Supporting Information

Organic-Inorganic Hybrids Assembled by

Bis(undecatungstophosphate) Lanthanates and Dinuclear

Copper(II)–Oxalate Complexes

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Figure S1. ORTEP view of compound 1.

- Figure S2. The coordination environment of La in compound 1.
- **Figure S3.** Schematic illustration of the 3D π - π stacking framework of compound 1.

Figure S4. IR spectra of compounds 1-6.

Figure S5. TG curve of compound 1.

Figure S6. XRPD patterns of compounds 1-3.

Table S1-6. Selected bond lengths (Å) and angles (°) in compounds 1-6.



Figure S1. ORTEP view of compound **1** with thermal ellipsoids at 50% probability; all the potassium cations, lattice water molecules and hydrogen atoms are omitted for clarity. Symmetry transformations used to generate equivalent atoms: #1 1-x, 1-y, -z; #2 1-x, y, 0.5-z.



Figure S2. The coordination environment of La in compound **1**. Color codes: La, orange; O, red. Symmetry transformation used to generate equivalent atoms, which is similar to Figure S1.



Figure S3. Schematic illustration of the 3D π – π stacking framework of compound 1. Color codes: Cu, teal; O, red; N, blue; C, black; fictive atom, white.



Figure S4. IR spectra of compounds 1-6.



Figure S5. TG curve of compound 1. Heating rate: 10 deg min⁻¹, N₂ atmosphere.



Figure S6 (a). XRPD patterns for simulated (blue) and as-synthesized (black) samples of 1.



Figure S6 (b). XRPD patterns for simulated (blue) and as-synthesized (black) samples of 2.



Figure S6 (c). XRPD patterns for simulated (blue) and as-synthesized (black) samples

of **3**.

P(1)-O(2)	1.527(6)	P(1)-O(3)	1.532(7)
P(1)-O(11)	1.537(7)	P(1)-O(6)	1.547(6)
W(1)-O(28)	1.723(7)	W(1)-O(3)	2.457(7)
W(2)-O(35)	1.702(8)	W(2)-O(6)	2.440(7)
W(3)-O(8)	1.713(7)	W(3)-O(3)	2.511(6)
W(4)-O(38)	1.734(6)	W(4)-O(11)	2.465(6)
W(5)-O(17)	1.702(7)	W(5)-O(3)	2.399(6)
W(6)-O(29)	1.722(7)	W(6)-O(2)	2.367(7)
W(7)-O(23)	1.686(7)	W(7)-O(6)	2.439(6)
W(8)-O(26)	1.702(7)	W(8)-O(11)	2.507(6)
W(9)-O(34)	1.726(8)	W(9)-O(2)	2.374(7)
W(10)-O(32)	1.712(7)	W(10)-O(6)	2.423(6)
W(11)-O(33)	1.711(8)	W(11)-O(11)	2.413(7)
La(1)-O(30)	2.467(7)	La(1)-O(15)	2.472(6)
La(1)-O(24)	2.507(7)	La(1)-O(5)	2.513(6)
Cu(1)-N(2)	1.935(9)	Cu(1)-N(1)	1.973(8)
Cu(1)-O(40)	1.989(6)	Cu(1)-O(41)	1.996(6)
Cu(1)-O(8)	2.378(7)	Cu(1)-O(17)	2.548(7)
O(2)-P(1)-O(3)	88.4(3)	O(2)-P(1)-O(11)	111.0(4)
O(3)-P(1)-O(11)	101.8(4)	O(2)-P(1)-O(6)	110.1(4)
O(3)-P(1)-O(6)	71.0(3)	O(28)-W(1)-O(15)	103.7(3)
O(28)-W(1)-O(10)	90.0(3)	O(28)-W(1)-O(3)	164.9(3)
O(10)-W(1)-O(18)	72.2(2)	O(10)-W(1)-O(3)	71.2(2)
O(19)-W(2)-O(25)	105.4(3)	O(35)-W(2)-O(25)	101.5(4)
O(27)-W(2)-O(6)	109.2(4)	O(25)-W(2)-O(36)	156.9(3)
O(8)-W(3)-O(18)	107.7(4)	O(14)-W(3)-O(7)	157.4(3)
O(18)-W(3)-O(14)	103.6(3)	O(14)-W(3)-O(13)	84.9(3)
O(38)-W(4)-O(30)	82.0(3)	O(38)-W(4)-O(11)	163.8(3)
O(39)-W(4)-O(16)	80.6(3)	O(16)-W(4)-O(11)	69.8(2)
O(17)-W(5)-O(21)	102.9(3)	O(21)-W(5)-O(9)	86.8(3)
O(9)-W(5)-O(10)	89.5(3)	O(17)-W(5)-O(3)	170.3(3)
O(29)-W(6)-O(5)	101.4(3)	O(29)-W(6)-O(2)	171.9(3)
O(5)-W(6)-O(1)	163.5(3)	O(31)-W(6)-O(1)	84.3(3)
N(2)-Cu(1)-N(1)	82.0(4)	N(2)-Cu(1)-O(41)	179.0(3)
N(1)-Cu(1)-O(40)	173.4(3)	O(40)- $Cu(1)$ - $O(41)$	84.5(3)
N(1)-Cu(1)-O(41)	97.6(3)	N(1)-Cu(1)-O(8)	92.4(3)
O(40)-Cu(1)-O(8)	94.0(3)	O(41)-Cu(1)-O(8)	88.3(3)
O(30)-La(1)-O(30)#1	83.0(3)	O(30)-La(1)-O(15)	70.1(2)
O(30)-La(1)-O(5)	113.5(2)	O(15)-La(1)-O(15)#1	136.0(3)
O(24)-La(1)-O(5)	73.1(2)	O(30)-La(1)-O(24)	73.0(2)
O(24)#1-La(1)-O(24)	136.7(3)	O(15)-La(1)-O(5)	73.3(2)

