



Application Note AN-RS-001

Identifying polymers with Raman spectroscopy

Rapid, nondestructive determination of colored plastics

Despite its precision in analyzing polymers, Raman spectroscopy struggles to accurately identify colored plastics due to fluorescence interference from pigments and additives. Polymer identification results may be less reliable under these conditions.

Utilizing multiple excitation wavelengths, comprehensive reference libraries, and employing advanced techniques all improve the reliability of Raman analysis. Metrohm's Raman solutions

encompass all of these capabilities and provide fast, accurate polymer identification. This Application Note focuses on Metrohm's advanced XTR® technology which improves identification of substances by eXTRacting the Raman signal from spectra with strong, occluding background fluorescence. Several types of colored polymers are examined, showing the benefits of using 785 nm Raman spectroscopy with the novel XTR fluorescence rejection technique.

This Application Note describes the identification of poly(ethylene-vinyl acetate) – also known as PEVA, polystyrene (PS), and polypropylene (PP) in colored plastics with Raman spectroscopy.

Measurements with the handheld MIRA XTR Raman

spectrometer require no sample preparation and provide immediate and unambiguous results. Rapid and nondestructive determination takes place through application of the XTR algorithm followed by an automated library search.

All spectra were measured using MIRA XTR, at a wavelength of 785 nm and with Orbital Raster Scan (ORSTM), in auto-acquisition mode. Occluding fluorescence initiates XTR algorithms automatically, returning a high-resolution, baselined spectrum of the material.

All samples in this study were common household and office materials, tested through direct contact

using the intelligent Universal Attachment (iUA).

Metrohm's Illicit and General Chemicals Library is a comprehensive spectral database of common materials for accurate identification of mixed samples. Each sample was identified using this library in MIRA Cal software. A range of polymer standards is displayed in **Figure 1**, illustrating their distinct fingerprints in the Raman spectrum.

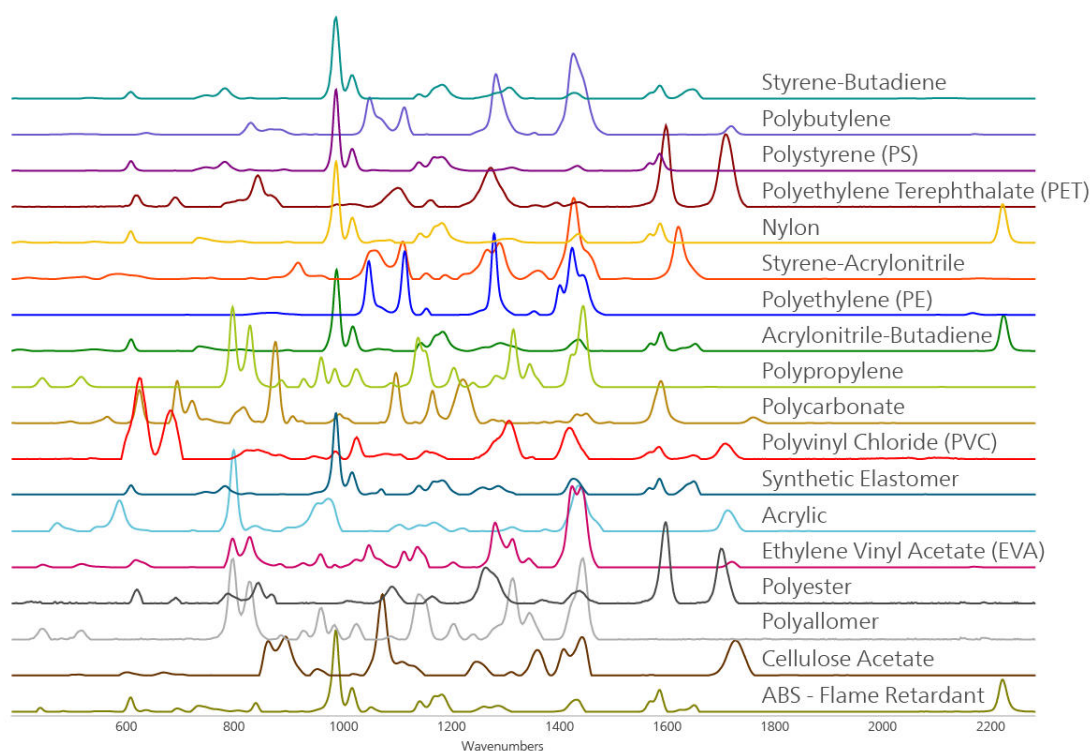


Figure 1. Stacked Raman library spectra for a wide range of polymer samples demonstrate how distinct the Raman fingerprint peaks are for each material.

RESULTS

The Raman spectra of various items composed of unknown polymers in different colors were collected

(Figure 2) and checked against the MIRA Illicit and General Chemicals Library.

