Experimental and Theoretical Analysis of the Vibrational Absorption (VA), Vibrational Circular Dichroism (VCD), Raman and Raman Optical Activity (ROA) Spectra of Amino Acids and Peptides in Aqueous Solution

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In this work we simulate the vibrational absorption (VA), vibrational circular dichroism (VCD), Raman and Raman optical Activity (ROA) spectra of amino acids and peptides in aqueous solution. The treatment of solvent, both explicitly and implicitly using a continuum model, is shown to be very important in treating amino acids and peptides, where H-bonding is very important. The treatment of the solvent using only the continuum treatment is shown to be inadequate. Finally the simulated VA, VCD, Raman and ROA spectra are compared to the experimental VA, VCD, Raman and ROA spectra of these small molecules and then also used to interpret the spectra of large molecules, for which the spectral simulations are not yet feasible.