Table S1. Selected bond lengths (Å) and angles (°) in compound 1^a .

^a Symmetry transformations used to generate equivalent atoms: #1 1-x, y, 0.5-z.

P(1)-O(19)	1.509(8)	P(1)-O(33)	1.518(8)
P(1)-O(23)	1.520(9)	P(1)-O(30)	1.546(9)
W(1)-O(6)	1.702(9)	W(1)-O(23)	2.452(7)
W(2)-O(13)	1.697(9)	W(2)-O(19)	2.361(8)
W(3)-O(11)	1.701(9)	W(3)-O(23)	2.411(8)
W(4)-O(4)	1.699(9)	W(4)-O(30)	2.443(8)
W(5)-O(8)	1.704(8)	W(5)-O(23)	2.506(7)
W(6)-O(1)	1.704(9)	W(6)-O(19)	2.359(8)
W(7)-O(29)	1.709(9)	W(7)-O(33)	2.447(9)
W(8)-O(25)	1.693(9)	W(8)-O(30)	2.490(7)
W(9)-O(35)	1.712(8)	W(9)-O(33)	2.407(7)
W(10)-O(2)	1.700(11)	W(10)-O(30)	2.419(9)
W(11)-O(17)	1.715(10)	W(11)-O(33)	2.455(9)
Pr(1)-O(41)	2.430(9)	Pr(1)-O(20)	2.473(8)
Pr(1)-O(18)	2.477(9)	Pr(1)-O(22)	2.438(8)
Cu(1)-N(2)	1.946(10)	Cu(1)-N(1)	1.961(9)
Cu(1)-O(40)	1.965(8)	Cu(1)-O(39)	1.979(8)
Cu(1)-O(8)	2.379(8)	Cu(1)-O(11)	2.564(8)
O(19)-P(1)-O(33)	111.9(5)	O(19)-P(1)-O(23)	110.6(5)
O(33)-P(1)-O(23)	107.2(5)	O(19)-P(1)-O(30)	110.5(4)
O(33)-P(1)-O(30)	109.0(5)	O(23)-P(1)-O(30)	107.4(5)
O(6)-W(1)-O(22)	103.6(4)	O(22)-W(1)-O(5)	93.1(4)
O(7)-W(1)-O(23)	70.6(3)	O(6)-W(1)-O(23)	165.7(3)
O(13)-W(2)-O(20)	101.8(4)	O(15)-W(2)-O(19)	72.8(3)
O(13)-W(2)-O(19)	171.0(4)	O(20)-W(2)-O(28)	163.5(4)
O(11)-W(3)-O(12)	101.5(4)	O(9)-W(3)-O(23)	73.4(3)
O(21)-W(3)-O(9)	89.0(3)	O(21)-W(3)-O(10)	156.9(4)
O(4)-W(4)-O(41)	105.5(4)	O(32)-W(4)-O(30)	69.5(3)
O(4)-W(4)-O(32)	96.0(4)	O(4)-W(4)-O(30)	163.5(4)
O(8)-W(5)-O(7)	103.0(4)	O(7)-W(5)-O(23)	72.4(3)
O(7)-W(5)-O(24)	89.7(4)	O(8)-W(5)-O(23)	172.1(4)
O(18)-W(6)-O(27)	92.9(4)	O(15)-W(6)-O(19)	72.4(3)
O(1)-W(6)-O(16)	95.6(4)	O(1)-W(6)-O(19)	172.0(4)
N(2)-Cu(1)-N(1)	82.5(4)	N(2)-Cu(1)-O(40)	174.1(4)
N(1)-Cu(1)-O(40)	95.9(4)	N(2)-Cu(1)-O(39)	97.5(4)
N(1)-Cu(1)-O(39)	179.2(4)	O(40)-Cu(1)-O(39)	84.0(3)
N(2)-Cu(1)-O(8)	92.4(4)	N(1)-Cu(1)-O(8)	92.3(4)
O(40)-Cu(1)-O(8)	93.3(3)	O(39)-Cu(1)-O(8)	88.5(3)
O(41)#1-Pr(1)-O(41)	82.3(4)	O(41)-Pr(1)-O(22)	70.7(3)
O(20)-Pr(1)-O(20)#1	81.1(3)	O(20)-Pr(1)-O(18)	74.1(3)

