Supporting materials

Crown ethers-like discrete clusters for sodium binding and gas adsorptions

Lan Deng,[a] Deng-Hui Ma,[a,b] Zhen-Lang Xie,[a] Rong-Yan Lin,[a] Zhao-Hui Zhou*,[a]

[a]*State Key Laboratory of Physical Chemistry of Solid Surfaces and Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, 361005, China, Tel: + 86-592-2184531; Fax: + 86-592-2183047* zhzhou@xmu.edu.cn
[b]*Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, Xiamen University*

Figure and Table Options

Figure S1. (a) Perspective view of $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**); 2D layered diagrams of $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**) in *a* (b) and *b* (c) axes respectively. Violet polyhedra represent Mo−O/N centers.

Figure S2. (a) The smallest asymmetric unit of the molecule in $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**); (b) Perspective view of $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), free and disordered water molecules were omitted for clarity. 2D packing diagrams of $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**) in *b* (c) and *c* (d) axes respectively.

Figure S3. (a) The smallest asymmetric unit of the molecule in $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**); (b) Perspective view of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**), free and disordered water molecules were omitted for clarity. 2D packing diagrams of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) in *a* (c) and *b* (d) axes respectively.

Figure S4. (a) Perspective view of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**), free and disordered water molecules were omitted for clarity. Packing diagrams of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) in *b* (b) and *c* (c) axes respectively.

Figure S5. MOF-like simplified topological nets in **1** ~ **4** in the *c*- (a ~ c) and *a*- (d) directions respectively. All spheres represent an integral Mo_6 unit.

Figure S6. Gases adsorption isotherms of $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**) at 298 K at different pressures for O_2 (a), CO_2 (b), H_2 (c), CH_4 (d), N_2 (e) respectively.

Figure S7. Gases adsorption isotherms of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) at 298 K at different pressures for O_2 (a), CO_2 (b), H_2 (c), CH_4 (d), N_2 (e) respectively.

Figure S8. Gases adsorption isotherms of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) at 298 K at different pressures for O_2 (a), CO_2 (b), H_2 (c), CH_4 (d), N_2 (e) respectively.

Figure S9. O_2 and CO_2 adsorption isotherms for **2** ~ **4** (a ~ c) respectively at 298 K and pressures of up to 1 bar.

Figure S10. N_2 adsorption-desorption isotherms of **2** ~ **4** at 77 K respectively.

Figure S11. Pore distributions for samples **2** ~ **4** using original H-K methods.

Figure S12. The SEM images of samples **2** ~ **4** (a ~ c) after gas adsorptions.

Figure S13. (a) TGA of $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**); (b) TGA of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**); (c) TGA of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) respectively.

Figure S14. Powder XRD curves for $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**, a), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**, b) and $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**, c) respectively.

Figure S15. IR spectra of $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) and $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) respectively.

Figure S16. FT-IR spectrum of 1H-1,2,3-triazole [$C_2H_3N_3$] in KBr plate.

Figure S17. Diffused reflectance spectra of solids $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) and $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) respectively.

Figure S18. EPR spectra of solids **2** ~ **4** (a ~ c) at 110 K respectively.

Figure S19. Solution ^{13}C NMR spectrum of pure trz.

Figure S20. Optimized individual conformers of **1-1** ~ **4-1** (a ~ d) respectively.

Figure S21. Local density of state (LDOS) and total density of state (TDOS) plots for compounds **1** ~ **4** (a ~ d), respectively.

Table S1. Crystallographic data and structural refinements for complexes $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**), $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) and $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) respectively.

Table S2. Selected hydrogen bond distances (Å) and angles (°) in $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**).

Table S3. Selected hydrogen bond distances (Å) and angles (°) in $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**).

Table S4. Comparisons of Na–O distances in **2** ~ **4** and some classical crown ethers.

Table S5. Selected bond distances (Å) and angles (°) in $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**).

Table S6. Selected bond distances (Å) and angles (°) in $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**).

Table S7. Selected bond distances (Å) and angles (°) in $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**).

Table S8. Selected bond distances (Å) and angles (°) in $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**).

Table S9. Comparisons of selected bond distances (Å) for $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**), $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**), $Na_3[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_3(trz)_3]\cdot 7.5H_2O$ (**5**),[1] $[Mo_8O_8(\mu_2\text{-}O)_{12}(Htrz)_8]\cdot 30H_2O$ (**6**),[1] $[Mo_8O_8(\mu_2\text{-}O)_{12}(Htrz)_8]\cdot 62H_2O$ (**7**),[2] $[MoO_3(1,2,3\text{-}Htrz)_{0.5}]$ (**8**),[3] $[Cu_3(Htrz)_2Mo_4O_{13}(OH)]\cdot 6H_2O$ (**9**),[3] $H_2[Cu_4(trz)_5(H_2O)_2][Mo_4Cu_4O_{26}]_{0.5}\cdot 3H_2O$ (**10**),[4] $[Cu_{24}(trz)_{16}(H_2O)Cl_4(HPMo_{12}O_{40})]$ (**11**),[5] Cu(trz) (**12**),[3] $[Cu_6(trz)_3I_3]_n$ (**13**),[6] $(Cu_5I_5)[Cu(trz)_2]^-$ (**14**),[7] $[Cu(trz)_2]$ (**15**),[8] $[Cu_3(trz)_2V_4O_{12}]$ (**16**),[9] $[Zn_{10}(trz)_{12}(TADIPA)_2(DMF)_4]\cdot DMF\cdot 6H_2O$ (**17**),[10] $[Zn_{10}(trz)_{12}(TPTA)_2(DMA)_2]\cdot 2DMA\cdot 4H_2O$ (**18**),[10] $[(Zn_3OH)_2(trz)_6\cdot Zn_6(OHOBDC)_6]\cdot 2NH_2(CH_3)_2$ (**19**),[11] $[(Zn_3OH)_2(trz)_6\cdot Zn_6(OBDC)_6]\cdot 2NH_2(CH_3)_2$ (**20**),[11] $[Zn_3(tp)_2(trz)_2]_n$ (**21**),[12] $Zn_5(trz)_6(NO_3)_4$ (**22**),[13] $Zn_3(trz)_2(bdc)_2\cdot 2DMAc$ $C_6H_4(OH)_2$ (**23**),[13] $[Ag_{29}(trz)_{18}][SiW_7W_5O_{40}](Ag_{29}SiW_{12})$ (**24**),[14] $H[Ag_{27}(trz)_{16}(H_2O)_4][(AsW_{12}O_{40})_2]$ (**25**),[15] $[Ag_{15}(trz)_8][AsW_{12}O_{40}]$ (**26**),[15] $H_3[Ag_{27}(trz)_{16}(H_2O)_6][SiW_{12}O_{40}]_2\cdot 5H_2O$ (**27**),[16] $H[Ag_{27}(trz)_{16}(H_2O)_4][PW_{12}O_{40}]_2\cdot 2H_2O$ (**28**),[16] $[Ag_{23}(trz)_{14}(H_2O)_2][HSiW_{12}O_{40}]$ (**29**),[16] $[Ag_{23}(trz)_{14}(H_2O)_2][PW_{12}O_{40}]$ (**30**),[16] $[Cd_3(trz)_3Cl_3]_n$ (**31**),[6] $\{[Cd_3(trz)_6]\cdot 6H_2O\}_n$ (**32**),[6] $Cd[HB(trz)_3]_2$ (**33**).[17]

Table S10. Detail calibrated adsorption data of O_2, N_2, H_2, CO_2 and CH_4 for $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**) at 298 K.

Table S11. Detail calibrated adsorption data of O_2, N_2, H_2, CO_2 and CH_4 for $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) at 298 K.

Table S12. Detail calibrated adsorption data of O_2, N_2, H_2, CO_2 and CH_4 for $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) at 298 K.

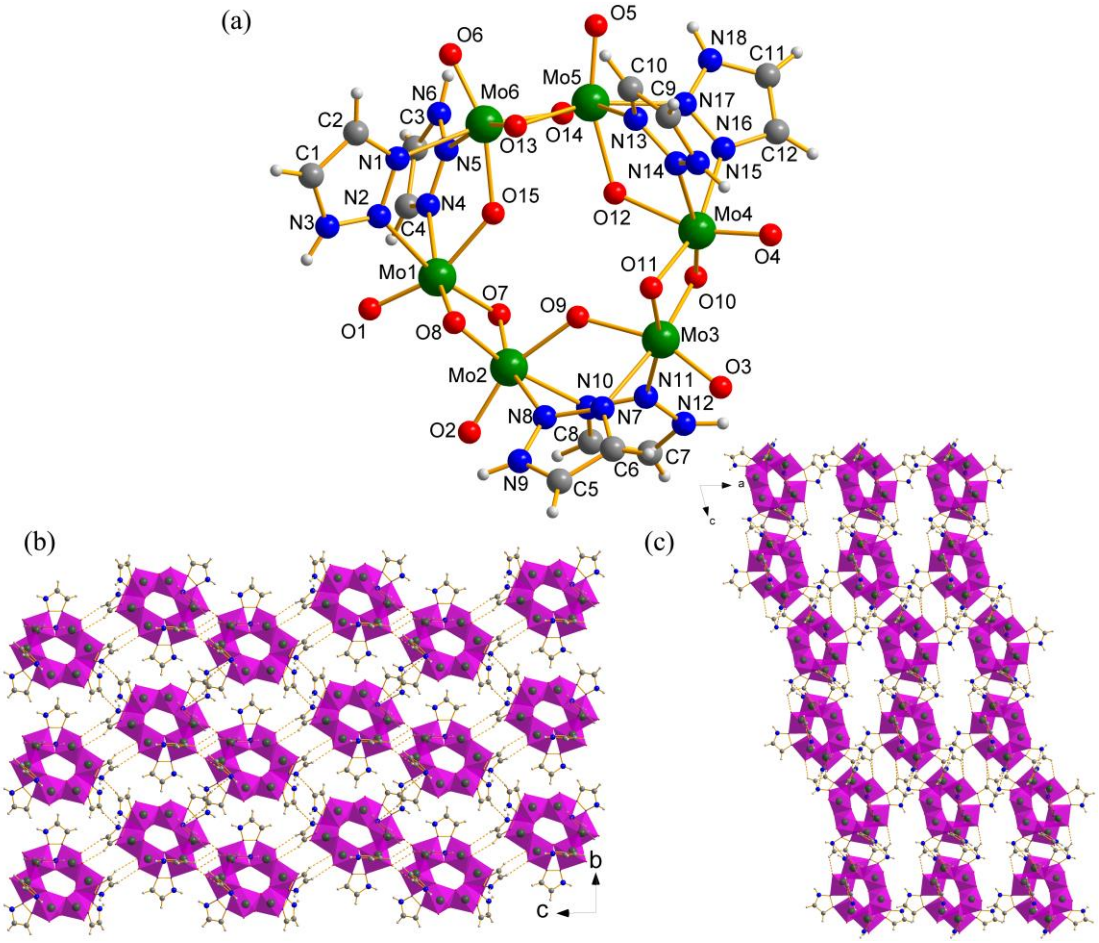
Table S13. Comparisons of O_2 and CO_2 adsorption data for **2** ~ **4** with some other reported porous materials at 1.0 bar under different temperatures.

Table S14. Bond valence calculations for complexes $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**), $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) and $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) respectively.

Table S15. Selected average bond lengths (Å) and NPA charge of different N donor and Mo atoms in the optimized individual conformers of **1-1** ~ **4-1**

complexes calculated at the B3LYP/def2SVP/LANL2DZ level of theory.

Table S16. Geometry optimized coordinates for compounds **1** ~ **4** and **1-1** ~ **4-1**, respectively.



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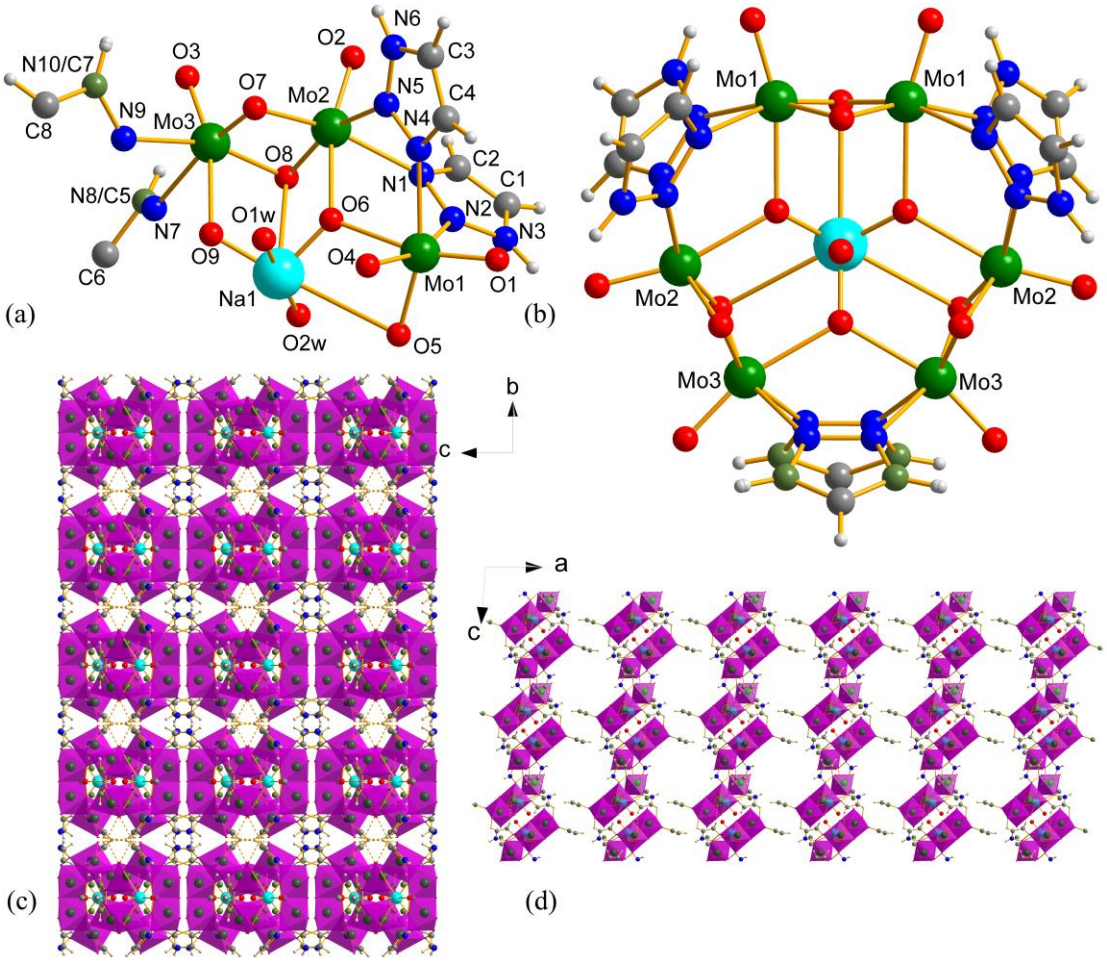


Figure S2. (a) The smallest asymmetric unit of the molecule in $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**); (b) Perspective view of $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), free and disordered water molecules were omitted for clarity. 2D packing diagrams of $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**) in *b* (c) and *c* (d) axes respectively.

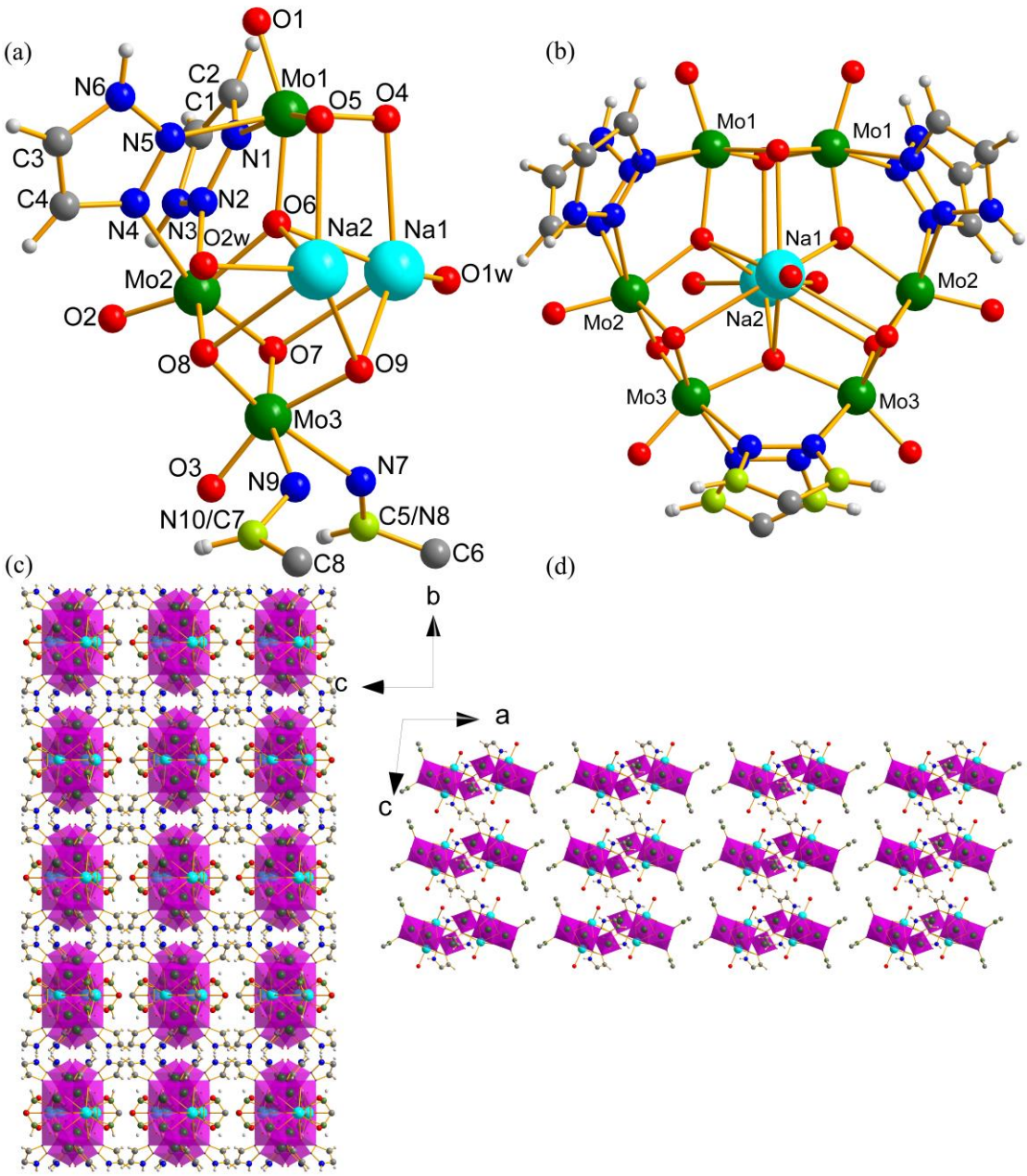
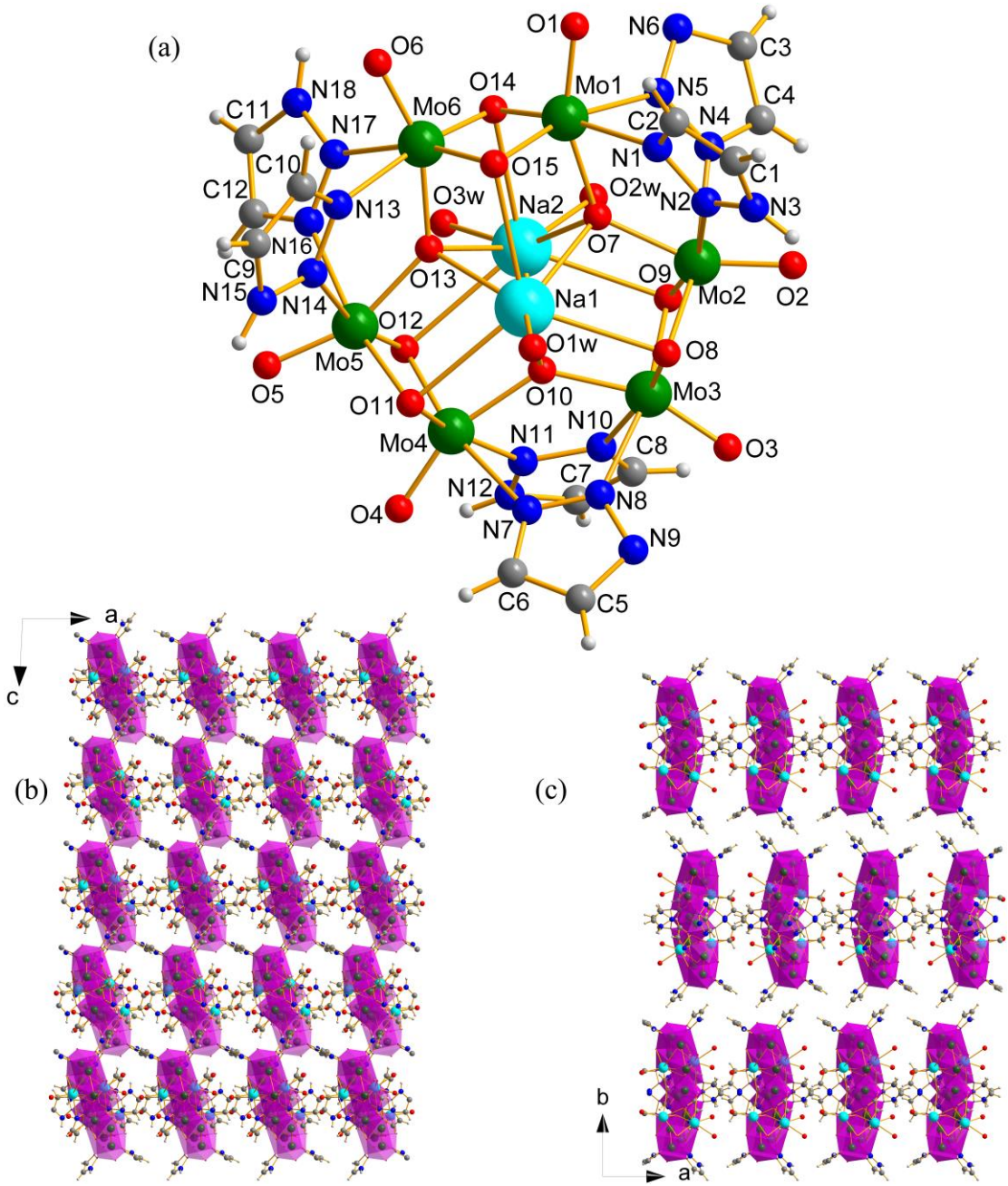


Figure S3. (a) The smallest asymmetric unit of the molecule in $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**); (b) Perspective view of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**), free and disordered water molecules were omitted for clarity. 2D packing diagrams of $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) in *a* (c) and *b* (d) axes respectively.



