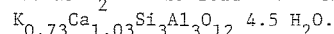


**08.4-01** CRYSTAL STRUCTURE OF A NEW ZEOLITE MINERAL. By E. Tillmanns and R. Fischer, Institut für Geowissenschaften, Joh. Gutenberg Universität, Postfach 3980, D-65 Mainz, Federal Republic of Germany.

The mineral has been found as clear colorless crystals in a limestone inclusion of a basalt from the Bellerberg near Mayen, Eifel, Germany. Electron-microprobe analysis gave  $\text{SiO}_2$  35.52,  $\text{Al}_2\text{O}_3$  30.13,  $\text{K}_2\text{O}$  6.80,  $\text{CaO}$  11.58 weight%, [84.03 %], the remainder of ~16 % was interpreted as  $\text{H}_2\text{O}$ . This leads to chemical formula



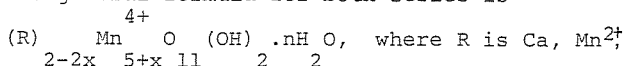
A single-crystal X-ray study shows the mineral to be triclinic, space group  $\text{P}\bar{1}$  with  $a=9.20(2)$ ,  $b=9.18(2)$ ,  $c=9.49(2)$  Å,  $\alpha=92.3(7)^\circ$ ,  $\beta=92.7(7)^\circ$ ,  $\gamma=90.1(7)^\circ$ ,  $Z=2$ .

The framework of  $\text{SiO}_4$  and  $\text{AlO}_4$  tetrahedra is essentially the same as in chabazite,  $\sim\text{CaAl}_2\text{Si}_4\text{O}_{12} \cdot 6\text{H}_2\text{O}$ , and contains double 6-rings (D6R) as secondary building units. Average T-O distances for the six different tetrahedra are 1.614, 1.611, 1.606 Å for Si-O and 1.743, 1.745 and 1.742 Å for Al-O distances indicating complete Si/Al ordering.

Chabazite apparently crystallizes in space group  $\text{R}\bar{3}\text{m}$  with  $a \sim 9.40$  Å and  $\alpha \sim 92^\circ$ , unit-cell dimensions that are very similar to those of the new mineral. Optical examinations (Majer, V. Yugoslav. Akad. Znanos. Umjetnos. (1953), 175) and structure refinements (Smith et al. Acta Cryst. (1964), 17, 374) have led to the suggestion that the true symmetry of chabazite is triclinic and the crystals are sextuply twinned. Although the tetrahedral frameworks are topologically equivalent in both structures, differences in detail, probably caused by Si/Al ordering, do exist and lead to changes in the occupation of non-framework positions.

**08.4-02** LAYER STRUCTURE IN POORLY CRYSTALLINE MANGANESE HYDROXIDES: BIRNESSITE AND RANCIEITE. By Soo Jin KIM, Department of Geological Sciences, Seoul National University, Seoul 151, Korea.

Birnessite and rancieite occur as poorly crystalline aggregate in terrestrial or marine manganese ores. Both minerals have similar layer structures, which consist of edge-shared ( $\text{MnO}_6$ ) octahedral layers and sheets of water molecules. They have hexagonal unit cells with variable dimensions, which depend on the water content and on the nature of cations between two layers. One out of six octahedral sites in the layers of linked ( $\text{MnO}_6$ ) is unoccupied. The mono- and divalent cations are systematically arranged above and below the vacancies in the octahedral layers and bounded with oxygens in both the ( $\text{MnO}_6$ ) layer and the sheet of  $\text{H}_2\text{O}$  molecules. Two solid solution series have been established between Ca and  $\text{Mn}^{2+}$  end members in natural samples. The general formula for both series is



Mg, Na, K, and n is about 3 for the rancieite series and 1.5 or less for the birnessite series. Three new mineral species have been established from this study. On the basis of above crystal-chemical relations, redefinition of birnessite and related minerals is proposed, and the validity of mineral takanelite (Nambu and Taniq̄a, 1971), which has been recognized as  $\text{Mn}^{2+}$  analogue of rancieite, is doubtful.

