

## Supplementary Material

### Synthesis, structure characterization, and properties of a new heterometallic coordination polymer containing two $\mu_3$ -bridging tridentate ligands

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**Table S1** List of structurally characterized (LH<sub>2</sub>)<sup>+</sup> containing compounds retrieved from CSD

No	Compounds	Space group	Ref Code
1	(LH <sub>2</sub> )(C <sub>6</sub> H <sub>4</sub> NO <sub>2</sub> )	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	PIPLOS
2	(LH <sub>2</sub> )(C <sub>4</sub> H <sub>5</sub> O <sub>4</sub> )	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	XUMMEA
3	(LH <sub>2</sub> ) <sub>2</sub> (Sal) <sub>2</sub> (H <sub>2</sub> O)	<i>P2<sub>1</sub>2<sub>1</sub>2</i>	HISMAZ
4	(LH <sub>2</sub> )(NAP)	<i>P2<sub>1</sub>2<sub>1</sub>2</i>	TEQCAW
5	(LH <sub>2</sub> ) <sub>2</sub> (C <sub>23</sub> H <sub>31</sub> N <sub>2</sub> O <sub>5</sub> )	<i>P2<sub>1</sub></i>	EDALEC
6	(LH <sub>2</sub> )(H <sub>2</sub> PO <sub>4</sub> )	<i>P2<sub>1</sub></i>	GEXRUW
7	(LH <sub>2</sub> )(C <sub>24</sub> H <sub>39</sub> O <sub>4</sub> )·5(H <sub>2</sub> O) <sub>3</sub>	<i>P2<sub>1</sub></i>	GOLWIN
8	(LH <sub>2</sub> )(C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>10</sub> P <sub>2</sub> )·2H <sub>2</sub> O	<i>P2<sub>1</sub></i>	HMADPH
9	(LH <sub>2</sub> )[H <sub>2</sub> AsO <sub>4</sub> ]	<i>P2<sub>1</sub></i>	KORSAL02
10	(LH <sub>2</sub> )[H <sub>2</sub> PO <sub>3</sub> ]	<i>P2<sub>1</sub></i>	POPNAJ
11	(LH <sub>2</sub> )[HgI <sub>4</sub> ]	<i>P2<sub>1</sub></i>	XENFAZ
12	(LH <sub>2</sub> )(C <sub>2</sub> HCl <sub>2</sub> O <sub>2</sub> )	<i>P2<sub>1</sub></i>	YOTMUQ
13	(LH <sub>2</sub> ) <sub>3</sub> (C <sub>3</sub> H <sub>4</sub> O <sub>7</sub> P)	<i>P1</i>	SEFQOJ
14	(LH <sub>2</sub> )(C <sub>22</sub> H <sub>29</sub> N <sub>4</sub> O <sub>2</sub> )	<i>P1</i>	YATJUZ
15	(LH <sub>2</sub> )(MEC)·CH <sub>3</sub> OH	<i>Cc</i>	TERLEK
16	(LH <sub>2</sub> ) <sub>3</sub> [PMo <sub>12</sub> O <sub>40</sub> ]·5H <sub>2</sub> O	<i>Cc</i>	WIYXEH
17	(LH <sub>2</sub> )[ReO <sub>4</sub> ]	<i>Pca2<sub>1</sub></i>	DUBXII
18	(NH <sub>4</sub> )(LH <sub>2</sub> )[MoO <sub>4</sub> ]	<i>P3c1</i>	CUFSII
19	[K(LH <sub>2</sub> )(MoO <sub>4</sub> )]	<i>P3c1</i>	<b>This work</b>
20	(LH <sub>2</sub> )I	<i>I2<sub>1</sub>3</i>	BUZFUX
21	[WS <sub>4</sub> Ag·LH <sub>2</sub> ·2DMF] <sub>n</sub>	<i>Pmn2<sub>1</sub></i>	ZOLJUF
22	(LH <sub>2</sub> )(Hfura)	<i>P<math>\bar{1}</math></i>	PIPLIM
23	(LH <sub>2</sub> ) <sub>2</sub> (nds)	<i>P<math>\bar{1}</math></i>	PIPMOT
24	(LH <sub>2</sub> )(ctrz)	<i>P<math>\bar{1}</math></i>	AHEXOC
25	H <sub>2</sub> [LH <sub>2</sub> ] <sub>0.5</sub> [Cd(phen) <sub>3</sub> ][Cd(H <sub>2</sub> O)(phen) <sub>2</sub> ] <sub>2</sub> (V <sub>16</sub> O <sub>38</sub> Cl) <sub>0.5</sub> {[Cd(H <sub>2</sub> O)(phen) <sub>2</sub> ] <sub>2</sub> (V <sub>16</sub> O <sub>39</sub> Cl) <sub>0.5</sub> ·2H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	CAPKUA
26	(LH <sub>2</sub> )(DFHB)	<i>P<math>\bar{1}</math></i>	CUYBIJ
27	(LH <sub>2</sub> )(SSal)·0.5H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	GADYUI
28	[Ag(mna)] <sub>6</sub> <sup>6-</sup> ·4Na <sup>+</sup> ·2(LH <sub>2</sub> ) <sup>+</sup> ·10H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	ENERIY
29	Na <sub>2</sub> [LH <sub>2</sub> ][Ni(OH) <sub>3</sub> Mo <sub>6</sub> O <sub>18</sub> (LH <sub>2</sub> )]·11.75H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	IBOQIC
30	(LH <sub>2</sub> ) <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> )·H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	IHUFQG
31	(LH <sub>2</sub> )(η <sup>5</sup> -C <sub>3</sub> H <sub>4</sub> COOH)Mn(CO) <sub>3</sub>	<i>P<math>\bar{1}</math></i>	PEHDEN
32	(LH <sub>2</sub> )(MEF)·H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	RUVNEC01
33	(LH <sub>2</sub> )(FLR)	<i>P<math>\bar{1}</math></i>	TEQKAE
34	(LH <sub>2</sub> )(FLU)·H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	TEQYEW
35	(LH <sub>2</sub> )(INDH)(IND)·H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	TERKOT
36	(LH <sub>2</sub> )(TOL)	<i>P<math>\bar{1}</math></i>	TERLIO
37	(LH <sub>2</sub> )(napq)	<i>P<math>\bar{1}</math></i>	VATVAP
38	(LH <sub>2</sub> ) <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> )·2H <sub>2</sub> O	<i>P<math>\bar{1}</math></i>	ZASKIQ
39	(LH <sub>2</sub> )(2mpa)	<i>P<math>\bar{1}</math></i>	XUMLUP
40	(LH <sub>2</sub> )(IBU)	<i>P2<sub>1</sub>/c</i>	CUGPIF
41	(LH <sub>2</sub> )(srtid)]·H <sub>2</sub> O	<i>P2<sub>1</sub>/c</i>	DOPYUE
42	(LH <sub>2</sub> )(SSal)	<i>P2<sub>1</sub>/c</i>	GADXUH
43	(LH <sub>2</sub> )(gmfb)	<i>P2<sub>1</sub>/c</i>	GICHUW
44	(LH <sub>2</sub> )(tfa)	<i>P2<sub>1</sub>/c</i>	SAFXAA
45	(LH <sub>2</sub> )(IBU)	<i>P2<sub>1</sub>/c</i>	TEQYIA
46	(LH <sub>2</sub> )(DIC)	<i>P2<sub>1</sub>/c</i>	TUDPIR01
47	(LH <sub>2</sub> )(dmtc)	<i>P2<sub>1</sub>/c</i>	YUFMAN
48	(LH <sub>2</sub> )(mal)	<i>P2<sub>1</sub>/c</i>	XUMMAW
49	(LH <sub>2</sub> )(Haba)	<i>P2<sub>1</sub>/c</i>	PIPLUY

