

08.4-18 THE ORDERING PATTERNS OF THE THALLIUM SULPHOSALTS' STRUCTURES. By T. Balić Žunić, Department of Mineralogy and Petrology, Faculty of Science, University of Zagreb, Zagreb, Yugoslavia.

When the bonding patterns of the thallium sulphosalts are examined, mainly the differences and the great variety of types come into view. If, on the other hand, in the description of the coordination polyhedra the complete surrounding of the thallium and of the arsenic and antimony atoms by the sulphur atoms is taken into account and not only the atoms at the standard bonding distances, the structural relationships in this class of compounds become obvious from their general ordering patterns.

Accepting these criteria, among the hitherto solved structures we observe the group of Tl-As sulphosalts related to orpiment, the group of Tl-Sb sulphosalts related to stibnite and the three special classes. Besides the pure Tl sulphosalts, the Tl/Pb sulphosalts can be also included in this scheme, because of the similar coordinations these two elements assume in the sulphosalt structures.

Related to the structure of orpiment (Morimoto, Min. Journal (1954) 1, 160) are the structures of lorandite (TlAsS₂)

(Fleet, Z. Kristallogr. (1973) 138, 147), imhofite (TlAs₃S₅)

(Divjaković and Nowacki, Z. Kristallogr. (1976) 144, 323), hutchinsonite (TlPbAs₅S₉) (Takeuchi et al., Z. Kristallogr.

(1965) 121, 321) and synthetic TlPbAs₃S₆ (Balić Žunić and Engel, in press). Related to the structure of stibnite

(Hofmann, Z. Kristallogr. (1933) 86, 225) are the structures of parapirotite (TlSb₅S₈) (Engel, Z. Kristallogr. (1980)

151, 203) and pierrotite (Tl(Sb,As)₅S₈) (Engel et al., in

press), Tl₈Pb₄Sb₂₁As₁₉S₆₈ (Nagl, Z. Kristallogr. (1979) 150, 85) and synthetic TlSb₃S₅ (Gcstojić et al., Z. Kristallogr.

The mentioned Tl-As sulphosalt structures show the orpiment-like double layers or portions of them with the Tl(Pb) and As atoms occupying the same type of positions, therefore having the same type of surrounding which is sevenfold and in the form of an octahedron with one split vertex or a trigonal prism with one centered face. The Tl-Sb sulphosalts, however, show in their structures the layers with the stibnite-like structure mutually interconnected by the Tl(Pb) coordination polyhedra which consist of 9 S atoms closing a trigonal prism with all the faces centered. The surrounding of the Sb(As) atoms in the stibnite-like portions is octahedral. Some of the Sb atoms are present in the interconnecting zones therefore having the same surrounding as the Tl atoms.

We see that the two Sb/As sulphosalts mentioned here show the features common to the Sb sulphosalts, but the structure of rebulite (Tl₅Sb₅As₈S₂₂) (Balić Žunić et al., Z. Kristallogr. (1982) 160, 109) cannot be simply related to the group of Sb nor the group of As sulphosalts. The explanation for this may be found considering the mineralogical relations it shows with the Tl/Hg sulphosalts simonite (Engel et al., Z. Kristallogr. (1982) 161, 159) and probably vrbaita.

The other two sulphosalt structures, that of ellisite (Tl₃AsS₃) (Gostojić, Z. Kristallogr. (1980) 151, 249) and of synthetic Tl₃SbS₄ (Gcstojić et al., Z. Kristallogr. (1981)

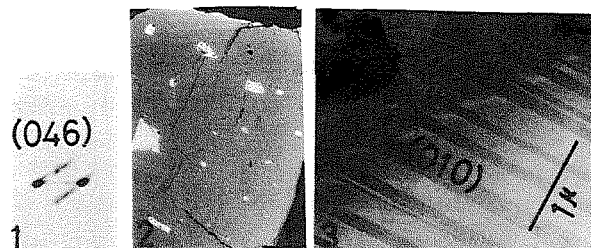
157, 299) also show no direct relation to the groups of structures previously described although the total surrounding of the As and Sb atoms is octahedral. The reason is, obviously, in the high proportion of Tl which dictates the structural pattern.

08.4-19 Crystallographic Investigation of Anorthoclase from Mt. Erebus, Antarctica
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An anorthoclase of chemical composition An₁₉Ab₆₃Or₁₈ from Mt. Erebus, Antarctica was studied by X-ray diffraction and transmission electron microscopy. Almost all specimens are twinned according to the albite law and in addition pericline twinning was observed in the quenched rim region.

In order to obtain high resolution, X-ray diffraction experiments were carried out in the synchrotron radiation laboratory at National Laboratory of High Energy Physics, Tsukuba, Japan. Using bright and coherent monochromatic X-ray from SR, the X-ray coherent and incoherent twin domains of albite were observed. By XMA and TEM no exsolution was detected. These facts may indicate that this anorthoclase was grown under high temperature and high pressure and that, if a monoclinic phase exists in this region, the twinings were caused by the monoclinic-triclinic phase transition and the stress in the rapid cooling.

Fig. 1 is a part of X-ray diffraction pattern, Fig. 2 is a composition photograph of XMA and Fig. 3 is a TEM photograph.



08.4-20 CRYSTAL STRUCTURE OF NEFEDOVITE, Na₅Ca₄(PO₄)₄F. By E.A. Pobedinskaya, M. Sebaï, G.I. Dorokhova and A.P. Khomyakov. Moscow State University, Faculty of Geology, USSR.

The structure of the new mineral nefedovite of khibin region has been studied. For the solution of the structure have been applied X-ray reflections collected using 2θ-θ method on single automatic diffractometer "Syntex P1". Previously triclinic system has been suggested for the mineral, but the refined parameters a₀=11.644(2), c₀=5.396(1), Z=2 and lattice symmetry showed the similarity of nefedovite with the previously studied compound of tetragonal system 4[NaTRSiO₄]NaX (X=OH, F). The structure has been determined analogously in groups I4/m and I4̄ and refined by the least-squares method in group I4̄ to better result R=7.3% in anisotropic approximation without consideration of absorption.

Basic orthophosphate structure is formed by clusters of four Ca coordinated by nine oxygens in two levels along the c-axis. Na-polyhedra between the clusters connect them to each other.