

Supplementary Information

Incorporating transition metal ions into uranium oxide hydrates: the role of Zn(II) and the effect of the addition of Cs(I) ions

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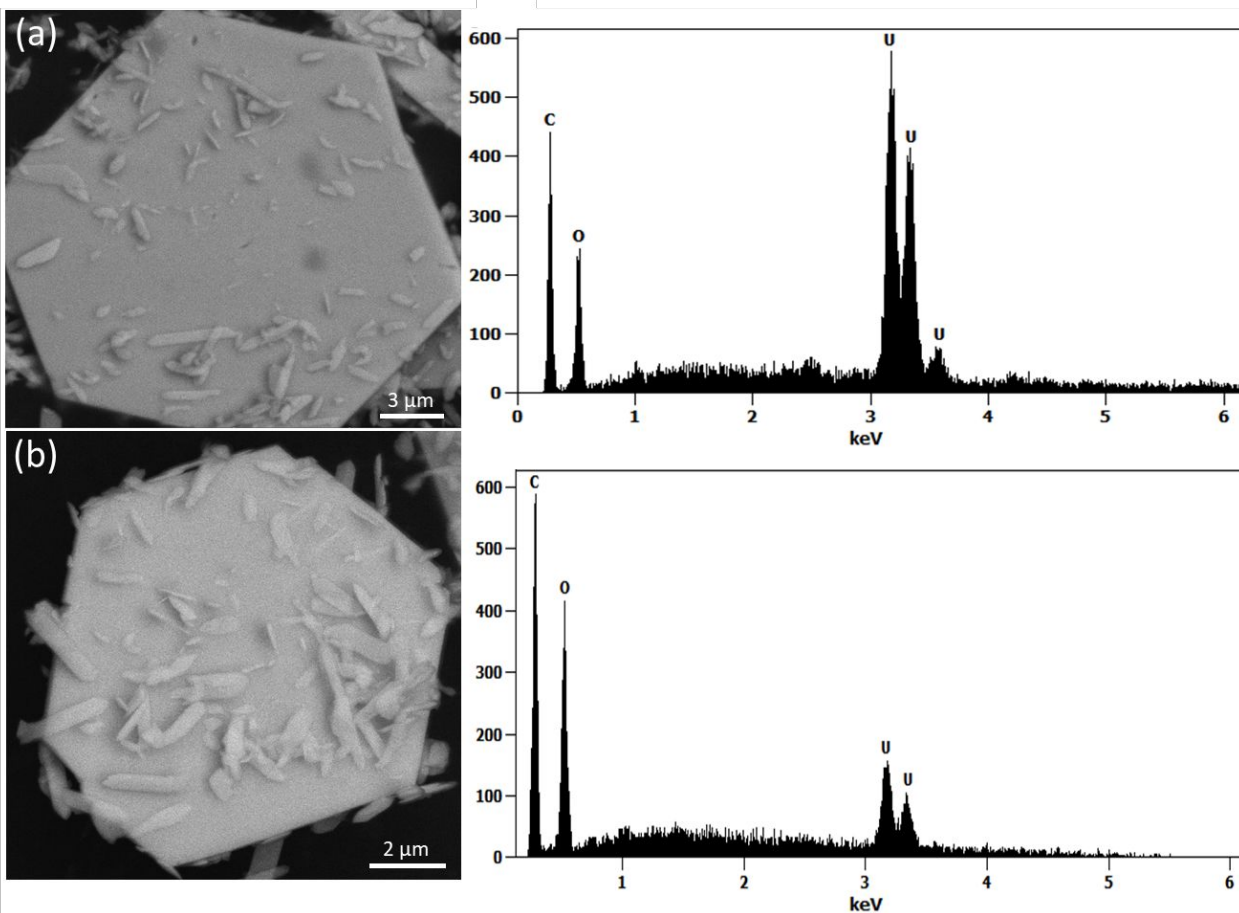


Figure S1. SEM-EDS of the minor phase isolated from the synthesis of both **UOHF-Zn** and **UOH-Zn**: an SEM image (a) and the corresponding EDS spectrum (b) of the hexagonal plate-like crystals confirming the presence of only U and O in the crystal.