50	(LH <sub>2</sub> )(chdc)	<i>P</i> 2 <sub>1</sub> / <i>c</i>	PIPMIN
51	(LH <sub>2</sub> )(2-anb)	<i>P</i> 2 <sub>1</sub> / <i>c</i>	VIPXUQ
52	(LH <sub>2</sub> )(Hdcba)	<i>P</i> 2 <sub>1</sub> / <i>n</i>	PIPMAF
53	(LH <sub>2</sub> )(Hcpa)	<i>P</i> 2 <sub>1</sub> / <i>n</i>	PIPMEJ
54	(LH <sub>2</sub> ) <sub>2</sub> (buta)	<i>P</i> 2 <sub>1</sub> / <i>n</i>	PIPMUZ
55	[LH <sub>2</sub> ] <sub>2</sub> {(LH <sub>2</sub> )CrMo <sub>6</sub> O <sub>18</sub> (OH) <sub>3</sub> }	<i>P</i> 2 <sub>1</sub> / <i>n</i>	ROQTAU
56	[WS <sub>4</sub> Ag·LH <sub>2</sub> ·H <sub>2</sub> O] <sub>n</sub>	<i>P</i> 2 <sub>1</sub> / <i>n</i>	ZOLKAM
57	(LH <sub>2</sub> )(C <sub>25</sub> H <sub>25</sub> N <sub>7</sub> O <sub>8</sub> P)·0.5(C <sub>2</sub> H <sub>6</sub> O)	<i>C</i> 2/ <i>c</i>	IWIXIW
58	(LH <sub>2</sub> )(C <sub>25</sub> H <sub>25</sub> N <sub>7</sub> O <sub>8</sub> P)	<i>C</i> 2/ <i>c</i>	IWIXOC
59	(LH <sub>2</sub> ) <sub>2</sub> [V <sub>10</sub> O <sub>28</sub> {Mn(H <sub>2</sub> O) <sub>5</sub> } <sub>2</sub> ]·2H <sub>2</sub> O	<i>C</i> 2/ <i>c</i>	LOYDOU
60	(LH <sub>2</sub> )Br	<i>R</i> $\bar{3}$	BUZGAE
61	(LH <sub>2</sub> )F	<i>R</i> $\bar{3}$	BUZGEI
62	(LH <sub>2</sub> )Cl	<i>R</i> $\bar{3}$	LH2C10
63	(LH <sub>2</sub> )(4HBA)	<i>Pbca</i>	CIKQIY
64	(LH <sub>2</sub> )CHO <sub>2</sub>	<i>Pbca</i>	UREWAQ
65	(LH <sub>2</sub> ) <sub>2</sub> [SiF <sub>6</sub> ]	<i>P</i> $\bar{3}$	ELUZUG
66	(LH <sub>2</sub> ) <sub>2</sub> SO <sub>4</sub>	<i>P</i> $\bar{3}$	YIYGEU

**Abbreviations used:** LH<sub>2</sub> = 1,3-dihydroxy-2-(hydroxymethyl)propan-2-aminium, C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub> = nicotinate, C<sub>4</sub>H<sub>5</sub>O<sub>4</sub> = succinate, Sal = salicylate, 4HBA = 4-Hydroxybenzoic acid, NAP = naproxen, DIC = diclofenac, MEF = mefenamate, FLR = flurbiprofen, FLU = flufenamic acid, IBU = ibuprofen, IND = indomethacin, TOL = tolfenamic acid, MEC = meclofenamic acid, Hfura = 2-furoic acid, Haba = 4-aminobenzoic acid, Hdcba = 2,4-dichlorobenzoic acid, Hcpa = 4-chlorophenoxyacetic acid, chdc = 1,4-cyclohexanedicarboxylic acid, nds = 1,5-naphthalenedisulfonic acid, buta = butane-1,2,3,4-tetracarboxylic acid, 2-anb = 2-amino-4-nitrobenzoate, ctrz = Cetirizine, phen = 1, 10'-phenanthroline, DFHB = 5-(2,4-difluorophenyl)-2-hydroxybenzoate, srtld = seratrodist, mna = 2-Mercaptonicotinate, napq = 2-oxido-1,4-naphthoquinone, dmte = N,N-dimethyldithiocarbamylacetate, C<sub>2</sub>O<sub>4</sub> = oxalate, DMF = Dimethylformamide, 2mpa = (2-methylphenoxy)acetate, mal = malonate, SSal = sulfosalicylate, gmfb = gemfibrozil, (C<sub>25</sub>H<sub>25</sub>N<sub>7</sub>O<sub>8</sub>P) = [3-[2-(4-benzoylpiperazin-1-yl)-2-oxoacetyl]-4-methoxy-7-(3-methyl-1,2,4-triazol-1-yl)pyrrolo[2,3-c]pyridin-1-yl]methyl dihydrogen phosphate, (η<sup>5</sup>-C<sub>5</sub>H<sub>4</sub>COOH)Mn(CO)<sub>3</sub> = cymantrenecarboxylate, tfa = trifluoroacetate.

