Determination of Enantiomeric Excess in Hydrolysis and Epoxidation Reaction by Fourier Transform VCD Spectroscopy : The Comparison of Real-time Reaction Monitoring and Simulation

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The first use of Fourier transform vibrational circular dichroism (FT-VCD) to follow changes in the per cent enantiomeric excess (%EE) of chiral molecules in time using a flow-cell sampling apparatus is reported. FT-VCD, as opposed to dispersive scanning VCD, eliminates the need to scan the VCD spectrum in time to monitor the % EE at more than one spectral location. The first use of partial least squares (PLS) chemometric analysis to determine %EE values from kinetic sets of VCD spectral data is also reported. These two advances have been used to monitor simultaneously changes in the fractional composition and the % EE of a mixture of two different chiral molecules which are Epichlorohydrine and Glycidol. This simulates the progress of the Hydrloysis and Epoxidation reaction from a chiral reactant to a chiral product where the %EE of both molecules can change with time.