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Description and crystal structure of albrechtschraufite, $MgCa_4F_2[UO_2(CO_3)_3]_2 \cdot 17\text{-}18H_2O$

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Abstract Albrechtschraufite, $MgCa_4F_2[UO_2(CO_3)_3]_2 \cdot 17\text{-}18H_2O$, triclinic, space group $P\bar{1}$, $a=13.569(2)$, $b=13.419(2)$, $c=11.622(2)$ Å, $\alpha=115.82(1)$, $\beta=107.61(1)$, $\gamma=92.84(1)°$ (structural unit cell, not reduced), $V=1774.6(5)$ Å^3, $Z=2$, $D_c=2.69$ g/cm^3 (for 17.5 H$_2$O), is a mineral that was found in small amounts with schröckingerite, $NaCa_3F[UO_2(CO_3)_3]$ $(SO_4) \cdot 10H_2O$, on a museum specimen of uranium ore from Joachimsthal (Jáchymov), Czech Republic. The mineral forms small grain-like subhedral crystals (≤ 0.2 mm) that resemble in appearance liebigite, $Ca_2[UO_2(CO_3)_3] \cdot \sim 11H_2O$. Colour pale yellow-green, luster vitreous, transparent, pale bluish green fluorescence under ultraviolet light. Optical data: Biaxial negative, $nX=1.511(2)$, $nY=1.550(2)$, $nZ=1.566(2)$, $2V=65(1)°$ ($\lambda=589$ nm), $r < v$ weak. After qualitative tests had shown the presence of Ca, U, Mg, CO$_2$ and H$_2$O, the chemical formula was determined by a crystal structure analysis based on X-ray four-circle diffractometer data. The structure was later on refined with data from a CCD diffractometer to $R1=0.0206$ and $wR2=0.0429$ for 9,236 independent observed reflections. The crystal structure contains two independent $[UO_2(CO_3)_3]^{4-}$ anions of which one is bonded to two Mg and six Ca while the second is bonded to only one Mg and three Ca. Magnesium forms a $MgF_2(O_{carbonate})_3(H_2O)$ octahedron that is linked via the F atoms with three Ca atoms so as to provide each F atom with a flat pyramidal coordination by one Mg and two Ca. Calcium is 7- and 8-coordinate forming CaFO$_6$,

CaF$_2$O$_2$(H$_2$O)$_4$, CaFO$_3$(H$_2$O)$_4$ and CaO$_2$(H$_2$O)$_6$ coordination polyhedra. The crystal structure is built up from $MgCa_3F_2[UO_2(CO_3)_3] \cdot 8H_2O$ layers parallel to (001) which are linked by $Ca[UO_2(CO_3)_3] \cdot 5H_2O$ moieties into a framework of the composition $MgCa_4F_2[UO_2(CO_3)_3] \cdot 13H_2O$. Five additional water molecules are located in voids of the framework and show large displacement parameters. One of the water positions is partly vacant, leading to a total water content of 17-18H$_2$O per formula unit. The $MgCa_3F_2[UO_2(CO_3)_3] \cdot 8H_2O$ layers are pseudosymmetric according to plane group symmetry *cmm*. The remaining constituents do not sustain this pseudosymmetry and make the entire structure truly triclinic. A characteristic paddle-wheel motif $Ca[UO_2(CO_3)_3]_4Ca$ relates the structure of albrechtschraufite partly to that of andersonite and two synthetic alkali calcium uranyl tricarbonates.

Introduction

In the course of a study of schröckingerite, $NaCa_3F$ $(SO_4)[UO_2(CO_3)_3]_2 \cdot 10H_2O$ (Mereiter 1986a), a specimen from Joachimsthal (Jáchymov, Czech Republic) was obtained from the Naturhistorisches Museum Wien (NHM Wien specimen A.a. 6740). According to evidence and reported also by Nováček (1939) this particular specimen was part of the original material investigated by Albrecht Schrauf in his description of schröckingerite as a new mineral (Schrauf 1873). It consists of pitchblende and red dolomite as the matrix for a cover by scattered globular schröckingerite aggregates, and contains in one place an incrustation of a few milligrams of greenish yellow grain-like crystals, which were initially considered to be liebigite. When occasionally the optical properties of one of these crystals were determined by spindle-stage methods, the results indicated a new mineral to be present, which was confirmed by subsequent investigations, including a single-crystal structure determination (a distinct birefringence and a negative optic character with $2V$ about 65° were consistent with an uranyl tricarbonate containing these complexes in two

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orientations mutually inclined between 50 and 70°; and such a mineral was not known).

The mineral was named in honour of Dr. Albrecht Schrauf (1837–1897), custodian at the former Hof-Mineralien Cabinet, now Naturhistorisches Museum Wien, and professor of mineralogy at the University of Vienna. The mineral and its name were approved in 1983 by the Commission on New Minerals and Mineral Names (IMA no. 1983–078). Only a short conference abstract on the crystal structure of the mineral was subsequently published (Mereiter 1984) in the hope to find a method to synthesize the mineral, which was as yet unsuccessful. Due to various circumstances a full publication was postponed over the years until the retirement of the author and the forthcoming 90th anniversary of Prof. Josef Zemann brought new life to the matter.

Physical properties

Albrechtschraufite forms small grain-like crystals with sizes of ≤ 0.2 mm. On the holotype specimen NHM Wien A.a. 6740 the crystals form a thin incrustation that is surrounded by well-developed pseudohexagonal platelets of schröckingerite. For colour photographs of the specimen, see Online resource 1. The crystals resemble in appearance liebigite, which is well known from Joachimsthal (Ondruš et al. 1997). They are pale yellow-green in colour, transparent to translucent, and have a vitreous luster. Under ultraviolet light (long and shortwave) they fluoresce light-bluish green, similar to schröckingerite but less intense. The crystals are short prismatic in habit and incompletely developed due to intergrowths. The following forms could be identified on two crystals which were screened with an X-ray single-crystal diffractometer: {001}, {−101}, {100}, {−110}, and {1–11}. The fracture of the crystals is conchoidal, no distinct cleavage was noted. Density determined by flotation in dibromomethane/1,1,2,2-tetrabromoethane mixtures is about 2.7, while the calculated X-ray density is 2.69 g/cm^3 based on 17.5 H$_2$O per formula unit. Optically the mineral is biaxial negative with $nX=1.511(2)$, $nY=1.550(2)$, $nZ=1.566(2)$, $2V=65(1)°$ ($\lambda=589$ nm), $X^a=122°$, $X^b=100°$, $X^c=19°$, $Y^a=140°$, $Y^b=105°$, $Y^c=96°$, $Z^a=111°$, $Z^b=18°$, $Z^c=108°$ (estimated uncertainties for orientation angles 3°), dispersion $r < v$ weak, X almost colourless, Y and Z pale yellowish green, as determined by spindle stage methods (Bloss 1978) in combination with X-ray diffraction.

Chemical composition and X-ray powder pattern

The chemical formula, MgCa$_4$F$_2$[UO$_2$(CO$_3$)$_3$]$_2$·17-18H$_2$O, is mainly based on a crystal structure determination described below. Mg, Ca, and U were confirmed to be present by a qualitative analysis with the energy-dispersive detector

of a scanning electron microscope. CO$_2$ and H$_2$O were detected by microchemical tests. The theoretical chemical composition of the mineral for a water content of 17 H$_2$O is: MgO 2.82 %, CaO 15.70 %, UO$_3$ 40.03 %, CO$_2$ 18.48 %, H$_2$O 21.44 %, F 2.66 %. An X-ray powder photograph of some crystal fragments was recorded with a Gandolfi camera and Ni-filtered Cu$K\alpha$ radiation. The strongest low 2θ lines in this pattern corresponded qualitatively with the pattern calculated from the crystal structure model, which is shown in Fig. 1. The strongest and most characteristic 12 lines in this pattern are (d_{calc} in Å/(I)/hkl): 11.811/(98)/010; 10.283/(32)/01-1; 9.739/(100)/001 & 1-10; 7.841/(8)/110; 6.628/(46)/02-1; 6.527/(42)/1-1-1; 6.321/(82)/200; 6.215/(52)/011; 6.138/(48)/2-10; 5.927/(46)/21-1; 5.844/(25)/; 1-20; 5.759/(40)/11-2.