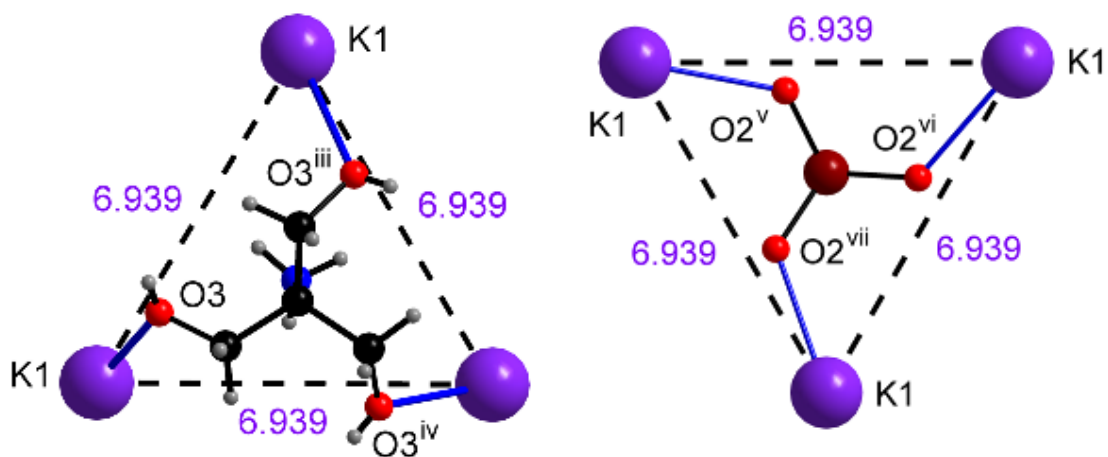
**Table S2** Selected bond lengths (Å) and bond angles (°) for **1**.

<i>Bond lengths</i> (Å)					
K1-O3	2.714(3)	N1-C1	1.495(6)	Mo1-O2 <sup>i</sup>	1.7563(16)
K1-O3 <sup>iii</sup>	2.714(3)	C(2)-O(3)	1.415(3)	Mo1-O2	1.7563(16)
K1-O3 <sup>iv</sup>	2.714(3)	C(1)-C(2)	1.528(3)	Mo1-O2 <sup>ii</sup>	1.7563(16)
K1-O2 <sup>v</sup>	2.8340(17)	C(1)-C(2) <sup>viii</sup>	1.528(3)	Mo1-O1	1.799(4)
K1-O2 <sup>vi</sup>	2.8340(17)	C(1)-C(2) <sup>ix</sup>	1.528(3)		
K1-O2 <sup>vii</sup>	2.8340(17)				
<i>Bond angles</i> (°)					
O3-K1-O3 <sup>iii</sup>	80.21(9)	O3-K1-O2#7	71.34(5)	C2-C1-C2 <sup>ix</sup>	110.6(2)
O3-K1-O3 <sup>iv</sup>	80.21(9)	O3#3-K1-O2#7	149.17(11)	C2 <sup>viii</sup> -C1-C2 <sup>ix</sup>	110.6(2)
O3 <sup>iii</sup> -K1-O3 <sup>iv</sup>	80.21(9)	O3#4-K1-O2#7	83.45(5)	O2 <sup>i</sup> -Mo1-O2	110.60(9)
O3-K1-O2 <sup>v</sup>	83.45(5)	O2#5-K1-O2#7	115.64(4)	O2 <sup>i</sup> -Mo1-O2 <sup>ii</sup>	110.60(9)
O3 <sup>iii</sup> -K1-O2 <sup>v</sup>	71.34(5)	O2#6-K1-O2#7	115.64(4)	O2-Mo1-O2 <sup>ii</sup>	110.60(8)
O3 <sup>iv</sup> -K1-O2 <sup>v</sup>	149.17(11)	O3-C2-C1	112.4(2)	O2 <sup>i</sup> -Mo1-O1	108.32(9)
O3-K1-O2 <sup>vi</sup>	149.17(11)	N1-C1-C2	108.4(2)	O2-Mo1-O1	108.32(9)
O3#3-K1-O2#6	83.45(5)	N1-C1-C2 <sup>viii</sup>	108.4(2)	O2 <sup>i</sup> -Mo1-O1	108.32(9)
O3#4-K1-O2#6	71.34(5)	N1-C1-C2 <sup>ix</sup>	108.4(2)		
O2#5-K1-O2#6	115.64(4)	C2-C1-C2 <sup>viii</sup>	110.6(2)		

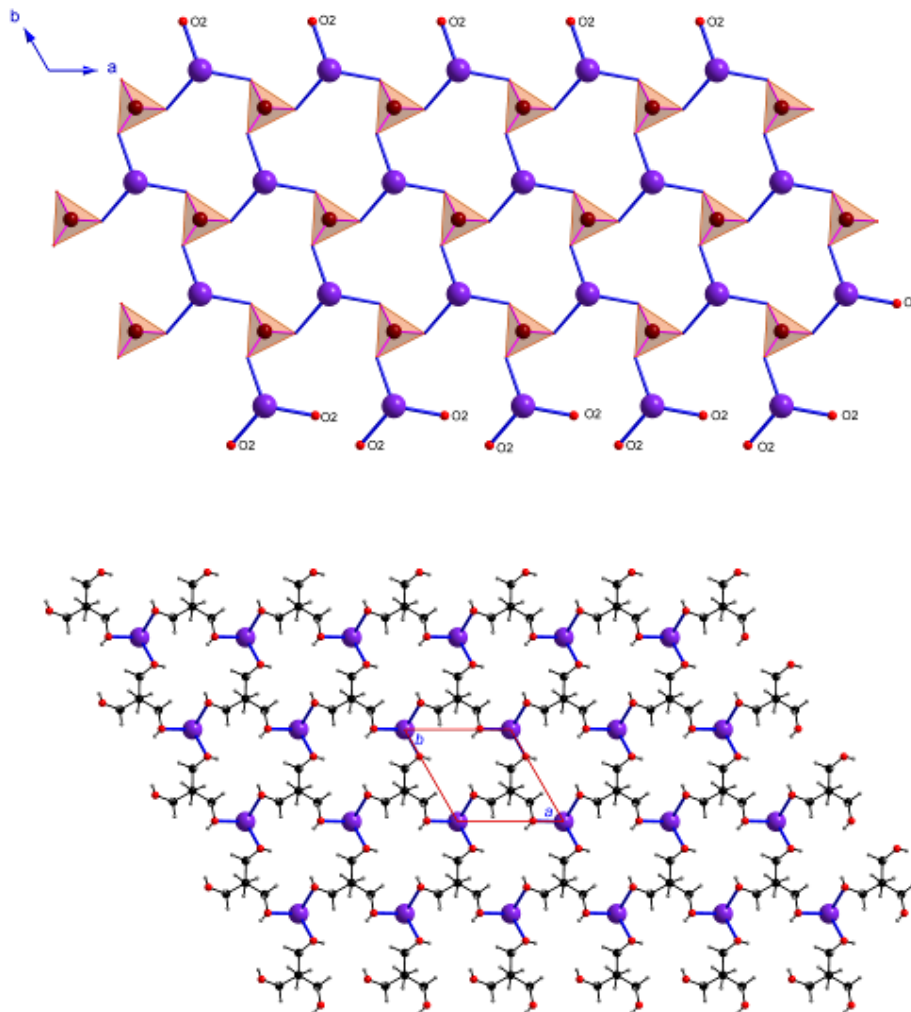
Symmetry codes for **1**: i) -y+1, x-y+1, z ii) -x+y, -x+1, z iii) -x+y, -x, z iv) -y, x-y, z v) -x+y, y-1, z-1/2 vi) x-1, x-y, z-1/2 vii) -y+1, -x+1, z-1/2 viii) -y+1, x-y, z ix) -x+y+1, -x+1, z

