NSF-RANN Trace Contaminants Abstracts

MASTER

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NSF-RANN TRACE CONTAMINANTS ABSTRACTS

Deborah S. Harnden, Editor
Robert H. Ross, Associate Editor

Prepared for the
National Science Foundation Research Applied to National Needs
Chemical Threats to Man and the Environment Program

by

Toxic Materials Information Center
Environmental Resource Center
Information Center Complex

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Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
for the
ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

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TRACE CONTAMINANTS NEWS

PERSONNEL CHANGES IN WASHINGTON OFFICE

Effective June 1977, Dr. Marvin Stephenson will resign as program manager for the Chemical Threats to Man and the Environment Program and will assume increased responsibilities as deputy division director of the Division of Advanced Research and Technology. His successor has not been named.

PERSONNEL CHANGES AT TOXIC MATERIALS INFORMATION CENTER

Deborah Harnden has moved to Baton Rouge, Louisiana, where her husband has accepted a position with Dow Chemical. Robert H. Moss will become editor and will assume day-to-day responsibility for *Trace Contaminants Abstracts*. Program participants are encouraged to contact Bob and report project news, meetings of interest, and notices of publications in order to make *Trace Contaminants Abstracts* a more effective communication tool for participants. Bob may be reached at (615)483-8611, ext. 3-0386.

PROGRAM MEMBER IS EDITOR OF BOOK

Dr. H. F. Walton has recently edited a book entitled *Benchmark Papers in Analytical Chemistry, Vol. 1: Ion-Exchange Chromatography*, published by Dowden, Hutchinson and Ross, Stroudsburg, Pennsylvania.

CHANGES IN THE PROGRAM DIRECTORY

Please notify Polly Purnell of the Environmental Response Center of any changes which may occur in your program, address, or personnel. Polly will also be happy to answer questions about program changes or Trace Contaminant publications. Program changes will be published in the newsletter so that directories may be kept up to date. Polly may be reached at (615)483-8611, ext. 3-0386.

FUTURE MEETINGS

National Pollution Conference, April 19-21, Atlanta, Georgia.
Write: WWEMA, 7900 Westpark Dr., McLean, Virginia 22101.

Environmental Control and Public Health Course, April 22 - October 15, Open Univ., England. Write: Post-experience Student Office, Open Univ., P.O. Box 76, Walton Hall, Milton Keynes MK7 6AA, England.

7th Annual Symposium on the Analytical Chemistry of Pollutants, April 24-27, Lake Lanier Island, Georgia. Write: Elaine McGarity, Environmental Research Lab., College Station Rd., Athens, Georgia 30601.

Inst. of Environmental Sciences Annual Meeting, April 25-28, Los Angeles, California. Write: Betty L. Peterson, Inst. of Environmental Sciences, 940 E. Northwest Highway, Mt. Prospect, Illinois 60056.

International Ozone Inst. Congress, May 4-6, Paris, France. Write: International Ozone Inst., European Committee Secretariat, 52 rue d'Anjou, 75384 Cedex 08 Paris, France.

1977 American Industrial Hygiene Conference, May 22-27, New Orleans, Louisiana. Write: Paul E. Toth, Ford Motor Co., American Rd. 444, Dearborn, Michigan 48121.

Joint Conference American Chemical Society and Canadian Institute of Chemistry, May 29-June 2, Montreal, Canada. Write: A. T. Winstead, ACS, 1155-16th St., N.W., Washington, D.C. 20036.

Trace Substances in Environmental Health Annual Meeting, June 7-9, Columbia, Missouri. Write: Delbert D. Hemphill, University of Missouri, Environmental Trace Substance Research Center, 411 Clark Hall, Columbia, Missouri 65201.

Air Pollution Control Association 70th Annual Conference & Exhibition, June 19-23, Toronto, Ont., Canada. Write: APCA, 4400 Fifth Ave., Pittsburgh, Pennsylvania 15213.

