

Raman spectroscopy coupled to Blind Source Separation Methods for deformation of surfactant mixtures

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Cleaning products and laundry detergents market has been constantly growing for several years. The legislative context and consumer's expectations require more environmentally friendly products. To ensure the product quality and composition, qualitative and quantitative analysis methods are thus required. However, laundry detergents contain up to 25 compounds which makes sample preparation and analysis difficult.

In this study, we focused on surfactant identification and quantification. These compounds represent the main part of detergent formulation with percentage up to 40%. Four surfactants classically used in laundry detergents were thus mixed to obtain 29 different mixtures. Samples were analyzed by Raman spectrometry. Three criteria were taken into account for Raman spectroscopy choice: little sample preparation, fast analyses and insensitivity to water in our mixtures. To identify and quantify each surfactant, two blind source separation (BSS) methods were evaluated on the acquired Raman spectra. The two BSS methods were Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS) and Independent Component Analysis (ICA). According to a design of experiments (DOE), influence of spectra preprocessing methods was investigated, as they can impact the predictive power of BSS methods. First results were quite satisfying. Raman analyses coupled to BSS methods are really interesting in the case of surfactant mixture deformation. These promising results allow expecting surfactant identification and quantification from real detergent samples.

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