the nearer neighbor atom exist. The peaks far from the origin with a constant height show less atomic interaction between the atoms with longer interatomic distances than a certain distance. They are comparable with the averaged peak in the common Patterson map. These procedures are considered to be useful in refining the coupling coefficients and calculations are in progress.

PS-08.04.22 STRUCTURES OF TWO TERNARY LAYERED TELLURIDES FeNb$_2$(μ$_n$-Te)$_6$(μ$_m$-Te) AND FeTe$_3$(μ$_n$-Te)$_6$(μ$_m$-Te) By S.X. Liu*, G.L. Cai, Z.M. Wang, J.L. Huang, Department of Chemistry; Fuzhou University, Fuzhou, Fujian 350002, China: State Key Laboratory of Structural Chemistry, Fuzhou, Fujian 350002, China.

The two ternary tellurides FeNb$_2$(μ$_n$-Te)$_6$(μ$_m$-Te) (I) and FeTe$_3$(μ$_n$-Te)$_6$(μ$_m$-Te) (II) were obtained by direct combination of the elements. They are two ternary chalcogenides crystallize in space group Pmmm with a=12.412(2), b=8.8173(9), c=7.596(2) Å, V=345.6 Å$^3$, Z=2, $\mu_{\text{r}}$=0.266, μ=2.1567 cm$^{-1}$, F(000)=682, D$_m$=7.238 g cm$^{-3}$ for (I) and a=12.377(3), b=3.7657(6), c=12.266(2) Å, V=338.9 Å$^3$, Z=2, $\mu_{\text{r}}$=0.2824, μ=0.0676 cm$^{-1}$, F(000)=760, D$_m$=9.894 g cm$^{-3}$ for (II). The crystal structures were solved by direct methods. Refinement was by full-matrix least-squares calculations with anisotropic thermal parameters. An occupancy factor of 0.5 for Fe atom on a mirror plane was proposed on the basis of peak heights in the difference Fourier map and thermal parameters for these two tellurides.

The two compounds are isomorphous and have a layered structure. In crystal FeNb$_2$(μ$_n$-Te)$_6$(μ$_m$-Te), every two niobium atoms form a pair Nb$_2$ with a Nb-Nb bond of 3.108(3) Å. Every iron atom is connected to two surrounding Nb$_2$ pairs, in which the Fe atom is 0.922 Å out of the square plane defined by the four Nb atoms. These FeNb$_4$ square pyramids are combined by sharing Nb-Nb edges to form an infinite metal cluster chain [Nb$_6$Fe$_6$]$_n$ along b axis, the distance between two Fe$_3$ atoms from two neighbouring square pyramids is 3.068 Å; on the other hand, each niobium atom is bonded to six tellurium atoms with a distorted octahedral stereochemistry while each iron atom is bonded to four tellurium atoms with a distorted tetrahedral one. These Nb$_6$-centred ocathdra and Fe-centred tetrahedra join via shared Te$_3$ triangular planes or Te$_2$-Te edges to form an infinite chain structure [Nb$_6$Fe$_6$]$_n$, along b axis. In addition, every two adjacent Nb$_6$-centred ocathdra from two adjacent chains are bridged in pairs by sharing a Te$_3$-Te$_2$ edge; every two neighbouring Fe-centred tetrahedra from two neighbouring chains are connected by a common tellurium atom. Therefore these polyhedra are combined to form an infinite sandwich perpendicular essentially to the c axis. The neighbouring sandwiches are held together by weak van der Waals interaction between Te atoms to form a layered structure in the crystal.

There are one μ$_n$-Te atoms and three μ$_m$-Te atoms in a formula FeNb$_2$Te$_4$ or FeTe$_3$Te$_4$.

This research was supported by the National Natural Science Foundation of China.

PS-08.04.23 STRUCTURE OF A NEW TERNARY LAYERED CHALCOGENIDE Ni$_2$Ta$_3$(μ$_n$-Te)$_6$(μ$_m$-Te) By B. Zhang, Z.M. Wang, S.X. Liu, J.L. Huang*, Department of Chemistry, Fuzhou University, Fuzhou, Fujian 350002, China: State Key Laboratory of Structural Chemistry, Fuzhou, Fujian 350002, China.

The new layered chalcogenide Ni$_2$Ta$_3$(μ$_n$-Te)$_6$(μ$_m$-Te) has been prepared by high-temperature reaction of the elements. Ni$_2$Ta$_3$Te$_6$ crystallizes with two formula units in a cell with dimensions a=4.749(2), b=3.768(1), c=10.074(2) Å, β=106.78(2)° in the monoclinic space group P 2$_1$/m. The structure was refined by full-matrix least-squares techniques with anisotropic temperature factors for all atoms to R=0.065 and Rs=0.044.

