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Thermodynamic Model for Borate in Elevated Temperature and High Ionic Strength Environments: Interaction Parameters for $B(OH)_3(aq)$

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In geological disposal of high level nuclear waste (HLW), borate is expected to be a significant player, owing to the following facts. First, relatively high concentrations of borate can be present in natural groundwaters such as brines associated with salt formations and formation waters. Second, borate is also released into the groundwater when borosilicate glass waste forms for HLW are corroded after canisters containing such waste forms are breached. Consequently, the presence of borate in the near-field of geological repositories can have three major potential impacts. The first potential major impact is that borate can form aqueous complexes with trivalent actinides [An(III)]. As a result, borate could become a potential transport agent for actinides by forming the An(III)-borate aqueous complexes. The second potential major impact is that borate can form solid species with actinides, as numerous actinide-bearing borate solid phases have been successfully synthesized in the literature, implying the possibility that actinides in waste could be transformed into, or be sequestrated as, actinide borates, if their solubility limits are reached. Additionally, the total boron concentration in the near-field is an important parameter for an evaluation of the possible occurrence of a nuclear criticality event. Hence the accurate knowledge of borate geochemistry under the conditions of various disposal concepts including high temperatures and high ionic strength is important to the evaluation of the role of borate in the performance assessment (PA). However, such knowledge is currently lacking.

In this study, we deleop a thermodynamic model for borate chemistry valid to high temperatures and high ionic strengths, with the Pitzer equations for activity coefficient calculations. As the interactions for the neutral borate species, $B(OH)_3(aq)$, are the foundation for the model, we present the interactions parameters related to $B(OH)_3(aq)$ in this work.

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