

Die beiden kurzen Kontaktabstände wachsen mit der Größe des Kations, wobei sich die Struktur des NH_4I_3 diesmal in den allgemeinen Gang einordnet.

Die hier vorgestellte Verbindungsreihe MI_3 , $M = \text{Tl}$, Rb , Cs , NH_4 verdeutlicht die strukturelle Flexibilität der Triiodidionen und -verbände. Diese geben den vom Kation diktierten Einflüssen nach, ohne daß der gemeinsame Strukturtyp verlassen wird.

Die Züchtung geeigneter Einkristalle haben die Herren cand. chem. G. Scholz und N. Behrendorf als Praktikumsaufgaben durchgeführt. Die Deutsche Forschungsgemeinschaft und der Fonds der Chemischen Industrie haben diese Arbeit durch Sachmittel unterstützt. Wir danken den Genannten.

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Structure of Strontium Tricarbonatodioxouranate(VI) Octahydrate

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Abstract. $\text{Sr}_2[\text{UO}_2(\text{CO}_3)_3] \cdot 8\text{H}_2\text{O}$, $M_r = 769.4$, monoclinic, $P2_1/c$, $a = 11.379(2)$, $b = 11.446(2)$, $c = 25.653(4)$ Å, $\beta = 93.40(1)^\circ$, $V = 3335.3(5)$ Å³, $Z = 8$, $D_x = 3.064$ g cm⁻³, $\text{Mo K}\alpha$, $\lambda = 0.71069$ Å, $\mu = 154$ cm⁻¹, $F(000) = 2832$, $T = 295$ K, final $R = 0.037$ for 3835 observed reflections. One eight-coordinated and three nine-coordinated Sr atoms, two $[\text{UO}_2(\text{CO}_3)_3]$ units with U in hexagonal bipyramidal coordination, thirteen Sr-bonded water molecules and three lattice water molecules per asymmetric unit build up a complicated framework structure. Sr–O distances are in the range 2.49(1)–2.92(1) Å; U–O(uranyl) is 1.784(13) Å, and U–O(carbonate) is 2.43(2) Å (averages).

Introduction. In a systematic study of uranyl carbonate minerals and related synthetic compounds (Mereiter, 1986) the title compound was of interest. It belongs to a series of salts $M_2[\text{UO}_2(\text{CO}_3)_3] \cdot n\text{H}_2\text{O}$, where $M = \text{Mg}$, Ca , Sr , Ba and certain combinations thereof and $n = 6$ to 18. These salts crystallize from aqueous solutions containing UO_2^{2+} and CO_3^{2-} in the molar ratio $\sim 1:3$, in which uranium is mainly present as the complex anion

$[\text{UO}_2(\text{CO}_3)_3]^{4-}$. The salts represent in part well known uranium secondary minerals, namely bayleyite, $\text{Mg}_2[\text{UO}_2(\text{CO}_3)_3] \cdot 18\text{H}_2\text{O}$, swartzite, $\text{CaMg}[\text{UO}_2(\text{CO}_3)_3] \cdot 12\text{H}_2\text{O}$, and liebigit, $\text{Ca}_2[\text{UO}_2(\text{CO}_3)_3] \cdot 11\text{H}_2\text{O}$ (Fron del, 1958; Alwan & Williams, 1980). The title compound (not yet identified as a mineral) was previously reported as a nonhydrate (Bachelet, Cheylan, Douis & Goulette, 1952; Jindra & Škramovský, 1966).

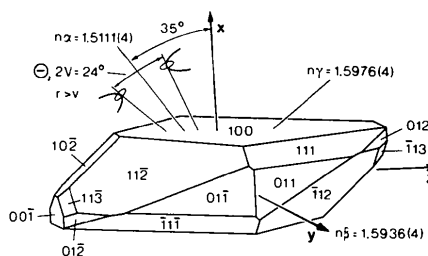


Fig. 1. Crystal of $\text{Sr}_2[\text{UO}_2(\text{CO}_3)_3] \cdot 8\text{H}_2\text{O}$ with optical data ($\lambda = 589$ nm). Pleochroism: n_α colourless, n_β and n_γ yellow. Fluorescence bright yellow-green in UV light. No cleavage.

