

# A Dawson-type $\{P_4W_{24}\}$ modified by phenylphosphonic acid with excellent proton conductivity

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**Proton conduction experiments:**

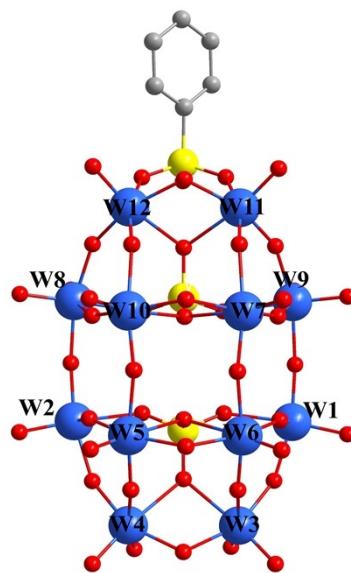
Firstly, the single crystals were uniformly ground into powder and then were put into a homemade mold with a radius of 3 mm to obtain circular pellets. And the thicknesses of the compound **1** was measured by a vernier caliper with 0.054 cm, respectively. Secondly, both sides of the pellets were coated with silver glue and dried naturally in air. And last, the pellets were fixed on the sample stage with gold wires. AC impedance measurements were performed on Solartron Analytical ModuLab 1260/1296 over the frequency ranging from 1 Hz to 10 MHz. The relative humidity was controlled by a STIK Corp CIHI-150BS3 incubator. Two silver electrodes were attached to both sides of the pellet to form four end terminals (quasi-fourprobe method). The measurements were carried out for 2 h at each testing temperature or RH. The ZsimpWin software was used to fit the equivalent circuit of the impedance data. The proton conductivity ( $\sigma$ ) and activation energy ( $E_a$ ) were calculated by the two following equations:

$$\sigma = L/RS \quad (1)$$

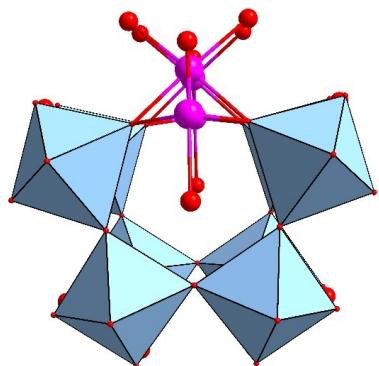
$$Ln \sigma T = Ln A - Ea/(K_b T) \quad (2)$$

where  $L$  is the thickness (cm) of the slice,  $S$  is the electrode area ( $\text{cm}^2$ ),  $R$  is the resistance ( $\Omega$ ),  $A$  is the pre-exponential factor,  $T$  represents the absolute temperature, and  $K_b$  is the Boltzmann constant ( $K_b = 8.63 \times 10^{-5}$  eV/K).

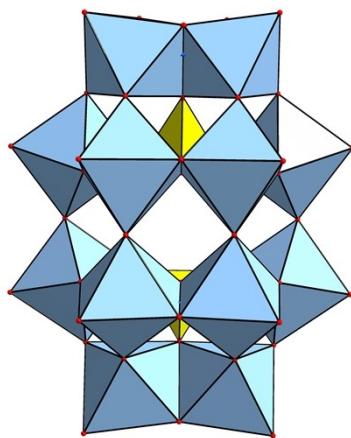
## Figures



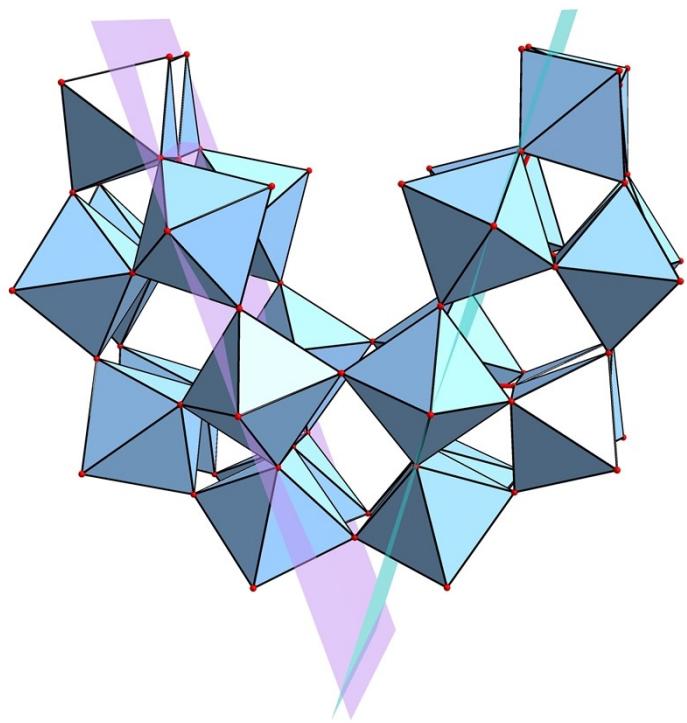
**Fig. S1.** The ball-and-stick representation of  $[P_2W_{12}O_{48}PhPO]^{14-}$ .



