

## <Supporting Information>

# Organic–Inorganic One-Dimensional Hybrid Aggregates Constructed from Aromatic-bisphosphonate-Functionalized Polyoxomolybdates

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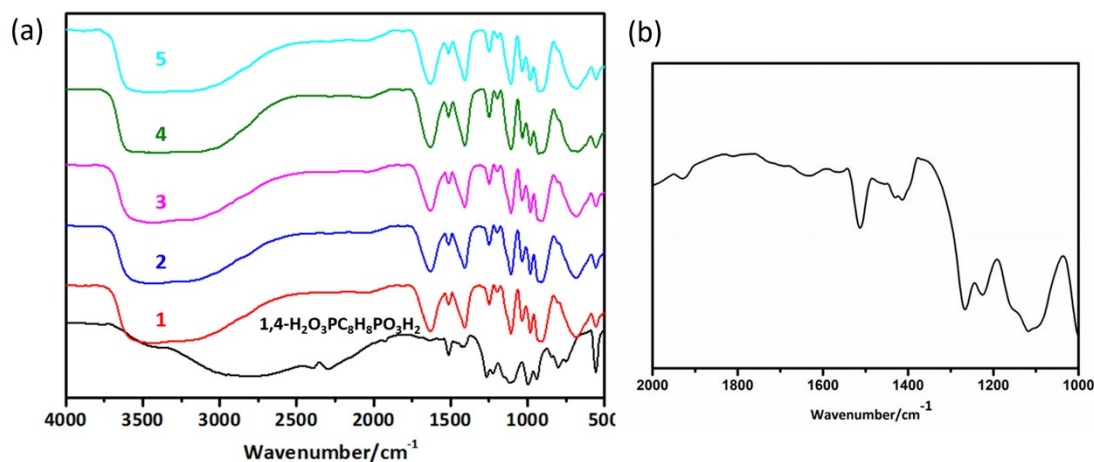
Table S8: Angel length of compound **1**.

## Physical measurements

IR spectra of all samples were recorded on a Bruker VERTEX 70 IR spectrometer using KBr pellets for solid sample palletized in the range 4000–400  $\text{cm}^{-1}$ . Raman spectra were performed on a Renishaw inVia with a red Spectra-Physics He–Ne laser (wavelength of 633 nm and 500 mW capacity). Thermogravimetric analyses (TGA) were measured by using a Mettler–Toledo TGA/SDTA 851<sup>e</sup> instrument in flowing  $\text{N}_2$  with a heating rate of 10  $^\circ\text{C min}^{-1}$ . Powder X-ray diffraction (PXRD) data were obtained on a Bruker D8 Advance instrument with Cu K $\alpha$  radiation ( $\lambda = 1.5418 \text{ \AA}$ ) in the angular range  $2\theta = 5\text{--}5^\circ$  at 293 K. C, H, and N elemental analyses were gain with an Elementar Vario EL cube CHNS analyzer. Photoluminescence properties were investigated on an EDINBURGH FLS 980 fluorescence spectrophotometer. Magnetic measurements were performed on a Quantum Design SQUID magnetometer.

## IR Spectrum

As shown in Fig. S1, the IR spectrum showed the skeletal vibrations between 500 and 4000  $\text{cm}^{-1}$  for five compounds, which is consistent with the result of single-crystal X-ray structural analysis. It also indicated that polyanions in 1–5 were isostructural. The five compounds have obvious characteristic absorption peaks at 600–1050  $\text{cm}^{-1}$ , which is the vibration of Mo–O and Mo–O–Mo in subunit  $\{\text{Mo}_5\text{O}_{15}\}$ . The absorption peaks of compounds 1–5 at 1050–1240  $\text{cm}^{-1}$  can be assigned to P–O vibrations. Strong superimposed peaks at about 1400–1600  $\text{cm}^{-1}$  are assigned to the stretching vibration of the aromatic ring and  $\text{NH}_4^+$  ions. In addition, the signal appearing at 1610–3500  $\text{cm}^{-1}$  are belonged to the flexural vibration and stretching of lattice and coordinated water molecules. Some assigned characteristic peaks of the samples are listed in Table S1.



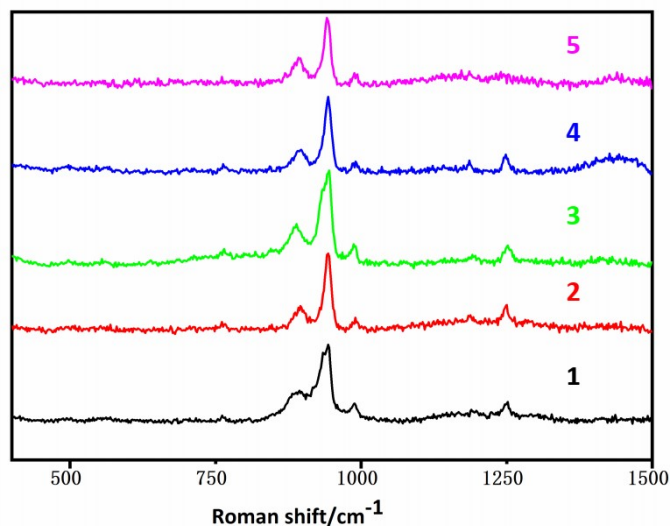
**Fig.S1.** (a) The IR of compounds 1–5 and ligand; (b) The IR of ligand between 2000–1000  $\text{cm}^{-1}$ .

**Table S1** Some assigned characteristic peaks of compounds 1–5.

Compounds	$\nu(\text{Mo-O})$	$\nu(\text{Mo-O-Mo})$	$\nu(\text{P-O})$	$\nu(\text{O-H})$	$\delta(\text{O-H})$
Ligand	--	--	1227(s), 1121(s)	--	--
1	1033(s), 982(s)	913(s), 686(s)	1194(m), 1105(s)	3425(s)	1628(s)
2	1034(s), 983(s)	908(s), 685(s)	1200(m), 1102(s)	3427(s)	1625(s)
3	1033(s), 979(s)	910(s), 687(s)	1195(m), 1101(s)	3425(s)	1621(s)
4	1031(s), 982(s)	912(s), 684(s)	1195(m), 1101(s)	3420(s)	1624(s)
5	1033(s), 980(s)	910(s), 685(s)	1192(m), 1106(s)	3421(s)	1620(s)

## Raman spectra

The Raman spectra in the solid state were carried out as a supplement to the IR test results. As shown in Fig. S2, the obvious characteristic Raman bands at 550–1000  $\text{cm}^{-1}$  are attributable to  $\nu(\text{Mo-O})$  and  $\nu(\text{O-Mo-O})$  vibrations of the POM skeleton, respectively. The peaks from 1000–1300  $\text{cm}^{-1}$  are mainly associated with the  $\nu(\text{P-O})$  vibrations. The signals of 1400–1410  $\text{cm}^{-1}$  were assigned to the  $\nu(\text{C-H})$  vibrations of the aromatic ring. Some assigned characteristic peaks of compounds **1**–**5** are listed in Table S2. IR and Raman spectra are consistent with the results of structural analysis.