Table S2. Selected bond lengths (Å) and angles (°) in compound 2^a .

O(18)-Pr(1)-O(18)#1 137.0(4) O(22)-Pr(1)-O(18) 114.2(3) ^{*a*} Symmetry transformations used to generate equivalent atoms: #1 2-x, y, 0.5-z.

1.516(8) 1.526(7) 1.694(8) 1.707(9) 1.706(10) 1.691(7) 1.699(8) 1.728(8) 1.700(8)	P(1)-O(32) P(1)-O(36) W(1)-O(13) W(2)-O(32) W(3)-O(32) W(4)-O(38) W(5)-O(38) W(6)-O(36)	1.537(8) 1.544(8) 2.346(8) 2.410(8) 2.450(8) 2.431(7) 2.458(8)
1.526(7) 1.694(8) 1.707(9) 1.706(10) 1.691(7) 1.699(8) 1.728(8) 1.700(8)	P(1)-O(36) W(1)-O(13) W(2)-O(32) W(3)-O(32) W(4)-O(38) W(5)-O(38) W(6)-O(36)	1.544(8) 2.346(8) 2.410(8) 2.450(8) 2.431(7) 2.458(8)
1.694(8) 1.707(9) 1.706(10) 1.691(7) 1.699(8) 1.728(8) 1.700(8)	W(1)-O(13) W(2)-O(32) W(3)-O(32) W(4)-O(38) W(5)-O(38) W(6)-O(36)	2.346(8) 2.410(8) 2.450(8) 2.431(7) 2.458(8)
1.707(9) 1.706(10) 1.691(7) 1.699(8) 1.728(8) 1.700(8)	W(2)-O(32) W(3)-O(32) W(4)-O(38) W(5)-O(38) W(6)-O(36)	2.410(8) 2.450(8) 2.431(7) 2.458(8)
1.706(10) 1.691(7) 1.699(8) 1.728(8) 1.700(8)	W(3)-O(32) W(4)-O(38) W(5)-O(38) W(6)-O(36)	2.450(8) 2.431(7) 2.458(8)
1.691(7) 1.699(8) 1.728(8) 1.700(8)	W(4)-O(38) W(5)-O(38) W(6)-O(36)	2.431(7) 2.458(8)
1.699(8) 1.728(8) 1.700(8)	W(5)-O(38) W(6)-O(36)	2.458(8)
1.728(8) 1.700(8)	W(6)-O(36)	
1.700(8)		2.468(8)
1 = 2 = (=)	W(7)-O(36)	2.486(7)
1.735(7)	W(8)-O(38)	2.489(7)
1.708(9)	W(9)-O(36)	2.405(8)
1.724(8)	W(10)-O(32)	2.431(7)
1.705(8)	W(11)-O(13)	2.370(7)
1.933(10)	Cu(14)-N(2)	1.970(10)
1.991(8)	Cu(14)-O(41)	1.992(8)
2.380(7)	Cu(14)-O(34)	2.561(7)
2.390(7)	Eu(1)-O(15)	2.401(8)
2.419(7)	Eu(1)-O(14)	2.436(9)
110.3(5)	O(38)-P(1)-O(36)	108.7(4)
107.7(4)	O(13)-P(1)-O(36)	111.0(4)
110.4(4)	O(32)-P(1)-O(36)	108.6(5)
73.4(3)	O(29)-W(1)-O(24)	92.9(3)
94.8(4)	O(28)-W(1)-O(13)	172.3(4)
72.7(3)	O(1)-W(2)-O(3)	104.8(4)
88.2(4)	O(1)-W(2)-O(32)	170.8(4)
