



Project Summary

Molecular Optical Spectroscopic Techniques for Hazardous Waste Site Screening

DeLyle Eastwood and Tuan Vo-Dinh

The U.S. Environmental Protection Agency is interested in field screening hazardous waste sites for pollutants in surface water, ground water, and soil. This report is an initial technical overview of the principal molecular spectroscopic techniques and instrumentation and their possible field-screening applications at hazardous waste sites. The goal of this overview is to describe the power and utility of molecular spectroscopic techniques for hazardous waste site screening and to define the main strengths, weaknesses, and applications of each major spectroscopic technique. These spectroscopic methods include electronic (ultraviolet-visible absorption and luminescence) and vibrational (infrared absorption and Raman scattering) techniques. A brief discussion is also given for some other techniques that rely on spectroscopic detection (colorimetry and fluorometry as well as immunoassay and fiber-optic chemical sensors).

The cost of instrumentation and analysis and the time needed for analysis are briefly addressed, and broad guidelines are given for three categories of instrumentation: portable, field deployable, and semi-field deployable. An outline of the spectroscopic principles and instrumentation for each particular spectroscopic technique is presented, and state-of-the-art approaches are described. Advantages, limitations, sensitivities, and examples of specific techniques and their applications to environmental pollutants are also discussed.

This Project Summary was developed by EPA's Environmental Monitoring Systems Laboratory, Las Vegas, NV, 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

The U.S. Environmental Protection Agency (EPA) is interested in field screening of hazardous waste sites for pollutants in surface and ground water as well as soil. Major reasons for this interest are to achieve improved cost effectiveness and to expedite remedial investigations at Superfund sites and thus reduce the time lag between sampling and the receipt of analytical data. Field analytical screening can also help to confine a detailed field investigation to those areas of a site which are truly contaminated and thus reduce the number of samples sent to the analytical laboratory, thereby providing more comprehensive environmental studies as well as more relevant data with reduced cost and time.

Often, for field screening, optical spectroscopic methods and experiments that are field deployable or portable provide attractive alternatives to more common EPA methods such as gas chromatography and mass spectrometry. Optical spectroscopic methods permit large number of samples to be screened, characterized, and prioritized in the field with little or no sample preparation. These screening techniques permit rapid response and considerable



cost savings because detailed analyses are required only for a selected subset of samples. Spectroscopic techniques may sometimes provide information on unusual sample types or on nonvolatile compounds that are of high-molecular weight or thermally labile. For functional groups or geometrical isomers, these techniques may also provide specific structural information complementary to methods such as gas chromatography. Spectroscopic techniques may also offer advantages for *in situ* measurements (with fiber optics), remote measurements, flow-through analyses, and nondestructive testing.

Each spectroscopic technique has certain advantages and disadvantages. Some may be more widely applicable, may be more feasible for field deployment using current technology, or may be more specific or sensitive for trace identification or classification. All of the techniques discussed in this report have the potential for field application either by themselves or in conjunction with appropriate separation or chromatographic steps. Recent rapid advances in computer hardware and software, chemometrics, and pattern recognition algorithms, although beyond the scope of this report, have also been combined with advances in spectroscopic instrumentation to improve the analysis of complex environmental pollutant mixtures and extract maximum information from data sets.

The main objective of this report is to provide a technical overview and assessment of the principal molecular spectroscopic techniques and instrumentation with applications for field screening at hazardous waste sites. These methods currently include UV-visible absorption and luminescence (electronic) spectroscopy as well as infrared absorption and Raman (vibrational) spectroscopy. For each method, a brief outline of the spectroscopic principles and instrumentation considerations is given to familiarize the reader with the present state-of-the-art approach. Advantages, limitations, sensitivities, and examples of specific techniques and their applications to environmental analyses are also discussed. Specific highlights are also given for adjunct techniques such as colorimetric and fluorometric analysis with chemical derivatization, spectroscopic immunoassay techniques, and fiber-optic chemical sensors. The range of possible applications of spectroscopic methods for field analysis is very broad and might include uses for identification, classification, semiquantitation, and quantitation.

