51	65.34(7)
O2–Mo2–N4	76.7(2)	O4–Mo11–Mo12	48.90(3)
O29–Mo2–Mo3	48.43(5)	O4–Mo11–K51	104.37(4)
O29–Mo2–K3	123.74(7)	O4–Mo11–K61	70.21(4)
O29–Mo2–O2	87.0(2)	O4–Mo11–O6	86.42(8)

O29–Mo2–O48	95.1(2)	O4–Mo11–O9	86.51(8)
O29–Mo2–O49	158.5(2)	O4–Mo11–N2	161.1(2)
O29–Mo2–N4	88.3(2)	O6–Mo11–Mo12	135.31(3)
O32–Mo2–Mo3	99.84(9)	O6–Mo11–K51	38.44(3)
O32–Mo2–K3	19.5(2)	O6–Mo11–K61	89.66(3)
O32–Mo2–O2	162.7(2)	O6–Mo11–O9	71.61(7)
O32–Mo2–O29	104.2(3)	O6–Mo11–N2	84.7(2)
O32–Mo2–O48	105.6(2)	O9–Mo11–Mo12	100.43(2)
O32–Mo2–O49	95.6(2)	O9–Mo11–K51	106.41(3)
O32–Mo2–N4	90.3(3)	O9–Mo11–K61	151.17(2)
O48–Mo2–Mo3	49.13(3)	O12–Mo11–Mo12	48.79(4)
O48–Mo2–K3	101.85(4)	O12–Mo11–K51	155.07(5)
O48–Mo2–O2	86.16(8)	O12–Mo11–K61	108.23(4)
O48–Mo2–O49	87.47(8)	O12–Mo11–O4	95.03(9)
O48–Mo2–N4	162.3(2)	O12–Mo11–O6	161.49(9)
O49–Mo2–Mo3	136.39(2)	O12–Mo11–O9	90.03(8)
O49–Mo2–K3	76.19(4)	O12–Mo11–N2	88.3(2)
O49–Mo2–O2	71.84(8)	O25–Mo11–Mo12	100.55(7)
O49–Mo2–N4	83.2(2)	O25–Mo11–K51	54.69(8)
N4–Mo2–Mo3	136.73(6)	O25–Mo11–K61	35.95(8)
N4–Mo2–K3	90.49(7)	O25–Mo11–O4	106.2(2)
Mo2–Mo3–K61	137.87(4)	O25–Mo11–O6	92.1(2)
O3–Mo3–Mo2	100.20(3)	O25–Mo11–O9	159.0(2)
O3–Mo3–K61	111.15(3)	O25–Mo11–O12	105.1(2)
O3–Mo3–N7	75.6(2)	O25–Mo11–N2	90.8(2)
O29–Mo3–Mo2	48.69(5)	N2–Mo11–Mo12	137.07(6)
O29–Mo3–K61	153.12(5)	N2–Mo11–K51	78.43(6)
O29–Mo3–O3	88.5(2)	N2–Mo11–K61	126.26(6)
O29–Mo3–O44	159.3(2)	N2–Mo11–O9	74.89(9)
O29–Mo3–O48	95.3(2)	O4–Mo12–Mo11	49.32(4)
O29–Mo3–N7	88.1(2)	O4–Mo12–O8	87.94(8)
O44–Mo3–Mo2	136.20(3)	O4–Mo12–O1A	87.88(9)
O44–Mo3–K61	43.00(4)	O4–Mo12–N9	163.7(2)
O44–Mo3–O3	71.04(8)	O8–Mo12–Mo11	98.74(2)
O44–Mo3–N7	84.0(2)	O8–Mo12–N9	77.38(9)
O48–Mo3–Mo2	49.11(3)	O12–Mo12–Mo11	49.05(3)
O48–Mo3–K61	103.17(3)	O12–Mo12–O4	95.68(9)
O48–Mo3–O3	88.30(8)	O12–Mo12–O8	86.16(9)
O48–Mo3–O44	87.23(8)	O12–Mo12–O1A	157.17(9)
O48–Mo3–N7	163.4(2)	O12–Mo12–N9	90.5(2)
O55–Mo3–Mo2	100.57(8)	O1A–Mo12–Mo11	136.95(3)
O55–Mo3–K61	50.68(9)	O1A–Mo12–O8	71.41(7)
O55–Mo3–O3	159.2(2)	O1A–Mo12–N9	80.8(2)
O55–Mo3–O29	105.9(2)	O23–Mo12–Mo11	99.39(7)
O55–Mo3–O44	93.2(2)	O23–Mo12–O4	104.2(2)
O55–Mo3–O48	104.8(2)	O23–Mo12–O8	161.9(2)
O55–Mo3–N7	89.7(3)	O23–Mo12–O12	105.7(2)
N7–Mo3–Mo2	136.82(6)	O23–Mo12–O1A	95.2(2)

