

**P.10.01.1***Acta Cryst.* (2005). A61, C367**Crystallosymmetric Structure and Evolution of the Mineral World**Nikolai P. Yushkin, *Institute of Geology of Russian Academy of Sciences (Ural Branch 54 Pervomaiskaya St., Syktyvkar, 167982, Russia.* E-mail: yushkin@geo.komisc.ru

The generalized theory of symmetry in application to mineralogy should certainly treat a mineral as an entire functional system, embracing its outer and inner environments, links, properties, external fields. In geological terms, the problem that seems most important is how to transfer symmetry investigations from the mineral individual to the entire mineral world. We are developing crystallosymmetric analysis of complex systems now (N. P. Yushkin "Crystallosymmetric Analysis of Complex Mineral Systems", Syktyvkar, 1985 which opens the possibility to study polymineral objects, such as rocks, ores, geospheres, etc., in terms of symmetry and provides principally new information for the understanding of their nature. To characterize the crystalline state of substances in polymineral systems, we introduced the concept of crystallosymmetric structure of systems.

Each geologic system composed of minerals is characterized by a strictly definite crystallosymmetric structure expressed by the constant parameters of the mineral species distribution within ranks of the symmetry system (categories, syngonies, point groups).

On the basis of obtained results a law of the geologic evolution of crystallosymmetric structure of mineral systems has been formulated. In the process of cosmic and geologic evolution the crystallosymmetric structure of mineral systems undergoes complication and qualitative changes; it's manifested in the increase of entropy of all symmetry characteristics, as well as in replacement of originally predominant cubic and orthorhombic minerals by monoclinic ones; decrease in the mineral substance symmetry occurs alongside with high and even increasing external morphology symmetry of the Earth and other mineral bodies.

**Keywords: symmetry of minerals, crystallosymmetric structure, evolution of symmetry**

**P.10.02.1***Acta Cryst.* (2005). A61, C367**Borophosphate: Crystal Chemistry, Systematic and Synthesis**Elena L. Belokoneva, Olga V. Dimitrova, *Moscow State University, Geological faculty, 119992 GSP2 Moscow, Leninskije Gory 1, Russia.* E-mail: elbel@geol.msu.ru

Borophosphate synthesis and characterization has been started only ~10 years ago. Significant contribution including first approach to structural chemistry [1] has been made in Germany. In our investigation among new borophosphates,  $\text{In}[\text{BP}_2\text{O}_8] \cdot 0.8\text{H}_2\text{O}$  relates to  $\text{M}^{\text{I}}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8] \cdot \text{H}_2\text{O}$  [1] and  $\text{Fe}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8] \cdot \text{H}_2\text{O}$  [2], has framework of In, B and P tetrahedra and most successful zeolite properties.

New systematic [3] uses B:P ratio (as in [1]) and besides topology and symmetry analysis of structural building blocks. When  $\text{B:P} > 1$ , B polyhedra in complex anion form structural blocks and its combination typical for the borates with the P tetrahedron in outside "decorating" (of high charge reason) or connecting role. When  $\text{B:P} \sim 1$ , low degree of condensation B and P polyhedra is typical with the borate anions topology and the same P tetrahedra role. When  $\text{B:P} < 1$  (most of the compounds) structural block of equal topology and local symmetry  $-4$  with the central B tetrahedron and four apical P tetrahedra may be detected in all the structures. Block can be full or deficient protonated. The condensation degree determines the systematic with the ortho, soro, chain, ribbon, layer or framework borophosphate anion. The higher pH is at hydrothermal synthesis, the higher is the condensation degree of blocks; low pH (acid condition) assists protonation of blocks. Topology and symmetry analysis demonstrates that in despite of the diversity, borophosphate form a single class of compounds. This work was supported by RFBS, project 02-03-33316.

[1] Kniep R., Engelhard H., Hauf C., *Chem. Mater.*, 1998, **10**, 2930. [2] Yilmaz A., Bu X., Kizilyalli M., Stucky G.D., *Chem. Mater.*, 2000, **12**, 3243. [3] Ruchkina A., Belokoneva E.L., *Russ. J. Inorg. Chem.*, 2003, **48**, 1812.