Experimental. Yellow crystals (Fig. 1), usual size ≤ 3 mm, severe subparallel intergrowth frequent, stable in air, grown by room-temperature evaporation of solutions containing 3.18 g Na_2CO_3 , 5.02 g $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ and 4.23 g $\text{Sr}(\text{NO}_3)_2$ in 100 g H_2O . Optical data, determined by spindle-stage methods (Bloss, 1981) and included in Fig. 1, suggested that CO_3 groups within the crystals are all oriented approximately parallel to $(10\bar{2})$. The leftmost quarter of a crystal of the shape shown was cut off approximately parallel to (100) to provide a chip of ~ 0.2 mm diameter for X-ray investigations. Preliminary cell and space-group information from precession photographs. Further work on Philips PW 1100 diffractometer using graphite-monochromatized $\text{Mo } K\alpha$ radiation. Unit-cell dimensions from 42 reflections, $5 < \theta < 20^\circ$. Data collected using ω scans, scan width 1° , scan rate 2° min^{-1} ; three standard reflections, $\pm 2\%$ variation. 5895 reflections measured, θ : $2 \rightarrow 25^\circ$, h : $-13 \rightarrow 13$, k : $0 \rightarrow 13$, l : $0 \rightarrow 30$; 3835 with $I > 3\sigma(I)$ considered observed and used in structure refinement. Absorption correction by Gaussian integration, transmission factors 0.136–0.257. Structure solved by Patterson and Fourier methods, H atoms not located. Refinement on F with anisotropic temperature factors only for Sr and U. Final $R = 0.037$, $wR = 0.038$, $w = [\sigma^2(F_o) + 0.00025F_o^2]^{-1}$, $(A/\sigma)_{\text{max}} = 0.05$, $\Delta\rho_{\text{max}} -1.0$ and $1.5 \text{ e } \text{Å}^{-3}$ in the vicinity of U. Isotropic extinction parameter $X = 0.00054$ according to definition of program *SHELX76* (Sheldrick, 1976), with which most calculations were carried out. Atomic scattering factors from *SHELX76*.

Discussion. Final positional parameters and isotropic temperature factors are given in Table 1, important bond lengths and angles in Table 2.* Fig. 2 shows the asymmetric unit of the structure and the atom-numbering scheme.

$\text{Sr}-\text{O}(W)$ bond distances ($W = \text{H}_2\text{O}$) are in the range 2.49 (1) to 2.92 (1) Å with mean values of 2.62 (14) Å for the eight-coordinated atom Sr(1) and 2.67 (12) Å for the nine-coordinated atoms Sr(2), Sr(3) and Sr(4). Next-largest $\text{Sr}-\text{O}(W)$ distances exceed 3.70 Å. The coordination figures of the four Sr atoms can with reservations be described as trigonal prisms which have two or three square faces capped by additional ligands. This type of coordination is frequently met in oxygen compounds of Sr (Fischer, 1970), a well known example is $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ (Wells, 1975).

* Lists of structure factors, anisotropic thermal parameters, coordination geometry of the water molecules, and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43147 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The two independent $[\text{UO}_2(\text{CO}_3)_3]$ units consist of essentially linear uranyl groups which are equatorially chelated by three bidentate CO_3 groups. The range and mean values of bond lengths and angles show, taking into account the standard deviations, a reasonable agreement with the more precisely determined dimensions of corresponding units in bayleyite, liebigite and schrockingerite, $\text{NaCa}_3[\text{UO}_2(\text{CO}_3)_3](\text{SO}_4)\text{F} \cdot 10\text{H}_2\text{O}$ (Mayer & Mereiter, 1986; Mereiter, 1982, 1986). Bond lengths of the units in these three compounds average $\langle \text{U}-\text{O} \rangle = 1.784$ (13) Å for uranyl O atoms, $\langle \text{U}-\text{O} \rangle = 2.430$ (18) and $\langle \text{C}-\text{O} \rangle = 1.298$ (9) Å for uranium-chelating carbonate O atoms, and $\langle \text{C}-\text{O} \rangle = 1.251$ (11) Å for the terminal carbonate O atoms, while the corresponding figures for the title compound are 1.784 (13), 2.427 (22), 1.290 (19) and 1.254 (7) Å. The pronounced distortions of the CO_3 groups in all these compounds – $\text{O}-\text{C}-\text{O}$ angles which face

