B195 Examination of Plastic Shopping Bags Using Attenuated Total Reflectance/ Fourier Transform Infrared Spectrometry (ATR/FTIR)

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After attending this presentation, attendees will understand how to obtain ATR infrared spectra from polymer films with high signal-to-noise ratios. Attendees will also understand the varied compositions of common plastic shopping bags and the capability of ATR/FTIR to differentiate shopping bags from different sources.

This presentation will impact the forensic science community by providing trace evidence examiners with knowledge of the composition of a common type of polymer material that may occur as forensic evidence. The presentation will also emphasize the value of paying attention to low levels of additives in polymeric products.

Plastic bags may appear in criminal investigations as packaging for many different types of evidence; however, only three publications have dealt with the forensic examination of plastic bags. Roux et al. analyzed a number of different types of bags (e.g., freezer bags, vegetable storage bags, sandwich bags, and general storage bags) purchased in Australia and in Asian countries.[1] Infrared spectrometry proved (along with visual examination) to be the most useful method for discriminating bags from different sources. Causin et al. examined shopping bags obtained from supermarkets in the Venice, Italy, area, using infrared spectrometry, thickness measurements, and differential scanning calorimetry.[2] The infrared spectra of the shopping bags fell into three categories: (1) pure polyethylene; (2) polyethylene containing calcium carbonate ($CaCO_3$); and, (3) polyethylene with a carbonyl stretch at 1740cm^{-1}. Hashimoto et al. analyzed plastic bags specially prepared by Japanese manufacturers using X-ray diffraction, infrared spectrometry and optical microscopy.[3]

This research used ATR/FTIR to examine shopping bags used in the United States and compare the results with previously published work.[1-3] Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA) were applied to the data to see if these methods yielded greater differentiation of the spectra compared to simple visual comparison. Forty different plastic shopping bags were obtained in the Washington, DC, area from supermarkets, department stores, restaurants, and hardware stores. ATR/FTIR spectra were obtained from five different non-printed areas on each bag. The ATR/FTIR spectra were obtained using a minimum of four layers of bag material to insure high signal-to-noise ratios to facilitate detection of the peaks of minor constituents. The spectra were scanned from 525cm^{-1} to 4,500cm^{-1} at 4cm^{-1} resolution; 128 scans were collected for each spectrum.

The shopping bags were found to be homogeneous and comprised of polyethylene, usually with an inorganic filler. Most of the shopping bags were found to contain $CaCO_3$. As Causin et al. found in the shopping bags they examined, the concentrations of $CaCO_3$ showed considerable variation.[2] Two of the bags contained talc and one bag contained both $CaCO_3$ and talc. Talc and $CaCO_3$ were confirmed by X-ray diffraction.

The spectral data from 525cm^{-1} to 1,800cm^{-1} were analyzed by PCA. Prior to PCA, the ATR /TIR spectra were scaled by setting the absorbances of the most intense peak of polyethylene to the same value. Some of the scaled spectra had significant baseline offsets; these were removed by taking the first derivative of the spectral data. Finally, the first-derivative data were autoscaled prior to PCA. The first factor extracted by PCA represented the quantity of $CaCO_3$ present in the bags, while the second factor represented the quantity of talc. LDA was performed using the extracted principal components and placed the ATR/FTIR spectra in seven groups with 100% accuracy.

Reference(s):

1. Roux C., Bull S., Goulding J., Lennard C. Tracing the source of illicit drugs through plastic packaging—a database. *J Forensic Sci* 2000:45(1):99–114.
2. Causin V., Marega C., Carresi P., Schiavone S., Marigo A. A quantitative differentiation method for plastic bags by infrared spectroscopy, thickness measurement and differential scanning calorimetry for tracing the source of illegal drugs. *Forensic Sci Int* 2006:164: 148-154.
3. Hashimoto T., Howitt D.G., Land D.P., Tullener F.A., Springer F.A., Wang S. Morphological and spectroscopic measurements of plastic bags for the purpose of discrimination. *J Forensic Sci* 2007:52(5):1082-1088.

Plastic Bags, Infrared Spectrometry, Principal Component Analysis

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