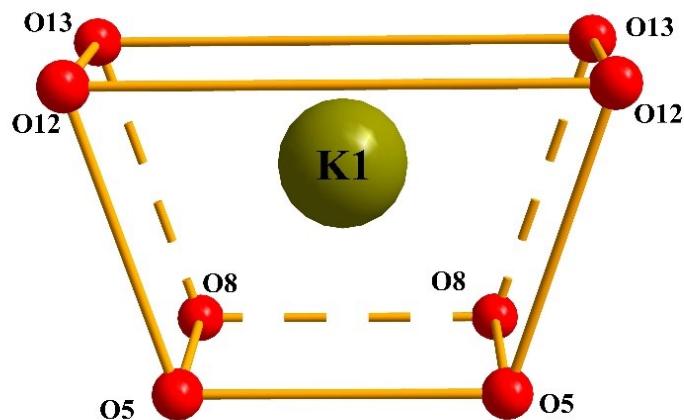
**Fig. S2.** The polyhedral/ ball-and-stick representation internal star-shaped cavity  $\{W_8Co_2O_{58}\}^{64-}$  of **1**.



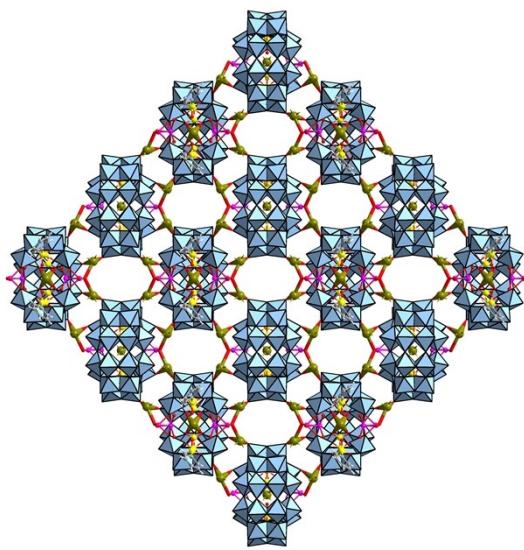
**Fig. S3.** The polyhedral/ball-and-stick representation of  $[\alpha\text{-H}_2P_2W_{12}O_{48}]^{12-}$  unit.



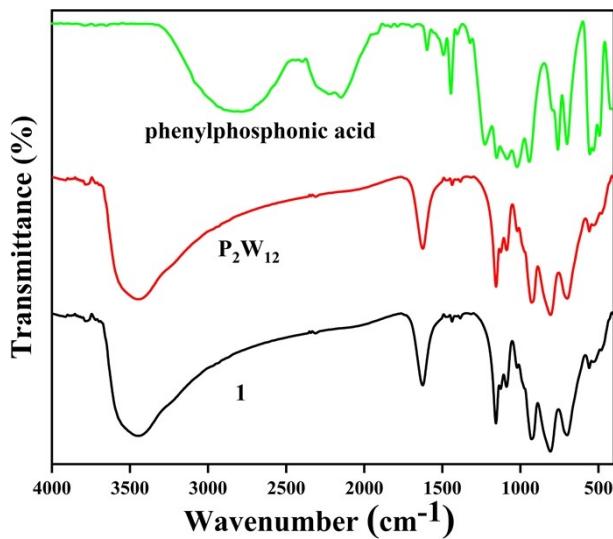
**Fig. S4.** The dihedral angle in the  $\{P_4W_{24}\}$  fragment is  $38.018^\circ$ .



