B92 Comparing X-Ray Diffractometry (XRD) and Fourier Transform Infrared (FTIR) Spectrometry for the Analysis of Forensic Evidence

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After attending this presentation, attendees will understand the value of XRD as a method of analysis applicable to a wide variety of forensic evidence, including soil, drugs, plastics, and papers. Attendees will become aware of instances in which XRD is superior to FTIR, particularly in providing compositional information about samples. Attendees will also become aware of the replacement of large XRD facilities with benchtop XRD units and the availability of new solid-state detectors that obviate the need for liquid nitrogen cooling.

This presentation will impact the forensic science community by increasing awareness of the value of XRD as a replacement for or supplement to FTIR in the analysis of certain types of forensic evidence.

Most forensic science laboratories tend to use FTIR as their go-to analytical method for the identification of unknown samples. The FTIR spectra of unknowns may be searched for in a variety of spectral libraries (e.g., drugs and polymers); even if no spectral match for the unknown is found, structural information about the unknown can be obtained. FTIR instruments are relatively inexpensive and well within the budgets of most forensic science laboratories. XRD has long been recognized as being similar to FTIR in the richness of the data it provides. For example, the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG) places XRD in the same category of analytical techniques as FTIR, Raman scattering, and mass spectrometry. In the past, XRD instrumentation was large (often requiring its own laboratory with attendant cooling units) and the detectors required liquid nitrogen cooling to function. New benchtop XRD instruments have reached the market; these have a small footprint and their new solid-state detectors eliminate the need for liquid nitrogen cooling. Forensic science laboratories should consider adding XRD to their repertory of analytical techniques. XRD can be particularly useful for the identification of minor crystalline constituents of samples where the infrared absorptions of these constituents are weak due to their low concentrations or where their absorptions are obscured by those of more abundant components of the samples.

To compare XRD and FTIR, two types of forensic samples were analyzed by both techniques. Sixteen different brands of trash bags and 28 different brands of black electrical tape were analyzed by both methods. These are two frequently encountered types of forensic evidence. The FTIR spectra of both the trash bags and the electrical tapes were dominated by absorptions of the polymers comprising the samples, with minor contributions from inorganic additives. In some cases, the infrared absorptions of the minor constituents were masked by the infrared absorptions of the polymer. The XRD patterns provided more information and better discrimination among samples than FTIR. For trash bags (composed primarily of polyethylene), the XRD patterns exhibited a clear distinction between Low-Density Polyethylene (LDPE) and Linear Low-Density Polyethylene (LLDPE). The trash bags were found to contain crystalline additives in varying concentrations (talc, calcite, or a combination of talc and calcite), while the electrical tapes contained a variety of additives whose XRD patterns were readily distinguished from one another. The differentiation of forensic samples is particularly important when questioned and known samples are compared in order to identify possible sources of the questioned samples.

This research demonstrates the value of XRD in analyzing forensic evidence, particularly when it is important to identify minor constituents whose infrared absorptions are very weak.

X-Ray Diffraction, FTIR, Analysis