

# Crystal Structure of NdNiO<sub>3</sub> at 123 and 292 K

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Well-shaped, small single crystals of the NdNiO<sub>3</sub> perovskite were grown under high oxygen pressure conditions in a belt-type press at 4 GPa. The reaction took place in sealed platinum capsules in the presence of KClO<sub>3</sub> as oxidizing agent. It seems that the choice of hydroxides of the involved cations as precursor reagents is crucial for the success of the crystal growth, *via* water vapor transport reactions. NdNiO<sub>3</sub> was investigated by X-ray powder and single crystal diffraction at 123 and 292 K: GdFeO<sub>3</sub> type, *Pbnm*,  $a = 538.10(7)$ ,  $b = 537.91(7)$ ,  $c = 760.26(10)$  pm,  $wR2 = 0.0434$ , 338  $F^2$  values, and 29 variables at 292 K. The low-temperature data gave no hint for a monoclinic distortion: *Pbnm*,  $a = 537.91(8)$ ,  $b = 538.49(8)$ ,  $c = 760.02(12)$  pm,  $wR2 = 0.0299$ , 338  $F^2$  values, and 29 variables. At room temperature, the Ni–O distances vary from 193.9 to 194.2 pm, and the O–Ni–O angles cover the range from 89.5 to 90.5°. Similar small distortions are observed for the NiO<sub>6</sub> octahedra at 123 K. Due to the strong orthorhombic distortion, the neodymium atoms have only nine oxygen neighbors at Nd–O distances from 236.0 to 295.7 pm.

**Key words:** High-Pressure Syntheses, High Pressure  
Crystal Growth, Crystal Structure