08. INORGANIC AND MINERALOGICAL CRYSTALLOGraphy

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NEW TYPE OF [Si₃O₈] LAYERS IN K₃Yb₃[Si₆O₁₆]₂(OH). By N.V. Belov, A.M. Dago, E.A. Podbedimskaya, D.Yu. Pochcarovsky, B.E. Strelkova, Faculty of Geology, Moscow State University, USSR.

Compound K₃Yb₃[Si₆O₁₆]₂(OH) was synthesised in the hydrothermal system K₂CO₃-Yb₂O₃-SiO₂-H₂O (T=450°C, P=950 atm., c K₂CO₃-Yb₂O₃-SiO₂ = 15-45%; c K₂O/SiO₂ = 1:1). The triclinic cell parameters of K₃Yb₃[Si₆O₁₆]₂(OH): a=6.868(2), b=11.434(6), c=11.454(8), α=88.52(3), β=90.91(5), γ=100.10(4)°, sp.gr. P1, Z=1. Anisotropically layers [Si₃O₈] were found in the structure, formed by 6-, 8- and 10-membered rings, was found in the structure of K₃Yb₃[Si₆O₁₆]₂(OH). The structure has been refined up to R=0.060. A new type of layers [Si₃O₈], formed by 6-, 8- and 10-membered rings, was found in the structure of K₃Yb₃[Si₆O₁₆]₂(OH). These layers are connected by Yb-octahedra into 3-dimensional framework. The large Yb-cations occupy the spaces inside the framework. The comparison of 1- and 2-dimensional tetrahedral [Si₃O₈] motifs indicates the possibility of the formation of layers in structures with "hard" cations (Zn, Cd, Yb) and bands in structures with "soft cations" (Ca, Na, Ba).

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CRYSTAL STRUCTURES OF THE GROUP OF Cd, Li, AND Cd,Li-BORATES. By E.V. Sokolova, Yu.K. Egorov-Tismanko, M.A. Simonov, N.V. Belov, Geological Department, Moscow State University, Moscow, USSR.

The crystal structures of a series of Cd-, Li- and Cd,Li-borates synthesized in the course of the investigation of hydrothermal crystallisation in the Li₂O(Na₂O)CdO·B₂O₃·H₂O systems have been determined as a further advance in the development of crystal chemistry of Cd-compounds.

Analyses of this series of compounds revealed the dependence of the character of crystal structures on the relative boron content. In Cd₄[B₄O₇(OH)]₂ each of two types of clusters forms its own original framework of Cd-octahedra, and the isolated 8-triangles give the structure an additional rigidity. Each of the 8-triangles belongs to both types of clusters. In the hexagonal LiCd[B₄O₇]-I modification the columns of Cd-hemioctahedra, placed edgewise, alternate with meta-chains of Li-tetrahedra along the c-axis. On the c-axis itself are threaded B₄O₇-triangles making the Cd,Li-framework more rigid. The two-layer closest packing of O atoms whose tetrahedral holes are filled with Cd,Li- and B cations, constitutes the basis of the triclinic LiCd[B₄O₇]-II modification. It is of interest that the Cd atoms attached to one of the faces of a tetrahedron attract the fifth O, resulting in the formation of a trigonal prism. B atoms are situated in triangles on the face of a closed-packed layer. In the Cd₄[B₂O₅] structure infinite chains, each of four Cd-octahedra in width, are separated by chains of empty octahedra. The [B₂O₅] pyro-groups linking together the discrete Cd-chains are located both above and under the empty octahedra. In the structure of the orthorhombic Li₃[B₅O₈(OH)₂]-I modification, B₄O₇-tetrahedra and B₂O₅-triangles form corrugated layers linked with each other by Li-tetrahedra paired along common edges as well as by hydrogen bonds. In the tetragonal Li₃[B₅O₈(OH)₂]-II modification the chains of [LiO₄] tetrahedra pierce the B-O framework of spiral-like [B₂O₅] chains.

Thus the boron-oxygen units are predominant when the content of B atoms is the largest. The cations play the subordinate role. When the content of B is relatively small, the B₂O₅-triangles serve only as connecting links for Cd,Li-units. The unusual coordination number 5 in two LiCd B₂O₅ modifications is associated with the requirements of commensurability of O-O-radicals and cations as well as of the balance of valency of anions.