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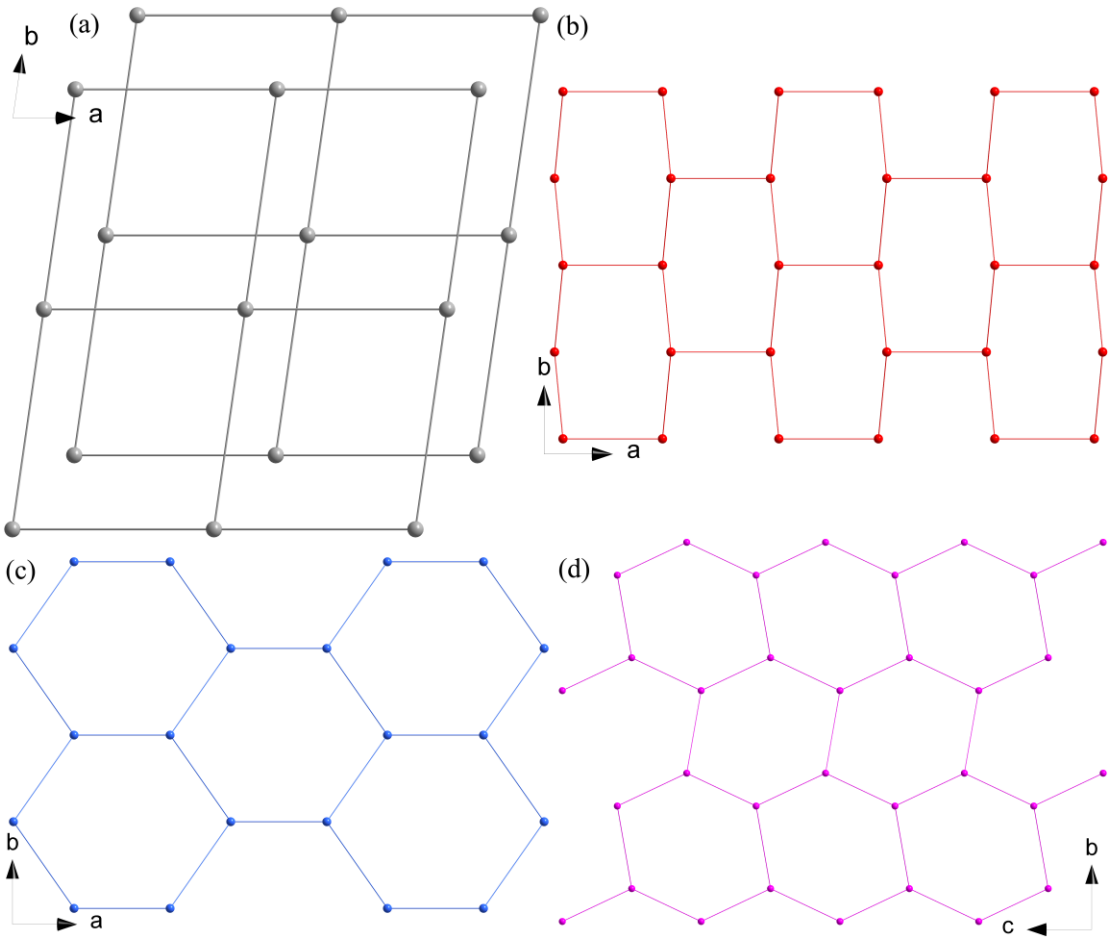


Figure S5. MOF-like simplified topological nets in **1** ~ **4** in the *c*- (a ~ c) and *a*- (d) directions respectively. All spheres represent an integral Mo_6 unit.

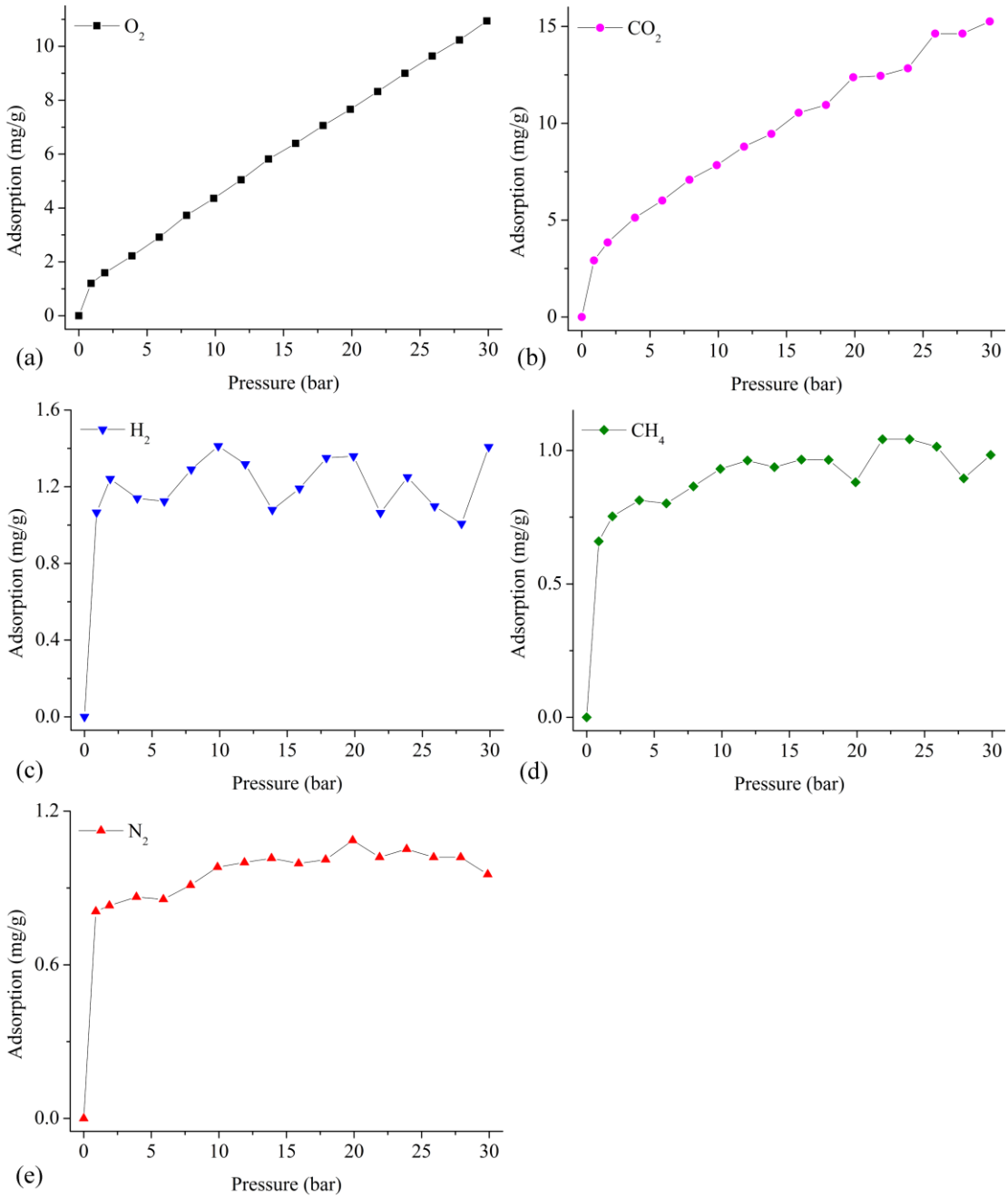
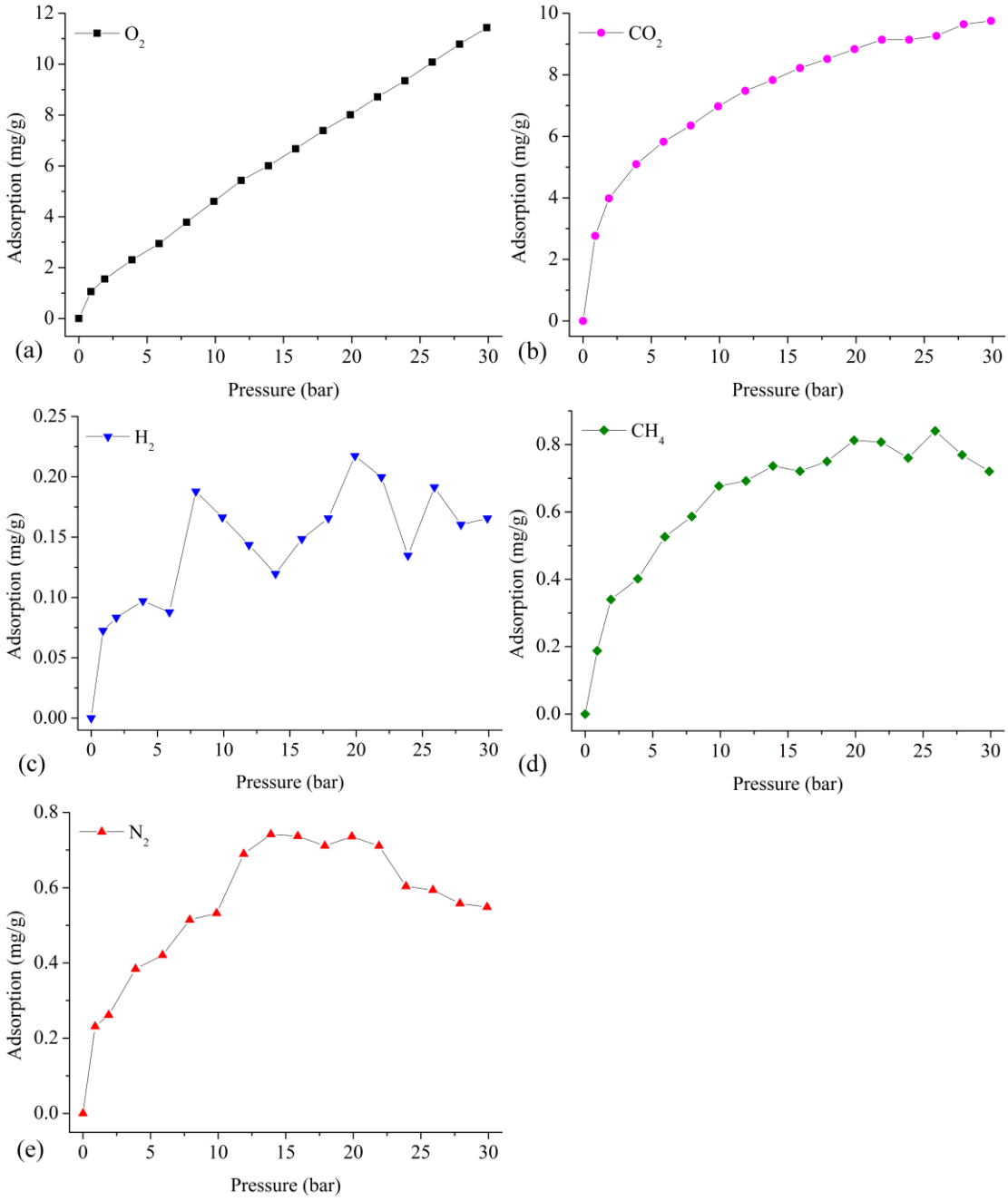


Figure S6. Gases adsorption isotherms of $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**) at 298 K at different pressures for O_2 (a), CO_2 (b), H_2 (c), CH_4 (d), N_2 (e) respectively.



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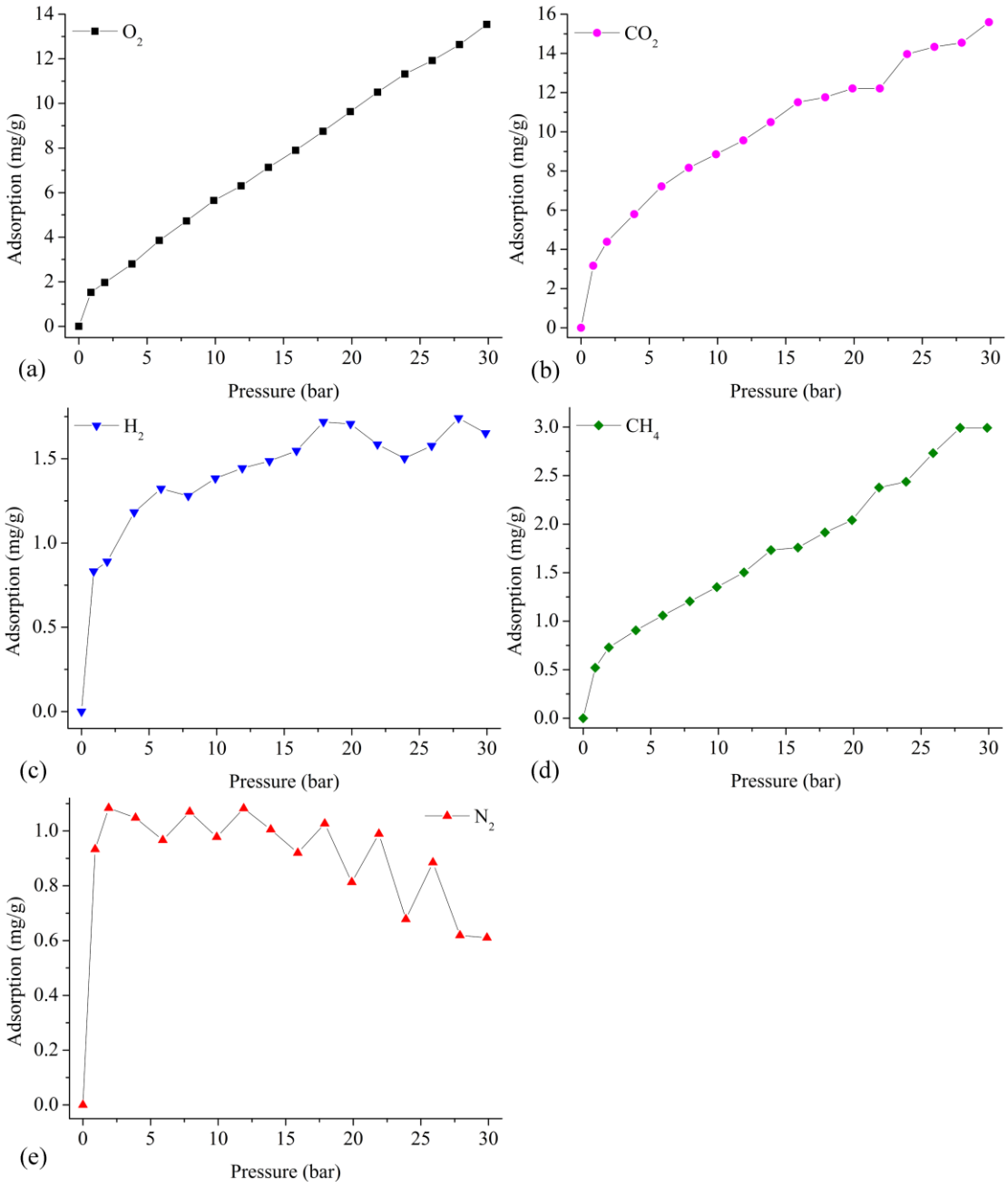

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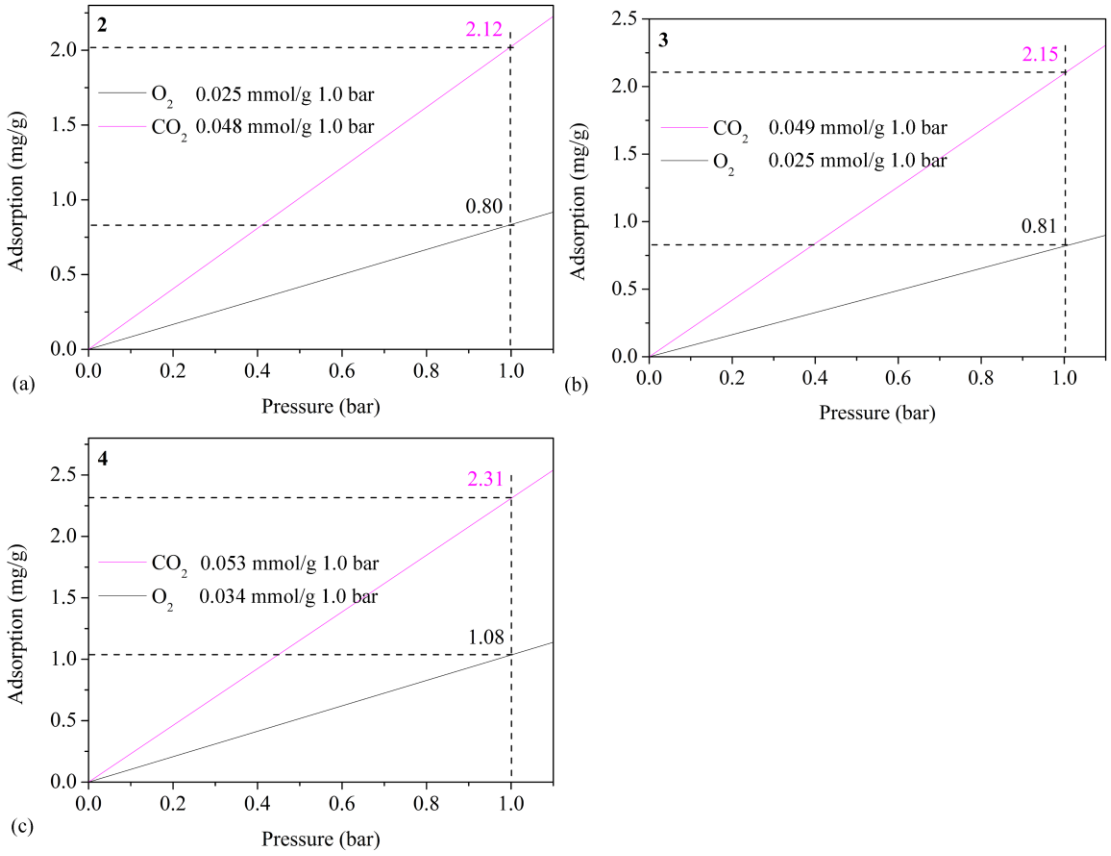


Figure S9. O_2 and CO_2 adsorption isotherms for **2** ~ **4** (a ~ c) respectively at 298 K and pressures of up to 1 bar.