**Fig. S5.** The coordination environment of the anion center K1.

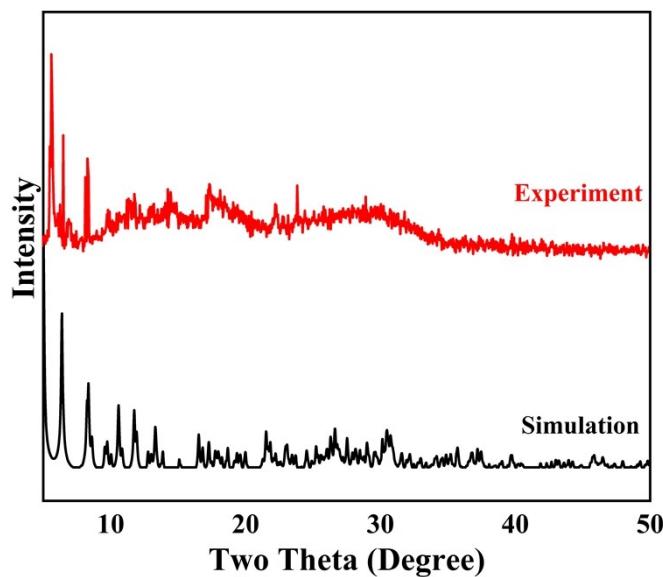


**Fig. S6.** The 3D structure of **1** linked by  $\text{K}^+$ .

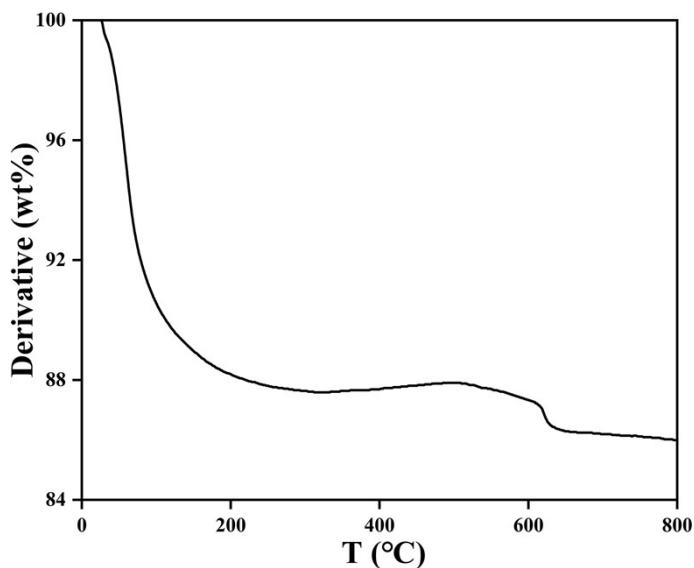


**Fig. S7.** The IR of compound **1**, phenylphosphonic acid and  $\{\text{P}_2\text{W}_{12}\}$ .

As shown in Fig. S7, the IR spectrum of compound **1** has distinct characteristic vibrational peaks in the region of  $4000 \text{ cm}^{-1} \sim 400 \text{ cm}^{-1}$ . The peaks at  $968$  and  $928 \text{ cm}^{-1}$  belong to the W–O<sub>t</sub> terminal vibration, and the peak at  $831 \text{ cm}^{-1}$  are associated with W–O bridges vibrations.<sup>S1</sup> The P–O vibrational bands in **1** appear at  $1157$ ,  $1127$ , and  $1022 \text{ cm}^{-1}$  in comparison with the P–O vibration bands of phenylphosphonic acid molecules at  $1132$ ,  $1129$  and  $1029 \text{ cm}^{-1}$ , which shows red shifts.<sup>S2</sup> The result suggests that the phenylphosphonic acid ligands are coordinated to the metal ions by means of the oxygen atoms.

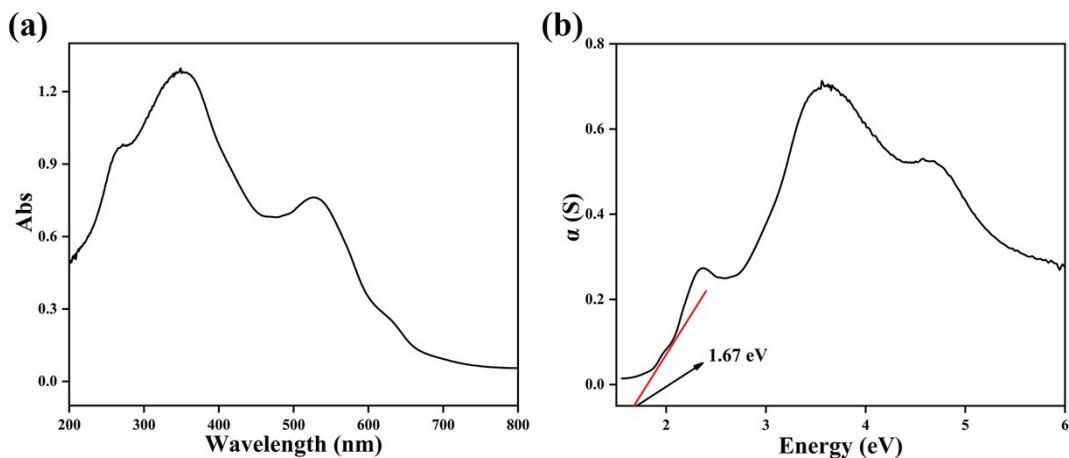


**Fig. S8.** The experimental, and simulated PXRD patterns of **1**.



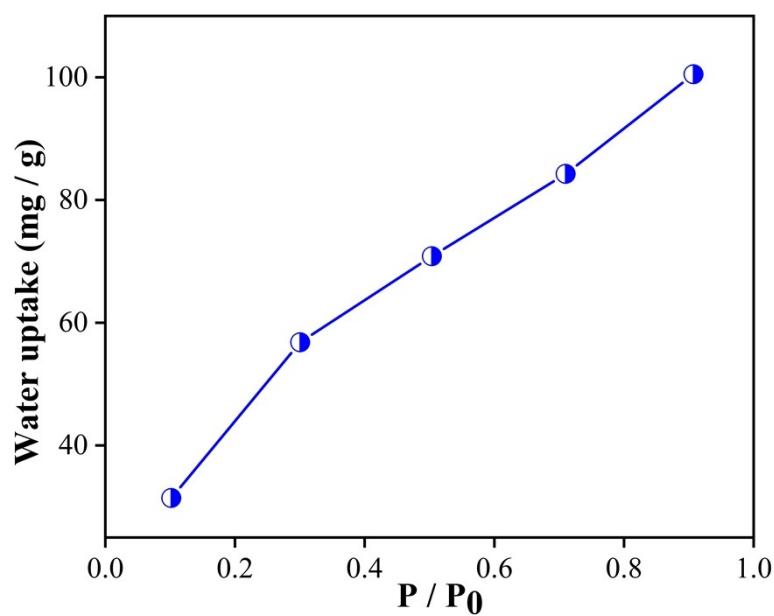
**Fig. S9.** The TGA curves of compound **1**.

