freely through the straight channels, the diameter of which is in the range from 2.64 to 3.30 Å. In this work the calculations, which allow to geometrically estimate the possibility of the location and movement of the molecules of xylene isomers and benzene in straight channels in zeolite ZSM-5 were carried out. We used the scanning method in 3 rotational and 3 translational degrees of freedom. All the distances between the atoms of a molecule and the surrounding atoms of the crystal were calculated for each scanning point and were compared with the normal van der Waals contacts. It was assumed that a molecule may be located in the scanning point if considerably shortened intermolecular contacts are absent. The calculation showed, that any of the considered molecules can be placed in a straight channel. However, only benzene and p-xylene molecules can move through such channel, because the overlapping of their van der Waals spheres with those of the channel atoms is acceptable (less 0.35 Å). The identity of the results obtained for the molecules of benzene and p-xylene indicates that the presence of substituent in para-position does not obstruct the movement of the molecule through the channel. Such calculations permit to estimate the geometry of available space.

PS-08.02.15 EVALUATION OF ZEOLITE FRAMEWORKS WITH THE VIEW TO CLASSIFICATION, ENUMERATION AND SOLUTION OF STRUCTURES.

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An overview of the current range of zeolite frameworks is presented as defined by their systematic relationships derived from their classification in terms of constituent 3-connected sheets. The application of the various methods for the classification and enumeration of zeolite frameworks and their usefulness in structure classification and solution is considered. Novel sets of hypothetical frameworks are evaluated, including a series for which the channel characteristics are pre-defined in two-dimensions.

08.03 - Minerals, Structure and Properties

PS-08.03.01 CRYSTAL CHEMISTRY OF THE CANCIRNITE LIKE MINERALS. By R.K.Rastsvetaeva,
Institute of Crystallography Russian Acad. of Sci., Moscow, Russia.

The structural peculiarities of afghanite, byttrite, liotite and the other minerals of the cancrinite group are investigated. A common system of describing the minerals of the cancrinite group by the letters A,B and C is suggested. The system is based on the arrangement of the six-membered rings around the rotation axes 3 along 2/3, 1/3, 2/3, 1/3, and 2/3, z and the screw axis 6 along 0, 0, z of space group P63mc. The letters correspond to the axes positions. The arrangement of these rings determines the form of the cavities and channels in the structures of this group of minerals. Three types of cavities are found in the structure of cancrinite (AB...), byttrite (ACBC...), and liotite (ACBABC...). The structure of afghanite (ACACBABC...) is characterized by combining the minimal cancrinite and maximal liotite cavities. A correlation between the chemical composition and the sizes and forms of the cavities is found.

PS-08.03.02A STUDY ON HOKULTOLITE SYNTHESIS AND ITS CRYSTALLOGRAPHIC ANALYSIS. Shu-Cheng Yu* and Jian-Sheng Lee, Department of Earth Sciences, National Cheng-Kung University, Tainan, Taiwan

Hokultolite is a mineral of hot spring deposit considered to be a solid solution of barite (BaSO₄) and angesite (PbSO₄). Natural occurrences of hokultolite reported in literature include Hokuto, Taiwan and Shibukure near Akita, Japan. The chemical composition of hokultolite from Taiwan was found to be from 21 mol% PbSO₄ to 32 mol% PbSO₄.

Synthetic hokultolite samples with different chemical composition were grown in the present study with the starting materials of solutions of Pb(NO₃)₂, Ba(NO₃)₂, and (NH₄)₂SO₄. Two different growth processes were carried out at 95 -100°C and ambient pressure conditions, with growth time of 3-4 days.

Optical microscopy and X-ray diffraction analysis suggest that the growth process significantly affects the crystallinity, growth rate and crystal size of the synthetic hokultolite. With two different growth processes, one process produced the sample with 59-71 mol% PbSO₄, and the other 73-80 mol% PbSO₄, with their corresponding average crystal size being less than 0.5 mm and greater than 0.5 mm, respectively. Extinction anomaly observed in optical microscopy study suggests that the grown materials may exhibit chemical/structural domain in the hokultolite crystal lattice.