Crystal structure determination

X-ray single-crystal data were initially measured with a Philips PW1100 four-circle diffractometer equipped with a scintillation detector and graphite monochromatized Mo$K\alpha$ radiation. A larger number of tiny crystal fragments (< 0.15 mm) had to be tested before one with acceptable reflection profiles and sufficient reflection intensities could be found, which was then used for data collection by θ-2θ scans up to $\theta_{max}=25°$. The raw data consisting of 6,255 independent reflections were corrected for absorption using an analytic method (Gaussian integration) and approximate boundary faces to describe the basic shape of the crystal. Assuming the mineral to have the chemical formula of the calcium uranyl tricarbonate liebigite, the structure was solved with direct and Fourier methods (Shelx76; Sheldrick 2008). The refinement (Shelx76; Sheldrick 2008) with anisotropic temperature factors but without hydrogen atoms converged at $R1=0.031$ for 4,347 independent reflections with $I>3\sigma(I)$. The assignment of the cation and fluorine positions was based on the height of their Fourier peaks and crystal chemical interpretation followed by least-squares refinement of their population parameters. Later on, a new data set was measured with this crystal when a Bruker Smart CCD diffractometer (Mo$K\alpha$ radiation, graphite monochromator) became available. This time eight sets of 602 ω-scan frames with different φ-settings and $\Delta\omega=0.3°$ / 40 s per frame were recorded and integrated with the program SAINT up to $\theta_{max}=30°$ (Bruker 2002). The 56,860 data were corrected for $\lambda/2$ effects and for absorption using the multi-scan method and the program SADABS (Bruker 2002). Merging provided 10,366 independent reflections of which 9,236 were observed ($I>2\sigma(I)$). The structure refinement (SHELXL-97; Sheldrick 2008) commenced with the previous model but tried to include also hydrogen atoms in order to get at least qualitative information about hydrogen bonding. This was possible only for the 13 cation-bonded water molecules which were refined as idealized rigid groups (O-H=0.80 Å, H-O-H=

Fig. 1 Most characteristic part of the X-ray powder pattern of albrechtschraufite calculated from the crystal structure data for CuKα radiation (λ=1.5418 Å) and a reflection half width of 0.15° giving *hkl* indices of the strongest reflections
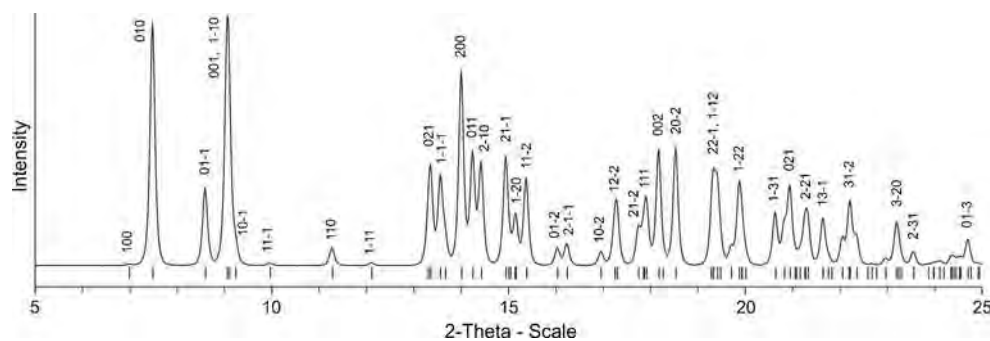
108°, $U_{iso}(H)=1.2 \times U_{eq}(O)$) in *x,y,z* and orientation using AFIX 6 restraints of program SHELXL-97 (Sheldrick 2008). In three cases additional distance restraints had to be applied for reasonable results. After optimization of the hydrogen atoms, they were in the final refinement only moved with their oxygen atoms but not rotated (AFIX 3). Also refined was the occupation factor of water molecule W(18), which was too close to a centre of inversion for full occupation. Moreover, the site occupation factors of Mg, Ca, F and the remaining water molecules were probed with the result that all showed full occupation by their respective atom species within narrow limits of error (refined population factors for Mg 1.008(5); for Ca 1.007–1.016(3); for fluorine 1.020–1.024(8), but 1.236–1.241(9) when calculated as O). In the final refinement all these population factors were fixed at 1 except for the water oxygen atom W(18) (final occupancy 0.29(1)). This refinement converged at the very satisfying results presented in Table 1 together with other crystallographic data. Throughout this work a triclinic structural unit cell in space group $P\bar{1}$ was used in order to give important structural features simple Miller indices. The conventional reduced cell has space group $P\bar{1}$, *a*=11.622(2), *b*=13.390(2), *c*=13.569(2) Å, *α*=71.81 (1), *β*=72.39(1), *γ*=64.44(1)°. The transformation matrix structural to reduced cell is (001/011/-100). Atomic parameters of the non-hydrogen atoms are given in Table 2. For brevity the oxygen atoms of the water molecules were denoted by "W". Selected bond lengths and bond angles are listed in Table 3. A complete list of the atomic parameters including U_{ij} and hydrogen atoms is given in Online Resource 1. A CIF with structural data has been deposited and may be obtained from Fachinformationszentrum Karlsruhe, 76344 Eggenstein-Leopoldshafen, Germany (fax: (+49)7247-808-666; e-mail: crysdata@fiz-karlsruhe.de, http://www.fiz-karlsruhe.de/request_for_deposited_data.html) on quoting the ICSD number 424660.

Description of the crystal structure

Uranyl tricarbonate groups

The crystal structure contains two independent $[UO_2(CO_3)_3]^{4-}$ anions in which almost linear uranyl groups $[O=U=O]^{2+}$ are equatorially chelated by three CO_3 groups. The mean bond lengths of U(1) / U(2) are <U-O> = 1.786 / 1.796 Å for the uranyl oxygen atoms and <U-O> = 2.451 / 2.423 Å for the carbonate oxygen atoms. Burns (2005) reported for 1.783 and 2.460 Å as typical mean values for (2+6) coordinated U^{6+} in mineral structures. The $U(CO_3)_3$ fragments of both anions are slightly puckered and show r.m.s. deviations from planarity of 0.048 Å for U(1) and 0.095 Å for U(2). The six independent carbonate groups have distorted triangular shapes with small O-C-O bond angles toward uranium and large ones for the rest, <O-C-O> = 114.6° and 122.7°, respectively. Their deviation from planarity is insignificant (0.002(3)–0.008(3) Å). Their C-O bond lengths vary from 1.250(4) to 1.310(3) Å and average to 1.283 Å, in good agreement with C-O=1.284(18) Å reported by Zemann (1981) in a review on the crystal chemistry of carbonate minerals. The C-O bonds to the oxygen atoms coordinating uranium average at 1.294 Å and to the terminal oxygen atoms at 1.260 Å. Unlike the U-O bonds, there is no significant difference between the mean C-O bond length of U(1) and U(2). The cation coordination of the two uranyl tricarbonate groups differs distinctly: That of U(1) is bonded to 2 Mg and 6 Ca, while that of U(2) is bonded to only 1 Mg and 3 Ca (Fig. 2). In compensation for this imbalance the $[UO_2(CO_3)_3]^{4-}$ anion of U(2) accepts a larger number of hydrogen bonds. In schröckingerite (Mereiter 1986a) the uranyl tricarbonate group is bonded via the carbonate oxygen atoms to 6 Ca and 3 Na, of which 3 Ca share edges with the UO_6 hexagon while each 1 Ca and 1 Na are bonded to the three terminal carbonate oxygen atoms. In liebigite the uranyl tricarbonate group is bonded to 4 Ca, of which 2 Ca share edges with the UO_6 hexagon, one Ca shares an edge with a CO_3 group and one is bonded to a terminal carbonate oxygen atom (Mereiter 1982). Compared with these two and three further alkali calcium uranyl tricarbonates (see below) the terminal CO_3 oxygen atoms of U(1) are unusual because they all are bonded to two divalent cations instead of at most one monovalent and one divalent cation.

Magnesium and calcium

Magnesium has an octahedral coordination by two F-atoms in *cis* arrangement, three carbonate O atoms in *facial* arrangement, and by the water molecule W(1). This MgF_2O_3W octahedron shares an $O_{carbonate}$ edge with a centrosymmetric

Table 1 Data collection and structure refinement details for albrechtschraufite

Empirical formula	$MgCa_4F_2[UO_2(CO_3)_3]_2 \cdot 17.29 H_2O^a$
Formula weight	1434.25
Temperature	297(2) K
Wavelength	0.71073 Å
Space group	$P\bar{1}$ (No. 2)
Unit cell dimensions (structural cell, not reduced, see text)	a=13.569(2) Å
	b=13.419(2) Å
	c=11.622(2) Å
	α=115.82(1)°
	β=107.61(1)°
	γ=92.84(1)°
Volume	1774.6(5) Å^3
Z	2
Density (calc. for above formula)	2.684 g/cm^3
Absorption coefficient	9.849 mm^{-1}
F(000)	1358
Crystal size	0.08×0.06×0.04 mm, yellow fragment
Θ range	1.61° to 30.03°
Index ranges	$-19 \leq h \leq 19$, $-18 \leq k \leq 18$, $-16 \leq l \leq 16$
Reflections collected/unique	56860/10366 [R_{int}=0.0302, R_{sigma}=0.0203]
Absorption correction	multi-scan (program SADABS)
Max. and min. transmission factors	0.69–0.55
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10366 / 0 / 498
Goodness-of-fit on F^2	1.112
Final R indices [$I>2\sigma(I)$]^b	R1=0.0206, wR2=0.0429 (9236 data)
R indices (all data)	R1=0.0267, wR2=0.0452 (10366 data)
Extinction coefficient	0.00074(5)
Largest diff. peak and hole	1.06 and -0.87 e Å^{-3}

^{a} 17.29 H$_2$O correspond to the X-ray site occupation factors of the water oxygen atoms, of which W(18) is partly vacant and has a refined occupancy of 0.29(1)

^{b} $R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$, $wR2 = [\Sigma(w(F_o^2 - F_c^2)^2) / \Sigma(w(F_o^2)^2)]^{\frac{1}{2}}$, $w = 1/[\sigma^2(F_o^2) + (0.0160P)^2 + 3.358P]$., $P = (F_o^2 + 2F_c^2)/3$

Table 2 Atomic coordinates and equivalent isotropic displacement parameters (Å$^2 \times 10^3$) for albrechtschraufite excluding hydrogen atoms

