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Application News

No.A456

Spectrophotometric Analysis

Identification of Multi-Component Contaminant using Advanced Contaminant Analysis Program

When conducting contaminant analysis, it is often the case that the contaminant consists of a mixture of substances. A spectrum search for component mixtures typically requires that the search criteria be changed to identify components other than the principle constituent, and this necessitates some degree of expertise in reading spectra. The Contaminant Analysis Program developed by Shimadzu, as introduced in Application News No. A400, is effective in just such cases. Here, we introduce the contaminant analysis program which is included in the new LabSolutions IR software.

Upgraded Contaminant Analysis Program

LabSolutions IR incorporates the new version of the contaminant analysis program with greatly enriched features. This version of the contaminant analysis program offers two key improvements over its predecessor, as described below.

(1) Enhanced contaminant database now consisting of 553 spectra
Identification of many more contaminants is now possible, greatly reducing the number of "no hit" search results.

(2) Adoption of new algorithm to improve search accuracy
Previously, "hits" were sometimes designated for nonexistent inorganic components. The newly implemented search algorithm greatly improves identification accuracy, particularly with respect to inorganic substances.

The ease of use of the Contaminant Analysis Program is illustrated by the following windows for launching and selecting the easurement method used.

Fig. 1 Window for Launching Contaminant Analysis Program

Click the "Contaminant Analysis Program" command button shown in Fig. 1 to start the analysis program. Then, just click the appropriate method button in the measurement method section window shown in Fig. 2.

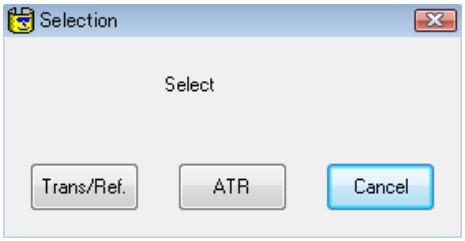

Fig. 2 Measurement Method Selection Window

The time spent conducting analysis by the conventional manual search method typically requires 20 minutes or more depending on the sample. Using this program, however, requires nothing more than selecting the measurement method. Analysis results are often obtained within seconds.

Analytical Results for Resin

Various types of additives are added to resin materials to enhance their material properties. The addition of these additives may result in their peaks overlapping those of the resin peaks, thereby complicating and adding a level of difficulty to the analysis. Here we introduce the results of analysis of vinyl chloride resin (PVC). Measurement was conducted by the single reflection ATR method. The measurement conditions are shown in Table 1, and the obtained ATR spectrum is shown in Fig. 3.

Table 1 Instrument and Analytical Conditions

Instruments	: IRPrestige-21, DuraSamplIR-II
Resolution	: 4 cm^{-1}
Accumulation	: 45
Apodization	: Happ-Genzel
Detector	: DLATGS

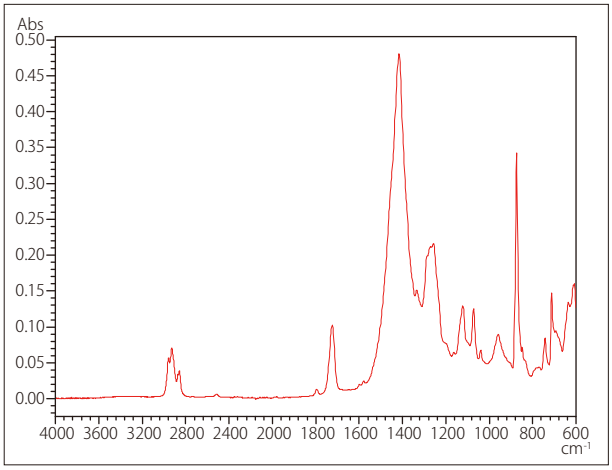

Fig. 3 ATR Spectrum of PVC Resin

The analytical results obtained using the Contaminant Analysis Program with respect to the ATR spectrum of Fig. 3 are shown in Fig. 4 and Fig. 5.

