

Application News

Fourier Transform Infrared Spectrophotometer IRXross™
Infrared Microscope AIMSight™
Infrared Raman Microscope AIRSight™

Analyzing Various Plastics —Benefits of Bundled KnowItAll® Software—

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User Benefits

- ◆ FTIR spectrophotometers are analytical instruments that are useful for determining the composition of microplastics and recycled plastics.
- ◆ KnowItAll database software can search for multiple components in mixtures or analyze functional groups at specific peaks.
- ◆ With a single click, optional KnowItAll bundle can automatically receive data from FTIR control software for quick spectral analysis.

Introduction

There is a great variety of plastic products being used all around us. Plastics are lightweight, strong, and easy to process, but they cause a variety of problems throughout the world. For research into solving the challenges of microplastics and recycled plastics, it is first important to determine the types of plastic materials involved. Of the many analytical instruments used to analyze plastics, Fourier transform infrared (FTIR) spectrophotometers are especially popular because they can analyze plastics easily without complex pretreatment steps, such as dissolving plastics in a solvent.

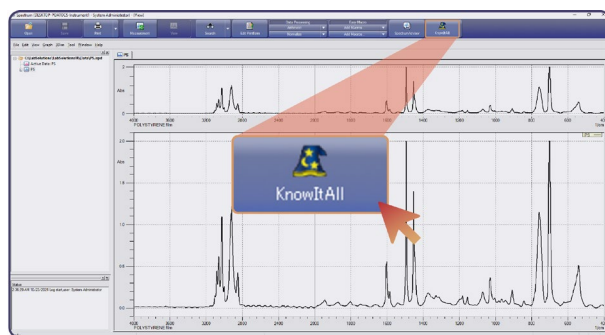
This article describes using John Wiley & Sons, Inc. KnowItAll software for plastic analysis. KnowItAll has an extensive library for a wide variety of data analysis, such as searching for multiple components to identify and determine the percentage of chemical components contained in plastics or identifying functional groups attributable to specific spectral peaks (partial structural analysis). Furthermore, KnowItAll is bundled with Shimadzu LabSolutions™ IR software for FTIR analysis and AMsolution infrared microscope software. Clicking the [KnowItAll] button in the Shimadzu software automatically sends the active spectral data to the KnowItAll software, ensuring quick analysis.

Infrared Spectral Analysis

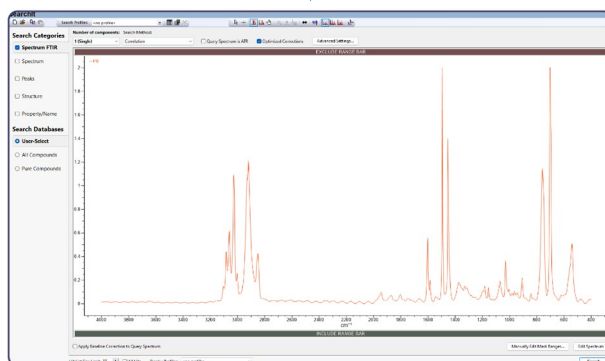
Due to the increased number of databases available in recent years for analyzing FTIR spectra, database search software with improved algorithms, and easier operability, it is now easy for anyone to search for infrared spectra and instantly display results on a computer screen. However, there can be problems interpreting spectrum search results if fully matching spectra in the database are not found. Even if similar results are found, there may be problems due to dissimilar peaks included in the spectra. Therefore, using difference spectra is recommended for such cases (FTIR TALK LETTER Vol. 22). FTIR TALK LETTER Vol. 24, 25, and 26 also provide advice on how to use the standard spectral search functionality included in LabSolutions IR and AMsolution software more effectively.

In addition to the standard functionality, KnowItAll bundle (Fig. 1) is recommended for users who want to automatically search for multiple components or functional groups of peaks. After acquiring an infrared spectrum, simply clicking the [KnowItAll] button automatically sends the spectrum active in LabSolutions IR or AMsolution software to the KnowItAll [SearchIt] window. In addition to easily comparing the match level of infrared spectra, the mixture analysis functionality in SearchIt can analyze mixtures based on the selected number of components. Also, ID Expert can determine the quality of infrared spectra loaded for searches. Analyzelt can display a list of all functional groups for any peak clicked.

