Three-body Effects in Calcium(II)-ammonia Solutions: Molecular Dynamics Simulations

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Molecular dynamics simulations have been performed with and without three-body corrections at an average temperature of 240 K using a flexible ammonia model. The system consists of one calcium ion and 215 ammonia molecules. The calcium(II)-ammonia interactions were newly developed, based on *ab initio* calculations with a basis set of double zeta quality. The role of three-body interactions on the structural and dynamical properties of the solution has been investigated. The presence of three-body corrections leads to the reduction of the first shell coordination number of Ca(II) in liquid ammonia from 9 to 8, the increase of the size of the solvation shell by 0.33 Å and the disappearance of the second solvation shell.

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