N7–Mo3–K61	79.71(7)	O23–Mo12–N9	88.6(2)
O3–Mo4–Mo5	98.24(2)	N9–Mo12–Mo11	139.47(6)
O21–Mo4–Mo5	48.89(4)	O8–Mo13–Mo14	100.96(2)
O21–Mo4–O3	86.28(9)	O8–Mo13–N3	76.47(9)
O21–Mo4–O44	156.78(9)	O15–Mo13–Mo14	48.95(5)
O21–Mo4–N12	88.6(2)	O15–Mo13–O8	87.69(8)
O31–Mo4–Mo5	100.9(2)	O15–Mo13–O1A	158.78(9)
O31–Mo4–O3	160.9(2)	O15–Mo13–O42	95.2(2)
O31–Mo4–O21	106.0(2)	O15–Mo13–N3	91.3(2)
O31–Mo4–O44	95.5(2)	O1A–Mo13–Mo14	136.87(3)
O31–Mo4–O47	105.8(2)	O1A–Mo13–O8	71.35(7)
O31–Mo4–N12	89.7(2)	O1A–Mo13–N3	80.8(2)
O44–Mo4–Mo5	135.71(3)	O42–Mo13–Mo14	49.10(3)
O44–Mo4–O3	70.72(8)	O42–Mo13–O8	89.01(8)
O44–Mo4–N12	82.8(2)	O42–Mo13–O1A	87.87(9)
O47–Mo4–Mo5	49.33(4)	O42–Mo13–N3	163.8(2)
O47–Mo4–O3	87.04(8)	O52–Mo13–Mo14	98.6(2)
O47–Mo4–O21	95.5(2)	O52–Mo13–O8	160.5(2)
O47–Mo4–O44	86.69(9)	O52–Mo13–O15	105.0(2)
O47–Mo4–N12	162.0(2)	O52–Mo13–O1A	94.5(2)
N12–Mo4–Mo5	137.52(8)	O52–Mo13–O42	104.3(2)
N12–Mo4–O3	75.8(2)	O52–Mo13–N3	88.2(2)
O19–Mo5–Mo4	136.15(3)	N3–Mo13–Mo14	140.18(5)
O19–Mo5–O41	71.09(7)	Mo13–Mo14–K32	119.46(7)
O19–Mo5–N15	83.6(2)	Mo13–Mo14–K8	153.40(5)
O21–Mo5–Mo4	48.81(6)	K32–Mo14–K8	39.35(5)
O21–Mo5–O19	159.6(2)	O15–Mo14–Mo13	48.85(4)
O21–Mo5–O41	88.9(2)	O15–Mo14–K32	129.29(5)
O21–Mo5–O47	94.8(2)	O15–Mo14–K8	151.5(2)
O21–Mo5–N15	87.3(2)	O15–Mo14–O16	159.69(9)
O41–Mo5–Mo4	98.72(3)	O15–Mo14–O42	95.0(2)
O47–Mo5–Mo4	48.64(4)	O15–Mo14–O45	87.84(9)
O47–Mo5–O19	87.59(9)	O15–Mo14–N13	90.4(2)
O47–Mo5–O41	85.26(8)	O16–Mo14–Mo13	135.67(2)
O47–Mo5–N15	159.2(2)	O16–Mo14–K32	68.90(4)
O51–Mo5–Mo4	100.3(2)	O16–Mo14–K8	36.4(2)
O51–Mo5–O19	93.6(2)	O16–Mo14–O45	72.03(7)
O51–Mo5–O21	105.1(2)	O16–Mo14–N13	82.4(2)
O51–Mo5–O41	160.9(2)	O26–Mo14–Mo13	99.08(9)
O51–Mo5–O47	106.0(2)	O26–Mo14–K32	26.1(2)
O51–Mo5–N15	93.4(3)	O26–Mo14–K8	64.3(2)
N15–Mo5–Mo4	136.03(7)	O26–Mo14–O15	104.1(2)
N15–Mo5–O41	74.0(2)	O26–Mo14–O16	94.8(2)
O11–Mo6–Mo7	49.28(4)	O26–Mo14–O42	105.8(2)
O11–Mo6–O19	88.20(9)	O26–Mo14–O45	161.5(2)
O11–Mo6–O41	84.20(8)	O26–Mo14–N13	89.2(2)
O11–Mo6–N16	160.3(2)	O42–Mo14–Mo13	48.93(4)
O18–Mo6–Mo7	48.87(5)	O42–Mo14–K32	105.92(4)