Table 1. Atomic coordinates and isotropic thermal parameters

	x	y	z	$B(\text{Å}^2)$
Sr(1)	0.81157 (10)	0.07388 (10)	0.08681 (4)	1.64 (3)†
Sr(2)	0.51304 (9)	0.26086 (10)	0.11385 (4)	1.48 (3)†
Sr(3)	0.45730 (10)	0.61617 (10)	0.13575 (4)	1.53 (3)†
Sr(4)	0.16313 (10)	0.79146 (10)	0.17865 (4)	1.69 (3)†
U(1)	0.28478 (4)	0.25102 (4)	-0.02337 (2)	0.95 (1)†
O(1)	0.4030 (7)	0.2558 (7)	-0.0655 (3)	1.6 (2)
O(2)	0.1635 (7)	0.2539 (7)	0.0187 (3)	2.0 (2)
C(1)	0.3639 (10)	0.4696 (11)	0.0224 (4)	1.4 (2)
O(3)	0.2921 (7)	0.4610 (7)	-0.0201 (3)	1.4 (2)
O(4)	0.3983 (7)	0.3711 (7)	0.0407 (3)	1.7 (2)
O(5)	0.3947 (8)	0.5678 (8)	0.0413 (3)	2.2 (2)
C(2)	0.3706 (10)	0.0396 (10)	0.0270 (4)	1.2 (2)
O(6)	0.3950 (7)	0.1428 (7)	0.0444 (3)	1.8 (2)
O(7)	0.2970 (7)	0.0394 (7)	-0.0138 (3)	1.8 (2)
O(8)	0.4148 (7)	-0.0516 (8)	0.0459 (3)	2.2 (2)
C(3)	0.1204 (10)	0.2322 (10)	-0.1104 (4)	1.4 (2)
O(9)	0.1649 (7)	0.1428 (7)	-0.0857 (3)	1.9 (2)
O(10)	0.1528 (7)	0.3291 (8)	-0.0923 (3)	2.1 (2)
O(11)	0.0514 (7)	0.2172 (8)	-0.1502 (3)	2.2 (2)
U(2)	0.71589 (4)	0.61849 (4)	0.26341 (2)	1.00 (1)†
O(12)	0.6210 (7)	0.6367 (7)	0.3161 (3)	1.7 (2)
O(13)	0.8115 (8)	0.5984 (8)	0.2123 (3)	2.3 (2)
C(4)	0.6085 (10)	0.4052 (10)	0.2261 (4)	1.3 (2)
O(14)	0.6890 (7)	0.4069 (7)	0.2647 (3)	1.6 (2)
O(15)	0.5737 (7)	0.5061 (8)	0.2103 (3)	1.8 (2)
O(16)	0.5659 (7)	0.3113 (7)	0.2087 (3)	1.9 (2)
C(5)	0.6279 (10)	0.8321 (11)	0.2183 (5)	1.6 (2)
O(17)	0.5929 (7)	0.7329 (7)	0.2012 (3)	2.0 (2)
O(18)	0.7128 (7)	0.8277 (8)	0.2536 (3)	2.0 (2)
O(19)	0.5872 (8)	0.9268 (8)	0.2012 (3)	2.5 (2)
C(6)	0.9094 (10)	0.6044 (10)	0.3411 (4)	1.4 (2)
O(20)	0.8812 (7)	0.7024 (8)	0.3179 (3)	2.1 (2)
O(21)	0.8559 (7)	0.5140 (8)	0.3203 (3)	2.2 (2)
O(22)	0.9790 (7)	0.5979 (8)	0.3807 (3)	2.3 (2)
W(1)	0.5947 (7)	0.0439 (7)	0.1140 (3)	1.5 (2)
W(2)	0.6483 (7)	0.2300 (7)	0.0291 (3)	1.9 (2)
W(3)	0.7660 (7)	0.2548 (8)	0.1409 (3)	1.9 (2)
W(4)	0.6201 (7)	0.4689 (7)	0.1073 (3)	1.7 (2)
W(5)	0.3568 (7)	0.4104 (7)	0.1503 (3)	1.7 (2)
W(6)	0.3776 (7)	0.8302 (7)	0.1358 (3)	1.8 (2)
W(7)	0.3412 (7)	0.6448 (7)	0.2249 (3)	1.8 (2)
W(8)	0.2037 (7)	0.6206 (8)	0.1152 (3)	2.1 (2)
W(9)	0.8470 (7)	-0.0056 (8)	0.1893 (3)	2.3 (2)
W(10)	0.9297 (9)	0.1796 (9)	0.0185 (4)	3.6 (2)
W(11)	0.1395 (8)	0.8912 (8)	0.0820 (4)	3.1 (2)
W(12)	0.0694 (7)	0.5924 (8)	0.2102 (3)	2.3 (2)
W(13)	0.0674 (8)	0.8293 (9)	0.2693 (3)	3.1 (2)
W(14)	0.1257 (7)	0.3734 (8)	0.1118 (3)	2.2 (2)
W(15)	0.8939 (9)	0.4449 (9)	0.1207 (4)	3.6 (2)
W(16)	0.0971 (9)	0.5800 (9)	0.0120 (4)	3.8 (2)

