High-Temperature Synthesis, Crystal Structure, and Properties of the New Sodium Rare-Earth Oxide Borates \( \text{Na}_2\text{RE}_2(\text{BO}_3)_2\text{O} \) \((\text{RE} = \text{Dy, Ho})\)

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Dedicated to Professor Hubert Schmidbaur on the occasion of his 70th birthday

The new monoclinic oxide borates \( \text{Na}_2\text{RE}_2(\text{BO}_3)_2\text{O} \) \((\text{RE} = \text{Dy, Ho})\) were synthesized using standard solid-state reactions in the temperature range 900 – 950 °C. They are isotypic to the known phases \( \text{Na}_2\text{RE}_2(\text{BO}_3)_2\text{O} \) \((\text{RE} = \text{Y, La, Nd, Sm-Gd, Er})\). The single crystal X-ray structure determination of \( \text{Na}_2\text{Dy}_2(\text{BO}_3)_2\text{O} \) revealed: \( P2_1/n \), \( a = 1063.9(1) \), \( b = 626.2(1) \), \( c = 1025.3(1) \) pm, \( \beta = 117.76(1)^\circ \), \( Z = 4 \), \( R1 = 0.0221 \), \( wR2 = 0.0402 \) (all data). The corresponding lattice parameters of \( \text{Na}_2\text{Ho}_2(\text{BO}_3)_2\text{O} \) determined from powder data are \( a = 1061.2(5) \), \( b = 623.7(2) \), \( c = 1022.5(3) \) pm, and \( \beta = 117.7(1)^\circ \). The structure consists of infinite sheets of \( \text{REO}_8 \)-polyhedra in the \( bc \)-plane, which are seperated by sodium atoms. The \( \text{BO}_3 \)-groups are isolated forming layers in the \( bc \)-plane. The results of IR-spectroscopic investigations, temperature-resolved in-situ powder-diffraction measurements, and DTA/TG measurements on \( \text{Na}_2\text{Dy}_2(\text{BO}_3)_2\text{O} \) are also presented.

Key words: Solid-State Synthesis, Oxide Borates, Crystal Structure