71.6(3)	O(6)-W(3)-O(10)	104.6(4)
91.5(4)	O(6)-W(3)-O(32)	169.9(4)
72.6(3)	O(33)-W(4)-O(30)	88.8(3)
103.5(3)	O(34)-W(4)-O(38)	171.0(3)
70.3(3)	O(17)-W(5)-O(30)	99.8(4)
84.1(3)	O(17)-W(5)-O(38)	164.7(3)
69.8(3)	O(15)-W(6)-O(35)	92.7(4)
99.4(4)	O(23)-W(6)-O(36)	163.9(4)
81.7(5)	O(40)-Cu(14)-O(41)	85.5(3)
177.9(4)	N(1)-Cu(14)-O(19)	94.2(4)
96.6(4)	N(2)-Cu(14)-O(19)	92.7(3)
96.1(4)	O(40)-Cu(14)-O(19)	87.1(3)
171.8(4)	O(41)-Cu(14)-O(19)	95.4(3)
135 8(3)	O(16)-Eu(1)-O(15)	71 5(3)
	1.700(3) $1.735(7)$ $1.708(9)$ $1.724(8)$ $1.705(8)$ $1.933(10)$ $1.991(8)$ $2.380(7)$ $2.390(7)$ $2.419(7)$ $110.3(5)$ $107.7(4)$ $110.4(4)$ $73.4(3)$ $94.8(4)$ $72.7(3)$ $88.2(4)$ $71.6(3)$ $91.5(4)$ $72.6(3)$ $103.5(3)$ $70.3(3)$ $84.1(3)$ $69.8(3)$ $99.4(4)$ $81.7(5)$ $177.9(4)$ $96.6(4)$ $96.1(4)$ $171.8(4)$ $135.8(3)$	1.700(6) $W(7)-O(30)$ $1.735(7)$ $W(8)-O(38)$ $1.708(9)$ $W(9)-O(36)$ $1.705(8)$ $W(11)-O(13)$ $1.933(10)$ $Cu(14)-N(2)$ $1.991(8)$ $Cu(14)-O(41)$ $2.380(7)$ $Cu(14)-O(34)$ $2.390(7)$ $Eu(1)-O(15)$ $2.419(7)$ $Eu(1)-O(14)$ $110.3(5)$ $O(38)-P(1)-O(36)$ $107.7(4)$ $O(13)-P(1)-O(36)$ $107.7(4)$ $O(13)-P(1)-O(36)$ $110.4(4)$ $O(22)-W(1)-O(24)$ $94.8(4)$ $O(28)-W(1)-O(13)$ $72.7(3)$ $O(1)-W(2)-O(32)$ $71.6(3)$ $O(6)-W(3)-O(10)$ $91.5(4)$ $O(6)-W(3)-O(10)$ $91.5(4)$ $O(6)-W(3)-O(32)$ $72.6(3)$ $O(33)-W(4)-O(38)$ $70.3(3)$ $O(17)-W(5)-O(38)$ $69.8(3)$ $O(15)-W(6)-O(35)$ $99.4(4)$ $O(23)-W(6)-O(36)$ $81.7(5)$ $O(40)-Cu(14)-O(19)$ $96.6(4)$ $N(2)-Cu(14)-O(19)$ $96.1(4)$ $O(41)-Cu(14)-O(19)$ $171.8(4)$ $O(41)-Cu(14)-O(19)$

Table S3. Selected bond lengths (Å) and angles (°) in compound $\mathbf{3}^{a}$.

O(16)-Eu(1)-O(29)	73.9(2)	O(15)-Eu(1)-O(15)#1	81.0(4)
O(15)-Eu(1)-O(29)	115.1(3)	O(14)#1-Eu(1)-O(14)	136.7(4)

^a Symmetry transformations used to generate equivalent atoms: #1 1-x, y, 1.5-z.

