

Abstract

# Multivariate Analysis as a Tool to Identify Concentrations from Strongly Overlapping Gas Spectra <sup>†</sup>

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Multivariate analysis (MVA) was introduced in the early 20th century and first applied in psychology under the name of Multiple Factor Analysis (MFA). It is based on principle component analysis (PCA) and can be of great use in other research fields as well. MVA results in a reduction of unnecessary data, thereby reducing the error and simplifying further processing. The method of Partial Least Square Regression (PLS) can be applied after PCA to link the measured data with target values.

In this work, we will apply MVA on spectroscopic data of gas mixtures in the Mid-IR in order to calculate the concentrations of compounds with strongly overlapping absorption spectra. This is a common challenge in broadband spectroscopy. Photoacoustic spectroscopy (PAS) in the wavelength region of 3200 nm to 3500 nm serves as an example detection technique. We will apply the analysis to measurements of different organic compounds and show the possibilities offered by MVA. After preprocessing of the raw photoacoustic data, approximately 1300 equally spaced wavelengths are selected. PCA is used to reduce the whole spectrum to only a few Principle Components (PC) and afterwards PLS regression serves to recalculate the spectra and determine concentrations.



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