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Thermodynamic properties of potassium chloride aqueous solutions

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Potassium chloride is a ubiquitous salt in natural fluids, being the second most abundant dissolved salt in many geological aqueous solutions after sodium chloride. It is a simple solute and strong electrolyte easily dissociating in water, however the thermodynamic properties of KCl aqueous solutions were never correlated with sufficient accuracy for a wide range of physicochemical conditions. In this communication we propose a set of parameters for a Pitzer-type model which allows calculation of all necessary thermodynamic properties of KCl solution, namely excess Gibbs free energy and derived activity coefficient, apparent molar enthalpy, heat capacity and volume, as well as osmotic coefficient and activity of water in solutions.
The system KCl-water is one of the best studied aqueous systems containing electrolytes. Although extensive experimental data were collected for thermodynamic properties of these solutions over the years, the accurate volumetric data became available only recently, thus making possible a complete thermodynamic formulation including a pressure dependence of excess Gibbs free energy and derived properties of the KCl-water liquids. Our proposed model is intended for calculation of major thermodynamic properties of KCl aqueous solutions at temperatures ranging from freezing point of a solution to 623 K, pressures ranging from saturated water vapor up to 150 MPa, and concentrations up to the salt saturation. This parameterized model will be further implemented in geochemical software packages and can facilitate the calculation of aqueous equilibrium for reactive transport codes.