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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 (ΔC_p) during the glass transition in a series of $(75q)\text{B}_2\text{O}_3-(75(1-q))\text{SiO}_2-15\text{Na}_2\text{O}-10\text{CaO}$ glasses. ΔC_p represents the difference between the liquid C_{pl} and the glass C_{pg} and is usually approximated as the configurational heat capacity ($C_{p,\text{conf}}$), particularly for relative strong inorganic system. As determined by differential scanning calorimetry (DSC), ΔC_p is found to increase non-linearly when substituting B₂O₃ for SiO₂. By using Raman spectroscopy we investigate whether and how the increase in ΔC_p 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 ΔC_p , 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 ΔC_p 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 ΔC_p as a function of composition. In the boron-rich compositions, the presence of six-membered borate rings with one and two [BO_{4/2}]⁻ groups are responsible for the increase of ΔC_p with B₂O₃ content.