2nd International Conference on Environmental Mutagens, July 11-15, Edinburgh, Scotland. Write: Secretary-General, Dr. P. Brookes, Inst. of Cancer Research, Pollards Wood Research Station, Nightingales Ln., Chalfont St. Giles, Bucks HP8 4SP, England.

Conference on Air Quality Meteorology and Atmospheric Ozone, August 1-6, Boulder, Colorado. Write: A. L. Morris, President, Ambient Analysis, Inc., P.O. Box 4056, Boulder, Colorado 80302.

2nd International Symposium on Aquatic Pollutants, September 26-28, Noordwijkerhout, The Netherlands. Write: George L. Baughman, Environmental Research Laboratory, U.S. Environmental Protection Agency, College Station Road, Athens, Georgia 30601 (404)546-3145.

C11
Optically Pumped Superfluorescent NaI Molecular Laser

Remesian, R.A.; Perist, F.L.; Pye, J.L.

Microwave Laboratory, U.S. Panson Laboratories of Physics, Stanford University, Stanford, CA 94305

PRCBE BC: (415) 497-6226 (Pye)

J. Appl. Phys., 47(4), 1515-1517; 1976, April

OPTICAL PUMPING; SCILUM; QUANTITATIVE MEASUREMENTS; LASERS; ELECTRICAL DISCHARGE MATHES; FLASH-LAMP PUMPING METHODS; PUMP ABSORPTION; PUMPED GAS; SPONTANEOUS INTENSITY; QUENCHING; SUPERFLUORESCENCE; E-X-BAND TRANSITIONS; LASER OSCILLATION; A-X-BAND TRANSITIONS; PUMP SATURATION; LASER GAIN; LASER SATURATION INTENSITY; ALKALI DIPOLE SYSTEMS; ANALYTICAL METHODS; ANALYSIS

Optical pumping is a convenient method to quantitatively study new potential lasers prior to attempting the more difficult electrical discharge and flash-lamp pumping methods. By optically pumping the pump absorption and saturation intensity, induced laser gain and laser saturation intensity, and the effects of quenching and buffer gas pressure can be measured. When an NaI molecule is optically pumped at 0.673 and 0.659 micrometers, a superfluorescent laser emission on a series of green and yellow molecular I-X-band transitions and laser oscillation in the near infrared on A-X-band transitions are obtained. Pump saturation, laser gain, and laser saturation intensity are reported. NaI is representative of the other alkali diatomic systems which have molecular emission bands extending from the visible into the infrared.

C22
Identification of the SF₆ Transitions Pumped by a CO₂ Laser

McBowell, R.S.; Galbraith, R.W.; Frcha, R.J.; Contrell, C.D.; Birkley, F.E.

Los Alamos Scientific Laboratory, Los Alamos, NY 87545; MIT Lincoln Laboratory, Lexington, MA 02171

PRCBE BC: (617) 462-6660 (Birkley)

Rev. Commun., 17(2), 176-181; 1976

SUPERFLUORESCENCE; LASERS; NONLINEAR ABSORBERS; SUPER ISOTOPES; ROTATIONAL STATES; RESONANCE; LASER LINES; J-VALUES; OCTAHEDRAL SYMMETRY TYPES; TRANSITIONS; VIBRATIONAL QUANTUM STATE; SPONTANEOUS-TCP MOLECULES; MOLE-LOCKERS; SATURABLE ABSORBERS; PERIAPLOIDIES; ANALYTICAL METHOD; METHOD DEVELOPMENT; ANALYSIS

