

Supporting Information for

Hydroxy- and alkoxy-bridged dinuclear uranyl Schiff base complexes: Hydrolysis, transamination and extraction studies

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Experimental Section:

X-ray Crystallography: Crystals of **1**·(DMF)₂ and **2**·(DMF)₂ were obtained in good yield from DMF at room temperature. Quality crystals could also be obtained from d₆-DMSO as **1**·(DMSO)₂ and **2**·(DMSO)₂. X-ray diffraction data were collected at -80 °C on a Bruker SMART APEX CCD X-ray diffractometer unit using Mo-K α radiation from crystals mounted in Paratone-N oil on glass fibers. SMART (v 5.624) was used for preliminary determination of cell constants and data collection control. Determination of integrated intensities and global cell refinement were performed with the Bruker SAINT Software package using a narrow-frame integration algorithm. The program suite SHELXTL (v 5.1) was used for space group determination, structure solution, and refinement.¹ Refinement was performed against F² by weighted full-matrix least square, and empirical absorption corrections (SADABS²) were applied. The *tert*-butyl groups on **2b** molecule are disordered over two (60 and 40 %) and restraints were applied to make chemically equivalent bonds approximately equal in the disordered fragments. H atoms were placed at calculated positions using suitable riding models with isotropic displacement parameters derived from their carrier atoms. Crystal data, selected bond distances and angles, are provided in Tables 1 - 3. Crystallography data for structural analysis of compounds **1**·(DMF)₂ and **2**·(DMF)₂ have been deposited with the Cambridge Crystallographic Data Center as CCDC nos. 656874 and 662434, respectively. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, U. K. (phone + 44 1223 336408; fax + 44 1223 336033).

Table S1. Crystal Data for **1**·(DMF)₂ and **2**·(DMF)₂.

Compounds	1 ·(DMF) ₂	2 ·(DMF) ₂
Empirical formula	C ₂₃ H ₃₀ N ₄ O ₁₀ U ₂	C ₈₇ H ₁₄₃ N ₁₁ O ₂₃ U ₄
Fw	998.57	2663.240
Wavelength (Å)	0.71073	0.71073
Crys syst	Monoclinic	Triclinic
Space group	P 21/n	P-1
a (Å)	11.797(3)	16.636(2)
b (Å)	9.784(2)	16.641(2)
c (Å)	24.594(5)	20.421(3)
α (deg)	90.00	104.963(3)
β (deg)	94.811(4)	93.128(3)
γ (deg)	90.00	103.839(3)
V (Å ³)	2828.7(1)	5262.2(1)
Z	4	2
density calcd (mg/m ³)	2.345	1.682
abs coeff (mm ⁻¹)	11.495	6.205
F(000)	1840	2588
Cryst size (mm ³)	0.1x0.1x0.05	0.1x0.5x0.05
Reflns collected	18601	36319
Indep reflns	4058 (R _{int} = 0.0687)	15175 (R _{int} = 0.1222)
Refinements method	Full-matrix least squares on F ²	Full-matrix least squares on F ²
GOF of F ²	0.858	0.868
Final R indices [I>2σ(I)]	R ₁ = 0.0272, wR ₂ = 0.0539	R ₁ = 0.0451, wR ₂ = 0.901
R indices (all data)	R ₁ = 0.0364, wR ₂ = 0.0557	R ₁ = 0.0686, wR ₂ = 0.967
Largest diff peak and hole (e/ Å ³)	1.177 and -0.691	1.811 and -1.632

Table S2. Selected bond distances for **1**·(DMF)₂ and **2**·(DMF)₂.

