

08.X-4 THE CLASSIFICATION OF MINERALS

by Glauco Gottardi, Università di Modena, Italy. A full report on the history of the classification of minerals was given by Lima-de-Faria(1983). Nowadays minerals are classified on the basis of their chemistry, structure or both. The most complete type of a purely chemical classification is Hey's "Index"; this is certainly a useful tool for every mineralogist, but has never been considered, even by its author, as a basic way for classifying minerals. A purely structural way was proposed by Lima-de-Faria(1983); his guideline is to "group the inorganic crystal structures first by category of their structural units (SU), which may be isolated atoms, finite groups, infinite chains, sheets or frameworks". The atoms, which pertain to a structure without being in the SU, are called interstitial and are considered separately. Chemistry and structure are the basis of most chemical classifications proposed and used to present, even though unintentionally in many cases. Strunz adopts this double criterion in his "Tabellen"; he subdivides the minerals chemically in 9 classes, and then groups them structurally within each class; his deep and pragmatical intuition allowed him to produce the most widely adopted classification: but the same criteria with similar chemical classes are present in much older handbooks, where minerals with the same symmetry and morphology are grouped, therefore anticipating the concept of "equal structure". Some proposals may be useful for stimulating further work. Firstly, a structural classification is unavoidable nowadays, but with the disadvantage of having galena and rocksalt in the same box; therefore a previous chemical subdivision in Strunz's 9 classes, or something of this kind, is necessary. Secondly, if we put minerals with the same structure in the same box, we must define clearly what "equal structure" means. Low coordination polyhedra (lato sensu) are certainly very important in this context, and high coordination ones are not, but where is the limit between low and high coordination? Moreover, if triangles, tetrahedra and octahedra are "accepted" polyhedra, and all three are present in a structure, have we to use all three in the classification or not? After making this choice, everything must be referred to these elements, and the topologic symmetry (aristosymmetry of Megaw) of these elements as arranged in the structure should be considered. Lastly, we should not forget that our final aim is a classification of minerals (or in general of inorganic structures): so every enumeration of possible structures can be considered as a useful basis, but one should avoid burdening the classification with a lot of empty boxes corresponding to possible structures never found in real crystals. For the same reasons, the classification of different classes, say borates and silicates, could be organized in a slightly different way, as done previously.

08.X-5 STANDARDIZED STRUCTURE DATA AS AN AID FOR THE SYSTEMATIC CRYSTAL CHEMISTRY OF INORGANIC AND METALLIC COMPOUNDS. By E. Parthé, Laboratoire de Cristallographie aux Rayons X, Université de Genève, 24, quai Ernest Ansermet, CH-1211 Genève 4, Switzerland.

One of the important tasks of systematic crystal chemistry is the recognition and the grouping of identical or quasi identical crystal structures. Owing to the lack of a standard for the description of crystal structures, positional coordinates of two identical structures may not show any correspondence whatsoever. There are numerous examples in the literature where identical crystal structures were not recognized as being isotypic but were described as different structure types. This happened even in Strukturberichte, where the types DO_{11} (Fe_3C) and DO_{20} ($NiAl_3$) actually correspond to the same structure type.

We propose a standardized form for presenting crystal structure data which makes use of the Hermann-Mauguin space group settings as given in the International Tables for Crystallography, Vol. A. as a choice both for the unit cell and the Wyckoff sets of atom coordinates. However, the use of International Tables alone is not sufficient to describe structure data in a unique way. For the unit cell an additional selection rule based on its metric may have to be used. Further structure descriptions can be obtained by

- a shift of origin of the coordinate system
- a rotation of the coordinate system and
- an inversion of the basis vector triplet.

For space groups without axial polarity up to 24 different descriptions for one structure can occur. To make a selection from these different structure descriptions a standardization parameter is calculated for each description. It corresponds to the sum of the distances from the origin of the unit cell to all atom sites in one particularly chosen asymmetric unit, calculated from the fractional coordinates alone by assuming that the unit cell is a cube of unit length. The structure description for which the standardization parameter has the smallest value is taken as standard. Details of this standardization procedure can be found in a recent publication (E. Parthé & L.M. Gelato (1984), Acta Cryst. A40,).

The application of the standardization procedure to published structure data has permitted not only the equivalence of atom coordinates of different compounds, already known to be isotypic, to be demonstrated, but has also revealed new cases of isotypism.

The examples to be discussed include the structural relationship between the η carbides, Ti_4Ni_2O and Ti_2Ni , the isotypism between $Ca_{31}Sn_{20}$ and $Pu_{31}Rh_{20}$ and between $Gd_3Cu_4Ge_4$ and $Li_4Sr_3Sb_4$ and finally the interpretation of the Mo_2IrB_2 structure as a substitution derivative of the Y_3Co_2 type.

It would be of great help for anyone undertaking systematic crystal chemical studies if the crystal structure data were to be available in standardized form. As long as there is no generally adopted policy of publishing structure data in standardized form only, it would be most useful if the crystallographic data bases were presented in such a way as to allow the easy recognition of isotypic (or isopuntal) structures by a simple comparison of the list of atom coordinates.