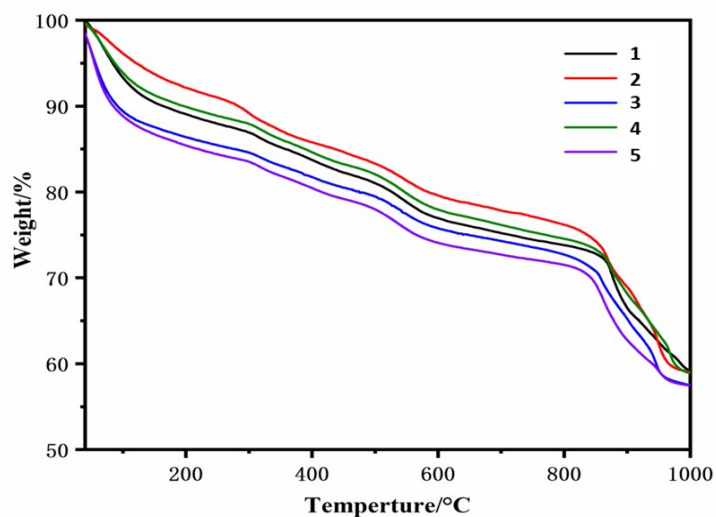


**Table S2** Some assigned characteristic Raman peaks of compounds **1**–**5**.

compounds	$\nu(\text{Mo-O})$	$\nu(\text{Mo-O-Mo})$	$\nu(\text{P-O})$
<b>1</b>	986, 936	886, 765	1187, 1248
<b>2</b>	986, 940	880, 764	1187, 1245
<b>3</b>	988, 938	882, 767	1188, 1250
<b>4</b>	989, 936	884, 765	1185, 1245
<b>5</b>	988, 940	883, 761	1186, 1249

### Thermogravimetric Analysis (TGA)

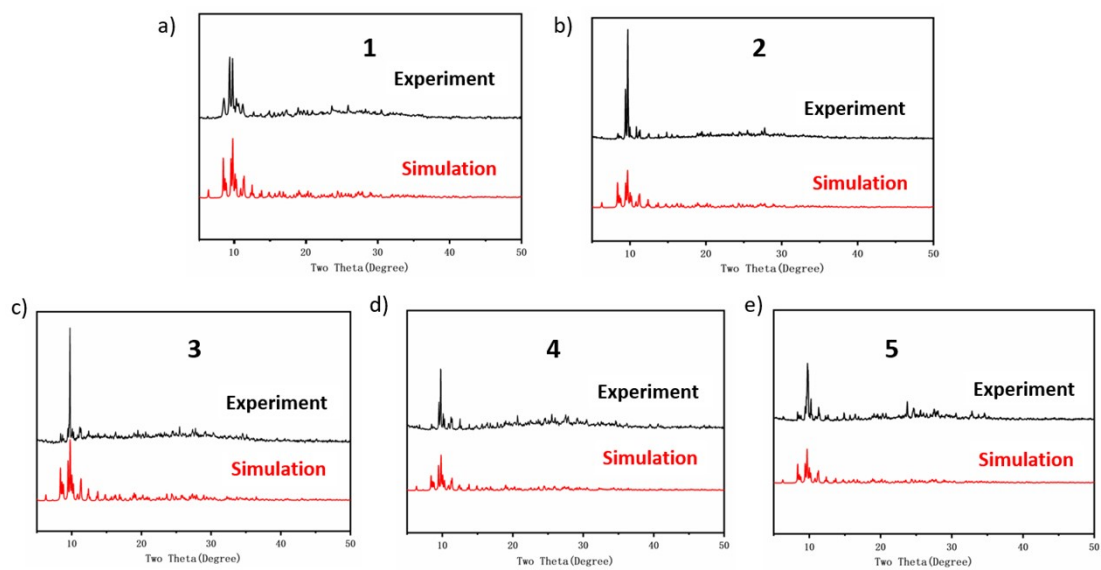
Under the protection of  $\text{N}_2$ , TGA curves of compounds **1**–**5** have been measured in the range of 25–1000  $^\circ\text{C}$ . As shown in Fig. S3, five compounds showed two consecutive weight loss changes. The first step is that the actual weight loss of **1**, is about 26.5 %, **2** is about 24.2 %, **3** is about 27.8 %, **4** is about 26.6 %, and **5** is about 28.7 % in the temperature range of 25–850  $^\circ\text{C}$ , which correspond to the loss of crystal water, coordination water, structural water, and the decomposition of the ammonium counter-cation and partial organic phosphonic acid fragments in **1**–**5**, respectively. In the second step, the mass loss is between 850–1000  $^\circ\text{C}$ , the actual weight loss of **1** is about 14.2 %, **2** is about 15.5 %, **3** is about 14.7 %, **4** is about 14.1 %, and **5** is about 13.8 %, which correspond to the loss of the remaining of organic phosphonic acid fragments, and the decomposition of the POMs skeleton.



**Fig. S3.** The TGA curves of compounds 1–5.

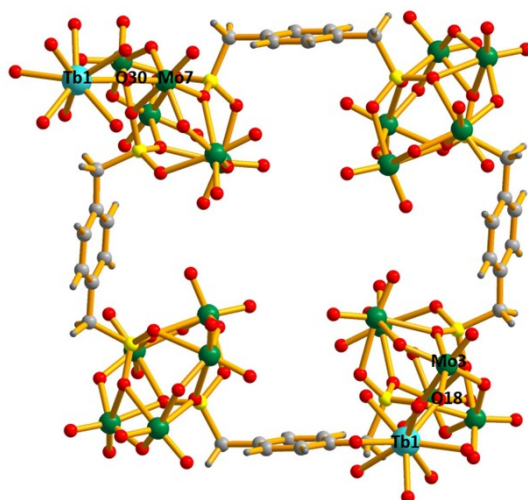
### PXRD

As shown in Fig. S4, the experimental PXRD patterns for five POMs are consistent with the simulated patterns obtained from X-ray single-crystal diffraction, which indicate that the samples are pure. The differences of peak intensity between the experimental and simulated patterns might be due to the anisotropic effects of crystal.

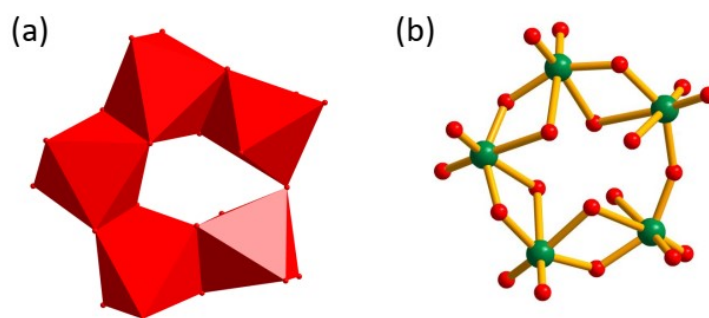


**Fig.S4.** The PXRD of compounds 1–5.

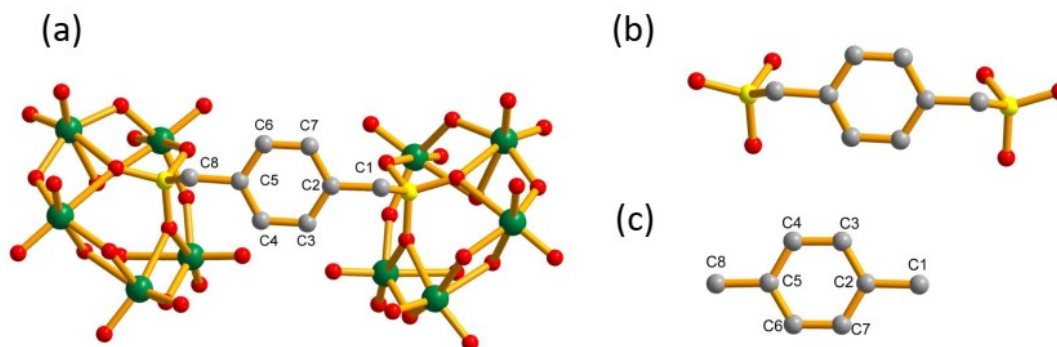
**Additional crystal structural pictures.**



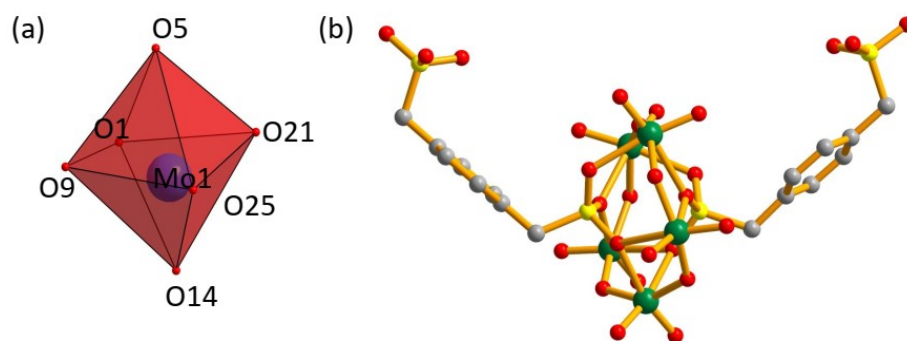
**Fig. S5.** Connection mode of between two Tb atoms in **1b** unit.