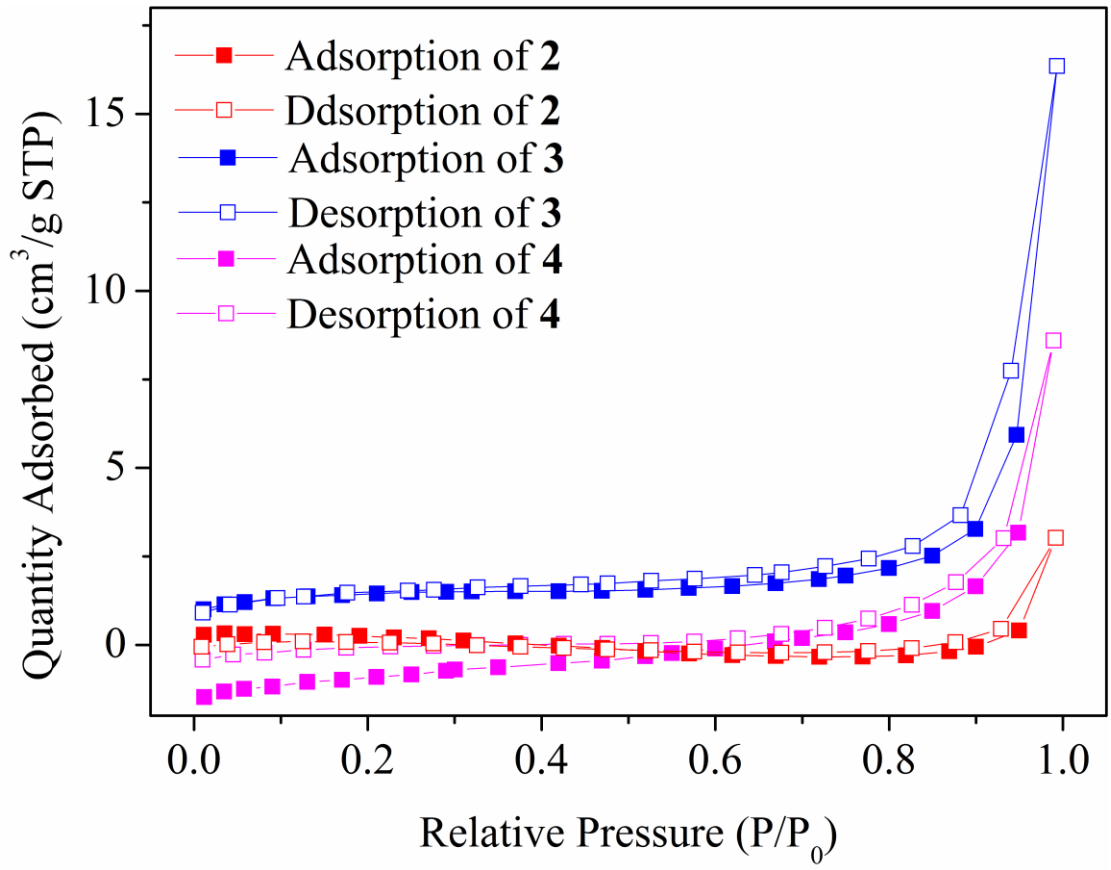


Figure S10. N_2 adsorption-desorption isotherms of **2** ~ **4** at 77 K respectively.

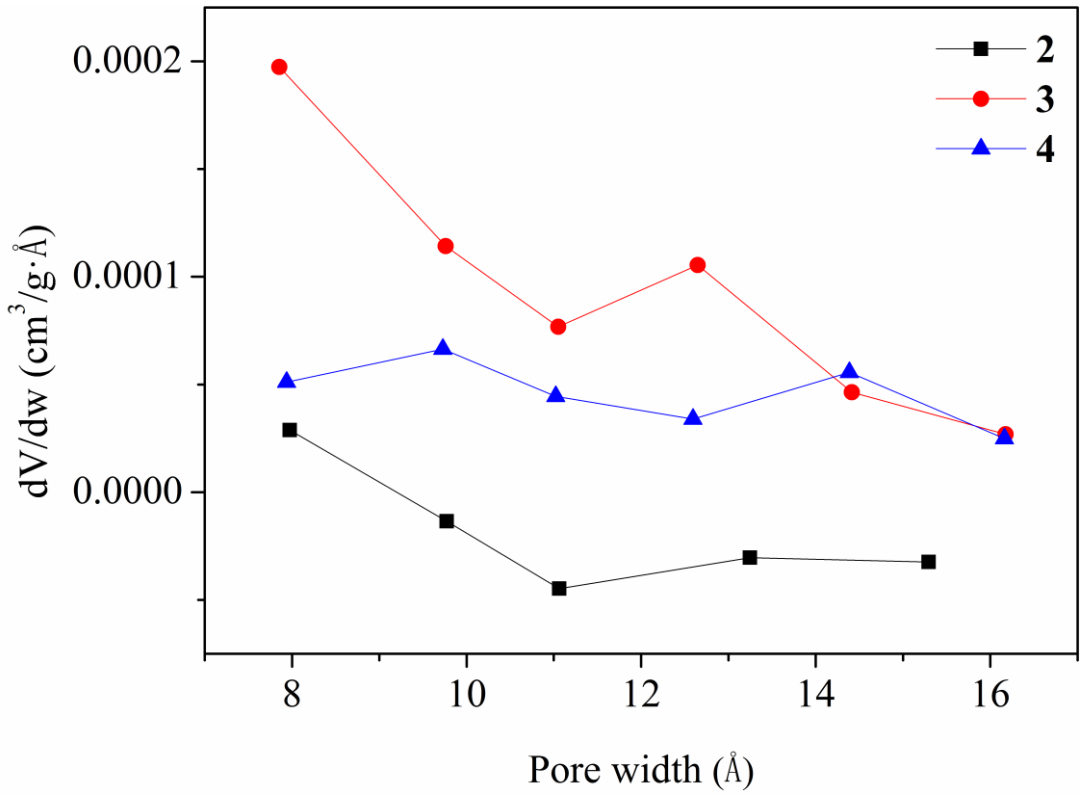


Figure S11. Pore distributions for samples **2** ~ **4** using original H-K methods.

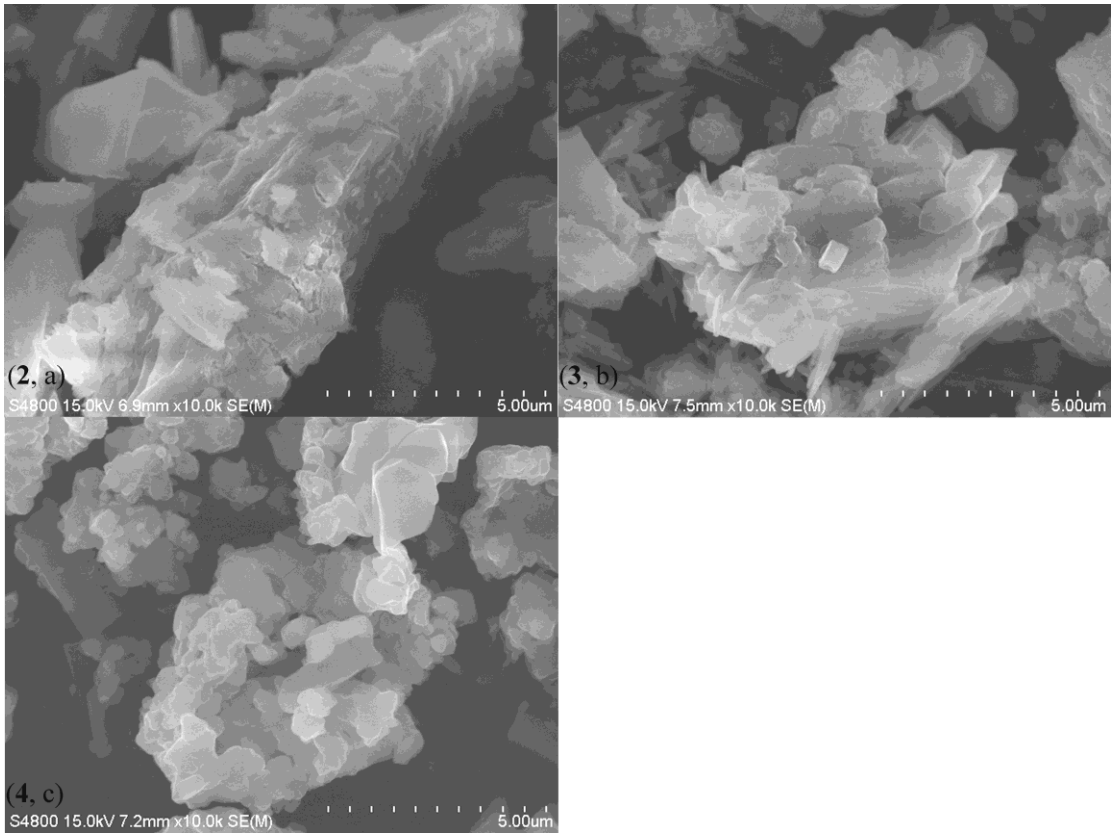
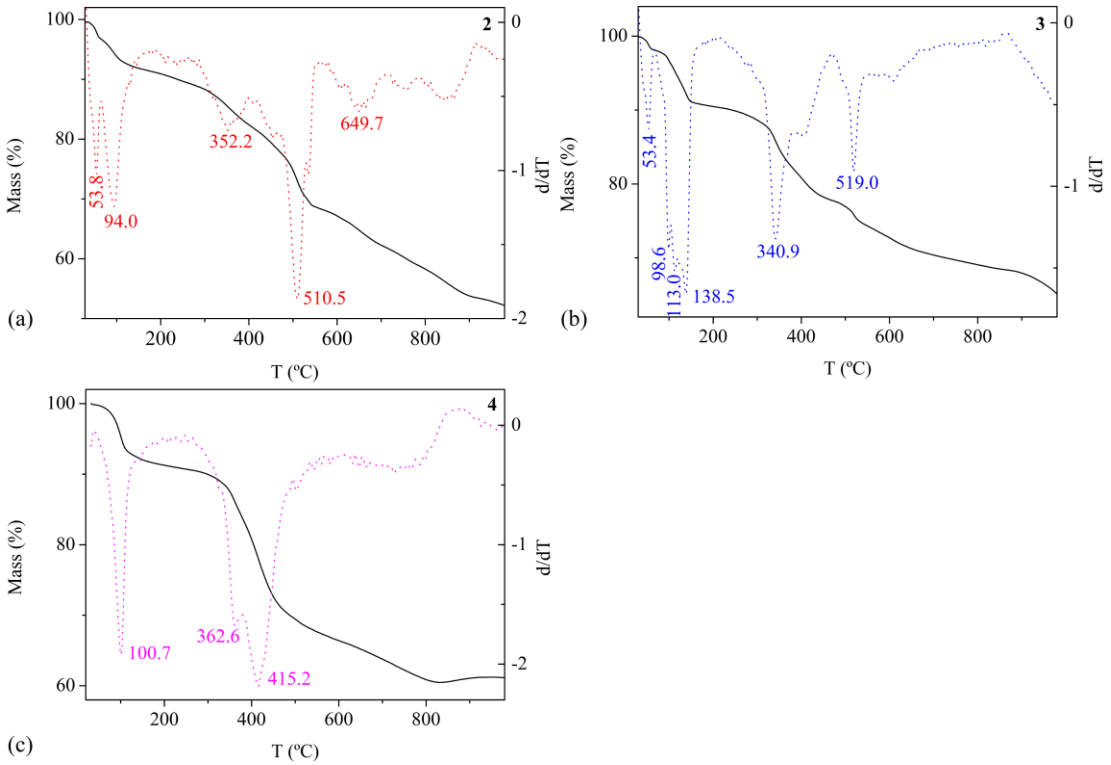


Figure S12. The SEM images of samples **2** ~ **4** (a ~ c) after gas adsorptions.



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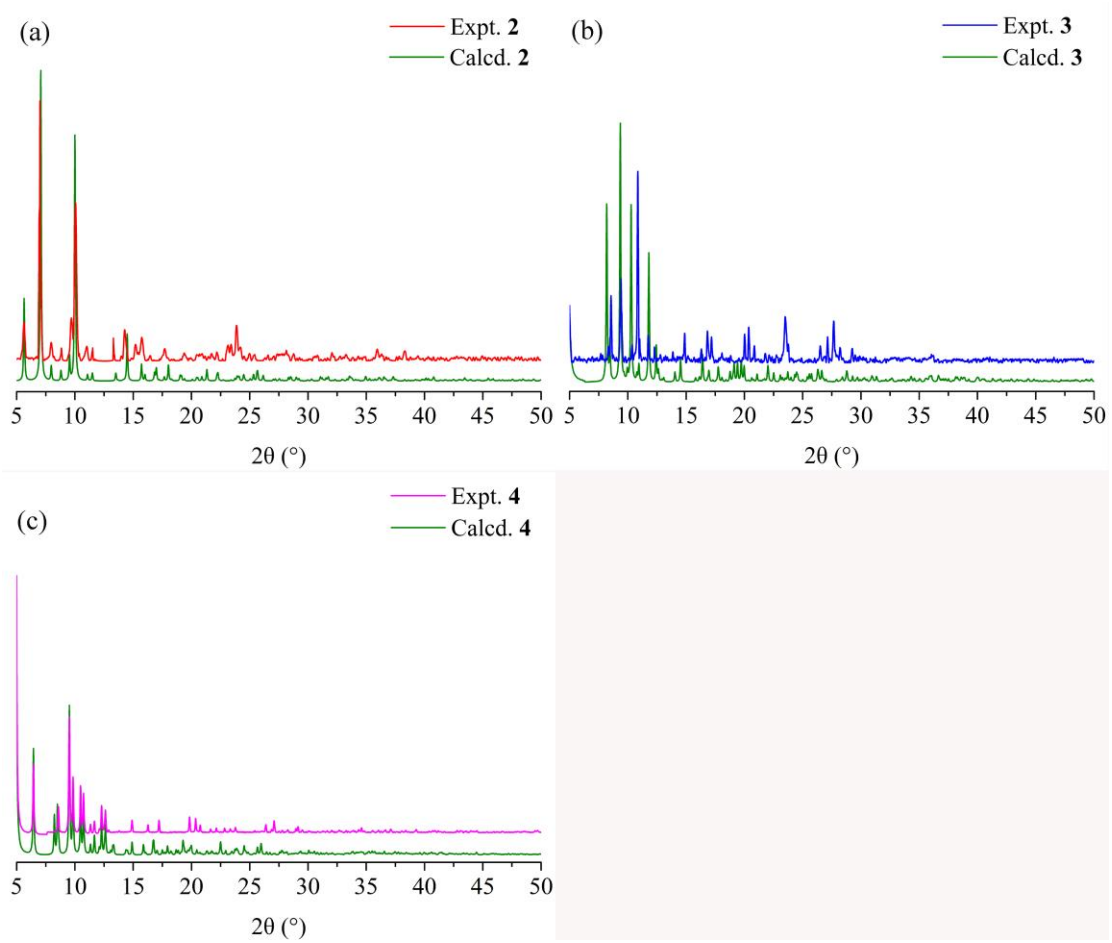

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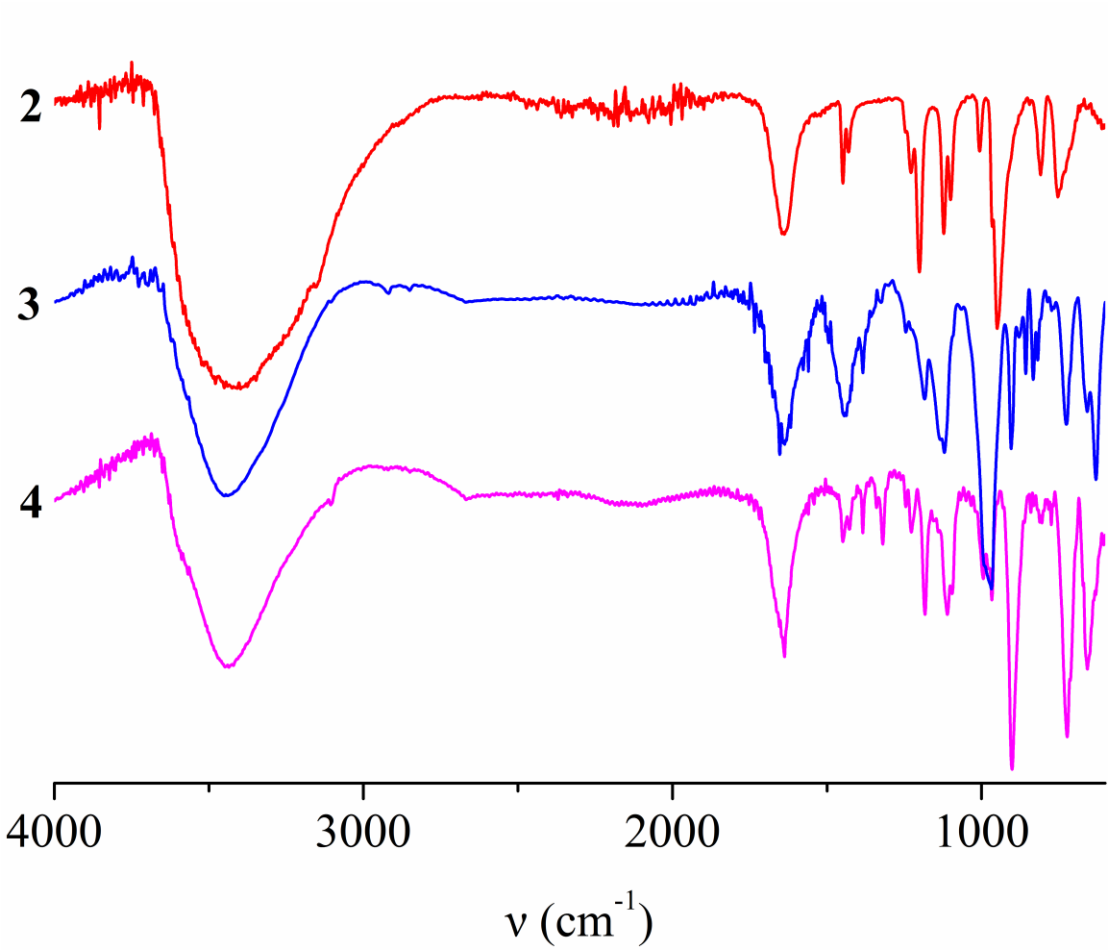

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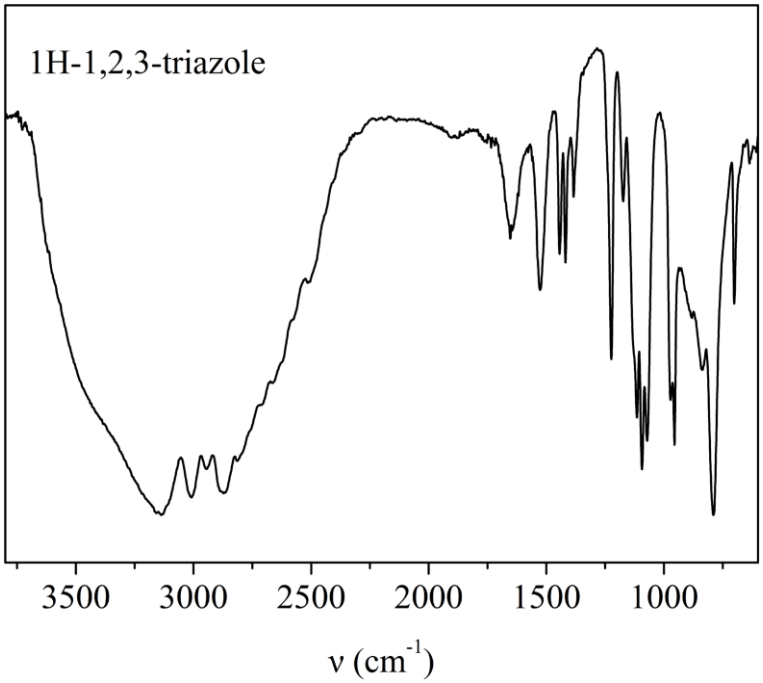

Figure S16. FT-IR spectrum of 1H-1,2,3-triazole [$C_2H_3N_3$] in KBr plate.