Sulfur hexafluoride (SF₆) is of interest to the

laser community as a nonlinear absorber of 10.6 micrometer CO₂ laser radiation; as a medium for self-induced transparency (SIT); and most recently as a medium for laser separation of sulfur isotopes. Interpretation of these numerous experiments is hindered by the fact that until now it has been impossible to specify precisely the SF₆ rotational states that are in resonance with the laser lines. A complete assignment for the J-values and octahedral symmetry types of all transitions from the vibrational ground state of SF₆ that lie within plus or minus 1.5 cm⁻¹ (0.05 CH⁻¹) of the 12C 16O2 P(10), P(18), and P(20) laser lines is presented. The SF₆ absorptions nearest these three laser frequencies are R(20)A(2)(20), P(13)A(2)(24), and an F(2) component of P(54) or P(60), respectively. An improved set of molecular constants also allows a more accurate estimate of the J-values of the SF₆ absorptions in the vicinity of other CO₂ laser lines. This method is also applicable to other spherical-top molecules (such as C₆₀) used as passive mode-lockers or saturable absorbers and to other hexafluorides.

C23
Particle Size Distribution and Chemical Composition of Coal-Tar Fumes

Hittle, B.C.; Stukel, J.J.

U.S. Army Construction Engineering Research Laboratory, Champaign, IL 61820; University of Illinois, Urbana, IL 61801

PRCBE BC: (217) 333-6561 (Stukel)

Am. Ind. Hyg. Assoc. J., 37(4), 192-204; 1976, April

PARTICULATES; COAL; COAL-TAR FUMES; SIZE DISTRIBUTION; CHEMICAL COMPOSITION; PHYSICAL CHARACTERISTICS; DISPERSED; CRYSTALLINE PARTICLES; FLUORESCENCE; POLYCYCLIC AROMATIC HYDROCARBONS; PNEUMOTOMY; ANTIDUCTURE; 3,4-DICUMYLURE; ANALYSIS

The chemical and physical characteristics of coal-tar fumes emitted from coal-tar spreading applications were studied. Two experiments were performed. Coal-tar fume particle size distribution was determined in the first experiment. The primary compounds found in the tar fumes and their relative concentrations were identified in the second experiment. The particulate samples were composed of spherical liquid droplets occasionally interspersed with solid crystalline-like particles and were highly fluorescent. The tar fumes consisted of polycyclic aromatic hydrocarbons, phenanthrene and anthracene being the most prevalent. Methylated polycyclic aromatic hydrocarbons were also found. 3,4-Dibenzopyrene was not present in the fumes.

(4) Long-Path Scattering with Tunable Lasers

Finley, F.E.; So, F.T.

Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, MA 02173

PRIME NO: (617) 462-6600

Presented at the 8th Materials Research Symposium - Methods and Standards for Environmental Measurement, Gaithersburg, MD, September 20-26, 1976; 1976

TUNABLE LASER; SIGNAL REFLECTION; DIFFERENTIAL ABSORPTION; QUANTITA TIVE ANALYSIS; NITROGEN CYCLE; NITROGEN FICIDE; SULFUR FICIDE; CARBON FICIDE; OZONE; MONITORING; FIELD STUDIES; IR-SALT LASER; HUMIDITY; DIFFUSED DETECTORS; ATMOSPHERIC TURBULENCE; SYSTEM SENSITIVITY; FREQUENCY MODULATION; AIR QUALITY; ANALYSIS

By using a tunable laser whose signal is reflected from a distant target, differential absorption of the laser power can permit a quantitative determination of the integrated pollutant concentration. Many molecular atmospheric pollutants, such as NO, NO₂, SO₂, CO, and O₃, have already been monitored by this technique. Tunable lasers in the ultraviolet, visible, and infrared regions of the electromagnetic spectrum have been employed. The laser source is a Ti-salt type. This laser is useful for field studies because of its small size, ruggedness and ease of wavelength tunability. The diode laser is mounted in a closed-cycle cryogenic cooler, and its emission is collimated by an Al-coated parabolic mirror, 12 cm in diameter. The beam is transmitted down-range to a retro reflector which reflects it back towards the parabolic mirror, which refocuses it onto the infrared detector situated behind a chalcogenide cell. In order to minimize the effects of atmospheric turbulence on system sensitivity, a derivative spectroscopic technique is employed in which the laser is frequency-modulated at 10 kHz at the pollutant gas absorption line. This system was used at the FCC water test range in Bedford, MA where an experimental detection limit of 5 ppb of CO has been established. The sensitivity and accuracy of these measurements are considered in detail, and a discussion of the long-path measurements in comparison with point sampling results are presented in order to evaluate the potential of the long-path laser monitor for providing more reliable and acceptable quantitative measurements of air quality.