Atom	x	y	z	U_{eq}
Mg	0.41979(7)	0.42236(8)	0.02416(10)	12.1(2)
Ca(1)	0.48138(4)	0.14003(4)	−0.01359(6)	12.0(1)
Ca(2)	0.26561(4)	0.28073(5)	0.11208(6)	16.1(1)
Ca(3)	0.14312(4)	0.49698(5)	0.00952(6)	14.7(1)
Ca(4)	0.84563(5)	−0.14801(5)	0.60690(7)	21.6(1)
F(1)	0.42284(13)	0.30237(14)	0.07639(18)	16(1)
F(2)	0.28315(13)	0.42011(14)	0.04822(18)	17(1)
U(1)	0.785960(8)	0.222723(8)	0.024224(10)	11.9(1)
O(1)	0.74685(18)	0.15651(19)	−0.1575(2)	23(1)
O(2)	0.82393(19)	0.2874(2)	0.2066(2)	25(1)
C(1)	0.6367(2)	0.3698(2)	0.0125(3)	13(1)
O(3)	0.73351(16)	0.39875(18)	0.0304(3)	22(1)
O(4)	0.61109(16)	0.27159(17)	0.0015(2)	20(1)
O(5)	0.57073(16)	0.43339(17)	0.0070(2)	16(1)
C(2)	0.7097(2)	0.0058(2)	−0.0043(3)	15(1)
O(6)	0.65044(16)	0.07884(17)	−0.0028(2)	19(1)
O(7)	0.80697(16)	0.03892(18)	0.0097(3)	21(1)
O(8)	0.67681(17)	−0.08996(17)	−0.0198(2)	20(1)
C(3)	0.9999(2)	0.3096(2)	0.0624(3)	16(1)
O(9)	0.97519(16)	0.21572(18)	0.0643(3)	21(1)
O(10)	0.92175(16)	0.36065(18)	0.0483(2)	20(1)
O(11)	1.09083(16)	0.34862(17)	0.0737(2)	18(1)
U(2)	0.712257(8)	0.029017(8)	0.409056(10)	13.8(1)
O(12)	0.61179(19)	0.0290(2)	0.4798(2)	27(1)
O(13)	0.81365(18)	0.02859(19)	0.3390(2)	24(1)
C(4)	0.6096(3)	0.1523(3)	0.2797(3)	20(1)
O(14)	0.6776(2)	0.1997(2)	0.4022(2)	34(1)
O(15)	0.58873(18)	0.04167(18)	0.2163(2)	21(1)
O(16)	0.56460(19)	0.20789(19)	0.2235(2)	23(1)
C(5)	0.6672(2)	−0.2150(2)	0.2593(3)	14(1)
O(17)	0.61595(18)	−0.15313(17)	0.2135(2)	20(1)
O(18)	0.73345(18)	−0.15961(18)	0.3839(2)	20(1)
O(19)	0.65280(17)	−0.32068(17)	0.1888(2)	18(1)
C(6)	0.8780(2)	0.1388(2)	0.6711(3)	18(1)
O(20)	0.84375(19)	0.03029(18)	0.6060(2)	23(1)
O(21)	0.82359(19)	0.19240(18)	0.6130(2)	24(1)
O(22)	0.95725(18)	0.1897(2)	0.7792(2)	25(1)
W(1)	0.4944(2)	0.5398(2)	0.2360(3)	36(1)
W(2)	0.16162(17)	0.16731(19)	0.1731(2)	21(1)
W(3)	0.3992(2)	0.2770(2)	0.3111(3)	36(1)
W(4)	0.16557(19)	0.1755(2)	−0.1257(3)	30(1)
W(5)	0.2896(4)	0.4597(3)	0.3224(3)	84(2)
W(6)	0.03802(17)	0.58768(18)	0.1502(2)	20(1)
W(7)	0.1406(2)	0.3647(2)	−0.2292(3)	31(1)
W(8)	0.26404(19)	0.6352(2)	0.2451(3)	32(1)
W(9)	0.9554(4)	−0.2792(4)	0.6310(4)	82(2)
W(10)	0.9648(2)	−0.1445(3)	0.4849(3)	57(1)

counterpart and is linked via its two F atoms with the coordination polyhedra of Ca(1), Ca(2) and Ca(3) by corner-, edge-, and corner-sharing links (Fig. 3). The Mg-F bonds, <Mg-F> = 1.955 Å, are by ca. 0.16 Å shorter than the four Mg-O bonds, <Mg-O> = 2.118 Å, which is about twice the difference of the ionic radii of F and O (Shannon 1976). The bond valence sum for Mg is 2.00 v.u. with 0.36 and 0.37 v.u. for the two Mg-F bonds (Brese and O'Keeffe 1991). Comparable MgF$_2$O$_4$ octa-

Table 2 (continued)

Atom	x	y	z	U_{eq}
W(11)	0.9914(2)	−0.0199(2)	0.8123(3)	38(1)
W(12)	0.6816(2)	−0.0963(3)	0.6487(3)	39(1)
W(13)	0.7301(3)	−0.3298(3)	0.4698(5)	89(2)
W(14)	0.4693(3)	0.7833(3)	0.3448(5)	73(1)
W(15)	0.9132(6)	0.5259(4)	0.3904(5)	130(3)
W(16)	0.6569(7)	0.4376(4)	0.3695(7)	170(4)
W(17)	0.1280(4)	0.5998(5)	0.4224(5)	98(2)
W(18)	0.5118(16)	0.5130(15)	0.4582(14)	99(8)

"W" denote oxygen atoms of water molecules. W(18) is partly vacant and has a refined occupancy of 0.29(1)

U_{eq} is one third of the trace of the orthogonalized U_{ij} tensor

hedra are uncommon among minerals disregarding (F,OH)-bearing silicates. An example with similar bond distances but with a *trans* arrangement of F is uklonskovite, NaMg(SO$_4$)F·2H$_2$O (Sabelli 1985), while *cis*-MgF$_2$O$_4$ octahedra are found in the unusual and complicated crystal structures of wagnerite, Mg$_2$(PO$_4$)(F,OH) (Coda et al. 1967; Ren et al. 2003).

The calcium atoms in albrechtschraufite are 7- to 8-coordinate and form the following polyhedra with an increasing number of water molecules: Ca(1)FO$_6$, Ca(2)F$_2$O$_2$W$_4$, Ca(3)FO$_3$W$_4$, Ca(4)O$_2$W$_6$. The Ca(1)FO$_6$ polyedron is a distorted monocapped trigonal prism, the rest forms bicapped trigonal prisms that may be also seen as distorted square antiprisms. The mean bond lengths Ca-(F,O,W) are 2.38 Å for Ca(1) and 2.45 Å for Ca(2), Ca(3), and Ca(4). The latter value agrees well with the 2.46 Å observed for three CaFO$_5$W$_2$ polyhedra of schröckingerite (Mereiter 1986a).

Fluorine

The fluorine atoms F(1) and F(2) are coordinated by one Mg and two Ca at distances that are by 0.05 to 0.18 Å shorter than the next shortest cation-(O,W) bonds of the respective polyhedra. The bond valence sums of F(1) and F(2) are 0.96 and 0.99 v.u. (Brese and O'Keeffe 1991). This supports the refined structure model, which gave no hint for a significant substitution of F by OH. F(2) has an almost flat coordination with an offset of 0.082 Å from the Mg-Ca(2)-Ca(3) plane while F(1) is modestly pyramidal with a 0.436(2) Å offset from its Mg-Ca(1)-Ca(2) plane. The sums of the three bond angles are 347.8° for F(1) and 359.5° for F(2). In schröckingerite, fluorine is in a more pyramidal FCa$_3$ coordination with <Ca-F> = 2.317 Å and an offset of 0.71 Å imparted by an cage-like Ca$_3$F(SO$_4$) unit in which the three Ca are cyclically linked by both anions (Mereiter 1986a). In the crystal structure of sheldrickite, NaCa$_3$F$_3$(CO$_3$)$_2$·2H$_2$O (Grice et al. 1997), one of the three F atoms has a coordination resembling F(2) in albrechtschraufite.