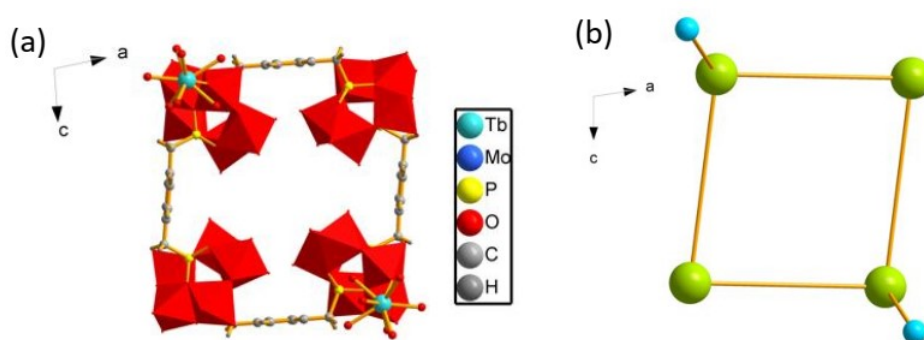
**Fig. S6.** (a) The polyhedral representation of the {Mo<sub>5</sub>O<sub>15</sub>} unit; (b) The ball-and-stick representation of the {Mo<sub>5</sub>O<sub>15</sub>} unit.



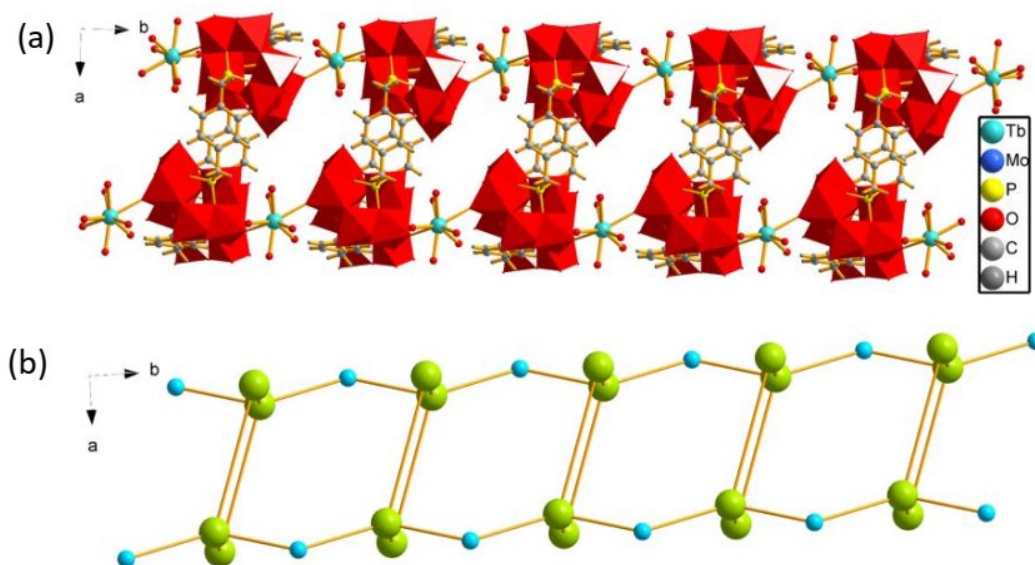
**Fig. S7.** (a) The ball-and-stick representation of {Mo<sub>10</sub>O<sub>30</sub>(1,4-O<sub>3</sub>PCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>PO<sub>3</sub>)} fragment; (a) The ball-and-stick representation of {1,4-O<sub>3</sub>PCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>PO<sub>3</sub>} fragment; (c) The ball-and-stick representation of {CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>} fragment.



**Fig. S8.** (a) The coordination mode of  $\text{Mo}^{16+}$ ; (b) Connection mode of between two  $\text{H}_2\text{O}_3\text{PCH}_2\text{C}_6\text{H}_4\text{CH}_2\text{PO}_3\text{H}_2$  ligands and  $\{\text{Mo}_5\text{O}_{15}\}$  unit.

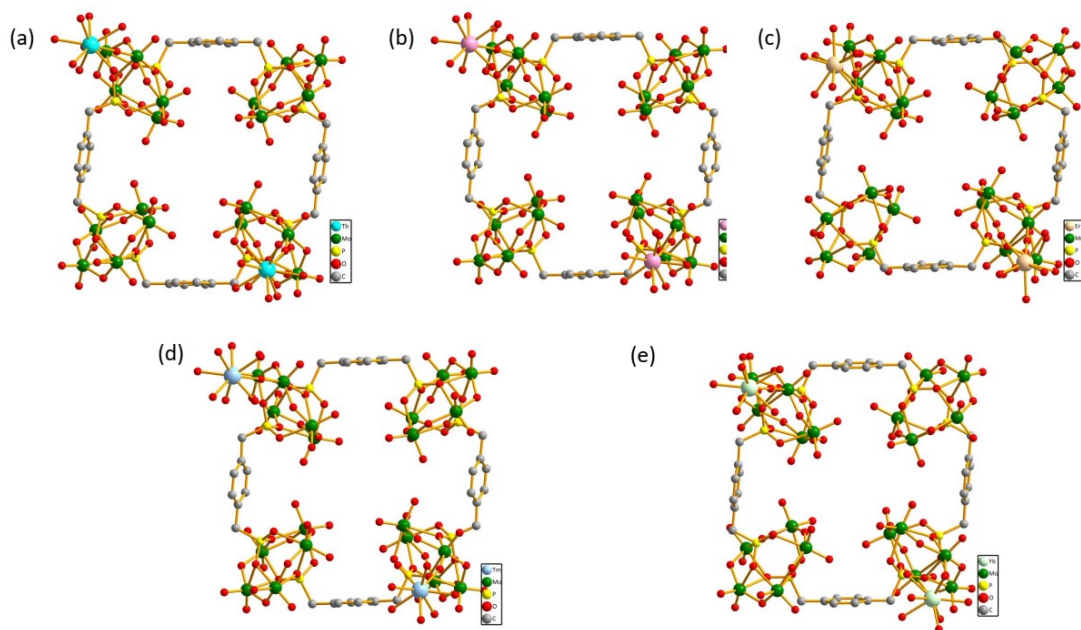


**Fig. S9.** (a) A view along the  $b$  axis of **1**; (b) A simplified view along the  $b$  axis of the **1**.

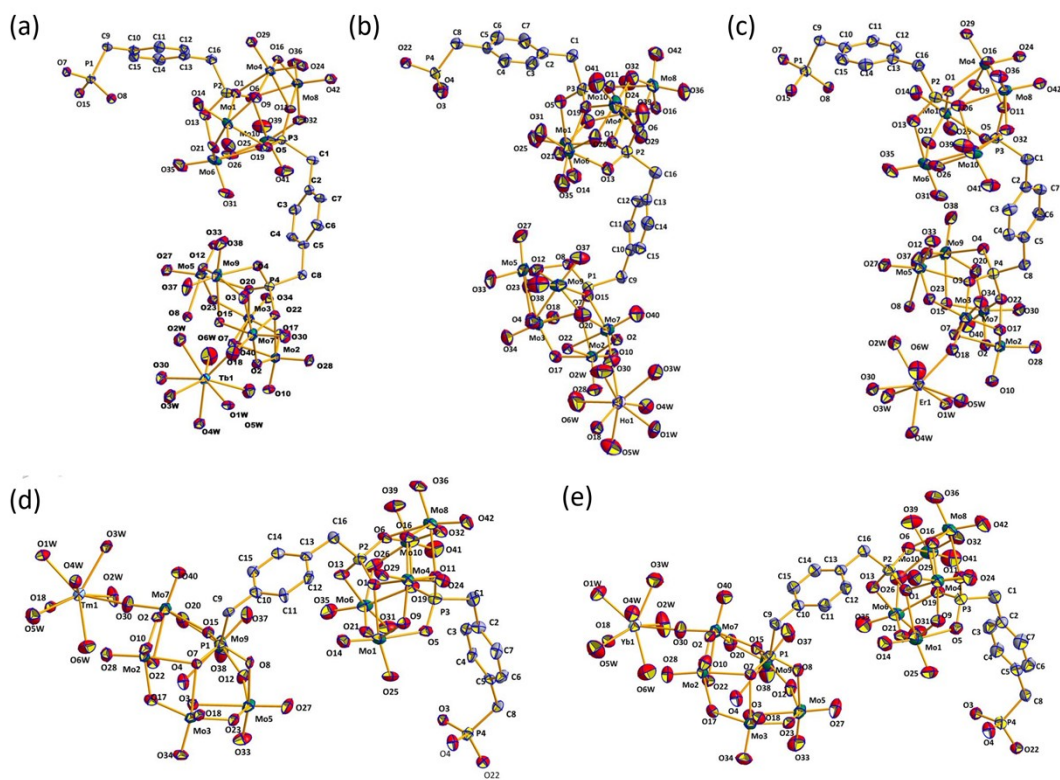


**Fig. S10.** (a) 1-D chain along the  $c$  axis of **1**; (b) A simplified view along the  $c$  axis of the 1-D chain of **1**.





