BRUKER

Forensic Analysis

● Gathering Evidence by IR and Raman Spectroscopy

Innovation with Integrity

FT-IR

Forensic Sciences apply Infrared and Raman spectroscopic methods for many years to analyze all types of unknown samples. These methods are proven to reveal the chemical composition of material suspected to be illicit or dangerous within seconds.

Microspectroscopy even allows to identify small pieces of trace evidence and to provide insight into the structure of complex samples like paint chips.

Bruker Optics offers suitable solutions for typical analytical questions in Forensics. This covers devices for micro- and macroscopic samples, for dedicated use or with flexibility for a broader range of applications.

- **Identification of Illicit Substances:**
  - Drugs
  - Explosives
  - Hazards

- **Determination of the Chemical Composition of Trace Evidence:**
  - Fibers
  - Particles
  - Paint chips

- **Detection of Forgery:**
  - Counterfeit money
  - Document falsification
  - Art forgery

Identifying the Unknown

Forensic science has to analyze samples that are challenging with regards to their diversity, composition and size. Typical sample types are illicit materials like drugs and explosives, trace evidence found at a crime scene like fibers or paint chips, and documents suspected to be counterfeit.

A high percentage of the seized drug samples are laced and therefore difficult to identify, new drug substances appear almost monthly and the amount of different substances is innumerable. Furthermore, many samples like fibers are microscopically small and cannot be analyzed by conventional means.

For all of these different substance classes and sample types IR-spectroscopy is a powerful tool that can identify an unknown sample in just a few seconds. Very complex samples like laced drugs or so called legal highs can be identified with dedicated spectral libraries and powerful tools like mixture analysis. With FT-IR microscopy, it is even possible to identify samples in the micrometer range and to analyze the individual components of a multi-layered paint chip.

Raman spectroscopic analysis of forensic samples provides complementary information to the obtained IR-results. While infrared spectroscopy allows to measure virtually any type of sample the particular strength of Raman is its higher specificity for certain substances. Furthermore Raman allows non-invasive measurements in vials and depth-profiling analysis of structured materials. These features make the method quite powerful for identifying pigments and for analyzing suspect material inside a glass vial or plastic packaging.

Infrared Spectroscopy

The IR-spectrum of any sample reflects its molecular composition – just like a chemical fingerprint (figure 1). Both, organic and inorganic chemical components contribute to the sample spectrum. Therefore the IR-method is very suitable to identify both pure compounds and complex materials. Furthermore the quantification of individual components inside the analyzed material is feasible.
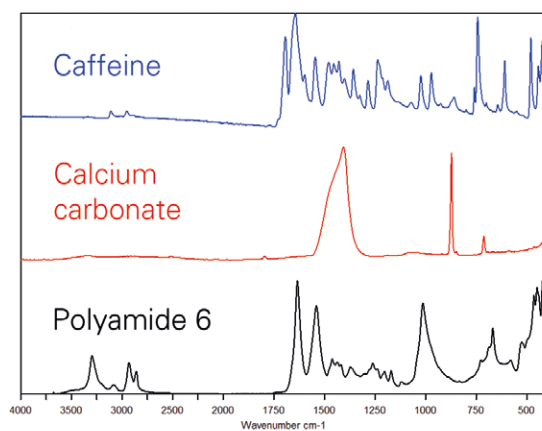

Fig.1: The IR-spectrum is a chemical fingerprint that allows identification of organic, inorganic and polymeric materials.

For most samples the FT-IR analysis is performed without sample preparation and without the need of any consumables. Measurement times are typically below 1 minute.

Prepared to Keep Track

Drug Analysis: Increasing Complexity

Suspected drug material has to be identified both in forensic laboratories but also in the field e.g. at known drug trading areas, clubs or music festivals. Accordingly the analysis might not only be performed by forensic scientists but also by law enforcement, security and safety organizations. This is a challenging task since the number of psychoactive substances is steadily increasing (figure 3). So called legal highs and "research chemicals" are derivatives from illicit drugs in order to bypass existing bans. Moreover, drugs are often laced to optimize profits or to combine the effects of certain active ingredients.

Fig. 2: ALPHA-P FT-IR spectrometer.

The ALPHA has proven to generate reliable results and therefore been accredited by CAST (Centre for Applied Science and Technology in the UK) for the identification of Ketamine and Mephedrone.