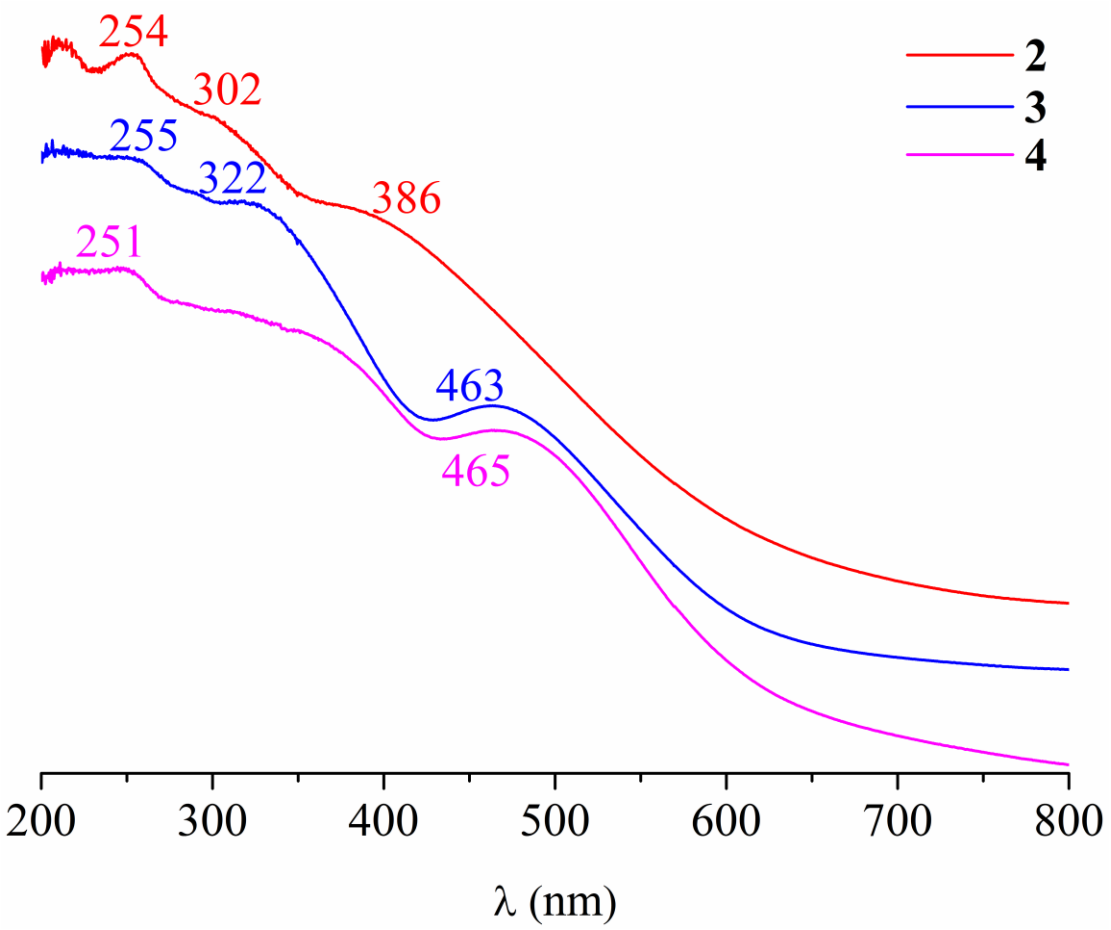

Figure S17. Diffused reflectance spectra of solids $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) and $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 9H_2O$ (**4**) respectively.

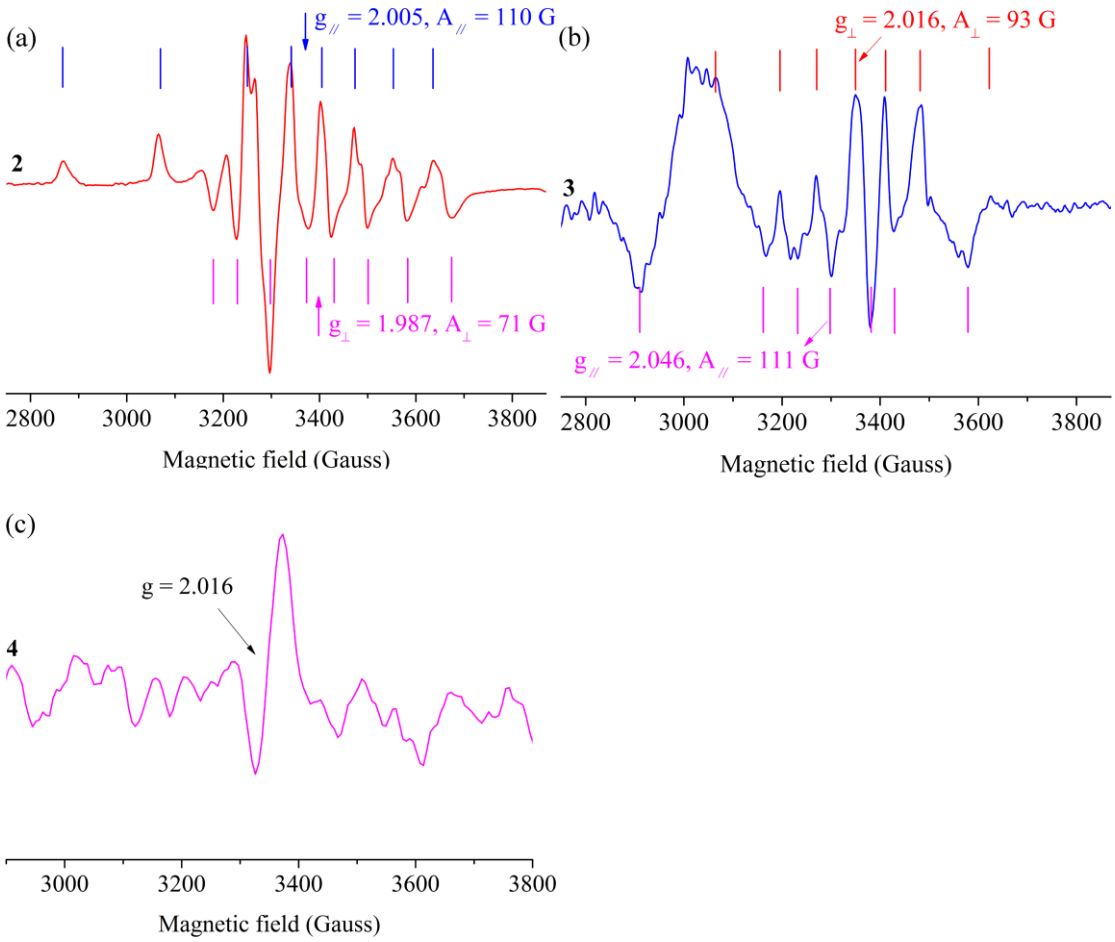

Figure S18. EPR spectra of solids **2** ~ **4** (a ~ c) at 110 K respectively.

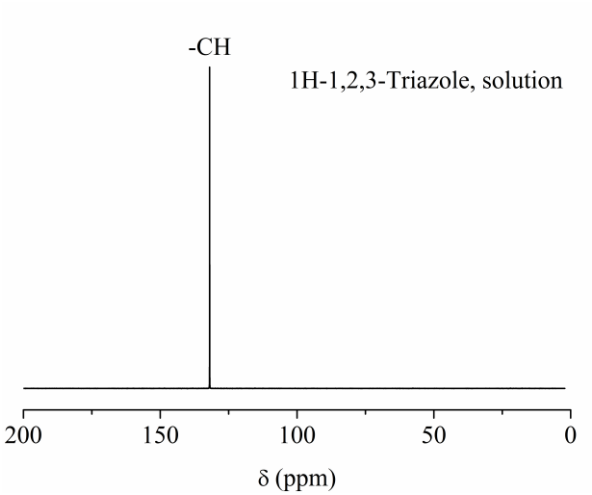

Figure S19. Solution ^{13}C NMR spectrum of pure Htrz.

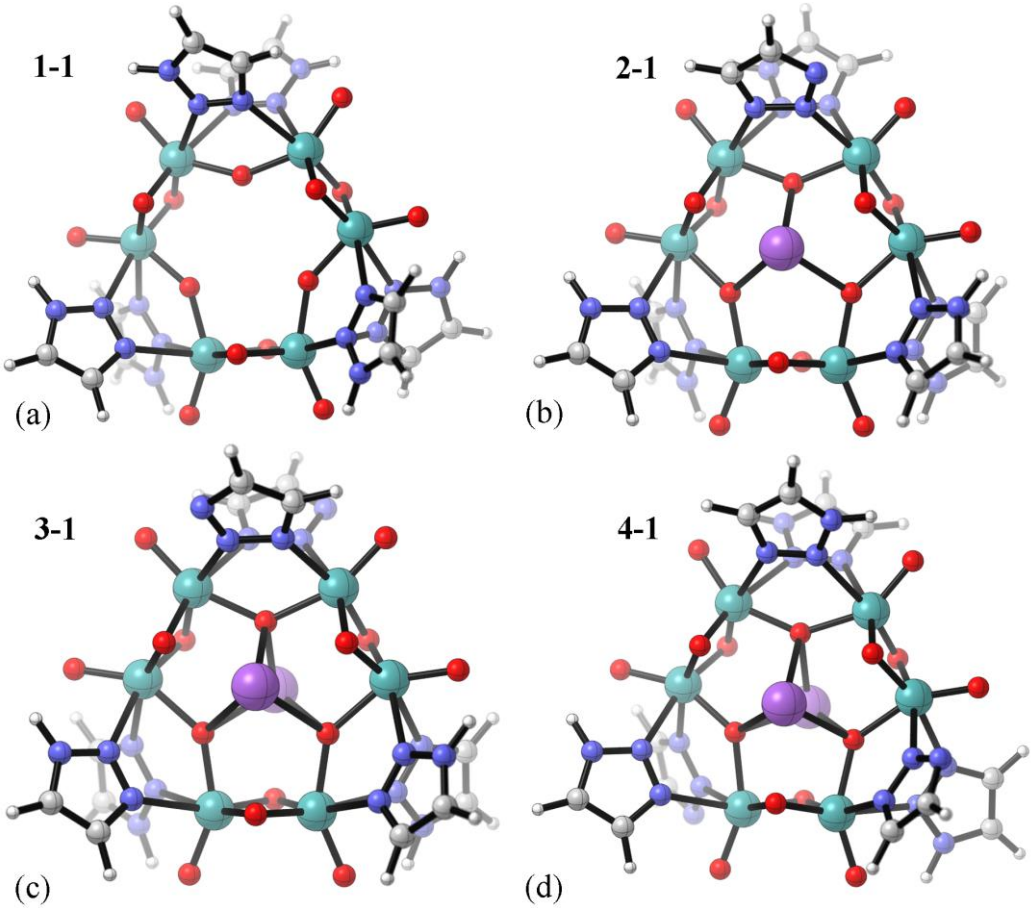

Figure S20. Optimized individual conformers of **1-1** ~ **4-1** (a ~ d) respectively.

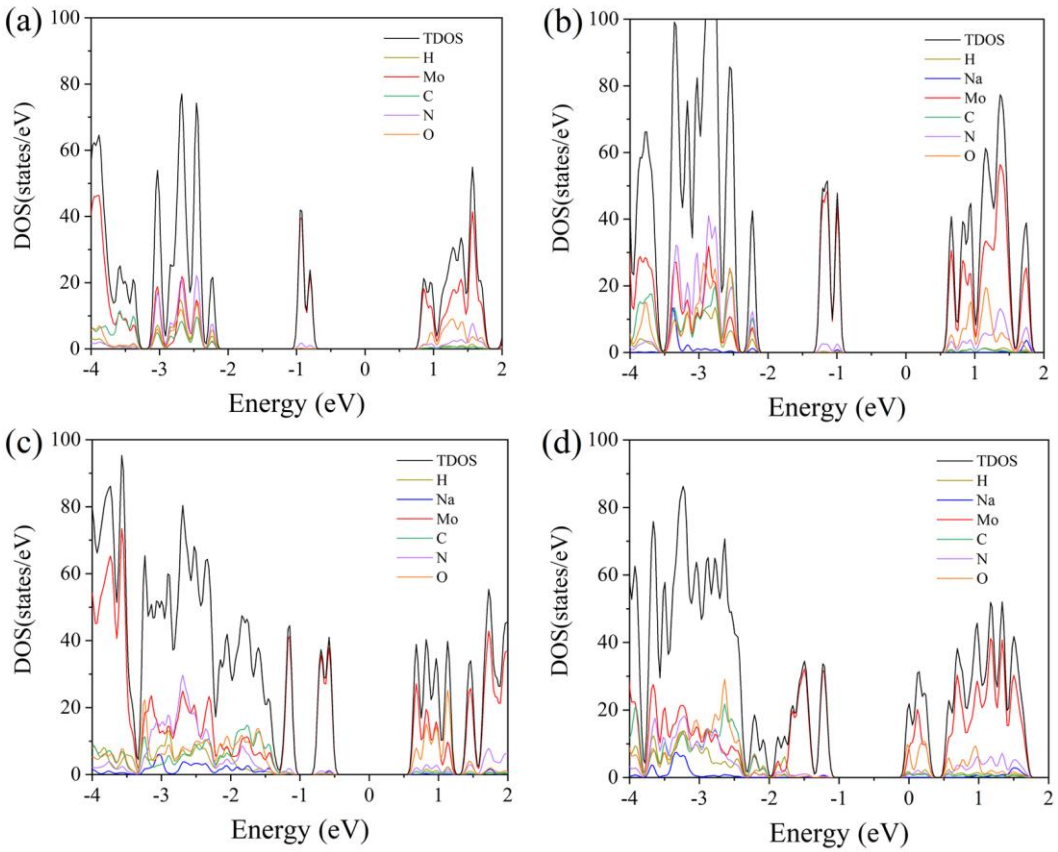

Figure S21. Local density of state (LDOS) and total density of state (TDOS) plots for compounds **1** ~ **4** (a ~ d), respectively.

Table S1. Crystallographic data and structural refinements for complexes $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**), $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) and $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) respectively.

Identification codes	**1**	**2**	**3**	**4**
Empirical formula	$C_{12}H_{48}Mo_6N_{18}O_{30}$	$C_{12}H_{41}Mo_6N_{18}NaO_{27}$	$C_{12}H_{36}Mo_6N_{18}Na_2O_{25}$	$C_{12}H_{114}Mo_6N_{18}Na_2O_{64}$
Formula weight	1500.3	1468.2	1454.1	2156.7
Temperature/K	100.0(1)	100.0(1)	228.0(1)	223.1(1)
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	$P\bar{1}$	$C\,2/m$	$C\,2/m$	$P\,2_1/c$
a/Å	10.7349(4)	25.0562(5)	38.068(3)	9.2936(3)
b/Å	11.4546(4)	20.0622(3)	20.884(2)	35.6369(1)
c/Å	19.5856(6)	11.1147(2)	9.5142(7)	21.4763(7)
α/°	89.050(3)	90	90	90
β/°	75.634(3)	94.591(2)	96.778(7)	92.824(3)
γ/°	81.845(3)	90	90	90
Volume/Å^3	2309.0(1)	5569.2(2)	7511.0(1)	7104.2(4)
Z	2	4	4	4
ρ_{calc}g/cm^3	1.769	1.530	1.168	1.236
μ/mm^{-1}	13.544	11.356	1.029	1.088
F(000)	1176.0	2452.0	2526.0	2528.0
Crystal size/mm^3	0.10 × 0.02 × 0.01	0.20 × 0.20 × 0.1	0.30 × 0.10 × 0.05	0.40 × 0.20 × 0.08
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2θ range for data collection/°	7.798 to 149.72	5.65 to 132.922	4.456 to 56.94	4.388 to 54.468

Index ranges	$-13 \le h \le 13$, $-14 \le k \le 13$, $-24 \le l \le 23$	$-29 \le h \le 29$, $-23 \le k \le 23$, $-13 \le l \le 12$	$-49 \le h \le 48$, $-26 \le k \le 27$, $-11 \le l \le 11$	$-11 \le h \le 11$, $-42 \le k \le 45$, $-26 \le l \le 26$
Reflections collected	26401	23822	30018	83022
Independent reflections	9024 [R_{int} = 0.0795, R_{σ} = 0.0702]	5004 [R_{int} = 0.0258, R_{σ} = 0.0175]	8780 [R_{int} = 0.1157, R_{σ} = 0.1325]	14721 [R_{int} = 0.1179, R_{σ} = 0.1085]
Data/restraints/parameters	9024/0/469	5004/16/259	8780/7/267	14721/16/505
Goodness–of–fit on F^2	1.106	1.039	0.891	0.982
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0606, wR_2 = 0.1671	R_1 = 0.0561, wR_2 = 0.1692	R_1 = 0.0678, wR_2 = 0.1420	R_1 = 0.0847, wR_2 = 0.2081
Final R indexes [all data]	R_1 = 0.0694, wR_2 = 0.1741	R_1 = 0.0617, wR_2 = 0.1772	R_1 = 0.1377, wR_2 = 0.1685	R_1 = 0.1322, wR_2 = 0.2344
Largest diff. peak/hole/e ·Å^{-3}	2.02/-1.42	1.68/-2.50	0.91/-0.47	0.85/-0.55

Table S2. Selected hydrogen bond distances (Å) and angles (°) in $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**).

D–H ··· A	D–H(Å)	H ··· A(Å)	D ··· A(Å)	D–H ··· A(°)
C1–H1 ··· N6[a]	0.93	2.57	3.489(1)	169
C3–H3A ··· O2[b]	0.93	2.45	3.130(1)	130
C4–H4 ··· O7[b]	0.93	2.60	3.480(1)	158
C6–H6A ··· O3[c]	0.93	2.54	3.337(1)	143
C9–H9A ··· N18[d]	0.93	2.57	3.480(1)	167
C11–H11 ··· O3[e]	0.93	2.55	3.132(1)	121

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

Table S3. Selected hydrogen bond distances (Å) and angles (°) in $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**).

D–H ··· A	D–H(Å)	H ··· A(Å)	D ··· A(Å)	D–H ··· A(°)
C1–H1 ··· O3[a]	0.93	2.53	3.196(1)	129
C2–H2 ··· O2[a]	0.93	2.54	3.299(1)	140

Symmetric codes: (a) ½ – *x*, ½ – *y*, 1 – *z*.

Table S4. Comparisons of Na–O distances in **2** ~ **4** and some classical crown ethers.

Compounds	Receptors	Na–O (Å)
2		$2.226(4)_{av}$
3	Mo_6O_9	$2.561(6)_{av}$
4		$2.582(7)_{av}$
1·**HB**·$2NaPF_6$[18]	benzo-15-crown-5	2.302(1) ~ 2.477(1)
2·$NaClO_4$[19]	aza-18-crown-6	2.430 ~ 2.581
1·$NaNO_2$[20]	aza-18-crown-6	2.44_{av}

HB = hydrogen bond

Table S5. Selected bond distances (Å) and angles (°) in $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**).

