

## Electronic supplementary information

### Crystal structures of uranyl complexes with isobutyrate and isovalerate anions

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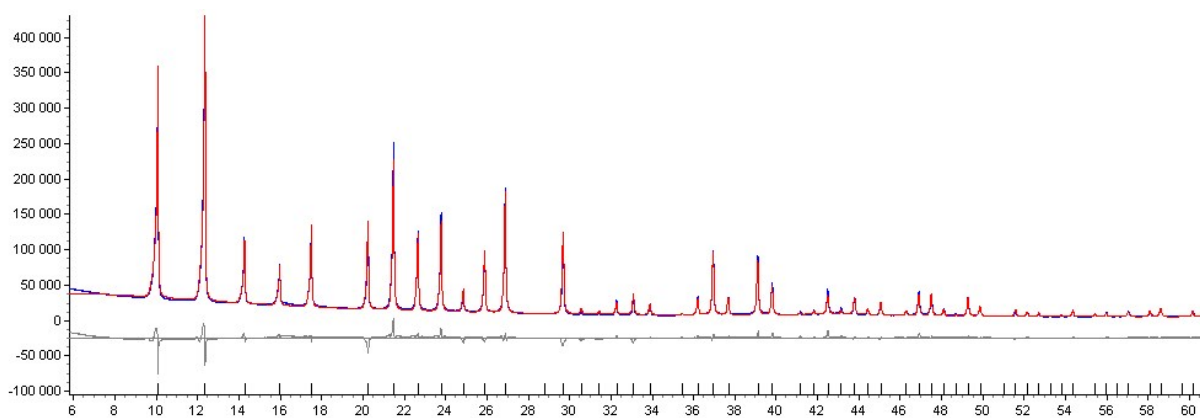


Fig. S1. The simulated (red line) and experimental (black line) XRD patterns of Cs[(UO<sub>2</sub>)(i-C<sub>3</sub>H<sub>7</sub>COO)<sub>3</sub>] (II) and their difference (grey line).

