

The crystal structure of single crystalline $\text{PrCa}_4\text{O}[\text{BO}_3]_3$

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$\text{PrCa}_4\text{O}[\text{BO}_3]_3$ belong to a structure family of Rare earth calcium oxoborates $\text{REX}_2\text{Z}_2\text{O}[\text{BO}_3]_3$ with $\text{RE} = \text{Er, Y, Gd, Sm, Pr, La}$ and $\text{X, Z} = \text{Ca}$ on two different *Wyckoff* sites. The materials have non-linear optical properties and show piezo- and pyroelectricity up to high temperatures. This means, the materials are promising candidates for sensor applications under extreme conditions [1]. Due to the numerous substitution possibilities of the differently coordinated cation sites (RE, X, Z), this result in a large chemical variability that can be used to improve desired properties [2].

The presented work, shows the structure solution and refinement of $\text{PrCa}_4\text{O}[\text{BO}_3]_3$ from single crystal X-ray diffraction data. A $\text{PrCa}_4\text{O}[\text{BO}_3]_3$ single crystal was grown by the Czochralski method. With an $\langle 010 \rangle$ oriented $\text{GdCa}_4\text{O}[\text{BO}_3]_3$ crystal seed, a $\text{PrCa}_4\text{O}[\text{BO}_3]_3$ crystal with a cylinder length of 20 mm, a diameter of 15 mm, and weight of 23.1 g was obtained.

The crystal structure was solved from single crystal X-ray diffraction data in the monoclinic crystal system with space group $C1m1$ (No. 8). The lattice parameters are $a = 8.1293(6) \text{ \AA}$, $b = 16.062(1) \text{ \AA}$, $c = 3.6023(2) \text{ \AA}$ and $\beta = 101.371(2)^\circ$, with a two formula units per unit cell. The structure solution is of high quality with final R - and wR_2 -values of below 3.8 %. A disorder between Pr of the RE site and Ca of X and Z site have been refined. The Pr/Ca disorder is up to 6.0 % and fits well within the demonstrated dependency of the disorder on the rare-earth ion radius found for other rare-earths in $\text{REX}_2\text{Z}_2\text{O}[\text{BO}_3]_3$ [2].

[1] Möckel R., Reuther C., Götze J. REECOB: 20 years of rare earth element calcium oxoborates crystal growth research. Journal of Crystal Growth, 371, 70-76 (2013)

[2] Münchhalfen M., Schreuer J., Reuther C., Mehner E., Stöcker H. Elastic, piezoelectric, and dielectric properties of rare-earth calcium oxoborates $\text{RCa}_4\text{O}(\text{BO}_3)_3$ ($R = \text{Er, Y, Dy, Gd, Sm, Nd, La}$). Journal of Applied Physics, 130, 095102-1 - 095102-12 (2021)