Table S4. Selected bond lengths (Å) and angles (°) in compound 4^a .

P(1)-O(12)	1.517(11)	P(1)-O(7)	1.553(10)
P(1)-O(11)	1.533(10)	P(1)-O(22)	1.562(11)
W(1)-O(32)	1.720(12)	W(1)-O(12)	2.466(10)
W(2)-O(28)	1.710(11)	W(2)-O(11)	2.347(10)
W(3)-O(29)	1.734(10)	W(3)-O(22)	2.477(10)
W(4)-O(25)	1.740(10)	W(4)-O(12)	2.478(9)
W(5)-O(26)	1.708(11)	W(5)-K(1)	3.939(5)
W(6)-O(30)	1.723(11)	W(6)-O(7)	2.433(10)
W(7)-O(34)	1.692(12)	W(7)-O(11)	2.350(10)
W(8)-O(15)	1.695(11)	W(8)-O(22)	2.494(9)
W(9)-O(33)	1.720(14)	W(9)-O(22)	2.370(11)
W(10)-O(35)	1.712(10)	W(10)-O(7)	2.396(9)
W(11)-O(36)	1.682(15)	W(11)-O(7)	2.436(11)
Cu(14)-N(2)	1.942(13)	Cu(14)-O(41)	2.000(10)
Cu(14)-N(1)	1.963(12)	Cu(14)-O(25)	2.353(10)
Cu(14)-O(40)	1.984(10)	Cu(14)-O(26)	2.579(10)
Gd(1)-O(17)	2.378(9)	Gd(1)-O(16)	2.413(9)
Gd(1)-O(20)	2.381(9)	Gd(1)-O(27)	2.431(10)
O(12)-P(1)-O(11)	111.3(6)	O(12)-P(1)-O(22)	108.6(6)
O(12)-P(1)-O(7)	108.4(6)	O(11)-P(1)-O(22)	110.5(6)
O(11)-P(1)-O(7)	110.3(6)	O(7)-P(1)-O(22)	107.7(6)
O(2)-W(1)-O(12)	69.7(4)	O(32)-W(1)-O(20)	103.1(5)
O(20)-W(1)-O(14)	94.3(5)	O(32)-W(1)-O(12)	165.5(5)
O(1)-W(2)-O(11)	80.0(4)	O(28)-W(2)-O(1)	95.1(4)
O(28)-W(2)-O(4)	102.6(5)	O(28)-W(2)-O(11)	170.3(5)
O(21)-W(3)-O(22)	70.4(4)	O(29)-W(3)-O(21)	95.7(5)
O(29)-W(3)-O(14)	101.6(5)	O(29)-W(3)-O(22)	163.9(5)
O(2)-W(4)-O(12)	73.1(4)	O(2)-W(4)-O(10)	87.5(5)
O(25)-W(4)-O(2)	102.4(5)	O(25)-W(4)-O(12)	172.1(5)
O(5)-W(5)-O(12)	73.3(4)	O(26)-W(5)-O(10)	100.2(5)
O(4)-W(5)-O(5)	87.6(4)	O(26)-W(5)-O(12)	170.4(5)
O(39)-W(6)-O(7)	71.3(4)	O(1)-W(6)-O(23)	90.8(5)
O(30)-W(6)-O(39)	101.1(5)	O(30)-W(6)-O(7)	170.7(5)
N(2)-Cu(14)-N(1)	81.4(6)	O(40)-Cu(14)-O(41)	85.4(4)
N(2)-Cu(14)-O(40)	96.1(5)	N(2)-Cu(14)-O(25)	93.8(5)
N(1)-Cu(14)-O(40)	172.4(5)	N(1)-Cu(14)-O(25)	92.5(5)
N(2)-Cu(14)-O(41)	178.3(5)	O(40)-Cu(14)-O(25)	94.8(4)
N(1)-Cu(14)-O(41)	97.0(5)	O(41)-Cu(14)-O(25)	87.0(5)

O(17)-Gd(1)-O(20)	71.8(3)	O(20)-Gd(1)-O(20)#1	134.8(5)
O(17)-Gd(1)-O(16)	115.2(3)	O(17)-Gd(1)-O(27)	73.7(4)
O(16)-Gd(1)-O(27)	73.4(4)	O(27)#1-Gd(1)-O(27)	137.2(5)
^a Symmetry transformations used to generate equivalent atoms: #1 1-x, y, 1.5-z.			