The TGA curves of compound **1** have been determined in the range of 25 ~ 800 °C under the protection of N<sub>2</sub>. The TGA curves for **1** exhibits two discrete stages of mass loss. From 30 °C to 200 °C, the first weight loss of 12.44% was due to the loss of 48 crystalline water molecules. The weight loss observed in the second step, which occurred at 200 ~ 800 °C, was mainly due to the escape of 10 coordinated water molecules and 2 phenylphosphonic acid ligands.



**Fig. S10.** (a) The UV spectrum of compound **1**. (b) The K-M function of **1**.

Within the scope of 200–800 nm, UV analyse was performed on solid samples. In Fig. S10., **1** shows three absorption analogy bands at 268, 348, and 527 nm. The strong absorption peaks at 268 and 348 nm belong to the charge transfer from the ligand to the tungsten metal. The absorption peak at 527 nm corresponds to the d-d transition of the tungsten ion. The band gap energy of compound **1** was calculated from the Kubelka-Munk equation to be 1.67 eV, suggesting that it has potential semiconducting properties.



**Fig. S11.** Water adsorption isotherm of compound **1**.

## Tables

**Table S1.** Summary of proton conductive crystals based on POMs.

Compounds	Conductivity (S cm <sup>-1</sup> )	Temperature (K)	Relative humidity (%)	Reference
K <sub>4</sub> Na <sub>4</sub> H <sub>11</sub> [KCo <sub>2</sub> (H <sub>2</sub> O) <sub>10</sub> P <sub>4</sub> W <sub>24</sub> O <sub>92</sub> {(PhPO) <sub>2</sub> }·48H <sub>2</sub> O	<b>1.59 × 10<sup>-2</sup></b>	318	95	<b>This work</b>
[Ni <sub>8</sub> (OH) <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> (BDPCOOH) <sub>6</sub> ]	2.22 × 10 <sup>-3</sup>	353	100	S3
[Cu(en) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ] <sub>2</sub> {[Cu(en) <sub>4</sub> ][Cu(en) <sub>2</sub> ] <sub>5</sub> {[Cu(en) <sub>2</sub> ]KNb <sub>24</sub> O <sub>72</sub> H <sub>1</sub> <sub>0</sub> ] <sub>2</sub> }·6en·70H <sub>2</sub> O	1.35 × 10 <sup>-3</sup>	358	98	S4
[H <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>8</sub> {[Na(H <sub>2</sub> O) <sub>4</sub> ] <sub>2</sub> NaAs <sub>2</sub> W <sub>22</sub> (CH <sub>3</sub> COO) <sub>2</sub> O <sub>76</sub> Rh <sub>2</sub> (N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub> }·H <sub>2</sub> O	3.23 × 10 <sup>-4</sup>	338	80	S5
[Cu <sub>3</sub> (μ <sub>3</sub> -OH)(H <sub>2</sub> O) <sub>3</sub> (atz) <sub>3</sub> ] <sub>3</sub> [P <sub>2</sub> W <sub>18</sub> O <sub>62</sub> ] <sub>14</sub> H <sub>2</sub> O	4.42 × 10 <sup>-6</sup>	298	97	S6
[H <sub>2</sub> en] <sub>4</sub> [Ni <sub>5</sub> (OH) <sub>3</sub> (trzS) <sub>3</sub> (en)(H <sub>2</sub> O)(B-α-PW <sub>9</sub> O <sub>34</sub> )] <sub>1</sub> ·6H <sub>2</sub> O	1.30 × 10 <sup>-5</sup>	358	98	S7
Cu <sub>6</sub> (Trz) <sub>10</sub> (H <sub>2</sub> O) <sub>4</sub> [H <sub>2</sub> SiW <sub>12</sub> O <sub>40</sub> ] <sub>1</sub> ·8H <sub>2</sub> O	1.84 × 10 <sup>-6</sup>	368	95	S8
[Cu(debqdc) <sub>2</sub> ] <sub>2</sub> [HPW <sub>12</sub> O <sub>40</sub> ] <sub>1</sub> ·4H <sub>2</sub> O	3.23 × 10 <sup>-4</sup>	373	98	S9
Na <sub>2</sub> [Gd <sub>2</sub> (H <sub>2</sub> O) <sub>11</sub> ] <sub>2</sub> [Gd <sub>3</sub> (H <sub>2</sub> O) <sub>2</sub> (α-SiW <sub>11</sub> O <sub>39</sub> ) <sub>2</sub> ] <sub>2</sub> ·69H <sub>2</sub> O	3.54 × 10 <sup>-3</sup>	358	98	S10
[Ce <sup>III</sup> (H <sub>2</sub> O) <sub>6</sub> ] <sub>2</sub> {[Ce <sup>IV</sup> <sub>7</sub> Ce <sup>III</sup> <sub>3</sub> O <sub>6</sub> (OH) <sub>6</sub> (CO <sub>3</sub> )(H <sub>2</sub> O) <sub>11</sub> ] <sub>2</sub> [P <sub>2</sub> W <sub>16</sub> O <sub>59</sub> ]} <sub>3</sub>	2.65 × 10 <sup>-4</sup>	373	75	S11
Na <sub>5.5</sub> H <sub>6.5</sub> [(SbW <sub>9</sub> O <sub>33</sub> ) <sub>2</sub> {WO <sub>2</sub> (OH)} <sub>2</sub> {WO <sub>2</sub> }RuC <sub>7</sub> H <sub>3</sub> NO <sub>4</sub> ] <sub>1</sub> ·36H <sub>2</sub> O	2.97 × 10 <sup>-2</sup>	348	75	S12

