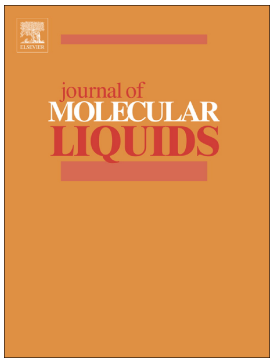

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Molecular dynamics in amorphous pharmaceutically important protic ionic liquid–benzalkonium chloride

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Abstract-In this paper; we report the dielectric measurements at ambient pressure to portray the molecular dynamics of a glass forming pharmaceutical as well as a protic ionic conductor, benzalkonium chloride [BaCl] by means of broadband dielectric spectroscopy. The measurement in macroscopic nature of a stochastic transport theory and of the electric modulus formalism stanchly reproduces the shape of the dispersion of the microscopic ionic movement in terms of translational and ionic diffusive motion of molecular ions. The situation is analogous to most ionic conductors, BaCl showed only single resolved peak in the electric modulus formalism and doesn't show any crystallisation tendency during cooling as well as heating. The temperature dependence of the conductivity relaxation has been fitted by single Vogel–Fulcher–Tamman (VFT) equation. It is found that the value of T_g observed from DSC is significantly higher than one obtained from the α-conductivity relaxation corresponding to 100 sec indicating that the structural $\tau_\alpha(T)$ is longer than conductivity $\tau_{\sigma\alpha}(T)$ for about 10 K. Finally, the results were compared with data for other protic ionic conductors like Procaine HCl, Procainamide HCl, Verapamile HCl, Lidocaine HCl, Tramadole HCl and Chlorpromazine HCl and found that BaCl is a good strong glass former.

Keywords: *Broadband dielectric spectroscopy; Protic Ionic Liquids; Amorphous materials; Active pharmaceutical ingredients; Density Function Theory; glass transition; thermodynamic parameters.*

1. Introduction

As of late, Ionic Liquids (ILs) as an active pharmaceutical ingredient (API) attracted scientific as well as industrial interest due to their tunable physical properties for enhancing