**Keywords: borophosphate, crystal chemistry and systematic, synthesis**

**P.10.02.2***Acta Cryst.* (2005). A61, C367**Crystallochemical Analysis of Halogenides and Chalcogenides of d-metals**Maxim V. Peskov, Vladislav A. Blatov, *Samara State University, Samara, Russia.* E-mail: helmut@sama.ru

A comparative crystallochemical analysis and classification are performed for 35 halogenides, 123 chalcogenides  $\text{M}_y[\text{TX}_4]$  (T is d-metal), and 1573 binary compounds  $\text{A}_x\text{B}_y$  using the program *IsoTest* of the *TOPOS* package. Two levels of structural relationship are considered: (i) 'grey' isomorphism, when a binary compound  $\text{A}_x\text{B}_y$  relates to a ternary compound  $\text{M}_y[\text{TX}_4]$  if some atoms M, T, or X are topologically equivalent; (ii) partial isotypism when a complex salt  $\text{M}_y[\text{TX}_4]$  is considered as a quasi-binary compound  $\text{M}_y[\text{T}]$  keeping the connectivity of initial net. The examples of 'grey' isomorphism for ternary compounds are found with  $\text{Tl}_2\text{Cl}_4$ ,  $\text{In}_2\text{Br}_4$ , magnetite, cristobalite, and  $\text{C}_3\text{N}_4$ . Partial isotypism is much more frequent; the following binary compounds participate in such relations: CsCl,  $\text{NdS}_2$ , NiAs, FeB,  $\text{BaF}_2\text{-HP}$ , PtS, sphalerite, fluorite,  $\text{PoCl}_2$ ,  $\text{BiF}_3$  (gananite),  $\text{ReO}_3$ . Many of the found correspondences are typical also for other anhydrous inorganic salts: orthosilicates, orthogermanates, arsenates, sulfates, selenates, molybdates, perchlorates, periodates, nitrates, carbonates, and borates.

Topological analysis of ionic arrays shows that in a half of the halogenides and almost in all the chalcogenides there are arrays related to close packings. Using the data on uniformity of these arrays the conclusions are made about their significant structure-forming role.

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**Keywords: comparative analysis, classification, inorganic compounds**

**P.10.02.3***Acta Cryst.* (2005). A61, C367**Crystal Structure of Two Related Selenites**Aitor Larrañaga<sup>a</sup>, J.L. Pizarro<sup>a</sup>, J.L. Mesa<sup>a</sup>, R. Olazcuaga<sup>b</sup>, M.I. Arriortua<sup>a</sup>, T. Rojo<sup>a</sup>, <sup>a</sup>Facultad de Ciencia y Tecnología, UPV/EHU, Apdo. 644, E-48080 Bilbao, Spain. <sup>b</sup>Institut de Chimie de la Matière Condensée de Bordeaux, 33608 Pessac, France. E-mail: nplavaa@lg.ehu.es

$\text{M}_3(\text{SeO}_3)_3 \cdot \text{H}_2\text{O}$  for  $\text{M} = \text{Mn, Co}$  have been synthesized using mild hydrothermal conditions under autogeneous pressure. The crystal structure of both compounds have been solved from X-ray single crystal data in  $\text{P} \bar{1}$  triclinic space group with  $Z = 2$ . The crystal structures of the  $\text{M}_3(\text{SeO}_3)_3 \cdot \text{H}_2\text{O}$  ( $\text{M} = \text{Mn, Co}$ ) consist of a three-dimensional framework formed by  $\text{MO}_6$  octahedra and  $(\text{SeO}_3)^{2-}$  selenite anions with trigonal pyramidal geometry. Both structures show the existence of zig-zag chains linked through  $\text{M}_2\text{O}_{10}$  dimeric units and  $\text{MO}_6$  octahedra and are inter-changeable by the rotation of these dimers and octahedra and a corresponding change of edge/corner sharing connectivity.

Taking into account the results of the luminescence and diffuse reflectance spectroscopies, the Dq and Racah (B and C) parameters have been calculated by fitting the experimental frequencies to an energy level diagram for octahedral  $d^5$  and  $d^7$  high spin Mn(II) and Co(II) ion systems.

Magnetic measurements show the existence of antiferromagnetic interactions in these compounds.

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**Keywords: synthesis, selenites, crystal structure and properties**

**P.10.02.4***Acta Cryst.* (2005). A61, C367-C368**Partial Substitution by Y, Pb or Bi in  $\text{Sr}_8\text{Ca}_6\text{Cu}_{24}\text{O}_{41}$** Oksana Romaniv<sup>a</sup>, Lev Akselrud<sup>a</sup>, Volodymyr Davydov<sup>a</sup>, Enrico