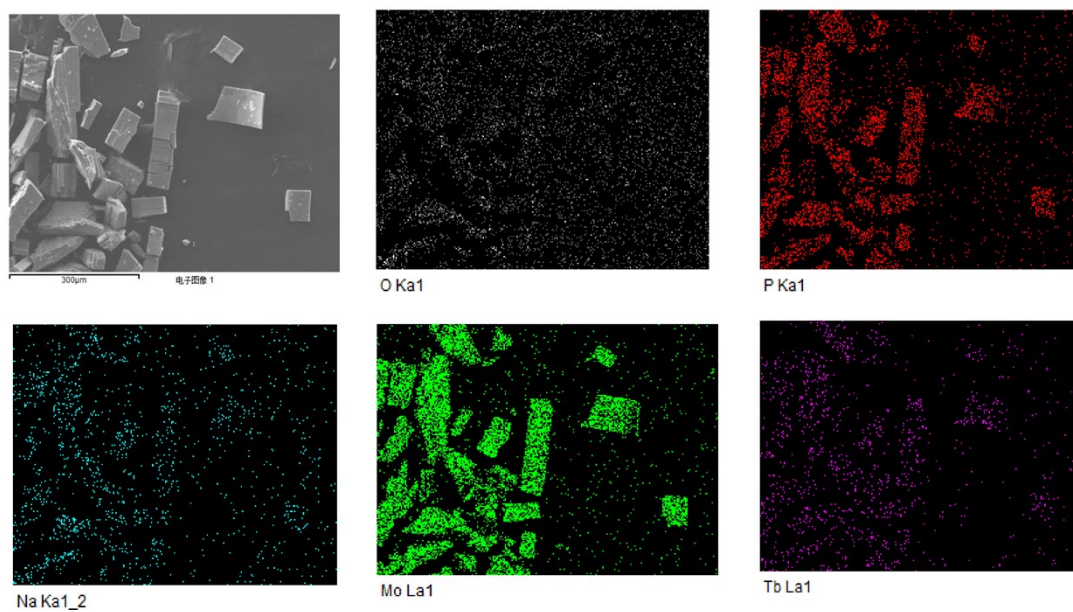
**Fig. S11** (a-e) The thermal ellipsoidal diagram of the asymmetric unit in the crystal structure of compounds 1-5.



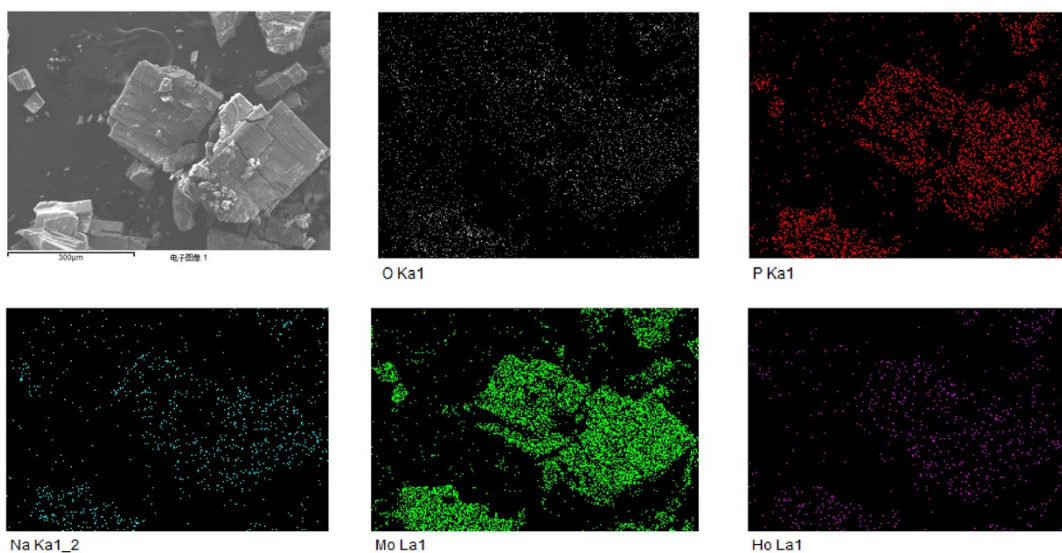
**Fig. S12** (a-e) Representative orped diagram of the asymmetric unit in the crystal structure of compounds 1-5. All the hydrogen atoms are omitted for clarity.

## SEM-EDX study

Scanning electron microscope (SEM) and energy dispersive spectroscopy (EDS) are presented for compounds **1–5**. The results show that the morphologies of **1–5** are shaped block, and these elements (O, P, Na, Mo, Ln) are present and distributed in the compounds **1–5** (Fig. S13-S17). The EDX elemental spectra for **1–5**, shown in Fig. S18, suggest the number ratio of Na, Mo, P, and Ln is about 1.05 : 7.28 : 3.02 : 0.66. Combined with the ratio of Mo, P, and Ln atoms determined in the anionic structural formula is 10 : 4 : 1, and the number is 20, 8, and 2, respectively, the number of Na is 2.88, which is about 3.

