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TOPOLOGICAL ORIGINS OF BOROSILICATE GLASS PROPERTIES

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Borosilicate glasses display a rich complexity of chemical behavior depending on the details of their composition and thermal history. Here, we investigate the topological principles of borosilicate glass chemistry covering the extremes from pure borate to pure silicate end members. To do so, we first introduce a two-state statistical mechanical model of boron speciation in which addition of network modifiers leads to a competition between the formation of nonbridging oxygen and the conversion of boron from trigonal to tetrahedral configuration. Using this model and temperature-dependent constraint theory, we derive a detailed topological representation of alkali-alkaline earth-borosilicate glasses that enables the accurate prediction of properties such as glass transition temperature, liquid fragility, hardness, and configurational heat capacity. The modeling approach enables a detailed understanding of the microscopic mechanisms governing macroscopic properties.