**08.4-03** THE CRYSTAL STRUCTURE AND TWINNING OF BARIUM URANYL PHOSPHATE HEXAHYDRATE (META-URANOCIRCITE), AND COMPARISON TO THE OTHER MEMBERS OF THE META-AUTUNITE MINERAL GROUP. By M. E. Zolensky and D. K. Smith, Department of Geosciences, The Pennsylvania State University, University Park, Pa., U.S.A.

As part of ongoing research to fully determine the structural relationships between the hydrated uranyl phosphates, the structure of  $\text{Ba}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot 6\text{H}_2\text{O}$  (meta-uranocircite) has been determined.

Cell parameters for meta-uranocircite were determined to be  $a = 9.81$ ,  $b = 9.91$ ,  $c = 16.92$  Å, and  $\gamma = 90.5^\circ$ . The space group was found to be  $\text{P}2_1$ , the lowest symmetry yet reported for a meta-autunite. Subsequent structure analysis showed meta-uranocircite to have the uranyl phosphate sheet structure common to all members of the meta-autunite group, with interlayer water and barium atoms disordered in roughly square-planar groups. Infra-red spectra of meta-uranocircite were collected and indicated no substitution of hydronium for interlayer water or for barium.

The grating-like twinning of meta-uranocircite was investigated and was found to be involved with a phase transition occurring at  $108^\circ \pm 1^\circ\text{C}$ . Meta-uranocircite has a strong  $\text{P}2_1/\text{nm}$  pseudocell, and the twin elements are mirrors present in the pseudocell, but which are not required by the true  $\text{P}2_1$  space group. The phase transition is accompanied by a loss of four water molecules, with the disappearance of twinning signaling an increase in symmetry. It is probable that above  $108^\circ\text{C}$  the dehydrated meta-uranocircite has a truly tetragonal cell as usually reported for the meta-autunite group minerals.

**08.4-04** THE CRYSTAL STRUCTURE OF FURONGITE. By Shen Jinchuan and Peng Zhizhong, The X-ray Laboratory of the Graduate School of Wuhan Geological College, Beijing, China.

Furongite is a new mineral discovered in China in 1974. Its crystal structure has been determined. From the report published in 1979, its triclinic unit-cell parameters are as follows:  $a = 17.87$ ,  $b = 14.18$ ,  $c = 12.18$  Å;  $\alpha = 67.8$ ,  $\beta = 77.5$ ,  $\gamma = 79.9^\circ$ . Its chemical formula, as reported, is  $\text{A}_{13}(\text{UO}_2)_7(\text{PO}_4)_{13}(\text{OH})_{14} \cdot 58\text{H}_2\text{O}$ ,  $Z = 1$ .

It is one of the minerals with the most complicated composition and structure in uranyl hydroxyl phosphates discovered so far. The sample under study comes from the oxidized zone of uranium deposits in Hunan Province of China. A total of 9184 independent reflections were measured in the  $\omega$ -2 $\theta$  mode over the range  $2\theta < 48$  (with a RIGAKU RASA-2 automated single-crystal diffractometer) at room temperature, Mo target.

The crystal structure analysis shows us that it has the space group  $\text{C}_i = \text{P}1$ , and there are at least 150 sets of atoms (no H account) in an asymmetric unit. The main cations in the structure have been obtained by the direct methods.

The crystal structure of furongite has a layer which consists of uranyl and ( $\text{PO}_4$ ) mainly; there is a lot of water between two layers. For comparison with other similar minerals, it is convenient to transform the unit cell to a new one which has the parameters  $a' = a - 2c = 19.227$ ,  $b' = b = 14.094$ ,  $c' = c = 12.102$  Å,  $\alpha' = 67.205$ ,  $\beta' = 115.642$ ,  $\gamma' = 94.506^\circ$ ,  $V = 2709.9$ . In this new orientation the direction of layer is parallel to (001). Based on this result, the physical properties of furongite could be explained perfectly. The determination of the structure will be helpful in the classification of uranium minerals, for the genesis of uranium deposits and in the study of uranium crystal chemistry.