s8b.m4.p5 **Different ways of establishing crystal structure interrelations: new examples.** *O.Yakubovich, **W.Massa. *Moscow Lomonosov State University, Vorob'evy Gory, 119899 Moscow, Russia. **Philipps-University, 35032 Marburg, Germany.
Keywords: crystal structure relationships, archetype.

A number of relationship varieties between crystal structures can be mentioned. Many of them have been described in the literature in terms of homologous, morphotropic, polysomatic (or accretional) series, polytypes or homeotypes, etc.

New examples of crystal structures, recently found by the authors, that seem to be different kinds of derivatives from simpler (basic) constructions, will be discussed. The refined crystal structure of the Ge-analogue of natisite $Na_2TiO[GeO_4]$ (R = 0.030) and the structure of a new V representative in the natisite raw of compounds $Na_3VFO_2[PO_4]$ (R = 0.016) differ mainly by the degree of the mixed anionic radical polymerization (layer or framework) and are symmetrically related with the interaction of the "group - subgroup" type. We have shown that structural transformations in the raw are conditioned by the character of chemical bonds in the anionic part and by the cationic sublattice ordering.

The new member in the lomonosovite family $Na_5Ti_2O_2(VO_4)[Si_2O_7]$ (R = 0.028) and a new Cu,Al fluoride disilicate $CuAl_2F_2[Si_2O_7]$ (R = 0.022) are interpreted in terms of the modular concept. When dividing the structure into several building blocks (characteristic associations of polyhedra), it is possible to notice the blocks origin and analyse the genetic relations between the present structure and its archetype. Two-dimensional seidozerite modules $\{Na_2Ti_2O_2[Si_2O_7]\}_{\infty\,\infty}$ alternate along the b axis with $\{Na_3VO_4\}_{\infty\,\infty}$ nets made by Na octahedra and V tetrahedra. We interpret the crystal structure of our Cu,Al fluoride disilicate as a polysome based on the topaz structure that is cut in two kinds of modules (*ABABA. . .*) and packed along the *b* axis with *C* and *C'* blocks. These *C* and *C'* blocks are formed by Cu pyramids and Si tetrahedra. Using the polysomatic approach we could model other hypothetical members of the two-modular mineral family in the frame of Cu, Al, Si, O, F composition with topaz as one end-member. The various polysomes arise from different ratios and sequences of the above mentioned *A*, *B*, *C* (*C'*) blocks.

A performed "genealogical" search in relation to the crystal structure of $K(Ti_{1-x}Cr_x)(O_{1-x}F_x)[PO_4]$ solid solution (R = 0.024) has shown that the KTP structure type is a derivative of the α-$CrPO_4$ one. The way of transformation can be described as an interstitial - omission interaction when α-$CrPO_4$ is treated as an archetype of the KTP structure. If one removes every second Cr atom along the *a* axis together with two O atoms and each second P atom along the *b* axis, a framework with $\{CrPO_4O\}^{2-}$ composition is formed. This framework is topologically identical with the $\{CrPO_4F\}^{-}$ framework in the structure of $KCrPO_4F$. Replacing some of the O atoms by F and filling the voids in the framework with K atoms, we arrive to the KTP structure type. $NaV_3[PO_4]_3$ is discussed as an intermediate on the way from α-$CrPO_4$ to KTP.

s8b.m4.p6 **Detection of Molecular Symmetry in the CambridgeStructural Database**. J.W. Yao, J.C. Cole, W.D.S. Motherwell, F.H. Allen, *Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, UK.*
Keywords: methods crystallography, data mining, data bases.

In the Cambridge Structural Database it has previously been difficult to investigate any relationship between molecular symmetry and crystal packing symmetry. Some basic rules for which the molecules are packed in the periodic orders have been summarised[1]. It has beenshown that molecular symmetry has an important relation with the packing of molecules in space groups for some certain cases[2].

In this study, an algorithm has been developed to find molecular point groups for any structural molecules in the CSD. The symmetry elements in a molecule are detected by finding the symmetry order from a topological check on the molecular graph and possible symmetry operations are then applied to the 3D coordinates of structure. The comparison for symmetry related atoms are made only for those topological equivalent atoms. The detected symmetry elements can be displayed superimposed on the molecule from the RPLUTO graphic interface.

This method has been applied to molecular structures in a number of space groups to investigate the relationship between molecular symmetry and the occupation of special positions of a given point symmetry in these space groups.

The program has been also extended to detect pseudo-symmetry in multiple molecules in an asymmetric unit, i.e. Z'>2.

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