O18–Mo6–O11	95.5(2)	O42–Mo14–K8	113.1(2)
O18–Mo6–O19	158.9(2)	O42–Mo14–O16	86.79(8)
O18–Mo6–O41	88.7(2)	O42–Mo14–O45	86.89(7)
O18–Mo6–N16	86.1(2)	O42–Mo14–N13	162.3(2)
O19–Mo6–Mo7	137.36(3)	O45–Mo14–Mo13	99.45(3)
O19–Mo6–O41	70.99(7)	O45–Mo14–K32	137.84(4)
O19–Mo6–N16	83.6(2)	O45–Mo14–K8	98.55(9)
O41–Mo6–Mo7	97.69(2)	O45–Mo14–N13	76.41(9)
O54–Mo6–Mo7	99.8(2)	N13–Mo14–Mo13	139.26(7)
O54–Mo6–O11	105.4(2)	N13–Mo14–K32	83.28(7)
O54–Mo6–O18	104.8(2)	N13–Mo14–K8	64.5(2)
O54–Mo6–O19	94.2(2)	Mo16–Mo15–K8	146.1(2)
O54–Mo6–O41	162.4(2)	Mo16–Mo15–K8A	131.68(7)
O54–Mo6–N16	93.1(3)	O7–Mo15–Mo16	49.31(3)
N16–Mo6–Mo7	134.97(7)	O7–Mo15–K8	114.5(2)
N16–Mo6–O41	76.2(2)	O7–Mo15–K8A	108.58(5)
O1–Mo7–Mo6	137.25(3)	O7–Mo15–O16	88.13(8)
O1–Mo7–O39	71.71(7)	O7–Mo15–O45	86.75(8)
O1–Mo7–N11	82.1(2)	O7–Mo15–N1	161.8(2)
O11–Mo7–Mo6	48.86(4)	O16–Mo15–Mo16	137.35(2)
O11–Mo7–O1	88.59(9)	O16–Mo15–K8	45.9(2)
O11–Mo7–O39	86.52(8)	O16–Mo15–K8A	56.41(5)
O11–Mo7–N11	162.2(2)	O16–Mo15–O45	71.50(7)
O18–Mo7–Mo6	48.81(5)	O16–Mo15–N1	82.45(9)
O18–Mo7–O1	157.98(9)	O20–Mo15–Mo16	99.39(7)
O18–Mo7–O11	95.0(2)	O20–Mo15–K8	52.0(3)
O18–Mo7–O39	86.82(9)	O20–Mo15–K8A	38.28(8)
O18–Mo7–N11	88.3(2)	O20–Mo15–O7	104.9(2)
O28–Mo7–Mo6	100.3(2)	O20–Mo15–O16	93.7(2)
O28–Mo7–O1	95.0(2)	O20–Mo15–O45	161.1(2)
O28–Mo7–O11	106.0(2)	O20–Mo15–O46	105.0(2)
O28–Mo7–O18	104.8(3)	O20–Mo15–N1	91.2(2)
O28–Mo7–O39	161.8(2)	O45–Mo15–Mo16	99.47(2)
O28–Mo7–N11	89.9(2)	O45–Mo15–K8	109.8(2)
O39–Mo7–Mo6	97.97(2)	O45–Mo15–K8A	124.18(4)
O39–Mo7–N11	76.24(9)	O46–Mo15–Mo16	49.03(4)
N11–Mo7–Mo6	137.09(6)	O46–Mo15–K8	145.1(2)
O1–Mo8–Mo1	135.79(3)	O46–Mo15–K8A	139.51(6)
O1–Mo8–O39	71.37(7)	O46–Mo15–O7	95.61(9)
O1–Mo8–N8	83.7(2)	O46–Mo15–O16	159.16(9)
O5–Mo8–Mo1	49.34(3)	O46–Mo15–O45	88.20(9)
O5–Mo8–O1	86.53(8)	O46–Mo15–N1	88.0(2)
O5–Mo8–O39	87.17(8)	N1–Mo15–Mo16	137.05(5)
O5–Mo8–N8	161.9(2)	N1–Mo15–K8	69.0(2)
O13–Mo8–Mo1	48.86(5)	N1–Mo15–K8A	78.95(7)
O13–Mo8–O1	158.86(9)	N1–Mo15–O45	75.55(9)
O13–Mo8–O5	95.20(9)	O7–Mo16–Mo15	49.14(3)
O13–Mo8–O39	87.65(8)	O7–Mo16–O14	85.13(8)

O13–Mo8–N8	88.5(2)	O7–Mo16–O40	87.38(8)
O22–Mo8–Mo1	99.96(8)	O7–Mo16–N6	160.7(2)
O22–Mo8–O1	94.0(2)	O14–Mo16–Mo15	98.23(2)
O22–Mo8–O5	105.9(2)	O40–Mo16–Mo15	136.42(3)
O22–Mo8–O13	105.7(2)	O40–Mo16–O14	71.35(7)
O22–Mo8–O39	160.1(2)	O40–Mo16–N6	83.8(2)
O22–Mo8–N8	90.0(2)	O46–Mo16–Mo15	48.72(4)
O39–Mo8–Mo1	99.98(2)	O46–Mo16–O7	95.15(9)
O39–Mo8–N8	75.2(2)	O46–Mo16–O14	88.29(9)
N8–Mo8–Mo1	137.39(5)	O46–Mo16–O40	159.23(9)
Mo10–Mo9–K7A	75.81(7)	O46–Mo16–N6	87.3(2)
O14–Mo9–Mo10	100.18(3)	O53–Mo16–Mo15	100.17(8)
O14–Mo9–K7A	159.83(4)	O53–Mo16–O7	106.0(2)
O14–Mo9–N14	76.1(2)	O53–Mo16–O14	161.5(2)
O17–Mo9–Mo10	48.84(4)	O53–Mo16–O40	94.0(2)
O17–Mo9–K7A	102.41(5)	O53–Mo16–O46	105.0(2)
O17–Mo9–O14	88.72(9)	O53–Mo16–N6	91.8(3)
O17–Mo9–O40	159.80(9)	N6–Mo16–Mo15	136.04(6)
O17–Mo9–O43	95.35(9)	N6–Mo16–O14	75.8(2)
O17–Mo9–N14	89.5(2)	O43–Mo9–O40	87.45(8)
O40–Mo9–Mo10	136.64(3)	O43–Mo9–N14	162.5(2)
O40–Mo9–N14	82.4(2)	O50–Mo9–Mo10	99.03(9)
O43–Mo9–Mo10	49.25(4)	O43–Mo9–Mo10	49.25(4)
O43–Mo9–K7A	75.17(5)	O43–Mo9–K7A	75.17(5)
O40–Mo9–O14	71.41(7)		

Table S7. Selected hydrogen bond distances (Å) and angles (°) in $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2 \cdot 7H_2O$ (**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 $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**).

Atom–Atom	**Distances/Å**	**Atom–Atom**	**Distances/Å**
Mo1–Mo2	2.5661(2)	Mo2–O1	2.164(7)
Mo1–O11	2.173(7)	Mo2–O22	1.941(6)
Mo1–O22	1.944(6)	Mo2–O2	1.941(6)
Mo1–O2	1.944(6)	Mo2–O4	1.701(7)
Mo1–O3	1.711(7)	Mo2–N23	2.156(7)
Mo1–N12	2.169(7)	Mo2–N24	2.156(7)
Mo1–N1	2.169(7)		

Table S9. Selected bond angles (°) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**).

