conference abstracts

s8b.m4.o5 **The method for comparing crystal structures by means of the graph theory.** V.A. Blatov, *Samara State University, Ac. Pavlov St. 1, Samara 443011, Russia.*
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A method for the classification of crystal structures and atomic packings is proposed, which is based on the representation of the system of interatomic bonds in a crystal as a finite 'reduced' graph. The novel concepts of 'topological isotypism', 'topological type', 'topological sort of atoms' are introduced to characterize topological likeness of crystal structures taken as a whole or of separate atomic packings. These concepts are similar to the terms 'isostructurality', 'structure type', 'crystallographic sort of atoms' normally used at the geometrical level of crystal structure description. The computer program *IsoTest* is worked out, allowing one to find automatically the topological similarity (topological isotypism) for large groups of stoichiometrically and structurally different compounds. An important features of *IsoTest* are (i) enumeration of all variants of topological representations of crystal structure or of choice of atomic packings in it irrespective of their crystal-chemical significance, (ii) automatic search for possible relations between different representations of different crystal structures, and (iii) determination of the type of an atomic packing at any degree of its distortion. Thus, all stages of crystal-chemical systematization may be automated.

The analysis was carried out of about 3000 crystal structures of anhydrous simple, double sulfates and molybdates, simple and complex sulfides, and other binary inorganic compounds. Numerous examples of topological isotypism within these groups of substances were found, which are frequently unexpected from traditional point of view. For instance, the following pairs are topologically equal: $K_2Mg_2(SO_4)_3$ and Th_3P_4; $Zr(SO_4)_2$ and $PbCl_2$; $Gd_2(MoO_4)_3$ and Rh_3P_2; etc. In many cases simple and complex compounds with similar composition have similar topology of crystal structures, for instance, $M_2(SO_4)_3$ and M_2S_3 (M=In) or M_2O_3 (M=Al,Ga,In,Fe,Cr); MSO_4 and MS (M=Zn, Ca, Sr, Ba, Fe, Co, Ni, Sn) or MO (M=Zn, Hg, Ca, Sr, Ba); Li_2SO_4 and Li_2S or Li_2O.

Topological similarity of crystal structures can be often explained in terms of atomic packings. The novel criteria of the search for the 'leading' packing in a crystal structure are proposed which are based on the concept of packing uniformity. We studied the topological features of all atomic packings in all the compounds mentioned above and found that the close packings distorted to some extent play the leading role in about 35% of crystal structures. It is shown that the packings not only of large anions, but also of large or heavy cations and the mixed packings can be frequently structure-forming. In many cases distorted close packings consist of complex atomic groups, in particular, of sulfate or molybdate ions.