

*Electronic Supplementary Information*

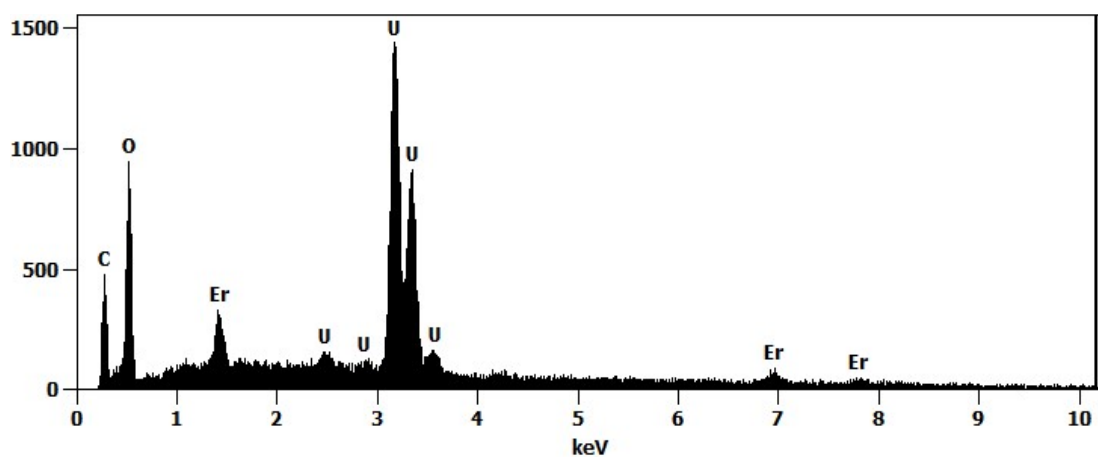
Uranium oxide hydrate frameworks with Er(III) or Y(III) ions:

Revealing structural insights leading to the low symmetry

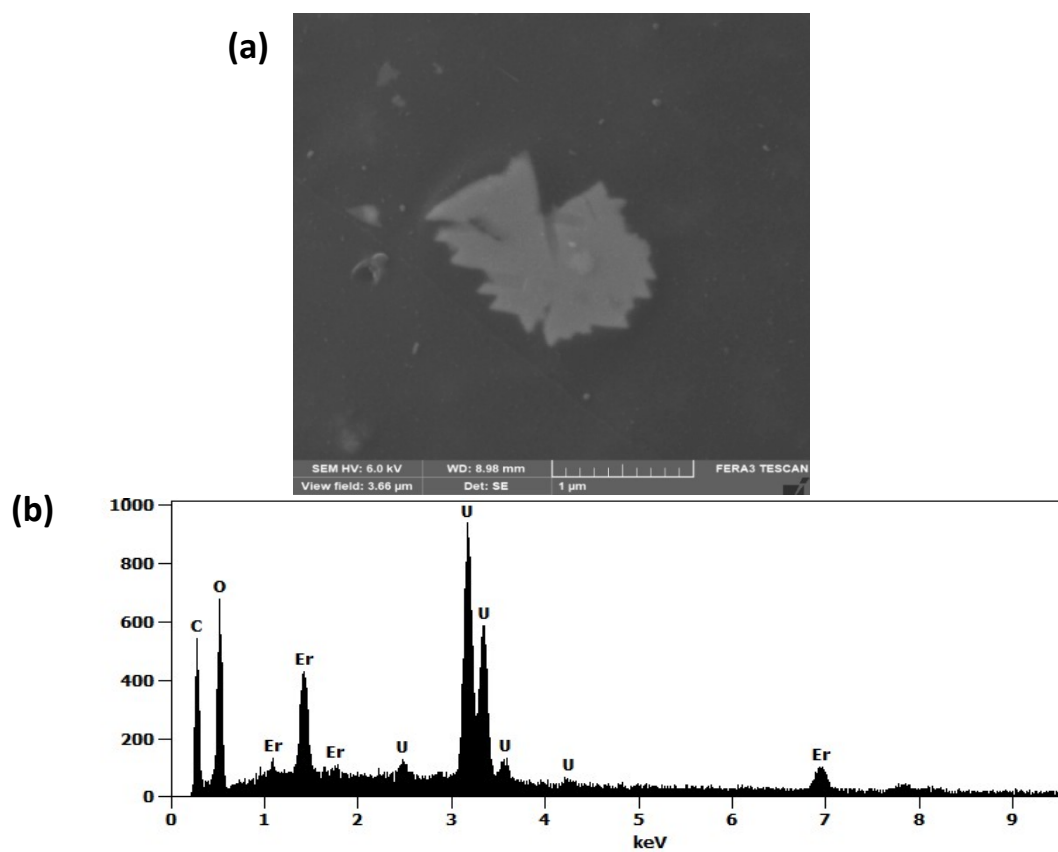
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**Figure S1.** Full EDS spectrum of UOF-Er.