$$\dagger B_{\text{eq}} = \frac{2}{3}\pi^2(U_{11} + U_{22} + U_{33}).$$

uranium measure about 114°, the rest about 123° – are a typical chelation effect. Least-squares-planes analysis shows that the U(1)(CO₃)₃ entity of the title compound has a similar flat conformation to liebigite and bayleyite. In comparison with them the U(2)(CO₃)₃ entity is more puckered. R.m.s. deviations of the atoms from the LS planes are 0.039 Å for U(1)(CO₃)₃ and 0.094 Å for U(2)(CO₃)₃.*

* See deposition footnote.

Table 2. Selected bond lengths (Å) and angles (°)

Sr coordination polyhedra			
Sr(1)—O(7 ⁱ)	2.54 (1)	Sr(2)—O(4)	2.56 (1)
Sr(1)—O(9 ⁱ)	2.50 (1)	Sr(2)—O(6)	2.55 (1)
Sr(1)—O(22 ⁱⁱ)	2.49 (1)	Sr(2)—O(12 ⁱⁱⁱ)	2.81 (1)
Sr(1)—W(1)	2.63 (1)	Sr(2)—O(16)	2.54 (1)
Sr(1)—W(2)	2.92 (1)	Sr(2)—W(1)	2.65 (1)
Sr(1)—W(3)	2.56 (1)	Sr(2)—W(2)	2.76 (1)
Sr(1)—W(9)	2.79 (1)	Sr(2)—W(3)	2.92 (1)
Sr(1)—W(10)	2.57 (1)	Sr(2)—W(4)	2.69 (1)
Mean	2.624	Sr(2)—W(5)	2.68 (1)
Sr(3)—O(1 ^{iv})	2.87 (1)	Mean	2.683
Sr(3)—O(5)	2.55 (1)	Sr(4)—O(11 ^v)	2.51 (1)
Sr(3)—O(15)	2.59 (1)	Sr(4)—O(14 ^{vi})	2.53 (1)
Sr(3)—O(17)	2.58 (1)	Sr(4)—O(21 ^{vi})	2.56 (1)
Sr(3)—W(4)	2.64 (1)	Sr(4)—W(6)	2.77 (1)
Sr(3)—W(5)	2.65 (1)	Sr(4)—W(7)	2.84 (1)
Sr(3)—W(6)	2.61 (1)	Sr(4)—W(8)	2.60 (1)
Sr(3)—W(7)	2.73 (1)	Sr(4)—W(11)	2.73 (1)
Sr(3)—W(8)	2.90 (1)	Sr(4)—W(12)	2.66 (1)
Mean	2.681	Sr(4)—W(13)	2.66 (1)
Mean	2.681	Mean	2.651
UO ₂ O ₂ polyhedra			
U(1)—O(1)	1.78 (1)	O(1)—U(1)—O(2)	177.1 (4)
U(1)—O(2)	1.80 (1)	O(1)—U(1)—O(3)—O(10)	88.0–94.2 (4)
U(1)—O(3)	2.41 (1)	O(2)—U(1)—O(3)—O(10)	87.8–89.9 (4)
U(1)—O(4)	2.45 (1)	O(2)—U(1)—O(4)	53.2 (3)
U(1)—O(6)	2.42 (1)	O(4)—U(1)—O(6)	64.9 (3)
U(1)—O(7)	2.44 (1)	O(6)—U(1)—O(7)	52.8 (3)
