

Structure of Flexible Chiral Molecules and Unconventional Solvents by Vibrational Circular Dichroism Spectroscopy

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Vibrational circular dichroism (VCD) unveils molecular conformational nuances by discerning absorption differences in right- and left-circularly polarized light within the infrared range. This subtle technique elucidates molecular interactions, especially those that are sensitive to hydrogen bonding, thereby offering particular insight into the structure of unconventional solvents. Interpreting VCD signals necessitates meticulous comparison with theoretical models. However, incorporating environmental effects posed challenges, now mitigated by advancements in computational modeling. Notably, simulating VCD spectra in highly structured liquids like Ionic Liquids (ILs) presented formidable hurdles due to pervasive long-range interactions. We have recently proposed a new methodology based on classical molecular dynamics simulations associated with the AMOEBA polarizable force field to calculate VCD spectra of flexible molecules [1]. A first study of a chiral and flexible molecule, namely phenylcyclohexanediol in a solvent of dimethyl sulfoxide (DMSO) was made successfully, leading to the calculation of infrared and VCD spectra. This work has now been extended to ILs, particularly spirocyclic pyrrolidinium with BF_4^- . Modeling both the infrared and VCD spectra for these systems reveals useful insights into their properties and the complex interactions with their environment.

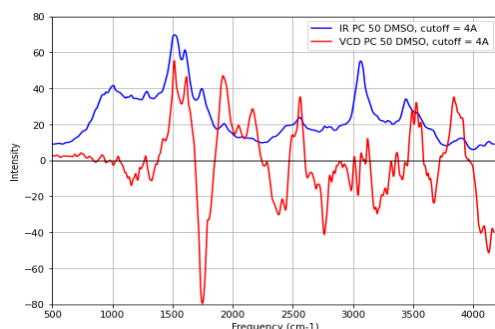


Figure 1. Infrared and VCD spectra of phenylcyclohexanediol in a box of solvent (DMSO)

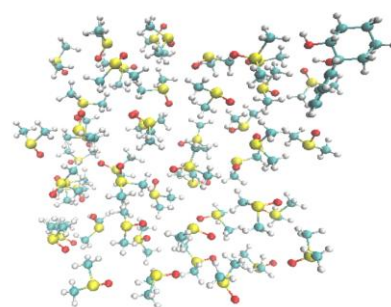


Figure 2. Phenylcyclohexanediol in a box of DMSO

Keywords: Vibrational circular dichroism (VCD); AMOEBA; polarization.