Rb₅In(MoO₄)₄: Crystal Structure of a Possible Laser Material

<u>Ekkehart Tillmanns</u>, Maria Wierzbicka, Uwe Kolitsch, *Institut für Mineralogie und Kristallographie, Universität Wien, Wien, Austria.* E-mail: ekkehart.tillmanns@univie.ac.at

The compounds $A_5M^{III}(XO_4)_4$ (A = Rb, K, TI; $M^{III} = REE$, Bi, Fe, In; X = Mo, W) crystallise in a variety of layered structure types, related to the mineral palmierite, $K_2Pb(SO_4)_2$ [1]. Some of the REE representatives are used as phosphors and laser materials [1].

During flux growth of alkali- M^{III} -silicates we have obtained the compound Rb₃In(MoO₄)₄ (I). Its crystal structure has been determined from single-crystal intensity data (Mo K α X-radiation, CCD area detector, 293 K) and refined in s.g. P2/c (no. 13) to R(F) = 0.0227 (a = 11.391(2), b = 7.983(2), c = 11.100(2) Å, $\beta = 113.74(3)^\circ$, V = 924.0(3) Å³, Z = 2). Compound I is characterised by a layered structure in which decorated kröhnkite-like [100] chains are built from a distorted InO₆ octahedron (<In-O> = 2.136 Å) corner-linked to two non-equivalent MoO₄ tetrahedra. The chains are similar to those in Ba₂Ca(HPO₄)₂(H₂PO₄)₂ [2]. Rb atoms separate these chains in different directions. Compound I is isotypic with Rb₅Er(MoO₄)₄ [3]. A calculated X-ray powder diffraction pattern demonstrates that the indexing and cell given for I on ICCD-PDF 26-1367 are incorrect. Financial support by the Austrian Science Foundation (FWF) (Grant P17623-N10) is gratefully acknowledged.

[1] Morozov V.A., Lazoryak B.I., Lebedev O.I., Amelinckx S., Van Tendeloo G., *J. Solid State Chem.*, 2003, **176**, 76. [2] Toumi M., Chabchoub S., Smiri-Dogguy L., Laligant Y., *Eur. J. Solid State Inorg. Chem.*, 1997, **34**, 1249. [3] Klevtsova R.F., Glinskaya L.A., *Dokl. Akad. Nauk SSSR*, 1976, **230**, 1337. Keywords: crystal structures, crystal growth, molybdenum compounds