

$Ga_2O_6 [PO_4]_3$. The dimers stringed on an two-hold axes form continuous chains along the Z axis in which the filled octahedra and the empty trigonal prisms are situated alternately. All the structure consists of a totality of indicated chains connected with each other by octahedra forming unique framework of the composition $Ga(PO_4)_2$ with large-scale spaces.

It is not difficult to notice that the obtained motive as composed from Ga-octahedra and PO_4 -tetrahedra carries a negative

charge equal to - 3 for compensation of which positive cations are required. The crystal chemistry analysis of interatomic distances indicates that such positive cations can be only protons transforming free terminal oxygen atoms of phosphate groups into hydroxylic ions. Thus, by taking into account the hydrogen atoms and the water molecules the presence of which in the structure is also confirmed by DT analysis and which are statistically arranged in the above indicated vacancies, the structural formula can be expressed as $GaH_3(PO_4)_2 \cdot 2,5 H_2O$.

and Ho form zigzag chains along the axis b being connected through the general rib with the nearest symmetrically equivalent polyhedra. Such chains of Ho-polyhedra form step (zigzag) layers, parallel to planes (001), being connected by general oxygen summits between them. The layers of Ho-polyhedra being associated by general summits and ribs of Na-polyhedra, B-tetrahedra and hydrogen bonds between them, form the framework structure of sodium and holmium borates.

08.2-59 THE CRYSTAL STRUCTURE OF SODIUM AND HOLMIUM BORATE. By G.G.Jafarov, G.K.Abdullayev. The Institute of Inorganic and Physical Chemistry of the Academy of Sciences, Azerbaijan SSR, Baku, USSR.

Sodium and holmium borate $NaHo[BO_2(OH)]_2OH$ was obtained under hydrothermal conditions in the system $HO_2O_3-Na_2O-H_2O$ at 400 C. The crystals are

transparent and are of lemon-yellow colour. The habitus of the crystals changes from shortly prismatic to isometric. The crystal structure was determined by single-crystal X-ray analysis (diffractometer, Mo radiation, 890 reflections, least squares refinement with anisotropic approximation, $R=0,083$). The cell dimensions are: $a=5,142(2)$, $b=6,434(4)$, $c=6,155(3)$ Å, $\beta=114,7(2)$, $Z=2$, $d_x=5,07$ g/cm³, space group $P2_1/m$. The structure has been

solved by the heavy atom method. The coordinations of Ho atoms have been determined from Patterson map. The localization of the remaining atoms (Na, O and B) was carried out from Fourier and difference electron density synthesis. The crystal structure of sodium and holmium borate consists of isolated $[BO_2(OH)]_2^{3-}$

tetrahedra ($B-O, 1,480-1,524$ Å) and coordination polyhedra of metallic cations. The sodium cations are inside the distorted bicapped trigonal prisms formed by two O atoms and six OH groups ($Na-O 2,204-2,613$ Å). The holmium cations are also inside the distorted eight coordinated polyhedra formed by four oxygen atoms and four OH groups. ($Ho-O 2,322-2,686$ Å) Na

08.2-60 STRUCTURAL ANALYSIS OF SUBSTITUTED BARIUM HOLLANDITES. By R.W. Cheary, J. Kwiatkowska and J. Hodge. School of Physics & Materials, New South Wales Institute of Technology, Sydney, N.S.W. 2007, Australia.

The structures of a number of polycrystalline barium hollandites have been determined by x-ray and neutron diffraction using the Rietveld method. The purpose of this work is to establish the structural conditions required for the successful immobilisation of radioactive waste within this group of compounds. In cesium substituted hollandites

(viz $[Ba_xCs_y][Al_{2x+y}Ti_{8-2x-y}]O_{16}$) the structural parameters for titanium, aluminium and oxygen do not change significantly with the level of cesium substitution. The only significant change occurs in the z parameter which defines the average Cs/Ba position. This increases with the level of Cs substitution indicating that these ions tend to occupy a more central location with respect to their coordinating oxygen ions. An analysis of the (Cs/Ba)-O bond length suggests a possible limit of structural stability corresponding to 0.25 cesium ions per unit cell. Electron microprobe results indicate that the level of cesium substitution is constrained by the condition that the total volume occupied per unit cell the cesium and barium remains substantially constant. Barium hollandites containing varying proportions and types of 3^+ ions on the octahedral sites have also been examined (viz $Ba_x[M_{2x}Ti_{8-2x}]O_{16}$, $M = Al, Ga, Fe$ and Ti) to determine how these affect the size of the barium site.