

## **Electronic Supplementary Information**

**For**

**Crystal structures of discrete, one-dimensional and cocrystalline copper(II)–  
uranyl(VI) systems: Influence of the reactant ratio in the competition between  
hydrogen bonds and coordinate bonds**

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## Electronic spectra

The electronic absorption spectra of compounds **1–4** and the corresponding mononuclear copper(II) compounds have been recorded. The compounds **1**, **3** and **4** are insoluble in common organic solvents except N,N-dimethylformamide (dmf) and unstable in the solution of dmf, as evidenced by the deposition of corresponding mononuclear compound from dmf solution. On the other hand, compound **2** is stable in acetonitrile solution. Therefore, while only diffuse reflectance spectra were recorded for **1**, **3** and **4**, both the solid state and solution (in acetonitrile) spectra were recorded for **2**. Spectral data along with some structural parameters are listed in Table S1. The spectra of **4** and the corresponding copper(II) compounds are shown in Fig. S1, while the spectra of other cases are shown in Figs. S2–S4.

It has been already mentioned that a correlation was proposed regarding the d-d band position of copper(II) as the function of shifting of the metal ion from the basal plane.<sup>1</sup> According to this correlation, the more the shifting of copper(II) from the basal plane, the less the energy of d-d transition. Although it was proposed long before, it was kept in darkness. Recently, we have reopened the issue and checked how it could be useful.<sup>2–5</sup> What we have already observed includes: (i) the correlation does not work for the copper(II) compounds derived from different ligands; (ii) the difference of  $\lambda_{\max}$  values of a copper(II)–diamagnetic compound and the corresponding mononuclear copper(II) compound matches well with the relative shifting of copper(II) in the two compounds in some cases, although inconsistency is observed in some other cases. In particular, in the  $\text{Cu}^{\text{II}}\text{U}^{\text{VI}}$  compounds, we have observed good correlation.<sup>3,4</sup> It is relevant therefore to check how much the correlation is valid in the present series of compounds.

As listed in Table S1, the d-d band of  $\{[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{U}^{\text{VI}}\text{O}_2)(\text{NO}_3)]_2[(\text{U}^{\text{VI}}\text{O}_2)_2(\mu\text{-HO})_2(\text{NO}_3)_4]\}_n$  (**4**) and the corresponding mononuclear compound  $[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{H}_2\text{O})]$  appears at 492 and 630 nm, respectively, *i.e.*, the band in **4** is blue shifted by a large 138 nm in comparison to the corresponding mononuclear copper(II) compound. The observation is well in line with the correlation because the copper(II) centre in **4** ( $d_{\text{Cu}} = 0.03 \text{ \AA}$ ) is much well pocketed in the basal plane in comparison to that in  $[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{H}_2\text{O})]$  ( $d_{\text{Cu}} = 0.204 \text{ \AA}$ ).<sup>3</sup> As already mentioned, another copper(II)–uranyl(VI) compound  $\{[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}]_2 \cdot \{(\text{U}^{\text{VI}}\text{O}_2)(\text{NO}_3)_2(\text{H}_2\text{O})_2\}\}$  (**2A**) has been reported previously.<sup>14</sup> Both the  $\lambda_{\max}$  (575 nm; Fig. S1) and  $d_{\text{Cu}}$  (0.087 Å) in **2A** are

