

# VIBRATIONAL CIRCULAR DICHROISM SPECTRA OF METHYL GLYCIDATE IN CHLOROFORM AND WATER: APPLICATION OF THE CLUSTERS-IN-A-LIQUID MODEL

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Infrared and vibrational circular dichroism (VCD) spectra of methyl glycidate, a chiral epoxy ester, were measured in  $\text{CCl}_4$  and water in the  $1000\text{ cm}^{-1} - 1800\text{ cm}^{-1}$  region. The experimental VCD spectra of methyl glycidate in water and in  $\text{CCl}_4$  show noticeable differences. In particular, there are strong VCD signatures at the water bending mode region, which can be attributed to chirality transfer from chiral methyl glycidate to water through hydrogen-bonding interactions. We applied the clusters-in-a-liquid model<sup>1</sup> where both implicit and explicit solute-solvent interactions are considered to simulate the experimental infrared and VCD features of methyl glycidate in  $\text{CCl}_4$  and water. All final geometry optimizations, frequency calculations, infrared and VCD intensity calculations were performed at the B3LYP-D3BJ/6-311++G(2d,p) level of theory where D3BJ is Grimme's empirical dispersion correction with damping factor.<sup>2</sup> We emphasize the link between the small methyl glycidate hydrates and the main long-lived species which exist in aqueous solution.

1 A. S. Perera, J. Thomas, M. R. Poopari, Y. Xu, *Front. Chem.* 2016, 4, 1-17. 2 S. Grimme, S. Ehrlich, L. Goerigk, *J. Comp. Chem.* 2011, 32, 1456-1465.