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. Recently, we 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]. The crucial element in these VCD simulations is determining the magnetic dipole moment, an intrinsic dynamical quantity. Highly flexible molecules turn out to be particularly interesting to study using this method, like 1-phenyl-1,2-cyclohexanediol (PC), that was successfully studied in a dimethyl sulfoxide (DMSO) solvent, leading to the calculation of both infrared and VCD spectra. Modeling both the infrared and VCD spectra for these systems reveals useful insights into their properties and the complex interactions with their environment, with the intention to extend this work to ILs and DES, like spirocyclic pyrrolidinium with BF4- and menthol acid acetic, respectively.

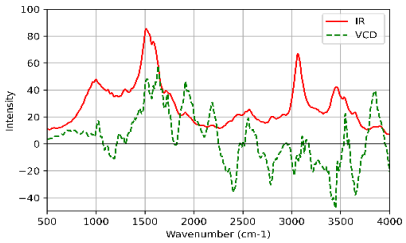

Figure 1. *Infrared and VCD spectra of PC in a box of solvent (DMSO)*

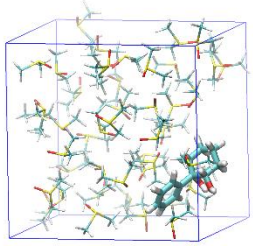

Figure 2. *Phenylcyclohexanediol in a box of DMSO*

References

[1] J. Bowles et al., Vibrational Circular Dichroism Spectroscopy with a Classical Polarizable Force Field: Alanine in the Gas and Condensed Phases. ChemPhysChem (2024).