FROM SENSING TO MAKING SENSE

Reference Spectra For The Identification Of Chemical Warfare Agent Simulants

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Infrared spectroscopy is one of the main approaches to detect and identify chemical warfare agents (CWAs). The technique is versatile, can be used in field conditions using portable instruments, and is capable of identifying small amounts of various agents. However, in real-world scenarios, many other compounds with similar chemical structures and properties (e.g., organophosphorus compounds from fertilizers and pesticides) are present that can obscure the spectral features from the material of interest. As a results, the measured infrared data consist of overlapping spectral contributions from many different compounds.

Extraction of relevant information from such convoluted spectra requires processing of the measured data. Such processing is often done using chemometric approaches such as principal component analysis (PCA), ordinary least square (OLS), partial least square (PLS) multivariate curve resolution (MCR), etc. However, no matter what approach is used, high-quality reference data is needed as input date to provide accurate deconvolution of the measured convoluted spectra. Without such high-quality input data, interpretation of the measured spectra is challenging at best and impossible at worst.

Our DTRA-funded project focuses on the high-temperature properties and chemistry of CWAs and their simulants. As part of this work, we are measuring high-resolution infrared spectra that are suitable as reference data during the analysis of raw data. The spectra are measured at various temperatures, ranging from 20 °C to 250 °C, with a spectral resolution of 0.1 cm-1.

Using a kinetic FTIR, our initial set of reference spectra has been measured for diisopropyl methylphosphonate (DIMP), a simulant for sarin. The high-resolution measurements required optimizing many aspects of the instrumental conditions. We will demonstrate how these reference spectra can be used during the analysis of infrared spectra to extract information about the identity of specific compounds and their concentrations.

Measuring high-resolution reference spectra of a wide range of relevant compounds will provide DTRA and other stake holders with the ability to monitor for the presence of chemical agents via infrared spectroscopy and performing reliable analysis of the data.

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