Atom–Atom–Atom	Angle/°	Atom–Atom–Atom	Angle/°
O11–Mo1–Mo2	105.41(9)	O22–Mo2–N23	164.6(2)
O22–Mo1–Mo2	48.62(7)	O2–Mo2–N24	164.6(2)
O2–Mo1–Mo2	48.62(7)	O4–Mo2–Mo1	97.6(3)
O2–Mo1–O11	89.5(2)	O4–Mo2–O1	158.4(3)
O22–Mo1–O11	89.5(2)	O4–Mo2–O2	106.1(2)
O22–Mo1–O2	93.0(3)	O4–Mo2–O22	106.1(2)
O22–Mo1–N12	164.0(2)	O4–Mo2–N23	88.6(2)
O22–Mo1–N1	86.2(3)	O4–Mo2–N24	88.6(2)
O2–Mo1–N12	86.2(3)	N23–Mo2–Mo1	135.1(2)
O2–Mo1–N1	164.0(2)	N24–Mo2–Mo1	135.1(2)
O3–Mo1–Mo2	97.0(3)	N24–Mo2–O1	76.2(2)
O3–Mo1–O11	157.6(3)	N23–Mo2–O1	76.2(2)
O3–Mo1–O22	105.7(2)	N23–Mo2–N24	89.2(4)
O3–Mo1–O2	105.7(2)	Mo2–O1–Mo14	119.4(3)
O3–Mo1–N1	89.8(2)	Mo2–O2–Mo1	82.7(3)
O3–Mo1–N12	89.8(2)	N2–N1–Mo1	124.3(4)
N12–Mo1–Mo2	134.56(9)	C1–N1–Mo1	129.0(7)
N1–Mo1–Mo2	134.56(9)	C1–N1–N2	106.7(7)
N1–Mo1–O11	74.56(9)	N1–N2–Mo21	122.6(4)
N12–Mo1–O11	74.56(9)	C3–N2–Mo21	130.9(7)
N12–Mo1–N1	90.1(4)	O22–Mo2–O1	88.5(2)
O1–Mo2–Mo1	103.97(8)	O2–Mo2–O22	93.2(4)
O2–Mo2–Mo1	48.71(7)	O2–Mo2–N23	86.8(3)
O22–Mo2–Mo1	48.71(7)	O22–Mo2–N24	86.8(3)
O2–Mo2–O1	88.5(2)		

Table S10. Selected hydrogen bond distances (Å) and angles (°) in $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-apz})_8]\cdot 20.5H_2O$ (**3**).

	D–H···A	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(°)
Intra	O1–H1···N1	0.85	1.99	2.630(2)	130
Intra	O1–H1···N2	0.85	2.05	2.664(2)	128
	N3–H3A···N3	0.88	2.28	2.961(2)	134
	N3–H3B···O3	0.88	2.48	3.108 (2)	129
	N3–H3B···O4	0.88	2.37	3.184 (2)	154

Symmetry codes: (a) *x*, -1 + *y*, *z*; (b) 1 + *x*, *y*, *z*; (c) *x,* 1 + *y, z*; (d) -1 + *x*, *y*, *z*; (e) 2 – *x*, 1 – *y*, 1 – *z*; (f) 1 – *x*, 1 – *y*, -*z*.

Table S11. Selected bond distances (Å) in $(Mo_8O_{26})_n \cdot 4n(3\text{-}H_2apz)$ (**4**).

Atom–Atom	Distances/Å	Atom–Atom	Distances/Å
Mo1–O5	1.902(4)	Mo3–O	1.903(4)
Mo1–O31	2.229(4)	Mo3–O12	1.692(5)
Mo1–O91	2.269(5)	Mo3–O16	1.726(4)
Mo1–O10	1.890(4)	Mo3–O42	2.078(4)
Mo1–O2	1.692(5)	Mo3–O51	2.125(4)
Mo1–O4	1.776(4)	Mo3–O61	2.300(4)
Mo2–O5	2.161(4)	Mo3–O	1.903(4)
Mo2–O6	1.880(4)	Mo3–O12	1.692(5)
Mo2–O3	1.767(5)	Mo4–O61	2.345(4)
Mo2–O91	1.935(5)	Mo4–O	1.923(5)
Mo2–O9	2.421(5)	Mo4–O91	2.205(5)
Mo2–O13	1.695(5)	Mo4–O10	2.003(5)
Mo3–O51	2.125(4)	Mo4–O15	1.718(5)
Mo3–O61	2.300(4)	Mo4–O17	1.703(5)

Table S12. Selected bond angles (°) in $(Mo_8O_{26})_n \cdot 4n(3\text{-}H_2apz)$ (**4**).

