Resolution enhancement of overlapping peaks in molecular spectra by derivative spectrometry method based on continuous wavelet transform

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Abstract

In this paper we consider a numerical differentiation algorithm based on the continuous wavelet transform for improving resolution of composite spectra. This approach provides the best contrast in differential curves as compared to the conventional derivative spectrometry. A main merit is that the wavelet-based technique gives stable estimations of derivative without using the regularization and on the other hand, it does not make peak shift. A comparative study of conventional derivative spectrometry based on the statistical regularization method and wavelet-based derivative spectrometry is made. Examples of the application of these for improving resolution of synthetic composite bands and real-world composite ones coming from molecular spectroscopy are given.

Keywords

Continuous wavelet transform, Derivative spectrometry, Resolution enhancement