This report is meant as a technical assessment and source document. This document can provide a basis for early

decision-making on potential spectroscopic techniques for field screening.

A table summarizes the applicability of each spectroscopic technique for field and laboratory use, together with advantages, limitations, sensitivity, current field availability, and estimated cost and time. It is hoped that this overview will allow an appreciation of the power and utility of molecular spectroscopic techniques for hazardous waste site screening.

Discussion and Conclusions

Spectroscopic approaches can provide valuable qualitative and quantitative information with substantial savings of time and money. Instruments and methods, developing rapidly in this growing area, can greatly improve environmental analytical technology. All of the spectroscopic methods have specific advantages and shortcomings and have potential applicability for particular environmental problems. Table 1 summarizes the advantages, limitations, and sensitivities with examples of specific techniques and their application to environmental pollutants. This table also includes definitions of portable, field-deployable and semi-field-deployable instruments and includes relative estimates of cost and time factors.

Ultraviolet-visible absorption spectroscopy is a mature technique that has good quantitative accuracy for single compounds after separation, or for simple mixtures. If it is used in conjunction with high-performance liquid chromatography using an optical multichannel analyzer as a detector, the entire spectrum for each chromatographic peak can be recorded. Its sensitivity is moderate and its specificity is low. Colorimetric reagents can greatly increase the specificity of the method and improve sensitivity by moving the spectrum of the reaction product into the visible region with high absorption coefficients. Ultraviolet-visible absorption spectroscopy is most useful for unsaturated compounds (aromatic or heterocyclic).

Ultraviolet-visible luminescence (fluorescence and phosphorescence), when applicable, can be the most sensitive spectroscopic technique for trace and ultratrace analysis, especially with laser excitation. It is useful in aqueous solutions to the part-per-billion to part-per-trillion level. Specific techniques most useful in the field include synchronous luminescence and room temperature phosphorescence. Luminescence is applicable to most polyaromatic compounds and their derivatives and can be made applied to many other compounds by using fluorometric reagents for chemical derivatization reactions. It can also be used with high performance liquid chroma-

tography and multichannel detection. Luminescence is much more selective for identification or classification purposes than ultraviolet-visible absorption but less selective than infrared or Raman spectroscopy. Its selectivity can be enhanced using various excitation and emission wavelengths and by time or phase resolution methods, and indirect detection methods such as fluorescence quenching or energy transfer.

Infrared absorption spectroscopy (dispersive and Fourier transform) has been used in field applications, especially for monitoring air pollutants using a gas cell, for characterizing oil or hazardous chemicals where structural information from group frequencies is useful and where sensitivity is not the critical factor. Infrared devices are also useful as real-time detectors with GC-FTIR and for specific quantitation applications such as oil and grease. Disadvantages include the need for sample preparation to eliminate water, which is the major interferent, some difficulties related to quantitation, and the moderate sensitivity of the technique. Lately, more compact, rugged instruments along with better sample preparation and signal processing techniques that are designed to increase the sensitivity of this method have made it more attractive for field use.

Raman spectroscopy complements infrared spectroscopy because it also provides structural information but with different selection rules. Raman spectroscopy is not sensitive to water and can use visible or near-infrared optical techniques. Until recently, Raman was considered to have several disadvantages for field use including complex instrumentation, need for laser excitation, fluorescence interferences in the visible, and relatively low sensitivity. These disadvantages have been somewhat reduced by the advent of more compact Raman spectrometers, smaller and/or near-IR lasers, and special, more sensitive Raman techniques. The most promising Raman technique for field use is surface-enhanced Raman spectroscopy in which Raman scattering efficiency can be enhanced by factors of as much as 10^6 for some compounds when a chemical is adsorbed on a special roughened metal (Cu, Ag, Au) surface. Although this technique may be promising for future field applications, it is not yet fully understood or developed and may not apply to all chemicals. The advantage of the technique is that it has the potential to combine the sensitivity of luminescence with structural information similar to that provided by infrared spectroscopy.