Table 3 Selected bond distances (Å) and angles (°) in albrechtschraufite

Mg–F(1)	1.951(2)	Ca(3)–F(2)	2.227(2)
Mg–F(2)	1.958(2)	Ca(3)–O(3)#2	2.404(2)
Mg–O(19)#1	2.099(2)	Ca(3)–O(10)#2	2.409(2)
Mg–O(5)	2.121(2)	Ca(3)–W(6)#4	2.430(2)
Mg–O(5)#2	2.124(2)	Ca(3)–W(6)	2.457(2)
Mg–W(1)	2.127(3)	Ca(3)–W(8)	2.487(3)
< Mg–(F,O,W) >	2.063	Ca(3)–W(7)	2.548(3)
		Ca(3)–O(11)#3	2.549(2)
Ca(1)–F(1)	2.272(2)	< Ca(3)–(F,O,W) >	2.439
Ca(1)–O(4)	2.341(2)		
Ca(1)–O(16)	2.350(2)	Ca(4)–W(13)	2.381(4)
Ca(1)–O(17)#1	2.386(2)	Ca(4)–O(20)	2.398(2)
Ca(1)–O(8)#1	2.408(2)	Ca(4)–W(11)	2.408(3)
Ca(1)–O(15)#1	2.411(2)	Ca(4)–W(9)	2.416(3)
Ca(1)–O(6)	2.461(2)	Ca(4)–W(10)	2.463(3)
< Ca(1)–(F,O) >	2.376	Ca(4)–W(12)	2.487(3)
		Ca(4)–O(18)	2.509(2)
Ca(2)–F(2)	2.319(2)	Ca(4)–W(2)#5	2.709(2)
Ca(2)–F(1)	2.321(2)	< Ca(4)–(O,W) >	2.471
Ca(2)–W(4)	2.370(3)		
Ca(2)–W(2)	2.479(2)	F(1)–Mg	1.951(2)
Ca(2)–W(5)	2.485(4)	F(1)–Ca(1)	2.272(2)
Ca(2)–W(3)	2.493(3)	F(1)–Ca(2)	2.321(2)
Ca(2)–O(11)#3	2.565(2)	F(2)–Mg	1.958(2)
Ca(2)–O(8)#1	2.574(2)	F(2)–Ca(2)	2.319(2)
< Ca(2)–(F,O,W) >	2.451	F(2)–Ca(3)	2.227(2)
U(1)–O(1)	1.781(2)	U(2)–O(12)	1.793(2)
U(1)–O(2)	1.790(2)	U(2)–O(13)	1.798(2)
U(1)–O(3)	2.478(2)	U(2)–O(14)	2.391(2)
U(1)–O(4)	2.461(2)	U(2)–O(15)	2.438(2)
U(1)–O(6)	2.445(2)	U(2)–O(17)	2.428(2)
U(1)–O(7)	2.435(2)	U(2)–O(18)	2.461(2)
U(1)–O(9)	2.481(2)	U(2)–O(20)	2.432(2)
U(1)–O(10)	2.408(2)	U(2)–O(21)	2.385(2)
< U(1)–O$_{uranyl}$ >	1.786	< U–O$_{uranyl}$ >	1.796
< U(1)–O$_{carbonate}$ >	2.451	< U–O$_{carbonate}$ >	2.423
C(1)–O(3)	1.278(3)	C(4)–O(14)	1.281(4)
C(1)–O(4)	1.286(3)	C(4)–O(15)	1.306(4)
C(1)–O(5)	1.274(3)	C(4)–O(16)	1.260(4)
< C(1)–O >	1.279	< C(4)–O >	1.282
C(2)–O(6)	1.296(3)	C(5)–O(17)	1.294(3)
C(2)–O(7)	1.310(3)	C(5)–O(18)	1.291(3)
C(2)–O(8)	1.254(3)	C(5)–O(19)	1.259(3)
< C(2)–O >	1.287	< C(5)–O >	1.281
C(3)–O(9)	1.299(3)	C(6)–O(20)	1.292(4)
C(3)–O(10)	1.298(3)	C(6)–O(21)	1.300(4)
C(3)–O(11)	1.262(3)	C(6)–O(22)	1.250(4)
< C(3)–O >	1.286	< C(6)–O >	1.281

Table 3 (continued)

|			
F(1)–Mg–F(2)	81.95(8)	Mg–F(1)–Ca(1)	127.27(9)
F(1)–Mg–O(5)	99.23(8)	Mg–F(1)–Ca(2)	105.57(8)
F(2)–Mg–O(5)#2	99.34(8)	Ca(1)–F(1)–Ca(2)	115.00(7)
O(5)–Mg–O(5)#2	79.14(9)		
F(1)–Mg–O(5)#2	172.83(10)	Mg–F(2)–Ca(3)	137.91(9)
F(2)–Mg–O(5)	177.00(9)	Mg–F(2)–Ca(2)	105.42(8)
O(19)#1–Mg–W(1)	174.15(10)	Ca(3)–F(2)–Ca(2)	116.21(7)
O(1)–U(1)–O(2)	179.10(11)	O(12)–U(2)–O(13)	179.54(11)
O(3)–U(1)–O(4)	51.87(6)	O(14)–U(2)–O(15)	53.94(8)
O(6)–U(1)–O(7)	53.43(7)	O(17)–U(2)–O(18)	52.81(7)
O(9)–U(1)–O(10)	52.72(7)	O(20)–U(2)–O(21)	53.68(7)
O(4)–U(1)–O(6)	65.37(7)	O(15)–U(2)–O(17)	65.87(7)
O(7)–U(1)–O(9)	72.82(7)	O(18)–U(2)–O(20)	65.21(7)
O(10)–U(1)–O(3)	64.12(7)	O(21)–U(2)–O(14)	68.53(8)
O(3)–C(1)–O(4)	114.8(2)	O(14)–C(4)–O(15)	115.8(3)
O(3)–C(1)–O(5)	122.8(2)	O(14)–C(4)–O(16)	122.6(3)
O(4)–C(1)–O(5)	122.4(2)	O(15)–C(4)–O(16)	121.6(3)
O(6)–C(2)–O(7)	114.7(2)	O(17)–C(5)–O(18)	114.5(2)
O(6)–C(2)–O(8)	123.1(3)	O(17)–C(5)–O(19)	122.8(3)
O(7)–C(2)–O(8)	122.2(3)	O(18)–C(5)–O(19)	122.7(3)
O(9)–C(3)–O(10)	113.5(2)	O(20)–C(6)–O(21)	114.1(3)
O(9)–C(3)–O(11)	123.8(3)	O(20)–C(6)–O(22)	124.1(3)
O(10)–C(3)–O(11)	122.7(2)	O(21)–C(6)–O(22)	121.8(3)

Water molecules

Albrechtschraufite contains 18 independent water molecules, the position of one of which is partly vacant. 13 water molecules are bonded to cations, namely W(1) to Mg and the twelve molecules W(2) through W(13) to Ca(2), Ca(3) and Ca(4). The water molecules W(2) and W(6) are bridging two Ca with bond angles of Ca(2)-W(2)-Ca(4) = 140.9(1)° and Ca(3)-W(6)-Ca(3)#9 = 103.2(1)°. The remaining 11 molecules are bonded to only one cation at bond distances that are on the average a little larger than the respective cation-$O_{carbonate}$ bonds. Approximate hydrogen positions for the 13 cation-

bonded water molecules were derived with the help of the X-ray data, which showed that they all donate pairs of hydrogen bonds to neighbouring O and W atoms with W…(O,W) distances mostly in the range from 2.7 to 3.1 Å (Table 4). One half of these hydrogen bonds are donated to uranyl tricarbonate atoms, preferably to their terminal carbonate but also to uranyl oxygen atoms. The other half of these hydrogen bonds is donated to other water molecules of which three are Ca-bonded while the rest is directed to the water molecules W(14) through W(18), which are not cation bonded. These last five molecules have neighbours suitable for hydrogen bond donation, but because of their large displacement parameters speculations about them are not justified. Further information about these water molecules is given below.

Architecture

The structure of albrechtschraufite is dominated by a puckered layer of the composition $MgCa_3F_2[UO_2(CO_3)_3] \cdot 8H_2O$ formed by Mg, Ca(1), Ca(2), Ca(3), the two F atoms, the uranyl tricarbonate of U(1), and the water molecules W(1) through W(8). The basic building block of this layer comprised of two mutually centrosymmetric formula units is depicted in Fig. 3. The cations in this unit exhibit a puckered arrangement with Mg, Ca(1), Ca(2), Ca(3), F(1), and F(2) having offsets of 0.05, −0.55, 0.53, −0.26, 0.39, and 0.13 Å, respectively, from the least squares plane through their 10 metal atoms. The two-dimensional repetition of this building block generates the layer that is shown in Fig. 4 as extending parallel to (001) at z~0 (for a polyhedral representation of this layer see Online resource 1). It is clearly evident that this layer with respect to topology and the bonds within the layer has a distinct pseudosymmetry according to the orthorhombic plane group *cmm* with mirror and glide lines parallel to the base vectors **a**+**b**= 18.605 Å and **a-b**=19.551 Å and with **a**+**b** ^ **a-b**=89.36°. Due to the inclination of the *c*-axis (**c**^**c***=32.33°) subsequent $MgCa_3F_2[UO_2(CO_3)_3] \cdot 8H_2O$ layers are mutually shifted by 6.31 Å approximately parallel to [110]. The distance between the mean planes of the layers is $d(001)$=9.758 Å, which prevents any direct contact between them. Inspected in detail,

Fig. 2 Comparison of the cation coordination of the two $[UO_2(CO_3)_3]^{4-}$ anions in albrechtschraufite
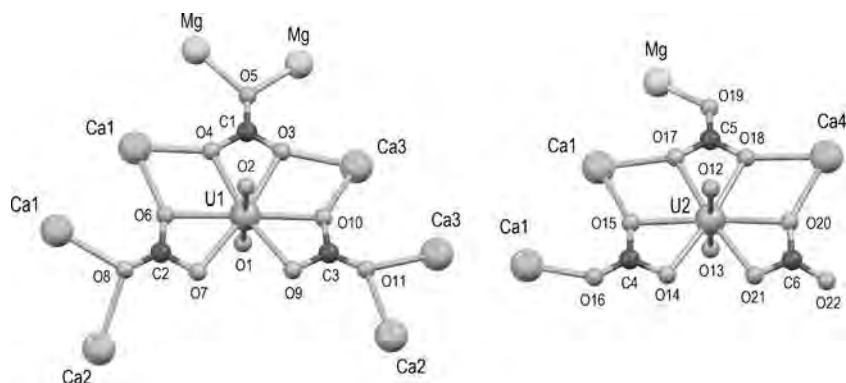
the layer shows at $x,y=\frac{1}{2},0$ and $x,y=0,\frac{1}{2}$ a violation of the pseudosymmetry because the couple of adjacent Ca(3) (centred at $x,y,z=0,\frac{1}{2},0$) is linked via two bridging water molecules W(6), whereas the couple of adjacent Ca(1) (centred at $x,y,z=\frac{1}{2},0,0$) is linked via two bridging C(4)O$_3$ belonging to the [UO$_2$(CO$_3$)$_3$] unit of U(2). The four anchor points by which one of these units [U(2)O$_2$(CO$_3$)$_3$] is attached to the MgCa$_3$F$_2$[UO$_2$(CO$_3$)$_3$]·8H$_2$O layer are marked in Fig. 4 by asterisks. Figures 5 and 6 show how this second uranyl tricarbonate unit makes a Ca(4)[U(2)O$_2$(CO$_3$)$_3$]·5H$_2$O moiety, which links the MgCa$_3$F$_2$[UO$_2$(CO$_3$)$_3$]·8H$_2$O layers perpendicular to (001) into a framework. It can be seen that the link of this moiety is very strong on one side by means of four cation-O$_{carbonate}$ bonds [O(15), O(16), O(17), O(19) linked with two Ca(1) and one Mg], while it is weak on the other side with only one comparatively long Ca(4)-W(2)-Ca(2) bridge of which Ca(4)-W(2)=2.709(2) Å is the longest Ca-(O,W) bond in the structure. However, the coherence of the MgCa$_3$F$_2$[UO$_2$(CO$_3$)$_3$]·8H$_2$O layers via the Ca(4)[U(2)O$_2$(CO$_3$)$_3$]·5H$_2$O bridges is strengthened by five hydrogen bonds donated by the water-rich Ca(4)O$_2$W$_5$ polyhedron to hydrogen bond acceptors of the adjacent MgCa$_3$F$_2$[UO$_2$(CO$_3$)$_3$]·8H$_2$O layer and by hydrogen bonds donated by the latter to the carbonate group C(6)O$_3$. In this way the MgCa$_3$F$_2$[UO$_2$(CO$_3$)$_3$]·8H$_2$O layers and the Ca[U(2)O$_2$(CO$_3$)$_3$]·5H$_2$O bridges form a framework with the composition MgCa$_4$F$_2$[UO$_2$(CO$_3$)$_3$]·13H$_2$O. The framework contains two kinds of cavities where the five water molecules W(14) through W(18) reside, which are not cation bonded. W(14) sits in a pocket of its own while W(15) through W(18) are in an irregular continuous channel extending at $y,z=\frac{1}{2},\frac{1}{2}$ along [100]. W(14) through W(17) were found to be fully occupied while W(18) is

