# Two-dimensional correlation spectroscopy : the power of power spectra.

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Power spectra are a powerful tool provided by two-dimensional correlation analysis. However, this tool is seldom used in practice. This work shows selected examples of using of the power spectra for the study of various kinds of samples with the aim to promote more common use of this tool. By examination of the power spectrum of specific sample, one can estimate the sensitivity of different molecular fragments on a given perturbation. Determination of the power spectra for smaller data subsets provides information on the dynamics of perturbation-induced spectral changes. If the experimental spectra of different samples in the same perturbation window are recorded, the comparison of the power spectra yields information on differences in the sensitivity of various samples on common perturbation. This possibility is particularly useful for studies of the spectra-structure correlations, interactions, and molecular dynamics. A comparison of the power spectra obtained by using different reference spectra provides information on the nature of spectral changes at different wavenumbers.

Słowa kluczowe

Two-dimensional correlation spectroscopy, 2D-COS, power spectrum, reference spectrum, near-infrared spectroscopy, NIR, hydrogen bonding, octyl alcohols, butyl alcohols–water mixtures, reorientation of liquid crystals

Adres publiczny

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