Other techniques that rely on spectroscopic detection and that greatly enhance

the utility of spectroscopic methods include colorimetry, fluorometry, immunoassay, and some fiber-optic chemical sensors. Fiber-optic sensors may also use some change in the optical properties of the fiber or cladding or may be used as probes for most of the spectroscopic techniques discussed.

Spectroscopic techniques are being used with increasing frequency for field screening, allowing rapid response and reduced costs for environmental monitoring programs. Such techniques also help to optimize sampling efforts and help to prioritize samples for more detailed analysis. Some spectroscopic methods can be

used in place without sampling, e.g., fiber-optic chemical sensors, whereas others can be used with portable instrumentation or field deployable instruments set up in a mobile laboratory. Recent instrumentation developments, such as more compact lasers, miniaturized optical hardware, new types of detectors such as charge-coupled devices, increased use of fiber optics, and better computer software for spectral data processing and pattern recognition have increased the utility of these spectroscopic methods.

Further research and development efforts are needed to improve the field applicability of current and new

spectroscopic analytical techniques, to make instruments more portable and compact. Also, new techniques that employ field-ready instruments need to be accompanied by detailed analytical protocols, appropriate standards, calibration criteria, and appropriate quality assurance for specific pollutant classes. Field spectroscopic instruments and methods are a rapidly improving and growing analytical area which can greatly improve environmental analytical technology.

A better appreciation of the conclusions, relative to the applicability of these spectroscopic techniques, can be obtained by reviewing Table I.

Table 1. Characteristics of Spectroscopic Techniques for Field Analysis

<i>Applicability</i>	<i>Advantages</i>	<i>Limitations</i>	<i>Sensitivity</i>	<i>Current Field Applicability</i>	<i>Related Lab Techniques & Sensors</i>
UV-vis Absorption					
<i>Polyaromatic Compounds (PACs)</i> <i>Dyes</i> <i>Colorimetric Reaction Products</i>	<i>Mature Technique</i> <i>Instrumentation Readily Available</i> <i>Good Quantitative Accuracy for Single Compounds and Simple Mixtures</i> <i>Few Interferences by Nonaromatics</i> <i>Spectral Data Available</i>	<i>Unspecific (Compared to IR and Luminescence)</i> <i>Extensive Sample Preparation</i> <i>Quantitation may be Affected by Solvent, Polarity, or Medium, Chemical Complexation</i>	<i>Moderate Sensitivity</i> <i>ppm - ppb in Favorable Cases</i>	<i>Portable</i> <i>- Hand-held Colorimeter</i> <i>- Colorimetric Kits</i> <i>Field Deployable. Instrumentation with Multichannel Detectors</i> <i>HPLC Detectors</i>	<i>UV-VIS Techniques</i> <i>- FT</i> <i>- Derivative</i> <i>LT Matrix Isolation</i> <i>Reflectance</i> <i>Photoacoustic Spectroscopy</i> <i>Fiber Optic Colorimetric Sensors</i> <i>Multichannel Detectors</i> <i>- Diode Arrays</i> <i>- CCDs</i>
UV-vis Luminescence (Fluorescence and Phosphorescence)					
<i>Polyaromatic Compounds</i> <i>Fluorescent Dyes</i> <i>Fluorometric Reaction Products</i> <i>PCBs</i> <i>Phenols</i> <i>Pesticides</i> <i>Semivolatiles</i> <i>Nonvolatiles</i> <i>Petroleum Oils</i>	<i>Most Sensitive Method for Trace and Ultratrace Analysis when Applicable</i> <i>Instrumentation Readily Available</i> <i>No Interference by Water</i> <i>Few Interferences by Nonaromatics</i> <i>Some Structural Specificity</i> <i>- Enhanced by Special Techniques</i>	<i>Limited to Compounds with Fairly High Luminescence Yields (Usually PACs, unless Derivatized)</i> <i>Relatively Unspecific for Structural Information (Compared to IR)</i> <i>Quantitation Complicated by Differences in Quantum Yields, Quenching, Microenvironments</i> <i>Limited Reference Spectra Available</i>	<i>Excellent Sensitivity</i> <i>ppb (pptillion or Less with Laser Excitation)</i> <i>Dependent on Quantum Yields</i>	<i>Portable Instruments Available</i> <i>Field Deployable Instruments Available</i> <i>Flow-through Oil-Water Monitors and HPLC with Multichannel Detectors</i> <i>Front Surface - RTP</i>	<i>Luminescence Techniques</i> <i>- Fluorescence</i> <i>- Phosphorescence</i> <i>- Synchronous</i> <i>- Time and Phase Resolution</i> <i>- Polarization</i> <i>- RT and LT</i> <i>- 3D</i> <i>- Microscopy</i> <i>Fiber Optic Fluorometric Sensors</i> <i>Multichannel Detectors</i> <i>- Diode Arrays</i> <i>- CCDs</i>

