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.

General information
State: Published
Organisations: Energy and Materials, Department of Chemistry
Contributors: Berg, R. W.
Pages: 1045-1075
Publication date: 2007
Peer-reviewed: Yes
Web of Science (2010): Impact factor 1.356
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.479 SNIP 0.656
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.469 SNIP 0.705
Scopus rating (2007): SJR 0.406 SNIP 0.586
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.444 SNIP 0.672
Scopus rating (2005): SJR 0.417 SNIP 0.724
Scopus rating (2004): SJR 0.427 SNIP 0.816
Scopus rating (2003): SJR 0.406 SNIP 0.635
Scopus rating (2002): SJR 0.503 SNIP 0.766
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.465 SNIP 0.738
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.355 SNIP 0.782
Scopus rating (1999): SJR 0.377 SNIP 0.649
Original language: English
Keywords: Vibration, Liquid, Conformational isomerism
Electronic versions:
DOIs:
10.1007/s00706-007-0760-9

Bibliographical note
Contains also original research results
Source: orbit
Source-ID: 207578
Research output: Research - peer-review › Journal article – Annual report year: 2007