$Ba_3YRu_{0.73(2)}Al_{1.27(2)}O_8$ and $Ba_5Y_2Ru_{1.52(2)}Al_{1.47(2)}O_{13.5}$: New Perovskite Ruthenates with Partial Octahedra Replacement

Barbara Schüpp-Niewa[a,b], Larysa Shlyk[a,c], Yurii Prots[d], Gernot Krabbes[a], and Rainer Niewa[b]

[a] IFW-Dresden, Leibniz-Institut für Festkörper- und Werkstoffforschung, Helmholtzstraße 20, 01069 Dresden, Germany
[b] Department Chemie, Technische Universität München, Lichtenbergstraße 4, 85747 Garching, Germany
[c] Department Physics & Astronomy, University of Kentucky, Lexington, KY 40506, USA
[d] Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden, Germany

Reprint requests to Prof. Dr. Rainer Niewa. Fax: +49 (89) 289 13762.
E-mail: rainer.niewa@ch.tum.de

Z. Naturforsch. **2007**, *62b,* 1383 – 1389; received June 11, 2007

Dark red single crystals of the new phases $Ba_3YRu_{0.73(2)}Al_{1.27(2)}O_8$ and $Ba_5Y_2Ru_{1.52(2)}Al_{1.47(2)}O_{13.5}$ have been grown from powder mixtures of $BaCO_3$, Y_2O_3, Al_2O_3, and RuO_2. The compositions given in the formulas result from the refinements of the crystal structures based on single crystal X-ray diffraction data (hexagonal $P6_3/mmc$ (No. 194), $Z = 2$, $Ba_3YRu_{0.73(2)}Al_{1.27(2)}O_8$: $a = 5.871(1)$, $c = 14.633(3)$ Å, $R1 = 0.035$, $wR2 = 0.069$ and $Ba_5Y_2Ru_{1.52(2)}Al_{1.47(2)}O_{13.5}$: $a = 5.907(1)$, $c = 24.556(5)$ Å, $R1 = 0.057$, $wR2 = 0.114$). $Ba_3YRu_{0.73(2)}Al_{1.27(2)}O_8$ crystallizes in a 6H perovskite structure, $Ba_5Y_2Ru_{1.52(2)}Al_{1.47(2)}O_{13.5}$ has been characterized as a 10H Perovskite. Due to similar spatial extensions of (Ru_2O_9) face-sharing pairs of octahedra and (Al_2O_7) vertex-sharing pairs of tetrahedra, both structures show partial mutual substitution of these units. Consequently, the title compounds may be written as $Ba_3Y(Ru_2O_9)_{1-x}(Al_2O_7)_x$, $x = 0.64(1)$ and $Ba_5Y_2RuO_6(Ru_2O_9)_{1-x}(Al_2O_7)_x$, $x = 0.74(1)$. This interpretation is supported by the results of electron probe microanalysis using wavelength-dispersive X-ray spectroscopy. An oxidation state of Ru close to +5 for the (Ru_2O_9) units, as can be derived from the distances d(Ru–Ru), additionally leads to similar charges of both the (Ru_2O_9) and the (Al_2O_7) units.

Key words: Crystal Structure, Solid State Synthesis, Ruthenium, Perovskite