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Implications for the Structural Origin of the Increase in Configurational Heat Capacity with Increasing B₂O₃ Content in Borosilicate Glasses

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In this work, we explore the structural origin of the compositional evolution of the jump in isobaric heat capacity (ΔCₚ) during the glass transition in a series of (75q)B₂O₃-(75(1-q))SiO₂-15Na₂O-10CaO glasses. ΔCₚ represents the difference between the liquid C_pl and the glass C_pg and is usually approximated as the configurational heat capacity (C_p,conf), particularly for relative strong inorganic system. As determined by differential scanning calorimetry (DSC), ΔCₚ is found to increase non-linearly when substituting B₂O₃ for SiO₂. By using Raman spectroscopy we investigate whether and how the increase in ΔCₚ is associated with changes in glass structure, particularly in the intermediate range order (IRO) structure. Raman bands in the medium-frequency region of 550-810 cm⁻¹ can be assigned to the vibrational modes of various superstructural units, reflecting the IRO. Our results demonstrate a possible link between the evolution of IRO structures and ΔCₚ, which reflects the number of minima in a multidimensional potential energy surface. In the silica-rich compositions, two types of borosilicate units exist, leading to the rapid increase of ΔCₚ with B₂O₃ content. In the compositions with similar concentration of B₂O₃ and SiO₂, the concentration of borosilicate units and borate superstructures change in an opposite way, leading to an approximate constant value of ΔCₚ as a function of composition. In the boron-rich compositions, the presence of six-membered borate rings with one and two [BO₄/2] groups are responsible for the increase of ΔCₚ with B₂O₃ content.