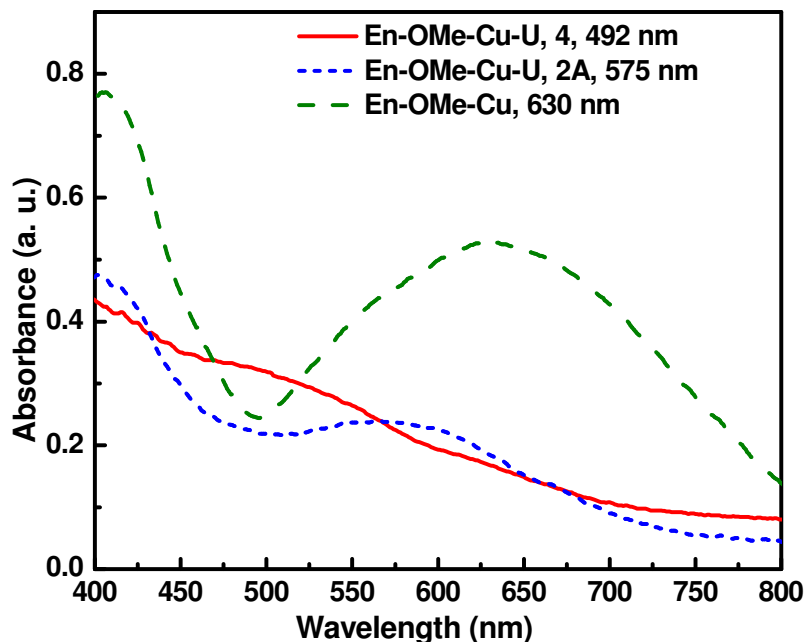
intermediate in comparison to those in  $[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{H}_2\text{O})]$  and **4**. So, the correlation works nicely in these three compounds derived from the same ligand; order of  $\lambda_{\text{max}}$  is  $[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{H}_2\text{O})]$  (630 nm) > **2A** (575 nm) > **4** (492 nm) and the order of  $d_{\text{Cu}}$  is  $[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{H}_2\text{O})]$  (0.204 Å) > **2A** (0.087 Å) > **4** (0.03 Å).

The  $d_{\text{Cu}}$  values of  $[\{\text{Cu}^{\text{II}}\text{L}^{\text{OEt-en}}\}_2\cdot\{\text{U}^{\text{VI}}\text{O}_2(\text{NO}_3)_2(\text{H}_2\text{O})_2\}]$  (**1**;  $d_{\text{Cu}} = 0.029$  Å) and  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-en}}\text{C}(\text{H}_2\text{O})]_6$  ( $d_{\text{Cu}} = 0.00$  Å) are not appreciably different, as are their  $\lambda_{\text{max}}$  values (567 and 565 nm for **1** and the mononuclear, respectively). The  $\lambda_{\text{max}}$  values of  $[(\text{U}^{\text{VI}}\text{O}_2)_2(\mu\text{-H}_2\text{O})_2(\text{NO}_3)_4]\cdot 4[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-py}}(\text{H}_2\text{O})]\cdot 2\text{MeCN}$  (**3**) and  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-py}}(\text{H}_2\text{O})]$  are 474 and 480 nm, respectively. Both the two types of copper(II) centres in **3** are well inside the  $\text{O}_4$  compartment, as evidenced by the small (0.034/0.038 Å)  $d_{\text{Cu}}$  values. On the other hand, it has not been possible to get a diffraction quality single crystal of  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-py}}(\text{H}_2\text{O})]$  and so the comparison of d-d band of **3** with the corresponding mononuclear compound is not possible. Regarding  $[\text{Cu}^{\text{II}}(\text{MeCN})\text{L}^{\text{OEt-pn}}(\text{U}^{\text{VI}}\text{O}_2)(\text{NO}_3)_2]$  (**2**) and the corresponding mononuclear compound  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-pn}}\text{C}(\text{H}_2\text{O})]$  (crystallographic information, selected bond lengths/angles and geometries of the hydrogen bonds of this compound are listed in Tables S2–S4, respectively, while crystal structure of this compound is shown in Fig. S5),<sup>7</sup> the  $d_{\text{Cu}}$  values in the former (0.176 Å) is much greater than in the latter (0.031 Å), revealing that  $\lambda_{\text{max}}$  of **2** should be significantly greater than that in  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-pn}}\text{C}(\text{H}_2\text{O})]$ . However, in contrast to the expectation,  $\lambda_{\text{max}}$  values in diffuse reflectance spectra are practically identical, 674 nm for **2** and 675 nm for  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-pn}}\text{C}(\text{H}_2\text{O})]$ . Even in solution spectra, significant difference of  $\lambda_{\text{max}}$  values does not occur;  $\lambda_{\text{max}}$  of **2** (625 nm) is greater by only 10 nm than that of  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-pn}}\text{C}(\text{H}_2\text{O})]$  (615 nm).

