Application Note AN-RS-008

Identification of monomers with Raman spectroscopy

Polymers are comprised of macromolecules that are in turn comprised of numerous identical or similar structural units that are referred to as monomers. This Application Note shows the convenient identification of conventional monomers within seconds using the portable Mira M-1 spectrometer. Monomers such as styrol, various alkyl methacrylates, divinylbenzene, ethylene glycol, phenol, terephthalic acid and urea have been investigated. Additives or inhibitors such as benzoquinone can be identified quickly and unambiguously.

INTRODUCTION

Today's industry, but also daily life, cannot be imagined without polymers. With the variety of the available polymers on the market, the number of monomers and especially additives, used to endow the polymers with special properties, is enormous.
Many polymer manufacturers, if not all, use their own special mixtures and additives, commonly carrying proper names, making it hard to get an idea of the function of certain additives. Nevertheless, all use the same monomers, which also means, that every polymer manufacturer will profit from a quick raw material check before feeding the raw materials into their polymerization process.
In this study, a library of commonly used monomers was built and subsequently used for the identification of unknown monomers.

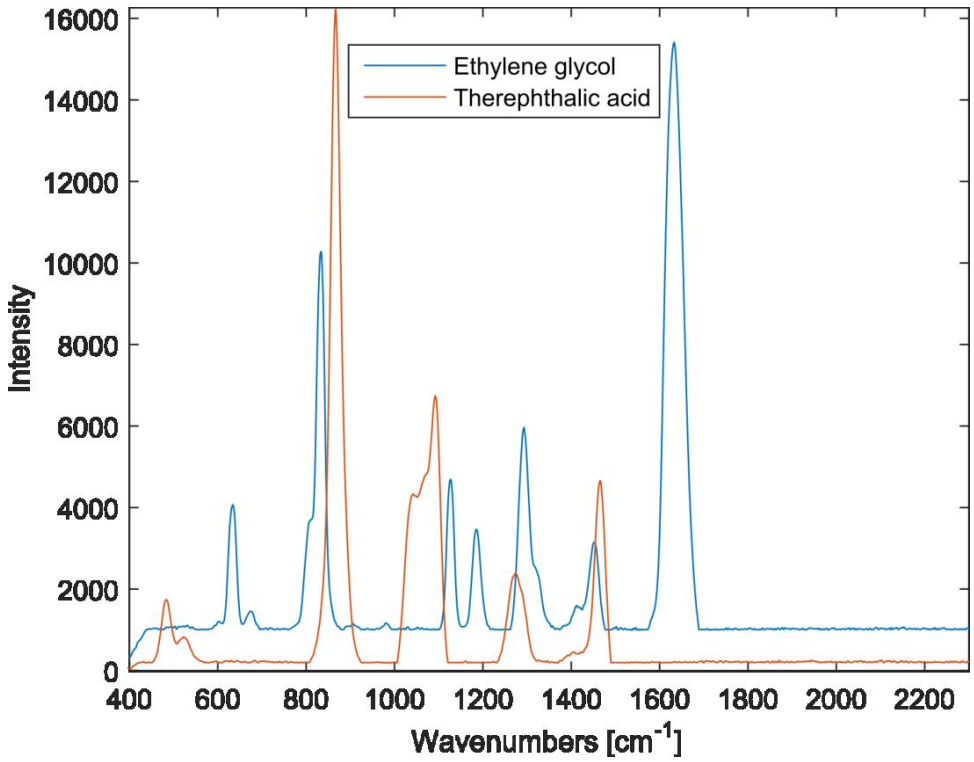

Figure 1. Raman spectra of ethylene glycol and therephthalic acid

EXPERIMENTAL

All spectra spectra were measured using the Mira M-1 handheld Raman spectrometer in auto-acquisition mode, i.e. integration times were determined automatically. A laser wavelength of 785 nm and the Orbital-Raster-Scan (ORS) technique were used. Some of the monomers were filled into vials and analyzed using the vial holder attachment, while other samples were analyzed directly in their plastic container using the long working distance (LWD) lens.
The following monomers were used in this study:

Monomer	Meas. mode	Usage
Divinylbenzene (DVB)	LWD	Styrene-DVB Copolymer (S-DVB)
Ethylene glycol	vial	Polyethylene terephthalate (PET)
Ethyl methacrylate	vial/LW	Paraloid B-72 (thermoplastic resin used for surface coatings and coservations
Formaldehyde	vial	Polyoxymethylene (POM), Bakelite, urea-formaldehyde (UF), melamine-formaldehyde (MF)
Urea	vial	Urea-formaldehyde (UF)
Hexamethylenetet ramine (HMTA)	vial	Hardening component for phenolic resins

