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Project Summary

Development of a Portable Monitor for Detection of Toxic Organic Compounds

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The objectives of this study were: (a) to design, construct, and deliver to EPA a prototype portable tunable atomic line molecular spectrometer (TALMS) benzene monitor, and (b) to locate matches of atomic lines and sharp molecular absorption features in other toxic organic compounds. TALMS is a newly developed, high resolution molecular absorption technique that is used in the ultraviolet-visible region of the optical spectrum to detect molecules in the gas phase. The dual beam prototype instrument was designed, constructed, tested and delivered to the Environmental Monitoring Systems Laboratory, Research Triangle Park, North Carolina, in December, 1983. It was designed for monitoring benzene with the Hg 253.7 nm line using the TALMS technique. The instrument consisted of three units: the optical unit (weight: 52 lbs, dimensions: 28 x 9 x 9"); the electronics unit (weight: 16 lbs, dimensions: 19 x 12.5 x 5.25"); and a power supply (weight: 14 lbs, dimensions: 12 x 8 x 8"). The total weight was 82 lbs. Tests of the performance of the benzene monitor showed linear response from the detection limit of approximately 40 ppm-v to 3000 ppm-v. Limited laboratory tests of a cryogenic concentration system for the unit were carried out.

Lamps for the volatile elements (As, Pb, Zn) that can be used with the TALMS technique are now available commercially from Heraeus, Hanau, West Germany. The magnetically contained lamps used with the TALMS technique were improved so that they are more stable, intense and have longer service lives.

Searches for locations of potential TALMS signals in o-, m-, p-xylenes, bromobenzene, benzene, and aniline were carried out using high and medium resolution absorption spectra as guides. TALMS signals were found for p-xylene with Si, Co, and Sb lines at 252.9 nm. No signals were found at this wavelength for o- or m-xylenes. TALMS signals were also found for bromobenzene at 270.2 nm (Pt) and 266.5 nm (Fe) and for aniline at 293.8 nm (Bi).

It is recommended that further searches for potential TALMS signals be carried out to extend the potential of the technique to other organic compounds and to decrease the detection limit for benzene. The investigation of a new related technique, Atomic Line Molecular Spectroscopy (ALMS) is recommended. It does not use the Zeeman effect, requires lighter equipment, and should have much lower detection limits. However, its selectivity would not be as great as that for TALMS.

This Project Summary was developed by EPA's Environmental Monitoring Systems Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

An analytical technique called Tunable Atomic Line Molecular Spectroscopy (TALMS) has been recently developed at

Lawrence Berkeley Laboratory. TALMS is essentially a high resolution, differential absorption spectroscopic technique. It is performed by splitting a source atomic emission spectral line into components with a magnetic field (Zeeman effect). A differential measurement is made between the absorption of a Zeeman component (or components) magnetically tuned to match a sharp analyte absorption feature and an unmatched Zeeman reference component(s). The sharp features in the absorption spectra of the organic compounds are due to rotational-vibrational fine structure in the electronic transitions. The difference in polarization between the split Zeeman components permits the matching and nonmatching wavelengths to be alternately selected and the absorption measured very rapidly with an electro-optical device called a Current Controlled Retardation Plate. The differential absorption is proportional to the amount of molecular species whose absorption line is matched by Zeeman component(s) of the source lamp. Therefore, calibration curves can be established following Beer's law.

TALMS is a high resolution (high selectivity) absorption spectroscopic technique. The high resolution is due to the narrow width of the atomic probe line, ca. 0.1 cm^{-1}, the location of which can be shifted by changing the magnetic field strength. The number of compounds that can be detected with TALMS is limited only by the presence of narrow, pseudo line structure in the absorption spectrum of the compound in the gas phase and the matching of an appropriate atomic emission line to this feature.

TALMS has a number of advantages as an analytical technique. It is a direct analysis technique requiring very little sample handling or preparation. Another feature of TALMS is its essential freedom from background interference. Since the difference in wavelength between the Zeeman components of the source emission line is typically 0.04 nm, any particle scattering or semi-continuous absorption will affect both components equally. Therefore, the differential absorption measurement will remove this interference from the total signal. The high resolution attainable with TALMS should result in high selectivity and unambiguous qualitative identification of compounds.