Inhibition of Corn and Sunflower Photosynthesis by Lead

Bazzaz, F.A.; Carlson, R.W.; Polfe, G.L.

Departments of Botany and Forestry, University of Illinois, Urbana, IL 61801

PRIME NO: (217) 233-6177

Physiol. Plant., 38, 326-329; 1975

CORN; SUNFLOWERS; LEAD CHLORIDE; TRANSPIRATION STREAM; PHOTOSYNTHESIS; LEAD; LEAD UPTAKE; TRANSPIRATION RATES; STOMATAL RESISTANCE; CARBON DIOXIDE; WATER VAPOR EXCHANGE; ANALYSIS

Detached corn and sunflower leaves supplied with PbCl₂ via the transpiration stream exhibited reduced rates of photosynthesis. The difference between species in the amount of Pb taken up was in direct proportion to their respective transpiration rates. For both species the reduction in photosynthesis and the amount of Pb taken up increased with increasing treatment concentrations. A corresponding reduction occurred in the rate of transpiration suggesting that stomatal resistance may be increased by Pb contamination. The pathways of CO₂ and water vapor exchange are discussed in relation to the effects of Pb on photosynthesis and transpiration.

TRANSPORT: IFA 947; L., MELIPHYTUS ARBUS L.

Application of the Unified Transport Model to the Movement of Pb, Cd, Zn, Cu, and S Through the Crooked Creek Watershed

Harro, J.H.; Lumboore, P.J.; Depovich, C.L.; Dixon, H.P.; Hanson, A.F.; Patterson, G.B.; Jackson, E.W.

Computer Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830

PRIME NO: (615) 803-0611, Ext. 3-6260

OVERVIEW-INTC-10, 52 p.; 1976, September

MODELS; MODELING; TRANSPORT MODELS; HEAVY METALS; LEAD; CADMIUM; ZINC; COPPER; SULFUR; WATERSHEDS; SOIL; HEAVY METAL ACCUMULATION; STREAMS; PLANT UPTAKE; HYDROLOGY; ; STREAMFLOW; COMPU:79 SIMULATION; ANALYSIS

Two versions of the Unified Transport Model (UTM) have been used to simulate movement of Pb, Cd, Zn, Cu and S through the Crooked Creek Watershed, a 1.3 mi. (2.2) forested headwaters area adjacent to a Pb mine and smelter in southeast Missouri. The Wisconsin Hydrologic Transport Model (WUTM) version was used to study accumulation of heavy metals in the soil and to simulate stream flow and heavy metal concentrations in the stream draining the watershed. The Terrestrial Ecology and Hydrology Model (TEHM) version was used to study heavy metal and SC₂ effects on the vegetation by considering plant uptake in a plant growth and decomposition model. The Soil Chemical Exchange of Heavy Metals (SCHEM) submodel in TEHM was used in a detailed comparison between results from a six-year simulation of heavy metal accumulation in the top soil layers and measured values. Agreement between simulated results from both versions of the UTM and measured values is satisfactory.

GEOGRAPHICAL DESCRIPTION: OS, Missouri, Ozark Mountains, Crooked Creek Watershed

47)

Laser Spectroscopic Instrumentation and
Techniques: Long-Path Scattering by Resonance
Absorption

Winkley, P.-E.

