



Vibrational spectroscopy with handheld instruments: State-of-the Art Instrumentation, Applications and Future Aspects

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INTRODUCTION

Fourty years ago Raman and FT-IR spectrometers almost occupied a separate room and NIR spectrometers were just about to quit the phase as add-ons to UV-VIS or IR spectrometers, respectively, and appear as stand-alone instruments. The following four decades were characterized by a multiplicity of exciting hard- and software developments for vibrational spectroscopy but apart from opening the lab to the process by the introduction of light-fiber optics, special probes and chemometric evaluation routines the techniques remained a domain for scientists. In contrast, the development of miniaturized, handheld instruments has not only led to a further extension of the range of applications by on-site and in-the-field measurements but also shows promise that these instruments may in the future be used by non-traditional user environments.

EXPERIMENTAL AND INSTRUMENTAL

The presentation will provide an overview on the latest instrumental developments of handheld spectrometers, discuss the pros and cons of the different techniques and will highlight the advantages of on-site measurements by means of selected application examples with the focus on near-infrared spectroscopy.

RESULTS AND DISCUSSION

The discussed application examples range from the on-site measurement and quantitative characterization of geological rock samples via classification of polymers for recycling purposes to the authentication of food and pharmaceuticals and should serve as guide lines for the implementation of handheld spectrometers as routine tools. Finally, the transfer of spectra that have been measured on two different laboratory FT-NIR spectrometers to the format of handheld instruments by measuring only a few samples with both spectrometer types will be demonstrated. Thus, despite the extreme differences in spectral range and resolution, data sets which have been collected and calibrations which have been developed thereof, respectively, over a long period on a

laboratory instrument can be conveniently transferred to a handheld system without the requirement for elaborate complete rescanning and recalibration of spectra.