Although not shown here, the same data analysis and evaluation capabilities described for infrared spectra are also available for Raman spectra.



Click the LabSolutions IR [KnowItAll] button.



Data is automatically sent to SearchIt (standard spectral analysis functionality) in KnowItAll.

Key Functionality Included in KnowItAll

- Mixture analysis for analyzing mixtures
- ID Expert for analyzing spectra
- Analyzelt for analyzing functional groups
- Building spectral databases
- Creating reports, etc.

Fig. 1 KnowItAll Bundle
(Example of Functionality Integrated with LabSolutions IR)

Instruments Used and Measurement Parameters

A system with a QATR™ 10 single-reflection ATR accessory installed in the sample compartment of an IRXross Fourier transform infrared spectrophotometer was used. The system is shown in Fig. 2 and measurement parameters are listed in Table 1.



Fig. 2 IRXross™ FTIR Spectrophotometer with QATR™ 10 Accessory

Table 1 Measurement Parameters

System:	IRXross and QATR 10 (diamond)
Resolution:	4 cm ⁻¹
Number of Scans:	45
Apodization Function:	SqrTriangle
Detector:	DLATGS

■ Analysis of Microplastics —Functional Group Analysis

The contamination of rivers and oceans by microplastics is occurring globally, causing concerns about how microplastics affect living organisms. In recent years, there have been various monitoring surveys and studies into microplastics, such as how they are distributed throughout the world. The following describes analyzing microplastics using the single-reflection ATR method. The acquired infrared spectrum and corresponding library search results are shown in Fig. 3. The standard Shimadzu library was used to determine that the material was polypropylene (PP). However, there were peaks in the 3,600 to 3,100 cm⁻¹ wavenumber range and near 1,700 cm⁻¹ and the 1,300 to 1,000 cm⁻¹ wavenumber regions that did not match the library data. Therefore, Analyzelt from the bundled KnowItAll was used to search for the corresponding functional groups. First, the results that confirmed the attribution of PP peaks are shown in Fig. 4. The functional group analysis enabled information about the functional groups, peak ranges, peak intensity, and vibration modes to be determined. Differing peaks were easily confirmed based on the predicted peak positions displayed on the spectrum. Then the peaks that did not match PP were successively selected to display corresponding reference results (Fig. 5). That inferred that the peaks in the 3,600 to 3,100 cm⁻¹ region were from an O-H group and the peaks near 1,700 cm⁻¹ and 1,300 to 1,000 cm⁻¹ were from the C=O and C-O groups. Given that none of those functional groups are present in PP structures, it suggests they were caused by changes in the infrared spectral pattern due to PP degradation (denaturing).

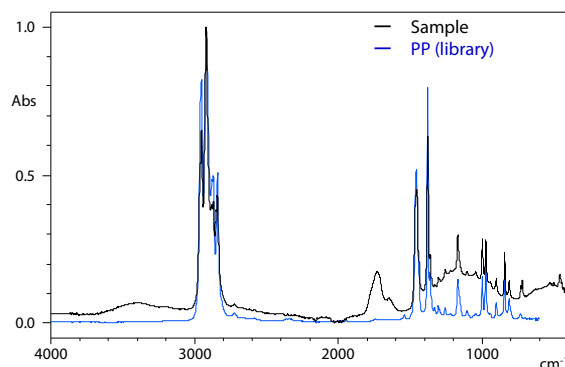


Fig. 3 Search Results Using a Standard Library

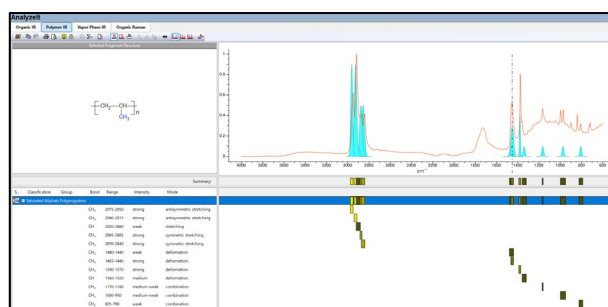


Fig. 4 KnowItAll Bundle : Functional Group Analysis Results (PP)