close to a centre of inversion (0.64 Å) and only partly occupied (population parameter 0.29(1)). The channel is wider near $x,y,z=0,\frac{1}{2},\frac{1}{2}$ and narrower near $\frac{1}{2},\frac{1}{2},\frac{1}{2}$. All water molecules in this channel show large displacement ellipsoids elongated parallel to the channel axis (this includes even the Ca-bonded channel wall molecule W(5)). Although these water molecules appear to be anchored in the framework via hydrogen bonds, it is possible that they show some zeolitic behaviour. The chemical formula MgCa$_4$F$_2$[UO$_2$(CO$_3$)$_3$]$_2$·17-18H$_2$O used in the title takes this aspect into account.
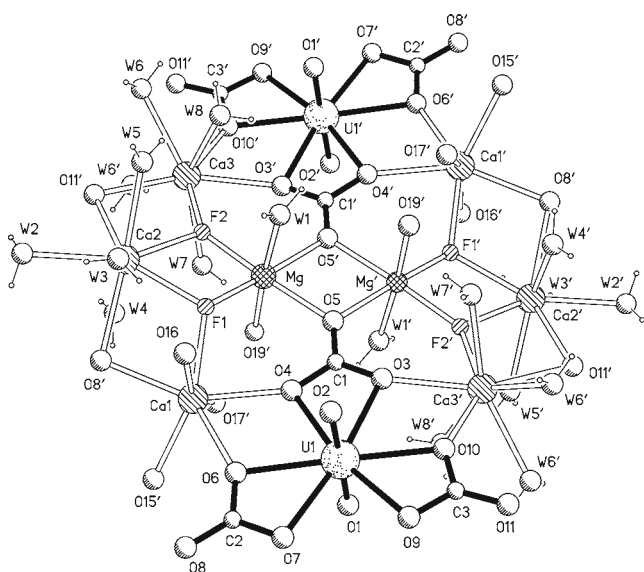
Structural relationships

Together with schröckingerite, NaCa$_3$F[UO$_2$(CO$_3$)$_3$](SO$_4$)·10H$_2$O, albrechtschraufite is the only other known uranium

Table 4 Hydrogen bonds (Å, °) according to the structure refinement

D-H···A	d(H···A)	d(D···A)	<(DHA)
W(1)-H(1A)···W(14)	2.31	3.028(5)	150.0
W(1)-H(1B)···W(16)	2.40	3.038(8)	137.7
W(1)-H(1B)···W(18)	1.97	2.702(15)	151.0
W(2)-H(2A)···O(7)#1	2.03	2.811(3)	163.2
W(2)-H(2B)···O(9)#3	1.93	2.714(3)	164.7
W(3)-H(3A)···O(16)	2.01	2.776(4)	159.6
W(3)-H(3B)···W(12)#5	2.11	2.886(4)	164.3
W(4)-H(4A)···O(13)#1	2.09	2.883(3)	170.0
W(4)-H(4B)···O(22)#9	1.96	2.756(3)	174.0
W(5)-H(5A)···W(8)	2.11	2.865(5)	157.9
W(5)-H(5B)···W(16)#8	2.29	3.046(8)	158.6
W(5)-H(5B)···W(18)#8	2.40	2.971(19)	128.8
W(6)-H(6A)···O(22)#8	1.93	2.723(3)	173.2
W(6)-H(6B)···W(17)	2.18	2.953(5)	163.2
W(7)-H(7A)···O(19)#1	2.08	2.835(3)	157.0
W(7)-H(7B)···W(15)#2	2.06	2.805(6)	155.5
W(8)-H(8A)···O(21)#8	1.96	2.761(3)	175.4
W(8)-H(8B)···W(14)	2.16	2.922(4)	160.1
W(9)-H(9A)···O(2)#11	2.31	3.055(4)	155.0
W(9)-H(9B)···W(15)#10	1.99	2.738(6)	156.1
W(10)-H(10A)···O(13)#11	2.15	2.948(4)	175.5
W(10)-H(10B)···W(7)#1	2.28	2.995(4)	148.4
W(11)-H(11A)···O(7)#11	2.19	2.989(3)	176.9
W(11)-H(11B)···O(22)	2.30	3.039(4)	153.9
W(12)-H(12B)···O(1)#13	2.27	3.034(4)	160.1
W(12)-H(12A)···W(14)#10	2.64	3.434(6)	174.0
W(13)-H(13A)···O(19)	2.52	3.173(6)	139.8
W(13)-H(13B)···W(16)#10	2.21	2.813(6)	132.2

Fig. 3 The layer-forming building block MgCa$_3$F$_2$[UO$_2$(CO$_3$)$_3$]·8H$_2$O of albrechtschraufite consisting of two centrosymmetric formula units. Mg and Ca coordination completed. Primes indicate the symmetry operation 1-x,1-y,-z

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z; #2 -x+1,-y+1,-z; #3 x-1,y,z; #5 -x+1,-y,-z+1 #7 x,y+1,z; #8 -x+1,-y+1,-z+1; #9 x-1,y,z-1; #10 x,y-1,z; #11 -x+2,-y,-z+1; #13 x,y,z+1; W-H=0.80 Å

Fig. 4 Perspective view of a MgCa$_3$F$_2$[UO$_2$(CO$_3$)$_3$]·8H$_2$O layer in albrechtschraufite extending at z~0 parallel to (001) with completed coordination of Mg and Ca. The four asterisks on the lower left mark the four carbonate oxygen atoms O(16)-O(15)-O(17)-O(19) by which an interlayer moiety Ca[U(2)O$_2$(CO$_3$)$_3$] ·5H$_2$O is attached to the layer via two CO$_3$ groups bridging one Mg and two Ca(1)
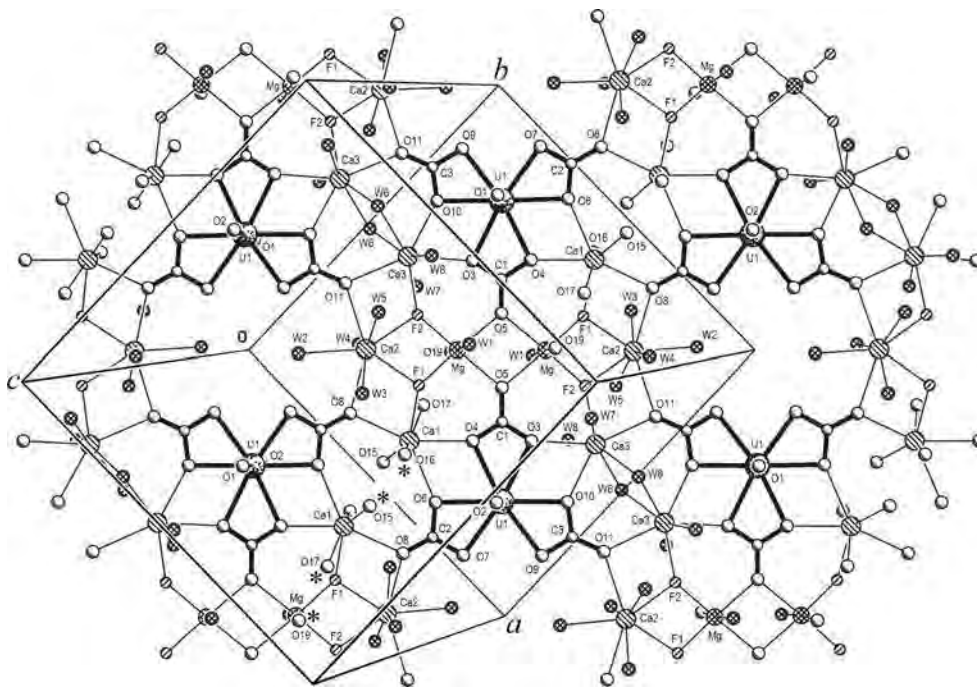
mineral containing stoichiometric fluorine. While schröckingerite is an important and widespread secondary uranyl carbonate mineral occasionally forming larger caliche-type deposits (Sheridan et al. 1962; Chernikov and Dorfman 2004), albrechtschraufite is at present only a mineralogical curiosity. Apart from their common main constituents Ca, F, [UO$_2$(CO$_3$)$_3$] and H$_2$O the structures of the two minerals do not have much in common. Schröckingerite has a pronounced layer structure with well-balanced cation-anion and hydrogen bond interactions and forms very thin plates of triclinic pseudohexagonal symmetry and a perfect cleavage. Albrechtschraufite in turn has a somewhat unbalanced structure with compact parts

