A Priori Prediction of the Standard State Partial Molar Volume of Aqueous Electrolytes to High Temperatures and High Pressures

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Fundamental understanding of industrial and natural processes requires reliable pressure and temperature dependence of chemical equilibria in aqueous solutions (1). Applications of these processes require high temperature data where experimental data are scarce. The standard state partial molar volume is an important property because it directly relates to changes in chemical potential with pressure. In the present study, the standard state partial molar volumes of aqueous solutions are predicted for chlorides, hydroxides, and sulfates of the alkali metals, alkali earth metals, and the first-row transition metals from unified theory of electrolytes (1) to high temperatures and pressures. The only required input to the model is the thermodynamic properties at 298.15 K and 0.1 MPa. Good agreement is observed between the available experimental data for standard state partial molar volumes and the corresponding values from the present model to well within the uncertainties of the experimental data up to 623.15 K and 1000 MPa. The present model is also compared with the correlations of Sedlbauer–O'Connell–Wood (2) and SUPCRT92 (3).

References

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