Table S5. Selected bond lengths (Å) and angles (°) in compound 5^a .

P(1)-O(40)	1.516(7)	P(1)-O(39)	1.538(7)
P(1)-O(22)	1.518(7)	P(1)-O(33)	1.547(7)
W(1)-O(18)	1.688(7)	W(1)-O(40)	2.441(7)
W(2)-O(27)	1.720(7)	W(2)-O(22)	2.344(6)
W(3)-O(10)	1.707(6)	W(3)-O(40)	2.478(6)
W(4)-O(31)	1.698(7)	W(4)-O(33)	2.433(6)
W(5)-O(3)	1.733(7)	W(5)-O(22)	2.348(6)
W(6)-O(36)	1.714(7)	W(6)-O(39)	2.441(7)
W(7)-O(30)	1.698(7)	W(7)-O(33)	2.485(7)
W(8)-O(17)	1.702(7)	W(8)-O(40)	2.445(6)
W(9)-O(4)	1.701(7)	W(9)-O(33)	2.430(7)
W(10)-O(5)	1.710(8)	W(10)-O(39)	2.444(7)
W(11)-O(7)	1.698(7)	W(11)-O(39)	2.393(7)
Cu(14)-N(1)	1.940(9)	Cu(14)-N(2)	1.989(9)
Cu(14)-O(11)	1.966(7)	Cu(14)-O(10)	2.392(7)
Cu(14)-O(12)	1.988(8)	Cu(14)-O(17)	2.596(7)
Yb(8)-O(21)	2.326(7)	Yb(8)-O(1)	2.331(7)
Yb(8)-O(19)	2.338(6)	Yb(8)-O(2)	2.350(7)
O(40)-P(1)-O(22)	111.0(4)	O(40)-P(1)-O(33)	107.3(4)
O(40)-P(1)-O(39)	108.8(4)	O(22)-P(1)-O(33)	110.2(4)
O(22)-P(1)-O(39)	110.3(4)	O(39)-P(1)-O(33)	109.2(4)
O(13)-W(1)-O(40)	70.8(3)	O(38)-W(1)-O(13)	81.0(3)
O(18)-W(1)-O(19)	104.7(3)	O(18)-W(1)-O(40)	165.3(3)
O(26)-W(2)-O(22)	73.3(3)	O(27)-W(2)-O(23)	95.9(3)
O(27)-W(2)-O(22)	172.1(3)	O(1)-W(2)-O(23)	161.2(3)
O(13)-W(3)-O(40)	72.5(3)	O(13)-W(3)-O(29)	90.5(3)
O(10)-W(3)-O(9)	102.7(3)	O(10)-W(3)-O(40)	172.8(3)
O(15)-W(4)-O(33)	69.2(3)	O(34)-W(4)-O(15)	82.5(3)
O(31)-W(4)-O(32)	99.1(3)	O(31)-W(4)-O(33)	164.4(3)
O(26)-W(5)-O(22)	72.7(2)	O(3)-W(5)-O(24)	101.2(3)
O(2)-W(5)-O(26)	95.2(3)	O(3)-W(5)-O(22)	171.6(3)
O(8)-W(6)-O(39)	70.9(3)	O(23)-W(6)-O(37)	90.9(3)
O(36)-W(6)-O(39)	170.7(3)	O(16)-W(6)-O(37)	156.8(3)
N(1)-Cu(14)-O(11)	96.1(4)	O(12)-Cu(14)-N(2)	96.4(4)
N(1)-Cu(14)-O(12)	178.9(3)	N(1)-Cu(14)-O(10)	93.6(3)
O(11)-Cu(14)-O(12)	84.5(3)	O(11)-Cu(14)-O(10)	94.3(3)
N(1)-Cu(14)-N(2)	82.8(4)	O(12)-Cu(14)-O(10)	87.2(3)

O(11)-Cu(14)-N(2)	173.0(3)	N(2)-Cu(14)-O(10)	92.7(3)
O(21)-Yb(8)-O(21)#1	80.4(4)	O(21)-Yb(8)-O(1)	115.5(2)
O(1)#1-Yb(8)-O(1)	80.2(3)	O(21)-Yb(8)-O(19)	71.7(2)
O(1)-Yb(8)-O(19)	74.0(2)	O(19)-Yb(8)-O(19)#1	135.7(3)
	1	1	

^{*a*} Symmetry transformations used to generate equivalent atoms: #1 1-x, y, 0.5-z.