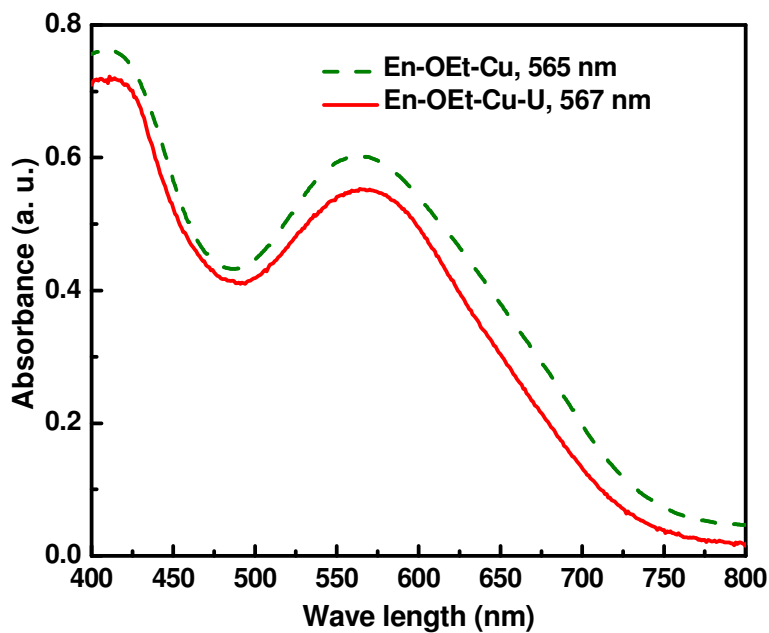
**Table S1** The comparison of the d-d band position and the displacement of the copper(II) centres from their least-squares N(imine)<sub>2</sub>O(phenoxo)<sub>2</sub> basal plane in **1–4** and the corresponding mononuclear systems

Compounds	$\lambda_{\max}$ /nm	$\Delta\lambda_{\max}^a$ /nm	$d_{\text{Cu}}/\text{\AA}$
$[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-en}}\text{C}(\text{H}_2\text{O})]^b$	565	----	0.00
$[\{\text{Cu}^{\text{II}}\text{L}^{\text{OEt-en}}\}_2 \cdot \{(\text{U}^{\text{VI}}\text{O}_2)(\text{NO}_3)_2(\text{H}_2\text{O})_2\}]$ ( <b>1</b> )	567	2	0.029
$[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-pn}}\text{C}(\text{H}_2\text{O})]^c$	615	----	0.031
$[\text{Cu}^{\text{II}}(\text{MeCN})\text{L}^{\text{OEt-pn}}(\text{U}^{\text{VI}}\text{O}_2)(\text{NO}_3)_2]$ ( <b>2</b> )	625	10	0.176
$[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-py}}(\text{H}_2\text{O})]$	480	----	----
$[(\text{U}^{\text{VI}}\text{O}_2)_2(\mu\text{-H}_2\text{O})_2(\text{NO}_3)_4] \cdot$ $4[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-py}}(\text{H}_2\text{O})] \cdot 2\text{MeCN}$ ( <b>3</b> )	474	6	0.038 (Cu1) 0.034 (Cu2)
$[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{H}_2\text{O})]$	630	----	0.204
$\{[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{U}^{\text{VI}}\text{O}_2)(\text{NO}_3)]_2$ $\cdot [(\text{U}^{\text{VI}}\text{O}_2)_2(\mu\text{-HO})_2(\text{NO}_3)_4]\}_n$ ( <b>4</b> )	492	138	0.030
$[\{\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}\}_2 \cdot \{(\text{U}^{\text{VI}}\text{O}_2)(\text{NO}_3)_2(\text{H}_2\text{O})_2\}]^d$ ( <b>2A</b> )	575	55	0.087

