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 $FeTa_2Te_4$.

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

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

 Copyright © 1993 International Union of Crystallography