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Synthesis and Crystal Structure of $(Sb_{1/3}Zn_{2/3})GaO_3(ZnO)_3$

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Keywords: Zink oxides; Antimony; Crystal structure

A high temperature (1350 °C) route in sealed platinum tubes was used for the synthesis of pure powders of $(Sb_{1/3}Zn_{2/3})GaO_3(ZnO)_3$. Single crystals of the compound were grown from a K_2MoO_4 flux.
$(Sb_{1/3}Zn_{2/3})GaO_3(ZnO)_3$ consists of an alternate stacking of $[(Sb_{1/3}Zn_{2/3})O_2]^-$ and $[(GaZn_3)O_4]^+$ units corresponding to CdI_2 and wurtzite structure type motifs, respectively. Inversions of the ZnO_4-tetrahedra occur (i) at the octahedral layers and (ii) halfway in the wurtzite type regions where trigonal bipyramidal coordinated cations build the boundary. The crystal structure has been determined by electron diffraction, HR-TEM and single-crystal X-ray diffraction. $(Sb_{1/3}Zn_{2/3})GaO_3(ZnO)_3$ crystallises trigonal ($P3_112$; No. 151; a = 5.60 Å, c = 42.02 Å). The compound described here has the structural characteristics as other known members of the general formula $ABO_3(ZnO)_m$ with m = integer, but an ordering of the cations within the $[(Sb_{1/3}Zn_{2/3})O_2]$- octahedral layer leading to a superstructure.[1]

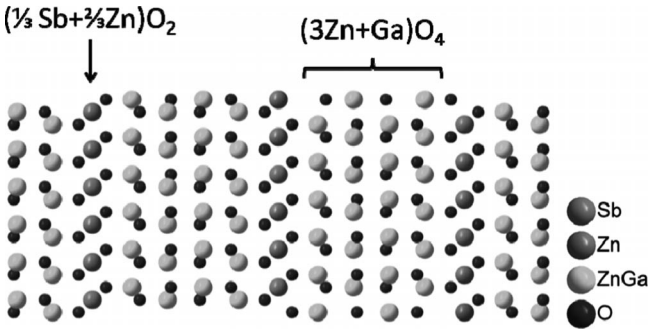

Figure 1. Crystal Structure of $(Sb_{1/3}Zn_{1/3})GaO_3(ZnO)_3$.

[1] I. Keller, W. Mader, *Z. Anorg. Allg. Chem.* **2010**, *636*, 1045–1049.

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Synthesis and Crystal Structure of $ZnSbO_2I$

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Colorless single crystals of $ZnSbO_2I$ were obtained by reaction of ZnO, Sb_2O_3 and ZnI_2 in a stoichiometric ratio of 1:1:1. Water was added and the mixture was tempered in Teflon-lined autoclaves at 120°C for 13 days. The structure was solved by single-crystal X-ray diffraction. The compound crystallizes in the monoclinic space group $P2(1)/m$, with a = 5.25(5) Å, b = 8.47(9) Å, c = 7.47(2) Å, β = 94.4(3) °, V = 331.94 Å^3 and Z = 4. The crystal structure refinement based on 813 reflections converged at $R1$ = 3.76% and $wR2$ = 0.0964, respectively. The structure consists of puckered layers of distorted $[ZnO_3I]$ tetrahedra and strings of Sb^{3+}cations coordinated by four oxygen atoms as described by *Warzycha* for $ZnSb_2O_3X(OH)$.[1]

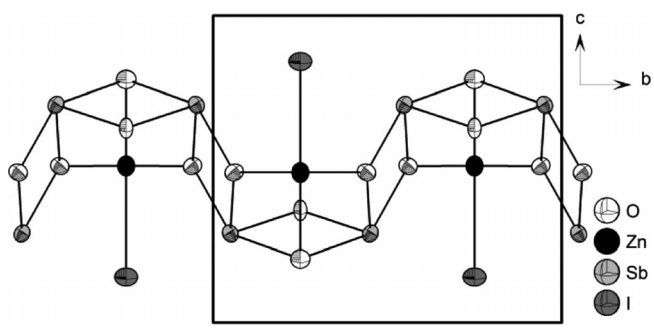

Figure 1: Structure of $ZnSbO_2I$ viewed along [100]

[1] K. Warzycha, *Dissertation*, University of Regensburg, **2010**.

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