(around the MgCa$_3$F$_2$ fragment) as well as wide open parts and likewise with water-free and water-rich Ca coordination polyhedra. And it represents a hybrid between a layer and framework structure that shows zeolitic features. Liebigite, Ca$_2$[UO$_2$(CO$_3$)$_3$]·~11H$_2$O, orthorhombic, space group Bba2 (Mereiter 1982), which has ½ MgF$_2$ less and 1½ H$_2$O more than albrechtschraufite per uranyl tricarbonate unit, exhibits a strongly puckered grate-like layer structure that behaves more like a honeycomb framework and is also comparatively stable despite the presence of zeolitic water molecules. In this structure, a carbonate group shares an edge with a Ca coordination polyhedron, a feature missing in albrechtschraufite and schröckingerite.

Fig. 5 Structure of albrechtschraufite in projection parallel to [100]. The five asterisks emphasize those atoms by which a Ca[U(2)O$_2$(CO$_3$)$_3$]·5H$_2$O moiety links two MgCa$_3$F$_2$[UO$_2$(CO$_3$)$_3$]·8H$_2$O layers via cation-oxygen bonds. W(15) through W(18) occupy the infinite channel along [100]
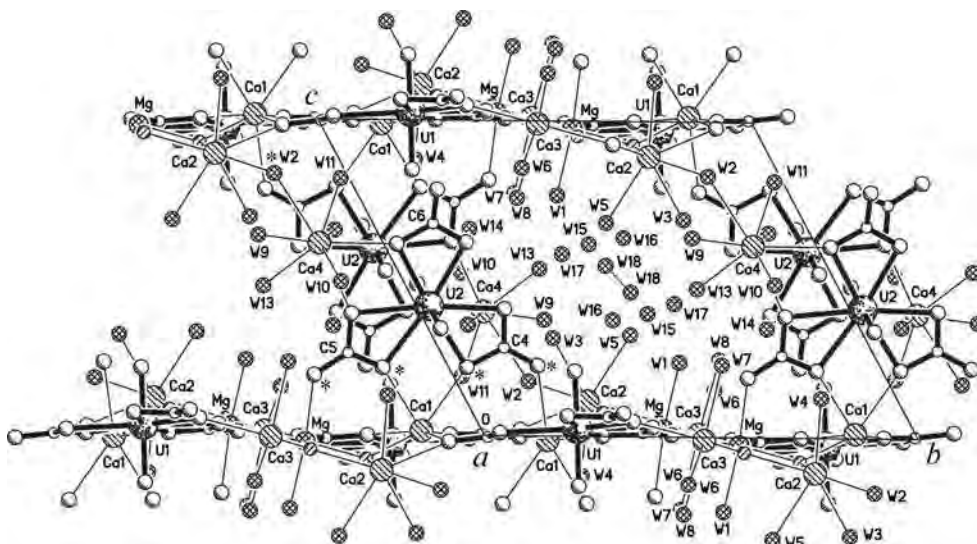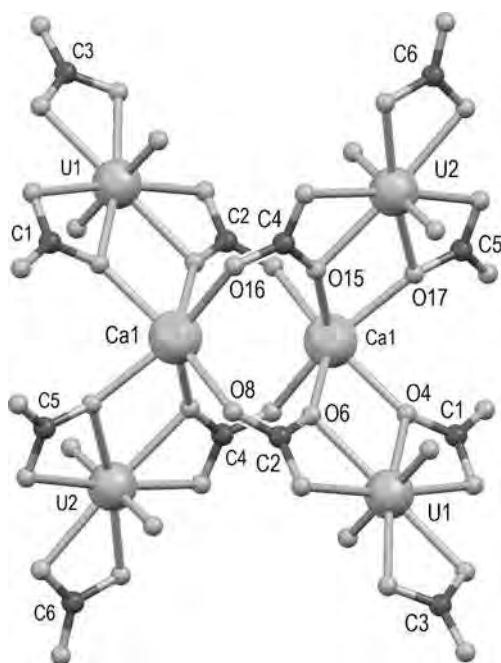
Fig. 6 Structure of albrechtschraufite in projection parallel to [010]. The $U(CO_3)_3$ moieties of U(1) and U(2) are inclined to each other by 59°
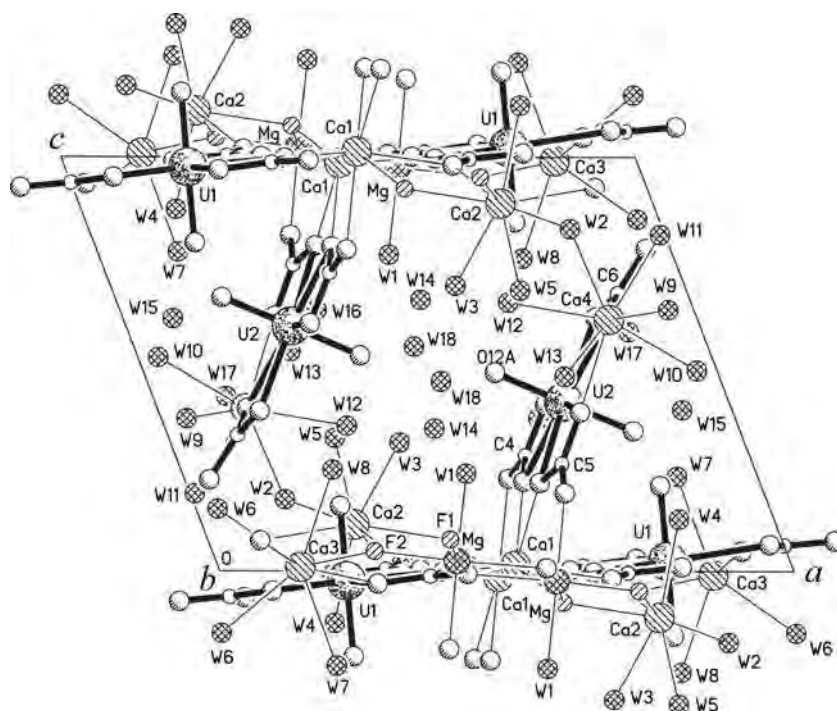
Andersonite, $Na_2Ca[UO_2(CO_3)_3]\cdot\sim6H_2O$, trigonal, space group $R\text{-}3m$, has a sturdy framework structure consisting of oval buckyball-like cages formed by six Na, six Ca and six $[UO_2(CO_3)_3]$ units (Coda et al. 1981). It is

Fig. 7 The paddle-wheel motif in albrechtschraufite which is shared with the crystal structures of andersonite and two synthetic alkali uranyl tricarbonates of formula type $A_2Ca_3[UO_2(CO_3)_3]_2\cdot nH_2O$ (A=Na, K). Ca (1)-Ca(1)=3.950 Å. In dinuclear transition metal complexes like Cu $(CH_3COO)_2\cdot H_2O$ only the four bridging groups of C(2) and C(4) would represent the then small paddle-wheel with Cu-Cu=2.65 Å

interesting to note that this structure has the same kind of compact link of two Ca ions via four bridging carbonate groups of four $[UO_2(CO_3)_3]$ units, which is present in albrechtschraufite for two adjacent Ca(1) linked via bridging two $C(2)O_3$ and two $C(4)O_3$ groups (Fig. 7). This is an important structural motif called the paddle-wheel structure, which is characteristic for dinuclear tetracarboxylate-bridged transition metal complexes with metal-metal bonding, e.g. $Cu(CH_3COO)_2\cdot2H_2O$ (Wells 1986). This paddle-wheel motif is also present in two synthetic alkali calcium uranyl tricarbonate hydrates of orthorhombic symmetry. It occurs in them within pseudotetragonal layers $\{Ca[UO_2(CO_3)_3]\}^{2-}$ with an egg-crate like structure (Vochten et al. 1994; Hughes-Kubatko and Burns 2004). At variance with albrechtschraufite, where each uranyl tricarbonate unit takes part in only one paddle-wheel motif, the units of the alkali calcium uranyl tricarbonates take part in two, which links them into a framework (andersonite) or a square grid (last two compounds).

From the aspect of structural relationships an unexpected feature of albrechtschraufite is the magnesium coordination in the form of an MgF_2O_3W octahedron. In highly hydrated uranyl compounds magnesium is normally present as a hexaquo complex MgW_6 and swartzite, $CaMg[UO_2(CO_3)_3]\cdot12H_2O$, or bayleyite, $Mg_2[UO_2(CO_3)_3]\cdot18H_2O$, are only two out of more examples (Mereiter 1986b; Mayer and Mereiter 1986). Moreover edge-sharing of two Mg-centered octahedra having two carbonate oxygen atoms as linkers is uncommon, albeit known from hydromagnesite, $Mg_5(CO_3)_4(OH)_2\cdot4H_2O$ (Akao and Iwai 1977).

