**Vibrational Circular Dichroism - It's easier than it looks**

Arvi Rauk

Department of Chemistry

University of Calgary

Calgary, Alberta, CANADA, T2N 1N4

**Abstract**

Vibrational Circular Dichroism (VCD) is the equivalent in the infrared region, of electronic circular dichroism (ECD, or CD) in the UV/visible region. The physical basis of VCD is the same as ECD, in that the intensity and sign of the signal are determined by the scalar product of an electric and magnetic dipole transition moment. In VCD the transition is between two vibrational levels of the same ground state vibrational mode while in ECD, the transition is between two electronic states. However, the theoretical description of VCD is complicated by the fact that most molecules have closed shell electronic ground states, and within the Born-Oppenheimer approximation, do not have non-zero magnetic dipole vibrational transition moments. Thus, the theory of VCD takes us beyond the BO approximation to include some coupling between the nuclear and electronic wavefunctions. As it happens, the rather complicated looking theory is rather easy to apply and early frustrations were not due to inability to calculate accurate transition moments, but rather due to a poor description of the vibrational motion itself. The problems went away with the advent of DFT methods that permitted the calculation of accurate forcefields and normal modes. Calculation of VCD spectra is now as routine as the calculation of IR spectra and is implemented in major electronic structure codes such as Gaussian and ADF. This lecture will provide some examples of application of VCD calculations to solve interesting conformational problems.