1			
Mo1–Mo2	2.570(4)	Mo5–O13	1.954(6)
Mo1–O8	1.967(7)	Mo5–O14	1.958(6)
Mo1–O7	1.955(7)	Mo5–O5	1.712(6)
Mo1–O15	1.958(7)	Mo5–N17	2.238(6)
Mo1–O1	1.728(8)	Mo5–N13	2.214(7)
Mo1–N4	2.245(7)	Mo4–O11	1.955(6)
Mo1–N2	2.240(9)	Mo4–O12	2.071(5)
Mo2–O8	1.974(5)	Mo4–O10	1.951(6)
Mo2–O9	1.973(5)	Mo4–O4	1.712(6)
Mo2–O7	1.969(6)	Mo4–N16	2.221(7)
Mo2–O2	1.707(6)	Mo4–N14	2.202(7)
Mo2–N10	2.212(7)	Mo6–O15	1.968(5)
Mo2–N8	2.217(7)	Mo6–O13	1.951(6)
Mo2–Mo7	2.572(5)	Mo6–O14	1.964(6)
Mo3–Mo4	2.5700(8)	Mo6–O6	1.711(6)
Mo3–O9	1.985(5)	Mo6–N5	2.237(6)
Mo3–O11	1.967(5)	Mo6–N1	2.224(7)
Mo3–O10	1.965(6)	O8–Mo7	1.961(7)
Mo3–O3	1.729(6)	O7–Mo7	1.962(7)
Mo3–N11	2.227(7)	O15–Mo7	1.944(7)
Mo3–N7	2.222(7)	O1–Mo7	1.741(7)
Mo5–Mo6	2.5569(9)	N4–Mo7	2.246(8)
Mo5–O12	2.059(5)	N2–Mo7	2.230(8)
O8–Mo1–Mo2	49.41(2)	O10–Mo4–Mo3	49.21(2)
O8–Mo1–N4	164.6(3)	O10–Mo4–O11	97.9(2)
O8–Mo1–N2	86.6(3)	O10–Mo4–O12	87.7(2)
O7–Mo1–Mo2	49.34(2)	O10–Mo4–N16	88.6(2)
O7–Mo1–O8	98.3(3)	O10–Mo4–N14	162.5(3)
O7–Mo1–O15	91.6(3)	O4–Mo4–Mo3	107.8(2)
O7–Mo1–N4	87.3(3)	O4–Mo4–O11	105.5(3)
O7–Mo1–N2	167.1(3)	O4–Mo4–O12	159.6(2)
O15–Mo1–Mo2	96.7(2)	O4–Mo4–O10	105.5(3)
O15–Mo1–O8	90.0(3)	O4–Mo4–N16	88.6(3)
O15–Mo1–N4	75.4(3)	O4–Mo4–N14	89.9(3)
O15–Mo1–N2	76.5(3)	N16–Mo4–Mo3	137.11(2)
O1–Mo1–Mo2	106.1(3)	N14–Mo4–Mo3	134.11(2)
O1–Mo1–O8	103.8(3)	N14–Mo4–N16	83.5(2)
O1–Mo1–O7	104.0(3)	O15–Mo6–Mo5	96.50(2)
O1–Mo1–O15	157.2(3)	O15–Mo6–N5	75.3(2)
O1–Mo1–N4	88.6(3)	O15–Mo6–N1	76.6(2)
O1–Mo1–N2	86.2(3)	O13–Mo6–Mo5	49.13(2)
N4–Mo1–Mo2	136.1(3)	O13–Mo6–O15	89.8(2)
N2–Mo1–Mo2	135.8(3)	O13–Mo6–O14	97.8(2)
N2–Mo1–N4	85.1(3)	O13–Mo6–N5	164.6(2)
O8–Mo2–Mo1	49.2(2)	O13–Mo6–N1	86.5(3)

O8–Mo2–N10	165.7(2)	O14–Mo6–Mo5	49.22(2)
O8–Mo2–N8	88.7(2)	O14–Mo6–O15	90.6(2)
O8–Mo2–Mo7	48.97(2)	O14–Mo6–N5	86.4(2)
O9–Mo2–Mo1	95.51(2)	O14–Mo6–N1	166.6(2)
O9–Mo2–O8	89.9(2)	O6–Mo6–Mo5	105.2(2)
O9–Mo2–N10	76.4(2)	O6–Mo6–O15	158.3(3)
O9–Mo2–N8	75.9(2)	O6–Mo6–O13	104.3(3)
O9–Mo2–Mo7	95.18(2)	O6–Mo6–O14	103.4(3)
O7–Mo2–Mo1	48.86(2)	O6–Mo6–N5	89.0(3)
O7–Mo2–O8	97.6(2)	O6–Mo6–N1	87.7(3)
O7–Mo2–O9	90.2(2)	N5–Mo6–Mo5	135.15(2)
O7–Mo2–N10	86.7(2)	N1–Mo6–Mo5	135.42(2)
O7–Mo2–N8	164.8(2)	N1–Mo6–N5	86.4(3)
O7–Mo2–Mo7	49.01(2)	Mo1–O8–Mo2	81.4(2)
O2–Mo2–Mo1	107.0(2)	Mo7–O8–Mo2	81.6(2)
O2–Mo2–O8	103.3(3)	Mo2–O9–Mo3	131.4(3)
O2–Mo2–O9	157.4(3)	Mo4–O11–Mo3	81.9(2)
O2–Mo2–O7	105.7(2)	Mo1–O7–Mo2	81.8(2)
O2–Mo2–N10	88.5(3)	Mo7–O7–Mo2	81.7(3)
O2–Mo2–N8	86.1(3)	Mo1–O15–Mo6	132.0(3)
O2–Mo2–Mo7	107.3(2)	Mo7–O15–Mo6	132.0(3)
N10–Mo2–Mo1	135.1(2)	Mo5–O12–Mo4	127.6(3)
N10–Mo2–N8	84.1(3)	Mo6–O13–Mo5	81.8(2)
N10–Mo2–Mo7	135.2(2)	Mo5–O14–Mo6	81.4(2)
N8–Mo2–Mo1	137.4(2)	Mo4–O10–Mo3	82.1(2)
N8–Mo2–Mo7	137.2(2)	N18–N17–Mo5	125.8(5)
O9–Mo3–Mo4	96.48(2)	N16–N17–Mo5	122.7(5)
O9–Mo3–N11	76.2(2)	N5–N4–Mo1	120.3(5)
O9–Mo3–N7	76.6(2)	N5–N4–Mo7	119.8(5)
O11–Mo3–Mo4	48.86(2)	C4–N4–Mo1	132.8(6)
O11–Mo3–O9	89.9(2)	C4–N4–Mo7	133.3(6)
O11–Mo3–N11	165.3(2)	N17–N16–Mo4	121.9(5)
O11–Mo3–N7	88.1(2)	C12–N16–Mo4	131.7(6)
O10–Mo3–Mo4	48.74(2)	N4–N5–Mo6	120.5(5)
O10–Mo3–O9	90.6(2)	N6–N5–Mo6	127.9(5)
O10–Mo3–O11	97.0(2)	N11–N10–Mo2	121.0(5)
O10–Mo3–N11	88.1(2)	C8–N10–Mo2	130.3(6)
O10–Mo3–N7	166.2(2)	N7–N8–Mo2	121.3(5)
O3–Mo3–Mo4	106.58(2)	N9–N8–Mo2	129.1(5)
O3–Mo3–O9	156.9(2)	N10–N11–Mo3	119.7(5)
O3–Mo3–O11	104.6(3)	N12–N11–Mo3	131.8(6)
O3–Mo3–O10	105.0(3)	N8–N7–Mo3	119.6(5)
O3–Mo3–N11	87.2(3)	C6–N7–Mo3	132.9(5)
O3–Mo3–N7	85.9(3)	N14–N13–Mo5	121.9(5)
N11–Mo3–Mo4	136.49(2)	C10–N13–Mo5	130.2(7)
N7–Mo3–Mo4	136.75(2)	N13–N14–Mo4	122.6(5)
N7–Mo3–N11	84.0(2)	N15–N14–Mo4	126.9(6)
O12–Mo5–Mo6	93.22(2)	N1–N2–Mo1	120.0(5)
O12–Mo5–N17	75.1(2)	N1–N2–Mo7	119.7(5)
O12–Mo5–N13	74.7(2)	N3–N2–Mo1	130.3(6)

O13–Mo5–Mo6	49.05(2)	N3–N2–Mo7	130.6(6)
O13–Mo5–O12	88.3(2)	N2–N1–Mo6	120.0(5)
O13–Mo5–O14	97.9(2)	C2–N1–Mo6	132.2(6)
O13–Mo5–N17	162.8(3)	O8–Mo7–Mo2	49.38(2)
O13–Mo5–N13	85.9(3)	O8–Mo7–O7	98.2(3)
O14–Mo5–Mo6	49.40(2)	O8–Mo7–N4	165.5(3)
O14–Mo5–O12	87.8(2)	O8–Mo7–N2	87.0(3)
O14–Mo5–N17	86.3(2)	O7–Mo7–Mo2	49.26(2)
O14–Mo5–N13	162.0(3)	O7–Mo7–N4	87.1(3)
O5–Mo5–Mo6	107.0(2)	O7–Mo7–N2	167.7(3)
O5–Mo5–O12	159.7(3)	O15–Mo7–Mo2	97.0(2)
O5–Mo5–O13	105.1(3)	O15–Mo7–O8	90.6(3)
O5–Mo5–O14	105.0(3)	O15–Mo7–O7	91.8(3)
O5–Mo5–N17	89.8(3)	O15–Mo7–N4	75.7(3)
O5–Mo5–N13	90.9(3)	O15–Mo7–N2	77.0(3)
N17–Mo5–Mo6	135.04(2)	O1–Mo7–Mo2	105.6(3)
N13–Mo5–Mo6	134.15(2)	O1–Mo7–O8	103.5(3)
N13–Mo5–N17	85.2(2)	O1–Mo7–O7	103.2(3)
O11–Mo4–Mo3	49.27(2)	O1–Mo7–O15	157.4(4)
O11–Mo4–O12	87.6(2)	O1–Mo7–N4	88.3(3)
O11–Mo4–N16	162.2(2)	O1–Mo7–N2	86.1(3)
O11–Mo4–N14	85.6(2)	N4–Mo7–Mo2	135.9(3)
O12–Mo4–Mo3	92.61(1)	N2–Mo7–Mo2	136.2(3)
O12–Mo4–N16	76.1(2)	N2–Mo7–N4	85.3(3)
O12–Mo4–N14	75.3(2)		

Table S6. Selected bond distances (Å) and angles (°) in $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**).

2			
Mo1–Mo1[1]	2.5639(1)	Mo3–O8	1.934(6)
Mo1–Na1	3.273(6)	Mo3–N9	2.173(7)
Mo1–O6	2.178(5)	Mo3–N7	2.192(7)
Mo1–O4	1.933(5)	Mo3–O3	1.690(6)
Mo1–O5	1.938(5)	Mo2–Na1	3.2603(2)
Mo1–O1	1.682(6)	Mo2–O6	2.184(5)
Mo1–N4	2.199(7)	Mo2–O7	1.938(6)
Mo1–N2	2.212(7)	Mo2–O8	1.939(6)
Mo3–Mo2	2.5652(9)	Mo2–N5	2.203(6)
Mo3–Na1	3.253(5)	Mo2–N1	2.200(8)
Mo3–O9	2.177(4)	Mo2–O2	1.690(6)
Mo3–O7	1.945(5)		
Mo1[1]–Mo1–Na1	66.94(4)	O2–Mo2–O7	105.6(3)
O6–Mo1–Mo1[1]	89.62(1)	O2–Mo2–O8	105.5(3)
O6–Mo1–Na1	25.91(2)	O2–Mo2–N5	92.0(3)
O6–Mo1–N4	77.2(2)	O2–Mo2–N1	91.1(3)
O6–Mo1–N2	76.3(2)	Mo3[1]–Na1–Mo3	70.71(1)
O4–Mo1–Mo1[1]	48.45(1)	Mo3–Na1–Mo2	46.39(5)
O4–Mo1–Na1	80.0(2)	Mo3[1]–Na1–Mo2	115.67(2)
O4–Mo1–O6	85.5(2)	Mo3[1]–Na1–Mo2[1]	46.39(5)
O4–Mo1–O5	96.1(2)	Mo3–Na1–Mo2[1]	115.67(2)
O4–Mo1–N4	86.6(2)	Mo2–Na1–Mo2[1]	152.0(2)
O4–Mo1–N2	161.0(3)	O6[1]–Na1–Mo3	136.3(4)
O5–Mo1–Mo1[1]	48.58(1)	O6[1]–Na1–Mo3[1]	79.6(2)
O5–Mo1–Na1	59.6(2)	O6–Na1–Mo3[1]	136.3(4)
O5–Mo1–O6	83.7(3)	O6–Na1–Mo3	79.6(2)
O5–Mo1–N4	160.5(3)	O6–Na1–Mo2[1]	135.5(3)
O5–Mo1–N2	87.2(2)	O6–Na1–Mo2	36.59(2)
O1–Mo1–Mo1[1]	106.4(2)	O6[1]–Na1–Mo2	135.5(3)
O1–Mo1–Na1	165.9(3)	O6[1]–Na1–Mo2[1]	36.59(2)
O1–Mo1–O6	164.0(3)	O9–Na1–Mo3	36.37(1)
O1–Mo1–O4	105.2(3)	O9–Na1–Mo3[1]	36.37(1)
O1–Mo1–O5	106.5(3)	O9–Na1–Mo2[1]	79.37(1)
O1–Mo1–N4	91.3(3)	O9–Na1–Mo2	79.36(1)
O1–Mo1–N2	91.6(3)	O5–Na1–Mo3	144.64(7)
N4–Mo1–Mo1[1]	134.33(2)	O5–Na1–Mo3[1]	144.64(7)
N4–Mo1–Na1	102.16(2)	O5–Na1–Mo2	98.94(1)
N4–Mo1–N2	84.2(3)	O5–Na1–Mo2[1]	98.94(1)
N2–Mo1–Mo1[1]	135.16(2)	O8–Na1–Mo3	36.24(1)
N2–Mo1–Na1	85.70(2)	O8[1]–Na1–Mo3	99.4(2)
Mo2–Mo3–Na1	66.95(7)	O8[1]–Na1–Mo3[1]	36.24(1)
O9–Mo3–Mo2	89.8(2)	O8–Na1–Mo3[1]	99.4(2)
O9–Mo3–Na1	26.0(2)	O8[1]–Na1–Mo2[1]	36.27(1)
O9–Mo3–N7	76.1(3)	O8–Na1–Mo2[1]	145.1(2)
O7–Mo3–Mo2	48.54(2)	O1W–Na1–Mo3	78.6(4)

O7–Mo3–Na1	79.65(2)	O1W–Na1–Mo3[1]	78.6(4)
O7–Mo3–O9	85.3(3)	O1W–Na1–Mo2	77.52(1)
O7–Mo3–N9	85.5(2)	O1W–Na1–Mo2[1]	77.52(1)
O7–Mo3–N7	160.8(2)	O2W–Na1–Mo3[1]	103.3(4)
O8–Mo3–Mo2	48.62(2)	O2W–Na1–Mo3	103.3(4)
O8–Mo3–Na1	59.96(2)	O2W–Na1–Mo2[1]	102.74(1)
O8–Mo3–O9	84.1(3)	O2W–Na1–Mo2	102.74(1)
O8–Mo3–O7	96.2(2)	Mo1–O6–Mo2	119.3(2)
O8–Mo3–N9	160.0(3)	Na1–O6–Mo1	118.2(3)
O8–Mo3–N7	86.7(2)	Na1–O6–Mo2	117.1(3)
N9–Mo3–Mo2	133.21(2)	O1W–O6–Mo1	115.4(4)
N9–Mo3–Na1	101.04(2)	O1W–O6–Mo2	116.6(4)
N9–Mo3–O9	76.2(3)	Mo3[1]–O9–Mo3	119.7(4)
N9–Mo3–N7	85.4(2)	Na1–O9–Mo3	117.6(3)
N7–Mo3–Mo2	134.65(2)	Na1–O9–Mo3[1]	117.6(3)
N7–Mo3–Na1	85.5(2)	O1W–O9–Mo3	115.9(2)
O3–Mo3–Mo2	106.4(2)	O1W–O9–Mo3[1]	115.9(2)
O3–Mo3–Na1	166.3(3)	Mo1–O4–Mo1[1]	83.1(3)
O3–Mo3–O9	163.8(3)	Mo2–O7–Mo3	82.7(2)
O3–Mo3–O7	105.2(3)	Mo1–O5–Mo1[1]	82.8(3)
O3–Mo3–O8	106.5(3)	Mo1–O5–Na1	84.3(3)
O3–Mo3–N9	92.2(3)	Mo1[1]–O5–Na1	84.3(3)
O3–Mo3–N7	92.0(3)	Mo3–O8–Mo2	82.9(2)
Mo3–Mo2–Na1	66.66(1)	Mo3–O8–Na1	83.8(2)
O6–Mo2–Mo3	89.76(1)	Mo2–O8–Na1	83.97(2)
O6–Mo2–Na1	26.29(2)	N5–N4–Mo1	124.0(5)
O6–Mo2–N5	77.2(2)	C4–N4–Mo1	128.6(6)
O6–Mo2–N1	76.8(2)	N9[1]–N9–Mo3	124.18(2)
O7–Mo2–Mo3	48.78(2)	N10–N9–Mo3	127.5(6)
O7–Mo2–Na1	79.55(2)	C7–N9–Mo3	127.5(6)
O7–Mo2–O6	85.1(2)	N7[1]–N7–Mo3	123.37(2)
O7–Mo2–O8	96.3(2)	N8–N7–Mo3	125.8(8)
O7–Mo2–N5	85.8(2)	C5–N7–Mo3	125.8(8)
O7–Mo2–N1	161.1(2)	N1–N2–Mo1	123.8(5)
O8–Mo2–Mo3	48.44(2)	N3–N2–Mo1	125.2(6)
O8–Mo2–Na1	59.8(2)	N4–N5–Mo2	122.9(5)
O8–Mo2–O6	84.2(2)	N6–N5–Mo2	126.8(6)
O8–Mo2–N5	161.1(3)	N2–N1–Mo2	123.2(5)
O8–Mo2–N1	87.5(3)	C2–N1–Mo2	132.5(7)
N5–Mo2–Mo3	133.97(2)	O8–Na1–Mo2	36.27(1)
N5–Mo2–Na1	102.43(2)	O8[1]–Na1–Mo2	145.1(2)
N1–Mo2–Mo3	135.34(2)	O2–Mo2–Mo3	105.9(2)
N1–Mo2–Na1	86.5(2)	O2–Mo2–Na1	165.1(3)
N1–Mo2–N5	84.8(3)	O2–Mo2–O6	164.3(3)

Symmetric codes: [1] + *x*, 1 – *y*, +*z*.

Table S7. Selected bond distances (Å) and angles (°) in $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**).

3			
Mo3–Mo2	2.5809(1)	Mo1–O4	1.965(5)
Mo3–Na1	3.503(3)	Mo1–O5	1.955(5)
Mo3–Na2	3.573(4)	Mo1–N1	2.231(7)
Mo3–O9	1.958(2)	Mo1–O1	1.717(5)
Mo3–O7	1.961(4)	Mo1–N5	2.199(8)
Mo3–O8	1.946(5)	Mo2–Na1	3.5121(2)
Mo3–N9	2.246(5)	Mo2–Na2	3.554(2)
Mo3–N7	2.193(6)	Mo2–O6	1.955(5)
Mo3–O3	1.672(5)	Mo2–O7	1.982(5)
Mo1–Mo1[1]	2.5786(2)	Mo2–O8	1.960(5)
Mo1–Na1	3.506(4)	Mo2–N2	2.237(7)
Mo1–Na2	3.519(4)	Mo2–O2	1.704(5)
Mo1–O6	1.950(4)	Mo2–N4	2.239(7)
Mo2–Mo3–Na1	68.60(5)	N4–Mo2–Na1	116.9(2)
Mo2–Mo3–Na2	68.38(5)	N4–Mo2–Na2	78.9(2)
Na1–Mo3–Na2	57.22(9)	Mo3–Na1–Mo3[1]	61.44(6)
O9–Mo3–Mo2	96.20(2)	Mo3–Na1–Mo1	99.65(7)
O9–Mo3–Na1	41.28(2)	Mo3[1]–Na1–Mo1	122.91(1)
O9–Mo3–Na2	40.95(2)	Mo3–Na1–Mo1[1]	122.91(1)
O9–Mo3–O7	90.5(2)	Mo3[1]–Na1–Mo1[1]	99.64(7)
O9–Mo3–N9	76.2(2)	Mo1–Na1–Mo1[1]	43.15(5)
O9–Mo3–N7	76.8(2)	Na2–Na1–Mo3[1]	62.43(8)
O7–Mo3–Mo2	49.47(1)	Na2–Na1–Mo3	62.43(8)
O7–Mo3–Na1	49.24(1)	Na2–Na1–Mo1	61.36(9)
O7–Mo3–Na2	94.02(1)	Na2–Na1–Mo1[1]	61.36(9)
O7–Mo3–N9	165.17(2)	O9–Na1–Mo3[1]	32.45(5)
O7–Mo3–N7	86.7(2)	O9–Na1–Mo3	32.45(5)
O8–Mo3–Mo2	48.87(1)	O9–Na1–Mo1	104.29(2)
O8–Mo3–Na1	94.41(1)	O9–Na1–Mo1[1]	104.29(2)
O8–Mo3–Na2	49.85(2)	O6–Na1–Mo3[1]	104.88(2)
O8–Mo3–O9	90.8(2)	O6[1]–Na1–Mo3	104.88(2)
O8–Mo3–O7	97.93(2)	O6[1]–Na1–Mo3[1]	67.42(1)
O8–Mo3–N9	88.8(2)	O6–Na1–Mo3	67.42(1)
O8–Mo3–N7	166.8(2)	O6[1]–Na1–Mo1[1]	32.23(1)
N9–Mo3–Mo2	137.28(1)	O6[1]–Na1–Mo1	67.37(1)
N9–Mo3–Na1	117.31(1)	O6–Na1–Mo1[1]	67.37(1)
N9–Mo3–Na2	80.20(2)	O6–Na1–Mo1	32.23(1)
N7–Mo3–Mo2	135.93(1)	O7–Na1–Mo3	33.76(1)
N7–Mo3–Na1	79.20(2)	O7–Na1–Mo3[1]	92.85(1)
N7–Mo3–Na2	117.68(2)	O7[1]–Na1–Mo3[1]	33.76(1)
N7–Mo3–N9	84.0(2)	O7[1]–Na1–Mo3	92.85(1)
O3–Mo3–Mo2	107.0(2)	O7–Na1–Mo1[1]	133.67(1)
O3–Mo3–Na1	150.7(2)	O7[1]–Na1–Mo1[1]	93.22(1)
O3–Mo3–Na2	150.2(2)	O7[1]–Na1–Mo1	133.67(1)
O3–Mo3–O9	156.8(3)	O7–Na1–Mo1	93.22(1)