(Continued)

Table 1. Continued

<i>Applicability</i>	<i>Advantages</i>	<i>Limitations</i>	<i>Sensitivity</i>	<i>Current Field Applicability</i>	<i>Related Lab Techniques & Sensors</i>
UV-vis Luminescence (Fluorescence and Phosphorescence) (continued)					
	<p><i>Very Selective</i> - Enhanced by Time and Wavelength Variability</p> <p><i>Can Distinguish Geometrical Isomers</i></p>				<p><i>Fluorescence Quenching or Energy Transfer</i> - Indirect Ways to Measure Non-luminescent Molecules</p>
Synchronous Fluorescence					
<p><i>Increased Specificity for Individual PACs or PAC Classes in Complex Mixture</i></p> <p><i>Petroleum Oils</i></p> <p><i>Creosoles</i></p>	<p><i>Increased Specificity</i></p> <p><i>Less Spectral Overlap</i></p> <p><i>Classification of PAHs by Number of Rings</i></p> <p><i>Useful for Screening</i></p> <p><i>Combine with Other Luminescence Techniques</i></p>	<p><i>Decrease in Sensitivity with Narrower Bandpasses and Wavelength Offset</i></p> <p><i>Loss of Vibrational Structure in Spectrum</i></p> <p><i>Need Dual Scanning Monochromators</i></p> <p><i>Need Polychromatic Source</i></p>	<p><i>Good Sensitivity</i></p> <p><i>Slightly Lower than Fluorescence Emission</i></p> <p><i>Dependent on Instrumental Conditions</i></p> <p><i>Dependent on Stokes Shift of Compound</i></p>	<p><i>Portable Instruments under Development</i></p> <p><i>Field Deployable Instruments Available</i></p>	<p><i>LT Measurements</i></p> <p><i>Time and Phase Resolution</i></p> <p><i>Derivative</i></p> <p><i>Remote Monitor under Development</i></p> <p><i>Synchronous Phosphorescence</i></p>
Room Temperature Phosphorescence (RTP)					
<p><i>Most Luminescent PACs, PCBs, PAHs</i></p> <p><i>Directly or with Heavy Atom Perturber</i></p>	<p><i>Easy Sample Prep</i></p> <p><i>Eliminates Scatter and Fluorescence Background</i></p> <p><i>Longer Lifetimes than Fluorescence</i></p> <p><i>No Need for Cryogenic Instrumentation</i></p> <p><i>Useful for Screening</i></p> <p><i>Additional Selectivity Due to Perturber</i></p>	<p><i>Oxygen may Quench in Solution</i></p> <p><i>Less Structure than LTP</i></p> <p><i>Substrate/Technique Dependent</i></p> <p><i>Quantitation may be Complicated</i></p> <p><i>Limited Corrected Spectra Available</i></p>	<p><i>Good Sensitivity</i></p> <p><i>ppb in Favorable Cases</i></p> <p><i>Dependent on Quantum Yield of Compound</i></p> <p><i>Dependent on Efficiency of Perturber</i></p>	<p><i>Portable Instruments Under Development</i></p> <p><i>Field Deployable Instruments Available</i></p> <p><i>Front Surface</i></p> <p><i>Rigid Medium</i> - Filter Paper - TLC Plate</p> <p><i>Dosimetry</i></p> <p><i>Easy Sample Prep</i></p>	<p><i>Can Compare with LT Techniques for Optimization</i></p> <p><i>Time Resolution</i></p> <p><i>TLC</i></p> <p><i>Organized Medium</i> - Micelle Solution - Cyclodextrin</p>
Low Temperature Luminescence (Fluorescence and Phosphorescence)					
<p><i>Luminescent PACs</i></p> <p><i>PCBs</i></p>	<p><i>Higher Sensitivity, Specificity than RT</i></p> <p><i>Vibrational Structure</i></p> <p><i>Similar to Raman</i></p> <p><i>Quantitation Over 6 Orders of Magnitude</i></p> <p><i>Distinguish Isomers</i></p> <p><i>Very Selective</i> - Enhanced by Time and Wavelength Variability</p>	<p><i>Cryogenic Apparatus More Complicated</i></p> <p><i>Need Skilled Operator</i></p> <p><i>Less Reference Spectral Data than RT</i></p> <p><i>Some Analytes Matrix Dependent</i></p>	<p><i>Excellent Sensitivity</i></p> <p><i>pptrillion in Optimal Cases</i></p> <p><i>Improved with Laser</i></p>	<p><i>Limited Semi-Field Deployability</i></p>	<p><i>LT Techniques</i> - Shpolskii Spectra - Laser-line Narrowing - Site Selection - Matrix Isolation</p> <p><i>Low Temperatures</i> 77 K to 4 K</p>

