Einkristalle des Neodym(III)-*meta*-Borats $Nd(BO_2)_3$ und -*ortho*-Borats $Nd[BO_3]$

Single Crystals of the Neodymium(III) *meta*-Borate $Nd(BO_2)_3$ and *ortho*-Borate $Nd[BO_3]$

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Pale violet, transparent, air- and water-resistant single crystals of the neodymium oxoborates $Nd[BO_3]$ and $Nd(BO_2)_3$ emerged from reactions of Nd_2O_3, NdF_3 or $NdCl_3$, and B_2O_3 in variable molar ratios during attempts to synthesize neodymium halide borates (*e. g.* $Nd_2F_3[BO_3]$ or $NdCl(BO_2)_2$). The preparations were carried out at 700 °C in sealed tantalum capsules using CsCl as a flux, or at 850 °C in evacuated silica ampoules with an excess of $NdCl_3$ as fluxing agent. Neodymium *ortho*-borate λ-$Nd[BO_3]$ (orthorhombic, *Pnma*; $a = 573.51(5)$, $b = 505.64(4)$, $c = 809.16(7)$ pm; $Z = 4$) is isotypic with aragonite-type $CaCO_3$ containing *quasi*-planar, discrete $[BO_3]^{3-}$ triangles (d(B–O) = 138 pm, 3×) and Nd^{3+} in ninefold oxygen coordination (d(Nd–O) = 239 – 269 pm, CN = 9). In the crystal structure of neodymium *meta*-borate $Nd(BO_2)_3$ (NdB_3O_6; monoclinic, $C2/c$; $a = 983.24(9)$, $b = 809.32(7)$, $c = 637.71(6)$ pm, $\beta = 126.639(8)°$; $Z = 4$) both $[BO_3]^{3-}$ triangles (d(B–O) = 133 – 142 pm, CN = 3) and $[BO_4]^{5-}$ tetrahedra (d(B–O) = 145 – 149 pm, CN = 4) are present. They share common corners forming chains of the composition $^1_\infty\{([(B1)(O1)^e_{2/1}(O2)^e_{2/1}][(B2)(O1)^e_{1/1}(O2)^e_{1/1}(O3)^t_{1/1}]_2)^{3-}\}$ ($\equiv {}^1_\infty\{(BO_2)^-\}$) which run parallel to the [101] direction and are interconnected by Nd^{3+} cations in tenfold coordination of oxygen atoms (d(Nd–O) = 238 – 280 pm, CN = 10).

Key words: Neodymium, Oxoborates, Crystal Structures