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Sophisticated algorithms of analysis of spectroscopic data

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The accuracy and reliability of the analysis of spectroscopic data depend critically on the treatment in order to resolve strong peak overlaps, to account for continuum background contributions, and to distinguish artifacts to the responses of some detector types. Analysis of spectroscopic data can be divided to
1. estimation of peaks positions (peak searching)
2. fitting of peak regions.
One of the most delicate problems of any spectrometric method is that related to the extraction of the correct information out of the spectra sections, where due to the limited resolution of the equipment, the peaks as the main carrier of spectrometric information are overlapping. Conventional methods of peak searching based usually on spectrum convolution are inefficient and fail to separate overlapping peaks. The deconvolution methods can be successfully applied for the determination of positions and intensities of peaks and for the decomposition of multiplets. Several deconvolution algorithms are studied and and their efficiences compared in the contribution.
However before the application of deconvolution operation we need to remove the background from spectroscopic data. One of the basic problems in the analysis of the spectra is the separation of useful information contained in peaks from the useless information (background, noise). In order to process data from numerous analyses efficiently and reproducibly, the background approximation must be, as much as possible, free of user-adjustable parameters. Baseline removal, as the first preprocessing step of spectrometric data, critically influences subsequent analysis steps. The more accurately the background is estimated the more presicely we can estimate the existence of peaks. In the contribution we present a new algorithm to determine peak regions and separate them from peak-free regions. Subsequently it allows to propose a new baseline estimation method based on sensitive non-linear iterative peak clipping with automatic local adjusting of width of clipping window. Moreover automatic setting of peak regions can be used to confine intervals of fitting and to fit each region separately.

Primary author: MORHAC, Miroslav (Institute of Physics, Slovak Academy of Sciences)

Presenter: MORHAC, Miroslav (Institute of Physics, Slovak Academy of Sciences)

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