(Continued)

Table 1. Continued

<i>Applicability</i>	<i>Advantages</i>	<i>Limitations</i>	<i>Sensitivity</i>	<i>Current Field Applicability</i>	<i>Related Lab Techniques & Sensors</i>
Infrared (Dispersive)					
<p><i>Organic and Inorganic</i></p> <p><i>Determination of Specific Functional Groups</i></p>	<p><i>Highly Specific Structural Data on Group Frequencies</i></p> <p><i>Mature Technique</i></p> <p><i>Instrumentation Widely Available</i></p> <p><i>Spectral Libraries Available</i></p>	<p><i>Mid/low Sensitivity</i></p> <p><i>Water is Interferent</i></p> <p><i>Requires Special Optics/Solvents</i></p> <p><i>Quantitation Difficulties</i></p> <p><i>Weak Optical Sources and Detectors</i></p>	<p><i>Less Sensitive than UV-vis Absorbance</i></p> <p><i>Much Less Sensitive than Fluorescence</i></p> <p><i>ppthousand to ppm in Favorable Cases</i></p>	<p><i>Portable and Field Instruments Available</i></p> <p><i>Portable Unit with Gas Cell</i></p> <p><i>Quantitation of Grease and Oil</i></p> <p><i>ATR Attachments for Solids, Oils</i></p>	<p><i>FTIR</i></p> <p><i>GC/LC-FTIR</i></p>
Infrared (Fourier Transform)					
<p><i>Organic and Inorganic</i></p> <p><i>Determination of Specific Functional Groups</i></p> <p><i>Routinely Used for Real-Time GC and Vapor Analysis</i></p>	<p><i>Highly Specific Structural Data on Group Frequencies</i></p> <p><i>Instrumentation Widely Available</i></p> <p><i>Real-Time Flow through Vapor Applications - GC-FTIR</i></p> <p><i>Spectral Libraries Available</i></p>	<p><i>Less Sensitive than Luminescence</i></p> <p><i>Requires Special Optics/Solvents</i></p> <p><i>Can Tolerate Some Water (Background Subtraction)</i></p> <p><i>Organics Detection 1-10 ppthousand in Water</i></p>	<p><i>More Sensitive than Dispersive IR - Signal Averaging</i></p> <p><i>ppm to subppm in Favorable Cases</i></p>	<p><i>Field and Semi-field Deployable</i></p> <p><i>- With or Without GC</i></p> <p><i>- Volatiles/Semivolatiles</i></p> <p><i>Adaptable to Use with SFC</i></p>	<p><i>GC/LC-FTIR</i></p> <p><i>Matrix Isolation - LT for Sensitivity</i></p> <p><i>Microscopy</i></p>
Near Infrared					
<p><i>Single Compounds</i></p> <p><i>Simple Matrices</i></p> <p><i>Organics Overtones</i></p>	<p><i>Sources and Optical Materials Better than Mid-IR</i></p> <p><i>Optically Good Sensor Materials</i></p> <p><i>Can Distinguish Major Components of Simple Matrix</i></p> <p><i>Fewer Interferences than Mid-IR</i></p>	<p><i>Less Spectral Structure than Mid-IR</i></p> <p><i>- Overtone Overlap</i></p> <p><i>- Less Specificity</i></p> <p><i>- Interpretation Complicated</i></p> <p><i>Not Useful for Complex Matrices</i></p> <p><i>Signal Processing and Pattern Recognition Required</i></p>	<p><i>Low Sensitivity</i></p> <p><i>10-1 ppthousand</i></p>	<p><i>Portable Near-IR Instrument with Fiber Optic Probe</i></p> <p><i>Characterization of Oil</i></p> <p><i>Bulk Chemical Analysis</i></p>	<p><i>Surface/Pollutant Interaction Studies</i></p> <p><i>Near IR Sensors</i></p> <p><i>Process Control</i></p>