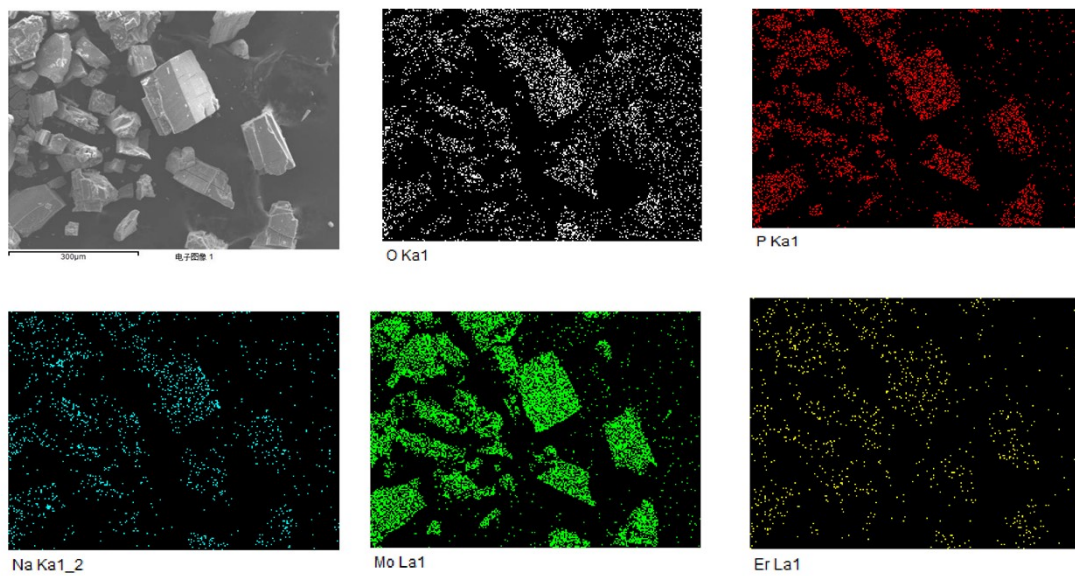


**Fig. S13** SEM-EDX element maps of **1**.

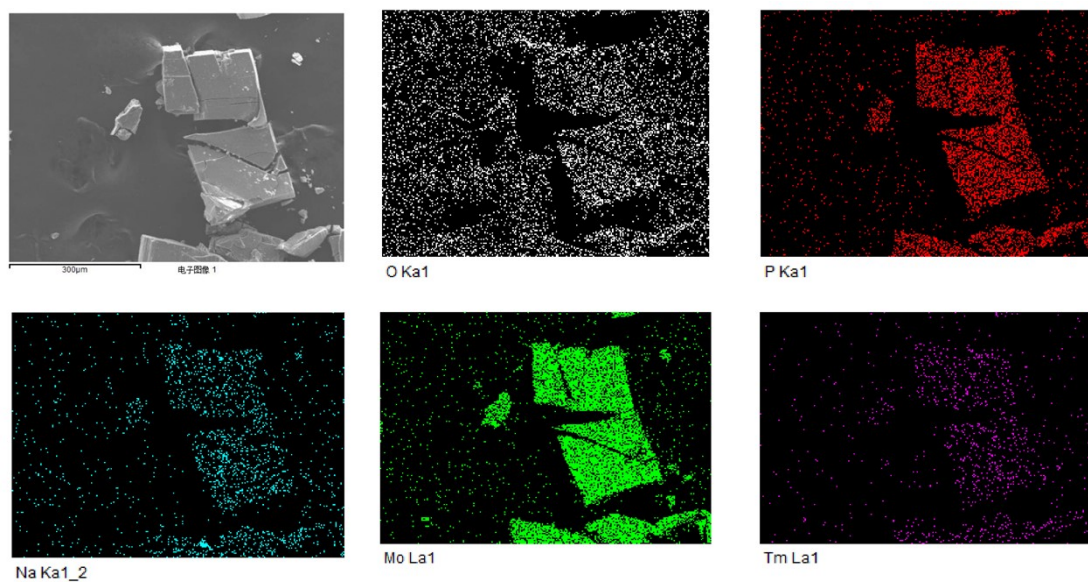


**Fig. S14** SEM-EDX element maps of **2**.

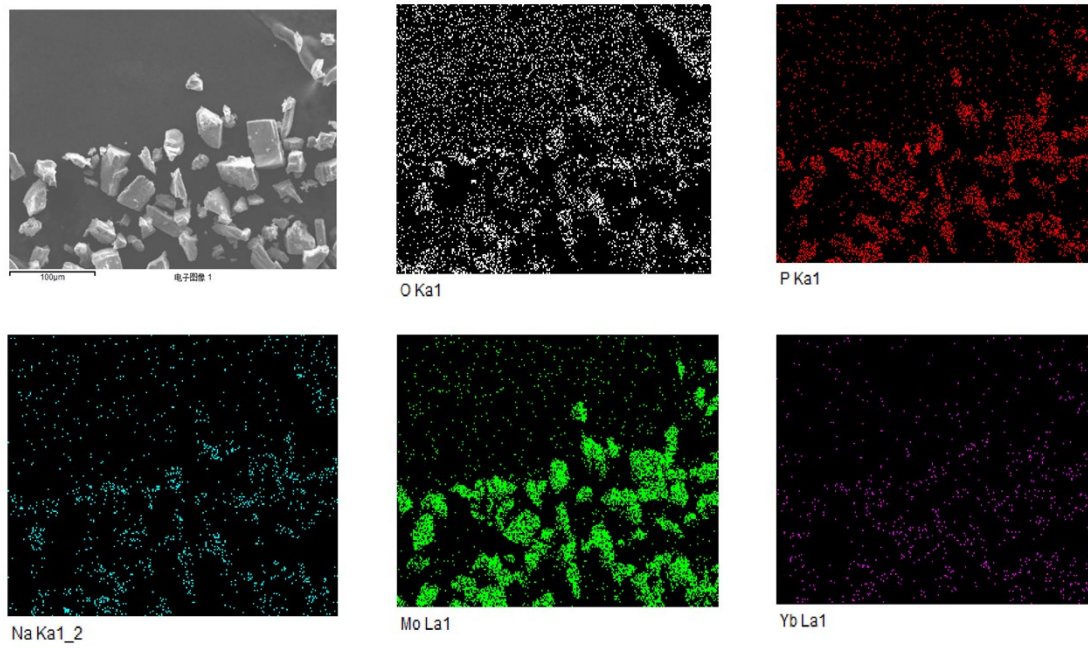




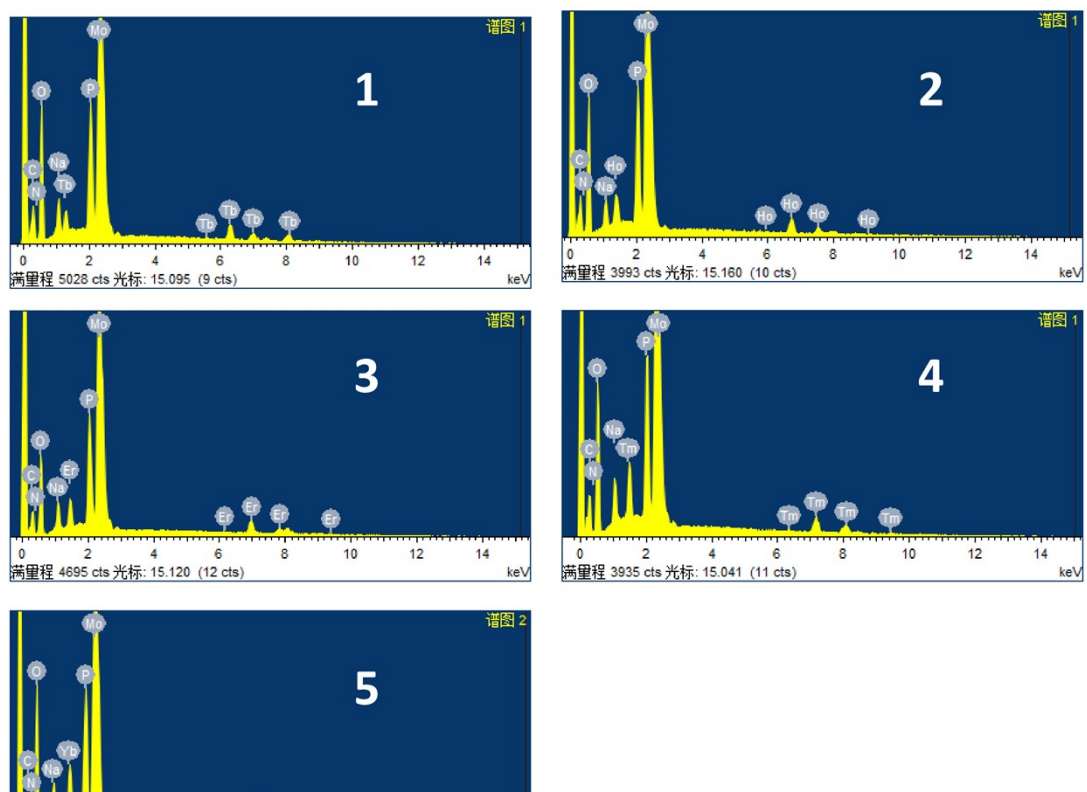
**Fig. S15** SEM-EDX element maps of 3.



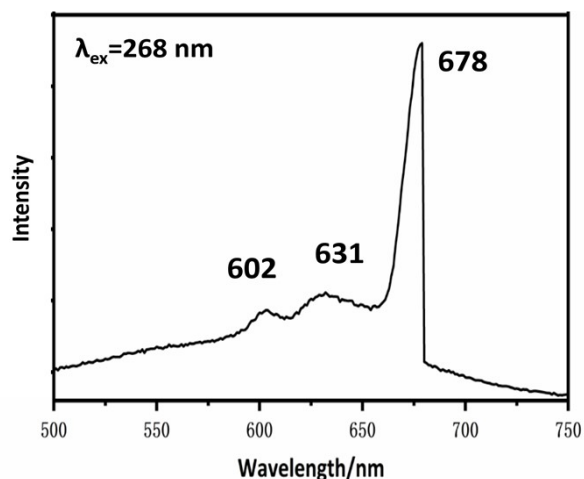
**Fig. S16** SEM-EDX element maps of 4.



