

APPLICATION NOTE

Solid Phase Microextraction (SPME) and HAPSITE ER: Detection of an Explosive and Several Explosive Taggants in Air

SUMMARY

HAPSITE® ER is a rugged, person-portable GC/MS instrument used for the detection of volatile and semivolatile organic compounds (VOCs and SVOCs). The HAPSITE ER SPME Sampling System, attached to the HAPSITE ER via its universal interface, provides the means to introduce SVOCs into the HAPSITE ER for separation and analysis. SPME is an effective sampling technique that has been successfully employed in fieldwork for the preconcentration of a variety of compounds. Many organic high explosives and explosive taggants can only be found in extremely low concentrations in the vapor phase due to their low volatilities. However, SPME vapor sampling will readily adsorb and concentrate these compounds. A study was carried out in order to evaluate SPME sampling and HAPSITE ER analysis of the explosive taggants:

- 2-Nitrotoluene (2-NT),
- 3-Nitrotoluene (3-NT),
- 4-Nitrotoluene (4-NT),
- 2,3-Dimethyl-2,3-dinitrobutane (DMNB),
- 2,4-Dinitrotoluene (2,4-DNT), and
- 2,6-Dinitrotoluene (2,6-DNT)

along with the explosive triacetone triperoxide (TATP) (see Table 1).

EXPERIMENTAL

A PDMS/DVB fiber was chosen for extraction of the taggants and explosive from air due to its ability to effectively adsorb nitropolyanion groups bonded to

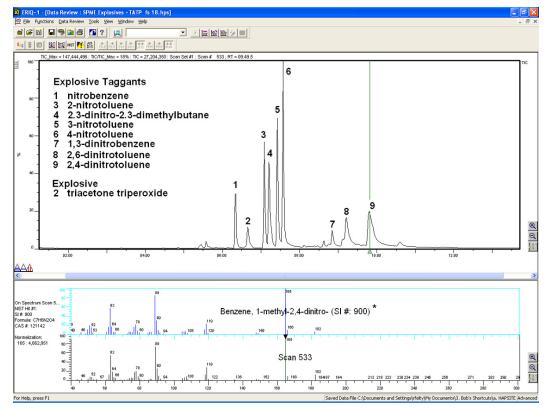
most of the compounds. Fifty nanograms (ng) of each taggant component of an EPA method 529 calibration standard, supplemented with an additional 100 ng of 2,4-DNT and DMNB, were injected into an empty 40 mL VOA vial to simulate sampling from air. Five hundred nanograms of the explosive, TATP, was also injected into the vial. A PDMS/DVB SPME fiber with protective fiber holder was inserted into the 40 mL VOA vial through the PTFE septum. The fiber was extended carefully and exposed to the sample for 10 minutes. Following exposure, the SPME fiber was carefully retracted, removed from the vial, and brought to the HAPSITE ER for analysis. The fiber holder was inserted into the SPME Sampling System desorption chamber. The fiber was then exposed inside the 250 °C desorption chamber which was attached to the injection port of the HAPSITE ER via the universal interface. A 15-minute sample separation and analysis run was carried out with the mass spectrometer scanning from 43 to 300 amu at a rate of 1.0 scan/sec. Method conditions and the resulting chromatogram are shown in Figure 1.

CONCLUSIONS

This study demonstrates the increased versatility of HAPSITE ER with the addition of the SPME Sampling System. Several semi-volatile explosive taggants and an explosive were extracted from an air sample with a SPME fiber and introduced into the HAPSITE ER for analysis.

| | Analyte Name | CAS Number | Retention Time |
|---|--------------------------------|---------------|-------------------|
| 1 | Nitrobenzene | 98-95-3 | 6:19.7 |
| 2 | Triacetone triperoxide | 17088-37-8 | 6:39.4 |
| 3 | 2-Nitrotoluene | 88-72-2 | 7:04.5 |
| 4 | 2,3-Dimethyl-2,3-dinitrobutane | 3964-18-9 | 7:12.8 |
| 5 | 3-Nitrotoluene | 99-08-1 | 7:25.2 |
| 6 | 4-Nitrotoluene | 99-99-0 | 7:34.6 |
| 7 | 1,3-Dinitrobenzene | 99-65-0 | 9:08.0 |
| 8 | 2,6-Dinitrotoluene | 606-20-2 | 9:12.1 |
| 9 | 2,4-Dinitrotoluene | 121-14-2 | 9:48.5 |

| Figure 1. Total Ion Chromatogram (TIC) of 8 Explosive Taggants and 1 Explosite |
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Column: Rtx-1MS (15 m x .25 mm x 1.0 µm) Column temperature program: 60 °C held for 0.5 minutes, ramp at 30 °C/min. to 160 °C, ramp at 24 °C/min. to 200 °C, hold for 10 minutes. * 1-methyl-2,4-dinitro-benzene is synonymous with 2,4-dinitrotoluene



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