Lincoln Laboratory, Massachusetts Institute of
Technology, Lexington, MA 02173

FAO/WHO: (17) 642-4404

Opt. Quant. Electron., 9, 145-147, 1976

TUNABLE LASER SPECTROSCOPY: LONG-PATH SCATTERING;
RESONANCE ABSORPTION SPECTROSCOPY; RARE EARTH
CALCULATION; TUNABLE INFRARED LASERS; AIR
POLUTION MONITORING; LONG-PATH SCATTERING;
APPLIED CASES; RESONANCE ABSORPTION; ANALYTICAL
TECHNOLOGY; REVIEW

Tunable laser spectroscopy has accentuated the
introduction of new measurement techniques,
particularly with regard to the wavelength
calibration. This paper highlights some of these
requirements and surveys laser spectroscopic
measurements which have already been performed in
the infrared. The rather unique properties of
tunable infrared lasers also make them useful for
air pollution monitoring. In particular, several
tunable laser techniques have been used for
long-path scattering of ambient gases in the
atmosphere by resonance absorption. The results
of these measurements are discussed. Table I is
a summary of laser methodology used for
detection of low molecular weight gases
implicated in air pollution. The spectra
obtained range from the single diatomic structure
of NO and CO to complex spectra associated with
molecules such as SO₂.

48)

Sensitivity of Vertebrate Embryos to Heavy Metals
as a Criterion of Water Quality. Phase III. Use
of Fish and Amphibian Eggs and Embryos as
Bioindicator Organisms for Evaluating Water
Quality

Birge, B.J.; Westerman, A.G.; Blach, J.A.

University of Kentucky, Water Resources Research
Institute Report No. 41, 27 p; PP-140-400; 1975

FAO/WHO: (606) 256-5500

University of Kentucky Water Resources Research
Institute Report No. 41, 27 p; PP-140-400; 1975

FISH EGGS: AMPHIBIAN EGGS; EMBRYOS; LARVAL
STAGES; BIOINDICATOR ORGANISMS; WATER QUALITY;
FRESH WATER; STREAM WATER; FISHING EFFICIENCY;
FISHING EFFICIENCY; EGG HATCHABILITY; AQUACULTURE
TECHNIQUE; GRAY TRIFIDEG; BAITING TECH; EGG
DEVELOPMENT; WATER QUALITY INDEX; BIOLOGICAL
POTENTIALITY; FRY; TERATOGENIC EFFECTS; MERCURY;
TRACE METALS; EGG MORTALITY; ANALYSIS; LONG-TERM
EFFECTS; CHADWICK CRYSTAL; FIC FICG;
DIC-SPOTTE TEST; HATCHING TEST

Fish and amphibian eggs, embryos and early
posthatched (larval) stages were evaluated as
bioindicator organisms with which to monitor the
quality of natural water resources. Eggs of 4
species were cultured in water collected from

each of 11 Inner Bluegrass rivers and streams.
The latter were chosen to represent water sources
varying in quality from extremely poor to good.
Selection was based on the sources and magnitude
of pollution, and the diversity and density of
aquatic populations. Cultures were maintained in
vitro, using 12-hr changes of water. Averaging
data for all 4 animal species, egg hatchability
(embryonic survival) ranged from 0% for the most
contaminated water to 50% for uncontaminated
water found to support a healthy aquatic biota.
Eggs of the squirrel treefrog and gray treefrog
were the most sensitive of 4 amphibian species
tested, and of a fish species, rainbow trout eggs
proved most susceptible to water contaminants.
Egg development provided an index to water
quality which compared favorably with independent
ecological indicators. In particular, the
frequencies of embryonic mortality recorded for
the 11 monitoring sites correlated with
reductions in density and species diversity of
aquatic populations. The results indicated that
eggs and embryos from a wide selection of fish
and amphibian species may be used as sensitive
indicators of water quality. Amphibian larvae and
early fish fry were considerably less sensitive
to variations in water quality. More
contaminated water sources which gave high rates
of embryonic mortality also produced high
frequencies of teratogenic development, affecting
up to 86% of the embryos which survived to
complete the hatching process. Defective
survivors were rare to absent in cultures where
egg hatchability exceeded 50%. The selected
water resources were analyzed for mercury and
other trace metals. Appreciable levels of
metallic contaminants were found in those water
sources which produced high levels of egg
mortality. Egg hatchability was precluded or
markedly reduced in all test waters where total
mercury reached 0.1 ppb or more.