P(1)-O(5) 1.462(13) P(1)-O(12) 1.575(12) P(1)-O(3) 1.495(12)P(1)-O(22) 1.583(12)1.701(13) W(1)-O(5) W(1)-O(15) 2.475(11)W(2)-O(26) 1.729(12)W(2)-O(22) 2.458(10) W(3)-O(27) W(3)-O(32) 1.692(13)1.950(13) W(4)-O(33) 1.704(13)W(4)-O(3)2.378(13)W(5)-O(21) W(5)-O(22) 1.715(13) 2.498(11) W(6)-O(3) W(6)-O(11) 1.712(13)2.346(12)W(7)-O(35) 1.728(14) W(7)-O(22) 2.377(11)W(8)-O(34) 1.722(13)W(8)-O(12) 2.375(11)W(9)-O(14) 1.715(14)W(9)-O(12) 2.423(13)W(10)-O(5) W(10)-O(7) 1.714(14)2.420(12)W(11)-O(41) 1.694(16) W(11)-O(12) 2.441(13)K(1)-O(20) K(1)-O(31) 2.405(13)2.420(12)K(1)-O(16) 2.458(12)K(1)-O(18) 2.480(12)Cu(1)-N(1)Cu(1)-O(2)1.90(2)2.009(14) Cu(1)-O(27) Cu(1)-N(2)1.940(17)2.393(13)Cu(1)-O(1)1.971(12)Cu(1)-O(7)2.560(13)O(5)-P(1)-O(3)O(5)-P(1)-O(22)111.3(7)109.9(7) O(5)-P(1)-O(12) 108.2(7)O(3)-P(1)-O(22) 108.9(7) O(3)-P(1)-O(12) 111.1(7)O(12)-P(1)-O(22) 107.3(7)O(29)-W(1)-O(5) 72.2(5) O(9)-W(1)-O(29)83.3(5) O(15)-W(1)-O(19) 99.2(7) O(15)-W(1)-O(5) 166.0(5)O(10)-W(2)-O(22) 69.5(4) O(26)-W(2)-O(10) 95.0(6) O(9)-W(2)-O(10) 82.8(5) O(26)-W(2)-O(22)163.0(5) O(8)-W(3)-O(6)87.3(6) O(29)-W(3)-O(6)87.9(5) O(27)-W(3)-O(29) 103.4(6) O(6)-W(3)-O(32)157.6(5) 95.9(5) O(18)-W(4)-O(13)O(17)-W(4)-O(3)72.6(5) O(13)-W(4)-O(3) 85.9(5) O(18)-W(4)-O(4)164.2(5)O(36)-W(5)-O(22) 71.3(5) O(32)-W(5)-O(24) 85.6(5) O(32)-W(5)-O(22) 86.4(5) O(21)-W(5)-O(22) 170.3(5) O(11)-W(6)-O(37) O(17)-W(6)-O(3) 73.2(5)93.3(6) O(11)-W(6)-O(17) 99.0(6) O(11)-W(6)-O(3)170.2(6) N(1)-Cu(1)-N(2)81.8(8) O(1)-Cu(1)-O(2)83.9(5) N(1)-Cu(1)-O(1)98.6(7) N(1)-Cu(1)-O(27)91.6(6)

N(2)-Cu(1)-O(1)

179.3(7)

N(2)-Cu(1)-O(27)

90.4(6)

Table S6. Selected bond lengths (Å) and angles (°) in compound 6^a .

N(1)-Cu(1)-O(2)	175.3(6)	O(1)-Cu(1)-O(27)	89.1(5)
N(2)-Cu(1)-O(2)	95.8(6)	O(2)-Cu(1)-O(27)	92.5(5)
O(20)-K(1)-O(20)#1	80.3(6)	O(20)-K(1)-O(31)	74.4(4)
O(31)#1-K(1)-O(31)	136.9(7)	O(31)-K(1)-O(16)	113.6(4)
O(20)-K(1)-O(16)	69.7(4)	O(20)-K(1)-O(18)	114.6(4)
	1		

^a Symmetry transformations used to generate equivalent atoms: #1 -x, y, 1.5-z.