

## Field-Portable GC/MS Characterization and Testing

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The purpose of the research reported here was to determine the detection, identification, and quantitation capabilities of a field-portable GC/MS instrument for classes of compounds of interest in homeland security and environmental monitoring applications. The instrument consisted of a low thermal mass gas chromatograph (LTM-GC) coupled to a cylindrical ion trap (CIT) mass spectrometer and packaged in a small footprint, ruggedized form factor. The vacuum system of the instrument was mounted on a shock-absorption platform within the instrument package for ruggedization.

Compounds studied included chemical weapons (CW) simulants, high explosives, pesticides, and related compounds. The instrumentation consisted of a low-thermal-mass (LTM) gas chromatograph coupled to a cylindrical ion trap (CIT) mass spectrometer. The instrument was also equipped with a direct-injection inlet which allowed desorption of samples from a solid-phase microextraction (SPME) fiber directly into the vacuum of the mass spectrometer.

Liquid injections of the CW simulants dimethyl methylphosphonate (DMMP, a G-agent simulant) and 2-chloroethyl ethyl sulfide (CEES, a mustard (H-agent) simulant) yielded absolute limits of detection (LODs) of approximately 2 pg for both compounds. With a chromatographic run-time of ~3.25 minutes, the total analysis time including sampling was under 10 minutes. Chromatographic and mass spectral quality will be illustrated during the presentation.

Research into the detection and identification of high explosives focused on optimization of the column temperature program and the temperatures of static heated zones of the instrument (i.e. the injector, guard columns, and CIT assembly), to minimize thermal degradation of the compounds while also minimizing analysis time. The LTM-GC allowed very rapid temperature ramping, so that even low volatility compounds such as trinitrotoluene (TNT) could be eluted in less than two minutes. Representative chromatograms and MS as well as MS/MS spectra will be presented.

The direct-SPME interface allowed for analysis of CW simulants and explosives via the mass spectrometer without prior GC separation. For both classes of compounds, desorption profiles of less than 30 seconds were achieved. Data illustrating the rapid desorption profiles of the analytes from the fiber will be shown as well as the resulting mass spectra.