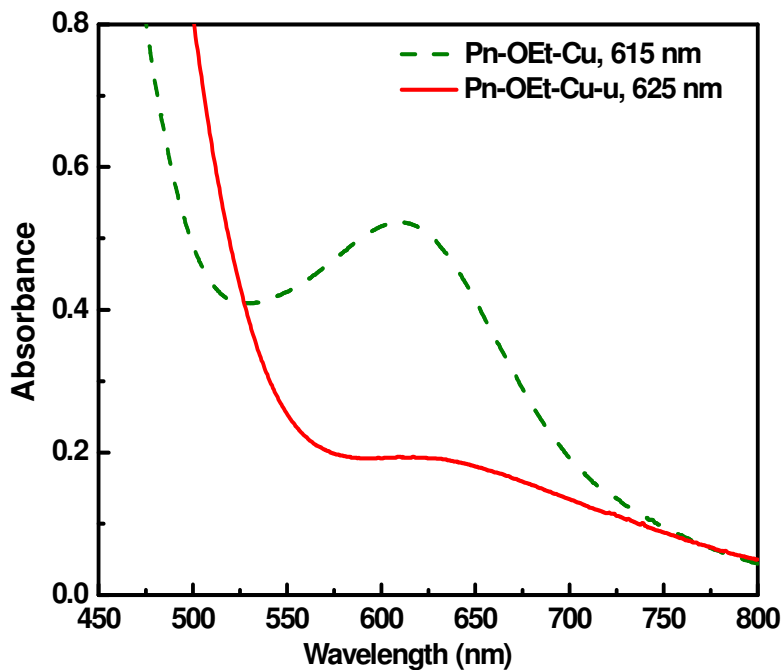
<sup>a</sup>Shifting amount of the copper(II) d-d band in **1–4** in comparison to that in  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-en/OEt-pn/OEt-py/OMe-en}}(\text{H}_2\text{O})]$ . <sup>b</sup>Ref 6. <sup>c</sup>Ref 7. <sup>d</sup>Ref 3.



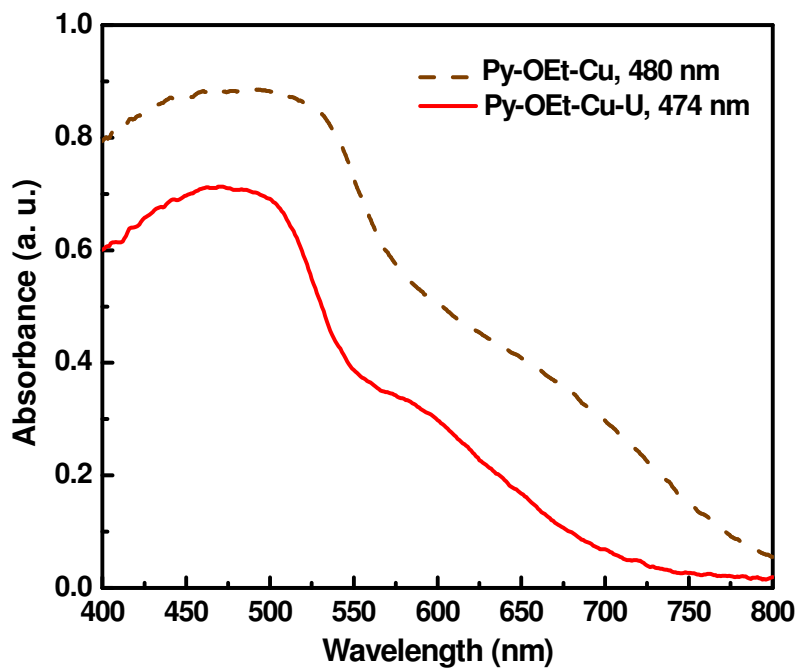
**Fig. S1** Diffuse reflectance spectra, in the range of 400–800 nm, of compound **4**, **2A** and the corresponding mononuclear copper(II) compound,  $[\text{Cu}^{\text{II}}\text{L}^{\text{OMe-en}}(\text{H}_2\text{O})]$ .



