Influence of spectral resolution, spectral range and signal-to-noise ratio of Fourier transform infra-red spectra on identification of high explosive substances

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Influence of spectral resolution, spectral range and signal-to-noise ratio of Fourier transform infra-red spectra on identification of high explosive substances

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Abstract

In the contemporary spectroscopy there is a trend to record spectra with the highest possible spectral resolution. This is clearly justified if the spectral features in the spectrum are very narrow (for example infra-red spectra of gas samples). However there is a plethora of samples (in the liquid and especially in the solid form) where there is a natural spectral peak broadening due to collisions and proximity predominately. Additionally there is a number of portable devices (spectrometers) with inherently restricted spectral resolution, spectral range or both, which are extremely useful in some field applications (archaeology, agriculture, food industry, cultural heritage, forensic science). In this paper the investigation of the influence of spectral resolution, spectral range and signal-to-noise ratio on the identification of high explosive substances by applying multivariate statistical methods on the Fourier transform infra-red spectral data sets is studied. All mathematical procedures on spectral data for dimension reduction, clustering and validation were implemented within R open source environment.

Keywords: FTIR spectroscopy, R Environment, resolution, synchrotron radiation

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