Zur Kristallchemie des ersten Blei-Zink-Silicium-Telluroxids: $PbZn_4SiTeO_{10}$

On the Crystal Chemistry of the First Lead Zinc Silicon Tellurium Oxyde $PbZn_4SiTeO_{10}$

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Single crystals of the new lead zinc silicon tellurium oxide $PbZn_4SiTeO_{10}$ have been prepared by solid state reaction in air. The compound is colourless and crystallizes in orthorhombic symmetry, space group D_{2h}^{16} Pnma, with the cell parameters: a = 6.542 (5), b = 15.624(4), c = 8.280(4) Å, Z = 4. The structure has been determined from a single crystal X-ray study and refined to the conventional values $R = 0.032$ and $wR(F^2) = 0.050$. Zn^{2+} and Si^{4+} show tetrahedral and Te^{6+} octahedral coordination by O^{2-}.The crystal structure is dominated by a $^{3}_{\infty}[Zn_4O_{10}]^{12-}$ framework with isolated TeO_6^{6+} and SiO_4^{4+} polyhedra. Pb^{2+} ions are incorporated in the network. The centres of negative charge of the lone pairs of Pb^{2+} are estimated by calculations of the Coulomb term of the lattice energy.

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