Bond distances of 1 ·(DMF) ₂ (Å)			
U1-O1	1.792(4)	U1-O2	1.783(4)
U1-O6	2.241(5)	U1-O7	2.380(5)
U1-O8	2.327(4)	U1-N1	2.544(5)
U2-O3	1.778(4)	U2-O4	1.794(4)
U2-O5	2.235(5)	U2-O7	2.364(4)
U2-O8	2.343(4)	U2-N2	2.579(5)
U2-O1D1	2.400(5)	U1-O1D2	2.461(4)
N1-C10	1.473(8)	N1-C11	1.272(8)
N2-C2	1.468(8)	N2-C3	1.286(8)
U1-U2	3.8693(8)		
Bond distances of 2 ·(DMF) ₂ (Å)			
U1-O1	1.762(6)	U1-O2	1.785(6)
U1-O5	2.221(6)	U1-O6	2.383(6)
U1-O8	2.389(6)	U1-N1	2.541(7)
U2-O3	1.766(6)	U2-O4	1.776(6)
U2-O6	2.341(6)	U2-O7	2.254(6)
U2-O8	2.375(6)	U2-N2	2.558(7)
U1-U2	3.9340(7)	U3-O9	1.774(6)
U3-O10	1.767(6)	U3-O13	2.227(6)
U3-O14	2.392(6)	U3-O16	2.341(6)
U3-N3	2.549(7)	U4-O11	1.764(6)
U4-O12	1.796(6)	U4-O14	2.352(6)
U4-O15	2.239(6)	U4-O16	2.338(6)
U4-N4	2.561(7)	U3-U4	3.8470(6)

Table S3. Selected bond angles for **1**·(DMF)₂ and **2**·(DMF)₂.

Bond angles of 1 ·(DMF) ₂ (deg)			
O1-U1-O2	178.7(2)	O1-U1-O6	90.76(2)
O2-U1-O8	91.90(2)	O6-U1-O8	154.81(2)
O7-U1-O8	68.84(2)	O3-U2-O4	179.5(2)
Bond angles of 2 ·(DMF) ₂ (deg)			
O1-U1-O2	179.0(3)	O1-U1-O5	88.0(3)
O1-U1-O6-	91.3(3)	O1-U1-O8	87.8(2)
O2-U1-O5	91.1(3)	O2-U1-O6	89.6(3)
O2-U1-O8	92.9(2)	O3-U2-O4	179.5(3)
O3-U2-O6	90.8(3)	O3-U2-O7	89.5(3)
O3-U2-O8	88.9(3)	O4-U2-O6	88.7(2)
O4-U2-O7	90.9(3)	O4-U2-O8	90.9(2)
O6-U2-O7	136.0(2)	O6-U2-O8	68.38(19)
O7-U2-O8	155.6(2)	O9-U3-O10	178.4(3)
O9-U3-O13	92.4(3)	O9-U3-O14	88.0(2)
O9-U3-O16	94.1(3)	O10-U3-O13	86.8(3)
O10-U3-O14	91.6(2)	O10-U3-O16	87.1(3)
O13-U3-O16	155.4(2)	O13-U3-O14	135.8(2)
O14-U3-O16	68.25(19)		