## Details of Instrumentation for characterization of **1**

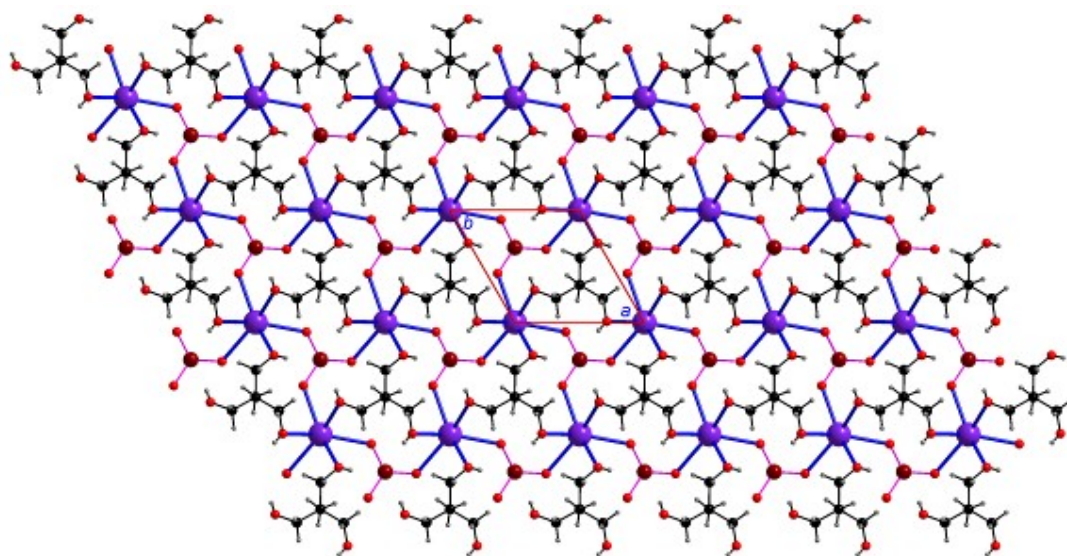
Infrared (IR) spectra of the solid samples diluted with KBr were recorded on a Shimadzu (IR Prestige-21) FT-IR spectrometer from 4000-400  $\text{cm}^{-1}$  at a resolution of 4  $\text{cm}^{-1}$ . Raman spectra of compounds in solid-state and in the aqueous medium were recorded by using an Agiltron PeakSeeker Pro Raman instrument with 785 nm laser radiation for excitation and laser power set to 100 mW. The samples for solution Raman spectra were taken in a quartz cuvette. The UV-visible spectrum of an aqueous solution of **1** was recorded using a Shimadzu UV-2450 double beam spectrophotometer using matched quartz cells. Isothermal weight loss studies were performed in a temperature-controlled electric furnace. Simultaneous thermogravimetry (TG) and differential thermal analyses (DTA) of a powdered sample of **1** were performed in alumina crucible in the temperature range of 30 °C to 600 °C, using a Netzsch STA-409 PC thermal analyzer, at a heating rate of 10°C/min. X-ray powder patterns were recorded on a Rigaku Miniflex II powder diffractometer using Cu-K $\alpha$  radiation with Ni filter. Conductivity measurements of **1** was carried out at room temperature using a Digital conductivity meter (LT-16) from Labtronics equipped with a standard conductometric cell composed of two platinum black electrodes. The piezoelectric property of **1** was studied using a composite piezoelectric oscillator from Mittal enterprises, New Delhi. The piezoelectric effect was measured qualitatively by application of 80 kHz frequency on the surface of a small crystal of size 15 $\times$ 7 $\times$ 2 mm<sup>3</sup> fixed on a contact plate with the aid of a tunable electromechanical oscillator. The electrical charge resulting from the applied mechanical force was measured and visualized using an oscilloscope. The measured piezoelectric effect of **1** was comparable with that of  $\alpha$ -quartz.



