

Determination of integrated intensities of overlapped IR bands by curve-fitting, Fourier self-deconvolution and a combination of both methods.

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Streszczenie

Curve-fitting, Fourier self-deconvolution, and a combination of these methods have been applied to determine integrated intensities of the bands arising from the C=O stretching mode of *n*-octanoic acid. When these bands are separated by more than an average band width, the most reliable results are supplied by curve-fitting. However, simple functions (Gauss or Lorentz) do not satisfactorily describe shapes of experimental bands, and more complex profiles should be used such as the sum or product of the Gauss and Lorentz functions or their convolution (Voigt profile). The applied Fourier self-deconvolution procedure assumes Lorentzian band shapes; therefore the determined intensities of the bands that deviate from this profile are always higher than the true values. An analysis combining the two methods mentioned above did not improve the results. The output bands from curve-fitting, with a high Lorentzian fraction, might have overestimated the band areas. Thus, the integration should be done over a limited wavenumber range. Our results clearly show that the band-shape function plays an important role during the determination of the integrated intensities using curve-fitting, Fourier self-deconvolution or a combination of both methods (referred to in this paper as the "combined method").

Słowa kluczowe

Curve-fitting, Fourier self-deconvolution, Integrated intensities, *n*-Octanoic acid

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