BaFe_{3.39(5)}Ru_{2.61(5)}O₁₁ and BaCo_{1.85(6)}Ru_{4.15(6)}O₁₁. Preparation, Crystal Structures, and Magnetic and Transport Properties of Quaternary Transition Metal Oxoruthenates

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Black plate-like single crystals of BaFe_{3.39(5)}Ru_{2.61(5)}O₁₁ and BaCo_{1.85(6)}Ru_{4.15(6)}O₁₁ were grown from a BaCl₂ flux [hexagonal, space group $P6_3/mmc$ (No. 194), Fe: a = 5.856(1), c = 13.587(1) Å, R1 = 0.029, wR2 = 0.084; Co: a = 5.842(1), c = 13.573(3) Å, R1 = 0.033, wR2 = 0.075]. The crystal structures contain two crystallographic sites with mixed Ru and Fe/Co occupation of different level in octahedral coordination and one site purely occupied by the respective 3d metal. The latter position is in trigonal bipyramidal coordination, with some indication for a displacement of the metal atom towards tetrahedral coordination. According to the charge balance, the ruthenium atoms are incorporated with different electronic situations in the two Ru containing sites. The Co compound may be described as containing Co^{2+} and Ru^{5+} next to Ru^{3+} . Magnetic susceptibility data support this assignment. According to magnetization measurements on oriented crystals, $BaCo_{1.85(6)}Ru_{4.15(6)}O_{11}$ is a soft ferromagnetic material with low coercive field and a spontaneous magnetization below $T_c = 105$ K. It behaves as an electric conductor. However, $BaFe_{3.39(5)}Ru_{2.61(5)}O_{11}$ is a narrow band semiconductor material with ferrimagnetic ordering at $T_c = 440$ K.

Key words: Oxoruthenates, Ferrates, Cobaltates, Magnetism, Crystal Structure

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