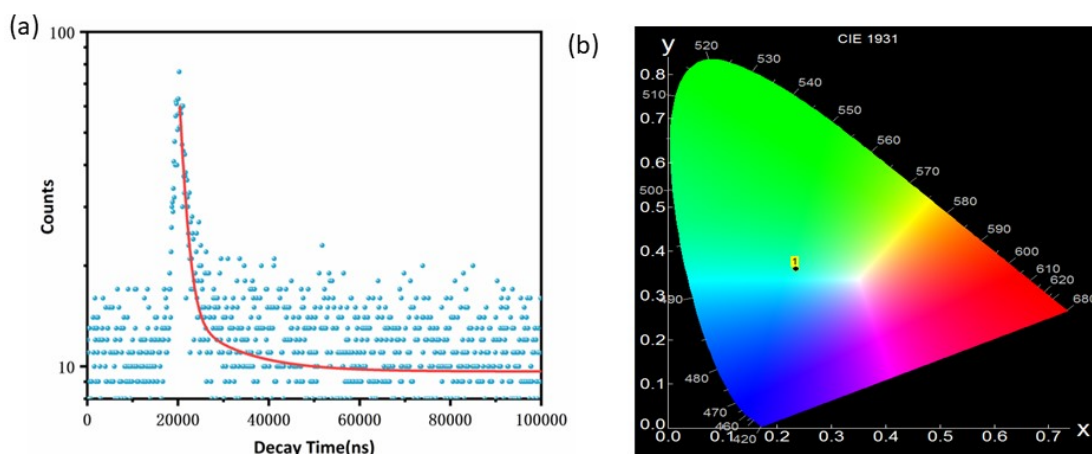
**Fig. S17** SEM-EDX element maps of 5.



**Fig. S18.** EDX elemental spectra of 1–5 showing the presence of Na, C, N, O, P, Mo, and Ln element in the lattice.



**Fig. S19** the emission spectrum of free ligand under excitation at 268 nm.



**Fig. S20.** (a) Decay time of ligand; (b) CIE chromaticity diagrams of compound **1**.

**Table S3.** Decay time of and compound **1** and ligand, and CIE chromaticity coordinate of compound **1**.

Compound	Decay time ( $\mu\text{s}$ )		(x, y)	
	$\tau_1$	$\tau_2$		
<b>1</b>	588.69 (100%)	-	0.23	0.36
Ligand	1.36 (54.06%)	11.35 (43.94%)	-	-

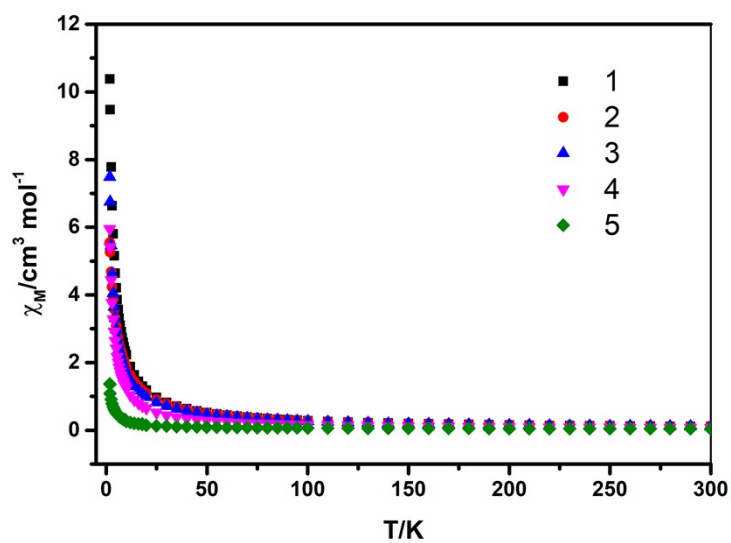


Fig. S21.  $\chi_M$  vs  $T$  curve of compounds 1–5.

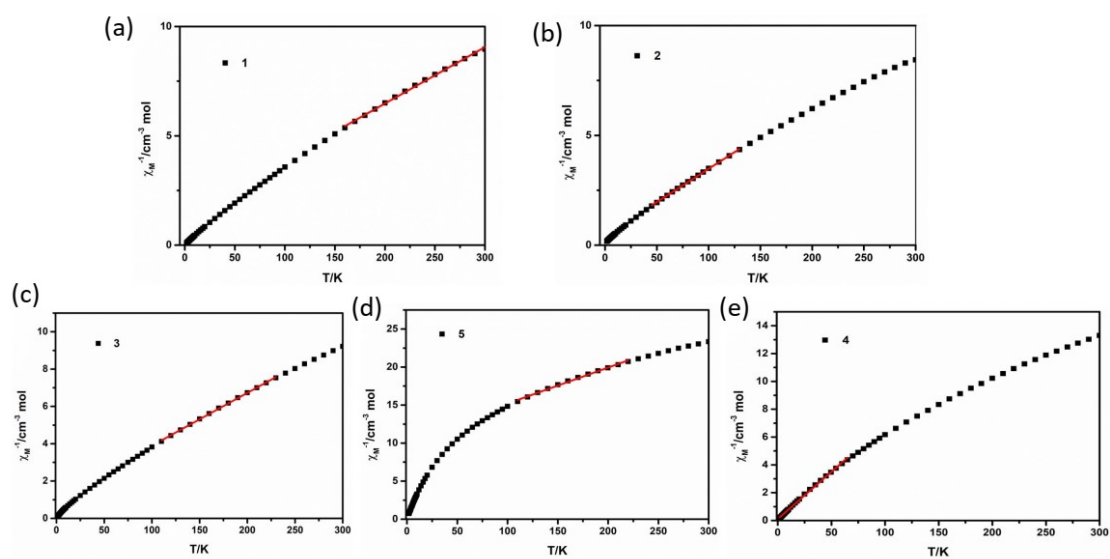


Fig. 22.  $\chi_M^{-1}$  vs  $T$  curve of compounds 1–5.

**Table S4. Crystallographic data of five compounds.**

Compound	1	2	3	4	5
Empirical formula	$N_5C_{32}H_{148}Mo_{20}Na_3O_{15}$ $2P_8Tb_2$	$N_5C_{32}H_{126}Ho_2Mo_{20}Na_3$ $O_{141}P_8$	$N_5C_{32}H_{164}Er_2Mo_{20}Na_3$ $O_{160}P_8$	$N_5C_{32}H_{142}Mo_{20}Na_3O_{149}$ $P_8Tm_2$	$N_5C_{32}H_{176}Mo_{20}Na_3O_{16}$ $6P_8Yb_2$
Formula weight	5588.87	5402.71	5749.65	5554.84	5869.31
Temperature/K	150	150	150	150	296
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$C2/c$	$C2/c$	$C2/c$	$C2/c$	$C2/c$
$a/\text{\AA}$	36.2646(11)	36.542(3)	36.542(3)	36.3225(11)	36.803(6)
$b/\text{\AA}$	11.0382(3)	11.0120(7)	11.0085(3)	10.9837(3)	11.0192(14)
$c/\text{\AA}$	37.7938(10)	37.666(3)	36.3183(10)	37.6737(11)	37.831(5)
$\beta/^\circ$	97.7710(10)	97.630(3)	98.0830(10)	97.8310(10)	97.728(5)
Volume/ $\text{\AA}^3$	14989.8(7)	15247(3)	14939.4(8)	14890.0(7)	15203(4)
Z	4	4	4	4	4
$\rho_{\text{calc}}/\text{cm}^3$	2.197	2.057	2.134	2.142	2.086
$\mu/\text{mm}^{-1}$	2.742	2.794	2.919	2.993	2.993
$2\theta$ range/ $^\circ$	4.506-50.2	4.498-50.198	4.36-50.2	4.366-50.198	4.356-50.2
	$-43 \leq h \leq 43$	$-44 \leq h \leq 41$	$-43 \leq h \leq 41$	$-43 \leq h \leq 43$	$-43 \leq h \leq 43$
Index ranges	$-13 \leq k \leq 12$	$-11 \leq k \leq 13$	$-11 \leq k \leq 13$	$-13 \leq k \leq 13$	$-13 \leq k \leq 12$
	$-42 \leq l \leq 45$	$-45 \leq l \leq 44$	$-24 \leq l \leq 45$	$-44 \leq l \leq 44$	$-45 \leq l \leq 45$
$F(000)$	9500.0	8972.0	9140.0	9148.0	9076.0
Reflections collected	53945	41348	37439	70129	62863
GoF( $F^2$ )	1.009	1.020	1.010	1.015	1.038
$R_1, wR_2 [I \geq 2\sigma(I)]$	0.0430, 0.0931	0.0441, 0.1125	0.0436, 0.1004	0.0536, 0.1031	0.0314, 0.0863
$R_1, wR_2$ [all data]	0.0593, 0.1023	0.0538, 0.1183	0.0548, 0.1069	0.0948, 0.1222	0.0364, 0.0898
Largest diff. peak/hole / $e \text{\AA}^{-3}$	2.17/-1.75	1.60/-1.70	1.88/-1.43	1.61/-1.40	1.75/-1.07

