Raman Spectroscopy and Ab-Initio Model Calculations on Ionic Liquids - DTU Orbit (15/01/2019)

Raman Spectroscopy and Ab-Initio Model Calculations on Ionic Liquids: Invited Review

A review of the recent developments in the study and understanding of room temperature ionic liquids are given. An intimate picture of how and why these liquids are not crystals at ambient conditions is attempted, based on evidence from crystallographical results combined with vibrational spectroscopy and ab-initio molecular orbital calculations. A discussion is given, based mainly on some recent FT-Raman spectroscopic results on the model ionic liquid system of 1-butyl-3-methylimidazolium ([C4mim][X]) salts. The rotational isomerism of the [C4mim]+ cation is described: the presence of anti and gauche conformers that has been elucidated in remarkable papers by Hamaguchi et al. Such presence of a conformational equilibrium seems to be a general feature of the room temperature liquids. Then the "localized structure features" that apparently exist in ionic liquids are described. It is hoped that the structural resolving power of Raman spectroscopy will be appreciated by the reader. It is of remarkable use on crystals of known different conformations and on the corresponding liquids, especially in combination with modern quantum mechanics calculations. It is hoped that these interdisciplinary methods will be applied to many more systems in the future. A few examples will be discussed.
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