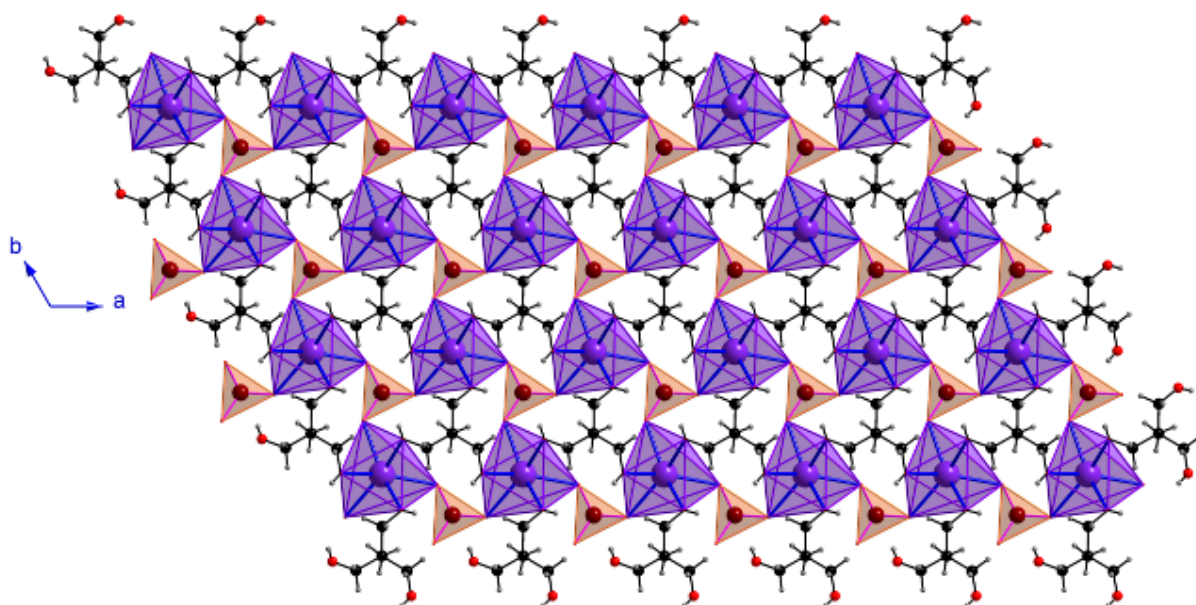
**Fig S1**  $\mu_3$ -tridentate binding mode of  $(\text{LH}_2)^+$  ligand (**left**) and  $(\text{MoO}_4)^{2-}$  (**right**) in **1** showing identical  $\text{K}\cdots\text{K}$  separations. Symmetry code: iii)  $-x+y, -x, z$  iv)  $-y, x-y, z$  v)  $-x+y, y-1, z-1/2$  vi)  $x-1, x-y, z-1/2$  vii)  $-y+1, -x+1, z-1/2$ .



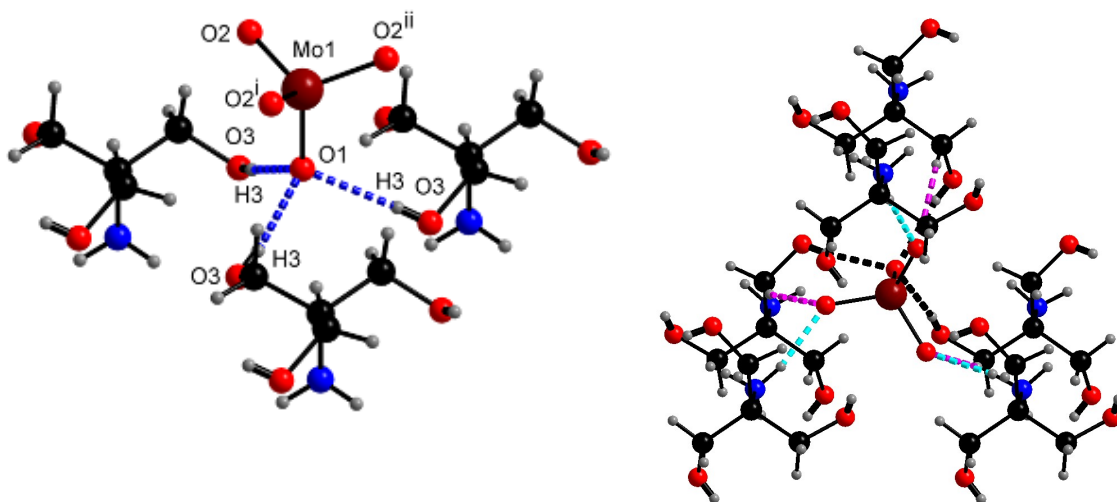
**Fig S2** A view along  $c$ -axis showing that  $(\text{MoO}_4)^{2-}$  is coordinated (via O2) to three different  $\text{K}^+$  ions. For clarity only  $\text{K}^+$  ions and the bridging  $(\text{MoO}_4)^{2-}$  (represented as polyhedra) are shown. O atoms of  $(\text{LH}_2)^+$  coordinated to  $\text{K}^+$  are not displayed (**top**). The bridging binding mode of  $(\text{LH}_2)^+$  (**bottom**). For a combined view of the binding of both ligands see **Fig S3**



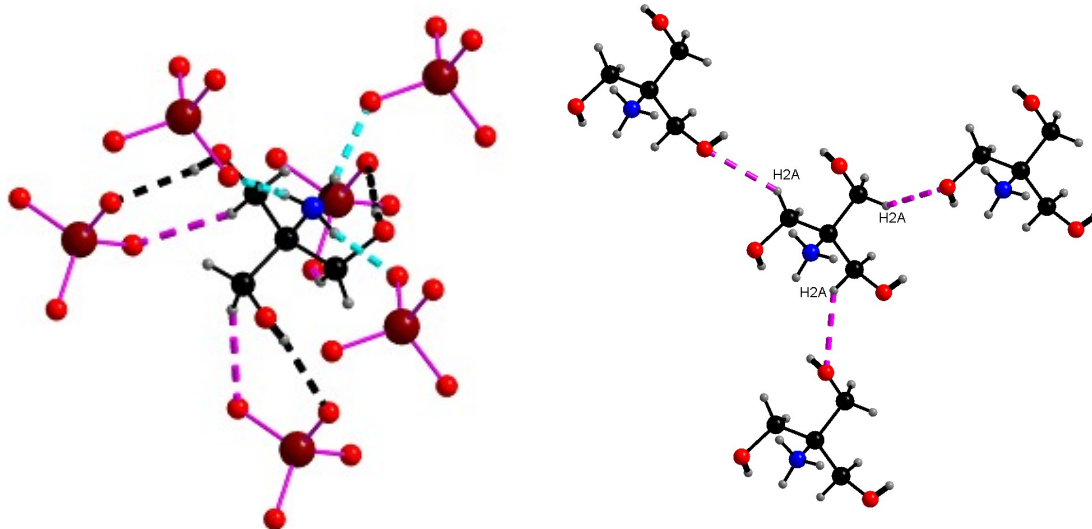
**Fig S3**  $\mu_3$ -bridging tridentate coordination modes of  $(LH_2)^+$  and  $(MoO_4)^{2-}$  resulting in hexa coordination around  $K^+$  and an extended structure



