08.4-01 CRYSTAL STRUCTURE OF A NEW ZEOLITE MINERAL. By E. Tillmanns and H. Fischer, Institut für Geowissenschaften, Johann Wolfgang 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 Sellierberg near Hayen, Eifel, Germany. Electron-microprobe analyses gave SiO₂, 35.52, Al₂O₃, 30.11, K₂O 6.80, C₄O 11.58 weight %. 0.45 mm, the remainder of 21.6 % was interpreted as H₂O. This leads to chemical formula (Na₃Ca₄,₃Ca₂Al₃,₃₄Al₂,₃O₁₂,₃H₂O.)

A single-crystal X-ray study shows the mineral to be trigonal, space group P6₃/m with a = 9.49(2), c = 9.023(7), y = 90.2(1)°, 13 = 2.

The framework of SiO₂ and Al₂O₃ tetrahedra is essentially the same as in chabazite-Si₁₂₄O₃₂₈H₄O, and contains double 3-rings (36R) as secondary building units. Average T-O distances for the six different tetrahedra are 1.614, 1.611, 1.606 A for Si₁₂O₃₂₈H₄O, and 1.745 and 1.742 A for Al₂O₃H₂O distances indicating complete SiAl ordering.

Chabazite apparently crystallizes in space group P6₃/m with a = 9.40 R, b = 9.20 R, c = 9.18 R, y = 90.5°. The crystal structure of furongite has a layer consisting of uranyl phosphate sheets common to all members of the meta-autunite group, with interlayer water and barium atoms ordered in roughly square-planar groups.

The crystal structure of furongite is established between Ca₂Mn₄₊₂OH₂₄(PO₄)₁₂.₅H₂O and Ca₂Mn₄₋₂OH₂₄(PO₄)₁₂.₅H₂O with the unit cell parameters a = 17.87, b = 14.18, c = 12.18 A; a = 67.8°, b = 77.5°, y = 79.9°. Its chemical formula, as reported, is Ca₁₂₂(PO₄)₁₃(OH)₁₄·5H₂O, 2 = 1.

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

Birnmesite and rancieite occur as poorly crystalline aggregates in terrestrial or marine manganese ores. Both minerals have similar layer structures, which consist of edge-shared (MnO₆) octahedral layers and sheets of water molecules. They have hexagonal unit cell with variable dimensions, which depend on the water content and on the nature of cations between the layers. Some differences in the octahedral sites in the layers of birnmesite are 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 (MnO₆) layers and the sheet of H₂O molecules. Two solid solution series have been established between Ca and Mn considering end members in natural samples.

The general formula for both series is

\[(R)\text{Mn}_n\text{O} \cdot (\text{OH})_m \cdot n\text{H}_2\text{O}, \quad \text{where} \ R = \text{Ca, Mn}^{2+}, \text{Mg, Na, K, and} n \text{is about } 3 \text{ for the rancieite series and } 1.5 \text{ or less for the birnmesite series. Three new mineral species have been established from this study. On the basis of above crystal-chemical relations, redefinition of birnmesite, divanadite, and rancieite is proposed, and the validity of mineral takanedi (Nambo and Togida, 1971), which has been recognized as Mn₄₂ analogue of rancieite, is doubtful.}

08.4-03 THE CRYSTAL STRUCTURE AND TWINNING OF BARIUM URYN PHOSPHATE HYDROXIDE (META-URANOCIRITE), AND COMPARISON TO THE OTHER MEMBERS OF THE META-AUTUNITE MINERAL GROUP. By H. E. Tillmanns 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 Ba(PO₄)₂·6H₂O (meta-uranocirite) has been determined.

Cell parameters for meta-uranocirite were determined to be a = 9.81, b = 9.91, c = 16.32A, and γ = 90.3°. The space group was found to be P2₁, the lowest symmetry yet reported for a meta-autunite. Subsequent structure analysis showed meta-uranocirite to have the uranyl phosphate sheet structure common to all members of the meta-autunite group, with interlayer water and barium atoms ordered in roughly square-planar groups. Infrared spectra of meta-uranocirite were collected and indicated no substitution of hydronium for interlayer water or for barium.

The grain-like twinning of meta-uranocirite was investigated and was found to be involved with a phase transition occurring at 108°C ± 1°C. Meta-uranocirite has a strong Bragg pseudodcell, and the twin elements are mirrors present in the pseudocell. The space group is parallelogrammic, with the presence of twinning implying an increase in symmetry. It is probable that above 108°C the dehydrated meta-uranocirite 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 Wun 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 A; a = 67.8°, b = 77.5°, y = 79.9°. Its chemical formula, as reported, is Ca₁₂₂(PO₄)₁₃(OH)₁₄·5H₂O, 2 = 1.

It is one of the minerals with the most complicated composition and structure in uranyl hydroxyl phosphates discovered so far. The single crystal study comes from the oxidized zone of uranium deposits in Hunan Province of China. A total of 9184 independent reflections were measured in the 0-2θ mode over the range 20 = 48° (with a RIGAKU RAS-2 automated single-crystal diffractometer) at room temperature, Mo target.

The crystal structure analysis shows that it has the space group C2 = P1, 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 (PO₄)₂⁻ 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' = 7.20, b' = 12.96, c' = 12.10 A; a' = 67.205°, b' = 77.5°, y' = 79.9°. 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.