O3–Mo3–O7	104.8(2)	O4–Na1–Mo3^{1}	133.43(1)
O3–Mo3–O8	103.9(3)	O4–Na1–Mo3	133.44(1)
O3–Mo3–N9	86.2(2)	O4–Na1–Mo1	33.83(1)
O3–Mo3–N7	86.7(3)	O4–Na1–Mo1^{1}	33.83(1)
Mo1^{1}–Mo1–Na1	68.43(3)	O1W–Na1–Mo3^{1}	114.2(3)
Mo1^{1}–Mo1–Na2	68.51(3)	O1W–Na1–Mo3	114.2(3)
Na1–Mo1–Na2	57.68(9)	O1W–Na1–Mo1	122.3(3)
O6–Mo1–Mo1^{1}	96.58(1)	O1W–Na1–Mo1^{1}	122.3(3)
O6–Mo1–Na1	41.29(1)	Mo1–Na2–Mo1^{1}	42.98(5)
O6–Mo1–Na2	41.88(1)	Mo1–Na2–Mo2	60.85(5)
O6–Mo1–O4	90.7(2)	Mo1^{1}–Na2–Mo2	98.56(9)
O6–Mo1–O5	90.3(2)	Na1–Na2–Mo1	60.96(9)
O6–Mo1–N1	76.7(2)	Na1–Na2–Mo1^{1}	60.96(9)
O6–Mo1–N5	75.5(3)	Na1–Na2–Mo2	60.72(6)
O4–Mo1–Mo1^{1}	49.01(1)	O9–Na2–Mo1	102.83(2)
O4–Mo1–Na1	49.42(2)	O9–Na2–Mo1^{1}	102.83(2)
O4–Mo1–Na2	94.38(2)	O9–Na2–Mo2	66.08(8)
O4–Mo1–N1	87.5(2)	O6–Na2–Mo1	32.19(1)
O4–Mo1–N5	165.2(3)	O6^{1}–Na2–Mo1	66.89(1)
O5–Mo1–Mo1^{1}	48.73(1)	O6^{1}–Na2–Mo1^{1}	32.19(1)
O5–Mo1–Na1	93.31(2)	O6–Na2–Mo1^{1}	66.89(1)
O5–Mo1–Na2	48.48(2)	O6^{1}–Na2–Mo2	102.95(2)
O5–Mo1–O4	97.2(2)	O6–Na2–Mo2	31.69(1)
O5–Mo1–N1	166.3(3)	O8–Na2–Mo1	92.33(1)
O5–Mo1–N5	88.0(3)	O8^{1}–Na2–Mo1^{1}	92.33(1)
N1–Mo1–Mo1^{1}	136.22(2)	O8–Na2–Mo1^{1}	131.79(2)
N1–Mo1–Na1	79.92(2)	O8^{1}–Na2–Mo1	131.79(2)
N1–Mo1–Na2	118.5(2)	O8^{1}–Na2–Mo2	130.23(2)
O1–Mo1–Mo1^{1}	107.2(2)	O8–Na2–Mo2	33.23(1)
O1–Mo1–Na1	150.7(2)	O5–Na2–Mo1^{1}	33.35(1)
O1–Mo1–Na2	149.8(2)	O5–Na2–Mo1	33.35(1)
O1–Mo1–O6	156.3(3)	O5–Na2–Mo2	92.32(1)
O1–Mo1–O4	104.8(3)	O2W^{1}–Na2–Mo1	125.0(4)
O1–Mo1–O5	105.1(3)	O2W^{1}–Na2–Mo1^{1}	99.8(4)
O1–Mo1–N1	86.0(3)	O2W–Na2–Mo1	99.7(4)
O1–Mo1–N5	87.0(3)	O2W–Na2–Mo1^{1}	125.0(4)
N5–Mo1–Mo1^{1}	136.4(2)	O2W–Na2–Mo2	86.1(2)
N5–Mo1–Na1	116.7(2)	O2W^{1}–Na2–Mo2	152.8(3)
N5–Mo1–Na2	78.72(2)	Mo3–O9–Mo3^{1}	132.1(3)
N5–Mo1–N1	84.5(3)	Mo3–O9–Na1	106.27(2)
Mo3–Mo2–Na1	68.23(6)	Mo3^{1}–O9–Na1	106.27(2)
Mo3–Mo2–Na2	69.16(7)	Mo3–O9–Na2	107.55(2)
Na1–Mo2–Na2	57.31(8)	Mo3^{1}–O9–Na2	107.55(2)
O6–Mo2–Mo3	96.36(1)	Mo1–O6–Mo2	133.1(2)
O6–Mo2–Na1	41.17(1)	Mo1–O6–Na1	106.5(2)
O6–Mo2–Na2	41.02(1)	Mo1–O6–Na2	105.9(2)
O6–Mo2–O7	90.23(2)	Mo2–O6–Na1	106.6(2)
O6–Mo2–O8	91.38(2)	Mo2–O6–Na2	107.30(2)
O6–Mo2–N2	76.0(2)	Mo3–O7–Mo2	81.76(2)
O6–Mo2–N4	75.8(3)	Mo3–O7–Na1	97.00(2)

O7–Mo2–Mo3	48.77(1)	Mo2–O7–Na1	96.82(2)
O7–Mo2–Na1	49.10(1)	Mo1–O4–Mo1[1]	82.0(3)
O7–Mo2–Na2	94.21(1)	Mo1–O4–Na1	96.7(2)
O7–Mo2–N2	88.1(2)	Mo1[1]–O4–Na1	96.8(2)
O7–Mo2–N4	165.0(3)	Mo3–O8–Mo2	82.73(2)
O8–Mo2–Mo3	48.40(2)	Mo3–O8–Na2	97.47(2)
O8–Mo2–Na1	93.88(1)	Mo2–O8–Na2	96.40(2)
O8–Mo2–Na2	50.37(2)	Mo1[1]–O5–Mo1	82.5(3)
O8–Mo2–O7	96.76(2)	Mo1–O5–Na2	98.2(2)
O8–Mo2–N2	166.5(3)	Mo1[1]–O5–Na2	98.2(2)
O8–Mo2–N4	89.2(2)	N9[1]–N9–Mo3	119.99(1)
N2–Mo2–Mo3	136.53(2)	C7–N9–Mo3	131.3(5)
N2–Mo2–Na1	79.76(2)	N10–N9–Mo3	131.3(5)
N2–Mo2–Na2	116.9(2)	N1–N2–Mo2	120.8(6)
N2–Mo2–N4	83.3(3)	N3–N2–Mo2	129.4(7)
O2–Mo2–Mo3	106.0(2)	N71–N7–Mo3	120.05(2)
O2–Mo2–Na1	149.8(2)	C5–N7–Mo3	132.6(6)
O2–Mo2–Na2	150.6(2)	N8–N7–Mo3	132.6(6)
O2–Mo2–O6	157.6(2)	N2–N1–Mo1	119.2(6)
O2–Mo2–O7	103.9(3)	C2–N1–Mo1	132.7(7)
O2–Mo2–O8	103.8(2)	N4–N5–Mo1	122.0(6)
O2–Mo2–N2	87.1(3)	N6–N5–Mo1	132.9(8)
O2–Mo2–N4	87.9(3)	N5–N4–Mo2	118.6(6)
N4–Mo2–Mo3	137.11(2)	C4–N4–Mo2	128.8(8)

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

Table S8. Selected bond distances (Å) and angles (°) in $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]$ ·9H_2O (**4**).

4			
Mo1–Mo6	2.6115(1)	Mo5–Mo4	2.6129(1)
Mo1–Na1	3.516(4)	Mo5–Na1	3.543(4)
Mo1–Na2	3.515(4)	Mo5–Na2	3.563(4)
Mo1–O7	1.949(5)	Mo5–O13	1.957(5)
Mo1–O15	2.079(7)	Mo5–O11	2.101(8)
Mo1–O14	2.063(7)	Mo5–N14	2.240(8)
Mo1–N1	2.259(8)	Mo5–O12	2.030(7)
Mo1–N5	2.231(8)	Mo5–O5	1.732(7)
Mo1–O1	1.727(6)	Mo5–N16	2.250(9)
Mo6–Na1	3.539(4)	Mo4–Na1	3.531(4)
Mo6–Na2	3.511(4)	Mo4–Na2	3.592(4)
Mo6–O15	2.074(7)	Mo4–O10	1.978(6)
Mo6–O14	2.051(6)	Mo4–O11	2.054(7)
Mo6–O13	1.966(5)	Mo4–O12	2.056(8)
Mo6–O6	1.714(6)	Mo4–N7	2.252(9)
Mo6–N13	2.234(8)	Mo4–O4	1.721(6)
Mo6–N17	2.234(9)	Mo4–N11	2.265(9)
Mo2–Mo3	2.6191(1)	Mo3–Na1	3.516(4)
Mo2–Na1	3.521(4)	Mo3–Na2	3.583(4)
Mo2–Na2	3.570(4)	Mo3–O10	1.954(6)
Mo2–O7	1.976(6)	Mo3–O8	2.019(8)
Mo2–O8	2.040(8)	Mo3–O9	2.103(8)
Mo2–O9	2.096(7)	Mo3–O3	1.731(6)
Mo2–N2	2.241(9)	Mo3–N10	2.242(9)
Mo2–N4	2.246(8)	Mo3–N8	2.224(9)
Mo2–O2	1.704(6)		
Mo6–Mo1–Na1	68.75(7)	O4–Mo4–Na2	150.4(3)
Mo6–Mo1–Na2	68.10(7)	O4–Mo4–O10	157.6(3)
Na2–Mo1–Na1	57.10(9)	O4–Mo4–O11	103.2(3)
O7–Mo1–Mo6	96.50(2)	O4–Mo4–O12	102.4(3)
O7–Mo1–Na1	41.91(2)	O4–Mo4–N7	87.0(3)
O7–Mo1–Na2	40.76(2)	O4–Mo4–N11	85.4(3)
O7–Mo1–O15	92.6(2)	N11–Mo4–Mo5	136.4(2)
O7–Mo1–O14	90.0(2)	N11–Mo4–Na1	118.7(2)
O7–Mo1–N1	77.4(3)	N11–Mo4–Na2	81.3(2)
O7–Mo1–N5	75.9(3)	Mo2–Mo3–Na1	68.27(7)
O15–Mo1–Mo6	50.96(2)	Mo2–Mo3–Na2	68.24(7)
O15–Mo1–Na1	50.75(2)	Na1–Mo3–Na2	56.50(9)
O15–Mo1–Na2	95.87(2)	O10–Mo3–Mo2	96.13(2)
O15–Mo1–N1	84.8(3)	O10–Mo3–Na1	41.31(2)
O15–Mo1–N5	165.7(3)	O10–Mo3–Na2	40.63(2)
O14–Mo1–Mo6	50.39(2)	O10–Mo3–O8	90.9(2)
O14–Mo1–Na1	95.18(2)	O10–Mo3–O9	91.0(2)
O14–Mo1–Na2	49.42(2)	O10–Mo3–N10	77.3(3)
O14–Mo1–O15	101.1(2)	O10–Mo3–N8	76.6(3)

O14–Mo1–N1	166.4(3)	O8–Mo3–Mo2	50.2(2)
O14–Mo1–N5	87.6(3)	O8–Mo3–Na1	49.64(2)
N1–Mo1–Mo6	135.3(2)	O8–Mo3–Na2	94.4(2)
N1–Mo1–Na1	78.9(2)	O8–Mo3–O9	101.2(3)
N1–Mo1–Na2	118.1(2)	O8–Mo3–N10	165.9(3)
N5–Mo1–Mo6	137.70(2)	O8–Mo3–N8	86.8(3)
N5–Mo1–Na1	117.7(2)	O9–Mo3–Mo2	51.29(2)
N5–Mo1–Na2	81.1(2)	O9–Mo3–Na1	95.94(2)
N5–Mo1–N1	84.4(3)	O9–Mo3–Na2	50.63(2)
O1–Mo1–Mo6	106.6(3)	O9–Mo3–N10	86.8(3)
O1–Mo1–Na1	150.9(3)	O9–Mo3–N8	165.5(3)
O1–Mo1–Na2	149.9(3)	O3–Mo3–Mo2	105.9(2)
O1–Mo1–O7	156.9(3)	O3–Mo3–Na1	150.7(3)
O1–Mo1–O15	103.0(3)	O3–Mo3–Na2	150.2(3)
O1–Mo1–O14	103.4(3)	O3–Mo3–O10	157.9(3)
O1–Mo1–N1	87.1(3)	O3–Mo3–O8	103.7(3)
O1–Mo1–N5	85.7(3)	O3–Mo3–O9	102.1(3)
Mo1–Mo6–Na1	67.81(7)	O3–Mo3–N10	85.7(4)
Mo1–Mo6–Na2	68.26(7)	O3–Mo3–N8	87.5(3)
Na2–Mo6–Na1	56.93(9)	N10–Mo3–Mo2	137.8(2)
O15–Mo6–Mo1	51.13(2)	N10–Mo3–Na1	118.5(3)
O15–Mo6–Na1	50.23(2)	N10–Mo3–Na2	81.6(2)
O15–Mo6–Na2	96.07(2)	N8–Mo3–Mo2	136.6(2)
O15–Mo6–N13	84.7(3)	N8–Mo3–Na1	79.9(2)
O15–Mo6–N17	164.8(3)	N8–Mo3–Na2	117.2(2)
O14–Mo6–Mo1	50.79(2)	N8–Mo3–N10	83.1(3)
O14–Mo6–Na1	94.72(2)	Mo1–Na1–Mo2	61.41(7)
O14–Mo6–Na2	49.47(2)	Mo1–Na1–Mo4	123.35(1)
O14–Mo6–O15	101.6(3)	Mo2–Na1–Mo4	100.15(9)
O14–Mo6–N13	166.2(3)	Mo3–Na1–Mo1	100.06(1)
O14–Mo6–N17	87.0(3)	Mo3–Na1–Mo2	43.70(5)
O13–Mo6–Mo1	96.64(2)	Mo3–Na1–Mo4	61.25(6)
O13–Mo6–Na1	41.54(2)	Na2–Na1–Mo1	61.42(1)
O13–Mo6–Na2	41.81(2)	Na2–Na1–Mo2	62.44(1)
O13–Mo6–O15	91.5(2)	Na2–Na1–Mo4	62.78(9)
O13–Mo6–O14	91.1(2)	Na2–Na1–Mo3	62.77(9)
O13–Mo6–N13	76.3(3)	O10–Na1–Mo1	104.70(2)
O13–Mo6–N17	75.7(3)	O10–Na1–Mo2	67.63(2)
O6–Mo6–Mo1	106.3(2)	O10–Na1–Mo4	32.52(1)
O6–Mo6–Na1	150.6(2)	O10–Na1–Mo3	32.21(2)
O6–Mo6–Na2	150.0(2)	O7–Na1–Mo1	32.22(1)
O6–Mo6–O15	102.7(3)	O7–Na1–Mo2	32.78(1)
O6–Mo6–O14	103.3(3)	O7–Na1–Mo4	104.76(2)
O6–Mo6–O13	157.0(3)	O7–Na1–Mo3	67.85(2)
O6–Mo6–N13	87.1(3)	O15–Na1–Mo1	36.19(2)
O6–Mo6–N17	87.2(3)	O15–Na1–Mo2	94.66(2)
N13–Mo6–Mo1	135.35(2)	O15–Na1–Mo4	135.1(2)
N13–Mo6–Na1	79.7(2)	O15–Na1–Mo3	136.10(2)
N13–Mo6–Na2	118.1(2)	O13–Na1–Mo1	67.89(2)
N13–Mo6–N17	84.4(3)	O13–Na1–Mo2	105.51(2)

N17–Mo6–Mo1	137.3(2)	O13–Na1–Mo4	67.39(2)
N17–Mo6–Na1	117.2(2)	O13–Na1–Mo3	105.05(2)
N17–Mo6–Na2	79.9(2)	O8–Na1–Mo1	94.15(2)
Mo3–Mo2–Na1	68.03(6)	O8–Na1–Mo2	35.23(2)
Mo3–Mo2–Na2	68.80(7)	O8–Na1–Mo4	93.32(2)
Na1–Mo2–Na2	56.57(9)	O8–Na1–Mo3	34.86(2)
O7–Mo2–Mo3	96.01(2)	O11–Na1–Mo1	135.9(2)
O7–Mo2–Na1	41.99(2)	O11–Na1–Mo2	135.33(2)
O7–Mo2–Na2	39.58(2)	O11–Na1–Mo4	35.47(2)
O7–Mo2–O8	91.5(2)	O11–Na1–Mo3	93.54(2)
O7–Mo2–O9	90.3(2)	O1W–Na1–Mo1	117.8(3)
O7–Mo2–N2	76.6(3)	O1W–Na1–Mo2	114.9(4)
O7–Mo2–N4	75.4(3)	O1W–Na1–Mo4	118.4(4)
O8–Mo2–Mo3	49.5(2)	O1W–Na1–Mo3	115.4(4)
O8–Mo2–Na1	49.56(2)	Mo1–Na2–Mo5	99.48(9)
O8–Mo2–Na2	94.4(2)	Mo6–Na2–Mo1	43.64(5)
O8–Mo2–O9	100.7(3)	Mo6–Na2–Mo5	61.22(7)
O8–Mo2–N2	85.7(3)	Na1–Na2–Mo1	61.47(9)
O8–Mo2–N4	164.9(3)	Na1–Na2–Mo6	61.96(9)
O9–Mo2–Mo3	51.5(2)	Na1–Na2–Mo5	61.48(1)
O9–Mo2–Na1	95.90(2)	O10–Na2–Mo1	103.94(2)
O9–Mo2–Na2	50.92(2)	O10–Na2–Mo6	104.42(2)
O9–Mo2–N2	165.7(3)	O10–Na2–Mo5	66.85(2)
O9–Mo2–N4	87.1(3)	O7–Na2–Mo1	31.98(1)
N2–Mo2–Mo3	134.7(2)	O7–Na2–Mo6	67.96(2)
N2–Mo2–Na1	78.4(2)	O7–Na2–Mo5	104.74(2)
N2–Mo2–Na2	116.2(2)	O14–Na2–Mo1	35.79(2)
N2–Mo2–N4	84.0(3)	O14–Na2–Mo6	35.59(2)
N4–Mo2–Mo3	138.11(2)	O14–Na2–Mo5	94.20(2)
N4–Mo2–Na1	117.2(3)	O13–Na2–Mo1	68.05(2)
N4–Mo2–Na2	80.4(2)	O13–Na2–Mo6	32.64(1)
O2–Mo2–Mo3	107.7(2)	O13–Na2–Mo5	31.46(1)
O2–Mo2–Na1	150.2(3)	O9–Na2–Mo1	93.97(2)
O2–Mo2–Na2	151.7(2)	O9–Na2–Mo6	135.3(2)
O2–Mo2–O7	156.3(3)	O9–Na2–Mo5	133.7(2)
O2–Mo2–O8	104.1(3)	O12–Na2–Mo1	134.06(2)
O2–Mo2–O9	103.8(3)	O12–Na2–Mo6	93.30(2)
O2–Mo2–N2	86.8(3)	O12–Na2–Mo5	34.63(2)
O2–Mo2–N4	86.2(3)	O3W–Na2–Mo1	126.5(6)
Mo4–Mo5–Na1	68.06(7)	O3W–Na2–Mo6	100.4(6)
Mo4–Mo5–Na2	69.17(7)	O3W–Na2–Mo5	85.5(4)
Na1–Mo5–Na2	56.44(9)	O2W–Na2–Mo1	100.2(7)
O13–Mo5–Mo4	96.46(2)	O2W–Na2–Mo6	126.1(7)
O13–Mo5–Na1	41.37(2)	O2W–Na2–Mo5	152.7(5)
O13–Mo5–Na2	40.39(2)	Mo4–O10–Na1	106.4(3)
O13–Mo5–O11	91.2(2)	Mo4–O10–Na2	107.7(3)
O13–Mo5–N14	75.9(3)	Mo3–O10–Mo4	131.8(3)
O13–Mo5–O12	91.7(2)	Mo3–O10–Na1	106.5(3)
O13–Mo5–N16	75.5(3)	Mo3–O10–Na2	108.2(3)
O11–Mo5–Mo4	50.25(2)	Mo1–O7–Mo2	132.6(3)

