Research paper

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Studies of Solvation behaviour of LiI prevailing in diverse solvent systems conductometrically and spectrometrically supported by ab-initio technique

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Abstract

Solvation nature of Lithium iodide (LiI) for both polar and nonpolar organic solvents *viz.*, acetonitrile and benzonitrile have been explored by effect of geometry, spectroscopic, conductometric, ab initio methods . Results of vibrational spectroscopic data were compared with experimental values. Centre of attraction is iodide anion on significant vibrational bands of benzonitrile. Fluorescence spectra provide a supporting to the mentioned facts. Ab initio calculations used for shaping the optimum location of Li^+ and I^- ions in ion-solvent interactions containing varying nitriles as solvent sphere. Emission band positions, intensity, shape of solvent-sensitive molecules in organic solvents of varying polarities are studied.

Keywords: Acetonitrile, Benzonitrile, Ion-solvation, Lithium Iodide, Vibrational wave numbers.

1. Introduction

The origin of exceptionally elevated solubility of anhydrous lithium iodide in organic solvent system has been a matter of some conjecture. This univalent salt of a small cation and a large anion must possess a favorable balance of lattice and solvation energies conducive to extensive solubility in a broad range of solvents. The solubility and stability of lithium iodide have encouraged its use in studies of salt effects in organic reactions. So it can be said that behaviour in which cations are solvated in solution retains interest for immeasurable applications. Acetonitrile has numerous uses,