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Quantitation of Chemical Warfare Agents using a Field-Ready Mass Spectrometer

ABSTRACT

This application note discusses the analysis of chemical warfare agents, as illustrated by two simulants, dimethyl methyl phosphonate (DMMP) and 2-chloroethyl ethyl sulfide (CEES). The analysis uses the Griffin 400 GC/MS (the Griffin 450 may also be used to perform the same analysis) to determine DMMP and CEES at levels of 22.5 pg/ μ L and 15.0 pg/ μ L, respectively.

INTRODUCTION

Sensitive and selective detection and identification of a wide variety of chemical species has become a necessity in many applications including the quantitation of chemical warfare (CW) agents, explosives, environmental pollutants, and other toxic industrial compounds and materials (TICs/TIMs). Field-deployable sensors are preferred in many instances, because valuable time, resources, and chemical information are conserved by performing analyses directly in the field, rather than retrieving samples to be studied at a later time in the laboratory. Griffin's family of compact, portable tandem mass spectrometers based on a cylindrical ion trap (CIT) mass analyzer^{1,2} has been developed to fulfill this need (see Figure 1).

The Griffin 400 - Mobile GC/MS/MS



EXPERIMENTAL

One applicable analysis method supported by the Griffin series of instruments is the analysis of chemical warfare agents. This is illustrated by analyzing the G-Agent simulant dimethyl methyl phosphonate (DMMP) and the Blister Agent simulant 2-chloroethyl ethyl sulfide (CEES). Standard samples of DMMP and CEES were prepared at various concentrations in isopropyl alcohol (IPA).

The field-ready CIT mass spectrometer used in this work was equipped with a low thermal mass gas chromatograph (LTM-GC), which works to quickly separate and introduce the sample to the analyzer. The complete system included a split/splitless injector, the LTM-GC, and the mass spectrometer.

The system used helium as the carrier gas. The injector was set in split mode, with a split ratio of 15:1 and a temperature of 250°C. All transfer lines were set at 250°C. All samples were injected using a volume of 1 μ L.

The samples were separated into their components using a Rts-1MS column, 30m x 0.25mm x 0.25 μ m (Restek, Bellefonte, PA), with a column flow of 1 mL/min. The separation used a temperature ramp that started at 50°C and rose at 20°C per minute to 118°C. From 118°C it rises at 50°C per minute to the final temperature of 280°C.

The sample components were ionized via electron ionization from a heated-filament electron source. The ionization time was set at 25ms.

RESULTS / DISCUSSION

The total ion chromatogram obtained for a 1 μ L injection of 1145 pg/ μ L DMMP solution is shown in Figure 2. The DMMP is separated from the solvent peaks and easily discernible from the baseline.

Figure 3 illustrates the mass spectrum obtained for DMMP. For quantitation of DMMP, the mass spectral peak areas for the ions at m/z 79, 94, 111, 124 and 126 were summed for each concentration using the reconstructed ion chromatogram (RIC) function in the Griffin software. The resulting peak was then integrated.

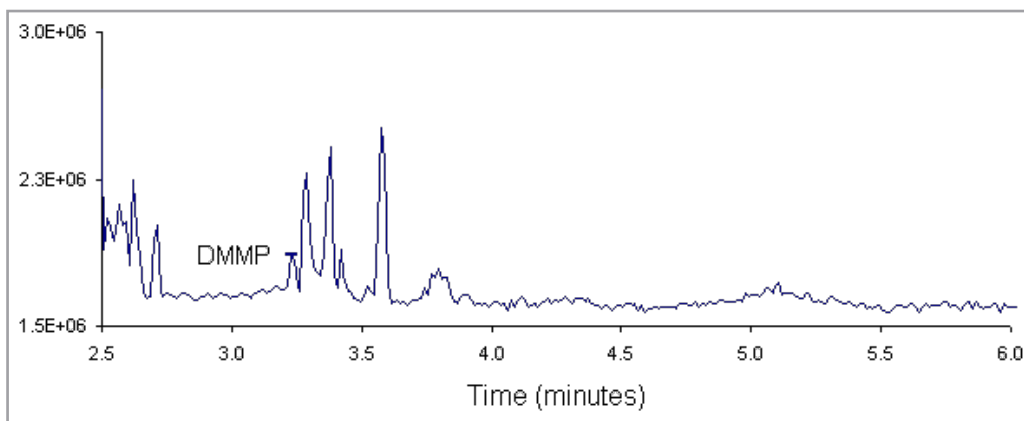


Figure 2. Total ion current trace for the DMMP solution.