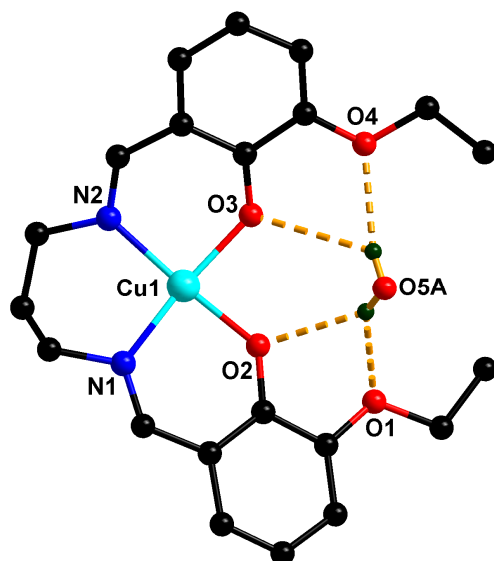
**Fig. S2** Diffuse reflectance spectra, in the range of 400–800 nm, of compound **1** and the corresponding mononuclear copper(II) compound,  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-en}}(\text{H}_2\text{O})]$ .



**Fig. S3** Electronic spectra of compound **2** and the corresponding mononuclear copper(II) compound,  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-pn}}(\text{H}_2\text{O})]$  in  $2 \times 10^{-3}$  (M) acetonitrile solution in the range of 450–800 nm.



**Fig. S4** Diffuse reflectance spectra, in the range of 400–800 nm, of compound **3** and the corresponding mononuclear copper(II) compound,  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-py}}(\text{H}_2\text{O})]$ .



**Fig. S5** Crystal structure of  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-pn}}\text{C}(\text{H}_2\text{O})]$ . All the hydrogen atoms except those of encapsulated water are omitted for clarity. Symmetry code: A,  $1 - x, -0.5 + y, 1.5 - z$ .

**Table S2** Crystallographic data for [Cu<sup>II</sup>L<sup>OEt-pn</sup>·(H<sub>2</sub>O)]

	[Cu <sup>II</sup> L <sup>OEt-pn</sup> ·(H <sub>2</sub> O)]
Formula	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub> Cu
Fw	449.98
Crystal color	Green
Crystal system	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>a</i> /Å	12.4930(17)
<i>b</i> /Å	10.3764(14)
<i>c</i> /Å	18.9139(18)
<i>α</i> /°	90.00
<i>β</i> /°	121.136(6)
<i>γ</i> /°	90.00
<i>V</i> /Å <sup>3</sup>	2098.6(4)
<i>Z</i>	4
<i>T</i> /K	296(2)
2 <i>θ</i> /°	3.80–50.34
<i>μ</i> /mm <sup>-1</sup>	1.075
<i>D</i> <sub>calcd</sub> /g cm <sup>-3</sup>	1.424
<i>F</i> (000)	940
absorption-correction	Multi-scan
index ranges	– 13 ≤ <i>h</i> ≤ 14 – 12 ≤ <i>k</i> ≤ 12 – 22 ≤ <i>l</i> ≤ 22
reflections collected	14318
independent reflections ( <i>R</i> <sub>int</sub> )	3762(0.0617)
<i>R</i> <sub>1</sub> <sup>b</sup> , <i>wR</i> <sub>2</sub> <sup>c</sup> ( <i>I</i> > 2σ( <i>I</i> ))	0.0448/0.0997
<i>R</i> <sub>1</sub> <sup>b</sup> , <i>wR</i> <sub>2</sub> <sup>c</sup> (for all <i>F</i> <sub>o</sub> <sup>2</sup> )	0.0729/0.1117

$${}^a R_1 = [\sum ||F_o| - |F_c|| / \sum |F_o|]. \quad {}^b wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum wF_o^4]^{1/2}.$$