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Supplementary information for:

Description and crystal structure of albrechtschraufite, MgCa$_4$F$_2$[UO$_2$(CO$_3$)$_3$]$_2$·17-18H$_2$O

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Content:

Photographs of albrechtschraufite (Fig. S1 and S2)

Polyhedral representation of a part of the crystal structure (Fig. S3)

Complete list of atomic parameters including H atoms and anisotropic displacement parameters U_{ij} (Table S1).
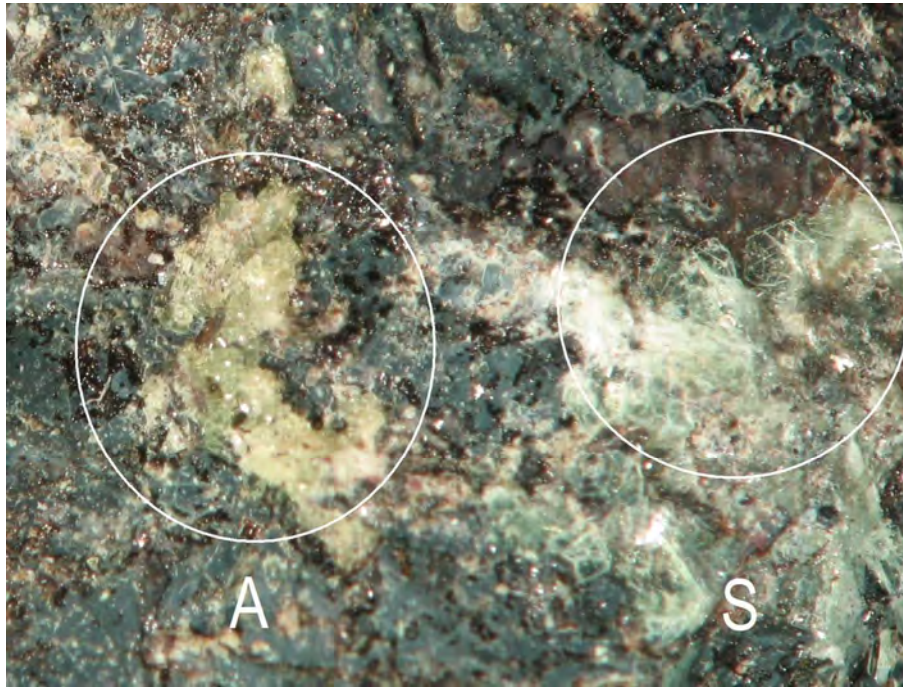
Fig S1. Albrechtschraufite (A) and schröckingerite (S) on massive uraninite on NHM Vienna specimen A.a. 6740. A pseudohexagonal plate of schröckingerite can be seen clearly on the upper right. Uraninite is shiny black in some areas or covered by a dark green oxidation layer in larger areas. Image width ca. 8 mm. The entire specimen (ca. 9 cm maximum dimension) is part of a vein and consists of massive uraninite (pitchblende) in the center bordered by seams of red iron-oxide stained coarse-grained dolomite. Photo Uwe Kolitsch.
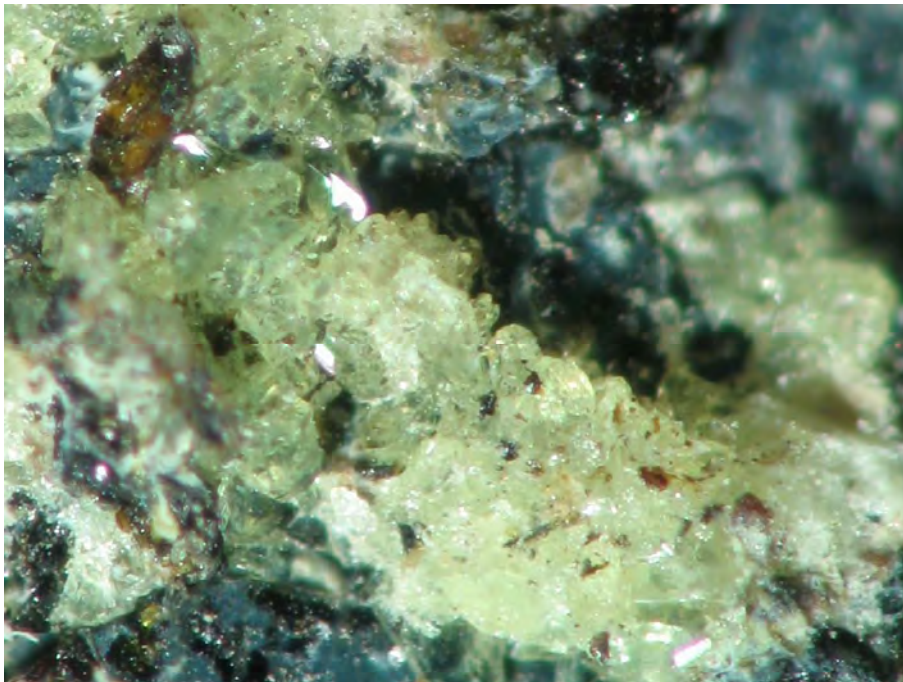
Fig. S2. A close-up view the albrechtschraufite in Fig. S1 showing an aggregate of pale yellowish-green crystals with glassy luster. Image width ca. 1.8 mm. Photo Uwe Kolitsch.
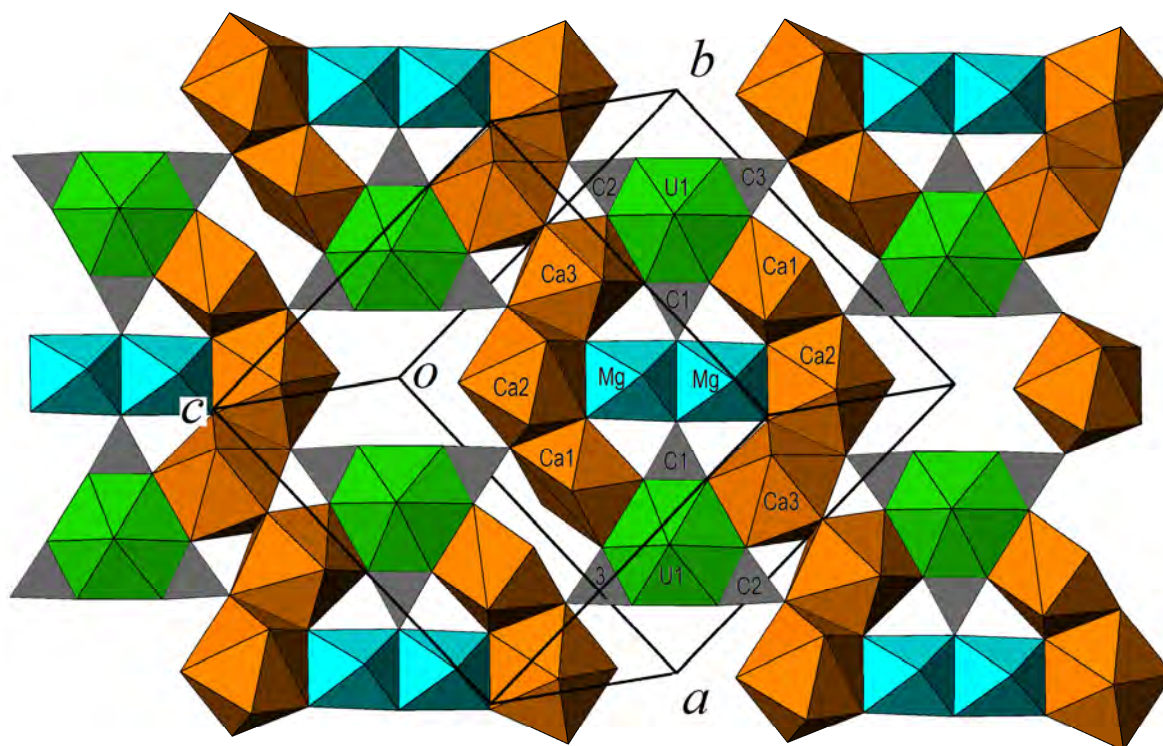
Fig. S3. Polyhedral representation of a $MgCa_3F_2[UO_2(CO_3)_3]\cdot 8H_2O$ layer in albrecht-schraufite extending at $z \sim 0$ parallel to (001). This drawing supplements Fig. 4 of the publication.

Table S1 Atomic coordinates, equivalent isotropic and anisotropic displacement parameters ($\text{Å}^2 \times 10^4$ for Mg, Ca, U; $\text{Å}^2 \times 10^3$ for C, O, H) for albrechtschraufite.

