

## MS14-P23 | STRUCTURAL ORDERING IN THE PYRITE-RELATED PHASES: $\text{PtSnS}$ , $\text{PtSnSe}$ AND $\text{PtSnTe}$

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The ternary  $\text{PtSnX}$  ( $X = \text{S}, \text{Se}$  or  $\text{Te}$ ) phases were prepared and their crystal structures were characterized using powder X-ray diffraction. The ternary compounds were synthesized from elements by solid state reactions using silica glass tube technique at  $600^\circ\text{C}$ . From earlier investigations it is known that the crystal structures of the title phases can be derived from the pyrite structure type ( $\text{FeS}_2$ ) by replacing of S-S the dumbbells by Sn-X heteroatomic anion pairs. Wehrich et al. (2004) suggested three ordering variants of these phases according to the relative orientation of Sn-X dumbbells: the cubic ulmannite type ( $P2_13$ ), the orthorhombic cobaltite type ( $Pca2_1$ ) and the trigonal type ( $R3$ ). Based on the DFT studies of Wehrich et al. (2004),  $\text{PtSnSe}$  and  $\text{PtSnTe}$  crystallizes in the cobaltite structure type, whereas the  $\text{PtSnS}$  prefers the trigonal one. A careful Rietveld analysis of powder X-ray diffraction patterns was performed in order to reveal the preferred structure type. The superstructure reflections indicating the structural ordering and apparent peak splitting in the diffraction patterns clearly indicated the cobaltite structure type for all prepared  $\text{PtSnX}$  phases. The cubic and trigonal structure models cannot fit satisfactorily the measured diffraction data. The crystal structure of title phases is based on a three-dimensional framework of corner-sharing distorted  $[\text{PtSn}_3\text{X}_3]$  octahedra. The Sn-X bond distances range from  $2.497(5) \text{ \AA}$  (in  $\text{PtSnS}$ ) to  $2.842(2) \text{ \AA}$  (in  $\text{PtSnTe}$ ).

[1] Wehrich, R. et al. (2004). J. Solid. State Chem. 177, 2591.