**Table S3** Bond lengths (Å) and bond angles (°) in the coordination environments of the copper(II) in compound [Cu<sup>II</sup>L<sup>OEt-pn</sup>·(H<sub>2</sub>O)]

Bond lengths		Bond angles	
Cu1–N1	1.963(3)	O3–Cu1–N1	169.89(11)
Cu1–N2	1.971(3)	O2–Cu1–N2	166.42(11)
Cu1–O2	1.912(2)	O2–Cu1–N1	91.61(11)
Cu1–O3	1.918(2)	O2–Cu1–O3	84.61(9)
		N2–Cu1–O3	91.22(11)
		N1–Cu1–N2	94.50(12)

**Table S4** The geometries (bond lengths in Å and bond angles in °) of the hydrogen bonds in [Cu<sup>II</sup>L<sup>OEt-pn</sup>·(H<sub>2</sub>O)]. Symmetry code: A, 1 – x, – 0.5 + y, 1.5 – z

D–H···A	D···A	H···A	D–H···A
O5A–H5AA···O1	2.966	2.271	146.95
O5A–H5AA···O2	3.021	2.345	143.97
O5A–H5BA···O3	3.153	2.655	124.68
O5A–H5BA···O4	2.929	2.182	166.01

**Table S5** Bond lengths (Å) and bond angles (°) of the coordination environments in **1**.  
Symmetry code is as in caption of Fig. 1

Bond lengths		Bond angles	
Cu1–N1	1.940(3)	N1–Cu1–O3	172.91(14)
Cu1–N2	1.939(3)	N2–Cu1–O2	169.74(14)
Cu1–O2	1.910(3)	N1–Cu1–O2	93.09(13)
Cu1–O3	1.916(3)	N2–Cu1–O3	93.06(13)
		N1–Cu1–N2	84.40(15)
		O2–Cu1–O3	90.54(11)
U1–O5	2.527(3)	O5–U1–O5A	179.999(1)
U1–O7	2.501(3)	O7–U1–O7A	179.999(1)
U1–O8	1.757(3)	O8–U1–O8A	180.0
U1–O9	2.410(3)	O9–U1–O9A	180.0
		O5–U1–O7	49.98(12)
		O5–U1–O7A	130.02(12)
		O5–U1–O8	93.33(14)
		O5–U1–O8A	86.67(14)
		O5–U1–O9	66.08(12)
		O5–U1–O9A	113.92(12)
		O7–U1–O8	86.41(15)
		O7–U1–O8A	93.59(15)
		O7–U1–O9	115.13(12)
		O7–U1–O9A	64.87(12)
		O8–U1–O9	87.56(13)
		O8–U1–O9A	92.44(13)

**Table S6** Bond lengths (Å) and bond angles (°) of the coordination environments in **2**.  
Symmetry code is as in caption of Fig. 2

