[MS36-05] Stacking Faults in the Cobalt Tellurium Oxo Phosphate Chloride Co2Te3O6(PO4)Cl. Iwan Zimmermann, Mats Johnsson

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The concept of using p-elements having a stereochemically active lone pair as e.g. Te4+,Se4+, Sb3+ was shown to be successful in finding new low dimensional materials. This synthesis strategy is often referred as “chemical scissors”, as the lone pair acts as a terminal ligand and helps to open up the crystal structure. [1] Compounds having low dimensional arrangements such as e.g. layers, chains or clusters have shown to exhibit interesting physical properties like e.g. frustrated magnetism.[2] Fe7(PO4)3Sb3O6Cl3 is one of few compounds in the transition metal oxo phosphate halide system having a lone pair element present, that is described up to now.[3] In this structure the iron atoms are arranged in one dimensional chains. The new compound Co2Te3O6(PO4)Cl crystallizes in the triclinic space group P-1 with the unit cell a = 5.1671(3) Å, b = 11.0523(8) Å, c = 19.1695(17), α = 98.34(1)o, β = 92.82(1)o, γ = 90.03(1)o.

The compound was obtained from a chemical transport reaction in evacuated and sealed silica tubes. The crystal structure is built up from charge neutral layers, which are stacked along the c-direction. Weak van der Waals interactions in between tellurium lone pairs and oxygen atoms that are protruding out from the layers are responsible for the cohesion of the layers. A doubling of the unit cell along b-direction could be shown due to one dimensional diffused scattering observed in the single crystal X-ray diffraction experiment. This results from stacking faults of the layers along the c-direction. A computer simulation was performed to prove that the stacking faults originate from two different possibilities of the layers to stack along the c-direction.

[1] Becker R., Johnsson M., Kremer R. K., Lemmens P. (2005) J. Solid State Chem.178, 2024–2029.
[2] Johnsson M., Törnroos K. W., Mila F., Millet P. (2000) Chem Mater.12, 2853–2857.
[3] Zimmermann I., Johnsson M., Lidin S. (2012) Eur J. Inorg, Chem.2012, 3971–3974.

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