Hydroquinone	vial	Polyether ether ketone (PEEK)
Methyl methacrylate (MMA)	LWD	Poly(methyl methacrylate) (PMMA)
Phenol	vial	Bisphenol-A (a precursor to polycarbonates and epoxide resins)
Styrene	vial	Polystyrene (PS), S-DVB
Therephthalic acid	vial	Polyethylene terephthalate (PET)

RESULTS AND DISCUSSION

To build the library, the samples were measured in vials but also with the LWD lens through amber bottles. Using the Mira Cal software, the spectra were investigated to check for visible differences between the monomers. Figure 2 shows an overlay of all the analyzed monomers.

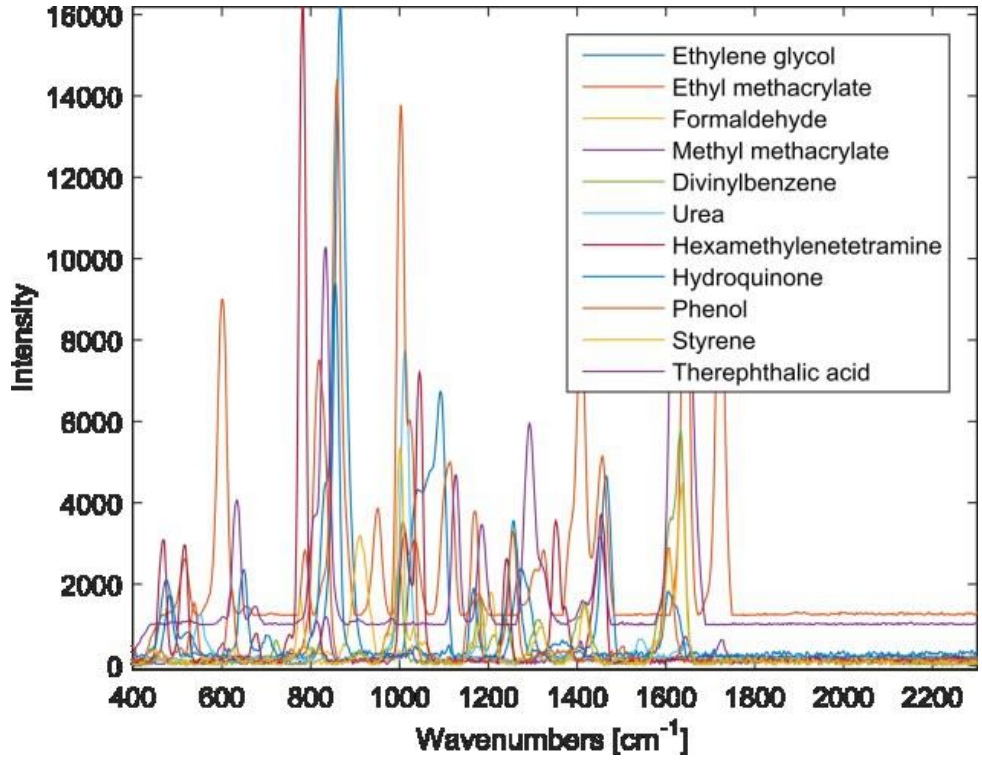

Figure 2. Overlay of the analysed monomers.

When using Mira in its autonomous mode, i.e., mode, without the use of the Mira Cal software, secure identification of the monomers was achieved, and the correlation coefficients were always greater 0.95.

CONCLUSIONS

This study shows that Mira M-1 can be used to unambiguously identify polymer raw materials used to produce commonly used polymers such as PET, POM and PEEK by measuring their spectra and matching them with a library. The identification takes just a few seconds. Additionally, additives or inhibitors such as benzoquinone can be quickly and unambiguously identified.

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CONFIGURATION

MIRA P Advanced

Le Metrohm Instant Raman Analyzer (MIRA) P est un spectromètre Raman portable performant qui s'utilise pour les déterminations rapides et non destructives et le contrôle des matériaux les plus divers, comme les principes actifs pharmaceutiques et les excipients. De très petite taille, le MIRA P est pourtant très robuste et dispose d'une structure de spectrographe haute efficacité, équipée de notre technologie « Orbital Raster Scan » (ORS) inédite. MIRA P satisfait aux prescriptions FDA 21 CFR partie 11.

Le Advanced Package comprend une lentille avec laquelle les matériaux peuvent être analysés directement ou dans leur conditionnement (classe de laser 3b), ainsi qu'un support de flacon pour analyser les échantillons dans des flacons en verre (classe de laser 1).