1st Detect

MMS-1000

HEADSPACE ANALYSIS OF BENZENE, TOLUENE, ETHYLBENZENE, AND XYLENE (BTEX) USING A MINIATURIZED ION TRAP MASS SPECTROMETER & EPA METHOD 8265

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ABSTRACT

The 1st Detect miniaturized mass spectrometer, MMS-1000™, was used to detect the presence of benzene, toluene, ethylbenzene, and xylene (BTEX) in air. Calibrated concentrations of standards were prepared to EPA method 8265 [1]. Samples were introduced through a membrane inlet and ionized with electron ionization (EI). The mass analyzer is a cylindrical ion trap design capable of performing MS/MS (MS^n) analyses.

INTRODUCTION

The components of BTEX are volatile organic compounds (VOCs) which are found in petroleum based products and are often used as solvents in industrial applications. Environmental contamination from these compounds can become a serious problem as they all have toxic effects and benzene is known to be a carcinogen.

The 1st Detect miniature mass spectrometer, MMS-1000, provides rapid on-line monitoring of VOCs in ambient air in a light weight, low power, affordable instrument coupled with a user-friendly software package.

This application note will detail the performance of the MMS-1000 for the analysis of VOCs, specifically BTEX, which includes performing calibration, acquiring mass spectra, and demonstrating orthogonal analysis with MS^n.

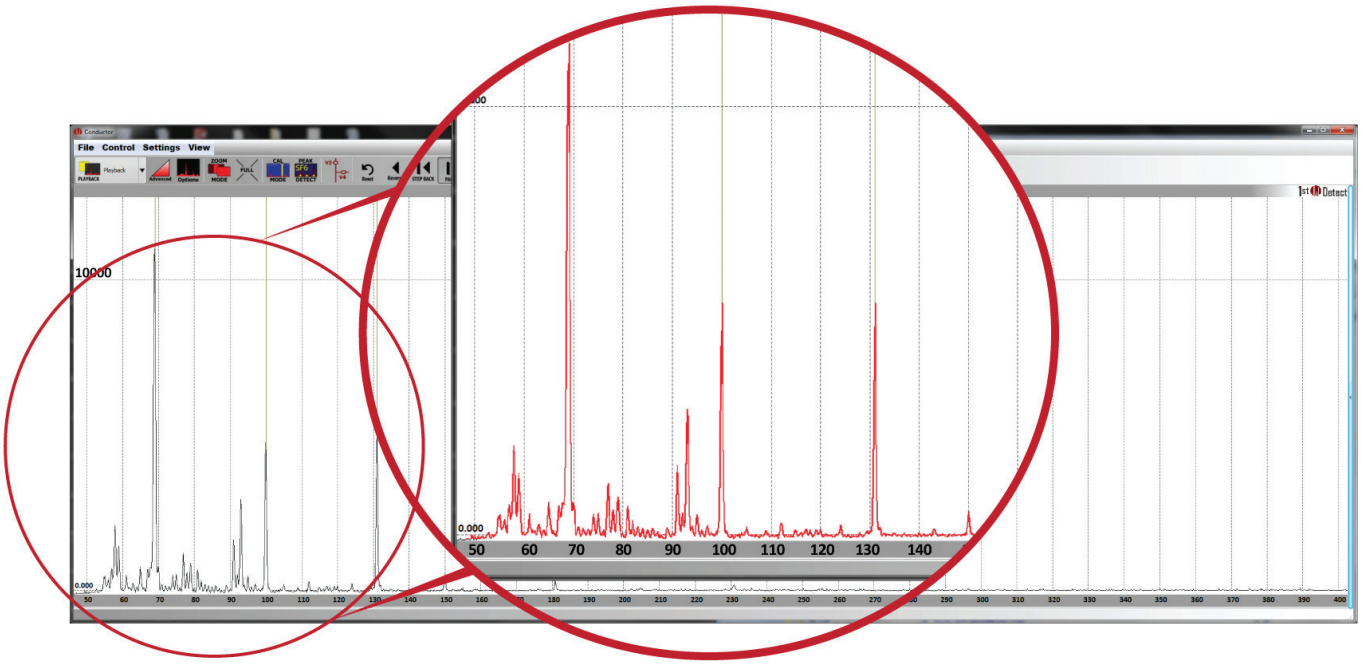

Figure 1: Mass spectrum of internal calibrant during auto-calibration sequence.
Inset: Demonstration of <0.4 amu full width half maximum resolution.