**Figure S2.** SEM-EDS of the minor phase isolated from the synthesis of UOF-Er: a secondary SEM image (a) and the corresponding EDS spectrum (b) confirming the presence of both U and Er in a  $\sim 2.5:1$  atomic ratio.

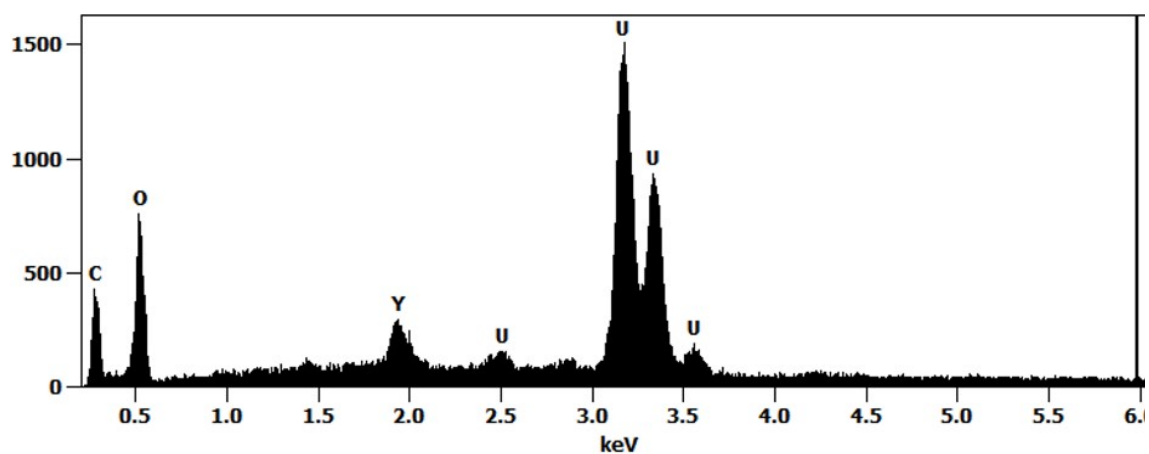


Figure S3. Full EDS spectrum of UOF-Y.

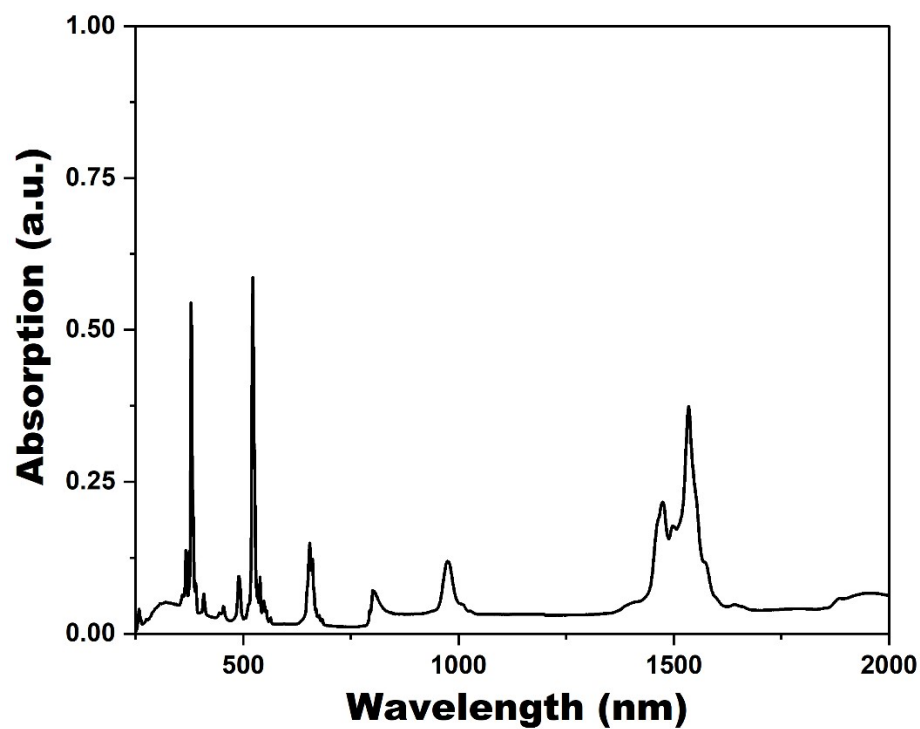


Figure S4. An absorption spectrum of  $\text{Er}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ .

**Table S1.** SEM-EDS results and metal ratios for both **UOF-Er** and **UOF-Y**, and minor phases.

Sample	Atom % U	Atom % Er	Atom % Y	U:Er/Y ratio
<b>UOF-Er</b>	17.1	2.99	-	5.7
<b>UOF-Er - minor phase</b>	13.06	5.45	-	2.4
<b>UOF-Y</b>	21.98	-	3.77	5.8
<b>UOF-Y - minor phase</b>	14.19	-	4.8	3.0

**Table S2.** Selected bond lengths (Å) and angles (°) for compounds **UOF-Er** and **UOF-Y**.

<b>UOF-Er</b>							
U1–O1	2.18(3)	U2–O5 <sup>3</sup>	2.40(3)	U3–O2	2.33(3)	U4–O1 <sup>6</sup>	2.36(3)
U1–O2	2.15(3)	U2–O6	1.74(3)	U3–O2 <sup>2</sup>	2.26(3)	U4–O10	2.24(4)
U1–O3	1.85(3)	U2–O7	1.72(3)	U3–O4	2.30(4)	U4–O11	1.90(3)
U1–O4	2.17(3)	U2–O8	2.53(3)	U3–O8	1.97(3)	U4–O12 <sup>4</sup>	2.28(3)
U1–O5	1.92(4)	U2–O8 <sup>3</sup>	2.39(3)	U3–O9	1.86(4)	U4–O12	2.28(3)
U1–O12 <sup>2</sup>	2.21(3)	U2–O10	2.29(3)	U3–O10	2.24(3)	U4–O13	2.40(3)
O3=U1=O5	176.0(15)	U2–O11	2.43(3)	U3–O18	2.36(3)	U4–O14	1.85(3)
		O6=U2=O7	178.2(16)	O8=U3=O9	175.0(14)	O11=U4=O14	174.5(15)
U5–O1 <sup>1</sup>	2.34(3)	U6–O13 <sup>5</sup>	2.08(4)	Er1–O14	2.22(3)		
U5–O4	2.30(3)	U6–O13	2.08(4)	Er1–O15 <sup>5</sup>	2.55(3)		
U5–O13 <sup>5</sup>	2.43(3)	U6–O18 <sup>5</sup>	2.05(3)	Er1–O16 <sup>7</sup>	2.37(3)		
U5–O15	1.84(3)	U6–O18	2.05(3)	Er1–O19	2.37(4)		
U5–O16	1.84(3)	U6–O19 <sup>5</sup>	2.14(4)	Er1–O20	2.33(4)		
U5–O17	2.39(7)	U6–O19	2.14(4)	Er1–O21	2.44(4)		
U5–O17 <sup>1</sup>	2.17(7)	O13–U6–O13 <sup>6</sup>	180.0	Er1–O22	2.36(4)		
U5–O18	2.37(3)			Er1–O23	2.25(3)		
O15=U5=O16	175.0(14)						
<b>UOF-Y</b>							
U1–O1	2.192(14)	U2–O5	2.358(13)	U3–O2 <sup>1</sup>	2.295(13)	U4–O1 <sup>2</sup>	2.341(13)
U1–O2	2.165(14)	U2–O6	1.760(14)	U3–O2 <sup>5</sup>	2.255(14)	U4–O10	2.210(13)
U1–O3	1.821(14)	U2–O7	1.785(14)	U3–O4 <sup>1</sup>	2.285(15)	U4–O11	1.884(13)
U1–O4	2.186(14)	U2–O8	2.481(13)	U3–O8	2.001(13)	U4–O12 <sup>6</sup>	2.244(14)
U1–O5	1.939(14)	U2–O8 <sup>1</sup>	2.369(13)	U3–O9	1.843(13)	U4–O12	2.275(13)
U1–O12 <sup>3</sup>	2.234(13)	U2–O10	2.318(13)	U3–O10	2.224(13)	U4–O13	2.399(14)
O3=U1=O5	176.5(6)	U2–O11	2.429(13)	U3–O18 <sup>4</sup>	2.378(13)	U4–O14	1.830(14)
		O6=U2=O7	178.8(6)	O9=U3=O8	173.3(6)	O14=U4=O11	176.6(6)
U5–O1 <sup>2</sup>	2.315(14)	U6–O13 <sup>4</sup>	2.063(14)	Y1–O14	2.260(14)		
U5–O4 <sup>9</sup>	2.283(13)	U6–O13	2.063(14)	Y1–O15	2.539(13)		
U5–O13	2.436(13)	U6–O18 <sup>4</sup>	2.038(13)	Y1–O16 <sup>5</sup>	2.348(13)		
U5–O15	1.829(13)	U6–O18	2.038(13)	Y1–O19	2.277(14)		
U5–O16	1.851(13)	U6–O19 <sup>4</sup>	2.200(13)	Y1–O20	2.336(14)		
U5–O17	2.21(3)	U6–O19	2.200(13)	Y1–O21	2.429(14)		
U5–O17 <sup>10</sup>	2.27(3)	O13–U6–O13 <sup>4</sup>	180.0(11)	Y1–O22	2.285(13)		
U5–O18	2.366(14)			Y1–O23	2.293(13)		
O15=U5=O16	174.0(6)						

