Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary data

Trinuclear $\{Sr[UO_2L_3]_2(H_2O)_4\}$ and Pentanuclear $\{Sr[UO_2L_3]_4\}^{2-}$ Uranyl Monocarboxylate Complexes (*L* – Acetate or *n*-Butyrate ion)

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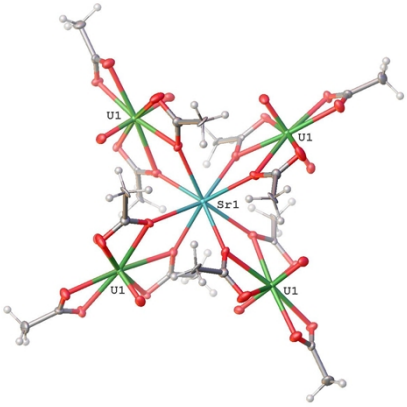

Figure S1. ORTEP view of a pentanuclear anionic complex $\{Sr[UO_2(CH_3COO)_3]_4\}^{2-}$ in the structure of **1** (p = 50%).

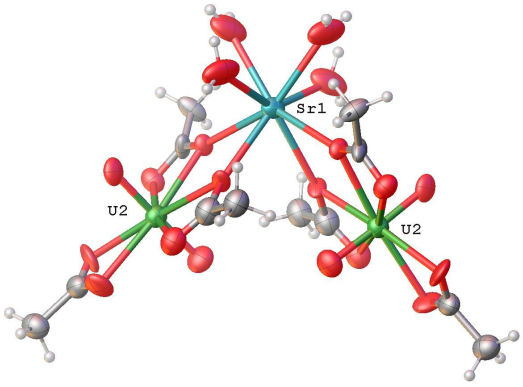

Figure S2. ORTEP view of a trinuclear neutral complex $\{Sr(H_2O)_4[UO_2(CH_3COO)_3]_2\}$ in the structure of **2** (p = 50%).

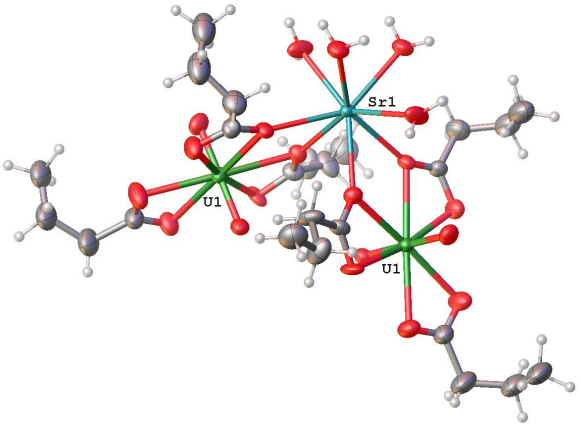

Figure S3. ORTEP view of a trinuclear neutral complex $\{Sr(H_2O)_4[UO_2(C_3H_7COO)_3]_2\}$ in the structure of **3** (p = 50%).

Table S1. Assignment of absorption bands in FTIR spectra of $Cs_2\{Sr[UO_2L_3]_4\}$ (**1**), $[Sr(H_2O)_6][UO_2L_3]_2\{Sr(H_2O)_4[UO_2L_3]_2\}_2$ (**2**) and $\{Sr(H_2O)_4[UO_2L_3]_2\}\cdot 2H_2O$ (**3**) *

Wave number, cm^{-1}			Assignment
1	**2**	**3**	
–	3436 s.	3493 s.	$\nu_s(H_2O)$, $\nu_{as}(H_2O)$
		2966 s.	$\nu_{as}(CH_3)$
2927 w.	2934 w.	2935 m.	$\nu_s(CH_3)$
–	–	2908 w.	$\nu_{as}(CH_2)$
2854 w.		2876 m.	$\nu_s(CH_3)$
–	1634 m.	1639 m.	$\delta(H_2O)$
1550 v.s.	1543 v.s.	1534 v.s.	$\nu_{as}(COO)$
1468 v.s. 1408 m.	1467 v.s. 1412 v.s.	1465 v.s. 1425 s.	$\nu_s(COO)$, $\delta_{as}(CH_3)$
–	–	1412 s.	$\delta(C_\alpha H_2)$
	1349 m.	1381 w.	$\delta_s(CH_3)$
–	–	1347 w.	$\omega(C_\alpha H_2)$
–	–	1315 m.	$\omega(C_\beta H_2)$
–	–	1261 m.	$tw(C_\alpha H_2)$
–	–	1212 w.	$tw(C_\beta H_2)$
–	–	1099 w.	$\nu(C_\beta C_\alpha)$
1052 w. 1018 w.	1052 m. 1016 m.	1080 w. 1051 w.	$\gamma(CH_3)$
–	–	955 w.	$\nu(C_\gamma C_\beta)$
922 v.s.	924 v.s.	926 v.s.	$\nu_{as}(UO_2)$
954 w.		903 m. 876 w.	$\nu(C_\alpha C)$
846 w.	847 w.	845 w.	$\nu_s(UO_2)$
–	–	806 w. 798 w.	$\gamma(C_\alpha H_2)$
–	–	754 w. 729 w.	$\gamma(C_\beta H_2)$
679 v.s.	681 v.s.	666 w. 643 w.	$\delta(COO)$
612 w.	612 s.	609 w.	$\gamma(COO)$
	534 w.	536 w. 530 w.	$\omega(COO)$

* v.s. – very strong, s. – strong, m. – medium, w. – weak.

