



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.

INTRODUCTION

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.

EXPERIMENTAL

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.

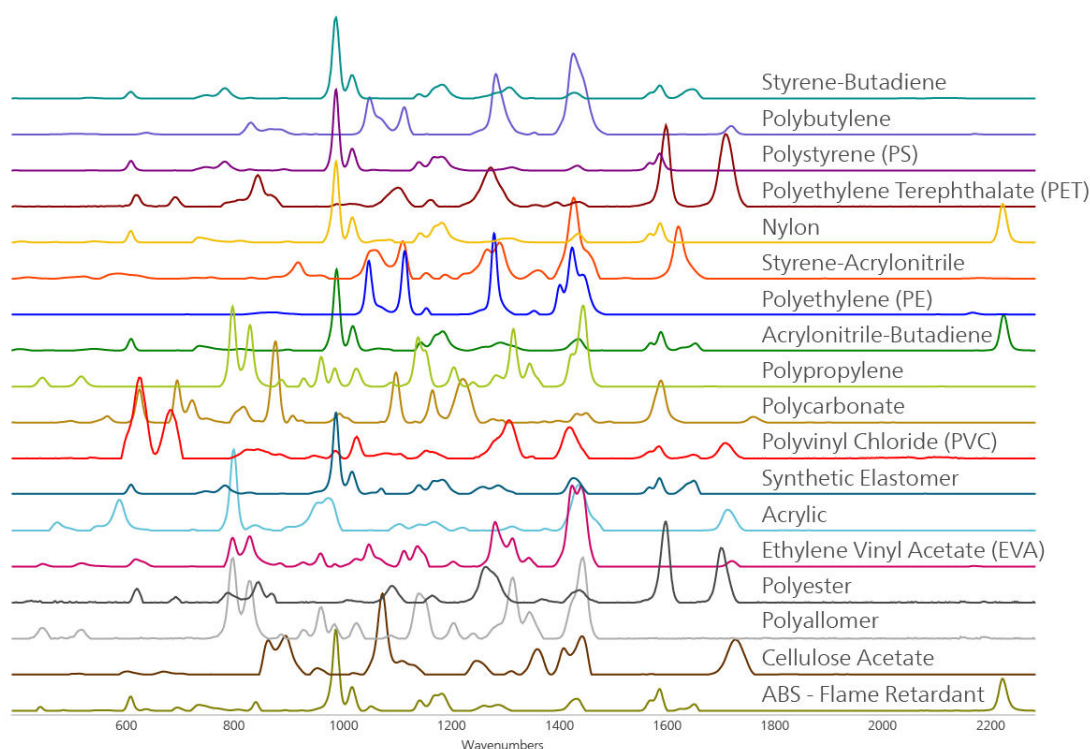


Figure 1. Stacked Raman library spectra for a wide range of polymer samples demonstrate how distinct the Raman fingerprint peaks are for each material.

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.

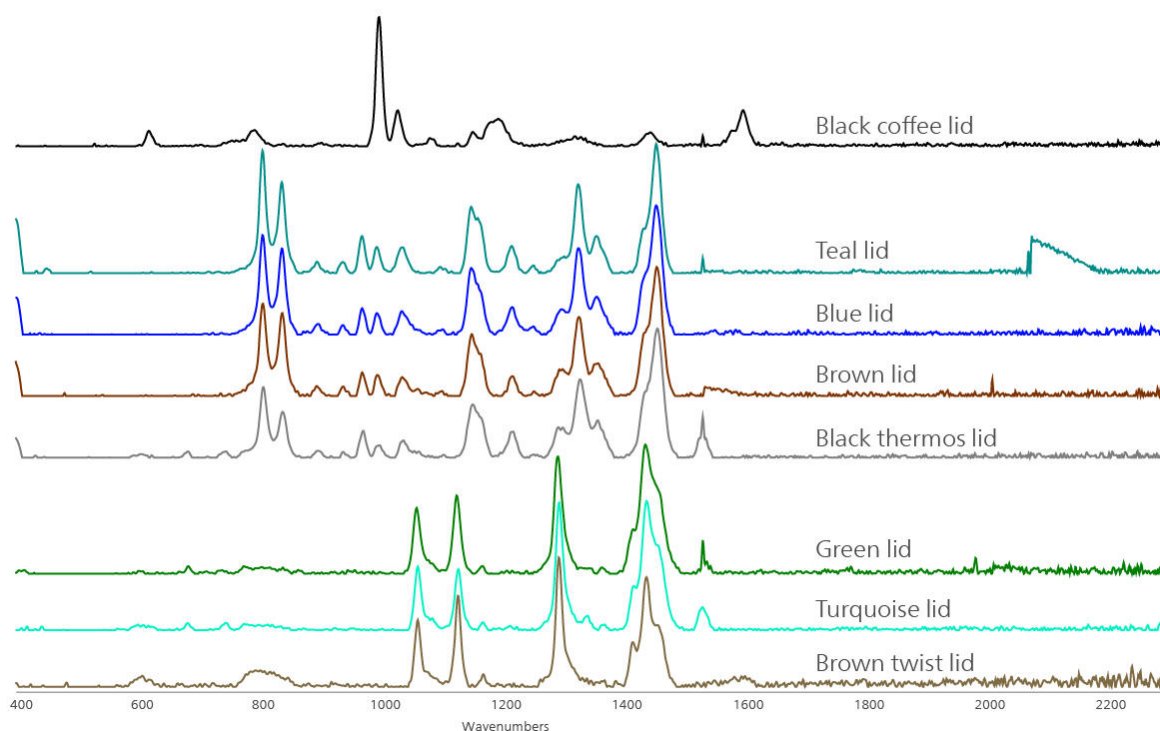


Figure 2. Resolved, stacked Raman spectra of various strongly colored plastics.