The title compound displays a new layered structure type. Every layer contains square pyramidal Ta atoms and tetrabedral Ni atoms each coordinated by Te atoms. There are two unique chains that run parallel to the b axis in the crystal. One chain consists of T$_{a}$-centred square pyramids that share Te-Te basal edge; the distance between two Ta atoms from the adjacent T$_{a}$-centred polyhedra is 3.708(1) Å (the b repeat). The square pyramidal coordination around Ta atom is unusual in the known tellurides. On the other hand, the other chain is made up of numbers of building blocks each consists of two edge-sharing Ni$_6$-centred tetrahedra. The coordination about Ni atom is distinctly distorted such that the Ni-Te bond lengths in tetrahedra are from 2.534 Å to 2.704 Å; the Te-Ni-Te angles from 92.4° to 122.45°. The distortion may be due to the Ni-Ni bonds described later. Every two neighbouring Ni$_6$-centred tetrahedra are related to each other by some complex operations including screw operation 2, [010], the closest distance between Ni atoms in adjacent tetrahedra is 2.586 Å, in each sandwich, each Ni atom is bonded to two neighbouring Ni atoms, forming two kinds of Ni$_6$ chains along the b axis with Ni-Ni bonds (2.532 Å and 2.722 Å respectively). The closest Ni-Ni distance in this compound is somewhat longer than the Ni-Ni distance of 2.492 Å in Ni metal. In each sandwich, every Ta atom between two adjacent Ni$_6$ chains is connected with five surrounding Ni atoms in the two Ni$_6$ chains, forming five Ta-Ni bonds of 2.661-2.846 Å. Hence there is a two-dimensional metal cluster in the ternary...
tellturide. 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.

This research was supported by the National Natural Science Foundation of China.

PS-08.04.24 EXPOSITION-DERIVED PHASEOUS INHOMOGENEITY OF POLYCOLOR TITANITE CRYSTALS FROM THE KHBINA ALKALINE MASSIF, KOLI PENINSULA, RUSSIA.

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

Unusual crystals of titanite with black heads have been found in a natro viability in rich sanidine of the khibina alkaline massif. The crystals are euhedral ones with prismatic faces [111] and [112], have been studied using detailed microscopic observation, chemical and electron microscope analyses.

Very narrow range of 2θ=26-27° is typical of the studied crystals which is quite different from all other khibina titanites where 2θ varies from 27° to 49°. Black colored spots are located at the sites of "s" axes exit. The crystals were found to have abnormal contents of Na₂O (5.2-5.7 wt%) as compared to average 1.2% for khibina titanite. Black colored parts contain also elevated contents of Na₂O (1.6-1.3 wt%) and SrO (0.5-0.7%) but lowered of FeO (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 homogenous entrance of these impurities into the crystal lattice of titanite perhaps.

In the following pattern: Ca⁴⁺→Na⁴⁺ in more light colored basal parts of the crystals many alternating lighter and darker bands are seen. The lighter bands contain Na₂O (5.2-5.7 wt%) FeO (0.7-1.0%) and SrO (0.5-0.7%), and the darker ones: Na₂O (1-3%), FeO (0.7-1.0%) and SrO (0.5-0.7%).

Rare xenomorphic micro-size inclusions of pyroclore were found within light colored parts of the crystals near the hibern 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 pyroclore grains or grain clusters sometimes as large as 1 mm. The formation of the pyroclore inclusions 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 IIi₃2 ⊙ VI₄ SEMICONDUCTING COMPOUNDS.

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There have been conflicting reports on the nature of the space group of a number of IIi₃2 ⊙ VI₄ semiconductors. These materials have been described in space group I₄2d as well as I₄.

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V in 8(d) 1 x,y,z
V in 8(g) -n x,y,z

In the present study, a detailed structural analysis of the following materials: Ca₂Al₂Si₄O₁₀, Mg₃Al₂Si₄O₁₀, Ca₂Ga₂Si₄O₁₀, Mg₃Ga₂Si₄O₁₀, Mn₂Al₂Si₄O₁₀ and Ti₂O₃Mg₂Si₄O₁₀ 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 mobility of x-ray diffractometry to distinguish subtle order-disorder details between neighboring elements of the periodic table have been considered throughout the analysis.

The purchase of the P3/F Nicolet diffractometer in which some of the intensity data were collected, was possible thanks to grants F-74 and TC-19 from CONICIT and CDDCH-ULA, respectively. This work was also possible thanks to grant C-235-90 from CDDCH-ULA.

PS-08.04.26 THE POSSIBLE QUALITATIVE SFOP-FORMULAS OF THE CHEMICAL ELEMENTS (CE) by O.E.Gorchalov* N.L.Lafrinova, N.L.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 32.6. In the most lengthy system there are four s, d, f blocks of CE, including 2, 1, 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 H₁₁, Ar₁₁₁₆. 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. 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 sfop. If the elements within the limits of the block are not distinguished, only 16 formulas of CC

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