

## 08.4-9 THE CRYSTAL STRUCTURE OF PARTHEITE

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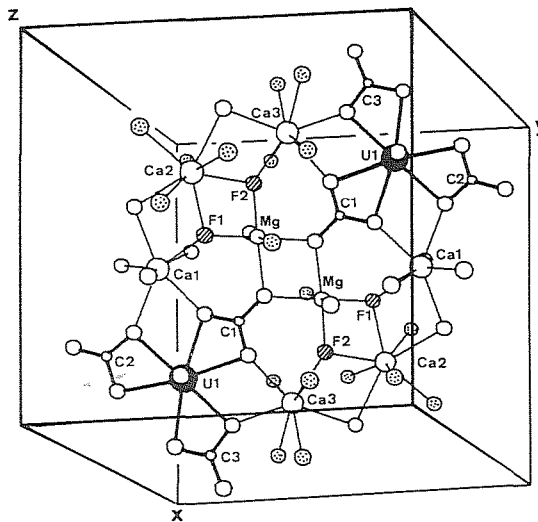
The mineral *parthéite* was discovered by H. Sarp (H. Sarp, J. Deferne, H. Bizouard and B.W. Liebich (1979), Bull. Suisse Min. Petr. 59, 5-13). The single crystal, kindly supplied by H. Sarp for our study was taken on the holotype sample (deposited in the Dpt. of Minéralogie, Muséum d'Histoire naturelle, Genève), originally located in ophiolites of the Taurus Mountain, Turkey. The structural study led to an R of 7% for 2012 reflections.

*parthéite* :  $\text{Ca}_2\text{Al}_4\text{Si}_4\text{O}_{15}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$ ,  $Z = 4$   
 space group :  $C2/c$   
 cell parameters :  $a = 21.555(3) \text{ \AA}$ ,  $b = 8.761(1) \text{ \AA}$ ,  
 $c = 9.304(2) \text{ \AA}$ ,  $\beta = 91.55(2)^\circ$   
 $D_m = 2.39 \text{ g/cm}^3$ ,  $D_x = 2.45 \text{ g/cm}^3$

The formula originally proposed was  $\text{CaAl}_2\text{Si}_2\text{O}_8 \cdot 2\text{H}_2\text{O}$ ,  $Z=8$ .

The structure consists of Al- and Si-centered oxygen tetrahedra ( $d(\text{Al-O}) = 1.753 \text{ \AA}$ ,  $d(\text{Si-O}) = 1.620 \text{ \AA}$ ) connected via corners to a framework of low density, built of 4, 6, 8 and 10 membered T-rings (T = Al, Si). Due to the presence of hydroxyl groups, the framework is interrupted at every second Al-site. The 10 membered rings form the perimeter of zig-zag channels of aperture 6.0 Å and 3.5 Å, which are filled by water molecules such as in *zeolites*.

The structure will be compared to those of other aluminosilicates of similar composition, such as *anorthite*  $\text{CaAl}_2\text{Si}_2\text{O}_8$  and *gismondite*  $\text{CaAl}_2\text{Si}_2\text{O}_8 \cdot 4\text{H}_2\text{O}$ . A detailed account of this work will appear in Z. Kristallogr.



Albrechtschraufite:  $\text{MgCa}_3\text{F}_2[(\text{UO}_2)(\text{CO}_3)_3] \cdot 8\text{H}_2\text{O}$  layer at  $z \sim 1/2$  as a part of the structure.  $\text{H}_2\text{O}$  oxygen atoms are dotted.

08.4-10 THE CRYSTAL STRUCTURE OF ALBRECHTSCHRAUFITE,  $\text{MgCa}_4\text{F}_2[(\text{UO}_2)(\text{CO}_3)_3]_2 \cdot 17\text{H}_2\text{O}$ . By K. Mereiter, Institut für Mineralogie, Kristallographie und Strukturchemie, Technische Universität Wien, Austria.

