Optical and Structural Properties of a Eu(II)-Doped Silico-aluminate with Channel Structure and Partial Site Occupation

Andreas Rief[a], Frank Kubel[a], and Hans Hagemann[b]

[a] Institute of Chemical Technologies and Analytics, Vienna University of Technology, Getreidemarkt 9/164-SC, A-1060 Vienna, Austria
[b] Dépt. de Chimie Physique, University of Geneva, 30, quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland

Reprint requests to Dr. A. Rief. E-mail: andreas.rief@tuwien.ac.at

Z. Naturforsch. **2007**, *62b,* 1535 – 1542; received June 14, 2007

A new barium silico-aluminate phase with the stoichiometry $Ba_{13.35(1)}Al_{30.7}Si_{5.3}O_{70}$ has been found and characterized. The compound crystallizes in the space group $P6_3/m$ (No. 176) with a = 15.1683(17), c = 8.8708(6) Å, V = 1767.5(4) Å^3, Z = 1, R_w = 0.026, 32 refined parameters. A 3-dimensional matrix of Al/SiO_4 tetrahedra with Ba(II) ions located in channels along the c axis builds up the structure. One of these channels is partially filled with Ba(II) ions (CN 6+3) in Wyckoff position 2*a*, leaving $\sim$ 1/3 of the positions empty. The second and third type of Ba(II) ions occupy channels orientated along the c axis with CN 4+2+2 and 4+3+1, respectively. The structure shows a rare clustered arrangement of six tetrahedra filled exclusively by Al(III) and therefore is an exception to Loewenstein's rule. The other tetrahedral positions show an Al to Si ratio of $\sim 4:1$. The Al/Si–O bond lengths in the tetrahedral Al/Si positions drawn *vs.* site occupation show linear behavior similar to the prediction by Vegard's rule for solid solutions. After doping with Eu(II) the compound shows bright orange-yellow luminescence with an unusual large shift of the Eu(II) emission band.

Key words: Disorder, Structure Refinement, Silico-aluminate, Luminescence, Channel Structure