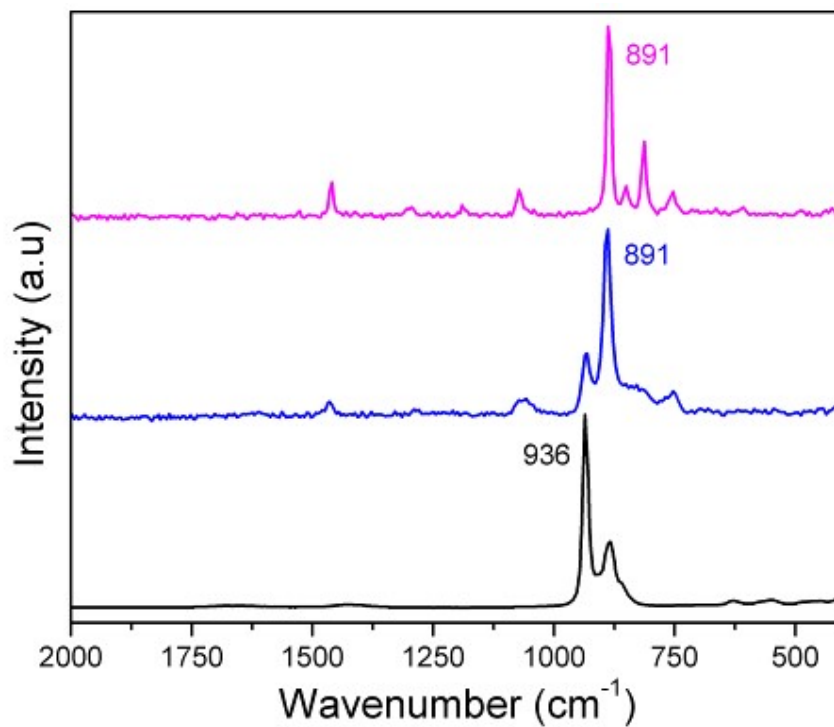
**Fig S4** A single layer of the hexagonal array in the (110) plane showing interlinked  $\{KO_6\}$  octahedra and  $\{MoO_4\}$  tetrahedra enclosing the organic cation in the cavity. In view of the three-fold symmetry of all the constituents, the  $\{MoO_4\}$  tetrahedra can also be considered in the cavity in a hexagonal array of interlinked  $\{KO_6\}$  octahedra and  $(LH_2)^+$  cations OR a hexagonal array of interlinked  $\{MoO_4\}$  tetrahedra and  $(LH_2)^+$  cations with a  $\{KO_6\}$  octahedron in the cavity.



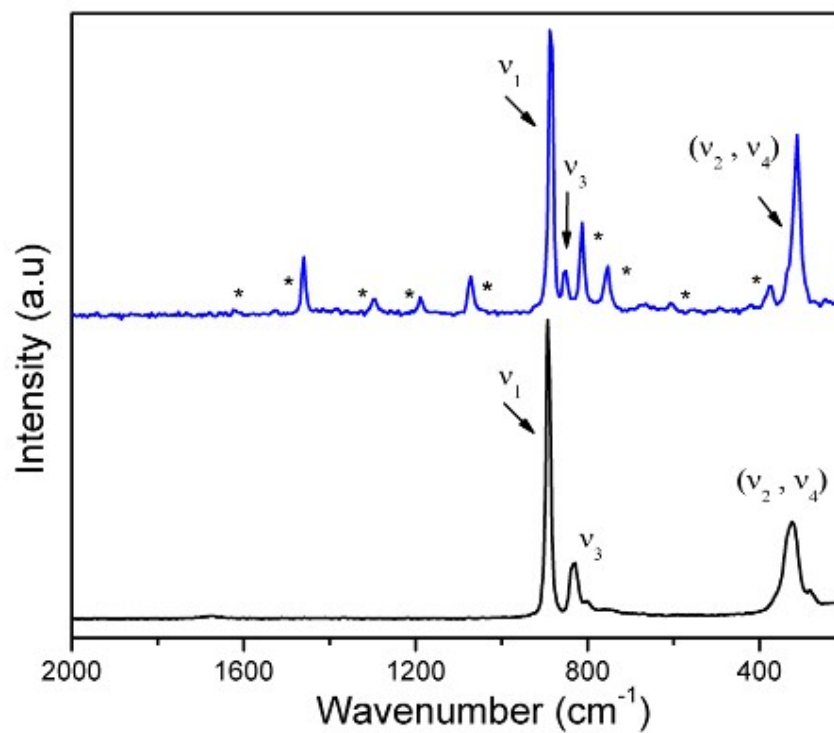
**Fig S5 A** H-bonding around the O1 site at (MoO<sub>4</sub>)<sup>2-</sup> (**left**) and linking of (LH<sub>2</sub>)<sup>+</sup> cations with (MoO<sub>4</sub>)<sup>2-</sup> (**right**)



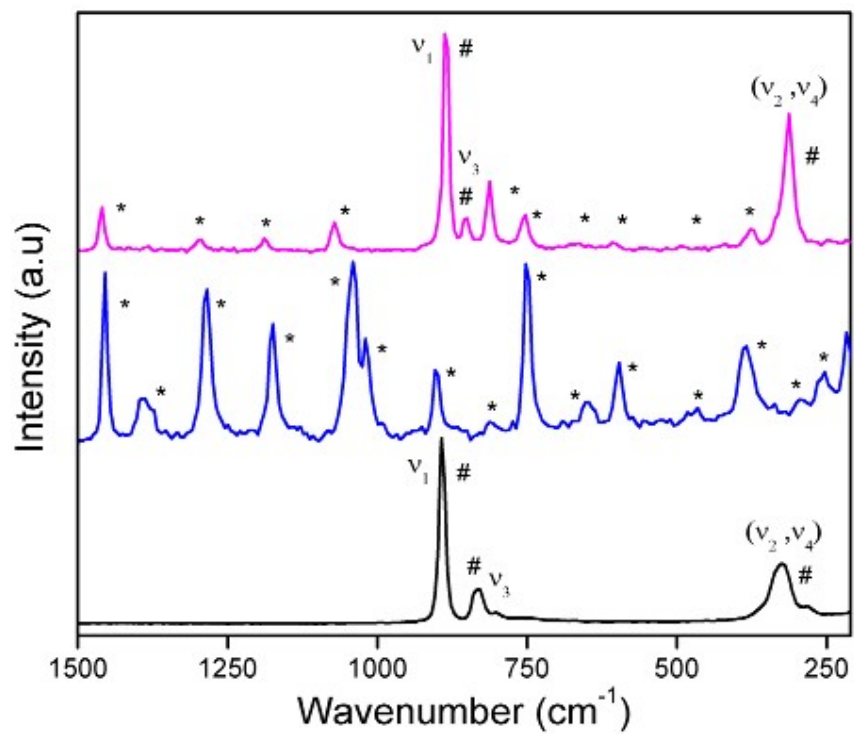
**Fig S5B** H-bonding around (LH<sub>2</sub>)<sup>+</sup> cation showing its linking with six symmetry related (MoO<sub>4</sub>)<sup>2-</sup> anions (**left**) and linking of (LH<sub>2</sub>)<sup>+</sup> cations with (LH<sub>2</sub>)<sup>+</sup> with the aid of C2-H2A...O3 interaction (**right**)