U(1)—O(9)	2.39 (1)	O(7)—U(1)—O(9)	65.1 (3)
U(1)—O(10)	2.42 (1)	O(9)—U(1)—O(10)	52.9 (3)
Mean U(1)—O(3)—O(10)	2.421	O(10)—U(1)—O(3)	71.1 (3)
U(2)—O(12)	1.79 (1)	O(12)—U(2)—O(13)	178.7 (4)
U(2)—O(13)	1.77 (1)	O(12)—U(2)—O(14)—O(21)	87.6–94.7 (4)
U(2)—O(14)	2.44 (1)	O(13)—U(2)—O(14)—O(21)	86.5–93.3 (4)
U(2)—O(15)	2.42 (1)	O(14)—U(2)—O(15)	53.2 (3)
U(2)—O(17)	2.44 (1)	O(15)—U(2)—O(17)	65.1 (3)
U(2)—O(18)	2.41 (1)	O(17)—U(2)—O(18)	52.7 (3)
U(2)—O(20)	2.47 (1)	O(18)—U(2)—O(20)	71.2 (3)
U(2)—O(21)	2.41 (1)	O(20)—U(2)—O(21)	52.9 (3)
Mean U(2)—O(14)—O(21)	2.433	O(21)—U(2)—O(14)	65.1 (3)
CO ₃ groups			
C(1)—O(3)	1.33 (2)	O(3)—C(1)—O(4)	113.5 (11)
C(1)—O(4)	1.27 (2)	O(3)—C(1)—O(5)	121.5 (11)
C(1)—O(5)	1.27 (2)	O(4)—C(1)—O(5)	125.0 (12)
C(2)—O(6)	1.29 (2)	O(6)—C(2)—O(7)	113.4 (11)
C(2)—O(7)	1.30 (2)	O(6)—C(2)—O(8)	123.9 (12)
C(2)—O(8)	1.25 (2)	O(7)—C(2)—O(8)	122.6 (12)
C(3)—O(9)	1.29 (2)	O(9)—C(3)—O(10)	114.9 (11)
C(3)—O(10)	1.25 (2)	O(9)—C(3)—O(11)	119.8 (11)
C(3)—O(11)	1.26 (2)	O(10)—C(3)—O(11)	125.2 (12)
C(4)—O(14)	1.31 (2)	O(14)—C(4)—O(15)	114.5 (11)
C(4)—O(15)	1.28 (2)	O(14)—C(4)—O(16)	121.5 (11)
C(4)—O(16)	1.25 (2)	O(15)—C(4)—O(16)	123.8 (12)
C(5)—O(17)	1.27 (2)	O(17)—C(5)—O(18)	114.5 (11)
C(5)—O(18)	1.29 (2)	O(17)—C(5)—O(19)	123.5 (12)
C(5)—O(19)	1.25 (2)	O(18)—C(5)—O(19)	122.0 (12)
C(6)—O(20)	1.30 (2)	O(20)—C(6)—O(21)	113.7 (11)
C(6)—O(21)	1.30 (2)	O(20)—C(6)—O(22)	123.2 (12)
C(6)—O(22)	1.25 (2)	O(21)—C(6)—O(22)	123.0 (12)

Symmetry code: none x, y, z ; (i) $1-x, -y, -z$; (ii) $2-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iv) $1-x, 1-y, z$; (v) $-x, 1-y, -z$; (vi) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$.

