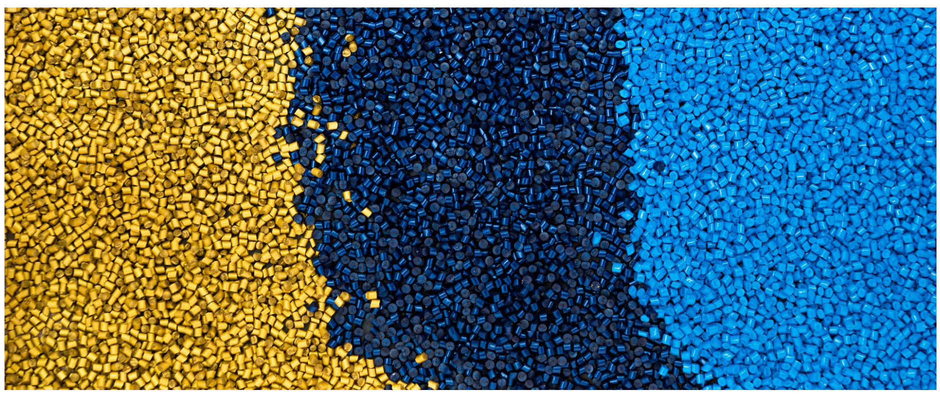
Application Note

Materials

Material Identification of Plastics Throughout Their Life Cycle by FTIR Spectroscopy

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



Authors

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Introduction

Understanding more about the life cycle of plastics is useful, considering how widely used they are in our daily lives. Once extracted from the ground, crude oil and natural gas are refined into multiple hydrocarbon products such as ethane and propane.[1] These products serve as the starting materials or building blocks of plastic pellets or nurdles, which are then used to produce plastic products. Depending on the final product, nurdles can be shaped and sized using different processes, such as plastic injection, molding machinery, and blowing. Finished plastic products include a vast range of items that are used in most sectors, including bottling of drinks and liquids, packaging materials, baby products, toys, textiles, construction, among many other sample-types.[2]

Once plastic products have been used, they can either be recycled or disposed of as waste in landfill or an incinerator. If there are any weaknesses in the collection and disposal practices of plastics, waste materials can end up in the environment (Figure 1). Littering and improper dumping of plastic waste also add to the amount of plastic in the environment.

For each step outlined in Figure 1, material identification is a critical quality assurance or safety control analysis that is widely performed in the plastic industry. The analysis of pre-production and produced materials ensures that the final product meets the quality and purity required for its intended purpose. Therefore, material identification is a requirement outlined in many industry standards. The same testing techniques are increasingly used to identify plastic waste in recycling centers, helping to maintain the quality of recycled plastics, and to identify plastic debris collected from the environment.

Fourier transform infrared (FTIR) spectroscopy is well suited to the identification of different types of plastic, providing reliable, high-quality data, and cost-effective analyses. This application note highlights how the Agilent Cary 630 FTIR spectrometer (Figure 2) provides an easy workflow for material identification throughout the life cycle of plastics.

Figure 2. Agilent Cary 630 FTIR spectrometer coupled with a diamond attenuated total reflectance (ATR) module.