**Table S2.** Bond Valence Sum (BVS) calculations of all the Co, P and W atoms in **1**.

Bond	Bond length	Bond Valence	Bond	Bond length	Bond Valence
Co1-O1W <sup>1</sup>	2.078(18)	0.352	Co2-O4W <sup>1</sup>	2.105(18)	0.328
Co1-O1W	2.078(18)	0.352	Co2-O4W	2.105(18)	0.328
Co1-O2W	2.02(3)	0.412	Co2-O5W	2.04(3)	0.390
Co1-O10	2.005(15)	0.429	Co2-O251	2.039(16)	0.391
Co1-O10 <sup>1</sup>	2.005(15)	0.429	Co2-O25	2.039(16)	0.391
$\Sigma(\text{Co1}) = 1.975$			$\Sigma(\text{Co2}) = 1.828$		
P1-O5	1.516(13)	1.269	P2-O12	1.509(13)	1.293
P1-O8	1.526(12)	1.235	P2-O13	1.513(12)	1.279
P1-O9	1.547(15)	1.167	P2-O20	1.535(14)	1.205
P1-O24	1.523(13)	1.245	P2-O39	1.579(15)	1.070
$\Sigma(\text{P1}) = 4.914$			$\Sigma(\text{P2}) = 4.864$		
P3-O30	1.549(16)	1.160	P4-O1	1.512(5)	1.282
P3-O32	1.565(18)	1.111	P4-O15	1.529(5)	1.225
P3-O48	1.544(15)	1.176	P4-O21	1.552(6)	1.151
P3-C1	1.78(2)	0.932	P4-C2	1.849(8)	1.117
$\Sigma(\text{P3}) = 4.380$			$\Sigma(\text{P4}) = 4.775$		

W1-O7	1.823(16)	1.303	W2-O2	1.847(14)	1.221
W1-O8	2.128(13)	0.572	W2-O3	1.968(12)	0.881
W1-O14	1.936(13)	0.960	W2-O5	2.127(11)	0.573
W1-O18	1.749(13)	1.592	W2-O28	1.731(12)	1.671
W1-O35	1.934(11)	0.965	W2-O31	1.954(12)	0.915
W1-O40	1.910(4)	1.030	W2-O41	1.909(4)	1.033
$\Sigma(W1) = 6.422$			$\Sigma(W2) = 6.294$		
W3-O9	2.298(13)	0.361	W4-O3	1.877(12)	1.126
W3-O14	1.896(11)	1.070	W4-O9	2.310(12)	0.349
W3-O21	1.948(14)	0.930	W4-O19	1.945(13)	0.937
W3-O26	1.701(16)	1.812	W4-O23	1.710(14)	1.769
W3-O27	1.934(13)	0.965	W4-O27	1.910(13)	1.030
W3-O42	1.904(3)	1.047	W4-O50	1.920(6)	1.003
$\Sigma(W3) = 6.185$			$\Sigma(W4) = 6.215$		
W5-O6	2.013(16)	0.780	W6-O4	1.987(16)	0.837
W5-O11	1.934(12)	0.965	W6-O11	1.943(12)	0.942
W5-O19	1.865(15)	1.163	W6-O21	1.865(15)	1.163
W5-O24	2.277(11)	0.382	W6-O24	2.303(12)	0.356
W5-O31	1.899(13)	1.061	W6-O34	1.727(14)	1.689
W5-O46	1.725(14)	1.698	W6-O35	1.905(11)	1.044
$\Sigma(W5) = 6.051$			$\Sigma(W6) = 6.032$		
W7-O4	1.838(16)	1.251	W8-O2	1.960(14)	0.900
W7-O15	1.954(12)	0.915	W8-O10	1.808(14)	1.357
W7-O17	1.832(12)	1.272	W8-O12	2.169(12)	0.512
W7-O20	2.307(12)	0.352	W8-O16	2.116(14)	0.590
W7-O33	2.10(2)	0.616	W8-O36	1.939(16)	0.953
W7-O45	1.721(12)	1.717	W8-O37	1.732(13)	1.667
$\Sigma(W7) = 6.124$			$\Sigma(W8) = 5.978$		
W9-O7	1.984(16)	0.843	W10-O6	1.807(16)	1.361
W9-O13	2.157(11)	0.528	W10-O15	1.928(12)	0.981
W9-O17	2.096(13)	0.623	W10-O16	1.812(13)	1.343
W9-O25	1.779(14)	1.468	W10-O20	2.299(12)	0.360
W9-O29	1.914(17)	1.019	W10-O22	2.08(2)	0.651
W9-O38	1.733(13)	1.662	W10-O43	1.748(13)	1.596
$\Sigma(W9) = 6.144$			$\Sigma(W10) = 6.291$		
W11-O29	1.914(15)	1.019	W12-O22	1.81(2)	1.350
W11-O32	2.049(18)	0.708	W12-O30	2.050(17)	0.706
W11-O33	1.78(2)	1.464	W12-O36	1.899(14)	1.061
W11-O39	2.274(14)	0.385	W12-O39	2.263(12)	0.397
W11-O44	1.975(19)	0.864	W12-O44	1.929(16)	0.979
W11-O51	1.733(16)	1.662	W12-O47	1.718(16)	1.731
$\Sigma(W11) = 6.102$			$\Sigma(W12) = 6.233$		

