The Madrid-2019 force field for electrolytes in water: An extension to the ions F^-, Br^-, I^-, Rb^+ and Cs^+

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In this work, we present an extension of the Madrid-2019 force field [1]. We have added to this extension the cations Rb+ and Cs+ and the anions F−, Br−, and I−. These ions were the remaining alkaline and halogen ions, not previously considered in the Madrid-2019 force field. The force field, denoted as Madrid-2019-Extended [2], does not include polarizability and uses the TIP4P/2005 [3] model of water and scaled charges for the ions. A charge of ±0.85e is assigned to monovalent ions. This new force field developed provides an accurate description of aqueous solution densities over a wide range of concentrations up to the solubility limit of each salt studied. Good predictions of viscosity and diffusion coefficients are obtained for concentrations below 2 m. Structural properties obtained with this force field are also in reasonable agreement with the experiment. The number of contact ion pairs has been controlled to be low so as to avoid precipitation of the system at concentrations close to the experimental solubility limit. We also present a comprehensive comparison of the performance for aqueous solutions of alkaline halides of force fields of electrolytes using scaled and integer charges. This comparison will help in the future to learn about the benefits and limitations of the use of scaled charges to describe electrolyte solutions.

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