Example: Analysis of a Street Sample

The free base of cocaine, called "crack" is only rarely available as a pure product. Figure 4 shows the mixture analysis of a real street sample that was measured with the ALPHA-P. It is obvious from the mixture analysis result, that the sample is also laced with the local anesthetic benzocaine. Additionally, there is a considerable amount of the pain reliever acetophenetidine (phenacetine) detectable that acts as a mild mood enhancer and is, due to its renal toxicity, also forbidden in most countries.
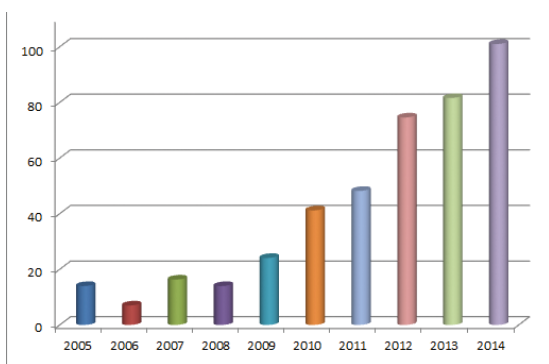
Fig. 3: EMCDDA reported number of new psychoactive substances discovered in Europe.

System for Substance Identification

The compact and rugged ALPHA-P FT-IR spectrometer (figure 3) is very suitable to quickly identify unknown substances irrespective of visual appearance or form. A full analysis takes less than a minute, including sampling, measurement and data evaluation. Due to simple handling, a clear software guided workflow and automated data evaluation the ALPHA can be operated by inexperienced users. For measurement the sample just needs to be pressed on the diamond ATR-crystal. After the measurement the sample's infrared spectrum is automatically matched to a database, just like identifying a human fingerprint.
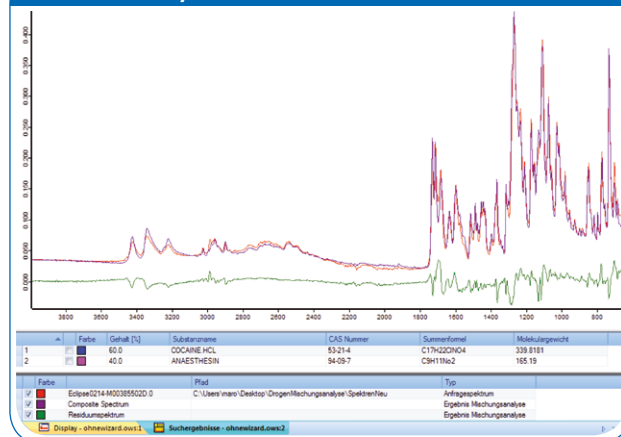
Fig. 4: Result of the mixture analysis of a street drug sample. The measure spectrum (red) is in high accordance with the composite spectrum (violet) which is the sum of cocaine base and lacing substances. The residual spectrum (green) shows the remaining spectral difference.

Explosives: Fast Identification

Explosives and their precursor substances need to be identified when suspect material is found in the public, during a house search or in security screenings at airports and borders. As is the case with drugs, there are also numerous substances and possible mixtures. For traces of explosive residues, ion mobility spectroscopy is the method of choice due to its outstanding sensitivity. When it comes to the analysis of visible amounts of any sample, FT-IR spectroscopy is much better suited, since it will provide information that is more specific and detailed. As an example, figure 5 shows the identification of a plastic explosive. The sample was identified as "NSP711", which is a plastic explosive based on 86 % PETN and 14 % plasticizer.
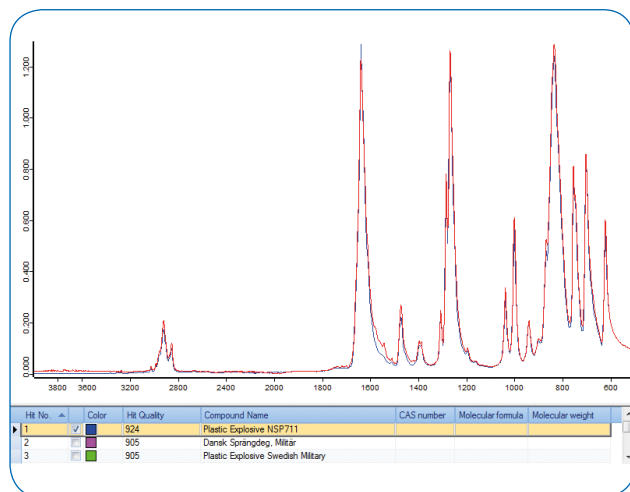

Fig. 5: Identification of a sample as plastic explosive.

