Verknüpfung von $(TeO_6)_6$- und $(TeO_6)_3(NiO_6)_3$-Sechsringen durch $TeNiO_9$-Oktaederdoppel in $Pb_3Ni_{4,5}Te_{2,5}O_{15}$

Connection of $(TeO_6)_6$ and $(TeO_6)_3(NiO_6)_3$ Hexagons by $TeNiO_9$ Octahedra Double in $Pb_3Ni_{4,5}Te_{2,5}O_{15}$

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Lead, Nickel, Tellurium Oxide, Crystal Structure

Single crystals of $Pb_3Ni_{4.5}Te_{2.5}O_{15}$ have been prepared by heating pellets of mixtures of PbO, TeO_2 and nickel hydroxide carbonate to 730 °C in air. X-ray investigations led to hexagonal symmetry, space group D_6^6-$P6_322$, lattice constants a = 10.2589(1), c = 13.554(5), Z = 4. Typical features of the crystal structure are face sharing $TeNiO_9$ octahedra doubles and planes of connected $(TeO_6)_6$ and $(TeO_6)_3(NiO_6)_3$ hexagons. The one-sided coordination of lead by oxygen is complemented by the lone pair of electrons. The lone pair positions are estimated by calculations of the Coulomb terms of lattice energy.

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