Understanding the effects of solvation is a prerequisite for controlling many processes in solutions such as liquid phase reactions, nucleation and crystallisation. Core level spectroscopy is one of the few techniques that can be used to probe molecular level interactions between organic solutes and solvents [1, 2]. Recently, we have shown that the N K-edge near edge X-ray absorption fine structure (NEXAFS) spectra combined with density functional theory calculations yield detailed information on the local structures of imidazole aqueous solutions [1].

Building on previous work [1] we have studied the structure of concentrated imidazole solutions by neutron scattering and core level spectroscopy. A structural model consisting of individually hydrated imidazole molecules was derived from neutron scattering data and the associated Monte Carlo empirical potential structural refinement (EPSR) simulation. Time dependent density functional theory (TD-DFT) calculations were carried out in ORCA on that structural model. The TD-DFT calculations accurately reproduce the peak positions and intensities of the N K-edge NEXAFS spectra of imidazole aqueous solutions. We note that the structural model from the EPSR simulation reproduces accurate N K-edge spectral features when compared to other structural models that we used including (i) monomeric imidazole (ii) a single imidazole molecule with an implicit solvent model (COSMO) (iii) a single imidazole molecule with explicitly added solvent molecules in the plane of the imidazole molecule. These studies confirm that the most important structural motifs are individually hydrated imidazole species, with little evidence for imidazole-imidazole self-association.


Keywords: Solvation, Neutron Scattering, NEXAFS