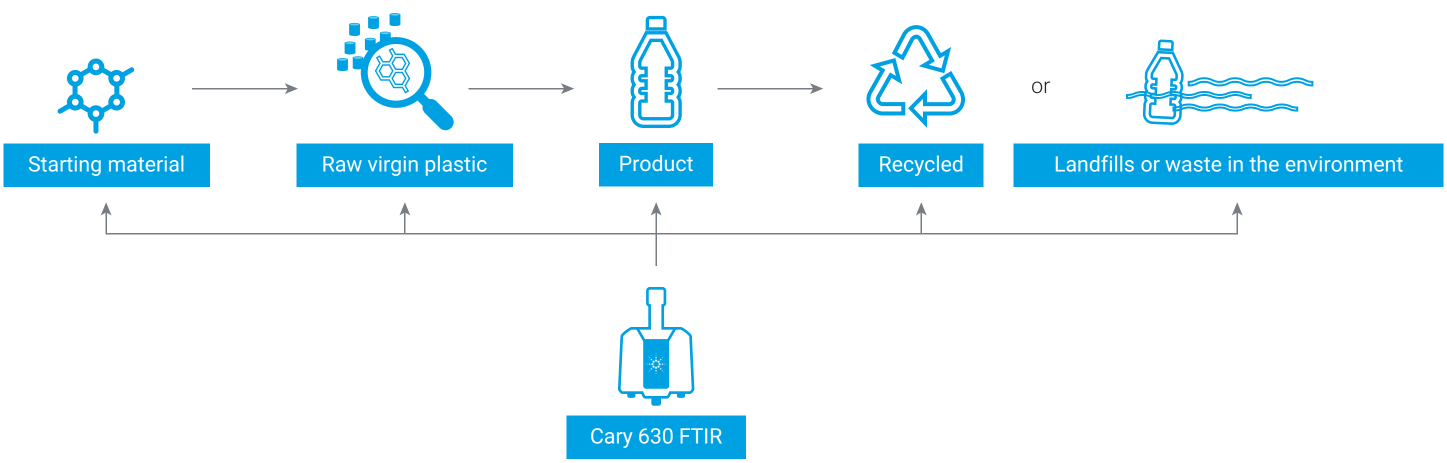


Figure 1. The life cycle of plastic. At each phase of a plastic's journey, material identification ensures reliable quality control and provides accurate safety requirements for starting materials and finished products. The Agilent Cary 630 FTIR with Agilent MicroLab software can be used to perform fast, easy, and reliable material identification workflows of different sample-types.

Experimental

Samples: Five samples were used in this study to cover four stages in the production, use, recycling, and disposal of plastics:

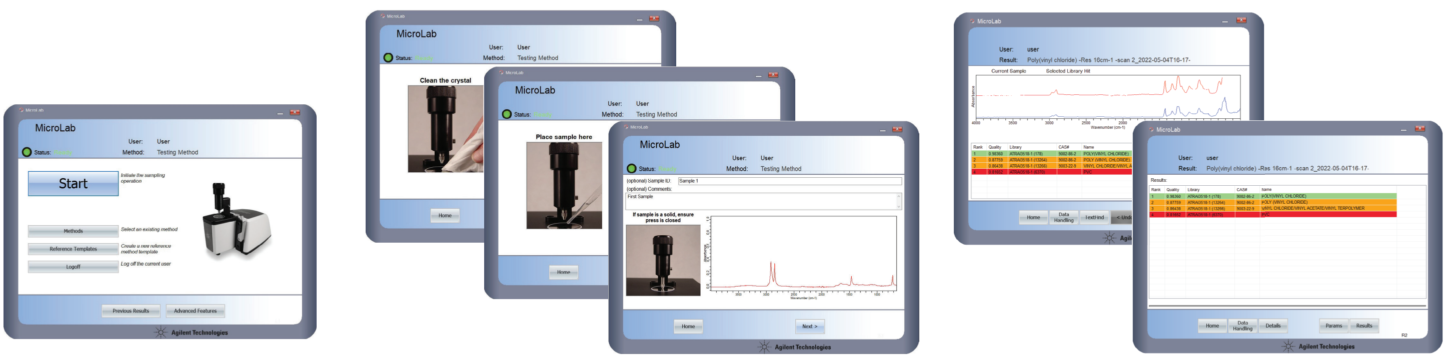
1. Plasticizer – starting material.
2. Nurdle – plastic raw material.
3. Coffee lid – plastic product.
4. Water bottle – recycled product.
5. Plastic debris – collected at random from Mordialloc Beach, Victoria, Australia.

Instrumentation: The Cary 630 FTIR spectrometer coupled with a diamond ATR module was used in this study (Figure 2).

Software: The Cary 630 FTIR spectrometer was controlled using Agilent MicroLab software, which uses a pictorial interface to guide users through the steps of the analysis, from sample introduction to reporting (Figure 3).