**Table S5. BVS values of Mo, P and Tb atoms of compound 1.**

Atom	BVS	Atom	BVS	Atom	BVS
Mo1	6.13	Mo6	6.09	P1	5.01
Mo2	6.14	Mo7	6.15	P2	4.94
Mo3	6.12	Mo8	6.18	P3	5.08
Mo4	6.04	Mo9	6.07	P4	5.01
Mo5	6.14	Mo10	6.06	Tb1	3.31

**Table S6. Bond length and BVS values of Ho, Er, Tm and Yb atoms in compounds 2-5.**

Bond	Bond length	Bond	Bond length	Bond	Bond length	Bond	Bond length
Ho1-O18 <sup>1</sup>	2.343(6)	Er1-O18 <sup>1</sup>	2.375(15)	Tm1-O18 <sup>1</sup>	2.334(8)	Yb1-O18 <sup>1</sup>	2.303(4)
Ho1-O30	2.337(6)	Er1-O30	2.302(16)	Tm1-O30	2.321(9)	Yb1-O30	2.311(5)
Ho1-O1W	2.353(6)	Er1-O1W	2.341(14)	Tm1-O1W	2.330(9)	Yb1-O1W	2.328(5)
Ho1-O4W	2.327(6)	Er1-O4W	2.316(14)	Tm1-O4W	2.295(9)	Yb1-O4W	2.292(5)



Ho1-O2W	2.361(7)	Er1-O2W	2.349(17)	Tm1-O2W	2.355(10)	Yb1-O2W	2.308(6)
Ho1-O3W	2.401(7)	Er1-O3W	2.381(17)	Tm1-O3W	2.407(9)	Yb1-O3W	2.372(6)
Ho1-O5W	2.387(8)	Er1-O5W	2.391(19)	Tm1-O5W	2.363(10)	Yb1-O5W	2.346(6)
Ho1-O6W	2.323(9)	Er1-O6W	2.320(18)	Tm1-O6W	2.322(11)	Yb1-O6W	2.300(7)

BVS(Ho1) = 3.31

BVS(Er1) = 3.26

BVS(Tm1) = 3.22

BVS(Yb1) = 3.29

**Table S7. Bond length of compound Co1.**

Bond	Bond length	Bond	Bond length	Bond	Bond length
Mo1-O1	2.379(6)	Mo2-O2	1.911(6)	Mo3-O3	2.173(6)
Mo1-O52	2.314(6)	Mo2-O7	2.272(6)	Mo3-O7	2.349(6)
Mo1-O9	1.907(6)	Mo2-O10	1.715(6)	Mo3-O17	1.902(6)
Mo1-O14	1.710(7)	Mo2-O17	1.919(6)	Mo3-O18	1.737(6)
Mo1-O21	1.918(6)	Mo2-O22	2.320(6)	Mo3-O23	1.934(6)
Mo1-O25	1.692(7)	Mo2-O28	1.703(6)	Mo3-O34	1.709(6)
Mo4-O1	2.222(6)	Mo5-O3	2.416(6)	Mo6-O13	2.243(6)
Mo4-O9	1.920(6)	Mo5-O8	2.258(6)	Mo6-O19 <sup>2</sup>	2.359(6)
Mo4-O11 <sup>2</sup>	2.358(6)	Mo5-O12	1.886(7)	Mo6-O21	1.905(7)
Mo4-O16	1.955(6)	Mo5-O23	1.946(6)	Mo6-O26	1.942(7)
Mo4-O24	1.715(7)	Mo5-O27	1.710(7)	Mo6-O31	1.704(7)
Mo4-O29	1.709(6)	Mo5-O33	1.697(7)	Mo6-O35	1.711(7)
Mo7-O2	1.944(6)	Mo8-O6	2.312(7)	Mo9-O4	2.309(7)
Mo7-O15	2.170(6)	Mo8-O11 <sup>2</sup>	2.309(6)	Mo9-O12	1.907(7)
Mo7-O20	1.909(7)	Mo8-O16	1.921(6)	Mo9-O15	2.418(6)
Mo7-O22	2.392(6)	Mo8-O32	1.911(6)	Mo9-O20	1.919(6)
Mo7-O30	1.728(7)	Mo8-O36	1.697(7)	Mo9-O37	1.719(7)
Mo7-O40	1.695(7)	Mo8-O42	1.708(7)	Mo9-O38	1.701(7)
Mo10-O6	2.418(6)	P1-O7	1.539(6)	P2-O1	1.540(7)
Mo10-O19 <sup>2</sup>	2.190(6)	P1-O8	1.512(6)	P2-O6	1.544(6)
Mo10-O26	1.962(7)	P1-O15	1.552(7)	P2-O13	1.513(7)
Mo10-O32	1.903(8)	P1-C9	1.787(9)	P2-C16	1.801(9)
Mo10-O39	1.720(8)	P3-O5	1.507(7)	P3-O19	1.548(7)
Mo10-O41	1.696(7)	P3-O11	1.535(6)	P3-C1	1.781(10)
P4-O3	1.556(7)	Tb1-O18 <sup>1</sup>	2.371(6)	Tb1-O2W	2.385(7)
P4-O4	1.512(6)	Tb1-O30	2.360(7)	Tb1-O3W	2.446(7)
P4-O22	1.546(6)	Tb1-O1W	2.376(6)	Tb1-O5W	2.400(7)
P4-C8	1.773(9)	Tb1-O4W	2.336(7)	Tb1-O6W	2.368(9)

**Table S8. Angel length of compound 1.**

Bond	Angel	Bond	Angel	Bond	Angel
O52-Mo1-O1	87.5(2)	O2-Mo2-O7	80.8(2)	O3-Mo3-O7	73.7(2)
O9-Mo1-O1	69.8(2)	O2-Mo2-O17	146.6(2)	O17-Mo3-O3	83.6(2)
O9-Mo1-O52	77.4(2)	O2-Mo2-O22	73.9(2)	O17-Mo3-O7	71.7(2)