Bond lengths		Bond angles	
Cu1–N1	1.973(4)	N1A–Cu1–O2	166.19(17)
Cu1–N2	2.392(8)	O2A–Cu1–O2	78.59(19)
Cu1–O2	1.968(3)	O2–Cu1–N1	91.29(16)
		N1–Cu1–N1A	97.0(3)
Cu1…U1	3.3025(8)	N2–Cu1–O2	97.62(19)
		N1–Cu1–N2	93.0(2)
		Cu1–O2–U1	96.69(13)
U1–O2	2.432(3)	O7–U1–O6	174.2(2)
U1–O3	2.514(4)	O2–U1–O5	174.13(12)
U1–O5	2.530(4)	O3–U1–O3A	159.6(2)
U1–O6	1.773(6)	O7–U1–O2	98.59(17)
U1–O7	1.737(5)	O6–U1–O2	86.34(18)
		O2–U1–O2A	61.66(15)
		O3–U1–O7	92.55(10)
		O3–U1–O6	86.47(10)
		O3–U1–O2A	68.53(12)
		O2–U1–O3	130.00(12)
		O5–U1–O7	87.24(19)
		O6–U1–O5	87.80(19)
		O2–U1–O5A	118.33(13)
		O3–U1–O5A	110.74(13)
		O3–U1–O5	49.84(13)
		O5–U1–O5A	61.01(18)

**Table S7** Bond lengths (Å) and bond angles (°) of the coordination environments in **3**.  
 Symmetry code is as in caption of Fig. 3

Bond lengths		Bond angles	
Cu1–N1	1.937(5)	N1–Cu1–O3	177.2(2)
Cu1–N3	1.947(5)	N3–Cu1–O2	174.57(19)
Cu1–O2	1.911(4)	N3–Cu1–O3	93.06(19)
Cu1–O3	1.916(4)	N1–Cu1–N3	84.2(2)
		N1–Cu1–O2	92.60(19)
		O2–Cu1–O3	90.16(17)
Cu2–N4	1.941(5)	N6–Cu2–O7	177.18(18)
Cu2–N6	1.956(5)	N4–Cu2–O8	174.7(2)
Cu2–O7	1.924(4)	N4–Cu2–O7	92.86(19)
Cu2–O8	1.918(4)	N6–Cu2–N4	84.3(2)
		O8–Cu2–O7	90.60(16)
		N6–Cu2–O8	92.2(2)
U1–O11	2.554(5)	O18–U1–O17	176.3(2)
U1–O12	2.549(5)	O12–U1–O19A	176.41(19)
U1–O14	2.520(5)	O19–U1–O15	179.23(18)
U1–O15	2.558(5)	O14–U1–O11	161.24(18)
U1–O17	1.749(5)	O18–U1–O19A	91.2(2)
U1–O18	1.746(5)	O17–U1–O19A	92.2(2)
U1–O19	2.346(4)	O19–U1–O18	89.6(2)
U1–O19A	2.334(5)	O19–U1–O17	93.1(2)
U1···U1A	3.9453(7)	O19–U1–O19A	65.1(2)
		O14–U1–O18	88.8(2)
		O17–U1–O14	91.2(2)
		O14–U1–O19A	66.05(17)
		O14–U1–O19	131.08(18)
		O12–U1–O18	85.9(2)
		O17–U1–O12	90.7(2)
		O12–U1–O19	116.95(18)
		O12–U1–O14	111.69(18)
		O18–U1–O11	90.4(2)
		O17–U1–O11	88.4(2)
		O19–U1–O11A	132.71(16)
		O19–U1–O11	67.65(17)
		O12–U1–O11	49.57(17)
		O18–U1–O15	90.4(2)
		O17–U1–O15	86.8(2)
		O19–U1–O15A	115.66(18)
		O14–U1–O15	49.70(18)
		O12–U1–O15	62.29(19)
		O11–U1–O15	111.58(18)
		U1–O19–U1A	114.9(2)

**Table S8** Bond lengths (Å) and bond angles (°) in the coordination environment of **4**. Symmetry code is as in caption of Fig. 4