Library generation: Sample 1 was identified via the Agilent ATR demo library. Samples 2 to 5 were identified via a user-generated library of polymers that was developed using the Polymer Sample Kit (Scientific Polymer Products, Inc.; catalog number 205; LOT number 600801012). The user generated spectral library contained ATR spectra of the most common polymers used in the plastic industry, including:

- Polystyrene (PS)
- Polypropylene (PP)
- High- and low-density polyethylene (HDPE and LDPE)
- Polyethylene terephthalate (PET)
- Polyvinyl chloride (PVC)
- Polycarbonate (PC)
- Poly (methyl methacrylate) (PMMA)
- Polyoxymethylene (POM)
- Polyamide (PA)
- Polytetrafluoroethylene (PTFE)



1 Start the analysis

2 Follow picture-driven software guidance

3 Instantly receive color-coded, actionable results

Figure 3. The intuitive Agilent MicroLab software makes finding answers with the Agilent Cary 630 FTIR spectrometer as easy as 1, 2, 3. The picture-driven software also reduces training needs and minimizes the risk of user-based errors.

The library search method applied the Similarity search algorithm using the parameters shown in 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, directly from the results screen.

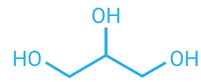
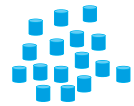
Table 1. Agilent Cary 630 FTIR–ATR operating parameters.

Parameter	Setting
Method	Library search
Library Used	User-generated polymers library (Agilent Internal Mini) and Agilent ATR demo library
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

The Cary 630 FTIR with diamond ATR sampling module was used to identify the five different samples that were representative of the life cycle of plastic. Using the Similarity algorithm to search the user-generated library spectral library, all five samples were identified with a hit quality index (HQI) of >0.97, with 1 being the highest theoretical value. As shown in Table 2, the HQI values were 0.99599 (plasticizer, glycerol), 0.99621 (plastic nurdle, LDPE), 0.97809 (coffee lid, PS), 0.98622 (water bottle, PET), and 0.98940 (weathered plastic, PP).

Table 2. Summary of plastic material identification analysis results obtained using the Agilent Cary 630 FTIR–ATR and Similarity search algorithm.

Sample Name	Image	Material Identification	Hit Quality Index
Plasticizer (Starting Material)		Glycerol	0.99599
Plastic Nurdle (Raw Material)		LDPE	0.99621
Plastic Product (Coffee Lid)		PS	0.97809
Recycled Plastic (Water Bottle)		PET	0.98622
Weathered Plastic (Waste)		PP	0.98940

For easy review of the data generated by the Cary 630 FTIR, the material identification results obtained for each sample are color-coded based on user defined confidence level thresholds (Figure 4). In this study, results with an HQI above 0.95 were color-coded in green, indicating a good spectral match and providing confidence in the identification of the material. Color-coding the results turns the Cary 630 FTIR system into an easy-to-use, turnkey solution that enables quick decision-making.

Figure 4. The Agilent Cary 630 FTIR spectrometer qualitative analysis of the five plastic samples (red traces) and library hits (blue traces). The table shows the hit quality, library used, and the hit name for each sample; (A) plasticizer; (B) nurdle; (C) coffee lid; (D) water bottle; (E) weathered plastic.

Conclusion

The Agilent Cary 630 FTIR spectrometer provided a simple-to-use solution for material identification of the raw materials used to make plastic through to recycled and waste plastic.

The Cary 630 FTIR and MicroLab software facilitated the quick and easy generation of a polymer library, which enabled the quick identification of plasticizer, nurdle, a cup lid, recycled water bottle, and plastic beach debris. All five samples were identified with a hit quality index (HQI) of >0.97, with 1 being the highest theoretical value. The MicroLab software applies color-coding to the identification results based on the HQI, making it quick and easy to review the quality of the data.

This study has shown the flexibility of the Cary 630 FTIR fitted with the ATR sampling module for material identification of samples as required by manufacturers, recyclers, or environmental researchers.

References

1. Rhodes, C. J. Plastic Pollution and Potential Solutions, *Sci. Prog.*, **2018** *101(3)*, 207–260. doi: 10.3184/003685018X15294876706211. Epub 2018 Jul 19. PMID: 30025551.
2. British Plastic Federation, Plastics Applications, accessed May 2023, https://www.bpf.co.uk/plastipedia/applications/Default.aspx

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

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