**Table S3.** Crystallographic data of compound **1**.

Compound	<b>1</b>
Empirical formula	C <sub>12</sub> H <sub>10</sub> Co <sub>2</sub> K <sub>5</sub> Na <sub>4</sub> O <sub>109</sub> P <sub>6</sub> W <sub>24</sub>
Formula weight	6901.74
Temperature / K	150.0
Crystal system	monoclinic
Space group	<i>C</i> 2/ <i>m</i>
a[Å]	35.2452(9)
b[Å]	21.1687(5)
c[Å]	21.4434(4)
α [Å]	90
β[Å]	90.1220(9)
γ[Å]	90
V[Å <sup>3</sup> ]	15998.8(6)
Z	4
ρcalcd [g/cm <sup>3</sup> ]	2.865
μ [mm <sup>-1</sup> ]	17.658
F (000)	12052.0
Index ranges	-42 ≤ h ≤ 41 -25 ≤ k ≤ 24 -25 ≤ l ≤ 25
Reflections collected	52886
Independent reflections	14645 [Rint = 0.0595, Rsigma = 0.0663]
data/restraints/parameters	14645/121/757
Goodness-of-fit on F <sup>2</sup>	0.995
R1, wR2 [I > 2σ(I)]	0.0845, 0.2179
R1, wR2 [all data]	0.0978, 0.2356

**Table S4.** Bond length of compound 1.

Bond	Bond length	Bond	Bond length	Bond	Bond length
W1-O7	1.823(16)	W2-O2	1.847(14)	W3-O9	2.298(13)
W1-O8	2.128(13)	W2-O3	1.968(12)	W3-O14	1.896(11)
W1-O14	1.936(13)	W2-O5	2.127(11)	W3-O21	1.948(14)
W1-O18	1.749(13)	W2-O28	1.731(12)	W3-O26	1.701(16)
W1-O35	1.934(11)	W2-O31	1.954(12)	W3-O27	1.934(13)
W1-O40	1.910(4)	W2-O41	1.909(4)	W3-O42	1.904(3)
W4-O3	1.877(12)	W5-O6	2.013(16)	W6-O4	1.987(16)
W4-O9	2.310(12)	W5-O11	1.934(12)	W6-O11	1.943(12)
W4-O19	1.945(13)	W5-O19	1.865(15)	W6-O21	1.865(15)
W4-O23	1.710(14)	W5-O24	2.277(11)	W6-O24	2.303(12)
W4-O27	1.910(13)	W5-O31	1.899(13)	W6-O34	1.727(14)
W4-O50	1.920(6)	W5-O46	1.725(14)	W6-O35	1.905(11)
W7-O4	1.838(16)	W8-O2	1.960(14)	W9-O7	1.984(16)
W7-O15	1.954(12)	W8-O10	1.808(14)	W9-O13	2.157(11)
W7-O17	1.832(12)	W8-O12	2.169(12)	W9-O17	2.096(13)
W7-O20	2.307(12)	W8-O16	2.116(14)	W9-O25	1.779(14)
W7-O33	2.10(2)	W8-O36	1.939(16)	W9-O29	1.914(17)
W7-O45	1.721(12)	W8-O37	1.732(13)	W9-O38	1.733(13)
W10-O6	1.807(16)	W11-O29	1.914(15)	W12-O22	1.81(2)
W10-O15	1.928(12)	W11-O32	2.049(18)	W12-O30	2.050(17)
W10-O16	1.812(13)	W11-O33	1.78(2)	W12-O36	1.899(14)
W10-O20	2.299(12)	W11-O39	2.274(14)	W12-O39	2.263(12)
W10-O22	2.08(2)	W11-O44	1.975(19)	W12-O44	1.929(16)
W10-O43	1.748(13)	W11-O51	1.733(16)	W12-O47	1.718(16)
Co1-O1W <sup>1</sup>	2.078(18)	Co2-O4W <sup>1</sup>	2.105(18)	P1-O5	1.516(13)
Co1-O1W	2.078(18)	Co2-O4W	2.105(18)	P1-O8	1.526(12)
Co1-O2W	2.02(3)	Co2-O5W	2.04(3)	P1-O9	1.547(15)
Co1-O10	2.005(15)	Co2-O251	2.039(16)	P1-O24	1.523(13)
Co1-O10 <sup>1</sup>	2.005(15)	Co2-O25	2.039(16)	P2-O12	1.509(13)
Co1B-O2W	1.85(3)	Co2B-O5W	1.79(3)	P2-O13	1.513(12)
Co1B-O3W	2.21(3)	Co2B-O6W	2.21(4)	P2-O20	1.535(14)
Co1B-O10	2.098(16)	Co2B-O251	2.097(16)	P2-O39	1.579(15)
Co1B-O10 <sup>1</sup>	2.098(16)	Co2B-O25	2.097(16)	P3-O30	1.549(16)
P3-O32	1.565(18)	P3-O48	1.544(15)	P3-C1	1.78(2)