O11–Mo5–Na1	50.00(2)	Mo1–O7–Na1	105.9(3)
O11–Mo5–Na2	95.4(2)	Mo1–O7–Na2	107.3(3)
O11–Mo5–N14	86.4(3)	Mo2–O7–Na1	105.2(3)
O11–Mo5–N16	164.7(3)	Mo2–O7–Na2	108.8(2)
N14–Mo5–Mo4	136.2(2)	Mo1–O15–Na1	93.1(2)
N14–Mo5–Na1	79.7(2)	Mo6–O15–Mo1	77.9(3)
N14–Mo5–Na2	116.2(2)	Mo6–O15–Na1	94.0(2)
N14–Mo5–N16	83.1(3)	Mo1–O14–Na2	94.8(2)
O12–Mo5–Mo4	50.7(2)	Mo6–O14–Mo1	78.8(2)
O12–Mo5–Na1	95.5(2)	Mo6–O14–Na2	94.9(2)
O12–Mo5–Na2	51.39(2)	Mo6–O13–Na1	106.2(2)
O12–Mo5–O11	100.7(3)	Mo6–O13–Na2	105.5(3)
O12–Mo5–N14	165.9(3)	Mo5–O13–Mo6	133.4(3)
O12–Mo5–N16	87.4(3)	Mo5–O13–Na1	106.7(3)
O5–Mo5–Mo4	106.3(2)	Mo5–O13–Na2	108.2(2)
O5–Mo5–Na1	150.8(3)	Mo2–O8–Na1	95.2(3)
O5–Mo5–Na2	150.7(2)	Mo3–O8–Mo2	80.4(3)
O5–Mo5–O13	157.3(3)	Mo3–O8–Na1	95.5(3)
O5–Mo5–O11	103.4(3)	Mo5–O11–Na1	93.7(3)
O5–Mo5–N14	87.6(3)	Mo4–O11–Mo5	77.9(3)
O5–Mo5–O12	102.4(3)	Mo4–O11–Na1	94.3(3)
O5–Mo5–N16	87.2(3)	N13–N14–Mo5	120.6(6)
N16–Mo5–Mo4	137.52(2)	N15–N14–Mo5	128.7(7)
N16–Mo5–Na1	116.8(2)	Mo2–O9–Mo3	77.2(3)
N16–Mo5–Na2	79.5(2)	Mo2–O9–Na2	93.2(2)
Mo5–Mo4–Na1	68.59(7)	Mo3–O9–Na2	93.5(3)
Mo5–Mo4–Na2	67.99(7)	Mo5–O12–Mo4	79.5(3)
Na1–Mo4–Na2	56.30(9)	Mo5–O12–Na2	94.0(2)
O10–Mo4–Mo5	96.14(2)	Mo4–O12–Na2	94.4(3)
O10–Mo4–Na1	41.12(2)	N14–N13–Mo6	119.6(6)
O10–Mo4–Na2	40.62(2)	C10–N13–Mo6	133.0(7)
O10–Mo4–O11	91.2(2)	N2–N1–Mo1	118.6(6)
O10–Mo4–O12	91.3(2)	C2–N1–Mo1	132.6(9)
O10–Mo4–N7	77.1(3)	N8–N7–Mo4	118.3(7)
O10–Mo4–N11	77.6(3)	C6–N7–Mo4	130.7(8)
O11–Mo4–Mo5	51.9(2)	N4–N5–Mo1	120.1(6)
O11–Mo4–Na1	50.20(2)	N6–N5–Mo1	129.7(8)
O11–Mo4–Na2	95.4(2)	N16–N17–Mo6	120.3(7)
O11–Mo4–O12	101.4(3)	N18–N17–Mo6	132.9(8)
O11–Mo4–N7	85.1(3)	N11–N10–Mo3	120.5(6)
O11–Mo4–N11	166.2(3)	C8–N10–Mo3	132.9(9)
O12–Mo4–Mo5	49.80(2)	N7–N8–Mo3	122.4(7)
O12–Mo4–Na1	95.36(2)	N9–N8–Mo3	130.1(8)
O12–Mo4–Na2	50.78(2)	N1–N2–Mo2	121.1(6)
O12–Mo4–N7	166.8(3)	N3–N2–Mo2	132.7(9)
O12–Mo4–N11	86.9(3)	N10–N11–Mo4	116.9(6)
N7–Mo4–Mo5	136.6(2)	N12–N11–Mo4	134.0(9)
N7–Mo4–Na1	79.9(2)	N5–N4–Mo2	120.0(6)
N7–Mo4–Na2	117.7(2)	C4–N4–Mo2	129.7(8)
N7–Mo4–N11	84.6(3)	N17–N16–Mo5	120.4(7)

O4–Mo4–Mo5	106.2(2)	C12–N16–Mo5	129.8(9)
O4–Mo4–Na1	151.0(3)		

Table S9. Comparisons of selected bond distances (Å) for $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**), $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**), $Na_3[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_3(trz)_3]\cdot 7.5H_2O$ (**5**),[1] $[Mo_8O_8(\mu_2\text{-}O)_{12}(Htrz)_8]\cdot 30H_2O$ (**6**),[1] $[Mo_8O_8(\mu_2\text{-}O)_{12}(Htrz)_8]\cdot 62H_2O$ (**7**),[2] $[MoO_3(1,2,3\text{-}Htrz)_{0.5}]$ (**8**),[3] $[Cu_3(Htrz)_2Mo_4O_{13}(OH)]\cdot 6H_2O$ (**9**),[3] $H_2[Cu_4(trz)_5(H_2O)_2][Mo_4Cu_4O_{26}]_{0.5}\cdot 3H_2O$ (**10**),[4] $[Cu_{24}(trz)_{16}(H_2O)Cl_4(HPMo_{12}O_{40})]$ (**11**),[5] Cu(trz) (**12**),[3] $[Cu_6(trz)_3I_3]_n$ (**13**),[6] $(Cu_5I_5)[Cu(trz)_2]^-$ (**14**),[7] $[Cu(trz)_2]$ (**15**),[8] $[Cu_3(trz)_2V_4O_{12}]$ (**16**),[9] $[Zn_{10}(trz)_{12}(TADIPA)_2(DMF)_4]\cdot DMF\cdot 6H_2O$ (**17**),[10] $[Zn_{10}(trz)_{12}(TPTA)_2(DMA)_2]\cdot 2DMA\cdot 4H_2O$ (**18**),[10] $[(Zn_3OH)_2(trz)_6\cdot Zn_6(OHOBDC)_6]\cdot 2NH_2(CH_3)_2$ (**19**),[11] $[(Zn_3OH)_2(trz)_6\cdot Zn_6(OBDC)_6]\cdot 2NH_2(CH_3)_2$ (**20**),[11] $[Zn_3(tp)_2(trz)_2]_n$ (**21**),[12] $Zn_5(trz)_6(NO_3)_4$ (**22**),[13] $Zn_3(trz)_2(bdc)_2\cdot 2DMAc\cdot C_6H_4(OH)_2$ (**23**),[13] $[Ag_{29}(trz)_{18}][SiW_7W_5O_{40}](Ag_{29}SiW_{12})$ (**24**),[14] $H[Ag_{27}(trz)_{16}(H_2O)_4][(AsW_{12}O_{40})_2]$ (**25**),[15] $[Ag_{15}(trz)_8][AsW_{12}O_{40}]$ (**26**),[15] $H_3[Ag_{27}(trz)_{16}(H_2O)_6][SiW_{12}O_{40}]_2\cdot 5H_2O$ (**27**),[16] $H[Ag_{27}(trz)_{16}(H_2O)_4][PW_{12}O_{40}]_2\cdot 2H_2O$ (**28**),[16] $[Ag_{23}(trz)_{14}(H_2O)_2][HSiW_{12}O_{40}]$ (**29**),[16] $[Ag_{23}(trz)_{14}(H_2O)_2][PW_{12}O_{40}]$ (**30**),[16] $[Cd_3(trz)_3Cl_3]_n$ (**31**),[6] $\{[Cd_3(trz)_6]\cdot 6H_2O\}_n$ (**32**),[6] $Cd[HB(trz)_3]_2$ (**33**).[17]

Complexes	M	Mo=O (Å)	Mo–μ_2-$O_{Mo–Mo}$(Å)	Mo–μ_2-$O_{Mo–trz–Mo}$ (Å)	M–N (Å)
1	Mo	$1.717(6)_{av}$	$1.961(6)_{av}$	$2.002(5)_{av}$	$2.225(7)_{av}$
2		$1.687(6)_{av}$	$1.938(6)_{av}$	$2.180(5)_{av}$	$2.197(7)_{av}$
3		$1.698(5)_{av}$	$1.961(5)_{av}$	$1.954(3)_{av}$	$2.225(7)_{av}$
4		$1.722(6)_{av}$	$2.065(7)_{av}$	$1.962(6)_{av}$	$2.244(9)_{av}$
Av		**$1.706(6)_{av}$**	**$1.981(6)_{av}$**	**$2.025(5)_{av}$**	**$2.223(8)_{av}$**
5	Mo	$1.727(5)_{av}$	$2.011(1)_{av}$	$1.959(9)_{av}$	$2.241(1)_{av}$
6		$1.688(4)_{av}$	$1.936(4)_{av}$	$2.157(3)_{av}$	$2.198(5)_{av}$
7		$1.683(7)_{av}$	$1.941(4)_{av}$	$2.148(3)_{av}$	$2.198(2)_{av}$
8		1.682(5)	$1.893(4)_{av}$	1.875(2)	2.433(5)
9		$1.730(3)_{av}$	$1.947(3)_{av}$		
10		$1.670(4)_{av}$	$1.888(9)_{av}$		
11		$1.662(7)_{av}$	$1.908(9)_{av}$		
Av		**$1.692(5)_{av}$**	**$1.932(5)_{av}$**	**$2.035(4)_{av}$**	**$2.268(3)_{av}$**
9	Cu				$1.952(4)_{av}$
10					$2.049(1)_{av}$
11					$1.881(9)_{av}$
12					$1.974(2)_{av}$
13					$1.929(1)_{av}$
14					$1.97(1)_{av}$
15					$2.181(5)_{av}$
16					$1.963(4)_{av}$
Av					**$1.987(3)_{av}$**
17	Zn				$2.101(4)_{av}$
18					$2.092(3)_{av}$
19					$2.080(8)_{av}$
20					$2.095(2)_{av}$
21					$2.050(3)_{av}$
22					$2.132(3)_{av}$
23					$2.065(4)_{av}$

Av		**2.088(4)$_{av}$**
24	Ag	2.146(4)$_{av}$
25		2.115(3)$_{av}$
26		2.13(3)$_{av}$
27		2.114(2)$_{av}$
28		2.126(2)$_{av}$
29		2.138(2)$_{av}$
30		2.145(2)$_{av}$
Av		**2.131(3)$_{av}$**
31	Cd	2.311(5)$_{av}$
32		2.351(6)$_{av}$
33		2.349(1)$_{av}$
Av		**2.373(4)$_{av}$**

Av represents average. List of abbreviations: H_4TADIPA = 5,5′-(1H-1,2,4-triazole-3,5-diyl)diisophthalic acid, DMF = *N*,*N*-dimethylformamide, H_4TPTA = [1,1′:3′,1″-terphenyl]-3,3″,5,5″-tetracarboxylic acid, DMA = *N*,*N*-dimethylacetamide; H_4DOBDC = 2,5-dihydroxyterephthalic acid, H_3OBDC = 2-hydroxyterephthalic acid; tp = terephthalate; H_2bdc = terephthalic acid, DMAc = *N*,*N*-dimethylacetamide.

Table S10. Detail calibrated adsorption data of O_2, N_2, H_2, CO_2 and CH_4 for $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**) at 298 K.

Gases	O_2		CO_2		CH_4		N_2		H_2	
Temperature (°C)	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
	0.901	1.20146	0.895	2.91417	0.900	0.65962	0.900	0.80859	0.900	1.06600
	1.910	1.59459	1.900	3.84683	1.910	0.75338	1.900	0.83135	1.910	1.24147
	3.900	2.22086	3.900	5.12808	3.900	0.81318	3.900	0.86466	3.910	1.13953
	5.900	2.91233	5.898	6.01419	5.899	0.80167	5.895	0.85572	5.910	1.12377
	7.897	3.72497	7.891	7.08482	7.899	0.86542	7.900	0.91075	7.900	1.29036
	9.890	4.36027	9.894	7.84100	9.895	0.93096	9.899	0.98113	9.901	1.41196
	11.893	5.04451	11.896	8.79690	11.899	0.96234	11.896	0.99932	11.900	1.31786
	13.900	5.81597	13.895	9.45548	13.893	0.93762	13.893	1.01587	13.901	1.07930
	15.894	6.39814	15.894	10.54885	15.895	0.96558	15.898	0.99552	15.907	1.19075
	17.900	7.05991	17.894	10.94648	17.897	0.96485	17.897	1.01067	17.903	1.35016
	19.896	7.66172	19.896	12.38102	19.897	0.88081	19.899	1.08557	19.905	1.35929
	21.899	8.32109	21.892	12.44916	21.895	1.04187	21.892	1.02015	21.900	1.06392
	23.897	8.99572	23.894	12.84092	23.895	1.04187	23.895	1.05164	23.903	1.25002
	25.894	9.63720	25.893	14.63140	25.897	1.01403	25.892	1.01958	25.904	1.09822
	27.896	10.23207	27.892	14.63140	27.897	0.89531	27.893	1.01958	27.902	1.00704
	29.897	10.93957	29.891	15.25720	29.896	0.98330	29.893	0.95286	29.905	1.40765

Table S11. Detail calibrated adsorption data of O_2, N_2, H_2, CO_2 and CH_4 for $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) at 298 K.

Gases	O_2		CO_2		CH_4		N_2		H_2	
Temperature (°C)	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
	0.900	1.05713	0.895	2.76303	0.900	0.18761	0.898	0.23097	0.900	0.07238
	1.900	1.55384	1.900	3.98258	1.910	0.34022	1.900	0.26136	1.900	0.08325
	3.900	2.30408	3.900	5.09627	3.900	0.40163	3.890	0.38401	3.910	0.09704
	5.890	2.94222	5.899	5.82859	5.900	0.52627	5.890	0.42085	5.910	0.08770
	7.899	3.78207	7.895	6.35108	7.896	0.58646	7.899	0.51454	7.900	0.18790
	9.897	4.60447	9.897	6.97763	9.899	0.67683	9.890	0.53204	9.901	0.16635
	11.900	5.43190	11.895	7.48048	11.900	0.69210	11.896	0.68936	11.905	0.14362
	13.895	6.00660	13.894	7.83025	13.895	0.73648	13.899	0.74183	13.912	0.11968
	15.896	6.67295	15.899	8.22129	15.894	0.72099	15.894	0.73707	15.900	0.14846
	17.900	7.38667	17.894	8.51607	17.894	0.75000	17.894	0.71126	17.903	0.16561
	19.894	8.01280	19.892	8.83445	19.899	0.81263	19.896	0.73580	19.906	0.21733
	21.894	8.71157	21.897	9.13997	21.897	0.80729	21.899	0.71102	21.905	0.19979
	23.894	9.34683	23.896	9.13997	23.898	0.76026	23.897	0.60355	23.904	0.13476
	25.893	10.07824	25.894	9.26432	25.897	0.84049	25.896	0.59378	25.901	0.19134
	27.898	10.78664	27.894	9.64255	27.894	0.76926	27.895	0.55800	27.904	0.16042
	29.896	11.43590	29.892	9.75213	29.898	0.72027	29.897	0.54853	29.900	0.16555

Table S12. Detail calibrated adsorption data of O_2, N_2, H_2, CO_2 and CH_4 for $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) at 298 K.

Gases	O_2		CO_2		CH_4		N_2		H_2	
Temperature (°C)	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
	0.900	1.52563	0.900	3.16372	0.897	0.51970	0.897	0.93336	0.902	0.83219
	1.900	1.96613	1.900	4.38676	1.900	0.72855	1.900	1.08367	1.900	0.89006
	3.900	2.79526	3.900	5.79246	3.900	0.90517	3.890	1.04798	3.900	1.18211
	5.899	3.85279	5.900	7.21671	5.892	1.05807	5.900	0.96659	5.890	1.32227
	7.895	4.72477	7.898	8.16657	7.891	1.20453	7.897	1.06992	7.899	1.27938
	9.896	5.64483	9.891	8.85294	9.894	1.35089	9.893	0.97765	9.908	1.38368
	11.896	6.30076	11.892	9.56203	11.899	1.50293	11.892	1.08237	11.901	1.44399
	13.893	7.13015	13.897	10.49088	13.897	1.73224	13.897	1.00510	13.905	1.48594
	15.896	7.89819	15.894	11.50677	15.895	1.75789	15.895	0.91991	15.904	1.54684
	17.894	8.74856	17.894	11.76114	17.896	1.91461	17.894	1.02700	17.903	1.71844
	19.896	9.63265	19.895	12.20985	19.894	2.04054	19.894	0.81302	19.904	1.70628
	21.894	10.50397	21.892	12.20985	21.892	2.37734	21.896	0.98947	21.903	1.58512
	23.894	11.31848	23.892	13.96626	23.895	2.43672	23.893	0.67786	23.903	1.50193
	25.893	11.91955	25.893	14.33316	25.895	2.73173	25.893	0.88494	25.906	1.57642
	27.895	12.63629	27.891	14.54317	27.895	2.99196	27.892	0.61879	27.902	1.74072
	29.895	13.54145	29.890	15.59483	29.895	2.99196	29.891	0.61035	29.901	1.65163

Table S13. Comparisons of O_2 and CO_2 adsorption data for **2** ~ **4** with some other reported porous materials at 1.0 bar under different temperatures.

Adsorbent	O_2 amount ($mmol \cdot g^{-1}$)	CO_2 amount ($mmol \cdot g^{-1}$)	Temperature (K)
2	0.0250	0.0482	298
3	0.0253	0.0489	298
4	0.0338	0.0525	298
MOF-177[21]	0.18		298
Cu(BDT)[22]	14.30		77
[Zn(dtp)][23]	12.39		77
[Zn(dtp)][23]		6.10	195
[Mg(TCPBDA)][24]		1.49	298
Fe_2(DOBDC)[25]		2.02	298
[Cu(tba)$_2$][26]		1.83	293
[Cu**L**][27]		4.95	298

List of abbreviations: H_2BDT = ditetrazole 1,4-benzeneditetrazol-5-yl; H_2dtp = 2, 3-di-1*H*-tetrazol-5-ylpyrazine; $TCPBDA^{2-}$ = *N*,*N*,*N*',*N*'-tetrakis(4-carboxyphenyl)-biphenyl-4'4-diamine; BOBDC = 2,5-dioxido-1,4-benzenedicarboxylate; tba = 4-(1*H*-1,2,4-triazol-1-yl)benzoate; H_2**L** = 5-(1*H*-tetrazol-1-yl)isophthalic acid

Table S14. Bond valence calculations for complexes $[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**), $Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**), $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**) and $Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**) respectively.

Complexes	Atoms	N	$\sum S_{ij}$	Δ
$[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_6]\cdot 15H_2O$ (**1**)	Mo1	5+	5.230	0.230
	Mo2	5+	5.386	0.386
	Mo3	5+	5.257	0.257
	Mo4	5+	5.263	0.263
	Mo5	5+	5.218	0.218
	Mo6	5+	5.394	0.394
	Mo	**5+**	**5.291**	**0.291**
$Na[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_5(trz)]\cdot 12H_2O$ (**2**)	Mo1	5+	5.351	0.351
	Mo2	5+	5.292	0.292
	Mo3	5+	5.363	0.363
	Mo	**5+**	**5.335**	**0.335**
$Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 10H_2O$ (**3**)	Mo1	5+	5.153	0.153
	Mo2	5+	5.078	0.078
	Mo3	5+	5.351	0.351
	Mo	**5+**	**5.194**	**0.194**
$Na_2[Mo_6O_6(\mu_2\text{-}O)_9(Htrz)_4(trz)_2]\cdot 49H_2O$ (**4**)	Mo1	5+	4.868	0.132
	Mo2	5+	4.899	0.101
	Mo3	5+	4.891	0.109
	Mo4	5+	4.862	0.138
	Mo5	5+	4.826	0.174
	Mo6	5+	4.926	0.074
	Mo	**5+**	**4.879**	**0.121**

Table S15. Selected average bond distances (Å) and NPA charge of different N donor and Mo atoms in the optimized individual conformers of **1-1** ~ **4-1** complexes calculated at the B3LYP/def2SVP/LANL2DZ level of theory.