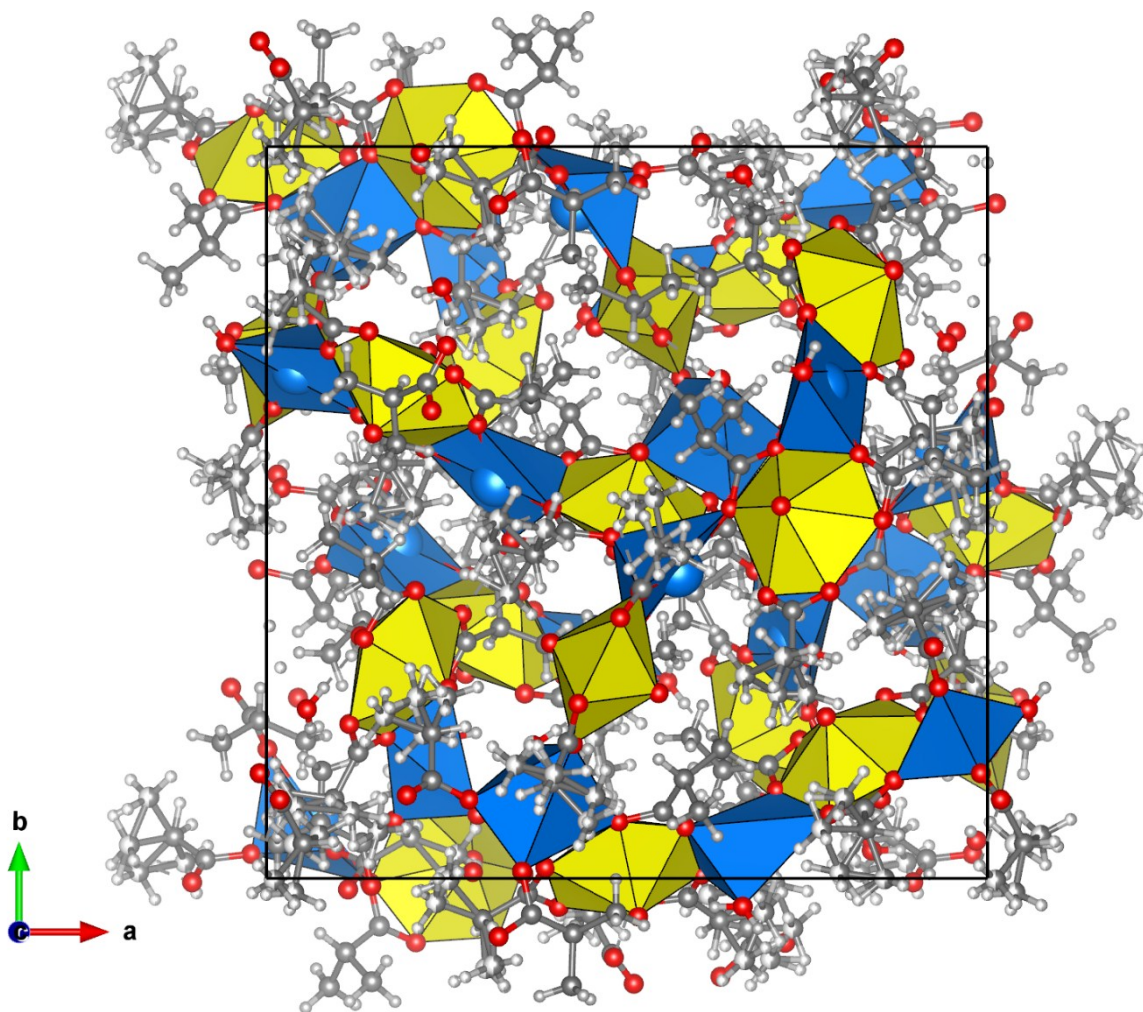


Fig. S2. Projection of crystal structure of  $\text{Na}[(\text{UO}_2)(i\text{-C}_3\text{H}_7\text{COO})_3] \cdot 0.7\text{H}_2\text{O}$  (I) on  $ab$  plane.

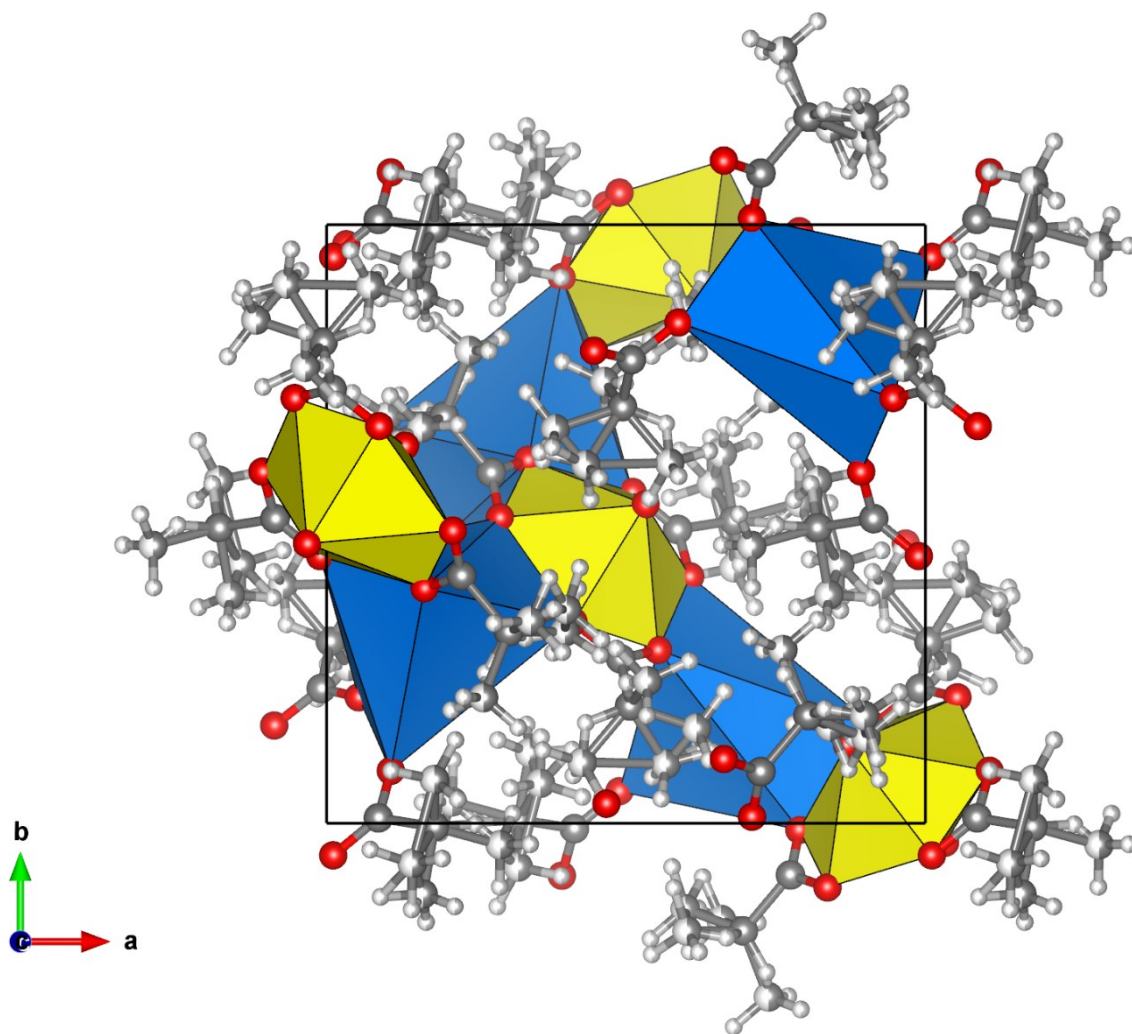


Fig. S3. Projection of crystal structure of Cs[(UO<sub>2</sub>)(*i*-C<sub>3</sub>H<sub>7</sub>COO)<sub>3</sub>] (II) on *ab* plane.