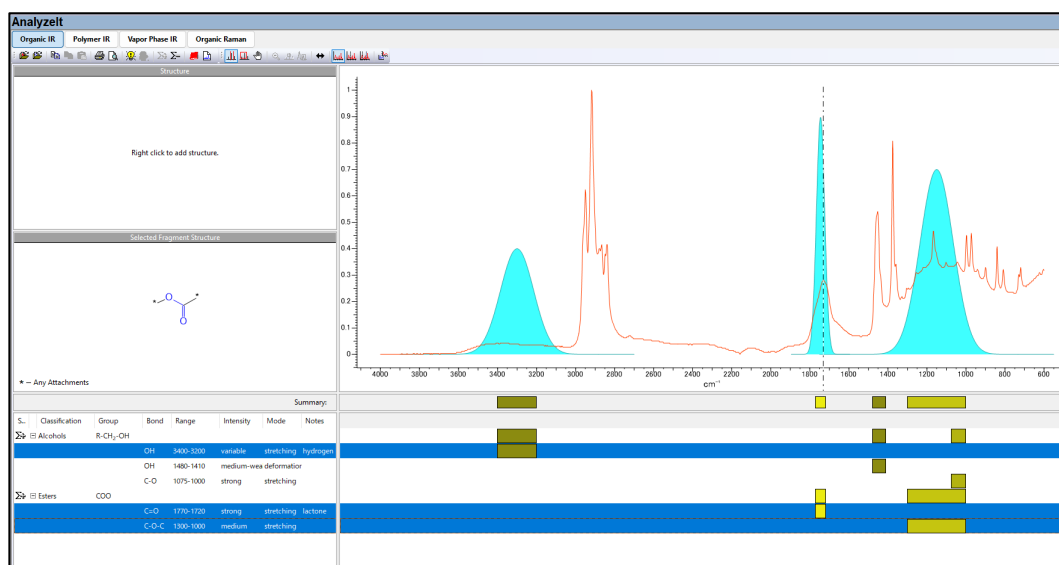


Fig. 5 KnowItAll Bundle : Functional Group Analysis Results (for Peaks that did not Match PP)

Shimadzu offers a proprietary library, the UV-Degraded Plastics Library, of infrared spectra for plastics degraded by ultraviolet light. It includes information about 14 types of plastics and infrared spectra acquired from samples exposed to ultraviolet rays for up to 550 hours (equivalent to about 10 years of UV exposure) using a super-accelerated weathering tester (Iwasaki Electric Co., Ltd.). This library was used for the search because of its applicability for analyzing microplastics. The search results (Fig. 6) show that the infrared spectrum from PP irradiated with ultraviolet rays for 150 hours was similar to the acquired spectrum, which confirmed that the sample was degraded PP. This demonstrates that Shimadzu's proprietary library can be used by any analyst to easily analyze microplastics.

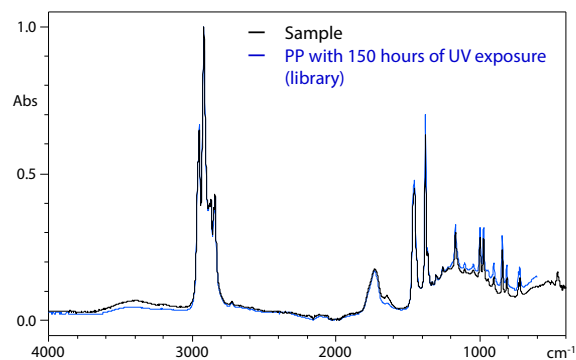


Fig. 6 UV-Degraded Plastics Library Search Results

■ Analysis of Recycled Plastic —Multi-Component Analysis

Recycled plastics are not composed of a single component but rather a composite of multiple materials. So infrared spectral analysis of plastics containing two or more types of components can be very complicated. For example, copolymers of polycarbonate (PC) and acrylonitrile butadiene styrene (ABS) offer the advantages of both PC and ABS polymers. They are used for a wide variety of applications, such as for automotive interior parts that require impact resistance, heat resistance, and superior formability, for office equipment, and even electrical parts due to their excellent performance as electrically insulative material.

Therefore, ID Expert from the bundled KnowItAll was used to analyze data measured with the single-reflection ATR method from a recycled PC/ABS material. This enabled the search results for everything from single or multiple components to be displayed automatically (Fig. 7). With multiple components, ID Expert can synthesize a composite spectrum from library spectra in the search results to display a residual spectrum based on measured data. Furthermore, the spectra can be linked to peak search or functional group analysis results that were not calculated by SearchIt data analysis.