Complexes	Bond Distances (Å)		NPA Charge		
	$Mo–N_{neutral}$	$Mo–N_{anion}$	Q_{Mo}	$Q_{N\text{-}neutral}$	$Q_{N\text{-}anion}$
1-1	2.435_{av}		0.998_{av}	-0.212_{av}	
2-1	2.413_{av}	2.264_{av}	0.969_{av}	-0.211_{av}	-0.291_{av}
3-1	2.399_{av}	2.235_{av}	0.942_{av}	-0.214_{av}	-0.273_{av}
4-1	2.388_{av}	2.250_{av}	0.945_{av}	-0.210_{av}	-0.290_{av}

Table S16. Geometry optimized coordinates for compounds **1** ~ **4** and **1-1** ~ **4-1**, respectively.

1			
Mo	9.797845339	7.421998322	7.366825012
Mo	7.421969778	3.544719927	11.6001938
Mo	10.660716	5.652893137	5.780763283
Mo	6.554768185	5.305920419	13.18735751
Mo	9.647420827	5.668480076	2.262223269
Mo	7.580426812	5.276325968	16.68808211
Mo	6.807966571	10.03428864	3.772931842
Mo	10.41091982	0.932783694	15.19868734
Mo	8.0896978	7.500294006	1.478845242
Mo	9.131108541	3.456159765	17.5021151
Mo	7.498020661	9.976586745	6.192231533
Mo	9.721467495	0.992722559	12.77942311
O	11.33028355	7.436634763	6.158945085
O	5.887145491	3.527470886	12.80614995
O	9.81935423	6.144044695	4.115997799
O	7.391780987	4.761486991	14.8509716
O	10.05262783	7.443311342	1.574659242
O	7.168546107	3.517723736	17.4024486
O	9.051441703	5.687487331	6.876731083
O	8.16708105	5.279744726	12.09450274
O	8.688118639	8.475200139	6.169586649
O	8.530881074	2.493278605	12.79887774
O	7.814098885	8.530072617	3.083579207
O	9.405270552	2.438647778	15.88787747
O	8.33091301	10.86290415	4.664362535
O	8.886859133	0.105502389	14.30461822
O	6.016635432	9.105107576	5.288343069
O	11.20209873	1.864098748	13.68184061
O	7.698093086	5.778242491	2.27889701
O	9.53620561	5.191493863	16.74878823
O	10.50923133	7.223289555	8.940240068
O	6.710357399	3.747033943	10.02783763
O	11.76304403	4.596371088	6.630945602
O	5.456678289	6.371606374	12.34164396
O	9.9646257	4.55168486	0.95391906
O	7.23425445	6.423146319	17.95770294
O	4.071291724	-0.008681141	3.391326475
O	13.14764494	10.97424384	15.57704922
O	5.110971823	-0.142452838	7.190884811
O	12.10824992	11.11285069	11.77916789
O	12.61418513	6.964045041	18.73801841
O	4.604255387	4.000658634	0.240291017
N	3.968979296	8.68812104	2.457452775
N	13.24134385	2.281328516	16.46898347
N	5.311276308	8.686211323	2.528138787
N	11.89894304	2.271648582	16.43105372

N	7.768659944	7.712165433	8.531547952
N	9.451193322	3.255070267	10.43639998
N	5.745296846	7.876319577	1.581194018
N	11.47704863	3.070024752	17.39171477
N	6.878945309	8.501606998	7.960628095
N	10.34255817	2.470756077	11.01247254
N	9.801100918	3.614724817	4.818903787
N	7.421831511	7.303227748	14.14200571
N	12.26283364	5.381980227	4.035601681
N	4.947787814	5.546478622	14.92743091
N	9.427594983	3.668728107	3.557468498
N	7.816122277	7.246094437	15.39595276
N	11.90794831	5.307052431	2.764920264
N	5.305831993	5.609762404	16.19725648
N	7.929879051	10.76617733	1.73496179
N	9.295918307	0.199289066	17.23492563
N	8.326409281	9.800990875	0.93216933
N	8.896269394	1.161497708	18.03990377
N	10.1897944	9.650660562	7.872915932
N	7.030687624	1.311189207	11.09277384
N	9.475250664	10.65826473	7.418939791
N	7.746480997	0.307455832	11.55258865
N	5.726392293	8.335275877	8.623971734
N	11.49355612	2.63280824	10.34551994
N	2.81493934	5.020767703	4.103377011
N	14.40340202	5.937487232	14.86201847
N	11.11158876	10.14721011	8.702493907
N	6.107834066	0.808560154	10.26812158
N	13.7040999	10.00626979	18.80914495
N	3.517567592	0.952558482	0.160619648
N	8.894249315	2.476083941	3.254093489
N	8.37628226	8.42797385	15.68702016
H	3.44746708	9.231133145	3.144950078
H	13.75072365	1.745751466	15.76666856
H	4.904120346	8.830274229	8.28425181
H	12.31571789	2.136281524	10.6836704
H	3.244154449	4.959111027	5.026335843
H	13.97502226	6.013789938	13.93975213
H	9.745390784	2.129483434	6.341648083
H	7.469116177	8.786564843	12.61653978
H	11.66612462	9.491688456	9.25633412
H	5.550962054	1.457604055	9.709095844
H	13.97894837	9.421403582	18.01864779
H	3.239514286	1.533935214	0.952403856
H	2.161707676	4.76039224	0.944397808
H	15.06587292	6.169340006	18.0208366
H	4.814372701	6.672390682	0.070106661
H	12.43077607	4.277278297	18.88415702
H	7.744235996	6.363852122	10.20676416
H	9.471987206	4.58813426	8.747835302

H	2.481479964	7.729541531	1.218213639
H	14.74717616	3.239237693	17.68463761
H	8.550909526	2.328698572	2.306693599
H	8.726742242	8.573003475	16.63200127
H	6.266734168	1.566339001	1.605542838
H	10.9598909	9.399212133	17.35713322
H	5.080140741	7.142365963	10.3220761
H	12.13608415	3.812153825	8.636313634
H	4.33385023	4.424242431	2.685401785
H	12.89954785	6.558482815	16.28540863
H	7.856843342	1.433113765	7.758532383
H	9.366962439	9.530400229	11.2276594
H	10.00861697	0.722823998	9.463215955
H	7.212040717	10.22588421	9.522509794
H	8.406722812	0.66057577	4.321290759
H	8.86265514	10.24094148	14.61584331
H	12.35548428	0.648265017	18.08621529
H	4.870715775	10.30813642	0.877738429
C	9.504818443	2.384872857	5.319722215
C	7.727349825	8.528482171	13.63331094
C	2.232988479	4.887986066	2.019283486
C	14.99107304	6.048490828	16.94559035
C	4.685961814	7.366624139	0.893984945
C	12.54690975	3.584836557	18.05774853
C	7.192849175	7.050524649	9.571750116
C	10.02472146	3.908188318	9.389484321
C	3.527966473	7.881244042	1.455979576
C	13.69701211	3.082956368	17.46798376
C	6.569434289	0.631298023	1.148744104
C	10.65682766	10.332392	17.81701021
C	5.865456501	7.438067132	9.636139897
C	11.35228554	3.521101976	9.326188556
C	3.305786357	4.706080216	2.875453245
C	13.92123766	6.256546315	16.0919891
C	8.323227665	0.477413982	7.963273019
C	8.899025301	10.48414312	11.01725568
C	9.381000993	0.156893922	8.793085575
C	7.839814806	10.79825054	10.18691263
C	8.899044617	1.636955351	4.324278288
C	8.362371934	9.267711833	14.61712319
C	7.161789209	0.386513374	-0.075872989
C	10.06307813	10.57251386	19.04178613
2			
Mo	4.603551	8.730613	9.521628
Mo	8.868149	8.22178	6.246881
Mo	7.178457	6.889044	7.637791
Mo	17.129953	18.760078	9.515879
Mo	21.393856	18.252623	6.240171
Mo	19.704819	16.920639	7.632102
Mo	19.587893	8.777758	1.563153

Mo	15.374062	8.203693	4.934515
Mo	17.053261	6.921876	3.483155
Mo	7.062613	18.808699	1.560806
Mo	2.84894	18.235708	4.932731
Mo	4.528007	16.953369	3.481995
Mo	19.566656	11.333688	1.562925
Mo	15.303492	11.840156	4.838882
Mo	16.991167	13.173311	3.446563
Mo	7.041253	1.301982	1.558562
Mo	2.778426	1.809998	4.836131
Mo	4.466904	3.141756	3.442825
Mo	4.583189	11.286815	9.52171
Mo	8.796634	11.860325	6.149747
Mo	7.117556	13.144371	7.60022
Mo	17.108612	1.253547	9.515994
Mo	21.322857	1.826758	6.143924
Mo	19.643412	3.109049	7.594938
O	6.114714	8.402691	8.353825
O	8.880286	7.680004	8.14473
O	7.032619	7.622772	5.823733
O	3.25447	8.013567	10.37399
O	10.00231	7.162054	5.425274
O	7.482309	5.174979	7.51395
O	18.640102	18.43429	8.345338
O	21.40535	17.714172	8.138503
O	19.558338	17.652637	5.817118
O	15.781121	18.042711	10.367909
O	22.528416	17.193222	5.418404
O	20.011377	15.207055	7.512218
O	18.080698	8.438166	2.750222
O	15.323681	7.670432	3.02588
O	17.218361	7.618197	5.31504
O	20.940956	8.08584	0.694288
O	14.30457	7.078011	5.744708
O	16.783861	5.197881	3.579512
O	5.555521	18.469219	2.747953
O	2.79909	17.702717	3.024141
O	4.69312	17.650152	5.313406
O	8.414796	18.114727	0.692318
O	1.780219	17.108984	5.742307
O	4.258273	15.229321	3.57736
O	18.055742	11.659577	2.733037
O	15.289987	12.380212	2.940892
O	17.13846	12.441418	5.261371
O	20.915359	12.051414	0.710757
O	14.168077	12.897678	5.662344
O	16.684389	14.886798	3.56692
O	5.531742	1.628385	2.72913
O	2.766367	2.347314	2.937366
O	4.613862	2.410706	5.258211

O	8.389285	2.020271	0.70614
O	1.643704	2.869625	5.65765
O	4.160507	4.855709	3.561117
O	6.091701	11.628086	8.336875
O	8.847981	12.397526	8.057454
O	6.95182	12.445483	5.770317
O	3.230073	11.979772	10.38977
O	9.865202	12.986215	5.338603
O	7.383453	14.868895	7.500836
O	18.615532	1.593127	8.328296
O	21.372955	2.360633	8.052273
O	19.478554	2.412625	5.763165
O	15.755853	1.945416	10.385107
O	22.392551	2.952198	5.333405
O	19.912724	4.832993	7.499052
O	8.251411	10.042825	6.668297
O	5.468997	10.014329	10.708215
O	3.860797	10.005385	8.207965
O	20.775291	0.009896	6.661969
O	17.994938	20.043327	10.702755
O	16.386251	20.034008	8.202401
O	15.921804	10.021104	4.41675
O	18.701752	10.050205	0.376237
O	20.309933	10.059481	2.876894
O	3.397968	20.052713	4.415098
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O	0.688932	4.786438	-0.058153
N	-1.26535	3.618642	1.716983
N	-2.540432	-2.923636	1.535611
N	-2.653753	-3.111666	-1.6311
N	-1.36703	3.783914	-1.45935
N	-2.41093	3.039055	1.54539
O	-4.548723	-1.84486	0.054248
N	-2.512845	3.202305	-1.621568
O	-4.463568	2.042483	0.078312
C	-1.364547	4.51562	2.729633
H	-0.516247	5.118649	3.042541
N	-3.265006	3.53759	2.415558
H	-4.227453	3.199671	2.363808
N	-1.348374	4.882251	-2.186189
H	-0.515394	5.46939	-2.104329
H	-4.346498	-2.972124	2.394201
C	-3.450706	-3.834957	-2.458856
H	-4.44635	-3.495869	-2.73261
C	-2.667033	4.470842	3.196273
H	-3.186795	5.004505	3.986976
C	-2.515123	5.034202	-2.860066
H	-2.711594	5.869578	-3.526331
C	-3.266696	3.934835	-2.481049
H	-4.274712	3.634656	-2.754841
Mo	2.64931	1.799372	0.027405
Mo	0.269017	-3.098639	0.078176
Mo	2.53689	-1.866324	0.022311
O	1.903241	-0.045772	0.155543
O	1.327468	-2.45351	1.525702
O	1.270821	-2.323027	-1.420405
O	3.933708	2.938764	0.042474
N	4.09454	0.589974	1.51795
N	-1.423045	-3.556955	1.700088
N	-1.535678	-3.742978	-1.460242
N	3.82421	0.592911	-1.488706
N	4.013269	-0.700692	1.441295
O	0.486741	-4.817953	-0.055924
N	3.790115	-0.743801	-1.488622
O	3.838356	-3.020569	0.132456
C	5.238036	0.925383	2.16563
H	5.517487	1.964285	2.31881
N	5.077314	-1.223785	2.014331
H	5.188303	-2.236199	1.916184
N	4.624378	1.053973	-2.419849
C	-1.54898	-4.427472	2.732474
H	-0.72624	-5.065471	3.044029
H	-0.775579	-5.490703	-2.04891
C	5.889505	-0.250841	2.494823
H	6.827516	-0.458399	3.001811
C	5.132303	-0.016945	-3.059021

H	5.827209	0.09089	-3.889906
C	4.608591	-1.165622	-2.466293
H	4.758192	-2.224145	-2.664626
Na	0.124153	0.014344	-1.295274
O	-1.037782	-1.617478	-0.116689
O	1.456386	2.403349	1.533995
O	1.346848	2.229069	-1.393926
C	-2.838767	-4.307082	3.220324
C	-2.757802	-4.981977	-2.807406
H	-3.370385	-4.796935	4.031234
H	-3.002444	-5.828922	-3.442406
N	-1.577757	-4.864842	-2.149856
N	-3.402864	-3.360434	2.430639
3-1			
Mo	1.275874	-2.864047	0.030101
Mo	-3.09408	0.38066	-0.034367
Mo	-1.287398	-2.861566	0.027569
O	-1.567952	-0.950634	0.034665
O	-0.004055	-2.651434	-1.451226
O	-0.006985	-2.872845	1.510789
N	3.042357	-2.532817	1.627869
N	-3.055028	-2.450168	-1.492689
N	3.057256	-2.44895	-1.485337
O	1.935826	-4.465682	-0.158105
N	-3.681473	-1.32627	-1.639802
O	-4.805388	0.635333	0.070472
O	-1.951541	-4.462294	-0.159829
N	-3.663056	-1.370546	1.512195
C	3.715356	-3.316233	2.508744
N	3.625577	-3.343178	-2.270137
N	-3.059105	-2.513353	1.622761
C	-4.671247	-2.816326	-2.937143
H	-5.286948	-3.384494	-3.628934
C	-4.693437	-1.493199	-2.527558
H	-5.358168	-0.67566	-2.794748
N	-3.633271	-3.357502	-2.254615
H	-3.276569	-4.312924	-2.177357
C	-3.711126	-3.276964	2.536075
H	-3.378855	-4.2819	2.782822
C	-4.782719	-2.536806	3.005714
H	-5.559029	-2.743086	3.737315
N	-4.697969	-1.366876	2.326873
H	-5.298361	-0.539653	2.311639
H	3.386815	-4.325362	2.743359
H	3.263228	-4.297567	-2.215924
Mo	3.094021	0.373531	-0.01071
Mo	-1.817552	2.638572	-0.000445
Mo	1.825416	2.636448	-0.03882
O	0.002667	1.80587	-0.052853
O	2.363169	1.339184	-1.497748

O	2.231536	1.304425	1.44018
N	3.647079	-1.390057	1.5244
N	0.677276	3.833135	-1.525731
N	3.689503	-1.325875	-1.61445
O	4.803519	0.62216	0.146135
N	-0.658536	3.877687	-1.474102
O	-3.005825	3.875178	-0.052449
O	3.016702	3.866635	0.071022
N	-0.666887	3.800522	1.506039
N	4.703773	-1.405511	2.310201
C	4.693584	-1.479154	-2.513347
H	5.358142	-0.658461	-2.771393
N	0.666614	3.849521	1.45004
C	0.092791	5.24207	-3.013157
H	0.212332	5.967998	-3.815144
C	-1.063658	4.763623	-2.396971
H	-2.117097	4.990936	-2.539011
N	1.153152	4.643835	-2.439147
C	1.074966	4.712848	2.393007
H	2.128595	4.939465	2.534273
C	-0.079958	5.172456	3.025992
H	-0.19769	5.878658	3.845681
N	-1.141742	4.585938	2.442439
H	5.311727	-0.583548	2.279354
Na	-0.009087	0.095924	-1.528353
Na	-0.000614	0.237626	1.548584
O	1.562854	-0.953313	0.034888
O	-2.305298	1.338415	-1.492379
O	-2.276781	1.308209	1.448714
C	4.661363	-2.793489	-2.949496
C	4.802423	-2.589061	2.96318
H	5.598373	-2.813319	3.667908
H	5.268125	-3.350256	-3.658261
4-1			
Mo	3.173878	-0.334178	-0.026293
Mo	2.319162	2.09699	-0.128376
Mo	0.694858	-3.049788	0.059187
Mo	-1.302568	2.843393	0.099075
Mo	-3.010269	0.914393	0.024619
Mo	-1.857	-2.580288	-0.039497
Na	-0.060927	-0.091845	-1.533049
Na	0.055857	-0.064631	1.518256
O	-1.73888	-0.549583	0.128201
O	1.378373	-1.191994	-0.113888
O	2.541596	0.832277	-1.55778
O	2.554921	0.892857	1.39001
O	0.361199	1.798269	-0.030807
O	-0.520932	-2.558136	-1.450221
O	-2.047199	1.846024	-1.414673
N	0.10822	3.944026	-1.482238

O	-0.544553	-2.602525	1.476599
O	-1.982283	1.769189	1.546448
O	-2.679708	-4.082439	0.025318
O	3.636322	3.226045	-0.072564
N	1.359272	3.675798	-1.68982
O	-2.071926	4.401396	0.058585
N	3.457846	-2.193797	-1.493863
N	-3.774294	-0.524615	-1.515797
N	3.271401	-1.952236	1.526601
N	1.451411	3.644481	1.462888
N	-3.611935	-1.945993	1.479379
O	4.888273	-0.31244	-0.132556
N	-3.341815	-1.791961	-1.546224
N	2.557629	-3.119085	-1.395342
O	-4.619867	1.55024	0.22155
N	-3.979932	-0.706218	1.420246
N	2.362274	-2.934421	1.572441
N	0.196568	3.896415	1.664388
N	3.001626	-4.202066	-1.998224
H	2.423533	-5.041458	-1.902174
N	-0.23167	4.965853	-2.24211
H	-1.185364	5.31966	-2.143987
O	0.94765	-4.7603	-0.092219
C	1.853955	4.539466	-2.611975
H	2.892532	4.50184	-2.930066
N	-3.918905	-2.472296	-2.505597
C	4.521073	-2.676193	-2.184367
H	5.40493	-2.069273	-2.360885
N	4.176717	-2.089739	2.464745
N	-5.149828	-0.584571	2.014075
H	-5.601311	0.330715	1.933264
C	0.080309	4.84629	2.626285
H	-0.889005	5.217361	2.948433
C	1.360661	5.185096	3.03028
H	1.740797	5.884991	3.769154
N	2.16515	4.407035	2.266159
H	3.182111	4.342362	2.187368
C	-4.673604	-0.384829	-2.504148
H	-5.177248	0.561292	-2.686259
C	-4.55871	-2.66028	2.136769
H	-4.461314	-3.733277	2.27888
C	4.233532	-3.988193	-2.520522
H	4.789166	-4.750451	-3.059227
C	0.822642	5.38558	-2.983096
H	0.762656	6.212792	-3.684836
C	-5.568757	-1.78153	2.491009
H	-6.511737	-1.913973	3.013741
C	-4.758063	-1.626457	-3.132912
H	-5.361079	-1.94488	-3.980988
C	3.853478	-3.198904	3.155477

H	4.447998	-3.538429	4.001381
C	2.700649	-3.743441	2.589249
H	2.115509	-4.626897	2.832634

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