Application Note

Environmental

Fast and Simple Material Identification of Plastic Debris Using FTIR Spectrometry

Polymer-type identification of beach samples using the Agilent Cary 630 FTIR with ATR

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Introduction

During the invention, development, and early production phases of synthetic plastics, only small quantities were produced, and dealing with waste-plastic was relatively controllable. Over the last few decades, however, plastic production has been growing faster than the production of any other materials. Nowadays, an estimated 400 million tons of plastic waste is produced every year, and a large portion of this waste ends up in the natural environment.[1]

In some recent studies, researchers have been investigating how plastic pollution impacts terrestrial ecosystems, including beach-ecosystems.[2,3] An important step in understanding the impact of plastic pollution on the environment is the advancement of analytical methods that can identify plastic waste and microplastic particles.

Fourier transform infrared (FTIR) spectroscopy is well-suited to the identification of different types of plastic, as it provides reliable performance, high-quality data, and cost-effective analyses. This study highlights how the Agilent Cary 630 FTIR spectrometer (Figure 1) provides a simple workflow that researchers can use for material identification of plastic debris. The workflow includes sample preparation, library generation, sample analysis, and data reporting.

Figure 1. Agilent Cary 630 FTIR spectrometer coupled with a diamond attenuated total reflectance (ATR) module.

Experimental

Samples

Plastic debris was collected at random from Mordialloc Beach, Victoria, Australia. A total of nine samples that had visibly degraded in the environment were selected for this study (Figure 2).

Figure 2. Plastic debris collected from a beach in Australia and analyzed in this study using the Agilent Cary 630 FTIR spectrometer.

Instrumentation

The Cary 630 FTIR spectrometer coupled with a diamond ATR module and controlled by Agilent MicroLab software was used in this study (Figure 1). The software guides the analyst through the analytical steps using a picture-driven interface. To maximize sample contact with the diamond crystal, a thin section of each hard plastic sample was generated using a blade (~ 2 mm). The sample was placed on the platform and measured directly by FTIR-ATR using the operating parameters given in Table 1.

Library generation

The plastic debris samples were identified by reference to a user-generated library of polymers that contained ATR spectra of the most common polymers used in the plastic industry. This library was developed using the Polymer Sample Kit (Scientific Polymer Products, Inc.; catalog number 205; LOT number 600801012), which includes polystyrene, polypropylene, high- and low-density polyethylene, polyethylene terephthalate, polyvinyl chloride, polycarbonate, poly (methyl methacrylate), polyoxymethylene, polyamides, and polytetrafluoroethylene.

The library search method used the Similarity search algorithm (Table 1). Spectral libraries can be easily created, maintained, and managed in the MicroLab software. A new library can be created in a few seconds. Spectra can be added to the library, either at the time of creation or at any other time, including directly from the results screen.

Table 1. Agilent Cary 630 FTIR–ATR operating parameters.

Parameter	Setting
Method	Library search
Library Used	User-generated polymers library (Agilent Internal Mini)
Search Algorithm	Similarity
Spectral Range	4,000 to 650 cm^{-1}
Background Scans	64
Sample Scans	64
Spectral Resolution	4 cm^{-1}
Background Collection	Air
Color-Coded Confidence Level Thresholds	Green (high confidence): >0.95 Yellow (medium confidence): 0.90 to 0.95 Red (low confidence): <0.90

Results and discussion

Despite the distinct colors of the different samples shown in Figure 2, eight of the nine plastic debris samples were identified as polypropylene, and one sample was identified as high-density polyethylene. The hit quality indices (HQI) for the polypropylene results were in the range of 0.94651 to 0.99405, and the HQI for high-density polyethylene was 0.97110, as shown in Table 2.

An HQI is automatically calculated for each library item and the value indicates how well the measured spectrum and the library spectrum match. The HQI is often used as a pass/fail criterium in material identification. The user-definable criteria that were applied in this study are described in Table 1 (color-coded confidence level thresholds).

Table 2. Summary of material identification results for the weathered plastic debris samples.