Spectral Databases

To be able to identify any unknown material comprehensive spectral databases are required. Bruker's ATR-FT-IR-COMPLETE library containing >26.000 spectra allows to determine the type of almost any material. Combined with specific libraries that are dedicated to drugs and explosives a very high identification power is achieved both for illicit substances and material that might be mistaken to be illegal or dangerous.

Bruker and TICTAC Communications Ltd offer a dedicated spectral library for new drugs, new psychoactive substances (NPS) and legal highs that enter the drug market. This library constantly is expanded by new drugs entering the market and regular updates are released.

Options for Mobile Use

Due to its small footprint the ALPHA is very suitable for use in mobile laboratories. The instrument can be powered by 12V from a car's cigarette lighter receptacle or using truck on-board voltage (24V). A rechargeable battery pack can be attached to the ALPHA with a dedicated transport panel and provides up to 8h of energy supply. With a tablet PC that can be attached on top of the instrument and a wireless connection adapter, it is possible to operate the ALPHA without disturbing cables or heavy computer hardware.

Fig. 6: The compact dimensions of the ALPHA allow easy transport. Independent operation is possible using mobility options like a battery pack and Wifi control.

Unveiling Trace Evidence

Analyze the Smallest Samples

Microspectroscopic methods have gained increasing popularity in forensic laboratories and are well-established for the analysis of samples that are too small or complex to be measured in a standard spectrometer. With FT-IR and Raman microscopy, it is possible to obtain spectra of extremely defined parts of the sample down to the micrometer range. As a result, only a very small amount of sample is required. By using the automated mapping feature, it is also possible to create two dimensional chemical images that visualize the distribution of chemical components in the sample. This feature is particularly helpful for the investigation of multi layered samples like for instance paint chips.

Identification of Fibers and Particles

Fibers and particles found at the crime scene can provide information about the criminal, e.g. about his clothing or specific places he has visited. Furthermore such traces might be compared to similar items retrieved from suspects and provide the link to the crime. Figure 7 shows the analysis of five different fiber samples that were measured and identified with the FT-IR microscope LUMOS. All the fibers are very thin with a diameter of about 25 µm and thus it is not possible to measure them with a macroscopic ATR unit. The polymer type was determined by a library search in the comprehensive ATR-FT-IR-COMPLETE-library. Even though the visual appearance of the fibers is very similar, only two of the fibers are made from the same polymer.
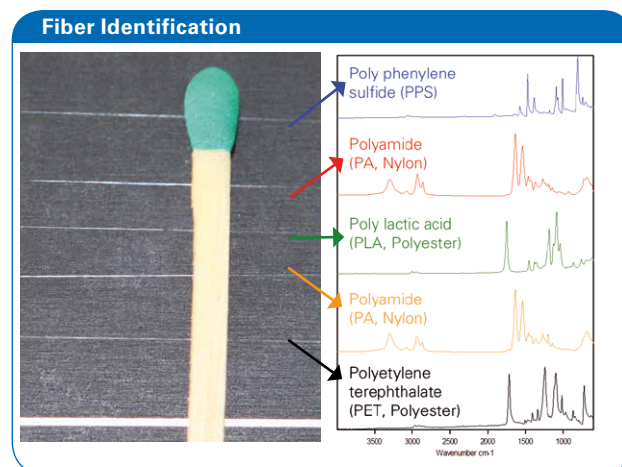

Fig. 8: LUMOS FT-IR microscope.

FT-IR Microscopy Made Easy

The LUMOS FT-IR microscope (figure 8) is an all in one solution with an integrated spectrometer, a high degree of motorization and a dedicated user-interface. Its 8x objective provides the measurement modes ATR, transmission and reflection with high quality visual inspection capabilities. The innovative motorized Attenuated Total Reflectance (ATR) crystal allows performing the complete measurement procedure fully automated including background and sample measurements. A high working distance and the unobstructed access to the sample stage facilitate an easy positioning of the sample. Its large field of view of 1.5 x 1.2 mm and the high depth of focus make sample inspection very comfortable. In combination with a motorized stage, fully automated mapping measurement can be performed.