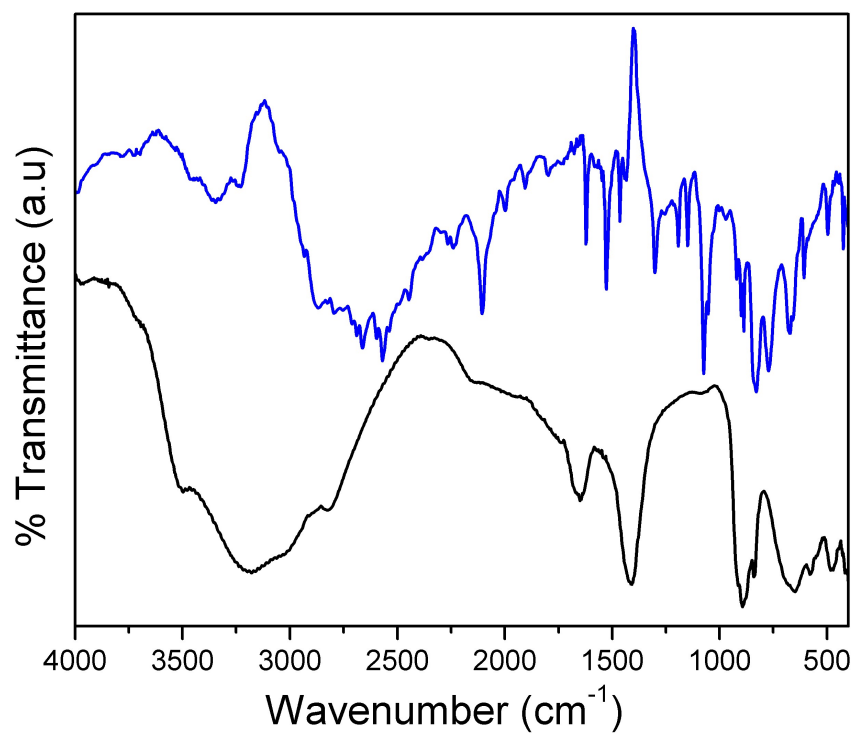
**Fig S6** Raman spectra of  $\text{K}_6[\text{Mo}_7\text{O}_{24}]\cdot 4\text{H}_2\text{O}$  (bottom), reaction mixture (pH ~6) of  $\text{K}_6[\text{Mo}_7\text{O}_{24}]\cdot 4\text{H}_2\text{O}$  and LH (middle) and  $[\text{K}(\text{LH}_2)(\text{MoO}_4)] \mathbf{1}$  (top).



**Fig S7** Raman spectra of  $[\text{K}(\text{LH}_2)(\text{MoO}_4)] \mathbf{1}$  (top) and  $\text{Na}_2\text{MoO}_4\cdot 2\text{H}_2\text{O}$  (bottom). \*bands of  $(\text{LH}_2)^+$  cation.



**Fig S8** Raman spectra of  $[\text{K}(\text{LH}_2)(\text{MoO}_4)] \mathbf{1}$  (top),  $(\text{LH}_2)\text{Cl}$  (middle) and  $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$  (bottom). \* are signals of  $(\text{LH}_2)^+$  cation. # are  $[\text{MoO}_4]^{2-}$  bands.



**Fig S9** IR spectra of  $(\text{NH}_4)_6[\text{Mo}_7\text{O}_{24}] \cdot 4\text{H}_2\text{O}$  (bottom) and  $[\text{K}(\text{LH}_2)(\text{MoO}_4)] \mathbf{1}$  (top).

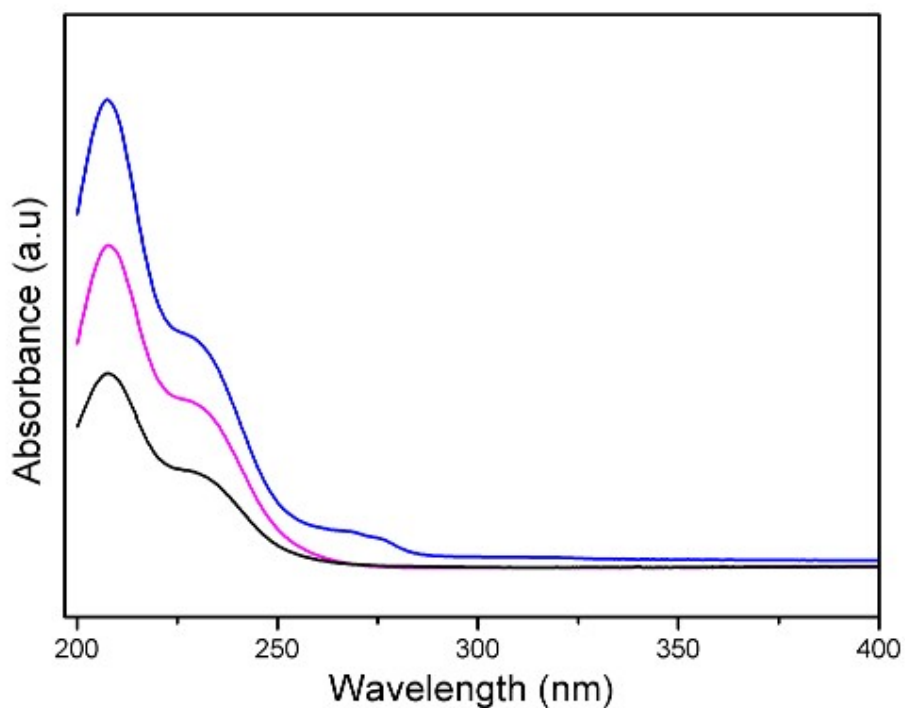


Fig S10 UV-Vis spectra of  $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$  (bottom), **1** (middle) and **2** (top).

