



Two-dimensional correlation analysis of hydrogen-bonded systems: basic molecules.

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Streszczenie

This review provides information on application of two-dimensional (2D) correlation spectroscopy to studies of the molecular structure and hydrogen bonding in basic molecules and their binary mixtures with water. The first part of this review is an introduction to 2D correlation analysis and includes detailed description how to calculate the synchronous and asynchronous spectra from the raw experimental data. An appropriate pretreatment is widely discussed and the MATLAB codes to perform these operations are given. In the second part, the applications of 2D correlation spectroscopy for explorations of basic molecules like aliphatic alcohols, N-methylacetamide (NMA), diols, amino alcohols, carboxylic acids, and water in the pure liquid phases are reviewed. Finally, the 2D correlation studies of binary mixtures of basic molecules with water are discussed. It has been shown that an application of 2D correlation analysis to the complex spectra makes it possible to obtain the information not readily seen in the original data.

Słowa kluczowe

Two-dimensional correlation spectroscopy, hydrogen bonding, Molecular structure, basic molecules, binary mixtures with water, near-infrared spectroscopy, infrared spectroscopy

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