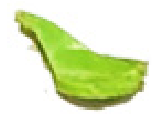
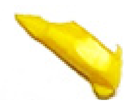
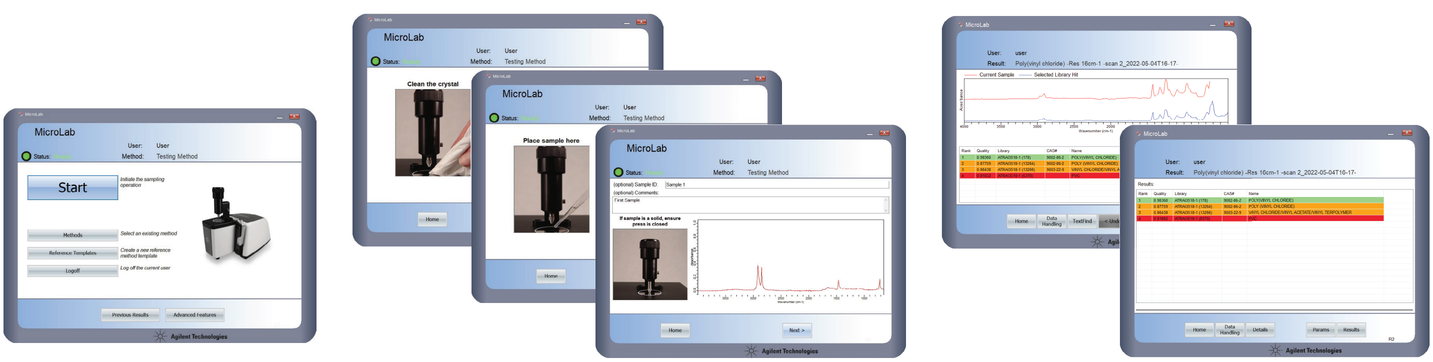
Sample Name	Image	Material Identification	Hit Quality Index
Turquoise Plastic		Polypropylene	0.98133
Green Plastic		Polypropylene	0.94651
Yellow Plastic		Polypropylene	0.98414
Blue Plastic 1		High-density polyethylene	0.97110
Blue Plastic 2		Polypropylene	0.99405
Orange Plastic 1		Polypropylene	0.98940
Red Plastic		Polypropylene	0.97501
Orange Plastic 2		Polypropylene	0.98414
Blue Plastic 3		Polypropylene	0.99034

Figure 3. Examples of the Agilent Cary 630 FTIR spectrometer qualitative analysis of plastic debris (red traces) and library hits (blue traces). The table shows the hit quality, library used, and the hit name for each sample. Color-coding the results based on the HQI can be used to define confidence levels, which helps users to interpret the results and reduces oversights that may lead to errors.

The color-coded material identification results obtained for each sample are displayed on the screen for ease of interpretation, as shown in Figure 3. This feature turns the FTIR system into a turnkey solution that enables quick decision-making.

The Cary 630 FTIR spectrometer is controlled using MicroLab software, which uses a pictorial interface to guide users through the steps of the analysis, from sample introduction to reporting (Figure 4).

The Cary 630 equipped with an ATR module can be used to generate libraries that are easy to update and optimize. MicroLab also offers multiple library search algorithms to account for different analytical needs, adding to the flexibility of the instrument.



1 Start the analysis

2 Follow picture-driven software guidance

3 Instantly receive color-coded actionable results

Figure 4. The intuitive Agilent MicroLab software workflow makes finding answers with the Agilent Cary 630 FTIR spectrometer quick and easy. The picture-driven software also reduces training needs and minimizes the risk of user-based errors.

Agilent solutions for environmental research

Agilent is advancing plastics and microplastics research across the world, offering a range of instruments, both benchtop and portable handheld, to analyze plastics and microplastics onsite, in laboratories, and outdoors in remote environments, delivering immediate and real-time results. In addition to the Agilent Cary 630 FTIR Spectrometer, Agilent also offers the following instruments:

Agilent 8700 Laser Direct Infrared (LDIR) Chemical Imaging System

Provides a sophisticated new approach to chemical imaging and spectral analysis for microplastics.

Agilent 4300 Handheld FTIR Spectrometer

The first of its kind instrument, employing lightweight ergonomics, ease-of-use, ruggedness, and flexibility in one system.

Agilent 4500 Series portable FTIR Spectrometer

Onsite analysis of incoming materials and outgoing finished products in the chemical, petrochemical, food, and polymer industries.

Agilent 5500 Series Compact FTIR Spectrometer

A compact, at-site analyzer, designed to provide accurate results rapidly and reliably, day after day.

Conclusion

The Agilent Cary 630 FTIR spectrometer fitted with an ATR sampling module provided a fast and simple method for the identification of nine samples of degraded plastic debris collected from a beach in Australia.

The intuitive, picture-guided Agilent MicroLab software was used to set up the method and build the user-generated library based on standard samples of commonly used polymers. Sample spectra acquired by the Cary 630 FTIR were automatically compared against spectra in the polymer library and the software identified polymer-type based on user-defined hit quality confidence limits.

The study demonstrated the capability of the Cary 630 FTIR with ATR for the quick identification of polymer-type waste plastics using a simple method tailored to the application.

Further information

– Agilent Cary 630 FTIR Spectrometer
– Agilent MicroLab Software
– Agilent MicroLab Expert Software
– FTIR Analysis & Applications Guide
– FTIR Spectroscopy Basics - FAQs
– ATR-FTIR Spectroscopy Overview
– Microplastics Technologies FAQs

References

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2. Andrady, A. L. Weathering and Fragmentation of Plastic Debris in the Ocean Environment, *Mar. Pollut. Bull.*, **2022**, 180:113761. doi: 10.1016/j.marpolbul.2022.113761. Epub 2022 Jun 1. PMID: 35665618
3. Lavers, J. L.; Rivers-Auty, J.; Bond, A. L. Plastic Debris Increases Circadian Temperature Extremes in Beach Sediments., *J. Hazard Mater.*, **2021**, 15; 416: 126140. doi: 10.1016/j.jhazmat.2021.126140. Epub 2021 May 17. PMID: 34492929

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