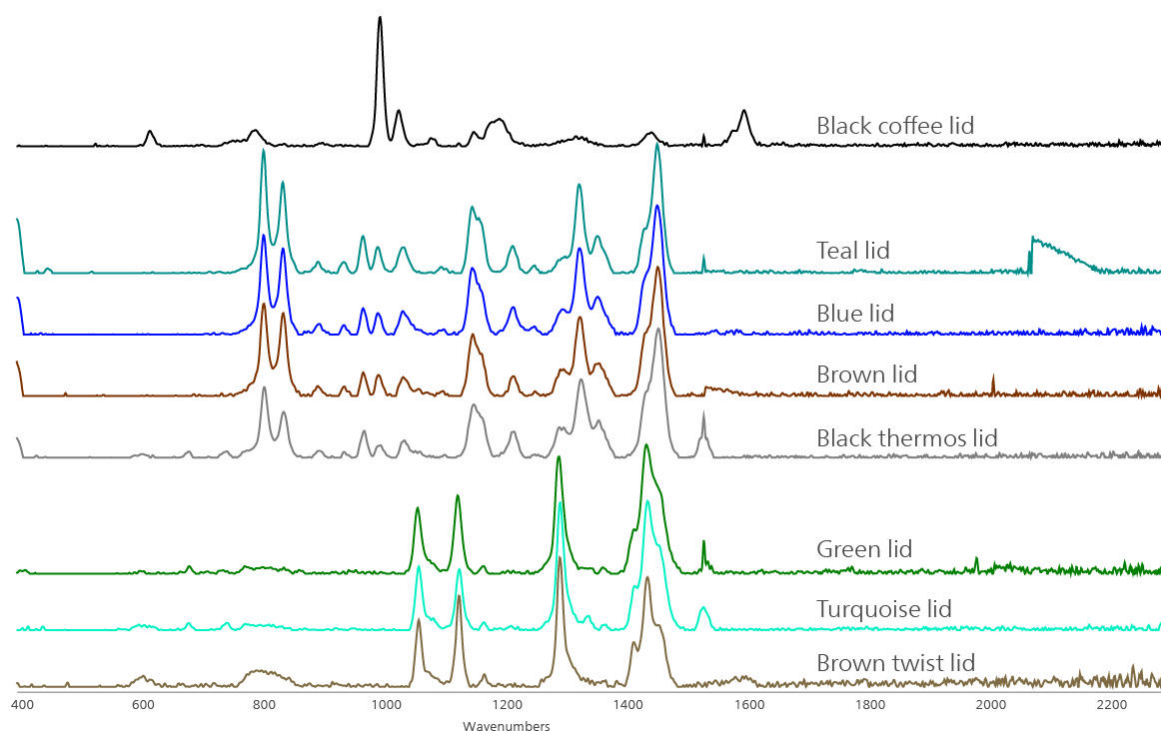


Figure 2. Resolved, stacked Raman spectra of various strongly colored plastics.

Results display on the device within seconds and include the name, CAS number, and HQI (Hit Quality Index) – a measure of the strength of correlation between sample and library spectra. **Figure 3**

demonstrates the accuracy of data collected from even strongly colored samples by comparing sample and library spectra.



Figure 3. A direct comparison of experimental and library spectra demonstrates the accuracy and resolution of both spectra and results. Each plastic sample matched to a single library spectrum with high HQI values.

CONCLUSIONS

Metrohm has unique solutions that overcome the problem of fluorescence while retaining all the

benefits of 785 nm interrogation — fast, accurate, nondestructive identification of colored polymers.

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CONFIGURATION



MIRA XTR Advanced

MIRA XTR is an alternative for high power 1064 nm systems. Powered by advanced computational processing, MIRA XTR uses a more sensitive 785 nm laser along with XTR algorithms to eXTRACT the Raman data from the sample fluorescence. MIRA XTR also features Orbital Raster Scanning (ORS) to provide better coverage of the sample increasing the accuracy of the results.

MIRA XTR Advanced package includes a Calibration Standard, Intelligent Universal Attachment, Right-angle Attachment, Vial Attachment, and MIRA SERS Attachment. A complete package for any type of analysis. Class 3B operation. MIRA XTR supports Metrohm handheld Raman libraries.



Intelligent Universal Attachment (iUA)

iUA is an intelligent 3-position collection optics accessory for MIRA systems. The iUA combines the flexibility of a universal attachment with the intelligent mode of operation of MIRA SmartTip Attachments. Each position indicates the ideal purpose of that position, i.e. surface, bag, or bottle.



MIRA Illicit and General Chemicals Library

MIRA (Metrohm Instant Raman Analyzer) library of illicit materials including drugs, TICs, TIMs, precursors, and general chemicals.