PS-08.03.03 THE X-RAY STUDY OF Fe₂I ORE MINERALS FROM THE PACIFIC OCEAN. By N.T.Dmitrieva,
Institute of ore deposits geology, mineralogy, petrology and geochemistry, Russian Acad Sci., Moscow.

The samples of natural Fe₂I oxide minerals from different types or oceanic basalt have been studied by X-ray and electron microprobe analyses. It is estimated that the dominating

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number of samples are the homogenous solid solutions of ulvospinel and magnetite. The unit cell parameters display the wide variations - from 8.490 ± 0.005 Å to 8.495 ± 0.005 Å. The latter value is close to the end member of the isomorphic series, indicating the existence of complete solid solution between ulvospinel and magnetite. Some samples reveal the exsolution intergrowths of ilmenite and titano-magnetite or hematite and titanomagnetite. The structure parameters have been correlated with geodynamic conditions of oceanic-continental formation.

PS-08.03.04 REFINEMENT OF EUOLUINITE STRUCTURE by Nicheng Shi, Ling Liao, Zhenheng Ma, X.Y. Xue Lab., China University of Geosciences, Beijing 100083, China.

Euolinite is a mineral discovered in China in 1985. It is the only natural silicate in which CaH10O8.
H2O·H2O·H2O·H2O structure was first determined by Geikie in 1968, but only the coordinates of oxygen atoms were obtained. Our lab, in 1974, obtained the structure of Euolinite and all oxygen coordinates of the ring of oxygen atoms were obtained. The structure of Euolinite was refined by Rietveld and the final R value was 10.02%.

PS-08.03.06 CRYSTAL STRUCTURE OF AN OCHREITE WITH SPACE GROUP P4 by T.S. Ma, N.C. Shi, and Q.F. Zeng, X.Y. Xue Lab., China University of Geosciences, Beijing 100083, China.

Ochreite with space group P41 occurred in ancient of Dajing, Shandong Province, China. Analysis by electron microscope gave: SiO2 54.48, TiO2 0.08, Al2O3 1.07, Fe2O3 3.86, MgO 9.81, FeO 10.37, CaO 16.26, Na2O 2.12, K2O 0.85, Cr2O3 0.002, and 9871.21 wt % corresponding to (Ca10.61, Fe2.04, Al0.03, Mg0.005, Si0.001)

PS-08.03.07 A NATURALLY OCCURING HYDROCARBON MINERAL. Mace H.A., and Peterson R.C.
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The mineral fichtelite (CaH4H2O) is a naturally occurring saturated hydrocarbon that is generally found in the remnants of pine-tree trunks in peat and lignite beds in the Fichtel Gebirge region of Germany. It is a fossil resin of abietic acid, which is a component of rosin found in pine trees.

Single crystals up to 4 mm were obtained from a mass of crystals (4 cm across), which existed on a piece of pine wood. The colorless, colourless fichtelites exhibited a platy habit with well-defined crystal faces. The monoclinic space group, C2, was obtained using precession techniques. Unit cell dimensions were determined to be ah = 10.706 Å, b = 7.485 Å, c = 10.823 Å and β = 105.64°.

The structure was determined by direct methods using 1229 unique reflections obtained with Mo-Kα X-ray. Full-matrix least-squares refinement of atomic positions and temperature factors produced an R = 0.059. The molecules, a hydrophenanthrene, consists of three non-linear fused six-membered rings in chair conformation, as well as an attached methyl group on the first ring, an isopropyl group on the third ring, and an angular methyl group. The position and isotropic temperature factors of all but one hydrogen were determined. All obtained bond lengths and angles were consistent with expected values.

The conversion of abietic acid to fichtelite is a result of chemical processes that result in the loss of the carboxylic acid group, as well as the saturation of the carbonyl group in the rings along with the gain of hydrogen atoms.

Small red crystals up to 1.5 mm were observed to be intergrown with the fichtelite. Work is currently being carried out to identify and crystal structure of this material.