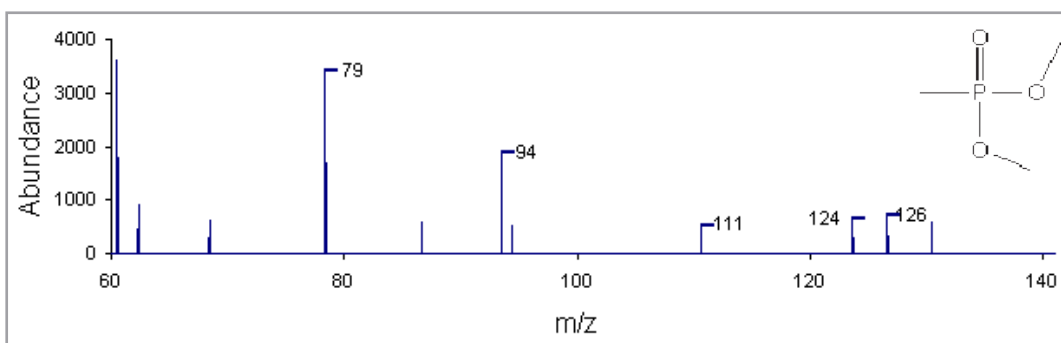


Figure 3. Mass spectrum of DMMP.

The total ion chromatograph obtained for a 1 μ L injection of 1070 pg/ μ L CEES Solution is shown in Figure 4. The CEES is well-separated from the solvent peaks and easily discernible from the baseline.

Figure 5 illustrates the mass spectrum obtained for CEES. For quantitation of CEES, the mass spectral peak areas for the ions at m/z 75 and 124 were summed for each concentration using the reconstructed ion chromatogram (RIC) function in the Griffin system software. The resulting peak was then integrated.

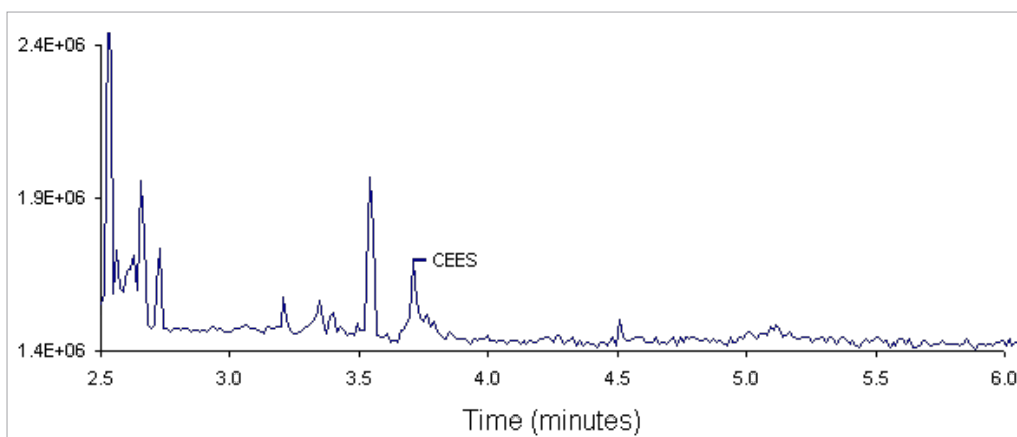


Figure 4. Total ion current trace for the CEES solution.