Atom	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg	0.41979(7)	0.42236(8)	0.02416(10)	121(2)	103(4)	106(4)	196(5)	95(4)	71(4)	33(3)
Ca(1)	0.48138(4)	0.14003(4)	-0.01359(6)	120(1)	101(2)	100(2)	176(2)	83(2)	45(2)	28(2)
Ca(2)	0.26561(4)	0.28073(5)	0.11208(6)	161(1)	140(3)	172(3)	242(3)	142(2)	92(2)	48(2)
Ca(3)	0.14312(4)	0.49698(5)	0.00952(6)	147(1)	109(2)	129(2)	244(3)	110(2)	79(2)	48(2)
Ca(4)	0.84563(5)	-0.14801(5)	0.60690(7)	216(1)	198(3)	226(3)	241(3)	132(3)	67(2)	67(2)
F(1)	0.42284(13)	0.30237(14)	0.07639(18)	16(1)	16(1)	15(1)	25(1)	14(1)	11(1)	8(1)
F(2)	0.28315(13)	0.42011(14)	0.04822(18)	17(1)	14(1)	18(1)	29(1)	16(1)	13(1)	8(1)
U(1)	0.785960(8)	0.222723(8)	0.024224(10)	119(1)	93(1)	100(1)	202(1)	95(1)	65(1)	34(1)
O(1)	0.74685(18)	0.15651(19)	-0.1575(2)	23(1)	24(1)	22(1)	24(1)	12(1)	9(1)	5(1)
O(2)	0.82393(19)	0.2874(2)	0.2066(2)	25(1)	24(1)	25(1)	25(1)	11(1)	8(1)	5(1)
C(1)	0.6367(2)	0.3698(2)	0.0125(3)	13(1)	11(1)	13(1)	20(1)	10(1)	7(1)	3(1)
O(3)	0.73351(16)	0.39875(18)	0.0304(3)	22(1)	12(1)	19(1)	47(1)	22(1)	15(1)	7(1)
O(4)	0.61109(16)	0.27159(17)	0.0015(2)	20(1)	13(1)	14(1)	41(1)	18(1)	12(1)	5(1)
O(5)	0.57073(16)	0.43339(17)	0.0070(2)	16(1)	12(1)	14(1)	29(1)	15(1)	10(1)	7(1)
C(2)	0.7097(2)	0.0058(2)	-0.0043(3)	15(1)	14(1)	15(1)	21(1)	12(1)	8(1)	4(1)

O(6)	0.65044(16)	0.07884(17)	-0.0028(2)	19(1)	13(1)	16(1)	34(1)	16(1)	11(1)	7(1)
O(7)	0.80697(16)	0.03892(18)	0.0097(3)	21(1)	12(1)	17(1)	42(1)	19(1)	13(1)	6(1)
O(8)	0.67681(17)	-0.08996(17)	-0.0198(2)	20(1)	18(1)	13(1)	37(1)	15(1)	14(1)	5(1)
C(3)	0.9999(2)	0.3096(2)	0.0624(3)	16(1)	14(1)	14(1)	24(1)	11(1)	9(1)	3(1)
O(9)	0.97519(16)	0.21572(18)	0.0643(3)	21(1)	13(1)	19(1)	43(1)	23(1)	12(1)	8(1)
O(10)	0.92175(16)	0.36065(18)	0.0483(2)	20(1)	12(1)	18(1)	39(1)	20(1)	12(1)	8(1)
O(11)	1.09083(16)	0.34862(17)	0.0737(2)	18(1)	11(1)	18(1)	29(1)	14(1)	9(1)	4(1)
U(2)	0.712257(8)	0.029017(8)	0.409056(10)	138(1)	146(1)	115(1)	132(1)	55(1)	29(1)	35(1)
O(12)	0.61179(19)	0.0290(2)	0.4798(2)	27(1)	25(1)	32(1)	28(1)	13(1)	12(1)	8(1)
O(13)	0.81365(18)	0.02859(19)	0.3390(2)	24(1)	23(1)	22(1)	22(1)	6(1)	10(1)	3(1)
C(4)	0.6096(3)	0.1523(3)	0.2797(3)	20(1)	24(2)	17(1)	19(1)	10(1)	6(1)	10(1)
O(14)	0.6776(2)	0.1997(2)	0.4022(2)	34(1)	49(2)	16(1)	20(1)	6(1)	-5(1)	9(1)
O(15)	0.58873(18)	0.04167(18)	0.2163(2)	21(1)	23(1)	14(1)	20(1)	7(1)	1(1)	4(1)
O(16)	0.56460(19)	0.20789(19)	0.2235(2)	23(1)	28(1)	21(1)	22(1)	13(1)	6(1)	12(1)
C(5)	0.6672(2)	-0.2150(2)	0.2593(3)	14(1)	12(1)	14(1)	17(1)	9(1)	5(1)	2(1)
O(17)	0.61595(18)	-0.15313(17)	0.2135(2)	20(1)	22(1)	13(1)	18(1)	6(1)	-1(1)	3(1)
O(18)	0.73345(18)	-0.15961(18)	0.3839(2)	20(1)	24(1)	15(1)	16(1)	7(1)	0(1)	4(1)
O(19)	0.65280(17)	-0.32068(17)	0.1888(2)	18(1)	21(1)	11(1)	20(1)	6(1)	5(1)	4(1)
C(6)	0.8780(2)	0.1388(2)	0.6711(3)	18(1)	19(1)	16(1)	17(1)	6(1)	6(1)	4(1)
O(20)	0.84375(19)	0.03029(18)	0.6060(2)	23(1)	27(1)	15(1)	19(1)	6(1)	-1(1)	3(1)
O(21)	0.82359(19)	0.19240(18)	0.6130(2)	24(1)	29(1)	15(1)	18(1)	5(1)	1(1)	4(1)
O(22)	0.95725(18)	0.1897(2)	0.7792(2)	25(1)	19(1)	22(1)	20(1)	4(1)	-1(1)	3(1)
W(1)	0.4944(2)	0.5398(2)	0.2360(3)	36(1)	45(2)	25(1)	26(1)	8(1)	2(1)	1(1)
W(2)	0.16162(17)	0.16731(19)	0.1731(2)	21(1)	17(1)	22(1)	31(1)	16(1)	10(1)	8(1)
W(3)	0.3992(2)	0.2770(2)	0.3111(3)	36(1)	29(1)	47(2)	41(2)	29(1)	13(1)	11(1)
W(4)	0.16557(19)	0.1755(2)	-0.1257(3)	30(1)	24(1)	24(1)	31(1)	6(1)	7(1)	11(1)
W(5)	0.2896(4)	0.4597(3)	0.3224(3)	84(2)	135(4)	67(3)	30(2)	14(2)	13(2)	66(3)
W(6)	0.03802(17)	0.58768(18)	0.1502(2)	20(1)	19(1)	17(1)	25(1)	10(1)	8(1)	4(1)
W(7)	0.1406(2)	0.3647(2)	-0.2292(3)	31(1)	24(1)	35(1)	31(1)	14(1)	10(1)	11(1)
W(8)	0.26404(19)	0.6352(2)	0.2451(3)	32(1)	23(1)	27(1)	34(1)	5(1)	10(1)	5(1)
W(9)	0.9554(4)	-0.2792(4)	0.6310(4)	82(2)	93(3)	81(3)	40(2)	12(2)	-1(2)	64(3)
W(10)	0.9648(2)	-0.1445(3)	0.4849(3)	57(1)	28(2)	82(3)	36(2)	7(2)	14(1)	-1(2)
W(11)	0.9914(2)	-0.0199(2)	0.8123(3)	38(1)	30(1)	32(1)	43(2)	22(1)	-4(1)	-3(1)
W(12)	0.6816(2)	-0.0963(3)	0.6487(3)	39(1)	42(2)	46(2)	45(2)	30(1)	23(1)	17(1)
W(13)	0.7301(3)	-0.3298(3)	0.4698(5)	89(2)	61(3)	42(2)	132(4)	46(3)	-10(3)	-13(2)
W(14)	0.4693(3)	0.7833(3)	0.3448(5)	73(1)	56(2)	47(2)	129(4)	38(2)	54(3)	15(2)
W(15)	0.9132(6)	0.5259(4)	0.3904(5)	130(3)	252(8)	44(2)	60(3)	11(2)	31(4)	32(4)
W(16)	0.6569(7)	0.4376(4)	0.3695(7)	170(4)	264(9)	42(3)	119(5)	33(3)	-23(5)	-30(4)
W(17)	0.1280(4)	0.5998(5)	0.4224(5)	98(2)	96(4)	115(4)	90(3)	69(3)	18(3)	-16(3)
W(18)	0.5118(16)	0.5130(15)	0.4582(14)	99(8)	122(16)	83(12)	39(8)	14(8)	-3(8)	-50(9)
H(1a)	0.5122	0.6073	0.2745	44						
H(1b)	0.5140	0.5184	0.2920	44						
H(2a)	0.1608	0.1028	0.1238	26						
H(2b)	0.1030	0.1779	0.1499	26						
H(3a)	0.4558	0.2679	0.3058	43						
H(3b)	0.3810	0.2362	0.3380	43						
H(4a)	0.1777	0.1190	-0.1776	35						
H(4b)	0.1049	0.1763	-0.1589	35						
H(5a)	0.2820	0.5183	0.3218	101						
H(5b)	0.3113	0.4720	0.4005	101						
H(6a)	0.0432	0.6544	0.1770	24						
H(6b)	0.0553	0.5772	0.2155	24						
H(7a)	0.1997	0.3635	-0.2282	37						
H(7b)	0.1096	0.3804	-0.2875	37						
H(8a)	0.2356	0.6826	0.2843	38						
H(8b)	0.3192	0.6665	0.2527	38						
H(9a)	1.0086	-0.2664	0.6934	99						

H(9b)	0.9598	-0.3278	0.5627	99
H(10a)	1.0258	-0.1165	0.5311	68
H(10b)	0.9616	-0.2035	0.4218	68
H(11a)	1.0456	-0.0268	0.8572	46
H(11b)	0.9974	0.0451	0.8289	46
H(12a)	0.6311	-0.1194	0.5795	46
H(12b)	0.6829	-0.0313	0.6962	46
H(13a)	0.6872	-0.3525	0.3945	107
H(13b)	0.7274	-0.3788	0.4910	107

"W" denote oxygen atoms of water molecules. W(18) is partly vacant and has a refined occupancy of 0.29(1).

U_{eq} is one third of the trace of the orthogonalized U_{ij} tensor.

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$