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.

Duncan Akporiaye

SINTEF-SI, P.O. Box 124 Blindern, N-0314 Oslo, Norway.

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

The structural peculiarities of afghanite, bystrite, liottite 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, z and 1/3, 2/3, z and the screw axis 6 along 0, 0, z of space group $P6_3mc$. 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...), bystrite (ACBC...) and liottite (ACBCBC...). The structure of afghanite (ACACBCBC...) is characterized by combining the minimal cancrinite and maximal liottite cavities. A correlation between the chemical composition and the sizes and forms of the cavities is found.

PS-08.03.02A STUDY ON HOKUTOLITE SYNTHESIS AND ITS CRYSTALLOGRAPHIC ANALYSIS Shu-Cheng Yu* and Jiann-Shing Lee, Department of Earth Sciences, National Cheng-Kung University, Tainan, Taiwan

Hokutolite is a mineral of hot spring deposit and considered to be a solid solution of barite ($BaSO_4$) and anglesite ($PbSO_4$). Natural occurrences of hokutolite reported in literature include Hokuto, Taiwan and Shibukure near Akita Japan. The chemical composition of hokutolite from Taiwan was found to be from 21 mol% $PbSO_4$ to 32 mol% $PbSO_4$.

Synthetic hokutolite samples with different chemical composition were grown in the present study with the starting materials of solutions of $Pb(NO_3)_2$, $Ba(NO_3)_2$ and $(NH_4)_2SO_4$. 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 hokutolite. With two different growth processes, one process produced the sample with 59-71 mol% $PbSO_4$ and the other 73-80 mol% $PbSO_4$, 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 exhibt chemical/structural domain in the hokutolite crystal lattice.

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

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

