MS14-P06 | ORDER-DISORDER IN THE ARSENOPALLADINITE, $Pd_8As_{2.5}Sb_{0.5}$, CRYSTAL STRUCTURE

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The crystal structure of the mineral arsenopalladinite, $Pd_8As_{2.5}Sb_{0.5}$, from the Kaarreoja River, Inari commune, Finnish Lapland, Finland, was solved on the basis of X-ray diffraction data collected from the single crystal. The two polymorph modifications established.

The both polymorphs are triclinic, space groups are *P*-1. The unit cell parameters are: *a*=7.3344(7) Å, *b*=7.3870(8) Å, *c*=7.5255(7), *α*=98.869(8)°, *β*=102.566(8)°, *γ*=119.10(1)°, *V*=331.19(1) $Å^3$, *Z*=4, *R1*=0.0481 for (**I**) and *a*=7.329(2) Å, *b*=7.384(2) Å, *c*=14.137(3) Å, *α*=95.983(4)°, *β*=92.027(4)°, *γ*=119.053(4)°, *V*=661.80(2) $Å^3$, *Z*=8, *R1*=0.0533 for (**II**).

A net of atoms parallel to the plane constitute the structure. As and Sb occupy separate sites in the structure and located in a triangular, 3^6 type, nets. Pd atoms separated in another nets: distorted triangular 3^6 and pentagon-triangular 3.5^3. The atomic nets of different orientation stack along the *c* axis.

All Sb atoms are ordered in one of the inversions centre (*1a* Wyckoff position) in the structure of the 7Å-asrenopalladinite. In the 14Å- asrenopalladinite Sb atoms disordered on to two positions. A half of Sb atoms occupie *1a* position, and a half – the *1h* position. In the result, one of the (As, Sb)-net is shifted in the *ab* plane caused stacking fault and doubling of the unit cell. The unit cell of the asrenopalladinite 7Å-polymorph contains 6 nets, the 14Å-polymorph contains 12 nets.

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