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.

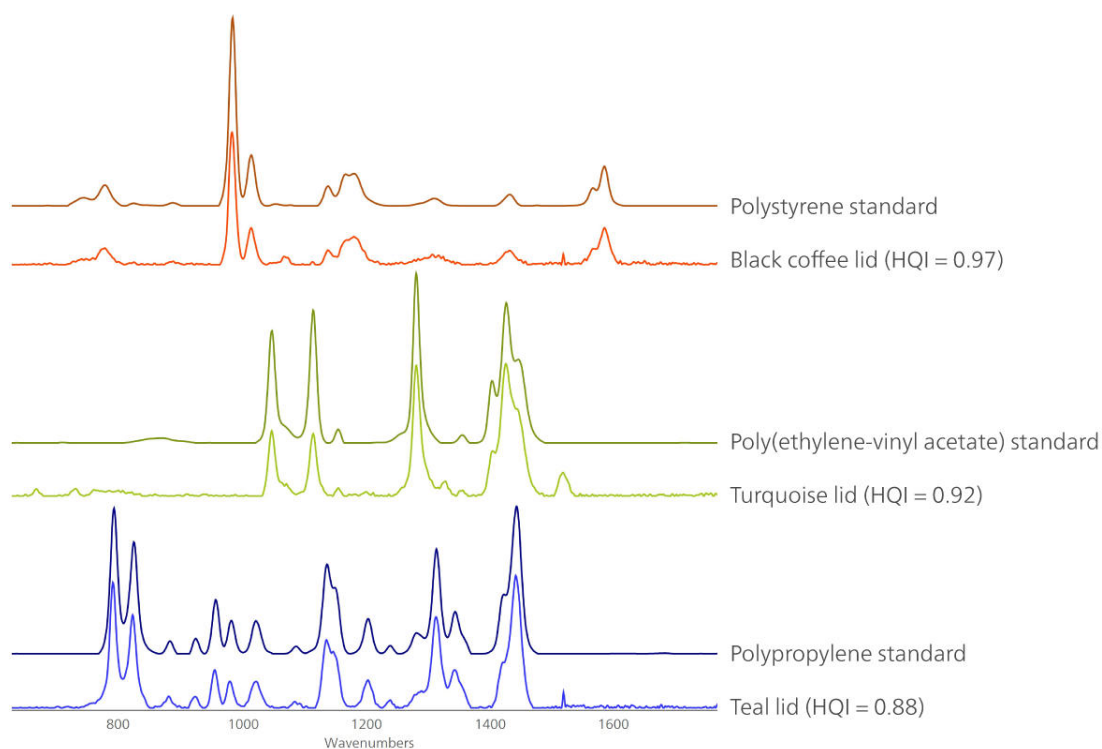


Figure 3. A direct comparison of experimental and library spectra demonstrates the accuracy and resolution of both spectra and results. Each plastic sample matched to a single library spectrum with high HQI values.

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 est une alternative pour les systèmes haute puissance 1 064 nm. Piloté par un traitement informatique avancé, MIRA XTR utilise un laser de 785 nm plus sensible ainsi que des algorithmes XTR pour extraire les données Raman de la fluorescence de l'échantillon. MIRA XTR dispose également d'un balayage de trame orbital (ORS, Orbital Raster Scanning) pour fournir une meilleure couverture de l'échantillon, améliorant ainsi l'exactitude des résultats.

Le pack MIRA XTR Advanced comprend un standard de calibrage, un embout universel intelligent, un embout à angle droit, un support de flacon et des accessoires SERS MIRA. Un package complet pour tous les types d'analyse. Fonctionnement en classe 3B. MIRA XTR prend en charge les bibliothèques Raman de Metrohm portables.



Embout universel intelligent (iUA)

L'iUA est un accessoire intelligent d'optique de collecte à 3 positions pour les systèmes MIRA. L'iUA combine la flexibilité d'un embout universel avec le fonctionnement intelligent des accessoires SmartTip de MIRA. Chaque position indique l'utilisation idéale de cette position, c'est-à-dire la surface, le sac ou le flacon.



Bibliothèque de produits chimiques généraux et illicites MIRA

Bibliothèque de substances illicites y compris drogues, TIC, MIT, précurseurs et produits chimiques généraux MIRA (Metrohm Instant Raman Analyzer).