08.1-01 INORGANIC STRUCTURE TYPES DESCRIBED BY FRAMEWORKS IN SPACE-GROUP TABLES. By E. Hellner, Institute of Mineralogy, University of Marburg, Lahnberge, D-3550 Marburg/L., Germany.

The tables will combine two different efforts of C. Hermann: the list of lattice complexes for each space group, contained in "Internationale Tabellen zur Bestimmung von Kristallstrukturen" (1935), and the detailed description of frameworks of structure types in "Strukturberichte", vols. 1 and 2. The base for the symbolism used for the description of frameworks and occupied voids are Hermann's symbols for lattice complexes (Z. Krist. <1960> 113, 142) which are expanded in "Space groups and lattice complexes"(NBS Monograph 194 (1973)', and the symbols for coordination polyhedra (Donnay et al., Z. Krist. <1964> 120, 364). There is one table for each space group. The head line contains a lattice-complex description of point positions and shows some homogeneous sphere packings, which occur in that space group (W. Fischer, Z. Krist. <1973> 138, 129, <1974> 140, 50). The tables will contain a detailed description of all known structure types until 1980. The cubic ones are tabulated in part IA. Part IB gives the corresponding list of all cubic homogeneous and heterogeneous frameworks, their properties (illustrated by drawings), and their grouping in main- and subclasses. Part II (in preparation)will list all deformed cubic structure types and those which may be derived from cubic ones by changing the stacking sequence.

08.1-02 MODULAR CRYSTALLOGRAPHY OF CHAIN SILICATES. By Yoshikazu Ohashi, Dept. of Geology, Univ. of Pennsylvania 19104, U.S.A.

One of the goals of systematic crystallography is to predict possible structures by analyzing geometrical regularities of the known structures. The concept of modular crystallography (Thompson, Amer. Min. vol. 63, 239, 1978) has been extended to 3-, 5-, and 7-tetrahedral repeat single chain silicates (pyroxenoids) as follows: (1) tetrahedral and octahedral beam modules are assumed to be similar to those found in the known structures, (2) possible ways of layer-module formation are analyzed, and (3) stackings of layer modules are examined. About half (A-F) of all possible combinations shown below are structures that have not been found.

Wollastonite	rhodonite		pyroxmangite
Pectolite	nambulite, marsturite		(C)
(A)	babingtonite		(D)
(*)	santaclaraite		(E)
Bustamite	(B)		(F)

(A) $ZY[Si_3O_8(OH)]$

(B) $Y_9[Si_{10}O_{28}(OH)_2]$

(C) $XY_6[Si_7O_{20}(OH)]$

(D) $ZY_5[Si_7O_{20}(OH)]$

(E) $Y_7[Si_7O_{20}(OH)](OH)H_2O$

$X=M^{+1}$

(F) $Y_{13}[Si_{14}O_{40}(OH)_2]$

$Y=M^{+2}$

(*) not new (same as pectolite)

$Z=M^{+3}$

Recently (A) has been found as the mineral cascandite, $CaScSi_3O_8(OH)$, (Merlino, priv. comm.). Expected powder patterns can be calculated for the hypothetical structures obtained from a distance least-squares method. This approach is useful not only to identify new species but also to provide systematic structural basis for Ca-Si-O-H minerals which are often too fine-grained for a single-crystal study.

08.1-03 GEOMETRICAL DECOMPOSITION OF SUBSTITUTION DERIVATIVES. By J. Lima-de-Faria, J.I.C.U., Alameda D.Afonso Henriques 41-4º E, 1000 Lisboa, Portugal.

We may consider the following question: are substitution derivatives geometrically decomposable in simple known structure types? For instance, is $A_p^oB_q^o[X_m]^c = A_p^o[X_m]^c + B_q^o[X_m]^c$ which are known structure types? A study of the geometrical decomposition of interstitial substitution derivatives of general formulas $A_p^oB_q^o[X_m]^{c/h}$ and $A_p^tB_q^t[X_m]^{c/h}$ (o for octahedral and t for tetrahedral interstices) has been

$Li^oIn^o[O_2]^c$ $Ti^o[O_2]^c$ $Ti^o[O_2]^c$

• Li, Ti
⊘ In, Ti
· O
□ Octahedral vacancy
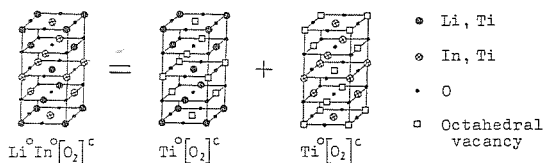
carried out, based on the proper layer description and on the standard representation of layered structures. Very simple descriptions of these structures were obtained, and it was concluded that there is a certain tendency for interstitial substitution derivatives to be geometrically decomposable in simple known structure types. This also expresses the tendency for atoms of the same kind to behave independently of the others, determining their own stability.

08.1-04 COMPARISON BETWEEN THE FRAMEWORK (BAUVERBAND) DESCRIPTION AND THE LAYER DESCRIPTION OF INORGANIC STRUCTURE TYPES: By E. Hellner, and E. Koch, Institute of Mineralogy, University Marburg, D-3550 Marburg, B.R.D., and by J. Lima-de-Faria and M.O. Figueiredo, J. I.C.U. Al. Af. Henriques, 41-4°E, 1000 Lisboa, Portugal.

A comparison is presented between the framework (Bauverband) description of crystal structure types, making use of lattice-complex symbols and coordination polyhedra, and the layer description, based on the characterization of layer patterns and stacking modes, and of coordination of the interstitial atoms. Illustrative examples are selected to show the capability of each symbolism to disclose interesting geometrical relationships, like polytypism, insertion, substitution, vacancy formation, ordering and distortion.

The need for establishing a useful compromise between the two extremes complete-but-complex and simple-but-ambiguous is stressed. The domains of convergence between both approaches are emphasized, thus making it worthwhile to undertake an agreement on a set of common symbols, as a starting point for an attempt towards a unified perspective on the systematics of inorganic crystal structures.