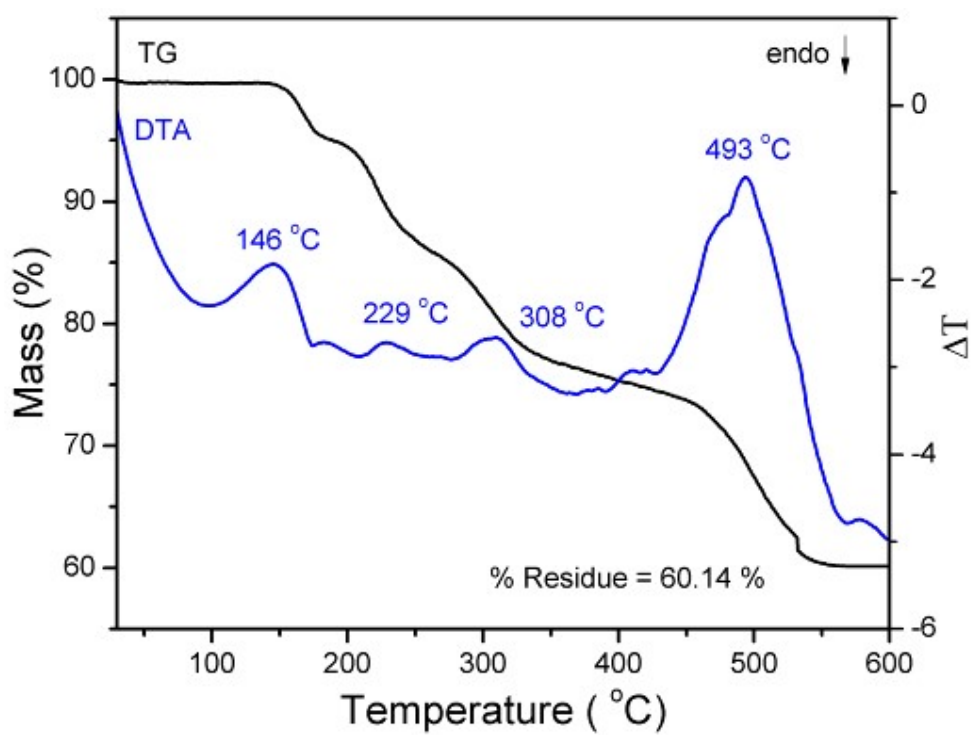
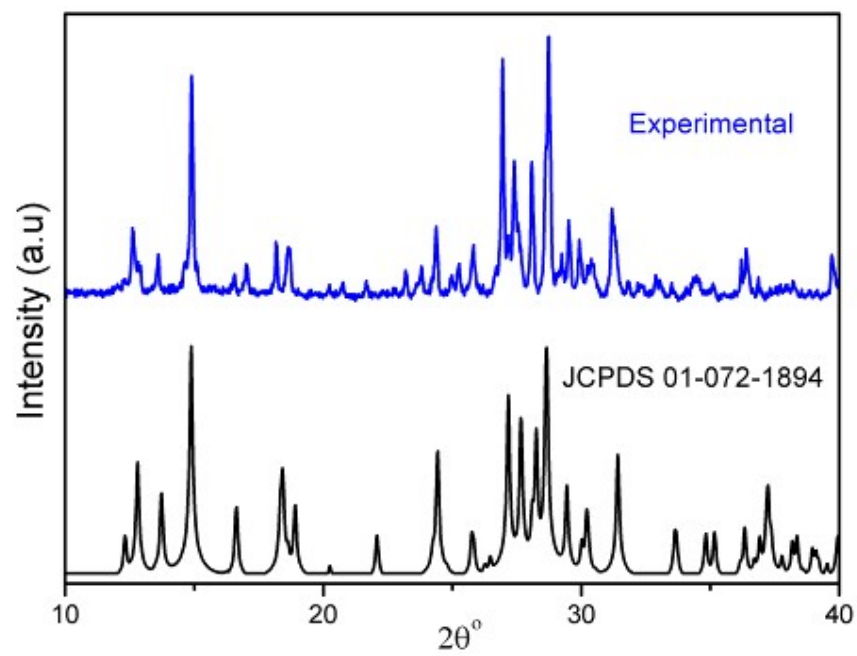


Fig S11 TG-DTA curves of **1**.



**Fig S12** X-ray powder patterns of K<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub> (**bottom**) and of the residue obtained after pyrolysis of [K(LH<sub>2</sub>)(MoO<sub>4</sub>)] **1** (**top**) at 800°C.

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: shelx

---

Bond precision:      C-C = 0.0033 A      Wavelength=0.71073

Cell:                      a=6.9394 (1)              b=6.9394 (1)              c=11.9594 (4)  
                                    alpha=90              beta=90              gamma=120

Temperature:              293 K

	Calculated	Reported
Volume	498.75 (2)	498.75 (2)
Space group	P 3 c 1	P 3 c 1
Hall group	P 3 -2" c	P 3 -2" c
Moiety formula	C4 H12 K Mo N O7	C4 H12 K Mo N O7
Sum formula	C4 H12 K Mo N O7	C4 H12 K Mo N O7
Mr	321.19	321.18
Dx, g cm <sup>-3</sup>	2.139	2.139
Z	2	2
Mu (mm <sup>-1</sup> )	1.745	1.745
F000	320.0	320.0
F000'	317.11	
h, k, lmax	9, 9, 16	9, 9, 16
Nref	954 [ 479]	929
Tmin, Tmax	0.564, 0.700	0.606, 0.746
Tmin'	0.527	

Correction method= # Reported T Limits: Tmin=0.606 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.94/0.97              Theta (max)= 29.576

R(reflections)= 0.0178 ( 906)

wR2(reflections)=  
0.0449 ( 929)

S = 1.309

Npar= 48

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

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● **Alert level C**

ABSTY02\_ALERT\_1\_C An \_exptl\_absorpt\_correction\_type has been given without  
a literature citation. This should be contained in the  
\_exptl\_absorpt\_process\_details field.  
Absorption correction given as MULTI-SCAN

PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	5	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	8	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....	8	Note
PLAT974_ALERT_2_C	Check Calcd Negative Resid. Density on Mol	-1.05	eA-3

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● **Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	3	Report
PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0	0.985	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature .... (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1C Constrained at	0.3333	Check
PLAT780_ALERT_1_G	Coordinates do not Form a Properly Connected Set		Please Do !
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
4 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check
- 
-

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### **Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### **Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