(Continued)

Table 1. Continued

<i>Applicability</i>	<i>Advantages</i>	<i>Limitations</i>	<i>Sensitivity</i>	<i>Current Field Applicability</i>	<i>Related Lab Techniques & Sensors</i>
Normal Raman Spectroscopy (NRS)					
<p><i>Organic and Inorganic Aqueous Solutions</i></p> <p><i>Biological Matrices</i></p> <p><i>Polymers</i></p>	<p><i>Specific as IR for Structural Information</i></p> <p><i>Different Selection Rules - Complements IR</i></p> <p><i>Fewer Interferences than IR in vis or near-IR Regions</i></p> <p><i>Water and Glass not Interferences</i></p> <p><i>Good Optics and Solvents Available</i></p> <p><i>Can Handle Unusual Sample Shapes/Sizes</i></p>	<p><i>Fluorescence Interference in UV-vis</i></p> <p><i>Requires Laser Source</i></p> <p><i>Relatively Complex Instrumentation</i></p> <p><i>Requires Skilled Operator</i></p> <p><i>Not as Mature as IR</i></p> <p><i>Relatively Poor Limits of Detection</i></p>	<p><i>Moderate Sensitivity 1000 - 20 ppm</i></p>	<p><i>Semi-field Deployable Instruments under Development</i></p>	<p><i>Research in:</i></p> <ul style="list-style-type: none"> - <i>Aqueous Solutions</i> - <i>Biological Matrices</i> - <i>Polymers</i> <p><i>Special Raman Techniques</i></p> <ul style="list-style-type: none"> - <i>SERS</i> - <i>Resonance</i> - <i>CARS</i> - <i>Microprobes</i> - <i>Microscopy</i> <p><i>LT Applications</i></p>
Surface Enhanced Raman Spectroscopy (SERS)					
<p><i>Many Pollutants</i></p> <p><i>Demonstrated for:</i></p> <ul style="list-style-type: none"> - <i>Pyridine</i> - <i>Hydrazine</i> - <i>PAHs</i> - <i>Pesticides</i> 	<p><i>Specific in Structural Information</i></p> <p><i>More Sensitive than Normal Raman</i></p> <p><i>As Sensitive as Luminescence in Favorable Cases</i></p> <p><i>No Interference by Water</i></p> <p><i>(See Also NRS)</i></p>	<p><i>Relatively New Tech.</i></p> <p><i>Surface/Substrate Material Dependent</i></p> <p><i>Reproducibility</i></p> <p><i>Requires Laser and Special Substrate</i></p> <p><i>Not all Analytes Enhanced Equally</i></p> <p><i>Few Spectral Libraries</i></p> <p><i>(See Also NRS)</i></p>	<p><i>Good Sensitivity for Selected Analytes</i></p> <p><i>ppm - ppb in Favorable Cases</i></p>	<p><i>Field Deployable Instrumentation under Development</i></p>	<p><i>Research to Optimize Techniques</i></p> <p><i>Microscopy</i></p> <p><i>Microprobes</i></p> <p><i>Surface Studies</i></p> <p><i>Fiber-Optic Sensors</i></p> <p><i>HPLC (under Development)</i></p> <p><i>Multichannel Detectors</i></p>

