ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

To

Binding of oxime group to uranyl ion: Uranyl complexes with 2-pyridyl ketoximes as ligands

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This work is dedicated to the loving memory of Malcolm H. Chisholm: A great scientist, a fantastic mentor and a precious friend.

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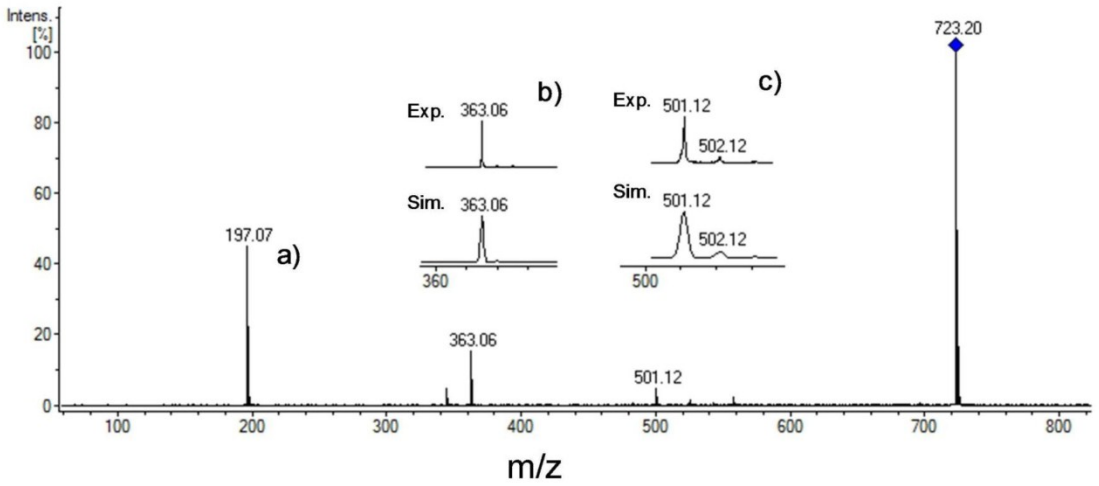

Fig. S1 Collision-induced fragmentation MS/MS spectra of $[UO_2(O_2CMe)(phpao)_2]^-$ ($UO_2C_{26}H_{21}N_4O_4$, *m/z*= 723.20) : a) The $phpao^-$ signal; b)$[UO_2(OH)_2(O_2CMe)]^-$ ($UO_2C_2H_5O_4$); c) $[UO_2(OH)_2(phpao)]^-$ ($UO_2C_{12}H_{11}N_2O_3$).