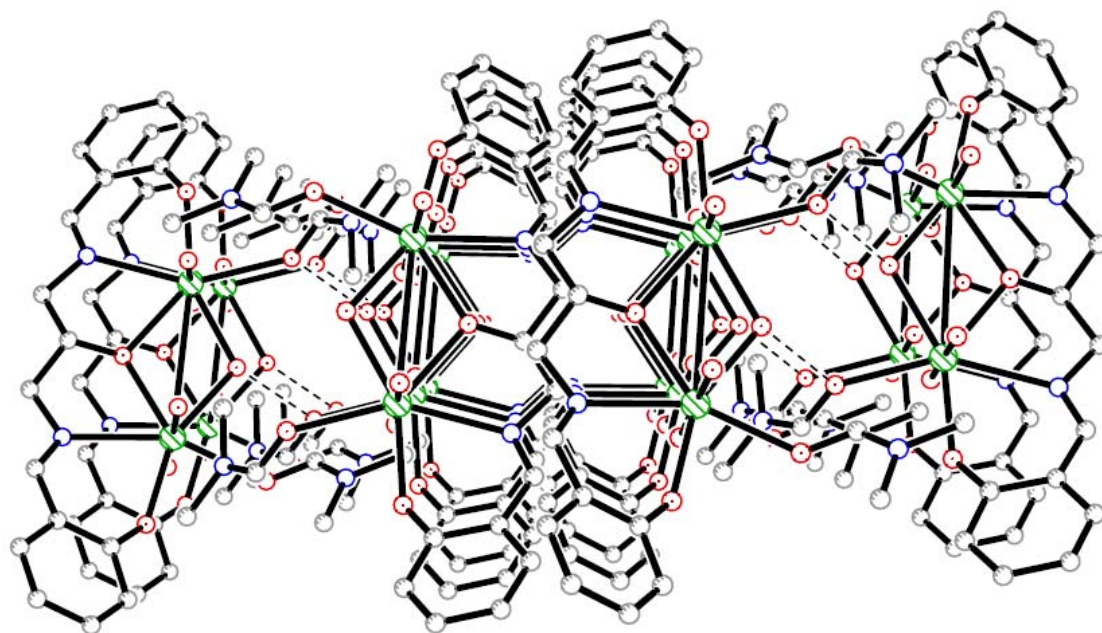


Fig S1. Packing diagram of **1** along the 'b' axis.

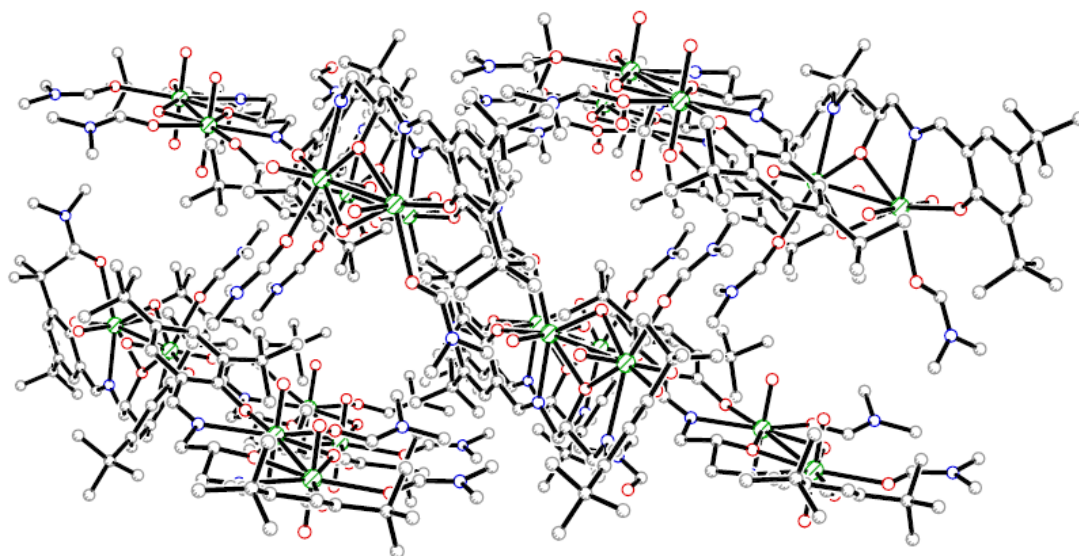


Fig S2. Packing diagram of **2** along the 'c' axis.

