A Strong Deviation from Vegard's Rule: X-Ray Powder Investigations of the Three Quasi-Binary Phase Systems BiOX–BiOY (X, Y = Cl, Br, I)

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The three quasi-binary phase systems BiOX–BiOY (X, Y = Cl, Br, I) have been investigated by X-ray powder methods. No quaternary phases were found in the three systems. BiOCl–BiOBr and BiOBr–BiOI form systems of unlimited mutual solubility. BiOCl–BiOI is a system of limited solubility at the iodine-rich side. In the BiOBr–BiOI system a strong deviation from Vegard's rule is observed with respect to one of the lattice parameters. A few methods to quantify such a deviation are briefly discussed and a possible explanation for the strong deviation in the BiOBr–BiOI system is proposed. Error calculations have been performed to estimate uncertainties in the concentration parameter *x* of the investigated mixtures. The crystal structure of BiOI has been re-determined by single crystal structure analysis.

Key words: Bismuth Oxide Halides, Vegard's Law, X-Ray Powder Diffraction