It has been ascertained that the structure does not contain cavities to take up more water molecules than those listed in Table 1. Therefore, the title compound is an octahydrate rather than a nonahydrate as previously reported (*cf. Introduction*). Low thermal parameters indicate all water molecules to be firmly anchored in the structure. Hydrogen bonds, derived by stereochemical considerations, show $W\cdots O$ and $W\cdots W$ distances in the range 2.62 (1) to 3.21 (1) Å, 25 of them are below 3.00 Å. According to their coordination three kinds of molecules can be distinguished: (i) $W(1)$ through $W(8)$ which bridge pairs of Sr atoms [$Sr-W-Sr = 92.7$ (4)– 102.9 (4)°] and donate pairs of hydrogen bonds; (ii) $W(9)$ through $W(13)$, each bonded to one Sr and involved in two to three hydrogen bonds; (iii) $W(14)$, $W(15)$ and $W(16)$, three lattice water molecules which are anchored by four to five hydrogen bonds.

Sr₂[UO₂(CO₃)₃].8H₂O possesses a complicated framework structure which is difficult to visualize. Two fundamental connection principles can be recognized. The first one is a finite S-shaped tetramer of Sr polyhedra which are directly tied together *via* the water molecules $W(1)$ through $W(8)$ by one edge- and two face-sharing links (Fig. 2). The second one is a zigzag ribbon parallel to [201] which is formed by both sorts of [UO₂(CO₃)₃] units and all those Sr polyhedra which are attached to them *via* bonds to carbonate O atoms (Fig. 3). Within this ribbon each unit is linked with two Sr *via* terminal carbonate O atoms and with two Sr *via* pairs of U-bonded carbonate O atoms, *i.e.* by polyhedral edge sharing. Despite many similarities in the environments of the two independent units, there is a difference between them in the relative position of one Sr. As a result, CO₃ groups belonging to U(1) are each bonded to two Sr, while the CO₃ groups belonging to U(2) are each bonded to three, one and two Sr, respectively. The only other direct links between the

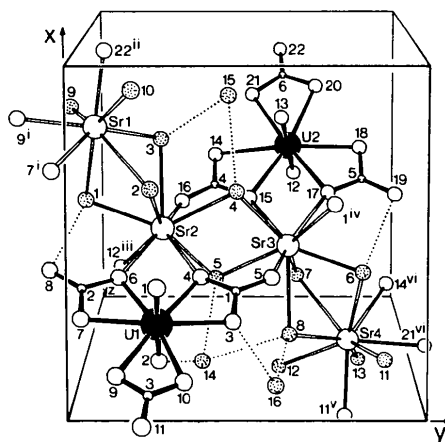


Fig. 2. View of the asymmetric unit. Water molecules and postulated hydrogen bonds are dotted, Sr-coordination figures completed. The symmetry code is defined in Table 2.

units and Sr are U(1)—O(1)—Sr(3) and U(2)—O(12)—Sr(2), *i.e.* via uranyl O atoms and thus perpendicular to the ribbons (not shown in Fig. 3).

