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Congruent melt terbium-rich borate Na₂Tb₂B₂O₇: Synthesis,

crystal structure, optical and magnetic properties

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Abstract: Single crystals of Na₂Tb₂B₂O₇ were successfully grown from a Na₂O -B₂O₃ - 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. Na₂Tb₂B₂O₇ belongs to monoclinic system, *P*₂₁/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)° and Z = 4. In the structure, the terbium atoms coordinate to eight oxygen atoms to form a TbO₈ polyhedra, which are connected through edge-sharing O atoms to form a layered [Tb₂(BO₃)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. Na₂Tb₂B₂O₇ exhibits high transparent in the range of 500 - 1500 nm. Meanwhile, it shows a green-emitting band due to the characteristic electronic ⁵D₄ to ⁷F₅ transitions of Tb³⁺ ions. Magnetic measurements show that Na₂Tb₂B₂O₇ exhibits typical paramagnetic behaviors from 2 K to 300 K.

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

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