Interpretation of two-dimensional correlation spectra: science or art.

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Streszczenie

It has been shown that the most common perturbations of conventional (one-dimensional) spectra such as random noise, baseline fluctuations, band position, and width changes may complicate two-dimensional (2D) correlation spectra, sometimes making them completely useless. In addition, two different physical causes may generate similar patterns for the synchronous and asynchronous spectra. Some of these effects, such as random noise and baseline fluctuations, can be eliminated from the input data, and one can recover the original appearance of 2D correlation spectra. The other effects, such as the frequency shift and bandwidth variation, cannot be removed from the experimental spectra. In this instance, the number and position of the correlation peaks can be elucidated by simulation studies. This report presents a few examples of typical patterns found in the synchronous and asynchronous spectra affected by those perturbations. Long streaks in 2D correlation spectra reveal extensive baseline fluctuations in the original data set. A simple offset often significantly reduces the extent of this effect. When no reasonable baseline correlations can be performed, the second derivative may solve this problem. In most cases, the perturbation-averaged spectrum is recommended as a reference. However, it has been proved that the calculation of 2D correlation spectra without any reference spectrum may also provide useful information, especially for data heavily influenced by noise or baseline fluctuations. In the majority of real-world systems, the spectral changes are a continuous function of applied perturbation. Thus, 2D correlation spectra yield information about the relative rate of intensity variations rather than the sequence of spectral events.

Adres publiczny

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