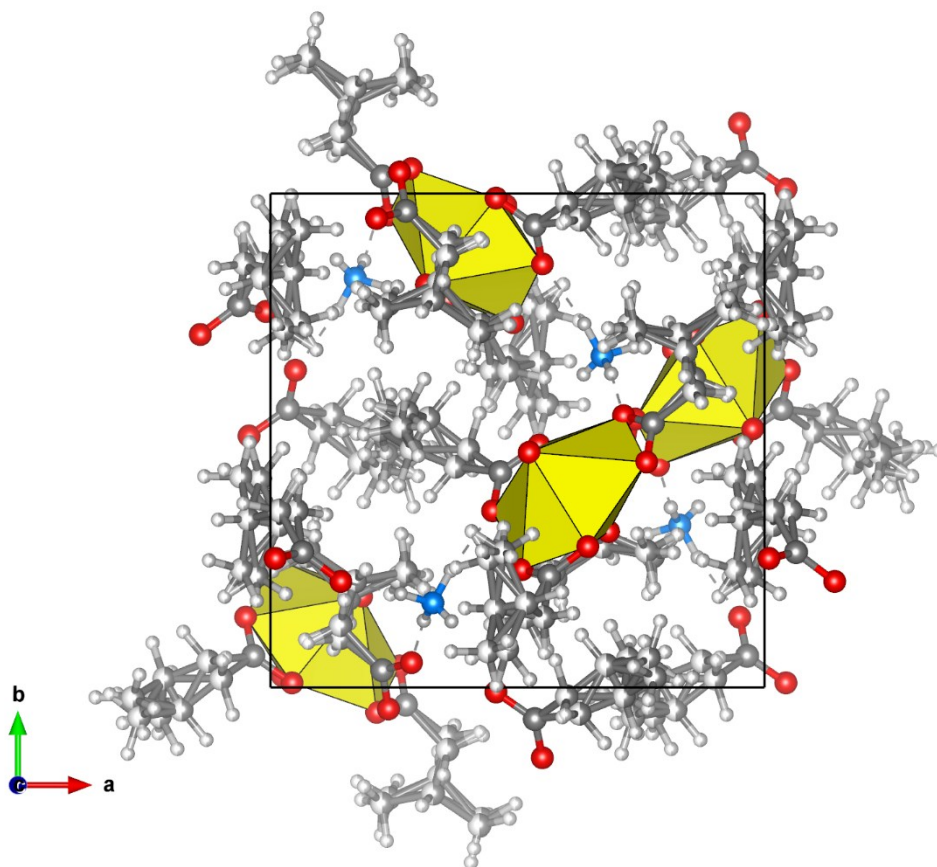


Fig. S4. Projection of crystal structure of  $(\text{NH}_4)[(\text{UO}_2)(i\text{-C}_4\text{H}_9\text{COO})_3]$  (**III**) on  $ab$  plane.

Table S1. Assignment of absorption bands in FTIR spectra of Na[(UO<sub>2</sub>)(*i*-C<sub>3</sub>H<sub>7</sub>COO)<sub>3</sub>]·0.7H<sub>2</sub>O (**I**), Cs[(UO<sub>2</sub>)(*i*-C<sub>3</sub>H<sub>7</sub>COO)<sub>3</sub>] (**II**) and (NH<sub>4</sub>)[(UO<sub>2</sub>)(*i*-C<sub>4</sub>H<sub>9</sub>COO)<sub>3</sub>] (**III**)\*

Wavenumber, cm <sup>-1</sup>			Assignment
I	II	III	
3428 m., br.			v(OH)
		3176 m., br.	v(NH)
2973 m. 2931 w.	2973 m. 2935 w.	2962 s. 2935 m. 2904 w.	v(CH)
2872 w.	2872 w.	2873 w.	
		1714 w. 1631 w.	δ(NH)
1614 w.			δ(OH)
1530 v.s.	1526 v.s.	1533 v.s.	v <sub>as</sub> (COO)
1486 s.	1485 s.	1462 v.s.	δ(CH)
1441 s.	1441 s.	1426 s.	v <sub>s</sub> (COO)
1379 w. 1364 w.	1379 m. 1365 m.	1410 s. 1387 m. 1371 m.	δ(CH)
1299 m.	1301 m. 1287 m.	1332 w. 1313 w. 1267 w. 1217 w.	tw(CH) ω(CH)
1169 w.	1170 w.	1169 w.	
1093 m. 1049 m.	1092 m.	1123 w. 1101 w.	v(C–C) γ(CH)
930 v.s.	929 v.s.	928 v.s.	v <sub>as</sub> (UO <sub>2</sub> )
880 w. 854 m. 779 w.	853 m. 773 w.	840 w. 809 w. 755 w. 736 w.	v(C–C) γ(CH)
661 w.	646 w.	657 w.	δ(COO)
	627 w.		γ(COO)
541 w.	542 w.	537 w.	ω(COO)

\* v.s. – very strong, s. – strong, m. – medium, w. – weak, br. – broad, v – stretching, δ – bending, ω – wagging, tw – twisting, γ – rocking.