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Congruent melt terbium-rich borate $Na_2Tb_2B_2O_7$: Synthesis, crystal structure, optical and magnetic properties

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Abstract: Single crystals of $Na_2Tb_2B_2O_7$ were successfully grown from a Na_2O - B_2O_3 - NaF flux, and its lanthanide homotypic compounds were synthesized using the solid-state reaction method and of pure phase according to the refinements of the X-ray diffraction patterns. $Na_2Tb_2B_2O_7$ belongs to monoclinic system, $P2_1/c$ space group, with cell parameters of a = 10.643(2) Å, b = 6.2724(13) Å, c = 10.247(2) Å, β = 117.72(3)^o and Z = 4. In the structure, the terbium atoms coordinate to eight oxygen atoms to form a TbO_8 polyhedra, which are connected through edge-sharing O atoms to form a layered $[Tb_2(BO_3)_2O]^{2-}$ sheets in the *bc* plane. Then the sheets are further linked along *a* direction to build three dimensional framework with the separation of Na^+ cations. $Na_2Tb_2B_2O_7$ exhibits high transparent in the range of 500 - 1500 nm. Meanwhile, it shows a green-emitting band due to the characteristic electronic $^5D_4$ to $^7F_5$ transitions of Tb^{3+} ions. Magnetic measurements show that $Na_2Tb_2B_2O_7$ exhibits typical paramagnetic behaviors from 2 K to 300 K.

Keywords: Borate; Crystal structure; Luminescent property; Magnetic property.