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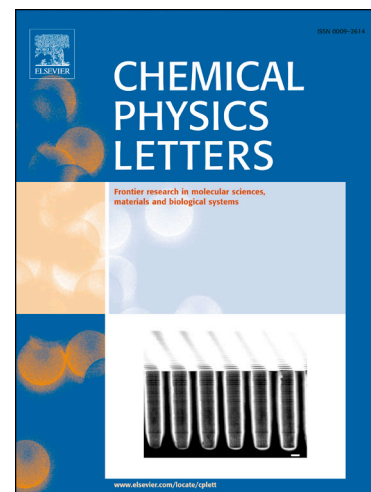
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Revisiting structure and dynamics of preferential solvation of K(I) ion in aqueous ammonia using QMCF-MD simulation

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Highlights

1. The used of QMCF-MD method to re-investigate of K(I) ion in aqueous ammonia system is successfully proving that alkali prefers to be solvated by water than ammonia
2. Four water and two ammonia molecules coordinated with K(I) ion in the first solvation shell and forming unsymmetrical octahedron structure.
3. The NBO analysis confirms a weak electrostatic interaction between ion and ligands where interaction between K(I) ion to H₂O is strongly than K(I) to NH₃

ABSTRACT

Structure and dynamics of preferential solvation of K(I) ion in aqueous ammonia have been re-investigated using ab initio quantum mechanical charge field (QMCF) molecular dynamics (MD) simulation. The average coordination number of the first solvation consists of 2 ammonia and 4 waters. The mean residence time is less than 2 ps confirming the rapid mobility of ligands. The distance evolution data shows the frequent of ligand exchanges. The second solvation shell shows a more labile structure. The NBO analysis of the first shell structure emphasizes that interaction of K(I)-H₂O is stronger than K(I)-NH₃. The Wiberg bond confirms a weak electrostatic of ion-ligand interaction.

Keyword: simulation, structure dynamics, QMCF, potassium, preferential

1. Introduction

Potassium ion in solution is still relevant to be studied since the ion in solvation system play the role in many aspects of life, such as K-channel in cell metabolism [1–4]. In liquid electrolytes, potassium ions will induce smaller solvated cations and causing a fast ionic conductivity with a high power [5]. The advantages of potassium properties are related to its capability as a charge carries and recently has

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