The dedicated OPUS Video-software is guiding the user through the whole measurement procedure and always provides the most suitable functions for the current measurement step. Also, the complete data evaluation is performed using the OPUS spectroscopic software. For identification of sample components spectrum search and mixture analysis are applied using the functionality of the OPUS/SEARCH package.

Fiber Identification

Fig. 7: Synthetic fibers on sampling plate and according spectra (right).

Structure of Paint and Varnish Chips

Pieces of car varnish are valuable trace evidence in case of hit and run accidents. By determination of the used materials it is possible to identify the car model involved in the accident. Also, when investigating potential art forgery the analysis of paint samples is required.

Analysis of Individual Layers in a Paint Sample

The IR-microscopic analysis of individual layers in a paint sample was performed using the ATR-technique. Measurement positions and the dimension of the measured area were defined individually for each layer. The measurement procedure including setting of the knife edge aperture was performed completely automated by the LUMOS.

Figure 9 shows the visual microscopic image of the paint sample with the corresponding spectra of four layers. The color coding of the measurement spots is according to the shown spectra. All layers, including the two white layers can be clearly distinguished by means of their spectra.
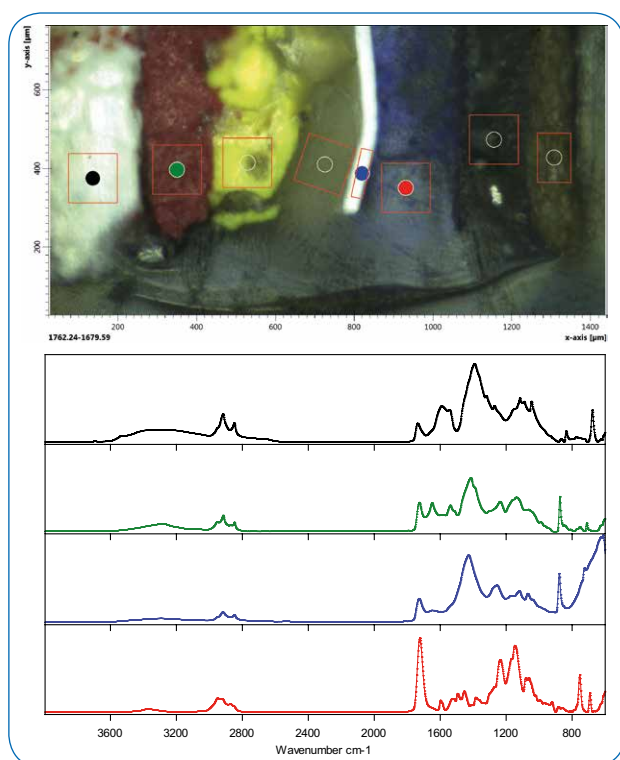

Fig. 9: Multilayered paint chip with indication of measurement positions and knife edge aperture settings. The color coding of the measurement spots corresponds with the color of the shown spectra.

Chemical Imaging of a Varnish Sample

By measuring regular grits of spectra in a defined sample area it is not only possible to identify individual components but also to determine their distribution. The result of such measurements are chemical images that show the content of a certain component in false colors superimposed with the visual microscopic image. The acquisition of spectra in a defined sample area can be performed by sequential measurement using a physical aperture that defines the obtained spatial resolution (mapping). A much increased speed of the analysis and an even higher spatial resolution can be achieved by using a microscope equipped with a Focal Plane Array (FPA) detector. The HYPERION 3000 is an imaging microscope that utilizes FPA detectors with up to 128 x 128 detector elements with each element generating a single spectrum.

As an example, the analysis of a four-layered varnish chip is shown in figure 10. Using the HYPERION 3000 an area of 340 x 340 µm was measured with a pixel resolution of 2.7 µm. The total acquisition time for the measurement of altogether 16384 spectra was 3 min at a spectral resolution of 4 cm^{-1}.
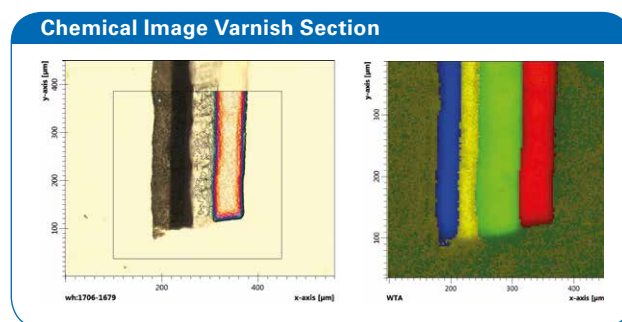
Chemical Image Varnish Section

Fig. 10: Left: Visual image and false color plot of the 4-layer varnish chip with the intensity distribution relating to the white layer. Right: Distribution of all varnish layers displayed in a WTA-plot.

