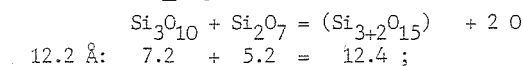


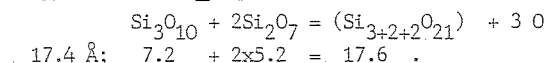
08.1-05 CRYSTAL CHEMISTRY OF Ca, R.E., AND Zr SILICATES, AS DERIVATIVES OF WOLLASTONITE CHAINS. By M. J. Chiragov, Department of Geology, The Azerbaijan State University, 370122 Baku, USSR.

Holmium silicate, $K_2H_2HoSi_3O_{10}$ (Chiragov (1979), Azerb. Univ. Geol. Bull.), is isostructural with $K_3YSi_3O_8(OH)_2$ (Ilyukin (1968), Dokl. Akad. Nauk USSR). Both are inosilicates and the Si_3O_{10} or $Si_3O_8(OH)_2$ groups that are part of their structures can be considered analogous to corresponding groups in the wollastonite chain, from the points of view of symmetry elements, bond angles and oxygen sharing with the cationic octahedron. Similar analogies exist in the arrangement of chains and distribution of cations in the structures of rhodonite $Mn_4CaSi_5O_{15}$ (Mamedov (1958), Dokl. Akad. Nauk Azerb. SSR), babingtonite $Fe^{+3}Fe^{+2}Ca_2Si_5O_{14}(OH)$, inesite $Mn_7Ca_2Si_{10}O_{28}(OH)_2 \cdot 5H_2O$, and pyroxmangite $Mn_3Fe_3CaSi_7O_{21}$. In these silicates the inosilicate groups bond themselves only to the octahedron of the Ca atom. Taking this peculiarity into account, the formation of chain types can be presented as follows:

in rhodonite, \underline{c} equals



in pyroxmangite, \underline{c} equals



Our conclusion is that, in silicate structures characterized by derivatives of the wollastonite chain, the basic motifs are the inosilicate groups Si_3O_{10} polymerized with octahedrons of large cations. We consider the scheme of formation of different structural types from simple structural units from this point of view.

08.1-06 CRYSTAL STRUCTURE PREDICTION BY ENERGY MINIMISATION. By C.R.A. Callow, A.N. Cormack, University College London, and F. Theobald, Laboratoire de Chimie Physique, Besançon, France.

This paper will show that calculations of crystal energetics for ionic solids coupled with efficient minimisation routines are capable of predicting the structure of complex inorganic solids, thereby promising to provide a valuable guide in structure refinements. The calculations we discuss are based on exact summations of both Coulomb and short-range components of the lattice energy. Energy minimisation may be performed with respect to all structural parameters. We illustrate the power of our method with two examples. The first concerns the recently discovered 'B' phases of VO_2 and TiO_2 (Marchand et al., Mat. Res. Bull. 15, 1129 (1980)). Energy minimisations were performed starting from an ideal model based on regular octahedra. The minimised structure shows distortions close to those observed in the X-ray refined model for VO_2 . A predicted structure for the analogous 'B' phase of TiO_2 is also presented; no experimental structure is yet available for this phase. Our second example is the mineral forsterite (Mg_2SiO_4) where again we show that distortions from idealised models are correctly predicted. We conclude with a discussion of potential future application of the technique to complex transition metal compounds and to minerals.

08.1-07 STRUCTURE BUILDING PRINCIPLES IN THE Pb-Bi-(Ag,Cu) SULPHOSALTS AND RELATED COMPOUNDS. By Emil Makovicky, Mineralog. Inst., Copenhagen, Denmark.

In comparison with As and Sb, (1) bismuth displays the smallest differences in the lengths of distinct categories of Bi-S bonds (resp. distances) and sometimes forms regular coordination octahedra; (2) the S-S dimensions of the full Bi-S coordination polyhedra differ least from those of the Pb-S polyhedra. In some sulphosalts differences between Pb and Bi are important and they are ordered (cosalite) whereas some are based on, or tolerate extensive mutual Pb-Bi substitution (lillianite, hegyptite, $PbBi_4S_7$, cannizzarite). Introduction of Se for part of S augments the geometrical tolerance for Pb-Bi variations over structural sites and the gamut of structure types. Structurally related compounds will also be quoted.

The structures of the Pb-Bi sulphosalts can be represented as modulated structures, usually based on somewhat deformed "galena-like" structure sliced in different crystallographic directions (slices parallel to (100) of PbS will be called T layers, those parallel to (111) of PbS will be called H layers). The combinations of several modulation operators create distinct structural types; the homologues in each series differ in the H/T match and/or layer thickness: (1) The cannizzarite homologous series with the structures composed of regularly alternating layers H and T which in one direction match after the vernier principle. (2) The galenobismutite homologues with the H and T layers broken into variably long strips by composition non-conservative glide planes. On the latter, zig-zag layers of additional atoms occur. Galenobismutite ($\approx CaFe_2O_4$), weibullite; a modified type: nuffieldite. (3) The cosalite homologous series with zig-zag layers of "galena-like" structure with H- and T- like portions alternating. The