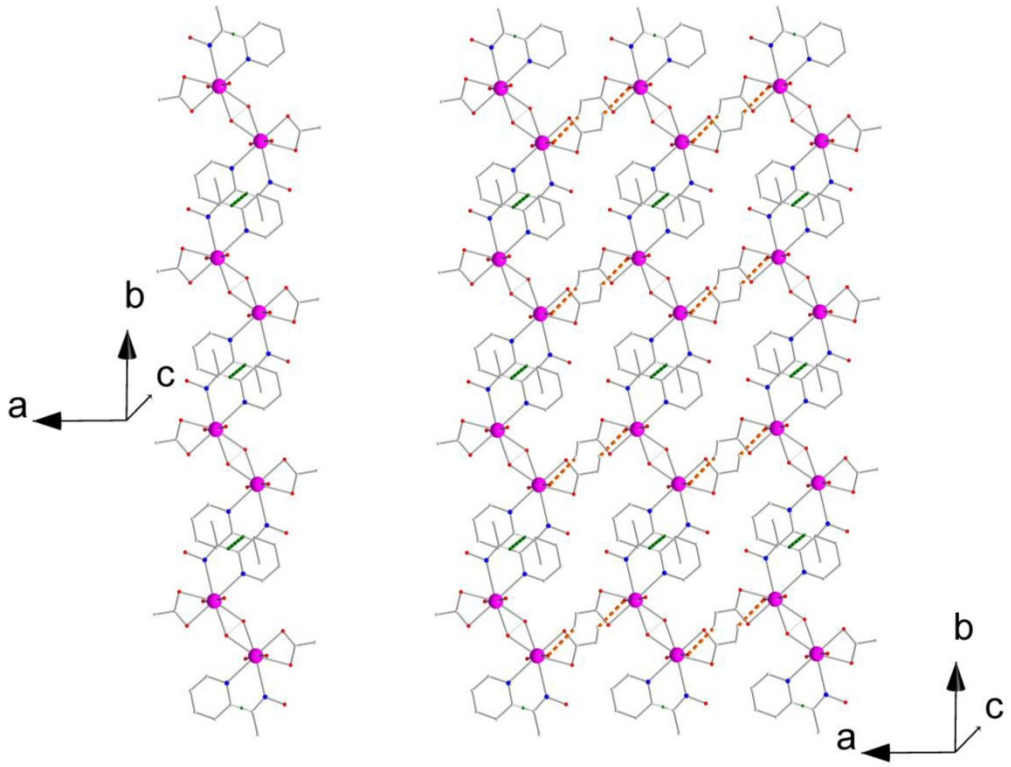

Fig. S2 Chains (left) along the *b* axis and 2D layers (right) parallel to the (001) plane for complex $[(UO_2)_2(O_2)(O_2CMe)_2(mepaoH)_2]$ (**3**). The dashed dark green and orange lines indicate π-π interactions and $C_{acetate\ methyl}$-H···O_{uranyl} H bonds.

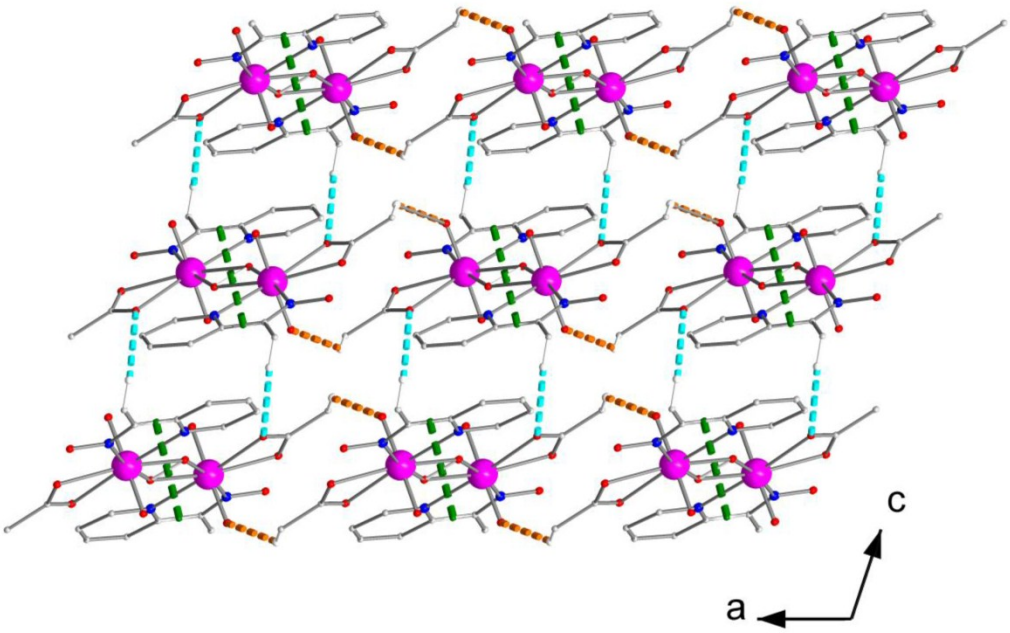

Fig. S3 A part of the 3D architecture in the crystal structure of complex $[(UO_2)_2(O_2)(O_2CMe)_2(mepaoH)_2]$ (**3**). The dashed dark green, turquoise and orange lines indicate π-π interactions, $C_{oxime\ methyl}$-H···$O_{coord.acetate}$ and $C_{acetate\ methyl}$-H···O_{uranyl} H bonds, respectively.

Table S1. Intermolecular H bonds in the crystal structures of **1**-**3**

Interaction D-H···A[a]	D···A (Å)	H···A (Å)	D-H···A(°)	Symmetry operation for A
		Complex **1**		
O6-H(O6)···O11	2.64	1.77	161.0	*x*, *y*, *z*
		Complex **2**		
C1[b]-H1(C1) ···C_g1	3.680(4)	3.17(5)	116(2)	-*x*+1, *y*+1, -*z*+1
		Complex **3**		
C1[c]-HB(C1)···O5	3.45	2.59	146.3	*x*, -*y*+0.5, *z+0.5*
C9[d]-HC(C9)···O3	3.28	2.55	131.9	-*x*+2, -*y*, -*z*

[a] D=donor, A=acceptor; [b] C1 is the methyl carbon atom of mepao$^-$, not labelled in Fig.4. [c] C1 is the methyl carbon of mepao$^-$, not labelled in Fig.6. [d] C9 is the methyl carbon atom of $MeCO_2^-$, not labelled in Fig.6.