08-Inorganic and Mineralogical Crystallography

There have been conflicting reports on the nature of the space group of a number of II III₂ square VI₄ semiconductors. These materials have been described in space group 14 2/m as well as 14 2.

<table>
<thead>
<tr>
<th>14 2/m [D₂h, N=12]</th>
<th>14 [C₄, N=82]</th>
</tr>
</thead>
<tbody>
<tr>
<td>II in 2(a) 4 0 0 0 0 0</td>
<td>II in 2(a) 4 0 0 0 0 0</td>
</tr>
<tr>
<td>III in 4(d) 4 0 0 0 0 0</td>
<td>III(i) in 2(b) 4 0 0 0 0 0</td>
</tr>
<tr>
<td>III in 2(d) 4 0 0 0 0 0</td>
<td></td>
</tr>
<tr>
<td>y in 8(l) 1 x x</td>
<td>y in 8(g) x x</td>
</tr>
<tr>
<td>z in 8(x)</td>
<td>z in 8(g) x x</td>
</tr>
</tbody>
</table>

In the present study, a detailed structural analysis of the following materials: CdAl₂S₄, HgSn₂S₄, HgGa₂S₄, HgAl₂Se₄, Zn₁₁Sn₆Se₄ and Mn₁₁Sn₆Te₄, 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 oxidation ordering scheme due to order-disorder phenomena was tried in all cases. The intrinsic inability of x-ray diffraction to distinguish subtle order-disorder details between neighboring elements of the periodic table have been considered throughout the analysis.

The purchase of the P3F Nicolet diffractometer in which some of the intensity data were collected, was possible thanks to grants F-74 and TC-19 from CONICIT and CDCHT-ULA, respectively. This work was also possible thanks to grant C-455-90 from CDCHT-ULA.

PS-08.04.25

THE POSSIBLE QUALITATIVE STOP-FORMULAS OF THE CHEMICAL ELEMENTS (CE) by O.E. Gorfahalova*, N.I. Stirmova, N.I. Kirilova, Department of Chemistry, All-Russian Institute for Scientific and Technical Information, Moscow, Russia

The most lengthy system 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 82. In the most lengthy system there are four 1,0 blocks of CE, including 11, 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 111, Ar 6b6. 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 31,14, in d-block 3,5,6,7,8(1-3), 1 2, in p-block 3,4,5,6,7,8. In the three of rows the same. While marking all of the group is omitted. The most general formulas of chemical compounds (CC) are being generated with four letters forp. If the elements within the limits of the block are not distinguished, only 15 formulas of CC

PS-08.04.24

EXOLUTION-DERIVED PSEUDOMORPHIC INHOMOGENEITY OF POLYCOLORED TITANITE CRYSTALS FROM THE KIBINA ALKALINE MASSIF, KOLA PENINSULA, RUSSIA. by M.L. Lapina* and B.I. Bovotukh, 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 riebeckiter of the Kibina alkaline massif. The crystals are columnar ones with prismatic faces 111 and 111, have been studied using detailed microscopic observation, chemical and electron microscope analyses.

Very narrow range of $2\theta$=26-27° is typical of the studied crystals which is quite different from all other Kibina titanites where $2\theta$ varies from 27° to 40°. Black colored spots are located at the sites of "a" at exit. The crystals were found to have abnormal contents of Na₂O (5.2-8.7 wt%) as compared to average 1.21% for Kibina titanite. Black colored parts contain also elevated contents of Na₂O (1.6-1.3 wt%) and SrO (0.5-0.7%) but lowered of Fe₂O₃ (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 homomorphic entrance of these impurities into the crystal lattice of titanite perhaps according to the following pattern: Ca\(_{14}\)Na\(_{4}\)Sr\(_{2}\)Fe\(_{2}\)O\(_{37}\)\rightarrow Na\(_{2}\)Na\(_{2}\)Sr\(_{2}\)Fe\(_{2}\)O\(_{37}\). In more light colored zones the crystals many alternating lighter and darker bands are seen. The lighter bands contain Na₂O=3.2-3.5%, Na₂O=2.8-1.0%, Fe₂O₃=8.1-10% and SrO=5%, and the darker ones: Na₂O=3.9-4.5%, Na₂O=0.8-1.0%, Fe₂O₃=10.8-12.2%, Fe₂O₃=9.3-12.2% and SrO=0.3%.

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

---

PS-08.04.25

ON THE STRUCTURE OF II III₂ square VI₄ SEMICONDUCTING COMPOUNDS.

J.M. Delgado
Department of Quimica, Facultad de Ciencias,
Universidad de Los Andes,
Mérida, Venezuela 5101