



Resolution enhancement in second-derivative spectra.

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Streszczenie

Derivative spectroscopy is a powerful tool for the resolution enhancement in infrared, near-infrared, Raman, ultraviolet-visible, nuclear magnetic resonance, electron paramagnetic resonance, and fluorescence spectroscopy. Despite its great significance in analytical chemistry, not all aspects of the applications of this method have been explored as yet. This is the first systematic study of the parameters that influence the resolution enhancement in the second derivative spectra. The derivative spectra were calculated with the Savitzky-Golay method with different window size (5, 15, 25) and polynomial order (2, 4). The results obtained in this work show that the resolution enhancement in the second derivative spectra strongly depends on the data spacing in the original spectra, window size, polynomial order, and peak profile. As shown, the resolution enhancement is related to variations in the width of the peaks upon the differentiation. The present study reveals that in order to maximize the separation of the peaks in the second derivative spectra, the original spectra should be recorded at high resolution and differentiated using a small window size and high polynomial order. However, working with the real spectra one has to compromise between the noise reduction and optimization of the resolution enhancement in the second derivative spectra.

Adres publiczny

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