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Application News

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Spectrophotometric Analysis

Investigation of Additives in Plastics by FTIR-ATR Spectroscopy

Commercially available plastic products contain polymers, such as polyethylene (PE) and polypropylene (PP), as their main components, in addition to various trace components that are added to enhance performance and maintain quality. Here we introduce an evaluation of additives used in plastic bags taking advantage of the high S/N ratio of the Shimadzu FTIR IRTracer-100 spectrophotometer.

Shimadzu IRTracer-100 FTIR Spectrophotometer and ATR Attachment MIRacle A

Single reflection ATR is commonly used as an infrared spectroscopy method for easy, non-destructive evaluation of additives in plastic products. Because measurement can be conducted without the need for pretreatment of the sample, the single reflection ATR method is widely used in various applications, including contaminant identification. As the depth of penetration of the infrared light into the sample surface using the ATR method is on the order of a few microns, this method can be used effectively, especially for additives that are localized on the sample surface.
As the content ratio of the target component becomes smaller, its peak intensity in the measured infrared spectrum will decrease accordingly, so an instrument with a high S/N ratio is required to obtain good evaluation results. The high 60000:1 S/N ratio of the Shimadzu FTIR IRTracer-100 ensures that clear and stable peak information is obtained from additives present even at trace levels. Fig. 1 shows an image of the Shimadzu FTIR IRTracer-100, and Fig. 2 shows an image of the MIRacle A Single Reflection ATR Accessory.

Fig. 1 Shimadzu IRTracer-100 FTIR Spectrophotometer

Fig. 2 MIRacle A Single Reflection ATR Accessory

Measurement

Using the single reflection ATR method, we measured the surface of commercially available plastic bags. A photograph of the plastic bags is shown in Fig. 3. The measurement conditions used are shown in Table 1, and the measurement results and spectrum search results are shown in Fig. 4.

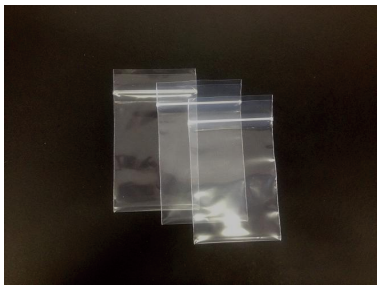

Fig. 3 Plastic Bags

Table 1 FTIR Measurement Conditions

Instruments	:	IRTracer-100, MIRacle A (Diamond prism – ZnSe support element)
Resolution	:	4 cm^{-1}
Accumulation	:	20
Apodization	:	Happ-Genzel
Detector	:	DLATGS

The results obtained from analysis of the plastic bag are consistent with the library spectrum of polyethylene, indicating that the principal component is polyethylene. Fig. 5 shows an expanded view in the vicinity of the baseline of Fig. 4. It is believed that the arrow-indicated peaks in the figure are derived from additives present in the plastic bags, and these are consistent with the spectra of aliphatic amides such as oleamide. Aliphatic amides are one type of substance added to resins to serve as a lubricant.

Also, after completing the measurement shown in Fig. 4, the plastic bag sample was removed from the ATR prism, and without washing the prism, another measurement was taken. The results are shown in Fig. 6. Here, the results resemble the spectrum of the aliphatic amide shown in Fig. 5, indicating the possible transfer of the additive in the plastic bag to the ATR prism.

