

dimensional 3-connected 10-gon nets (of a (10.3)- α type after A.F.Wells) acting as a template. For $N_W/N_T = 1/3$ it is this network which provides uniform interaction between template W (or W+S) components and $TO_{4/2}$ framework constituents. Conventionally one can subdivide the whole tetrahedral framework into two subsystems as if generated by different W,S subnets.

PS08.00.09 CRYSTAL CHEMISTRY OF SYNTHETIC 1:3 SILICATE AND GERMANATE PYROXENES M. Behruzi, E. Banerjee-Appel, F.D. Scherberich and Th. Hahn. Institut fuer Kristallographie, RWTH Aachen, D 52056 Aachen, Germany.

Binary systems of the type $LiAlGe_2O_6$ - $LiGaGe_2O_6$ show peritectic melting and increase of the melting temperatures with increasing atomic number of the three valent cations (Fe, Sc, In). All 1:3 pyroxenes crystallize only in the monoclinic form with the exception of $LiScGe_2O_6$ and $LiInGe_2O_6$ which can be synthesized in the monoclinic and orthorhombic enstatite types. The orthorhombic forms are the low temperature phases and undergo a sluggish but complete transition to the monoclinic form; the reverse transition is much more sluggish.

The monoclinic germanates show a rapid and reversible phase transition from the low temperature form (mostly P21/c) to the high temperature form (C2/c). The phase transitions give rise to a discontinuous increase of the a, c and β but decrease of the b axis. Furthermore, the symmetrically non-equivalent tetrahedral chains become equivalent and the tetrahedral chains stretch.

Special features of monoclinic pyroxenes: 1) The observed M^{3+} -O bond lengths are 0.985 of the calc. bond lengths. 2) The Li-O and Na-O bond lengths differ for the corresponding silicates and germanates 3) They are a linear function of the M^{3+} -O bond lengths. 4) The c axes of the Li and Na silicates are equal and a linear function of the M^{3+} -O. 5) The c-axes of the germanates are larger than those of the corresponding silicates. They are also a linear function of M^{3+} -O; for C2/c they are larger than for P21/c.

PS08.00.10 INORGANIC STRUCTURAL CHEMISTRY WITH CRYSTALLOGRAPHIC DATABASES. G.Bergerhoff and M.Berndt, University of Bonn, Germany

Application of a clearcut definition for the concept of isotypism to the crystallographic databases allows to find new and old relations between inorganic crystal structures. First of all data have to be standardized in order to get a uniform description of crystal structures. We started to apply STRUCTURE TIDY, the procedure of L.M.Gelato and E.Parth (J.appl.Cryst. 20 (1987) 139-143), to the ICSD (Inorganic Crystal Structure Database). But there are limits of this method if cell dimensions or coordinates are near specific values. In a second step, therefore, all structures within an isopointal group are compared with each other. The structural difference between structure (1) and structure (2) is now the degree Δ of isotypism, which is zero for complete coincidence (m = multiplicity).

$$\Delta = (((2^{1/2} * \Delta(c)) + 1) * \Delta(d)) - 1$$

where is $\Delta(c) = (\sum (m * ((x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2)^{1/2}) / \sum m$
 $\Delta(d) = a_1^2 * b_2 * c_2 / a_2^2 * b_1 * c_1$ where $a_1 > a_2, b_2 > b_1, c_2 > c_1$
 $\Delta(c)$ is the weighted mean difference of the coordinates of both structures, $\Delta(d)$ combines the relation between the cell dimensions of both structures. Δ is calculated and reduced to the minimum value by selecting the best fitting set of equivalent coordinates and cell choice. The comparison by means of the Δ value can also be expanded beyond the limits of an isopointal group. In course of the indexing process of the database the minimal Δ value is stored as a retrieval parameter in the revised version SICS (Standardized Inorganic Crystal Structures) of the ICSD. The user now can choose any structure and ask for isotypes within a preselected Δ range. For the effectivity of this way of retrieval several examples are given. This algebraic procedure has the advantage not to be dependent on theories of bonding and connec-

tions. For a real impression of the structures compared we use DIAMOND, a graphics system easily used in connection with the databases. Further information you may find in WWW: <http://www.rhrz.uni-bonn.de/~unc442/diamond.html>

PS08.00.11 STUDIES ON THE TEMPERATURE DEPENDENCE OF ELECTROCONDUCTIVITY FOR CRYSTALS OF PHLOGOPITE AND FLUOROPHLOGOPITE. Y.V. Ezhova, F.A. Scherbachenko, V.A. Kamakov, N.A. Hlopenko, Irkutsk State University, Irkutsk, Russia

The specific conductivity of natural (phlogopite) and synthetic (fluorophlogopite) micas has been studied as a function of temperature. This allowed to establish activation energies and a nature of charge carriers responsible for current in crystals under investigation.

The conductivity of Phlogopites in the temperature range 300-500 K is associated with aqua-pellicle impregnations and is characterized by activation energy of 0.15-0.20 eV. In the range 500 - 900 K the carriers are loosely bound ions of impurities with activation energy of 0.3-0.4 eV. Above 900 K the activation energy is about 3.0 eV and the charge carriers are most likely fluorine ions.

Within the considered interval of temperatures specific conductivity of fluorophlogopites is by two orders of magnitude lower than those of phlogopites. The differences in the magnitude and character of conductivity for these species of mica are explained by a high thermoresistance of fluorophlogopite. The latter is due to a substitution of hydroxygroups by fluorine ions, more firmly bound to lattice, and due to the nearly complete absence of molecular water in fluorophlogopite.

PS08.00.13 DETERMINATION OF SPACE GROUP AND STRUCTURE FOR SYNTHETIC SVABITE: $Ca_5(AsO_4)_3F$. P. Goodman, A. Schwartzman, School of Physics, University of Melbourne, Parkville, Vic. Australia 3052, B.Rodier, F. Lincoln, Department of Chemistry, University of Western Australia, Nedlands, W.A. Australia 6009; T.J. White, Ian Wark Research Institute, University of South Australia, The Levels, S.A., Australia 5098.

Although the structure of fluoro-apatite was established some 50 years ago¹, the chemical analogue with As replacing P has never been investigated structurally, due primarily to the fact that in its native form it is associated with numerous cation impurities. In this paper we present evidence to show that the As substitution causes the space group to shift from $P6_3/m$ to $P6_322$, as a result of a shift of the heavier cation from special to general positions. The structural change has been investigated in the solid solutions $Ca_5(As_xP_{1-x}O_4)_3F$, and it appears that the change occurs for $x > 0.5$, although a complete phase diagram has yet to be described.

Investigative methods include CBED and Rietveld refinements of powder x-ray data.

¹C.A.Beevers and D.B.McIntyre (1946) Mineralogical Mag. 27, 870.