the nearer neighbor atoms 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 assuming the coupling coefficients and calculations are in progress.

PS-08.04.22 STRUCTURES OF TWO TERNARY LAYERED TELLURIDES $FeNb_2(\mu_4\text{-}Te)_2(\mu_5\text{-}Te)$ AND $FeTa_2(\mu_4\text{-}Te)_2(\mu_5\text{-}Te)$ 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 $FeNb_2(\mu_4\text{-}Te)_2(\mu_5\text{-}Te)$ (I) and $FeTa_2(\mu_4\text{-}Te)_2(\mu_5\text{-}Te)$ (II) were obtained by direct combination of the elements. These two ternary chalcogenides crystallize in space group P mnn with a=12.412(2), b=3.8173(9), c=7.295(2) Å, V=345.6 Å^3, Z=2, Mr.=752.06, μ=216.87 cm^{-1}, F(000)=632, D_x=7.226 g.cm^{-3} for (I) and a=12.377(3), b=3.7687(6), c= 7.266(2) Å, V=338.9 Å^3, Z=2, Mr.=928.14, μ=507.66 cm^{-1}, F(000)= 760, D_x=9.094 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 isostructural and have a layered structure. In crystal $FeNb_2(\mu_4\text{-}Te)_2(\mu_5\text{-}Te)$, every two niobium atoms form a pair Nb_2 with a Nb-Nb bond of 3.108(5) 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 $\{Nb_2Fe\}_n$ along *b* axis, the distance between two Fe atoms from two neighbouring square pyramids is 3.968 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-centred octahedra and Fe-centred tetrahedra join via shared Te_3 triangular planes or Te-Te edges to form an infinite chain structure $\{Nb_2FeTe_4\}_n$ along *b* axis. In addition, every two adjacent Nb-centred octahedra from two adjacent chains are bridged in pairs by sharing a Te-Te 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_5-Te atom and three μ_4-Te atoms in a formula $FeNb_2Te_4$ or $FeTa_2Te_4$.

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PS-08.04.23 STRUCTURE OF A NEW TERNARY LAYERED CHALCOGENIDE $Ni_2Ta(\mu_4\text{-}Te)_2(\mu_5\text{-}Te)$ 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 $Ni_2Ta(\mu_4\text{-}Te)_2(\mu_5\text{-}Te)$ has been prepared by high-temperature reaction of the elements. Ni_2TaTe_3 crystallizes with two formula units in a cell with dimensions a=7.473(2), b=3.708(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 technique with anisotropic temperature factors for all atoms to R=0.053 and R_w=0.064.

The title compound displays a new layered structure type. Every layer contains square pyramidal Ta atoms and tetrahedral 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 Ta-centred square pyramids that share Te-Te basal edge; the distance between two Ta atoms from the adjacent Ta-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-centred tetrahedra. The coordination about Ni atom is distinctly distorted such that the Ni-Te bond lengthes in tetrahedra are from 2.534 Å to 2.704 Å; the Te-Ni-Te angles from 92.4° to 122.46° . The distortion may be due to the Ni-Ni bonds described later. Every two neighbouring Ni-centred tetrahedra are related to each other by some complex operations including screw operation 2_1 [010], the closest distance between Ni atoms in adjacent tetrahedra is 2.526 Å. In each sandwich, each Ni atom is bonded to two neighbouring Ni atoms, forming two kinds of Ni_n chains along the *b* axis with Ni-Ni bonds (2.526Å and 2.722Å 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_n chains is connected with five surrounding Ni atoms in the two Ni_n chains, forming five Ta-Ni bonds of 2.661-2.848Å. Hence there is a two-dimensional metal cluster in the ternary

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 EXSOLUTION-DERIVED PHASEOUS INHOMOGENEITY OF POLYCOLORED TITANITE CRYSTALS FROM THE KHIBINA ALKALINE MASSIF, KOLA PENINSULA, RUSSIA.

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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{$\bar{1}$11}, have been studied using detailed microscopic observation, chemical and electron microprobe analyses.

Very narrow range of +2V=26-27° 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 III_2 □ VI_4 SEMICONDUCTING COMPOUNDS.

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There have been conflicting reports on the nature of the space group of a number of II III_2 □ VI_4 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}^{11}, N° 121]				$I\bar{4}$ [S_4^2, 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)	$\bar{4}$..	0,½,¼
VI	in 8(i)	1	x,x,z	VI	in 8(g)	..m	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 lengthly 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 generaled 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 generaled with four letters sfdp. If the elements within the limits of the block are not distinguished, only 15 formulas of CC