CuU unit				U <sub>2</sub> unit							
Bond lengths		Bond angles		Bond lengths		Bond angles		Bond lengths		Bond angles	
Cu1–N1	1.902(9)	N1–Cu1–O3	178.3(4)	U1–O1	2.655(7)	O5–U1–O6	177.1(3)	U2–O10	1.726(8)	O10–U2–O11	177.2(4)
Cu1–N2	1.908(9)	N2–Cu1–O2	176.1(4)	U1–O2	2.400(7)	O3–U1–O7	170.1(3)	U2–O11	1.755(8)	O15–U2–O12A	177.0(3)
Cu1–O3	1.906(7)	O6C–Cu1–O18	172.84	U1–O3	2.392(7)	O2–U1–O9	167.1(3)	U2–O12	2.327(8)	O12–U2–O17	176.1(3)
Cu1–O2	1.912(7)	N1–Cu1–O2	96.0(4)	U1–O4	2.625(7)	O4–U1–O1	162.4(3)	U2–O17	2.527(8)	O13–U2–O16	159.6(4)
Cu1–O6C	2.625	N2–Cu1–O3	95.7(4)	U1–O5	1.730(7)	O2–U1–O7	123.4(3)	U2–O13	2.535(8)	O12A–U2–O11	88.7(3)
Cu1–O18	2.740	N1–Cu1–N2	86.0(4)	U1–O6	1.755(8)	O2–U1–O4	122.4(2)	U2–O16	2.498(19)	O11–U2–O17	87.4(3)
		O2–Cu1–O3	82.3(3)	U1–O7	2.478(7)	O3–U1–O1	123.0(2)	U2–O15	2.559(8)	O13–U2–O11	86.6(3)
		O6C–Cu1–O3	84.78	U1–O9	2.503(8)	O3–U1–O9	120.9(3)			O11–U2–O16	93.2(5)
		O6C–Cu1–O2	89.71			O9–U1–O1	115.9(3)	U2...U2A	3.8791(9)	O15–U2–O11	89.4(3)
		O6C–Cu1–N1	95.4			O7–U1–O4	114.1(3)			O11–U2–O12	94.3(3)
		O6C–Cu1–N2	93.5			O5–U1–O4	100.6(3)			O10–U2–O12A	93.3(3)
		O18–Cu1–O3	88.06			O6–U1–O3	96.8(3)			O10–U2–O12	88.2(4)
		O18–Cu1–O2	89.28			O5–U1–O3	86.0(3)			O10–U2–O13	93.3(3)
		O18–Cu1–N1	91.75			O7–U1–O1	65.0(3)			O10–U2–O16	86.0(5)
		O18–Cu1–N2	87.24			O6–U1–O1	81.8(3)			O10–U2–O15	88.5(3)
						O5–U1–O1	96.9(3)			O10–U2–O17	90.1(3)
Cu1...U1	3.466	Cu1–O2–U1	106.4(3)			O6–U1–O4	80.6(3)			O13–U2–O15	48.9(3)
		Cu1–O3–U1	107.0(3)			O5–U1–O2	86.1(3)			O13–U2–O17	110.3(3)
						O6–U1–O2	95.4(3)			O13–U2–O12	66.3(3)
						O3–U1–O2	63.2(2)			O13–U2–O12A	133.2(3)
						O5–U1–O7	87.1(3)			O15–U2–O12	114.8(3)
						O6–U1–O7	90.1(3)			O15–U2–O17	61.6(3)
						O5–U1–O9	82.1(3)			O15–U2–O16	110.6(4)
						O6–U1–O9	96.1(3)			O17–U2–O12A	116.0(3)
						O7–U1–O9	50.9(3)			O16–U2–O17	49.4(4)
						O3–U1–O4	60.3(2)			O16–U2–O12	134.0(4)
						O4–U1–O9	65.5(3)			O16–U2–O12A	67.2(4)
						O1–U1–O2	60.2(2)			O12–U2–O12A	67.6(3)
										U2–O12–U2A	112.4(3)

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- 7 Crystal structure of  $[\text{Cu}^{\text{II}}\text{L}^{\text{OEt-pn}}\text{C}(\text{H}_2\text{O})]$  is known: CSD Refcode: WUYGAZ and CCDC No. 739723. However, we have redetermined its single crystal structure.