Identification of Polymeric Samples FT-IR and Sadtler Database Search: An Example

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Abstract

The identification of polymer samples presents a unique challenge. Seldom does one encounter a single component system. Most commonly, one is faced with a fully formulated composition comprising the major polymer as well as organic (impact modifier, processing aid, plasticizer) and inorganic (filler, flame retardant) components. The use of FT-IR coupled with spectral searching of Bio-Rad's Sadtler FT-IR databases provides for an efficient methodology to the identification problem. This note presents a typical example for an unknown sample analyzed in our laboratory.

Methods

A thin slice of the unknown sample was obtained by microtoming. The FT-IR spectrum was acquired on an Analect FT-IR microscope. 64 scans were co-added at 4 cm^{-1} resolution. The sample was extracted in $CH Cl_3$.

The soluble residue was also run on the FT-IR microscope under similar conditions. Following partial dissolution in THF, the insoluble fraction was separated and run as a KBr pellet. 100 scans were co-added at 4 cm^{-1} resolution.

All FT-IR spectra were baseline corrected and converted to Sadtler's format. All spectra were also normalized using the Sadtler software. The Euclidean Distance algorithm was employed. The search range was set to a lower limit of 800 cm^{-1} for those samples analyzed by FT-IR microscopy due to reduced MCT detector range.

Analysis: Sadtler Databases Spectral Searching

The original sample spectrum was searched in the Monomers and Polymers Database. The results are shown in Figure 1. The Hit List showed the presence of PVC as the major component. The Hit Quality Index (HQI) indicated that the unknown sample had a different formulation than the PVC formulations available in the database.

Based on our preliminary identification, the sample was dissolved in THF to remove the PVC. The insoluble fraction spectrum, Figure 2, indicated the presence of an inorganic material. It was searched using the Inorganics and Polymer Additives Libraries. A good match to the spectrum of $CaCO_3$ was obtained. The $CH Cl_3$ extract spectrum was compared to the Hit List library spectra obtained for the original unknown sample.

It was concluded that only very small amounts of PVC were still present. The extract spectrum was then searched using the Monomers and Polymers and Plasticizers Databases. The results are illustrated in Figure 3. The material was identified as Elvaloy, a vinyl acetate/carbonmonoxide/ ethylene co-polymer*, which is a PVC compound modifier. The HQI value of 977 was attributed to baselining differences, residual PVC and the possibility of different monomer ratios in our materials than those present in the library compounds.

Conclusion

Based on the results below it was possible to identify the unknown sample as a PVC formulation containing $CaCO_3$ and Elvaloy modifier. The use of the Sadtler Spectral Databases enabled the immediate identification of the major polymeric component, the appropriate choice of extraction solvents and the identification of the additives.

Without the use of the spectral databases, a much more laborious procedure of manual spectral comparisons would have been necessary with no guarantee of success.

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Editor's Note

*This description of Elvaloy™ is taken from Index of Polymer Trade Names, VCH Publishers, New York, NY. Users of Bio-Rad's Sadtler databases will find that the Bio-Rad's editors include many important physical, chemicals, and commercial information properties with each spectrum.

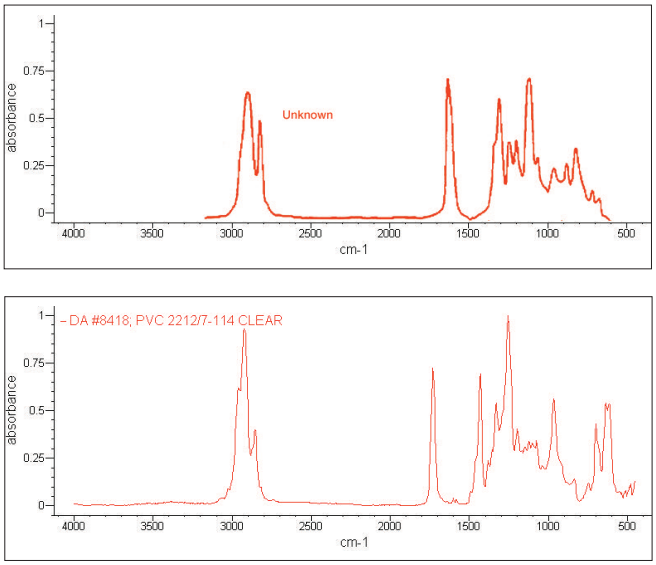

Fig. 1.

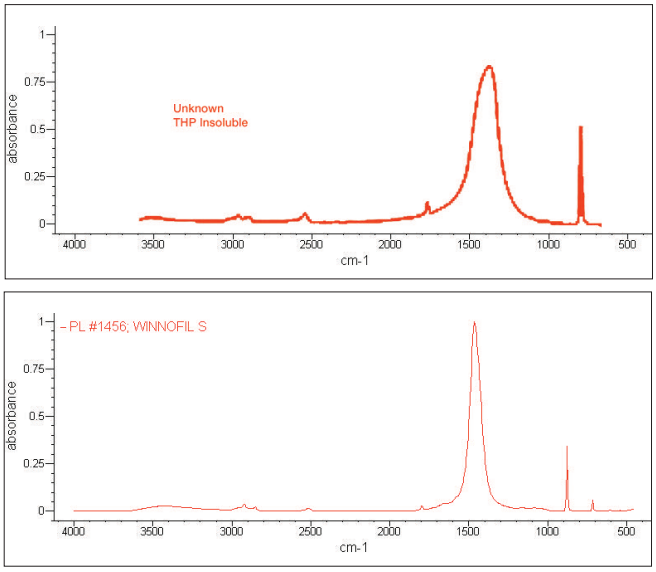

Fig. 2.

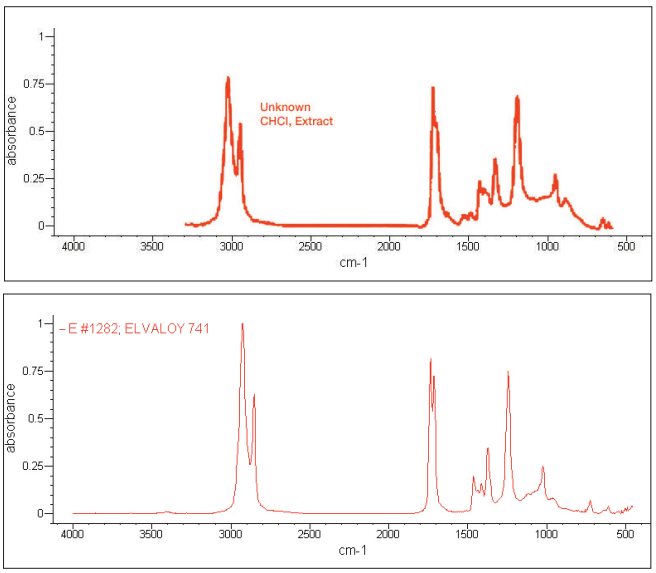

Fig. 3.

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