**Table S5.** Angles of compound 1.

Bond	Angle	Bond	Angle	Bond	Angle
O7-W1-O8	85.2(5)	O2-W2-O3	166.7(5)	O2-W3-O9	82.1(5)
O7-W1-O14	166.3(5)	O2-W2-O5	85.8(5)	O2-W3-O21	83.7(6)
O7-W1-O35	92.9(6)	O2-W2-O31	92.0(6)	O2-W3-O27	154.5(6)

O7-W1-O40	91.5(8)	O2-W2-O41	91.7(7)	O2-W3-O42	90.5(7)
O7-W1-O8	81.7(5)	O2-W2-O5	81.5(5)	O2-W3-O9	81.0(5)
O7-W1-O7	100.0(6)	O2-W2-O2	98.8(6)	O2-W3-O9	172.6(6)
O7-W1-O8	174.8(6)	O2-W2-O3	93.9(6)	O2-W3-O14	105.0(6)
O7-W1-O14	93.1(6)	O2-W2-O5	175.3(6)	O2-W3-O21	97.5(7)
O7-W1-O35	94.8(6)	O2-W2-O31	93.9(6)	O2-W3-O27	100.2(6)
O7-W1-O40	96.7(7)	O2-W2-O41	98.4(7)	O2-W3-O42	97.3(8)
O7-W1-O8	84.9(5)	O2-W2-O3	83.1(6)	O2-W3-O9	72.6(5)
O7-W1-O14	82.1(6)	O2-W2-O5	84.7(5)	O2-W3-O21	89.4(6)
O7-W1-O8	83.1(6)	O2-W2-O3	90.5(7)	O2-W3-O9	84.5(7)
O7-W1-O14	90.8(8)	O2-W2-O5	82.6(6)	O2-W3-O21	165.0(8)
O7-W1-O35	166.8(6)	O2-W2-O31	166.4(7)	O2-W3-O27	90.0(7)
O2-W4-O9	82.9(5)	O2-W5-O24	83.0(5)	O2-W6-O24	83.1(5)
O2-W4-O19	84.1(6)	O2-W5-O6	83.0(5)	O2-W6-O4	88.8(6)
O2-W4-O27	155.5(6)	O2-W5-O24	83.0(5)	O2-W6-O24	73.1(5)
O2-W4-O50	92.3(8)	O2-W5-O6	83.0(5)	O2-W6-O4	164.2(6)
O2-W4-O9	81.6(5)	O2-W5-O11	83.0(5)	O2-W6-O11	91.7(6)
O2-W4-O3	105.1(7)	O2-W5-O24	83.0(5)	O2-W6-O24	81.9(5)
O2-W4-O9	171.6(6)	O2-W5-O31	83.0(5)	O2-W6-O35	85.1(6)
O2-W4-O19	96.7(7)	O2-W5-O6	83.0(5)	O2-W6-O4	96.8(7)
O2-W4-O27	99.2(7)	O2-W5-O11	83.0(5)	O2-W6-O11	98.5(6)
O2-W4-O50	96.2(9)	O2-W5-O24	83.0(5)	O2-W6-O21	98.8(7)
O2-W4-O9	72.7(5)	O2-W5-O6	83.0(5)	O2-W6-O24	171.7(5)
O2-W4-O19	89.9(6)	O2-W5-O11	83.0(5)	O2-W6-O35	102.7(6)
O2-W4-O50	88.3(8)	O2-W5-O19	83.0(5)	O2-W6-O4	88.7(6)
O2-W4-O9	85.7(8)	O2-W5-O24	83.0(5)	O2-W6-O11	158.7(6)
O2-W4-O19	167.1(8)	O2-W5-O31	83.0(5)	O2-W6-O24	85.6(5)
O2-W7-O15	91.2(6)	O2-W8-O12	83.7(5)	O2-W9-O13	84.1(5)
O2-W7-O20	87.5(5)	O2-W8-O16	83.1(5)	O2-W9-O17	83.1(5)
O2-W7-O33	169.6(5)	O2-W8-O2	97.3(5)	O2-W9-O13	80.7(5)
O2-W7-O20	71.3(5)	O2-W8-O12	88.3(6)	O2-W9-O7	97.6(6)
O2-W7-O33	84.4(6)	O2-W8-O16	168.5(6)	O2-W9-O13	88.8(6)
O2-W7-O4	95.5(6)	O2-W8-O36	94.8(6)	O2-W9-O17	169.3(6)
O2-W7-O15	154.2(6)	O2-W8-O12	80.4(5)	O2-W9-O29	95.3(7)
O2-W7-O20	84.2(5)	O2-W8-O2	162.1(6)	O2-W9-O7	161.4(6)
O2-W7-O33	84.7(6)	O2-W8-O12	83.6(6)	O2-W9-O13	82.8(6)
O2-W7-O20	82.2(5)	O2-W8-O16	82.4(6)	O2-W9-O17	81.7(6)
O2-W7-O4	98.7(6)	O2-W8-O2	95.8(7)	O2-W9-O7	94.7(7)
O2-W7-O15	100.7(6)	O2-W8-O10	100.9(7)	O2-W9-O13	170.9(6)
O2-W7-O17	102.8(6)	O2-W8-O12	170.9(6)	O2-W9-O17	90.2(6)
O2-W7-O20	170.1(6)	O2-W8-O16	90.5(6)	O2-W9-O25	100.3(6)

