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Simulations of mean ionic activity coefficients and solubilities in aqueous electrolyte solutions[1]

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Aqueous electrolyte solutions play an important role in industrial, geochemical and biological applications. The mean ionic activity coefficients quantify the deviation of salt chemical potential from ideal solution behavior; experimental measurements are available for many salts over broad ranges of concentration and temperature, but there have been practically no prior simulation results, because if sampling difficulties for explicit-solvent electrolyte solutions. We have developed a new approach for determination of activity coefficients of aqueous electrolytes [1]. Common fixed-point-charge models for water and ions are unable to reproduce simultaneously activity coefficients and solubilities. Polarizable models perform better, but still predict an incorrect temperature dependence of these properties [2]. [1] Z. Mester and A. Z. Panagiotopoulos "Mean ionic activity coefficients in aqueous NaCl solutions from molecular dynamics simulations," *J. Chem. Phys.* **142**: 044507, 10 pp (2015). http://dx.doi.org/10.1063/1.4906320 [2] H. Jiang, Z. Mester, O. A. Moultos, I. G. Economou, and A. Z. Panagiotopoulos, "Thermodynamic and Transport Properties of H2O+NaCl from Polarizable Force Fields," J. *Chem. Theory Comput.* **11**: 3802-3810 (2015). http://pubs.acs.org/doi/abs/10.1021/acs.jctc.5b00421

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