As a result of previous Interagency Agreements EPA-80-D-X1014 and AD-89-F-2A008 with Lawrence Berkeley Laboratory, TALMS instruments were designed, constructed, and delivered to the Environmental Monitoring Systems Laboratory at Research Triangle Park, North Carolina. Two prototype instruments were delivered—a large laboratory instrument and a benzene monitor.

The goals of the present study were to: (a) design, construct, and deliver to the Environmental Monitoring Systems Laboratory, Research Triangle Park, North Carolina, a portable TALMS benzene monitor, and (b) to determine the spectral location of potential TALMS features in toxic organic compounds other than benzene. A portable TALMS instrument would be useful in field detection and monitoring for benzene and other toxic compounds. Determination of spectral locations of potential TALMS signals is necessary to optimize instrument performance and to extend the technique to other organic compounds.

The instrument design, construction, and testing are described in the report. The procedures and results of TALMS molecular absorption—atomic line matches and developments in lamp design and construction are also given. Appendices of the report include operating instructions for the TALMS portable monitor and detailed descriptions of the optical, mechanical, and electronic components.

Conclusions and Recommendations

Design and construction of a prototype transportable TALMS instrument for benzene detection was completed on schedule and delivered to the Environmental Monitoring Systems Laboratory at Research Triangle Park, North Carolina in December, 1983. It consisted of three modules: a sensing module, an electronics module and a power supply. The sensing module weighed 52 lbs (24 kg) and the electronics module and power supply weighed 16 lbs (7.3 kg) each. The electronics module is connected to the other units by an extension cord for convenient field use. The electronics module was designed to be powered by a 100-watt motor generator in the field. Instrument performance tests show that the instrument has a linear response over the range from the detection limit of 40 ppm-v up to 3000 ppm-v. This detection limit is too high for direct ambient air detection of benzene and some form of concentration technique will be required.

A new commercially available source (W. C. Heraeus GmbH, PEW, Hanau, West Germany) is available that allows As, Pb, and Zn lines to be used in this instrument in addition to the Hg lines for which it was designed. However, different interference filters or a monochromator would be required if these lamps were used. While this instrument was under construction, major advances were made in the assembly and operation of the magnetically confined atomic discharge lamps leading to more stable and intense emission.

Searches for TALMS signals in organic molecules were found to be slow and tedious due to lack of high resolution absorption spectra in the literature for most compounds. After considerable experimentation with a variety of lamps and medium resoltuion absorption spectra, TALMS signals were found for p-xylene (Si: 252.85 nm; Co: 252.9 nm; Sb: 252.85 nm; Pt: 273.4 nm; Pt: 248.7 nm); for bromobenzene (Pt: 270.2 nm; Fe: 266.5 nm); aniline (Bi: 293.8 nm); and for benzene (Si: 252.85 nm; Sb: 252.85 nm). No signals were found for o- or m-xylene. TALMS signals have now been found for benzene, bromobenzene, chlorobenzene, toluene, p-xylene, aniline, phenol, pyridine, and formaldehyde.

Since major decreases in detection limits are dependent upon the location of more intense analysis lines, it is recommended that more studies be carried out to locate new analysis lines for compounds of interest.

It is also recommended that the investigation of a new, related analytical technique called Atomic Line Molecular Spectroscopy (ALMS) be initiated. This technique involves absorption near the intense absorption bands of the vacuum ultraviolet region (180 to 220 nm) using one or more atomic lines. The advantages over the TALMS technique are much lower detection limits and a lighter instrument since only a small magnet and no squeezer are required. Selectivity will be decreased, but it may be adequate if absorption by several atomic lines is utilized.

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The complete report, entitled "Development of a Portable Monitor for Detection of Toxic Organic Compounds," (Order No. PB 84-229 673; Cost: $10.00, subject to change) will be available only from:
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5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650
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