BRAVO –
Advanced Data Acquisition and Evaluation in Handheld Raman Spectroscopy

The main benefit of handheld spectrometers is that the instrument itself can be taken to the sample and thus can be employed for various applications with high degree of flexibility. For routine applications like materials identification and verification, it is highly desirable to have as many functions as possible automated. A good example is the quality control of incoming goods using handheld Raman spectrometers, which allows analyzing materials directly through packaging[1].

There are also always many advanced applications where the instrument requirements will be user or application dependent. Previously most small handheld Raman systems lacked the flexibility to allow the user to optimize the data collection for the desired analysis. The handheld Raman spectrometer BRAVO features an advanced operation mode via remote control utilizing Bruker's comprehensive spectroscopy software OPUS. The remote control is accomplished via Wi-Fi or an Ethernet connection using a docking station. Consequently, in any case where a mobile or handheld instrument needs to be run untethered to electrical power supply, and has to require flexible data acquisition BRAVO is a very powerful solution.

With BRAVO there is the direct option to initiate measurements from the OPUS software and to subsequently run user defined evaluation processes. In addition, it is possible to set parameters such as integration time and number of co-added measurements manually. The settings can be stored in experiment files which can be assigned to a user or specific application.

What possibilities are coming up?

BRAVO measures Raman spectra in a quality typically only obtainable from powerful benchtop spectrometers[2]. This means that acquired spectra can be used for any kind of evaluation such as quantification or complex identification methods. At this stage, not only the mathematically processed data used for on board verifications based on the Sequentially Shifted Excitation (SSE™) method is available but also the raw data resulting from each laser excitation is accessible, which is often preferred for scientific applications[3].

The spectroscopy software suite OPUS combines a wide range of functionality for analytical and research applications with an intuitive design and highest degree of flexibility. Furthermore, additional software packages are available to meet the needs of specific applications[4]. The following examples provide insight into the many possibilities based on the remote control option and comprehensive OPUS spectroscopy software.

OPUS SEARCH

The OPUS SEARCH package is an advanced library searching tool capable of mixture analysis and represents a typical approach to identify the spectra of unknown materials. A typical example is given in Figure 1. Libraries can be setup by the user and many comprehensive databases are available. Typical applications include forensic investigations, detection of hazardous, materials characterization in the industrial environment, and analysis of objects in the field of art and cultural heritage[5].

OPUS IDENT

The OPUS IDENT package is an excellent comprehensive tool for reliable identification of raw materials, intermediates and finished products offering the highest flexibility for method setup. The combination of user defined data pre-treatment, selection of various methods for data evaluation and control of many more parameters make it the ultimate easy-to-use program for dedicated quality control solutions. Figure 2 shows the example of the differentiation of very similar oil samples using principle component analysis.

OPUS QUANT

OPUS QUANT is a state-of-the-art software package for setting up and validating quantification models utilizing advanced PLS based methods. Analogous to the setup of an IDENT method, the user is guided step-by-step in generating the quantification models. In Figure 3, an example of a calibration is given to determine the relative anhydrite content in gypsum.

Fig. 2: 3D score plot of an IDENT analysis of similar oil samples measured with the BRAVO. The colored spheres represent the areas in which the identification was successful, respectively. Very similar materials (yellow and blue spheres) can be addressed in sub libraries or assigned to one class.

Fig. 3: Calibration model for the relative anhydrite content in gypsum based on the evaluation of the symmetric SO_4 vibration.
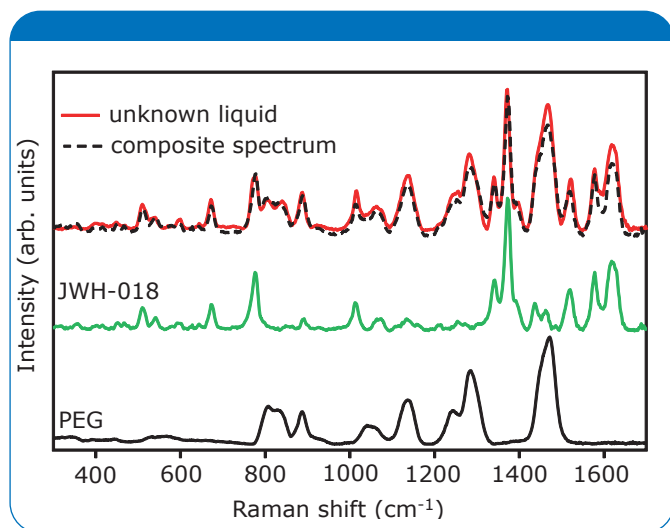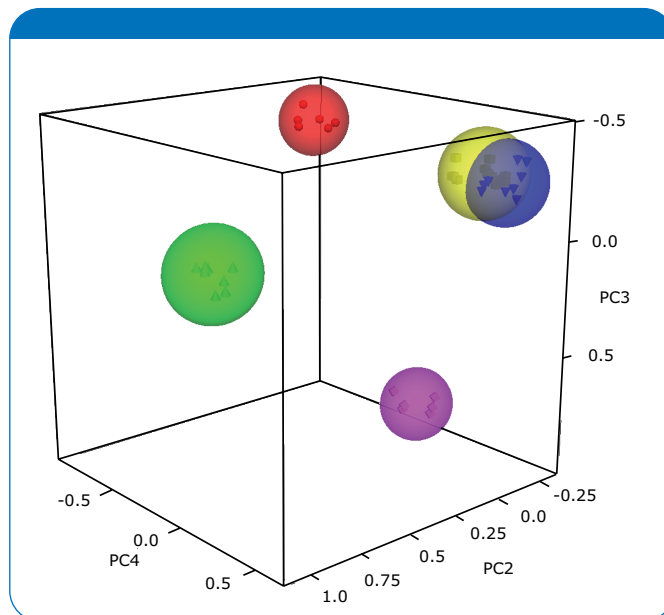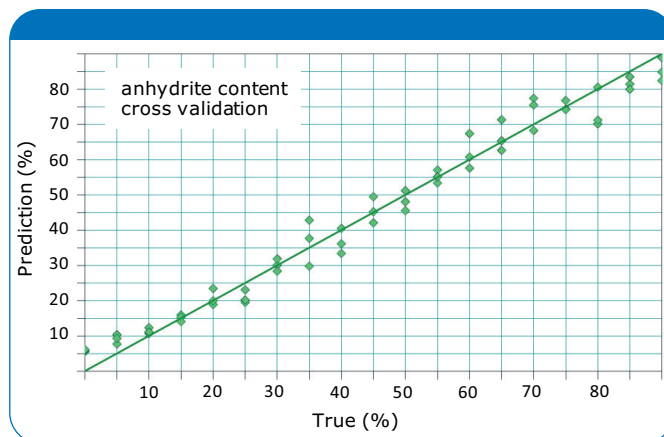

Figure 1: Example of the analysis of an unknown liquid (red spectrum). The mixture analysis based on the analysis of multiple libraries reveals the presence of two materials, polyethylene glycol (PEG) and the synthetic cannabinoid JWH-018. The calculated composition spectrum (dashed line) matches the query spectrum.

References
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[5] Conti et al., Portable Sequentially Shifted Excitation Raman spectroscopy as an innovative tool for in situ chemical interrogation of painted surfaces, Analyst (2016)