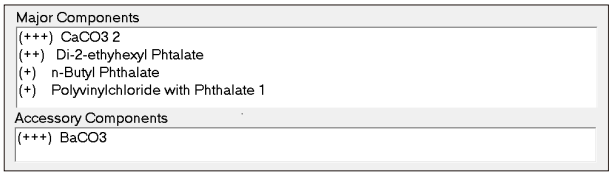

Fig. 4 Analytical Results 1

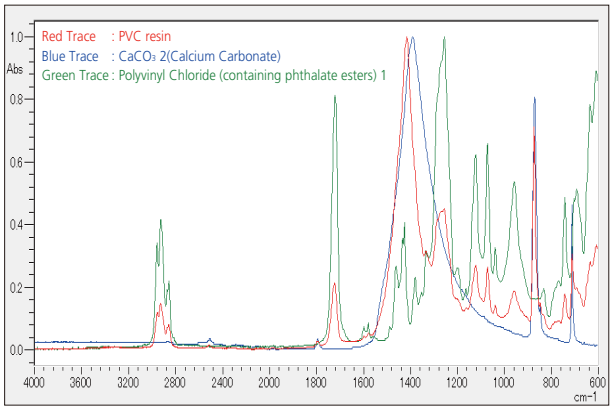

Fig. 5 Analytical Results 2

The analysis results indicated hits not only on the phthalic acid ester present in the PVC, but also on the calcium carbonate. The additives phthalic acid ester and calcium carbonate are commonly used as a plasticizer and non-reinforcing filler, respectively, in PVC products.

Analytical Results for Rubber

Rubber materials, like resin materials, commonly contain additives. Here, we introduce the results of analysis of ethylene propylene diene (EPDM) rubber. Measurement was conducted by the single reflection ATR method, and the obtained ATR spectrum is shown in Fig. 6

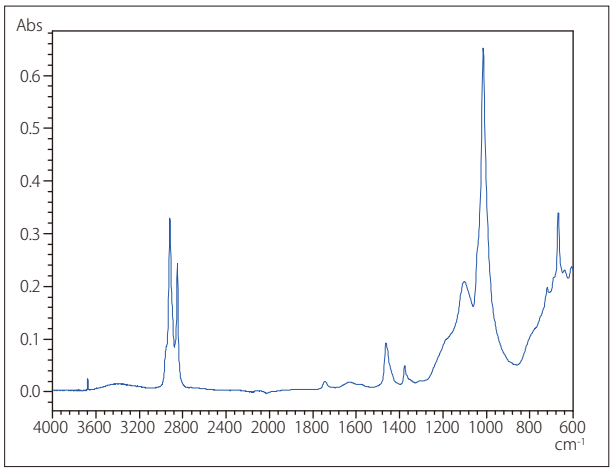

Fig. 6 ATR Spectrum of EPDM

The results of analysis of the obtained ATR spectrum using the Contaminant Analysis Program are shown in Fig. 7 and Fig. 8.

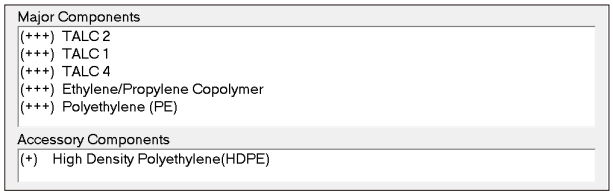

Fig. 7 Analytical Results 3

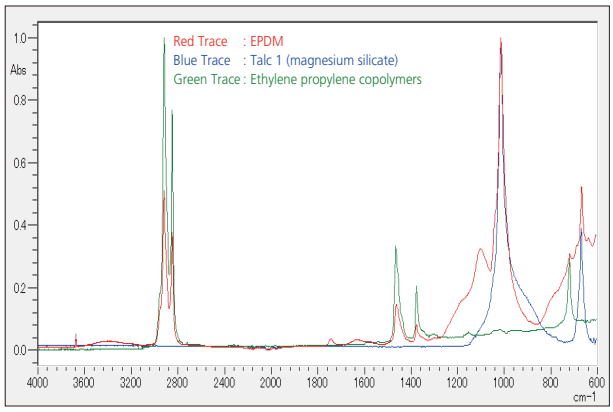

Fig. 8 Analytical Results 4

The analysis results indicated hits not only on the rubber substance ethylene-propylene, but also on the additive talc. It should be noted that with respect to EPDM, ethylene-propylene rubber (EPM) and EPDM polymer cannot be distinguished in the infrared spectrum[1)].

Conclusion

Here, we introduced examples of analysis of materials consisting of resin and rubber mixtures using the upgraded Contaminant Analysis Program. Resin and rubber materials often contain inorganic substances, but these inorganic substances can now be easily detected using the upgraded Contaminant Analysis Program. In cases where even more accurate confirmation of inorganic substances is required, the use of an instrument specifically designed for analysis of inorganic substances, such as an X-ray fluorescence spectrometer, is recommended for validation.

[References]
1) JIS K 6230 Rubber - Identification - Infrared spectroscopic method

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