EXPERIMENTAL

INSTRUMENTATION: The analysis was performed using the 1st Detect MMS-1000 mass spectrometer (1st Detect, Webster, Texas, USA) with a membrane inlet system and electron ionization. The membrane inlet for the system is capable of introducing chemicals in with concentrations of 50 ppb - 1000 ppm. Carrier/buffer gas for the system is ambient air. Note: All hardware, pumps, electronics, and software required for analysis are built into the chassis of the instrument.

SAMPLE PREPARATION: Stock solutions of each chemical component were prepared as described in EPA method 8265 in section 7.11. Samples of 500 ppb were made from stock solutions by diluting with dry UHP nitrogen.

MASS CALIBRATION: The MMS-1000 has a built-in auto-calibration system. The mass calibration can be executed at any time to ensure proper calibration is maintained throughout the analysis. Furthermore, the MMS-1000 maintains mass assignment by better than 0.2 amu over a 24 hr period to ensure daily analyses are properly calibrated.

MASS ANALYSIS: The MMS detector provides real time MS analysis of all four components of BTEX in air, simultaneously. Furthermore, by simply selecting the MS^n mode from a drop down tab, and clicking on the desired peak, MS/MS analysis is invoked, providing orthogonal analysis of the sample. Also, simple controls allow the user to select parameters such as the isolation window and the collision-induced dissociation (CID) power to be used to fragment the ion.

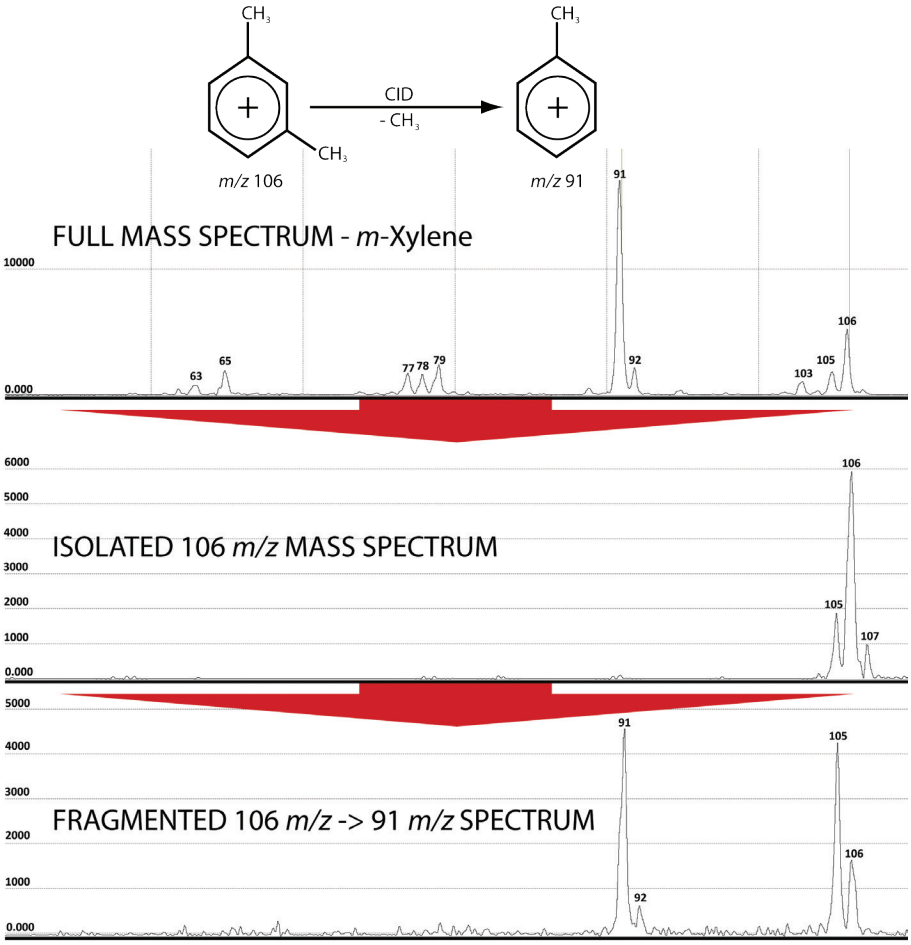

Figure 2: MS/MS of *m*-xylene. *m/z* 106 fragmented into *m/z* 91

CONCLUSION

This study illustrates the laboratory performance provided by the 1st Detect MMS-1000 chemical detector, while maintaining a small footprint and low power consumption. VOCs in the air can be monitored in real time with the MMS-1000. Furthermore, when a potential contaminant is identified through a single MS analysis, MS/MS can be performed to confirm identification and reduce false alarms.

References:

[1] EPA Test Method 8265, Volatile organic compounds in water, soil, soil gas, and air by direct sampling ion trap mass spectrometry (DSITMS), United States Environmental Protection Agency, March 2002

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