Substance identification algorithm by a set of secondary radiation spectra

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This paper is concerned with spectroscopy, specifically with problem of definition of substances by their spectra. The main goal is to increase selectivity and reliability of substances express analysis methods. It is suggested to use several spectra of similar or different nature simultaneously. Optimal algorithm of spectra set analysis is determined. The reason is to identify experimental spectra by known spectra in data base. It is suggested to extend least squares algorithm to provide method that uses several spectra. To provide equal use of several spectra the normalization by detected spectra or known spectra is suggested. On the basis of proposed objective function the classifier is obtained. New method is approved on the basis of visible and near ultraviolet range static Fourier spectrometer. ROC-analysis is applied to check method effective. Thus the best modification of the method is determined. Results can be applied to increase selectivity and reliability of devices that provide chemical express analysis.

Keywords: *spectroscopy, substance identification, chemical monitoring, ultraviolet spectra, least squares method, classification problem, ROC-analysis.*

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