Atom–Atom	Angle/°	Atom–Atom	Angle/°
O5–Mo1–O31	81.12(7)	O–Mo4–O61	74.55(7)
O5–Mo1–O91	71.69(8)	O–Mo4–O91	85.93(8)
O31–Mo1–O91	71.80(7)	O–Mo4–O10	152.34(8)
O10–Mo1–O5	144.0(2)	O91–Mo4–O61	73.04(6)
O10–Mo1–O31	81.37(8)	O10–Mo4–O61	82.59(7)
O10–Mo1–O91	73.00(8)	O10–Mo4–O91	72.47(7)
O2–Mo1–O5	106.6(2)	O15–Mo4–O61	87.78(9)
O2–Mo1–O31	84.63(9)	O15–Mo4–O	101.4(2)
O2–Mo1–O91	156.4(2)	O15–Mo4–O91	157.0(2)
O2–Mo1–O10	102.8(2)	O15–Mo4–O10	92.9(2)
O2–Mo1–O4	104.5(2)	O17–Mo4–O61	166.2(2)
O4–Mo1–O5	96.05(9)	O17–Mo4–O	98.0(2)
O4–Mo1–O31	170.86(9)	O17–Mo4–O91	95.2(2)
O4–Mo1–O91	99.06(9)	O17–Mo4–O10	100.9(2)
O4–Mo1–O10	96.3(2)	O17–Mo4–O15	105.2(2)
O5–Mo2–O9	80.03(6)	Mo1–O5–Mo2	108.0(2)
O6–Mo2–O5	76.56(8)	Mo1–O5–Mo31	146.8(2)
O6–Mo2–O91	143.4(2)	Mo31–O5–Mo2	105.05(8)
O6–Mo2–O9	76.97(7)	Mo2–O6–Mo31	108.47(9)
O3–Mo2–O5	156.20(8)	Mo2–O6–Mo41	111.2(2)
O3–Mo2–O6	100.3(2)	Mo31–O6–Mo41	89.25(6)
O3–Mo2–O91	98.5(2)	Mo3–O–Mo4	117.0(2)
O3–Mo2–O9	76.29(7)	Mo2–O3–Mo11	117.9(2)
O91–Mo2–O5	73.63(8)	Mo11–O9–Mo2	93.98(7)
O91–Mo2–O9	77.4(2)	Mo21–O9–Mo11	102.69(9)
O13–Mo2–O5	100.1(2)	Mo21–O9–Mo2	102.6(2)
O13–Mo2–O6	102.7(2)	Mo21–O9–Mo41	151.6(3)
O13–Mo2–O3	103.6(2)	Mo41–O9–Mo11	94.96(8)
O13–Mo2–O91	103.0(2)	Mo41–O9–Mo2	98.07(7)
O13–Mo2–O9	179.6(2)	Mo1–O10–Mo4	115.8(2)
O51–Mo3–O61	69.07(6)	C3–N4–N5	108.1(6)
O–Mo3–O51	87.76(7)	C2–N5–N4	109.0(5)
O–Mo3–O61	76.01(8)	C26–N1–N28	107.9(6)
O–Mo3–O42	157.81(9)	C24–N28–N1	110.1(5)
O12–Mo3–O51	95.9(2)	N28–C24–N29	122.7(6)
O12–Mo3–O61	163.84(9)	N28–C24–C25	107.1(6)
O12–Mo3–O	98.1(2)	N29–C24–C25	130.2(7)
O12–Mo3–O16	105.7(2)	N4–C3–C22	109.7(6)
O12–Mo3–O42	99.5(2)	N5–C2–N23	121.7(6)
O16–Mo3–O51	155.5(2)	N5–C2–C22	108.1(6)
O16–Mo3–O61	90.20(9)	N23–C2–C22	130.2(7)
O16–Mo3–O	100.1(2)	C3–C22–C2	105.0(6)
O16–Mo3–O42	87.98(9)	N1–C26–C25	109.0(6)
O42–Mo3–O51	77.10(7)	C26–C25–C24	105.9(6)
O42–Mo3–O61	83.40(7)	Mo1–O4–Mo33	171.3(3)

O5–Mo1–O31	81.12(7)	O–Mo4–O61	74.55(7)
O5–Mo1–O91	71.69(8)	O–Mo4–O91	85.93(8)
O31–Mo1–O91	71.80(7)	O–Mo4–O10	152.34(8)
O10–Mo1–O5	144.0(2)	O91–Mo4–O61	73.04(6)
O10–Mo1–O31	81.37(8)	O10–Mo4–O61	82.59(7)
O10–Mo1–O91	73.00(8)	O10–Mo4–O91	72.47(7)
O2–Mo1–O5	106.6(2)	O15–Mo4–O61	87.78(9)
O2–Mo1–O31	84.63(9)	O15–Mo4–O	101.4(2)
O2–Mo1–O91	156.4(2)	O15–Mo4–O91	157.0(2)
O2–Mo1–O10	102.8(2)	O15–Mo4–O10	92.9(2)
O2–Mo1–O4	104.5(2)	O17–Mo4–O61	166.2(2)
O4–Mo1–O5	96.05(9)	O17–Mo4–O	98.0(2)
O4–Mo1–O31	170.86(9)	O17–Mo4–O91	95.2(2)
O4–Mo1–O91	99.06(9)	O17–Mo4–O10	100.9(2)
O4–Mo1–O10	96.3(2)	O17–Mo4–O15	105.2(2)
O5–Mo2–O9	80.03(6)	Mo1–O5–Mo2	108.0(2)
O6–Mo2–O5	76.56(8)	Mo1–O5–Mo31	146.8(2)
O6–Mo2–O91	143.4(2)	Mo31–O5–Mo2	105.05(8)
O6–Mo2–O9	76.97(7)	Mo2–O6–Mo31	108.47(9)
O3–Mo2–O5	156.20(8)	Mo2–O6–Mo41	111.2(2)
O3–Mo2–O6	100.3(2)	Mo31–O6–Mo41	89.25(6)
O3–Mo2–O91	98.5(2)	Mo3–O–Mo4	117.0(2)
O3–Mo2–O9	76.29(7)	Mo2–O3–Mo11	117.9(2)
O91–Mo2–O5	73.63(8)	Mo11–O9–Mo2	93.98(7)
O91–Mo2–O9	77.4(2)	Mo21–O9–Mo11	102.69(9)
O13–Mo2–O5	100.1(2)	Mo21–O9–Mo2	102.6(2)
O13–Mo2–O6	102.7(2)	Mo21–O9–Mo41	151.6(3)
O13–Mo2–O3	103.6(2)	Mo41–O9–Mo11	94.96(8)
O13–Mo2–O91	103.0(2)	Mo41–O9–Mo2	98.07(7)
O13–Mo2–O9	179.6(2)	Mo1–O10–Mo4	115.8(2)
O51–Mo3–O61	69.07(6)	C3–N4–N5	108.1(6)
O–Mo3–O51	87.76(7)	C2–N5–N4	109.0(5)
O–Mo3–O61	76.01(8)	C26–N1–N28	107.9(6)
O–Mo3–O42	157.81(9)	C24–N28–N1	110.1(5)
O12–Mo3–O51	95.9(2)	N28–C24–N29	122.7(6)
O12–Mo3–O61	163.84(9)	N28–C24–C25	107.1(6)
O12–Mo3–O	98.1(2)	N29–C24–C25	130.2(7)
O12–Mo3–O16	105.7(2)	N4–C3–C22	109.7(6)
O12–Mo3–O42	99.5(2)	N5–C2–N23	121.7(6)
O16–Mo3–O51	155.5(2)	N5–C2–C22	108.1(6)
O16–Mo3–O61	90.20(9)	N23–C2–C22	130.2(7)
O16–Mo3–O	100.1(2)	C3–C22–C2	105.0(6)
O16–Mo3–O42	87.98(9)	N1–C26–C25	109.0(6)
O42–Mo3–O51	77.10(7)	C26–C25–C24	105.9(6)
O42–Mo3–O61	83.40(7)	Mo1–O4–Mo33	171.3(3)
O5–Mo1–O31	81.12(7)	O–Mo4–O61	74.55(7)
O5–Mo1–O91	71.69(18)	O–Mo4–O91	85.93(8)
O31–Mo1–O91	71.80(17)	O–Mo4–O10	152.34(8)

