

08-Inorganic and Mineralogical Crystallography

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telluride. And then the metal atoms are packed between layers of Te atoms to form a sandwich, the adjacent sandwiches are held together by weak van der Waals interaction between Te atoms.

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PS-08.04.24 EXOLUTION-DERIVED PHASEOUS INHOMOGENEITY OF POLYCOLORED TITANITE CRYSTALS FROM THE Khibina ALKALINE MASSIF, KOLA PENINSULA, RUSSIA.

by M.I.Lapina* and B.J.Boroutsky, *Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry (IGEM), Russia Academy of Sciences, Moscow.*

Unusual crystals of titanite with the black heads have been found in a natrolite vein in rischorrite of the Khibina alkaline massif. The crystals are cuneiform ones with prismatic faces $n\{111\}$ and $t\{111\}$, have been studied using detailed microscopic observation, chemical and electron microprobe analyses.

Very narrow range of $+2V=26-27^\circ$ is typical of the studied crystals which is quite different from all other Khibina titanites where $2V$ varies from 17° to 40° . Black colored spots are located at the sites of "a" axe exits. The crystals were found to have abnormal contents of Nb_2O_5 (5,2-6,7 wt%) as compared to average 1,21% for Khibina titanite. Black colored parts contain also elevated contents of Na_2O (1,6-1,9 wt%) and SrO (0,5-0,7%) but lowered of Fe_2O_3 (0,4-0,5%). Distribution of all elements throughout the black heads is fairly even which was confirmed by electron microscope studies and is suggestive of isomorphous entrance of these impurities into the crystal lattice of titanite perhaps according to the following pattern: $Ca^{2+}Ti^{4+} \rightarrow Na^+Nb^{5+}$. In more light colored basal parts of the crystals many alternating lighter and darker bands are seen. The lighter bands contain $Nb_2O_5=3,2-3,5\%$, $Na_2O=0,8-1,0\%$, $Fe_2O_3=0,8-1,0\%$ and $SrO=0,5\%$, and the darker ones: $Nb_2O_5=3,9-4,9\%$, $Na_2O=1,06-1,2\%$, $Fe_2O_3=0,9-1,2\%$ and $SrO=0,3\%$.

Rare xenomorphic micron-size inclusions of pyrochlore were found within light colored parts of the crystals near the hinter parts of the black heads. The number and size of such inclusions is evidently growing with the rising extent of secondary alterations of the host titanite and the size of pyrochlore grains or grain clusters sometimes is as large as 1 mm. The formation of the pyrochlore inclusions is assumed to be a result of Nb exsolution from Nb-titanite solid solution and subsequent recrystallization.

PS-08.04.25
ON THE STRUCTURE OF II III₂ □ VI₄
SEMICONDUCTING COMPOUNDS.

J.M. Delgado
Departamento de Química, Facultad de Ciencias,
Universidad de Los Andes,
Mérida, Venezuela 5101

There have been conflicting reports on the nature of the space group of a number of II III₂ □ VI₄ semiconductors. These materials have been described in space group $I\bar{4}2m$ as well as $I\bar{4}$:

$I\bar{4}2m$ [D_{2d}^1 , N° 121]				$I\bar{4}$ [S_4^1 , N° 82]			
II	in 2(a)	$\bar{4}2m$	0,0,0	II	in 2(a)	$\bar{4}$	0,0,0
III	in 4(d)	$\bar{4}$	0,½,¼	III(1)	in 2(b)	$\bar{4}$	0,0,½
				III(2)	in 2(c)	$\bar{4}$	0,¼,¼
VI	in 8(i)	1	x,x,z	VI	in 8(g)	1	x,y,z

In the present study, a detailed structural analysis of the following materials: $CdAl_2S_4$, $HgAl_2S_4$, $HgGa_2S_4$, $HgAl_2Se_4$, $ZnIn_2Se_4$ and $MnIn_2Te_4$, has been performed. High-quality single crystal x-ray diffraction data published in the literature and collected in our laboratory were used. Particular attention was paid to the behavior of the different structural refinements in which only superstructures reflections were employed. An attempt to establish the possible cation ordering scheme due to order-disorder phenomena was tried in all cases. The intrinsic inability of x-ray diffractometry to distinguish subtle order-disorder details between neighboring elements of the periodic table have been considered throughout the analysis.

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PS-08.04.26 THE POSSIBLE QUALITATIVE SFDP-FORMULAS OF THE CHEMICAL ELEMENTS (CE) by O.E.Gorchakova*, N.L.Smirnova, N.I.Kirillova, Department of Chemistry, All-Russian Institute for Scientific and Technical Information, Moscow, Russia

The most lengthy system of CE consists of 32 groups and 7 rows. After giving to every CE the number and group and row, we get the system of numerical binary designations of CE from 11 to Rn 32.6. In the most lengthy system there are four s,f,d,p blocks of CE, including 2,14,10,6 groups. CE within the limits of the block is marked by a 3-signs symbol: the letter of the block, the number of the group within the limits of the block, the number of the row. For example H s11, Ar p66. The third model of the system of CE is generated by use of 8 numbers of A and B groups: in s-block 1,2, in f-block 3(1-14), in d-block 3,4,5,6,7,8(1-3),1 2, in p-block 3,4,5,6,7,8. In the three of rows are the same. While marking all of the group is omitted. The most general formulas of chemical compounds (CC) are being generated with four letters sfdp. If the elements within the limits of the block are not distinguished, only 15 formulas of CC