Portable Infrared Spectroscopy Chemical Detectors for Identification of Unknown Liquids and Solids

Portable Fourier Transform Infrared spectroscopy (FTIR) chemical detectors are instruments used to identify unknown or suspect materials. Applications include investigations of clandestine labs, illegal dumping sites, suspected arson, identification of chemical spills, unlabeled containers or drums, and screening suspicious substances/packages. FTIR instruments may be used in combination with other technologies (e.g., Raman spectroscopy) to improve detection and confidence in identification.

Overview

Infrared spectroscopy (IR) deals with the infrared region of the electromagnetic spectrum, which includes light with longer wavelengths and lower frequencies than visible light. IR exploits the fact that molecules absorb specific frequencies of light that are characteristic of their structure. The pattern of light absorption is called a spectrum, which constitutes a fingerprint for that particular chemical (spectra is the plural of spectrum). Different types of IR instruments include non-dispersive, dispersive, photoacoustic, and Fourier Transform, the latter of which is the focus of this TechNote. FTIR instruments provide information about sample composition by attempting to match the spectral fingerprint of an unknown sample to a library containing spectral fingerprints for thousands of known compounds. Typically, computerized spectral matching algorithms select several candidate compounds from the library with spectral features most similar to the unknown sample. These are then ranked based on degree of similarity between the candidate and the unknown sample spectral features and display the ranked list to the user.

Portable FTIR instruments are smaller, easier-to-use, and less costly than their laboratory-sized counterparts. Most weigh less than five pounds (an older model in a transport case weighs 15 pounds) and run times vary from two to six hours. FTIR instruments consist of a display, control buttons, data ports, and a sampling arm (anvil). The smaller handheld units are ruggedized to withstand harsh environments, resistant to shock, and submersible for decontamination. FTIR instruments allow emergency responders to quickly confirm, rule out, or identify a suspect material.
**Instrument Features**
Selection considerations for portable FTIR instruments include ease and speed of sample analysis, and ease of use, including carrying, handling (some models have slip-resistant grips), and the quality of the button and screen interface.

**User Interface**
The smaller handheld FTIR instruments have relatively simple button interfaces with newer models also having touch screen capability. The ease of manipulating buttons and viewing the screen in personal protective equipment (PPE) and bright or dark situations is critical for use in potentially hazardous environments. Models that do not have back-illuminated buttons can be more difficult to use in low light, and the number of steps (button pushes) required to analyze a sample affects ease of use. To minimize overall size, portable FTIRs have relatively small screen sizes. Because of this, it is important that the screen has sufficient resolution, brightness, and clarity, and uses a font of sufficient size, particularly for data analysis or closer examination of spectra.

**Data Transmission/Communication**
Some FTIR instruments have only a cellular data transmission option, which could be limiting if there is a low or no cellular signal. Others have radio frequency wireless transmission capability, but there must be a clear line of sight. If data cannot be wirelessly transmitted, the data must be retrieved using an external drive such as an SD card. However, SD cards are tiny devices that can be difficult to manipulate while wearing heavy gloves.

**FTIR Applications and Complementary Instruments**
FTIR instruments can identify a wide range of chemical threats including toxic industrial chemicals, fuel products, fertilizers, pesticides, and drugs; however, a significant limitation of FTIR is that it is applicable only to compounds with covalent bonds. FTIR cannot be applied to elemental substances like metals (iron or aluminum), non-metals (sulfur or phosphorous), and salts (sodium or calcium chloride). In addition, FTIR is not a highly sensitive technique and is not effective for dilute solutions of chemicals with concentrations below about 10 percent.

Raman spectroscopy is also a rapid and nondestructive technique used to identify unknown material and is complementary to FTIR. Unlike FTIR, Raman is not affected by strong infrared absorbers like glass or water. Therefore, Raman measurements can be performed on material without removing it from its container for most translucent or transparent glass, bags, and envelopes. However, Raman does not work well on samples having colored components or compounds that fluoresce.

Both techniques are often employed during emergency responses to identify spills, residues, material in unlabeled containers, or other potential threat material. Identification of unknown solids and liquids from toxic industrial chemicals and drug precursors to explosives and chemical warfare agents is possible with FTIR and Raman spectroscopy. In practice, most emergency responders use both of these techniques. While little cost savings is realized, one product currently available does combine both FTIR and Raman into a single device.

**Data Manipulation and Output**
While FTIR instruments can readily identify most single component samples, multi-component and complex samples may be more difficult to accurately identify. More advanced data manipulations include spectral subtraction and spectral overlays, but the smaller handheld instruments require that these operations be conducted on a separate laptop computer. In addition, the ability to transmit data wirelessly is required to transmit results to incident command or for reach-back expert support.