

Abstract

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Classification of synthetic organic pigments by multivariate data analysis of FTIR spectra.

For the identification of pure synthetic organic pigments Fourier Transform Infrared (FTIR) spectroscopy has been established as a powerful analytical technique. Usually the identification of such pigments by FTIR is processed by comparing the spectrum of an unknown sample with the spectra present in a database. Those samples are difficult to be identified if they don't match with one of the library spectra, and even class assignments can be performed by experts' analysis only.

In this paper an approach is presented to facilitate classification of organic pigments by multivariate statistical analysis of their FTIR spectra. Partial least-squares discriminant analysis (PLS-DA) was applied to the pigments FTIR spectra, using 11 binary y -variables for pigment class definition.

The threshold of the discriminant variable \hat{y} could be optimized for each class. It is shown that application of the classification models to FTIR spectra of unknown paint samples gained very similar results as obtained from experts.