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Theory of model electrolyte solutions: assessing the short- and long-ranged contributions by molecular simulations

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Abstract

In this work, we conduct a comprehensive simulation study on Helmholtz energies for non-primitive model electrolyte solutions in order to assess fluid theories. Simulation data is obtained with two different methods. Using a new thermodynamic integration path, we calculate Helmholtz energy contributions arising from damped, short-ranged electrostatic pair potentials. The division of the potential into a damped, short-ranged and a long-ranged part using a complementary error function corresponds to the division of a standard Ewald sum. Additionally, we applied a standard thermodynamic integration method to obtain the full electrostatic contribution to the Helmholtz energy. We evaluate the analytical long-range contribution developed by Rodgers and Weeks [J. M. Rodgers and J. D. Weeks, *J. Chem. Phys.* **131**, 244108 (2009)] and find excellent agreement to our simulation data for any damping parameter $\alpha^* \geq 1.5$ for liquid-like densities. Further, the simulation data is compared to a third order perturbation theory we recently presented.

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