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 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-08.03.03 THE 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

number of samples are the homogenious solid solutions of ulvospinel and magnetite. The unit cell parameters display the wide variations −from 8.390 ± 0.005Å to 8.485 ± 0.005Å The latter value is close to the end member of the isomorphous series, indicating the existance of complete solid solution between ulvospinel and magnetite. Some samples reveal the exsolution intergrowth of ilmenite and titanomagnetite or hematite and titanomagnetite The structure parameters have been correlated with geodynamic conditions of oceanic-basalts formation.

PS-08.03.04 REFINEMENT OF SUOLUNITE STRUCTURE By Nicheng Shi*, Libing Liao, Zhesheng Ma, X-Ray Lab., China University of Geosciences, Beijing 100083, China.

Suolunite is a mineral discovered in China in 1965. It is the only natural silicate in which CaO:SiO₂:H₂O=1:1:1. Its structure was first determined by Weissenberg photographic method in 1965. But only x and y coordinates of nonhydrogen atoms were obtained. Our Lab. restudied its structure in 1974 and obtained all z coordinates of the nonhydrogen atoms. The deviation factors for F(hk0) and F(hkl) were 17.2% and 18.3% respectively. This study is to refine suolunite structure and to find out as much hydrogen atoms as possible. The intensity data of suolunite was collected on RASA-IIS Rigaku auto-four-circle diffractometer. MoKα radiation, graphite monochromator. 2θ range for data collection: 3° <2θ<120°. Intensity data were corrected for PL factor. 1519 intensities were collected in total and 1281 separate intensities, for which |F|>3δ|F|, were used in the refinement. The unit cell parameters of suolunite are: a=11.119(3)A, b=19.776(3)A, c=5.9900(8)A, V=1317.18(5)A³. Orthorhombic system. Space group is Fdd2. Dx=2.71g/cm³. The least-squares refinement reduces the R factor to 0.032 for anisotropic temperature factors. Coordinates of all nonhydrogen atoms and some hydrogen atoms were obtained. The refinement result indicates that z coordinates of all atoms in suolunite are away from 1/4, 1/2 and 3/4 to some extent. The bond lengths and bond angles showed that the double tetrahedra in suolunite are the most streched. The Si-O-Si angle of it is very close to 180°, which attracts attention from many crystalchemists.

PS-08.03.05 CRYSTAL STRUCTURE OF AN OMPHACITE WITH SPACE GROUP Pn By Z.S.Ma, N.C.Shi and Q.f.Zhang, X-Ray Laboratory, China University of Geosciences, Beijing 100083, China.

Omphacite with space group Pn occurred in eclogite of Zhucheng, Shandong Province, China. Analysis by electron microprobe gave: SiO₂ 54.409, TiO₂ 0.084, Al₂O₃ 9.207, FeO 3.285, MnO 0.012, MgO 10.317, CaO 16.264, Na₂O 5.123, K₂O 0.005, Cr₂O₃ 0.005, sum 98.712(wt %) corresponding to (Ca₀.₆₃Na₀.₃₆)₀.₉₉(Mg₀.₆₆Fe₀.₁₀Al₀.₃₆)₁.₀₂(Si₂O₆).

The crystal(0.25·0.6·0.32 mm in size) was selected and mounted on RASA-IIS Rigaku 4-circle automated diffractometer, with MoKα radiation, a graphite monochromator, a 2θ-ω scan, the scanning constant Δω=1.282+0.5tanθ, a speed of 4°/min. 1833 diffractions were collected in the range of 3° <2θ<65°, of which 905(F>3 σ |F|) were used for structure refining. The possible space group is P2/n or Pn. The Pn space group was confirmed by the results of structure refinement. a=9.607(4), b=8.774(4), c=5.245(1) Å, β= 106.63(3)°, V=423.62 Å³, Z=4. Dx=2.483 g/cm₃. The structure was solved by direct methods (SHELX-76). Atomic coordinates, occupancies, isotropic and anisotropic temperature factors were carried out which finally led to reduction of R to 0.051. The polyhedra of Ca-O, Na-O and Mg-O underwent stronger distortions(the ranges of bond length Ca-O 2.35~2.72 Å; Na-O 2.34~2.73 Å; Mg-O 1.97~2.14Å; Al-O 1.91~ 2.08 Å) than polyhedra of omphacite with P2/n, which caused the symmetry to be reduced. Probably, the occurrence of omphacite with Pn indicated it being of lower formation temperature than omphacite with P2/n.

PS-08.03.06 FICHTELITE.
A NATURALLY OCCURRING HYDROCARBON MINERAL.
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The mineral fichtelite ($C_{19}H_{34}$) 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 clear, colourless crystals exhibited a platy habit with well-defined crystal faces. The monoclinic space group, $P2_1$, was obtained using precession techniques. Unit cell dimensions were determined to be a = 10.7060 Å, b = 7.4585 Å, c = 10.8236 Å and β = 105.840°.

The structure was determined by direct methods using 1229 unique reflections obtained with Mo-Kα X-radiation. Full-matrix least-squares refinement of atomic positions and temperature factors produced an $R_w = 0.039$. The molecule, a perhydrophenanthrene, 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 carbons contained 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 determine the identity and crystal structure of this material.