

The Application of Vibrational Circular Dichroism (VCD) Spectroscopy to the Determination of the Stereochemistries of Chiral Molecules

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ABSTRACT :

The VCD spectra of chiral molecules are measured using a Fourier-Transform VCD instrument, and both enantiomers of the chiral molecules. Analysis of the experimental VCD spectrum of a chiral molecule is carried out using the Stephens quantum-mechanical VCD Theory, and *ab initio* Density Functional Theory (DFT) incorporated in the GAUSSIAN program. For all the molecules whose stereochemistries have been determined using VCD, the Absolute Configurations (ACs) and for conformationally flexible molecules, the structures of the conformations have been determined.

The molecules are: Troger's Base; perhydrotriphenylene; chiral sulfoxides; isopropylidene thiapanes which are glycosidase inhibitors; chromen-4-ones; 2,2-dimethyl biphenyl, 6,6, dicarboxylic acid and a Baeyer-Villiger oxidation product and a triarylamine heterohelicene.

The Natural Products quadrone, schizozygine, plumericin, prismatomerin, have been studied. The sex pheromone of the obscure mealybug has also been studied.

Pharmacological chiral molecules including Calcium Channel Antagonists have also been studied. One chiral transition-metal complex: the Chromium tricarbonyl complex of N-pivaloyl-tetrahydro quinoline has been studied.

Several of the chiral molecules whose ACs had been previously determined using Electronic CD (ECD) were proved by VCD to have opposite configurations. So VCD is more reliable than ECD! In addition, one chiral molecule whose AC had been determined using X-ray crystallography was proved by VCD to have an opposite AC.

The utilisation of VCD to determine the stereochemistries of molecules synthesized by asymmetric synthesis, provides understanding of the reactions used.