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Preferential Solvation of Li^+ in 18.45 % Aqueous Ammonia: A Born−Oppenheimer ab Initio Quantum Mechanics/Molecular Mechanics MD Simulation

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A molecular dynamics simulation using a mixed ab initio quantum mechanics/molecular mechanics formalism has been performed in order to obtain refined structural properties for a Li(I) ion in 18.45% aqueous ammonia solution. Using a double-ζ valence basis set for the quantum mechanically described first solvation shell including the ion, a tetrahedral structure with three water and one ammonia ligand is observed, in contrast to the octahedral structure with three water and three ammonia ligands predicted by classical pair potential simulation. This can be considered as further proof for the importance of nonadditive n-body effects for a proper description of ions in solution, even if they are only single charged. Further structural data and the preference for water ligands are discussed on the basis of detailed simulation results.