O10–Mo1–O5	144.0(2)	O91–Mo4–O61	73.04(6)
O10–Mo1–O31	81.37(8)	O10–Mo4–O61	82.59(7)
O10–Mo1–O91	73.00(8)	O10–Mo4–O91	72.47(7)
O2–Mo1–O5	106.6(2)	O15–Mo4–O61	87.78(9)
O2–Mo1–O31	84.63(9)	O15–Mo4–O	101.4(2)
O2–Mo1–O91	156.4(2)	O15–Mo4–O91	157.0(2)
O2–Mo1–O10	102.8(2)	O15–Mo4–O10	92.9(2)
O2–Mo1–O4	104.5(2)	O17–Mo4–O61	166.2(2)
O4–Mo1–O5	96.05(9)	O17–Mo4–O	98.0(2)
O4–Mo1–O31	170.86(9)	O17–Mo4–O91	95.2(2)
O4–Mo1–O91	99.06(9)	O17–Mo4–O10	100.9(2)
O4–Mo1–O10	96.3(2)	O17–Mo4–O15	105.2(2)
O5–Mo2–O9	80.03(6)	Mo1–O5–Mo2	108.0(2)
O6–Mo2–O5	76.56(8)	Mo1–O5–Mo31	146.8(2)
O6–Mo2–O91	143.4(2)	Mo31–O5–Mo2	105.05(8)
O6–Mo2–O9	76.97(7)	Mo2–O6–Mo31	108.47(9)
O3–Mo2–O5	156.20(8)	Mo2–O6–Mo41	111.2(2)
O3–Mo2–O6	100.3(2)	Mo31–O6–Mo41	89.25(6)
O3–Mo2–O91	98.5(2)	Mo3–O–Mo4	117.0(2)
O3–Mo2–O9	76.29(7)	Mo2–O3–Mo11	117.9(2)
O91–Mo2–O5	73.63(8)	Mo11–O9–Mo2	93.98(7)
O91–Mo2–O9	77.4(2)	Mo21–O9–Mo11	102.69(9)
O13–Mo2–O5	100.1(2)	Mo21–O9–Mo2	102.6(2)
O13–Mo2–O6	102.7(2)	Mo21–O9–Mo41	151.6(3)
O13–Mo2–O3	103.6(2)	Mo41–O9–Mo11	94.96(8)
O13–Mo2–O91	103.0(2)	Mo41–O9–Mo2	98.07(7)
O13–Mo2–O9	179.6(2)	Mo1–O10–Mo4	115.8(2)
O51–Mo3–O61	69.07(6)	C3–N4–N5	108.1(6)
O–Mo3–O51	87.76(7)	C2–N5–N4	109.0(5)
O–Mo3–O61	76.01(8)	C26–N1–N28	107.9(6)
O–Mo3–O42	157.81(9)	C24–N28–N1	110.1(5)
O12–Mo3–O51	95.9(2)	N28–C24–N29	122.7(6)
O12–Mo3–O61	163.84(9)	N28–C24–C25	107.1(6)
O12–Mo3–O	98.1(2)	N29–C24–C25	130.2(7)
O12–Mo3–O16	105.7(2)	N4–C3–C22	109.7(6)
O12–Mo3–O42	99.5(2)	N5–C2–N23	121.7(6)
O16–Mo3–O51	155.5(2)	N5–C2–C22	108.1(6)
O16–Mo3–O61	90.20(9)	N23–C2–C22	130.2(7)
O16–Mo3–O	100.1(2)	C3–C22–C2	105.0(6)
O16–Mo3–O42	87.98(9)	N1–C26–C25	109.0(6)
O42–Mo3–O51	77.10(7)	C26–C25–C24	105.9(6)
O42–Mo3–O61	83.40(7)	Mo1–O4–Mo33	171.3(3)

Table S13. Selected hydrogen bond distances (Å) and angles (°) in $(Mo_8O_{26})_n \cdot 4n(3\text{-}H_2apz)$ (**4**).

