



Quantitative Evaluation of IR and Corresponding VCD Spectra

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Contemporary literature does not explain the infrared and vibrational circular dichroism (VCD) spectra of chiral molecules from a classical perspective.^{1,2} As a result, the primary usage of VCD spectra is to determine the absolute configuration of a chiral molecule through comparison of experimental data and quantum mechanical calculations. Classical treatments of IR and VCD spectra can provide insight into the spectra. E.g., dispersion analysis based on wave optics and dispersion theory can be applied, which was extended by Born and Kuhn to include chiral substances. VCD dispersion analysis, as we devised it,³ uses pairs of coupled oscillators to quantitatively describe the dielectric function and the chiral admittance functions that make up IR and VCD spectra. Oscillator strength, damping, oscillator position, vertical distance between coupled oscillators, and the coupling constant are the five parameters used to model the dielectric functions and chiral admittance functions of α -Pinene and Propylene oxide. In most cases, this model is sufficient to achieve a good correspondence between experimental and simulated data. The coupling can also impact the conventional IR spectra of chiral compounds by shifting peaks and transferring oscillator strengths.

Keywords: Vibrational circular dichroism; Infrared spectroscopy; Dispersion Analysis.

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