The chemical image in figure 10 visualizes the intensity distribution of a spectral feature that is specific for the white layer. In order to combine all the different components in one image, a WTA-image was created (figure 10 right). The WTA model assigns the color of the dominant component to each individual image pixel thereby allowing displaying several components in one picture.

Unmask Counterfeits & Forgery

Falsification of Documents

FT-IR and Raman microscopy can help to detect cases of falsification of documents. Typical questions are the determination and characterization of inks on the document and the order in which they have been applied.

In figure 11 a document is shown where the number three was subsequently changed with another ball-pen of the same color into an eight. By automated FT-IR microspectroscopic mapping of a grid of 32 x 26 measurement points the complete number was analyzed. In the resulting spectra a band was detected that is only present in the left part of the number. This result is visualized in figure 11 where the chemical image resulting from this band is projected over the visual image. Since only the high intensity values are shown in color and all the other areas remain transparent, one can easily see the different chemical composition of the two halves of the eight.
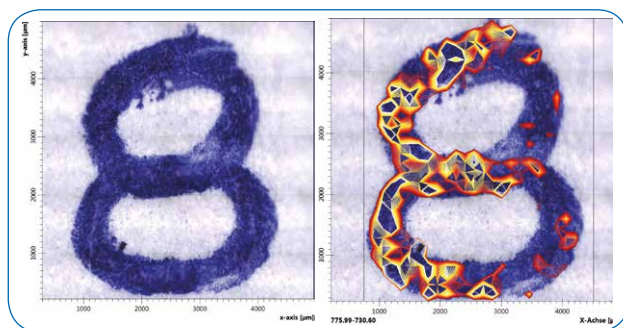

Figure 11: Visual image (left) and overlaid chemical image (right) of the forged eight.

Art Forgery

The investigation of an potentially forged art objects includes the judgement of art historians about plausibility of style and craftsmanship as well as the analysis of used materials by forensic methods. IR and Raman spectroscopy give insight into the range of chemical compounds that were used to create a certain piece or art and allow to compare these findings with the artistic materials that actually were available in the time of origin. Raman microspectroscopy is extremely powerful to selectively identify individual colors in paintings, particularly inorganic pigments. Moreover, it is very attractive as the analysis can be performed contact-free directly on the sample. Figure 12 shows the Raman spectra of a variety of pigments used in an ancient Nepalese painting. The measurements were performed with the SENTERRA Raman microscope setup as "open architecture" system that allows to analyze even very large samples.
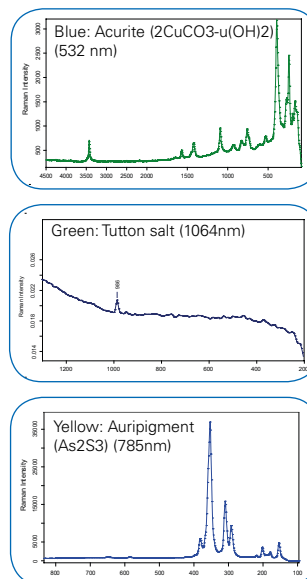

Figure 12: Determination of pigments used in an ancient Nepalese painting by the SENTERRA Raman microscope.

Reliable Raman Micro-Spectroscopy

The SENTERRA is a high performance Raman microscope spectrometer designed for demanding analytical applications in both - the R&D and routine laboratory. Its most important innovation is certainly the continuous calibration method, as it ensures highes wavenumber accuracy without the need for calibrations with external standards. Due to a very compact design the SENTERRA´s beam path is short resulting in a high sensitivity and stability.

Counterfeit Money

Materials used in paper currency, like fibers, inks and polymeric coatings can be characterized using IR and Raman spectroscopy. This "chemical fingerprint" can be utilized to detect suspected counterfeit money.

Bruker Optics is ISO 9001 and ISO 13485 certified.

Laser class 1

Technologies used are protected by one or more of the following patents: DE 102004025448; DE 19940981; US 5923422; DE 19704598