Cs_2NiO_2 Revisited. Crystal Structure and Magnetic Properties

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Single crystals as well as microcrystalline powders of Cs_2NiO_2 were obtained *via* the azide/nitrate route from appropriate mixtures of CsN_3, $CsNO_3$ and NiO. The single-crystal structure analysis confirmed that Cs_2NiO_2 crystallizes in the tetragonal space group $I4/mmm$ ($Z = 2$, $a = 4.4090(3)$, $c = 13.576(3)$ Å, $R1 = 0.036$, $wR2 = 0.093$). Above 45 K, Cs_2NiO_2 is paramagnetic, and an analysis based on the Curie-Weiss law has resulted in $\mu = 2.89$ μ_B paramagnetic units, $\theta = -30.8$ K and $T_N \sim 20$ K.

Key words: High-spin Nickel(II) Compounds, Linear Coordination, Antiferromagnetic Ordering, Azide/Nitrate Route