ABSTRACT

STUDY ON STRUCTURE AND DYNAMICS OF SOLVATION LITHIUM (I) ION USING QUANTUM MECHANICAL CHARGE FIELD (QMCF) MOLECULAR DYNAMICS SIMULATION

by

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The solvation of Li(I) in liquid ammonia has been investigated by an ab initio quantum mechanical charge-field molecular dynamics (QMCF-MD) simulation. Being the first simulation of a metal cation in liquid ammonia employing this methodology, the work yields a wide range of accurate structural and dynamical data. Li(I) is tetrahedrally coordinated by four ammonia molecules in the first solvation shell at a distance of 2.075 Å. Two ligand exchange attempts have been observed within 12 ps of simulation time. The second solvation shell shows a more labile structure with numerous successful exchanges. The results are in excellent agreement with experiments.

Keyword: solvation, Li^+, liquid ammonia, quantum mechanical charge field (QMCF), molecular dynamics simulation.