Determination of relative rate of spectral events by novel modification of two-dimensional correlation spectroscopy.

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Sign of two-dimensional (2D) correlation peaks provides information on sequence of spectral events. This information is related to molecular mechanism of changes in a given system. Recently, few papers addressing the problems with interpretation of the sign of 2D correlation peaks have been published. To overcome these problems, a modification of the generalized 2D correlation method has been proposed. This method compares variations in the dynamic spectrum with a linear change at a reference point. The rates of spectral responses at individual wavenumbers are proportional to magnitudes of the peaks in the slice of asynchronous spectrum at the reference point. This way, analysis of complex 2D contour plots is replaced by a simple examination of one-dimensional (1D) slice spectrum. In spite of reduced ability of the resolution enhancement, in special cases the proposed method provides information not accessible from the classical 2D correlation analysis. At first, the principles of this method are shown with the synthetic data. Next, the influence of spectral separation, band width and position changes on the slice spectrum is evaluated. Finally, the proposed approach is applied to the experimental spectra of two hydrogen-bonded systems.

Słowa kluczowe

2D correlation spectroscopy, Rate of spectral events, Simulated spectra, Hydrogen-bonded systems

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