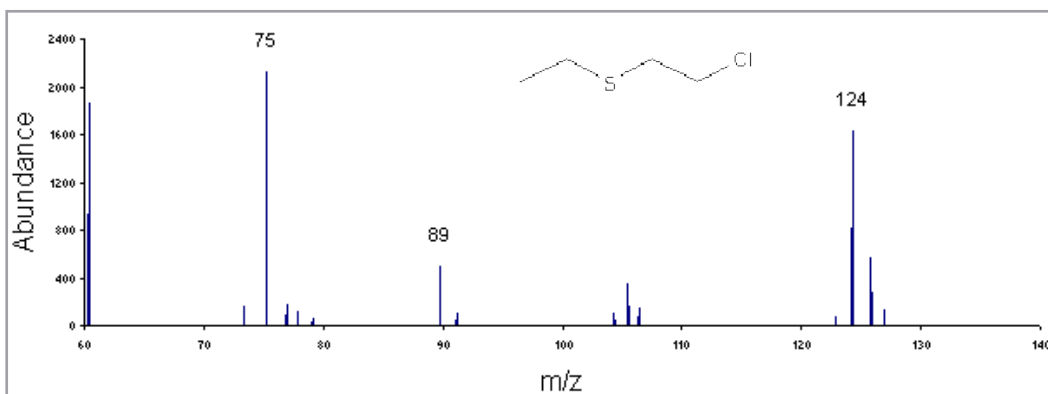


Figure 5. Mass spectrum of CEES

Figure 6 illustrates the calibration curve obtained for DMMP over the concentration range from 115pg/ μ L to 2290 pg/ μ L. This calibration curve, together with blank injections of IPA run under the conditions described previously, indicate a limit of detection (LOD) of 22.5pg/ μ L.

Figure 7 illustrates the calibration curve obtained for CEES over the concentration range from 107pg/ μ L to 2140 pg/ μ L. This calibration curve, together with blank injections of IPA run under the conditions described previously, indicate a limit of detection (LOD) of 15.0pg/ μ L.

As this experiment illustrates, chemical warfare agents as represented by the simulants DMMP and CEES are detectable to low levels using the Griffin 400 GC/MS. Combining this low level of detection with the portability of the Griffin 400 creates a combination that can be used in varying areas and conditions for quick analysis of samples.

These data represent typical results.

REFERENCES

1. Wells, J.M.; Badman, E.R.; Cooks, R.G. *Anal. Chem.* 1998, 70, 438-444.
2. Patterson, G.E.; Guymon, A.J.; Riter, L.S.; Everly, M.; Griep-Raming, J.; Laughlin, B.C.; Ouyang, Z.; Cooks, R.G. *Anal. Chem.* 2002, 74, 6145-6153.

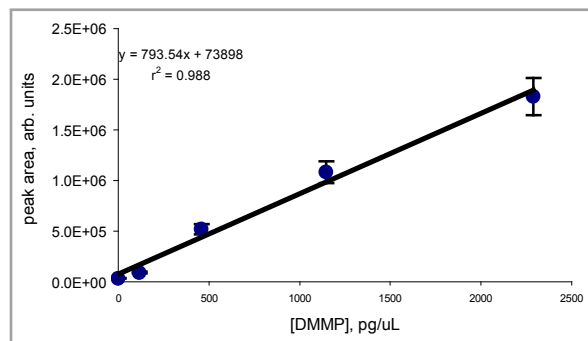


Figure 6. Calibration curve obtained for DMMP over the concentration range 115 pg/ μ L to 2290 pg/ μ L.

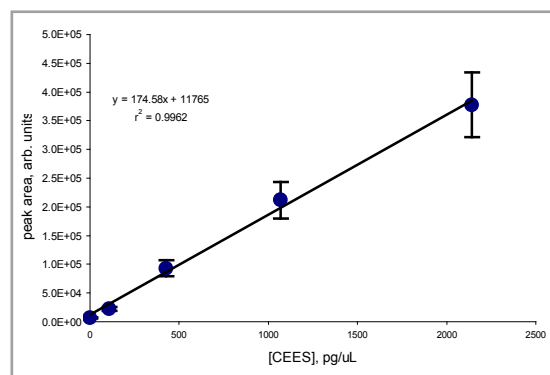


Figure 7. Calibration curve obtained for CEES over the concentration range 107pg/ μ L to 2140 pg/ μ L.