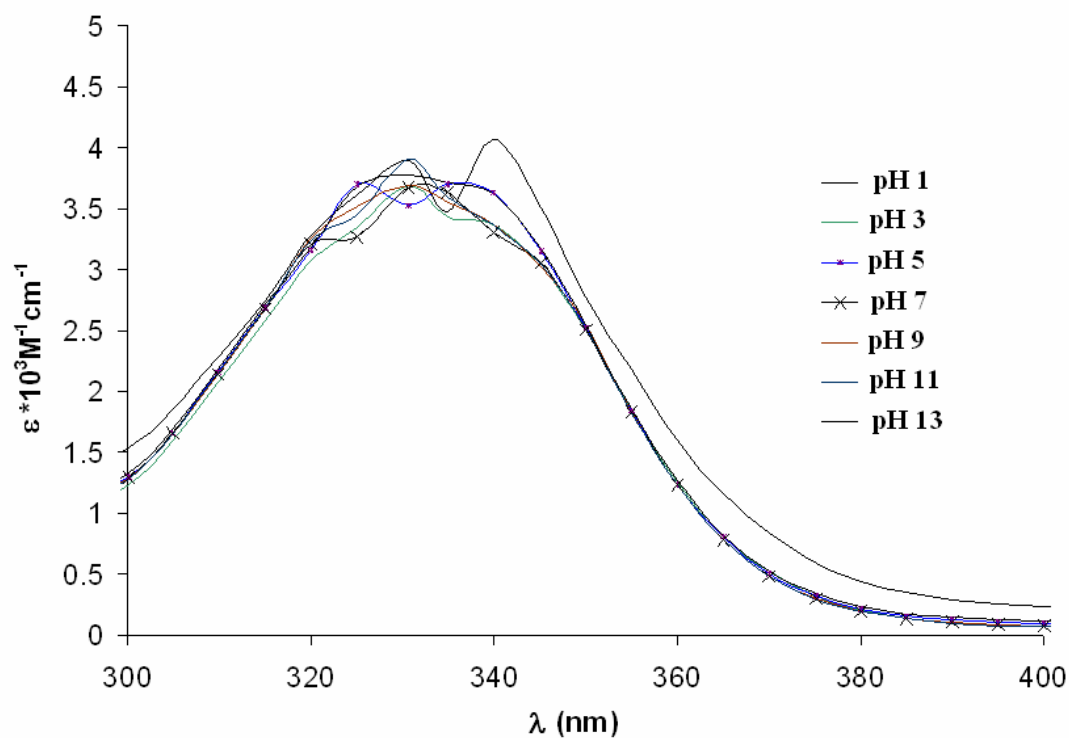


Fig S3. Hydrolysis profile of H₃L₂.