It can also calculate PC/ABS ratios (0.38:0.62) by optimal spectral fitting.

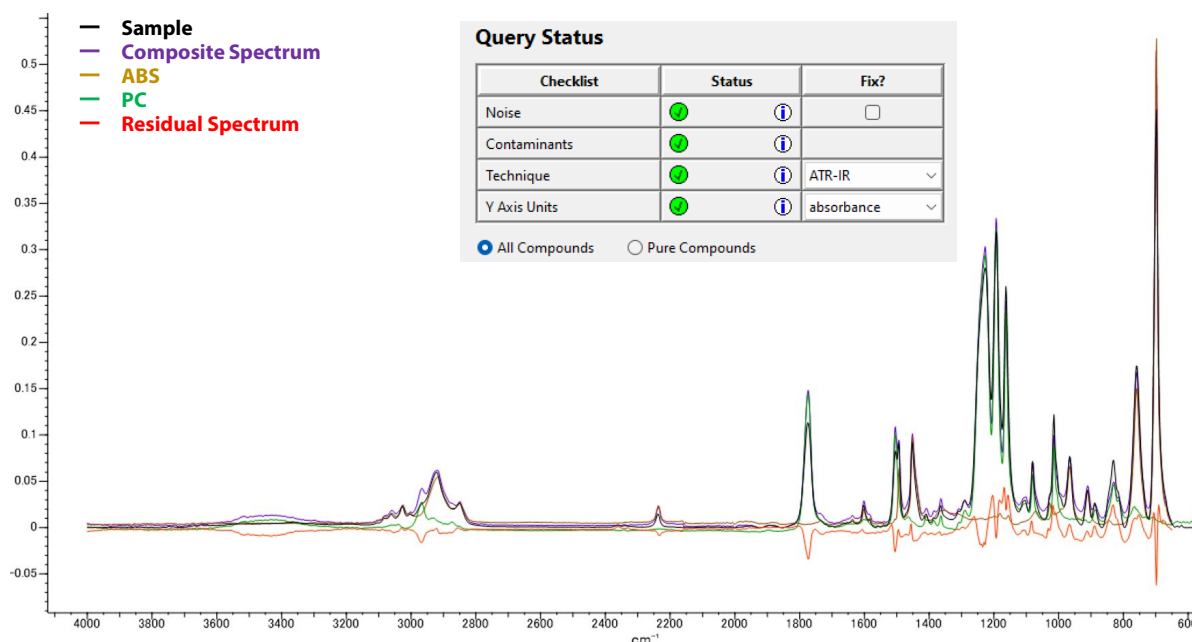
However, those ratios are calculated based on the infrared spectral area ratios without considering the molar absorption coefficient of the substances involved, which can differ from the actual ratios (PC:ABS = 0.25:0.75). Therefore, caution is required when using the ratio values.

In addition, ID Expert can automatically determine* the presence or absence of infrared spectral noise (based on estimated S/N values) and contaminants (defined as water vapor or carbon dioxide in the atmosphere). It also includes functionality for repeating searches.

* High noise or contaminants can be indicated with a red or yellow color by selecting the [Status] field inserted in Fig. 7.

■ Conclusion

An FTIR system in combination with a single-reflection ATR accessory can measure a variety of plastics. However, the analyst must be able to judge whether the software data analysis results are correct, which requires significant amounts of knowledge and experience. But with KnowItAll bundle described in this article, functional groups of specific peaks or multiple components can be easily analyzed, providing an effective way to improve the accuracy of data analysis.



1-Component Results		2-Component Results		3-Component Results		4-Component Results		Peak Results	Functional Groups
Score	Infrc Ratio	Name	Chemical Structure	Spectrum	<auto> (IR/ATR-IR)				
1	90.45	N.A.	Composite Spectrum						Composite spectrum
		0.62	Poly(acrylonitrile-co-butadiene-co-styrene)						ABS
		0.38	DFL-4038						PC
		N.A.	Residual Spectrum						Residual spectrum

Fig. 7 KnowItAll Bundle : ID Expert Search Results

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