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Statistical Mechanical Modeling of Lithium Borate Glass Structure and Topology

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Predicting the compositional evolution of the atomic-scale structure of oxide glasses is important for developing quantitative composition-property models. In binary borate glasses, the addition of network modifiers will either increase the connectivity by converting three-fold into four-fold coordinated boron, or decrease the connectivity by creating non-bridging oxygens. Here, based on ¹⁰B nuclear magnetic resonance spectroscopy data from literature, we present a statistical description of the compositional evolution of both intermediate range superstructures (e.g., boroxol rings) and short range Q_n species in lithium borate glasses. This is done by accounting for the relative enthalpic and entropic contributions to the bonding preferences. We show that the entire glass structure evolution can be predicted based on experimental structural information for only a few glass compositions in each series. The developed structural model can be combined with a previously established constraint theory model to also predict the glass transition temperature.