



CYCLE DE CONFÉRENCES DE CHIMIE

*Avec le concours de : Manufacture Française des Pneumatiques MICHELIN
Ecole Nationale Supérieure de Chimie de Clermont-Ferrand
Institut de Chimie de Clermont-Ferrand (ICCF UMR 6296)
U.F.R.S.T. Département de Chimie*

Vendredi 19 Juillet 2013 à 10 h (Hors cycle)

Salle C Bâtiment de Chimie - (Site des Cézeaux)

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Polarizabilities in ionic liquids

The molar polarisability is a significant electrical property of solvents; it measures the ease with which a molecular electron cloud reacts under the influence of an electric field, and is governed by the strength of nuclear charge centres controlling their electrons. The molar polarisability is thus of particular importance for ionic liquids because a delocalised and flexible cationic charge distribution is a key contributing factor for low electrostatic interactions between ions. Ab initio calculations of ionic liquids have reported effective molecular charges of cations and anions of much less than $\pm 1e$, which can be reproduced by incorporating polarisability effects in simulations. In contrast, we show that scaled partial charges are a cheap but dangerous byway to mimic polarisability effects. Overall, the polarisability creates induced dipoles, which accelerates the dynamics of the ionic liquids systems without major changes in structure or hydrogen bonding capabilities. This way, the agreement between results from molecular dynamics simulations and experiments are improved, in particular in the short-time regime as demonstrated by solvation dynamics spectroscopy data.