O9-Mo1-O21	143.6(3)	O7-Mo2-O22	80.7(2)	O17-Mo3-O23	152.4(3)
O14-Mo1-O1	86.6(3)	O10-Mo2-O2	99.0(3)	O18-Mo3-O3	156.5(3)
O14-Mo1-O52	174.1(3)	O10-Mo2-O7	89.3(3)	O18-Mo3-O7	86.2(3)
O14-Mo1-O9	100.8(3)	O10-Mo2-O17	101.2(3)	O18-Mo3-O17	101.8(3)
O14-Mo1-O21	99.8(3)	O10-Mo2-O22	168.5(3)	O18-Mo3-O23	93.8(3)
O21-Mo1-O1	81.9(2)	O17-Mo2-O7	73.2(2)	O23-Mo3-O3	73.5(2)
O21-Mo1-O52	79.0(3)	O17-Mo2-O22	81.4(2)	O23-Mo3-O7	86.9(2)
O25-Mo1-O1	168.5(3)	O28-Mo2-O2	100.3(3)	O34-Mo3-O3	96.8(3)
O25-Mo1-O52	83.3(3)	O28-Mo2-O7	166.4(3)	O34-Mo3-O7	166.2(3)
O25-Mo1-O9	101.4(3)	O28-Mo2-O10	103.9(3)	O34-Mo3-O17	97.8(3)
O25-Mo1-O14	102.6(3)	O28-Mo2-O17	100.3(3)	O34-Mo3-O18	105.0(3)
O25-Mo1-O21	102.9(3)	O28-Mo2-O22	86.5(3)	O34-Mo3-O23	100.1(3)
O1-Mo4-O11 <sup>2</sup>	73.1(2)	O8-Mo5-O3	88.6(2)	O13-Mo6-O19 <sup>2</sup>	87.3(2)
O9-Mo4-O1	73.3(2)	O12-Mo5-O3	84.3(2)	O21-Mo6-O13	80.2(3)
O9-Mo4-O11 <sup>2</sup>	87.0(2)	O12-Mo5-O8	80.6(3)	O21-Mo6-O19 <sup>2</sup>	83.9(2)
O9-Mo4-O16	151.2(3)	O12-Mo5-O23	144.7(3)	O21-Mo6-O26	145.8(3)
O16-Mo4-O1	81.4(2)	O23-Mo5-O3	67.8(2)	O26-Mo6-O13	78.0(3)
O16-Mo4-O11 <sup>2</sup>	72.4(2)	O23-Mo5-O8	77.5(2)	O26-Mo6-O19 <sup>2</sup>	69.0(3)
O24-Mo4-O1	158.5(3)	O27-Mo5-O3	168.7(3)	O31-Mo6-O13	172.7(3)
O24-Mo4-O9	98.8(3)	O27-Mo5-O8	84.7(3)	O31-Mo6-O19 <sup>2</sup>	85.5(3)
O24-Mo4-O11 <sup>2</sup>	86.7(3)	O27-Mo5-O12	103.5(3)	O31-Mo6-O21	99.9(3)
O24-Mo4-O16	99.9(3)	O27-Mo5-O23	101.8(3)	O31-Mo6-O26	98.5(3)
O29-Mo4-O1	96.1(3)	O33-Mo5-O3	84.0(3)	O31-Mo6-O35	102.4(4)
O29-Mo4-O9	101.3(3)	O33-Mo5-O8	172.4(3)	O35-Mo6-O13	84.6(3)
O29-Mo4-O11 <sup>2</sup>	164.2(3)	O33-Mo5-O12	100.0(3)	O35-Mo6-O19 <sup>2</sup>	168.3(3)
O29-Mo4-O16	94.8(3)	O33-Mo5-O23	98.3(3)	O35-Mo6-O21	102.9(3)
O29-Mo4-O24	105.1(3)	O33-Mo5-O27	102.4(4)	O35-Mo6-O26	101.0(4)
O2-Mo7-O15	81.5(2)	O112-Mo8-O6	80.9(2)	O4-Mo9-O15	88.1(2)
O2-Mo7-O22	71.7(2)	O16-Mo8-O6	79.3(2)	O12-Mo9-O4	79.4(3)
O15-Mo7-O22	74.3(2)	O16-Mo8-O11 <sup>2</sup>	74.2(2)	O12-Mo9-O15	82.3(2)
O20-Mo7-O2	151.4(3)	O32-Mo8-O6	73.8(3)	O12-Mo9-O20	143.4(3)
O20-Mo7-O15	74.7(3)	O32-Mo8-O11 <sup>2</sup>	81.0(3)	O20-Mo9-O4	77.8(3)
O20-Mo7-O22	86.6(3)	O32-Mo8-O16	145.8(3)	O20-Mo9-O15	68.8(2)
O30-Mo7-O2	98.4(3)	O36-Mo8-O6	87.9(3)	O37-Mo9-O4	172.1(3)
O30-Mo7-O15	160.0(3)	O36-Mo8-O11 <sup>2</sup>	167.3(3)	O37-Mo9-O12	98.9(3)
O30-Mo7-O20	98.6(3)	O36-Mo8-O16	98.0(3)	O37-Mo9-O15	84.0(3)
O30-Mo7-O22	86.6(3)	O36-Mo8-O32	101.7(3)	O37-Mo9-O20	99.8(3)
O40-Mo7-O2	96.8(3)	O36-Mo8-O42	105.0(4)	O38-Mo9-O4	85.3(3)
O40-Mo7-O15	97.2(3)	O42-Mo8-O6	167.0(3)	O38-Mo9-O12	103.8(3)
O40-Mo7-O20	101.7(3)	O42-Mo8-O11 <sup>2</sup>	86.5(3)	O38-Mo9-O15	170.0(3)
O40-Mo7-O22	166.3(3)	O42-Mo8-O16	100.1(3)	O38-Mo9-O20	102.4(3)

O40-Mo7-O30	102.6(3)	O42-Mo8-O32	101.4(3)	O38-Mo9-O37	102.6(4)
O192-Mo10-O6	72.6(2)	P1-O15-Mo7	130.4(4)	P4-O3-Mo3	130.2(3)
O26-Mo10-O6	86.7(2)	P1-O15-Mo9	133.6(3)	P4-O3-Mo5	132.0(3)
O26-Mo10-O19 <sup>2</sup>	72.4(3)	P1-O7-Mo2	126.6(3)	P4-O4-Mo9	120.7(4)
O32-Mo10-O6	71.4(2)	P1-O7-Mo3	129.3(3)	P4-O22-Mo2	126.0(3)
O32-Mo10-O19 <sup>2</sup>	83.4(3)	P1-O8-Mo5	120.6(3)	P4-O22-Mo7	128.1(3)
O32-Mo10-O26	151.5(3)	P2-O13-Mo6	121.1(4)	O181-Tb1-O1W	77.8(2)
O39-Mo10-O6	86.9(3)	P2-O6-Mo8	126.6(4)	O181-Tb1-O2W	71.7(2)
O39-Mo10-O19 <sup>2</sup>	156.4(3)	P2-O6-Mo10	127.1(4)	O181-Tb1-O3W	116.9(2)
O39-Mo10-O26	95.4(4)	P2-O1-Mo1	135.2(3)	O181-Tb1-O5W	73.3(2)
O39-Mo10-O32	101.3(4)	P2-O1-Mo4	129.3(3)	O181-Tb1-O1W	77.8(2)
O41-Mo10-O6	166.1(3)	P3-O5-Mo12	119.7(3)	O30-Tb1-O18 <sup>1</sup>	138.0(2)
O41-Mo10-O19 <sup>2</sup>	97.6(3)	P3-O11-Mo42	128.6(3)	O30-Tb1-O1W	138.9(2)
O41-Mo10-O26	99.8(4)	P3-O11-Mo82	126.3(4)	O30-Tb1-O2W	73.0(2)
O41-Mo10-O32	98.2(4)	P3-O19-Mo62	133.7(4)	O30-Tb1-O3W	72.4(3)
O41-Mo10-O39	104.5(4)	P3-O19-Mo10 <sup>2</sup>	128.5(4)	O30-Tb1-O5W	127.0(2)
O1W-Tb1-O2W	114.8(3)	O4W-Tb1-O2W	143.5(2)	O30-Tb1-O6W	70.2(3)
O1W-Tb1-O3W	72.1(2)	O4W-Tb1-O3W	80.8(2)	O5W-Tb1-O3W	141.2(2)
O1W-Tb1-O5W	74.2(2)	O4W-Tb1-O5W	74.4(2)	O6W-Tb1-O18 <sup>1</sup>	87.3(3)
O4W-Tb1-O18 <sup>1</sup>	144.4(2)	O4W-Tb1-O6W	96.4(3)	O6W-Tb1-O1W	145.1(3)
O4W-Tb1-O30	75.2(2)	O2W-Tb1-O3W	72.9(3)	O6W-Tb1-O2W	89.4(3)
O4W-Tb1-O1W	79.2(2)	O2W-Tb1-O5W	140.6(3)	O6W-Tb1-O3W	141.9(3)