O2-W7-O33	91.4(7)	O2-W8-O36	94.8(7)	O2-W9-O29	96.1(7)
O2-W10-O15	91.4(6)	O2-W11-O32	87.6(7)	O2-W12-O30	162.9(6)
O2-W10-O16	95.1(6)	O2-W11-O39	83.6(5)	O2-W12-O36	93.1(7)
O2-W10-O20	87.2(5)	O2-W11-O44	156.7(6)	O2-W12-O39	85.8(6)
O2-W10-O22	169.7(5)	O2-W11-O39	77.8(6)	O2-W12-O44	91.2(7)
O2-W10-O20	71.9(5)	O2-W11-O29	92.1(8)	O2-W12-O39	77.2(5)
O2-W10-O22	84.3(6)	O2-W11-O32	163.7(6)	O2-W12-O30	86.2(7)
O2-W10-O15	154.4(6)	O2-W11-O39	86.0(6)	O2-W12-O39	83.4(5)
O2-W10-O20	83.7(5)	O2-W11-O44	91.2(7)	O2-W12-O44	157.4(6)
O2-W10-O22	85.1(6)	O2-W11-O32	83.0(7)	O2-W12-O30	83.4(7)
O2-W10-O20	82.6(5)	O2-W11-O39	73.7(5)	O2-W12-O39	74.8(6)
O2-W10-O6	98.8(7)	O2-W11-O29	102.4(7)	O2-W12-O22	105.1(8)
O2-W10-O15	99.9(6)	O2-W11-O32	93.6(8)	O2-W12-O30	91.7(8)
O2-W10-O16	103.5(6)	O2-W11-O33	102.4(8)	O2-W12-O36	102.4(7)
O2-W10-O20	170.1(6)	O2-W11-O39	169.4(7)	O2-W12-O39	167.3(7)
O2-W10-O22	91.1(7)	O2-W11-O44	99.4(7)	O2-W12-O44	97.9(8)
O1W <sup>1</sup> -Co1-O1W	93.4(13)	O1W <sup>1</sup> -Co1B-O3W	162.2(13)	O1W <sup>1</sup> -Co2-O25 <sup>1</sup>	92.1(7)
O1W <sup>1</sup> -Co1-O1W	91.4(9)	O1W <sup>1</sup> -Co1B-O10 <sup>1</sup>	96.6(9)	O1W <sup>1</sup> -Co2-O4W	174.8(8)
O1W <sup>1</sup> -Co1-O1W <sup>1</sup>	91.4(9)	O1W <sup>1</sup> -Co1B-O10	96.6(9)	O1W <sup>1</sup> -Co2-O4W <sup>1</sup>	85.8(8)
O1W <sup>1</sup> -Co1-O1W <sup>1</sup>	87.1(7)	O1W <sup>1</sup> -Co1B-O3W	96.4(8)	O1W <sup>1</sup> -Co2-O4W	174.8(8)
O1W <sup>1</sup> -Co1-O1W	87.1(7)	O1W <sup>1</sup> -Co1B-O3W	96.4(8)	O1W <sup>1</sup> -Co2-O4W <sup>1</sup>	85.8(8)
O1W <sup>1</sup> -Co1-O1W	174.2(8)	O1W <sup>1</sup> -Co1B-O10	86.8(10)	O1W <sup>1</sup> -Co2-O25 <sup>1</sup>	92.3(9)
O1W <sup>1</sup> -Co1-O1W <sup>1</sup>	174.2(8)	O1W <sup>1</sup> -Co2-O4W	95.7(14)	O1W <sup>1</sup> -Co2B-O6W	160.1(13)
O1W <sup>1</sup> -Co1-O2W	94.4(7)	O1W <sup>1</sup> -Co2-O4W	92.9(8)	O1W <sup>1</sup> -Co2B-O25	97.7(9)
O1W <sup>1</sup> -Co1-O2W	94.4(7)	O1W <sup>1</sup> -Co2-O4W <sup>1</sup>	92.9(8)	O1W <sup>1</sup> -Co2B-O25 <sup>1</sup>	97.7(9)
O1W <sup>1</sup> -Co1-O10 <sup>1</sup>	91.9(8)	O1W <sup>1</sup> -Co2-O25	92.1(7)	O1W <sup>1</sup> -Co2B-O6W	96.4(8)
O1W <sup>1</sup> -Co2B-O6W	96.4(8)	O1W <sup>1</sup> -Co2B-O25 <sup>1</sup>	89.1(9)		

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