Cylindrical Ion Trap Mass Spectrometer for Chemical Warfare Agent Detection and Identification

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1. **REPORT DATE**
   01 OCT 2005

2. **REPORT TYPE**
   N/A

3. **DATES COVERED**
   -

4. **TITLE AND SUBTITLE**
   Cylindrical Ion Trap Mass Spectrometer for Chemical Warfare Agent Detection and Identification

5. **PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)**
   Night Vision/Electro Optics and Chemical/Biological/Explosives Detection Group Naval Surface Warfare Center, Crane Division Crane, IN 47522

6. **AUTHOR(S)**

7. **SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)**

8. **PERFORMING ORGANIZATION REPORT NUMBER**

9. **DISTRIBUTION/AVAILABILITY STATEMENT**
   Approved for public release, distribution unlimited

10. **SUPPLEMENTARY NOTES**

11. **ABSTRACT**

12. **SUBJECT TERMS**

13. **SECURITY CLASSIFICATION OF:**
    a. REPORT unclassified
    b. ABSTRACT unclassified
    c. THIS PAGE unclassified

14. **LIMITATION OF ABSTRACT**
    UU

15. **NUMBER OF PAGES**
    17

16. **NAME OF RESPONSIBLE PERSON**


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Standard Form 298 (Rev. 8-98)
Prepared by ANSI X39-18
Selective, Rapid Detection of Chemical Warfare Agents in Air by Ion Trap Mass Spectrometry

- **Requirements, field portable plus**
  - **Speed of analysis:** < 10 seconds
  - **Sensitivity:** LOD < 1 part per trillion by volume
  - **Selectivity:** samples are complex mixtures of organics

- **The Solution**
  - Miniature mass spectrometer
  - Ion trap with simple cylindrical electrodes
  - Rapid, selective membrane introduction of samples

- **Basis for Effort**
  - Detailed simulations of ion motion in ion traps
  - Decade-long study of ion trap performance
  - Collaboration between Purdue, Crane, and Griffin, a start-up company who will manufacture instruments
Methodology

- Selective Adsorption/Desorption
- Selective Ionization
- Selective Mass Analysis
- Selective Dissociation and MS/MS Analysis

Air Sample → Membrane → Selective Desorption → Selective Ionization → Mass Analysis → MS/MS Analysis

Thermal Release → Laser or CI → Ion trap (CIT)

Preconcentration of analytes → Detection → Data Analysis

**Multiple Stages of Selectivity**

- Selective Adsorption/Desorption
- Selective Ionization
- Selective Mass Analysis
- Selective Dissociation and MS/MS Analysis

Harnessing the Power of Technology for the Warfighter
Miniaturization of the Mass Spectrometer

BEEQ – Research grade laboratory Instrument
Size: Big
Weight: 4 tons
Power: 15,000 W

Mini-CIT Ver. 5.0
Size: 45 x 60 x 71 cm
Weight: 140 lbs
Power: 200 - 300 W

Modified ITS-40
Rugged
Transportable
Size: 200x 200x 100 cm
Weight: 800 lbs
Power: 4500 W

Mini-CIT Ver. 7.0
• Size 18cm x 28cm x 65 cm
• Weight: 60 lbs
• Power 120W
Current Commercial System

Griffin Analytical Technologies

Figure 3: a) Calibration curve for methyl salicylate using direct air sampling onto the membrane. b) Mass spectrum of methyl salicylate from an 8 ppb gas-phase standard.
Mini Mass Spec Monitoring of Menthol from Cough Drops in Air

Halls cough drops (12 mg menthol per drop) in air mini 5.0 with internal unheated membrane

Menthol
C_{10}H_{20}O
MW 156.27

m/z Thomson
Relative Intensity

55,57
69,71
95
78-87
109
123
156

Harnessing the Power of Technology for the Warfighter
Altoid in Air: Mini Mass Spec

Trap and Release MIMS

0.45 V peak height
Rise: 26 sec.
Fall: 26 sec.

0.9 V peak height
Rise: 30 sec.
Fall: 30 sec.
Membrane Introduction Test Set

- Flow-Bench with mass flow meters
- RTDs/Humidity sensors
- Variable membrane heater
- Vacuum chamber with variable pump
- Dual chamber vapor generator
- Automated testing
Mini-Mass Spectrometer

New Design

- Sample Inlet
- Filament
- Ion Lenses
- Cylindrical Ion Trap
  \[ r_0 = 2.5 \, \text{mm} \]

Current Design
Performance Characteristics:
Sensitivity and Resolution

1 pg of methyl salicylate in 1 µL methanol

Resolution ~100
Toluene with membrane inlet
MS$^n$ of Methyl Salicylate

CID: 0 V

CID: 0.02 V

CID: 0.02 V

CID: 0 V

Harnessing the Power of Technology for the Warfighter
Wavelets

- Wavelet transform
  - Definition
    \[ WT_x(a, \tau) = \frac{1}{\sqrt{a}} \int x(t) \psi^* \left( \frac{t - \tau}{a} \right) dt \]
  - Admissible condition
    \[ c_\psi = \int_0^\infty \frac{|\Psi(\omega)|^2}{\omega} d\omega < \infty \]
  - Inverse transform
    \[ x(t) = \frac{1}{c_\psi} \int_0^\infty \frac{da}{a^2} \int_{-\infty}^{\infty} WT_x(a, \tau) \frac{1}{\sqrt{a}} \psi \left( \frac{t - \tau}{a} \right) d\tau \]
Signal Processing of Data

Wavelet Filtering

Single scan of methyl salicylate

Original and processed data
Signal Processing of Data

Wavelet Filtering

Results after trend removal
CIT Automated Test Set

- Fully automated PXI based control system
- Control software written in LabVIEW
- Leak valve and membrane introduction system
- Couple with flow bench and vapor generator
Future Work

Multiplexed CIT

- System integration
- Performance optimization
- IMS-MS
- Multiplexed CIT
- Biological Capabilities
- Algorithm Development
Acknowledgements

Funding:
Integrated Detection of Hazardous Materials (IDHM) Program, a Department of Defense project managed jointly by Center for Sensing Science and Technology, Purdue University, and Naval Surface Warfare Center, Crane, Indiana

Dr. Cooks acknowledges the technical support of the Amy Instrumentation and Dr Robert Santini provided via the Indiana Instrumentation Institute (III).

Robert Santini, Andy Guymon, Chris Doerge, Mark Carlsen, Mike Everly, Jim Zimmerman, Alan Ronemus, Robert Fagan, Randy Rapogle, and Greg Hawkins.