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Statistical Mechanical Approach to Predict the Structure Evolution in Phosphate Glasses

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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 phosphate glasses, addition of network modifiers generally lead to depolymerization of the networks as described by the Q-speciation, but involves a variety of different network former/modifier interactions. Here, based on ^{31}P magic angle spinning nuclear magnetic resonance spectroscopy data from literature, we present a statistical description of the compositional evolution of Q-speciation in phosphate glasses with alkali, magnesium, and zinc modifiers by accounting for the relative enthalpic and entropic contributions to the bonding preferences.[1] 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. Finally, we also discuss the possibility to extend the statistical mechanical model to binary silicate and borate glasses.

[1] Bødker M. S., Mauro J. C., Goyal S., Youngman R. E., Smedskjaer M. M. Predicting Q-Speciation in Binary Phosphate Glasses using Statistical Mechanics. *J. Phys. Chem. B* **122**, 7609-7615 (2018).