(Continued)

Table 1. Continued

Applicability	Advantages	Limitations	Sensitivity	Current Field Applicability	Related Lab Techniques & Sensors
Resonance Raman					
PACs Absorbing in UV Phenols	Specific in Structure May Eliminate Fluorescence Background (See Also NRS)	Only Chromophore Vibrations Enhanced Limited to UV Absorbing Compounds - Mainly PACs Quantitation Difficult Not Comparable to Other Raman Techniques UV Laser Source Complex Instrumentation (See Also NRS)	Fair Sensitivity in Favorable Cases with Chromophore Vibrations	Many Practical Difficulties	Chromophore Characterization Biological Application

Definitions of portable, field deployable, and semi-field deployable as used in this table are:

Portable:

Battery powered
One person can carry
Little sample prep. (< 10 min.)
Instrument cost < \$30,000
Analysis cost < \$30

Field Deployable:

Generator powered
Compact, two people can lift (several instruments in mobile lab)
Relatively simple sample prep. (< 1 hr.)
Instrument cost \$30,000 to \$100,000
Analysis cost \$30 - \$200

Semi-field Deployable:

Can fit in mobile lab
Complex or fragile instrument
Often considerable sample prep. (> 1 hr.)
Instrument cost > \$100,000
Analysis cost > \$200

Definitions of abbreviations as used in this table are:

ATR	Attenuated Total Reflectance	PAC	Polyaromatic Compounds
CARS	Coherent Anti-Stokes Raman Spectroscopy	PAH	Polyaromatic Hydrocarbons
CCD	Charge-Coupled Device	PCB	Polychlorinated Biphenyls
FTIR	Fourier Transform-Infrared Spectroscopy	ppb/ppm	part per billion/part per million (mg/mL, µg/mL)
GC	Gas Chromatography	RTP	Room Temperature Phosphorescence
HPLC	High Performance Liquid Chromatography	SERS	Surface-Enhanced Raman Spectroscopy
IR	Infrared Spectroscopy	SFC	Supercritical Fluid Chromatography
LC	Liquid Chromatography	TLC	Thin-Layer Chromatography
LT	Low Temperature	UV-vis	Ultraviolet-Visible Spectroscopy
NRS	Normal Raman Spectroscopy		

DeLyle Eastwood is with Lockheed Engineering and Sciences Company, Las Vegas, NV 89119. Tuan Vo-Dinh is with Oak Ridge National Laboratory, Oak Ridge, TN 37831.

William H. Engelmann is the EPA Project Officer, (see below).

The complete report, entitled "Molecular Optical Spectroscopic Techniques for Hazardous Waste Site Screening," (Order No. PB91-195990/AS; Cost: \$23.00, subject to change) will be available only from:

National Technical Information Service

5285 Port Royal Road

Springfield, VA 22161

Telephone: 703-487-4650

The EPA Project Officer can be contacted at:

Environmental Monitoring Systems Laboratory

U.S. Environmental Protection Agency

Las Vegas, NV 89193-3478

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati, OH 45268

BULK RATE
POSTAGE & FEES PAID
EPA PERMIT NO. G-35

Official Business
Penalty for Private Use \$300

EPA/600/S4-91/011