<sup>1</sup>1-X,1-Y,1-Z; <sup>2</sup>2-X,2-Y,1-Z; <sup>3</sup>1-X,2-Y,1-Z; <sup>4</sup>2-X,2-Y,2-Z; <sup>5</sup>1-X,1-Y,1-Z; <sup>6</sup>+X,+Y,1+Z; <sup>7</sup>2-X,1-Y,1-Z

**Table S3.** BVS calculations for **UOF-Er**.

	<b>U1</b>	<b>U2</b>	<b>U3</b>	<b>U4</b>	<b>U5</b>	<b>U6</b>	<b>Er</b>	
<b>Occ</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	
<b>Sym</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>2</b>	<b>1</b>	
<b>CN #</b>	<b>6</b>	<b>7</b>	<b>7</b>	<b>7</b>	<b>7</b>	<b>6</b>	<b>8</b>	<b>Σ</b>
O1	0.78			0.56	0.57			<b>1.92</b>
O2	0.81		0.58 0.67					<b>2.06</b>
O3	1.44							<b>1.44</b>
O4	0.80		0.62		0.62			<b>2.03</b>
O5	1.31	0.51						<b>1.82</b>
O6		1.86						<b>1.86</b>
O7		1.89						<b>1.89</b>
O8		0.40	0.52 1.17					<b>2.09</b>
O9			1.50					<b>1.50</b>
O10		0.63	0.68	0.69				<b>2.01</b>
O11		0.48		1.34				<b>1.82</b>
O12	0.75			0.63 0.64				<b>2.02</b>
O13				0.52	0.48	0.95 0.95		<b>1.95</b>
O14				1.47			0.53	<b>2.00</b>
O15					1.50		0.22	<b>1.73</b>
O16					1.50		0.36	<b>1.86</b>
O17					0.80	0.52		<b>1.32</b> (OH)
O18			0.55		0.54	1.00 1.00		<b>2.09</b>
O19						0.84 0.84	0.35	<b>1.19</b> (OH)
O20							0.40	<b>0.40</b> (H <sub>2</sub> O)
O21							0.30	<b>0.30</b> (H <sub>2</sub> O)
O22							0.37	<b>0.37</b> (H <sub>2</sub> O)
O23							0.50	<b>0.50</b> (H <sub>2</sub> O)
<b>Σ</b>	<b>5.89</b>	<b>6.29</b>	<b>5.78</b>	<b>5.86</b>	<b>5.88</b>	<b>5.58</b>	<b>3.04</b>	

**Table S4.** BVS calculations for **UOF-Y**.

	<b>U1</b>	<b>U2</b>	<b>U3</b>	<b>U4</b>	<b>U5</b>	<b>U6</b>	<b>Y</b>	
<b>Occ</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	
<b>Sym</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	<b>0.5</b>	<b>1</b>	
<b>CN #</b>	<b>6</b>	<b>7</b>	<b>7</b>	<b>7</b>	<b>7</b>	<b>6</b>	<b>8</b>	<b>Σ</b>
O1	0.76			0.57	0.60			<b>1.93</b>
O2	0.80		0.62	0.68				<b>2.10</b>
O3	1.57							<b>1.57</b>
O4	0.77		0.64		0.64			<b>2.05</b>
O5	1.25	0.55						<b>1.80</b>
O6		1.76						<b>1.76</b>
O7		1.66						<b>1.66</b>
O8		0.43	0.55	1.10				<b>2.08</b>
O9			1.50					<b>1.50</b>
O10		0.59	0.72	0.74				<b>2.05</b>
O11		0.48		1.37				<b>1.85</b>
O12	0.70			0.70	0.64			<b>2.04</b>
O13				0.51	0.48	0.98	0.98	<b>2.95</b>
O14				1.54			0.51	<b>2.05</b>
O15					1.53		0.24	<b>1.78</b>
O16					1.47		0.41	<b>1.88</b>
O17					0.66	0.74		<b>1.39</b> (OH)
O18			0.53		0.57	1.03	1.03	<b>2.13</b>
O19						0.76	0.76	0.49 <b>1.24</b> (OH)
O20							0.42	<b>0.42</b> (H <sub>2</sub> O)
O21							0.32	<b>0.32</b> (H <sub>2</sub> O)
O22							0.49	<b>0.49</b> (H <sub>2</sub> O)
O23							0.47	<b>0.47</b> (H <sub>2</sub> O)
<b>Σ</b>	<b>5.85</b>	<b>6.02</b>	<b>5.78</b>	<b>6.08</b>	<b>5.93</b>	<b>5.54</b>	<b>3.35</b>	