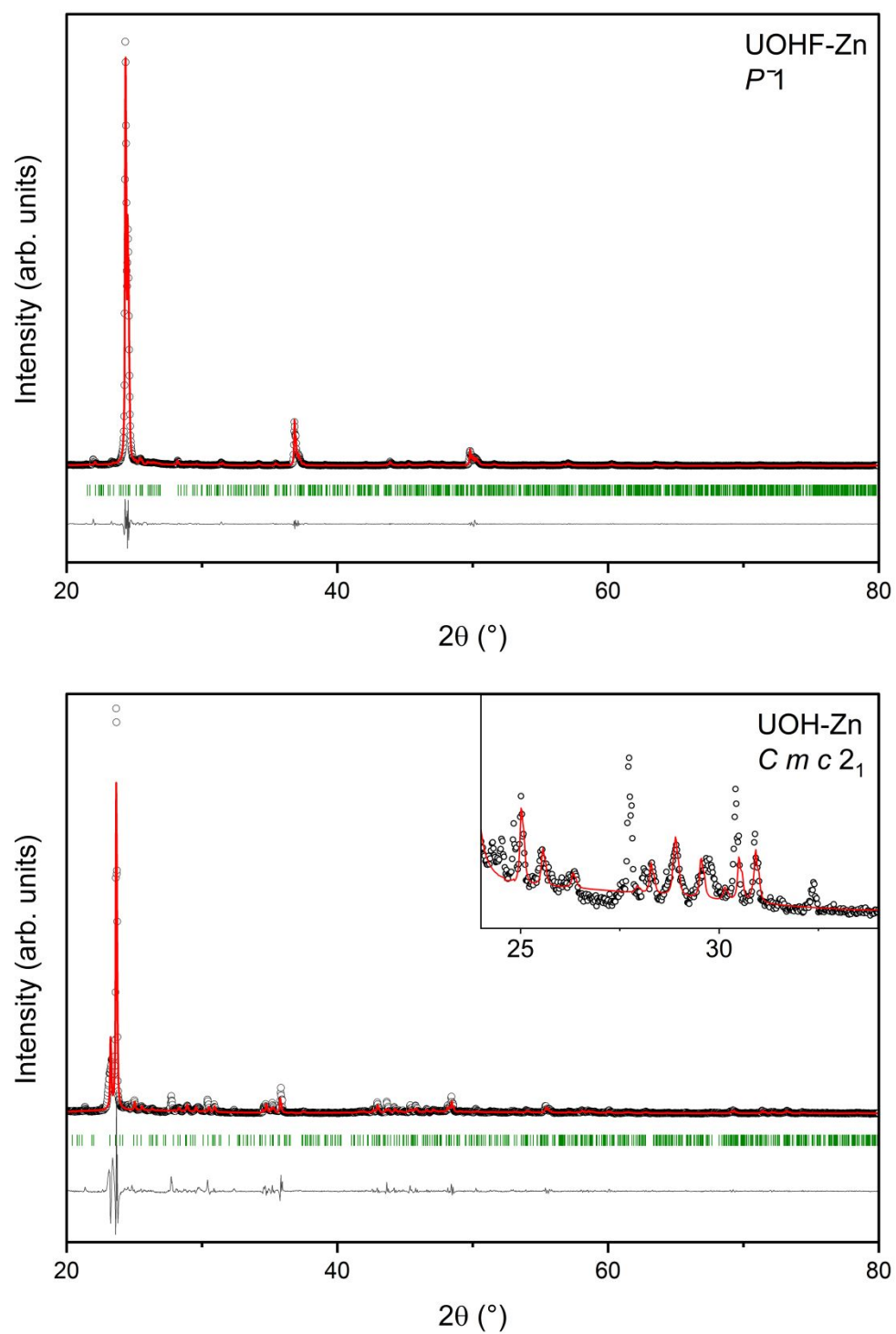


Figure S2. Powder XRD patterns of **UOHF-Zn** (top) and **UOH-Zn** (bottom) indexed with a Le Bail fitting method. Allowed hkl marks are shown in green, the collected data is shown as black circles and a fitting of the phase is shown as the red line.

Table S1. BVS calculations for **UOHF-Zn**

	U1		U2		U3		U4		U5		U6		Zn1		Zn2			
Occ	1		1		1		1		1		1		0.65		0.35			
Sym.	1		1		1		1		2		1		1		1			
CN #	7		7		6		7		6		7		6		5		Σ	
O1	1.64										0.25						1.89	
O2	1.73																1.73	
O3	0.51		1.26														1.78	
O4			1.54												0.35		1.89	
O5			0.64		0.66	0.76											2.07	
O6					1.48						0.41						1.89	
O7	0.57				1.22												1.79	
O8					0.73		0.66	0.68									2.08	
O9					0.79		0.65					0.66						2.10
O10							1.51										1.51	
O11	0.52	0.43					1.11										2.06	
O12							0.48		1.15	1.15	0.45							2.08
O13	0.56		0.66				0.81										2.03	
O14			0.49						1.18	1.18	0.45							2.12
O15									0.62	0.62							0.62 (H ₂ O)	
O16											1.48				0.43		1.91	
O17											1.44		0.42					1.87
O18			0.60		0.78						0.64						2.02	
O19											0.80						0.80 (H ₂ O)	
O20											0.45						0.45 (H ₂ O)	
O21											0.46		0.19	0.58			1.23 (OH)	
O22															0.41		0.41 (H ₂ O)	
O23															0.42		0.42 (H ₂ O)	
Σ	5.96		5.87		5.75		5.91		5.90		5.91		2.19		2.20			

Table S2. BVS calculations for **UOH-Zn**

	U1	U2	U3	U4	Cs1		Cs2		Zn1		
Occ	1	1	1	1	0.5		0.5		0.5		
CN #	7	7	7	7	11		8		6		Σ
O1	1.65								0.27		1.92
O2	1.72				0.15	0.15					2.02
O3	0.50	0.46		0.41							1.37 (OH)
O4	0.56			0.66							1.22 (OH)
O5	0.47	0.41	0.48								1.36 (OH)
O6	0.72	0.66	0.67		0.06	0.06					2.18
O7		1.56							0.38		1.94
O8		1.50			0.11	0.11	0.12	0.12			1.97
O9		0.55	0.41	0.51							1.47
O10		0.71	0.66	0.66			0.11	0.11			2.25
O11			1.62		0.14	0.14			0.24		2.14
O12			1.59				0.08	0.08			1.76
O13	0.35		0.45	0.47							1.27 (OH)
O14				1.72			0.15	0.15			2.01
O15				1.65							1.65
O16					0.09				0.27		0.36 (H ₂ O)
O17					0.15				0.33		0.47 (H ₂ O)
O18									0.37		0.37 (H ₂ O)
O19					0.03						0.03 (H ₂ O)
O20											0.00 (H ₂ O)
O21											0.00 (H ₂ O)
O22											0.00 (H ₂ O)
Σ	5.98	5.85	5.88	6.07	1.19		0.94		1.86		