	D–H···A	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(°)
Intra	N4–H4···O16[a]	0.88	2.03	2.852(8)	155
Intra	N5–H5···O10	0.88	1.80	2.671(7)	171
	N1–H1···O15[b]	0.88	2.07	2.813(8)	142
	N28–H28···O6	0.88	1.88	2.740(7)	165

Symmetry codes: (a) 2 – *x*,1 - *y*, 2 – *z*; (b) -1 + *x*,+*y*,-1 + *z*;

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

Complexes	Atoms	N	$\sum S_{ij}$	Δ
$Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 26H_2O$ (**1**)	Mo1	**5+**	**5.113**	**0.113**
	Mo2	**5+**	**5.232**	**0.232**
	Mo3	**5+**	**5.288**	**0.288**
	Mo4	**5+**	**5.264**	**0.264**
	Mo5	**5+**	**5.203**	**0.203**
	Mo6	**5+**	**5.075**	**0.075**
	Mo7	**5+**	**5.098**	**0.098**
	Mo8	**5+**	**5.263**	**0.263**
		5+	**5.192_{av}**	**0.192_{av}**
$K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2\cdot 7H_2O$ (**2**)	Mo1	**5+**	**5.274**	**0.274**
	Mo2	**5+**	**5.225**	**0.225**
	Mo3	**5+**	**5.244**	**0.244**
	Mo4	**5+**	**5.209**	**0.209**
	Mo5	**5+**	**5.144**	**0.144**
	Mo6	**5+**	**5.199**	**0.199**
	Mo7	**5+**	**5.183**	**0.183**
	Mo8	**5+**	**5.198**	**0.198**
		5+	**5.209_{av}**	**0.209_{av}**
$(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**)	Mo1	**5+**	**5.236**	**0.236**
	Mo2	**5+**	**5.236**	**0.236**
		5+	**5.236_{av}**	**0.236_{av}**
$(Mo_8O_{26})_n\cdot 4n(3\text{-}H_2apz)$ (**4**)	Mo1	**6+**	**6.067**	**0.067**
	Mo2	**6+**	**5.986**	**0.014**
	Mo3	**6+**	**5.965**	**0.035**
	Mo4	**6+**	**5.887**	**0.113**
		6+	**5.976_{av}**	**0.976_{av}**

Table S15 Comparisons of CO_2 adsorption data for **1**, **2** and **3** with some typical MOFs at 1 bar, 298 K.

Adsorbents	Common name	Amounts ($mmol \cdot g^{-1}$)
1	—	0.051
2	—	0.044
3	—	0.030
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; TCPBDA2 = N,N,N',N' -tetrakis(4--carboxyphenyl)-b iphenyl-4'4-diamine; DOBDC = 2,5-dioxido--1,4-benzenedicarboxylate

References

1. E. D. Bloch, D. Britt, C. Lee, C. J. Doonan, F. J. Uribe-Romo, H. Furukawa, J. R. Long and O. M. Yaghi, *J. Am. Chem. Soc.*, 2010, **132**, 14382–14384.
2. A. Phan, C. J. Doonan, F. J. Uribe-Romo, C. B. Knobler, M. O'Keeffe and O. M. Yaghi, *Accounts Chem. Res.*, 2010, **43**, 58–67.
3. F. Debatin, A. Thomas, A. Kelling, N. Hedin, Z. Bacsik, I. Senkovska, S. Kaskel, M. Junginger, H. Müller, U. Schilde, C. Jäger, A. Friedrich and H.-J. Holdt, *Angew. Chem. Int. Edit.*, 2010, **49**, 1258–1262.
4. M. Du, C. P. Li, M. Chen, Z. W. Ge, X. Wang, L. Wang and C. S. Liu, *J. Am. Chem. Soc.*, 2014, **136**, 10906–10909.
5. Y. E. Cheon, J. Park and M. P. Suh, *Chem. Commun.* , 2009, **36**, 5436–5438.
6. W. Lou, J. Yang, L. Li and J. Li, *J. Solid. State. Chem.*, 2014, **213**, 224–228.

Table S16. Detail calibrated adsorption data of O_2, CH_4, H_2, N_2 and CO_2 for $Na_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2 \cdot 26H_2O$ (**1**) at 298 K.

Gases	O_2		CO_2		CH_4		N_2		H_2	
Temperature (^oC)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)
25.0	0	0	0	0	0	0	0	0	0	0
	0.9	3.12896	0.9	2.26296	0.9	0.29402	0.9	1.61535	0.9	1.06597
	1.9	4.41539	1.9	5.24443	1.9	0.42723	1.9	1.84907	1.9	1.13681
	3.9	6.71136	3.9	6.75948	3.9	0.42634	3.9	1.82816	3.9	1.51252
	5.9	8.83502	5.9	8.83305	5.9	0.49042	5.9	2.09596	5.9	1.68547
	7.9	11.28441	7.9	10.0279	7.9	0.63139	7.9	2.2997	7.9	1.79344
	9.899	13.00532	9.899	10.51599	9.899	0.75219	9.899	2.29942	9.899	1.86436
	11.898	16.03821	11.898	12.38129	11.898	0.8594	11.898	2.56169	11.898	1.97806
	13.897	18.09408	13.897	12.76031	13.897	0.92508	13.897	2.68969	13.897	2.11509
	15.898	20.46554	15.898	14.61157	15.898	0.98235	15.898	2.81044	15.898	1.96378
	17.892	22.78616	17.892	14.6307	17.892	0.10458	17.892	2.54029	17.892	2.10285
	19.894	24.79334	19.894	16.17265	19.894	1.11984	19.894	2.73852	19.894	1.94762
	21.894	27.21597	21.894	16.4973	21.894	1.22295	21.894	2.78228	21.894	2.16093
	23.897	29.36634	23.897	17.1501	23.897	1.25047	23.897	2.94039	23.897	2.25783
	25.891	31.14864	25.891	19.4883	25.891	1.35201	25.891	2.96055	25.891	2.28429
	27.897	33.36281	27.897	20.37474	27.897	1.73615	27.897	2.96055	27.897	2.42783
	29.896	35.70517	29.896	21.12056	29.896	1.98079	29.896	3.32752	29.896	2.3886

