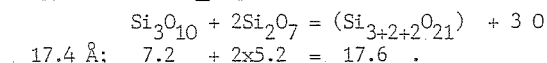08.1-05   CRYSTAL CHEMISTRY OF Ca, R.E., AND Zr
SILICATES, AS DERIVATIVES OF WOLLASTONITE CHAINS. By M.
J. Chiragov, Department of Geology, The Azerbaijan State
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Holmium silicate, $K_2H_2HoSi_3O_{10}$ (Chiragov (1979), Azerb.
Univ. Geol. Bull.), is isostructural with $K_3YSi_3O_8(OH)_2$
(Ilyukin (1968), Dokl. Akad. Nauk USSR). Both are ino-
silicates 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 dis-
tribution 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 pe-
culiarity into account, the formation of chain types can
be presented as follows:

in rhodonite, c equals

$$Si_3O_{10} + Si_2O_7 = (Si_{3+2}O_{15}) \quad + 2\ O$$
$$12.2\ \text{Å:} \quad 7.2 \quad + 5.2 \ = \ 12.4\ ;$$
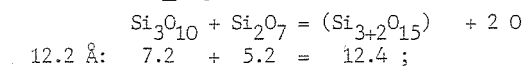
in pyroxmangite, c equals

$$Si_3O_{10} + 2Si_2O_7 = (Si_{3+2+2}O_{21}) \quad + 3\ O$$
$$17.4\ \text{Å;} \quad 7.2 \quad + 2\times5.2 \ = \ 17.6\ .$$

Our conclusion is that, in silicate structures charac-
terized by derivatives of the wollastonite chain, the
basic motifs are the inosilicate groups Si_3O_{10} polymer-
ized 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' pha-
se 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 categor-
ies 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, heyrov-
skyite, $PbBi_4S_7$, 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 represent-
ed 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 regu-
larly alternating layers H and T which in one direction
match after the vernier principle. (2) The galenobismu-
tite 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 addit-
ional atoms occur. Galenobismutite ($\approx CaFe_2O_4$), weibull-
ite; 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