

Monitoring Kinetics Using Near Infrared Spectra and Two-dimensional Correlation Spectroscopy

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Near Infrared (NIR) spectra has long been used in industry to monitor rates of reactions via calculation of analyte concentrations. However, the kinetic information is inherent in the data through spectral ratios. Two-dimensional correlation spectroscopy (2D-COS) is a spectral method that is based on changes (e.g. concentration) in time and is therefore uniquely suited for reaction monitoring. This method is especially useful in the understanding of how the reaction(s) proceeds. We will show the application of 2D-COS to synthetic kinetic data from different reaction orders to illustrate the method. We will then show application to real reactions of various orders. Finally, we will illustrate how 2D-COS will be of specific interest to developing optimized industrial reactions.