Analysis of Intermolecular Interactions by means of molecular Voronoi–Dirichlet polyhedra. Intermolecular interactions in the structures of **2** and **3** were analyzed using the method of molecular Voronoi–Dirichlet (VD) polyhedra. This method allows one to describe all types of interatomic interactions automatically from one background and without a human factor. The VD polyhedron of an atom is a convex polyhedron of minimum volume, containing this point, and bounded by perpendicular planes, which pass through middle points of segments, connecting this point with all other points. Therefore VD polyhedron represents the shape of an atom in a structure of a compound. Each face of a VD polyhedron belongs to two atoms, A and B, and can be characterized by a rank (RF), which is the number of chemical bonds in the shortest chain connecting A and B. Thus, RF = 1 for all covalent bonds, and RF = 2 for A and B atoms in the chain A–D–B. If a face of the VD polyhedron of atom A is generated with atom B from another molecule (or chain, or layer), the rank of the A…B contact is set to zero, because there is no bonding chain connecting A and B. Molecular VD polyhedron results from the integration of VD polyhedra of atoms comprising a molecule. During this procedure all inner faces, corresponding to covalent interactions (RF = 1) and intramolecular contacts (RF ≥ 2), vanish inside a molecular VD polyhedron. Therefore, the faceting of a molecular VD polyhedron is formed only by faces with RF = 0, and each of them corresponds to a given contact between two atoms of neighboring molecules. Partial contributions $\Delta_{A/Z}$ of each type of contacts can be unambiguously estimated in percents by calculating the relative surface areas $S_{A/Z}$ of the corresponding faces of molecular VD polyhedron.

See also for details:

1) Shevchenko, A.P. & Serezhkin, V.N. Stereoatomic model and structure of saturated hydrocarbon crystals // Russ. J. Phys. Chem. 2004. 78. P. 1598–1606.

2) Serezhkin, V. N.; Pushkin, D. V. & Serezhkina, L. B. Analysis of the Conformational Polymorph Crystal Structures by Means of Molecular Voronoi-Dirichlet Polyhedra // Crystallogr. Rep. 2010. 55. P. 554–562.

3) Serezhkin V.N., Serezhkina L.B. & Vologzhanina A.V. Voronoi-Dirichlet tesselation as a tool for investigation of polymorphism in molecular crystals with $C_wH_xN_yO_z$ composition and photochromic properties // Acta Crystallogr. 2012. B68. P. 305–312.

Table S2. Characteristics of intermolecular interactions in the structures of **2** and **3** calculated by the method of molecular VD polyhedra *

Type of contact *A*/*Z*	*k*	d_{min}–d_{max}, Å	$S_{A/Z}$, Å^2	$\Delta_{A/Z}$, %
$[Sr(H_2O)_6][UO_2L_3]_2\{Sr(H_2O)_4[UO_2L_3]_2\}_2$ (**2**)				
O/O	120	2.84–4.21	96.6	4.7
C/O	32	3.14–3.89	30.3	1.5
H/O	568	1.93–5.27	1072.1	52.7
H/C	84	2.67–4.09	70.9	3.5
H/H	496	2.05–5.56	764.8	37.6
Total	1300	1.93–5.56	2034.7	100.0
$\{Sr(H_2O)_4[UO_2L_3]_2\}\cdot 2H_2O$ (**3**)				
O/O	12	2.75–3.33	7.0	0.8
C/O	6	3.12–3.32	0.4	<0.1
H/O	206	1.90–4.19	363.9	39.4
H/C	32	2.61–4.27	21.9	2.4
H/H	346	1.91–5.01	529.2	57.4
Total	602	1.90–5.01	922.4	100.0

* All possible types of intermolecular contacts *A*/*Z* with the rank of VD polyhedra equal to zero are taken into account. *k* – number of contacts, *d* – range of interatomic *A*…*Z* distances, $S_{A/Z}$ – total area of faces of VD polyhedron, corresponding to contacts *A*/*Z*, and $\Delta_{A/Z}$ – partial contribution of *A*/*Z* interactions into the total area of faces of molecular VD polyhedron, corresponding to one formula unit of the compound.