

Experimental and simulation results (using the extended Madrid-2019 force field) for the maximum in density of 1m salt solutions containing the cations Rb^+ and Cs^+ : and the anions F^- , Br^- and I^- .

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We present the experimental validation of the temperature of the maximum in density (TMD) at constant pressure (1 bar) predicted by the recently proposed extension of the Madrid-2019 force field for electrolyte solutions containing F^- , Br^- and I^- anions and Rb^+ and Cs^+ cations [1]. To that aim the TMD for a number of salts comprising at least one of those ions have been measured by monitoring the temperature-dependent meniscus position in capillary glass tubes within the prescriptions reported in reference [2]. The experimental results are contrasted against Molecular Dynamics simulation in the isothermal-isobaric ensemble (NpT) results within the scale-charged framework provided by the extended Madrid-2019 force field. Drawbacks and future projections are also projected.

REFERENCES

- [1] S. Blazquez, M. M. Conde, J. L. F. Abascal and C. Vega, *J. Chem. Phys.*, 156 (2022) 044505.
- [2] L. F. Sedano, S. Blazquez, E. G. Noya, C. Vega and J. Troncoso, *J. Chem. Phys.* 156 (2022) 154502.

FIGURES

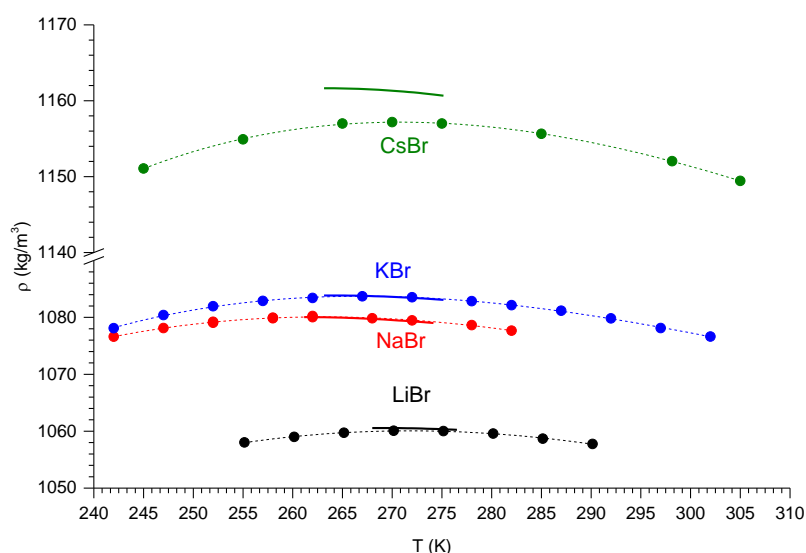


Figure 1: Experimental (continuous lines) and simulated (symbols) TMDs for alkaline bromides. Dashed lines stand for third order polynomial fitting to Molecular Dynamics results.