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Spectral line shape identification by using fractional derivative spectrometry

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Abstract

Before it is difficult to say about a peak shape without conducting additional research. Conventional nonlinear fitting methods based on the OLS approach are unsuitable to unambiguously assign the overlapped peaks. This implies that a composite band can be decomposed into elementary components of a given shape with the same integral reconstruction error with a large number of ways. A main drawback of this approach is the high variance of the spectral parameters to be estimated. This is due to the overlapping of individual components, which leads to the ambiguous fitting. In this paper we develop a simple mathematical tool in terms of fractional derivative (FD) to determine the overlapping peaks spectral parameters. It is possible due to several positive effects of FD connected with the behavior of its zero-crossing and maximal amplitude. For acquiring a stable and unbiased FD estimate we utilize the statistical regularization method. Along with the well-known distributions such as Lorentzian, Gaussian and their linear combinations the Tsallis distribution is used as a model to correctly resolve overlapped peaks. As exhaustive examples demonstrating a power of the method we estimate unresolved bands spectral parameters of synthetic and experimental infra-red spectra.

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Keywords

Derivative spectrometry, Fitting, Fractional derivative, Overlapping peaks