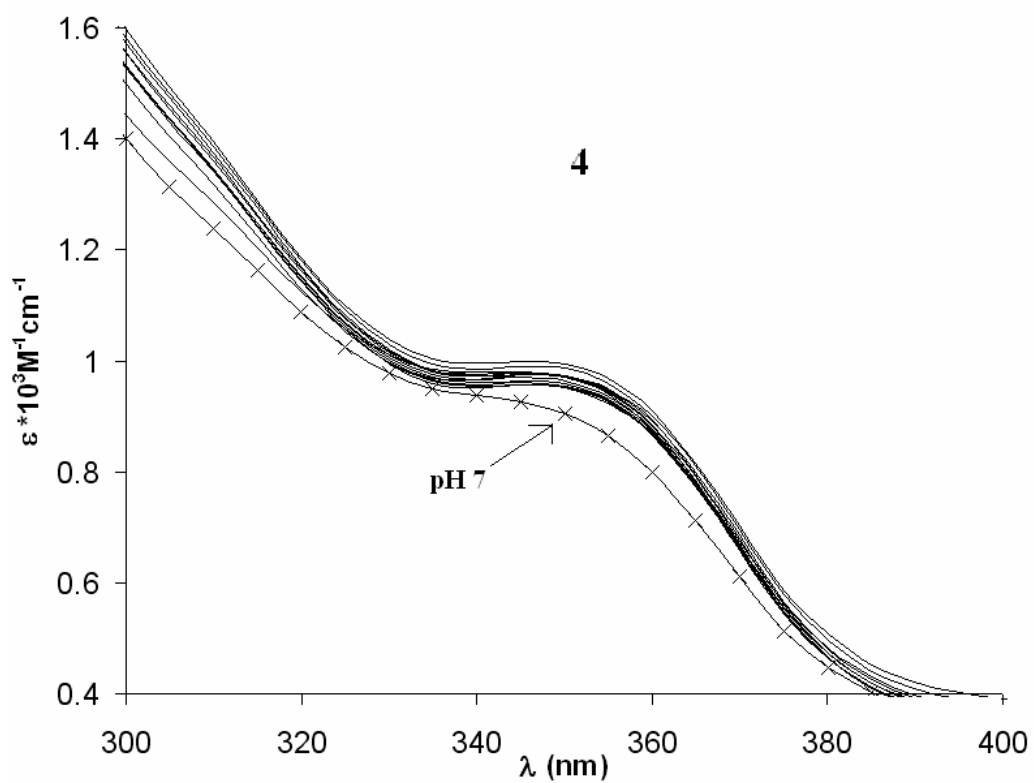


Fig S4. Hydrolysis profile of compound **4** (0.1 mM) dissolved in CHCl₃.

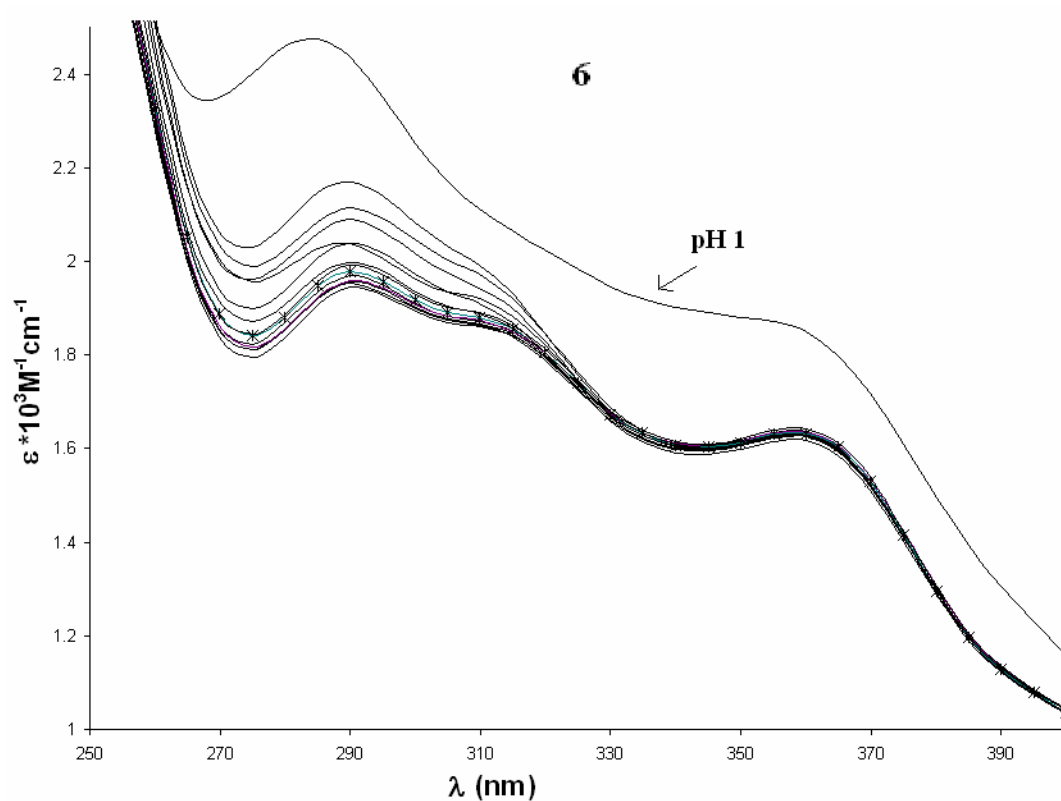


Fig S5. Hydrolysis profile of compound **6** (0.1 mM) dissolved in CHCl₃.

References:

- ¹ G. M. Sheldrick, 'SHELXTL PC, version 6.12, An Integrated System for Solving, Refining, and Displaying Crystal Structures from Diffraction Data; Siemens Analytical X-ray Instruments, Inc', 2001.
- ² G. M. Sheldrick, 'SADABS-An empirical absorption correction program; Bruker Analytical X-ray Systems ', 1996.