Albrechtschraufite is a new uranylcarbonate mineral which was recently detected on a specimen of schroekinggerite,  $\text{NaCa}_3(\text{UO}_2)(\text{CO}_3)_3(\text{SO}_4)\text{F} \cdot 10\text{H}_2\text{O}$ , from Joachimsthal, Bohemia. The crystal structure and chemical formula of the new mineral have been determined by single crystal X-ray diffraction methods: Space group  $P\bar{1}$ ,  $a = 13.562(3)$ ,  $b = 13.406(3)$ ,  $c = 11.636(3) \text{ \AA}$ ,  $\alpha = 115.75(2)$ ,  $\beta = 107.66(2)$ ,  $\gamma = 92.86(2)^\circ$ ,  $Z = 2$   $\text{MgCa}_4\text{F}_2[(\text{UO}_2)(\text{CO}_3)_3]_2 \cdot 17\text{H}_2\text{O}$ ; Least-squares refinement is presently at  $R = 0.045$  for about 4300 independent observed reflections. The crystal structure contains two independent complex anions  $[(\text{UO}_2)(\text{CO}_3)_3]^{4-}$ . The coordination octahedron around Mg is formed by two F, three carbonate oxygen atoms and one  $\text{H}_2\text{O}$ . The two F atoms exhibit flat to flat-pyramidal coordination, each by one Mg and two Ca. Calcium atoms are seven- and eight-coordinate:  $\text{Ca}(1)\text{F}_6$ ,  $\text{Ca}(2)\text{F}_2\text{O}_2(\text{H}_2\text{O})_4$ ,  $\text{Ca}(3)\text{F}_3(\text{H}_2\text{O})_3$  and  $\text{Ca}(4)\text{O}_2(\text{H}_2\text{O})_6$ . The structure can be described as being built up from layers of the composition  $\text{MgCa}_3\text{F}_2[(\text{UO}_2)(\text{CO}_3)_3] \cdot 8\text{H}_2\text{O}$  (see Figure) which are interconnected into a framework by another  $[(\text{UO}_2)(\text{CO}_3)_3]$  unit, one Ca, five Ca-bonded water molecules and four lattice water molecules. The mineral and its name have been approved by the IMA Commission on New Minerals and Mineral Names.

08.4-11 LOW- AND HIGH-TEMPERATURE CRYSTAL STRUCTURES OF  $\text{LiFeGe}_2\text{O}_6$ ,  $\text{LiFeSi}_2\text{O}_6$  AND  $\text{LiCrSi}_2\text{O}_6$ . By M. Behruzi \*, Th. Hahn \*, C.T. Prewitt\*\*, K. Baldwin\*\*, \* Institut für Kristallographie der RWTH Aachen, 5100 Aachen, FRG; \*\* Department of Earth & Space Sci., SUNY, Stony Brook, NY, USA.

The title compounds are monoclinic 1:3-pyroxenes. Single crystals of several mm diameter were grown from flux melts. The low  $\rightarrow$  high transformations  $P2_1/c \rightarrow C2/c$  were investigated by DTA and structure refinements at various temperatures. Common features are:  
 - very rapid transitions at  $500^\circ\text{C}$  ( $\text{LiFeGe}_2\text{O}_6$ ),  $-45^\circ\text{C}$  ( $\text{LiFeSi}_2\text{O}_6$ ) and  $70^\circ\text{C}$  ( $\text{LiCrSi}_2\text{O}_6$ ); disappearance of reflections with  $h+k \neq 2n$  within seconds;  
 - characteristic, abrupt changes of cell parameters:  $a$ ,  $c$ , and  $\beta$  increase,  $b$  decreases;  
 - in the low forms two distinct tetrahedral chains, in the high forms all chains symmetrically equivalent;  
 - at the transition the tetrahedral chains become more extended, i.e. the O3-O3-O3 angle increases;  
 - practically no changes of tetrahedra and M1-octahedra; the coordination number for Li (M2) increases from 5 to 6 for the silicates, remains 6 for germanate.  
 Distinguishing feature is the change of the tetrahedral chain angle: In  $\text{LiFeSi}_2\text{O}_6$  and  $\text{LiCrSi}_2\text{O}_6$  from about  $165^\circ$  to  $179^\circ$ , i.e. the S and O chains become fully extended; in  $\text{LiFeGe}_2\text{O}_6$  the S chain remains in S orientation (chain angle  $152^\circ$  to  $166^\circ$ ), the O chain flips over to S orientation (chain angle  $140^\circ$  to  $194^\circ$ , i.e. a rotation of  $54^\circ$ , involving atom movements of up to 1 Å). This change in orientation is observed here for the first time. These transitions will be compared with other pyroxene transitions.  
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