Table S17. Detail calibrated adsorption data of O_2, CH_4, H_2, N_2 and CO_2 for $K_8[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_8(3\text{-}apz)_4]_2 \cdot 7H_2O$ (**2**) at 298 K.

Gases	O_2		CO_2		CH_4		N_2		H_2	
Temperature (^oC)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)
25.0	0	0	0	0	0	0	0	0	0	0
	0.9	1.90564	0.9	1.93188	0.9	0.17755	0.9	1.30711	0.9	1.0482
	1.9	2.34313	1.9	4.46665	1.9	0.41781	1.9	1.71385	1.9	1.36448
	3.9	3.9577	3.9	6.54667	3.9	0.50646	3.9	1.74209	3.9	1.57429
	5.899	5.25999	5.899	8.63235	5.899	0.61781	5.899	1.6044	5.899	1.67095
	7.899	6.73363	7.899	10.28668	7.899	0.77755	7.899	1.76292	7.899	1.6949
	9.901	8.29548	9.901	10.89093	9.901	0.8957	9.901	1.76293	9.901	1.98097
	11.898	9.67019	11.898	11.63851	11.898	1.22909	11.898	1.80255	11.898	2.01146
	13.898	11.00709	13.898	12.85041	13.898	1.46978	13.898	1.83216	13.898	1.96403
	15.896	12.19266	15.896	13.70906	15.896	1.73113	15.896	1.85216	15.896	1.86834
	17.898	13.73702	17.898	13.94952	17.898	1.82363	17.898	1.88002	17.898	1.78302
	19.899	15.09458	19.899	14.12219	19.899	2.08517	19.899	1.92421	19.899	2.00387
	21.901	16.34802	21.901	14.37056	21.901	2.28722	21.901	2.03192	21.901	2.10909
	23.898	17.44163	23.898	14.45098	23.898	2.32213	23.898	2.13192	23.898	2.59101
	25.901	18.90777	25.901	14.62885	25.901	2.37824	25.901	2.28663	25.901	2.63133
	27.899	20.36395	27.899	14.94952	27.899	2.48864	27.899	2.29481	27.899	2.78893
	29.899	21.79289	29.899	15.04952	29.899	2.60172	29.899	2.31928	29.899	3.18588

Table S18 Detail calibrated adsorption data of O_2, CH_4, H_2, N_2 and CO_2 for $(NH_4)_4[Mo_8O_8(\mu_2\text{-}O)_8(\mu_2\text{-}OH)_4(3\text{-}apz)_8]\cdot 20.5H_2O$ (**3**) at 298 K.

Gases	O_2		CO_2		CH_4		N_2		H_2	
Temperature (^oC)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)	Pressure (bar)	Adsorption (mg/g)
25.0	0	0	0	0	0	0	0	0	0	0
	0.9	3.12896	0.9	1.32099	0.9	0.29402	0.9	1.82273	0.9	1.0967
	1.9	4.41539	1.9	4.52066	1.9	0.42723	1.9	2.31918	1.9	1.1027
	3.9	6.71136	3.9	6.71786	3.9	0.42634	3.9	2.43304	3.9	1.30016
	5.9	8.83502	5.9	8.7988	5.9	0.49042	5.9	2.3022	5.9	1.42839
	7.896	11.28441	7.896	10.89091	7.896	0.63139	7.896	2.07722	7.896	1.51916
	9.896	13.00532	9.896	12.01432	9.896	0.75219	9.896	2.94041	9.896	1.62
	11.897	16.03821	11.897	12.2066	11.897	0.8594	11.897	2.66057	11.897	1.6468
	13.893	18.09408	13.893	13.55591	13.893	0.92508	13.893	3.0166	13.893	1.7851
	15.896	20.46554	15.896	13.71729	15.896	0.98235	15.896	3.13906	15.896	1.81732
	17.896	22.78616	17.896	14.73724	17.896	0.10458	17.896	3.01442	17.896	1.83418
	19.895	24.79334	19.895	15.08271	19.895	1.11984	19.895	2.89226	19.895	1.79702
	21.894	27.21597	21.894	15.68434	21.894	1.22295	21.894	2.88822	21.894	1.9948
	23.897	29.36634	23.897	16.06625	23.897	1.25047	23.897	3.11785	23.897	1.66251
	25.895	31.14864	25.895	16.42758	25.895	1.35201	25.895	2.71309	25.895	1.64418
	27.894	33.36281	27.894	17.3163	27.894	1.73615	27.894	2.63758	27.894	1.70475
	29.897	35.70517	29.897	18.21973	29.897	1.98079	29.897	2.44146	29.897	1.7183