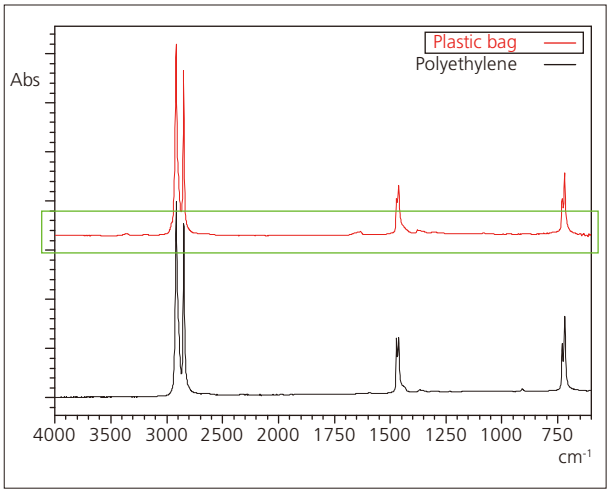

Fig. 4 Infrared Spectrum and Search Result for Plastic Bag

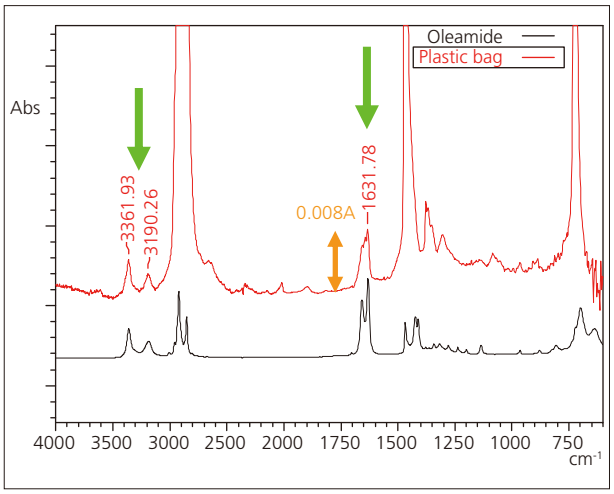

Fig. 5 Expanded Infrared Spectrum of Figure 4 and Spectrum of Oleamide

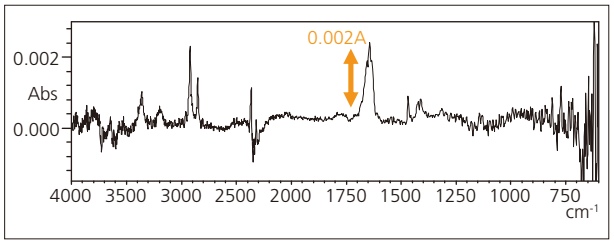

Fig. 6 Infrared Spectrum of Substance Transferred to ATR Prism

The peaks associated with the aliphatic amide that appeared in the measurement results of Figs. 5 and 6, respectively, show very weak intensity with absorbance values less than 0.010 A. Also, there is a peak in the vicinity of 1631 cm^{-1}, a region that easily reflects the presence of water vapor in the air. Deeming that purging the measurement system with dry air or nitrogen gas was unnecessary led to the clear detection of these minute peaks.

Investigation of Repeatability of Small Peaks

It is generally possible to gain an understanding of content level using the height and area value of the peak originating from the target component, but for small peaks derived from additives, it is important to grasp the measurement repeatability. Ten continuous repeat measurements were taken with a plastic bag sample in close contact with the ATR prism. The peak area values of the peak in the vicinity of 1631 cm^{-1} and the calculated CV values are shown in Table 2. The integration was repeated twenty times and one time, and these values were compared, respectively, with those obtained with the Shimadzu IRPrestige-21. The better stability of measurement values obtained with the IRTracer-100 is attributed to its higher S/N ratio.

Table 2 Peak Area and CV Values

	IRPrestige-21		IRTracer-100	
	No. of Integrations 20 times	No. of Integrations 1 times	No. of Integrations 20 times	No. of Integrations 1 times
Area value	1.034	0.956	1.039	1.034
	1.049	1.006	1.025	1.021
	1.034	1.138	1.015	0.957
	1.008	1.052	1.006	0.952
	1.029	0.888	0.991	1.055
	0.967	0.974	0.996	1.055
	0.983	0.965	1.001	0.940
	0.967	0.970	0.972	0.995
	0.972	1.038	0.972	0.995
	0.957	1.011	0.982	0.995
CV value %	3.46	6.72	2.19	4.16

*The displayed area values represent normalized values based on the average of 10 repeat measurements.

Conclusion

Here we introduced an evaluation of trace additives in plastic resin. The high S/N ratio of the Shimadzu FTIR IRTracer-100 enabled stable and clear acquisition of minute peaks originating from additives present at minute levels.

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