The combination of these two connection principles and their conjunction with numerous hydrogen bonds results in a framework structure (Fig. 4) in which the zigzag ribbons are aligned in planes parallel to (10 $\bar{2}$),

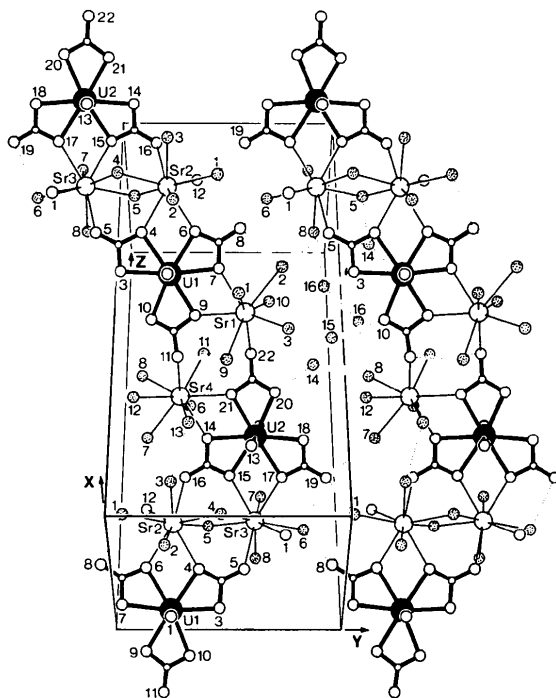


Fig. 3. Two Sr—[UO₂(CO₃)₃] zigzag ribbons extending along [201]. Water molecules and postulated hydrogen bonds are dotted. View direction inclined at about 45° to x and z axes.

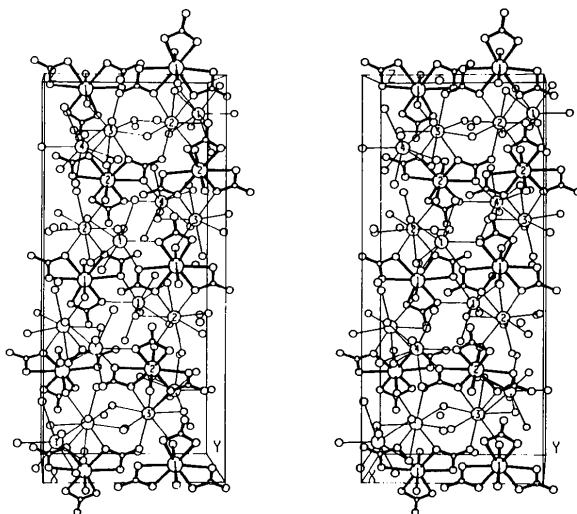


Fig. 4. Stereoscopic view of the structure along a^* .

but in which the cohesive forces are most effective parallel to (100), the plane parallel to which crystals of the title compound are most extended (Fig. 1). What remains to be mentioned is the presence of local pseudoinversions. One of them, the central point between Sr(2) and Sr(3) at $x \approx 0.49$, $y \approx 0.44$ and $z \approx 0.13$ (Fig. 2), relates quite well most atoms of the asymmetric unit. One major violation of this pseudo-symmetry concerns W(10), bonded to eight-coordinated Sr(1), which has W(12) and W(13), bonded to nine-coordinated Sr(4), as its counterparts.

A comparison of the structures of Mg₂[UO₂(CO₃)₃].18H₂O (bayleyite; Mayer & Mereiter, 1986), Ca₂[UO₂(CO₃)₃].11H₂O (liebigite; Mereiter, 1982) and Sr₂[UO₂(CO₃)₃].8H₂O reveals the following trends: (i) Increasing coordination numbers and increasing polyhedral condensation for divalent cations — isolated Mg(H₂O)₆ octahedra which are exclusively hydrogen bonded to [UO₂(CO₃)₃] units *versus* CaO₃(H₂O)₄ and CaO₄(H₂O)₄ polyhedra which are directly linked to [UO₂(CO₃)₃] units but not among themselves *versus* Sr(O₂H₂O)₈ and Sr(O₂H₂O)₉ polyhedra which are directly linked to [UO₂(CO₃)₃] units and among themselves as well. Thus, a transition takes place from an island-like structure in bayleyite *via* a layered structure in liebigite to a framework structure in the title compound. (ii) Decreasing number of lattice water molecules from 6 *via* 3 to 1.5 H₂O per formula unit.

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