GEOGRAPHICAL DESCRIPTION: KY, Kentucky, Cave Run,
Tom Branch, Wolf Run, East Hickman Creek, West
Hickman Creek, Gainaway Branch, Hickman Creek,
Sawby Branch, Kentucky River, Elkhorn Creek,
Steele's Run

TAXONOMIC: MICROPTERUS SALMOIDES; CAPASSINUS
NOVATUS; ICTALURUS PUNCTATUS; SALMO GAIARDII;
CASTROPHYRUS CAROLINENSIS; DUPO PUNCTATUS;
BAGROPTICUS; SYLA COPTOCEPHALA; SYLASQUIPPELLA

459

A Comparison of Factors Affecting Accuracy in Atomic Emission and Atomic Absorption Spectrometry Using a Graphite Furnace for Trace Metal Analysis in Water

Speck, H.S.; Baird, T.C.; O'Haver, T.C.

Institute for Materials Research, Analytical Chemistry Division, National Bureau of Standards, Washington, DC 20230; Department of Chemistry, University of Maryland, College Park, MD 20742

SPORR NO: (30)450-2610 (O'Haver)

Presented at the 9th Materials Research Symposium - Methods and Standards for Environmental Measurement, Gaithersburg, MD, September 20-24, 1976; 1976

SENSITIVITY; TRACE METALS; ATOMIC SPECTROSCOPY; GRAPHITE FURNACE ATOMIZER; FLAME TECHNIQUE; SPECTRAL INTERFERENCES; PHYSICAL INTERFERENCES; SPECTRAL INTERFERENCES; CORRECTION METHODS; ACCURACY; GRAPHITE FURNACE ATOMIC EMISSION SPECTROSCOPY; GRAPHITE FURNACE ATOMIC ABSORPTION SPECTROSCOPY; ANALYTICAL METHODS; ANALYSIS

The sensitivity required for the analysis of many metals in natural waters by atomic spectroscopy can only be obtained, in most cases, by the use of the graphite furnace atomizer. However, the circumstances necessary to obtain accurate analytical results with graphite furnace atomic spectroscopic techniques are far more rigid than with flame techniques. Chemical, physical, and spectral interferences are generally more serious with graphite furnace techniques. Therefore, correction methods must be applied to obtain accurate results. The techniques of Graphite Furnace Atomic Emission Spectrometry (GFES) and Graphite Furnace Atomic Absorption Spectrometry (GFAS) provide an interesting contrast in analytical methods. Interferences in the two techniques differ markedly in their severity, order of interference (additive or multiplicative), and method of correction. In this presentation, the effects of these interferences on the accuracy obtainable with both graphite furnace techniques are discussed, particularly for the analysis of trace metals in water.

419

Improved Accuracy in Background-Corrected Atomic Absorption Spectrometry

Zander, R.T.; O'Haver, T.C.

Chemistry Department, University of Maryland, College Park, MD 20742

SPORR NO: (30)450-614 (O'Haver)

Presented at the 9th Materials Research Symposium - Methods and Standards for Environmental Measurement, Gaithersburg, MD, September 20-24, 1976; 1976

BACK-GROUND CORRECTED ATOMIC ABSORPTION SPECTROSCOPY; MOLECULAR ABSORPTION; PARTICULATE LIGHT SCATTERING; ANALYTICAL METHODS; TWO-LINE METHOD; BACKGROUND; CORRECTED NOISE METHOD; FIS-CORRECTION; PURE ATOMIC ABSORPTION; BACKGROUND INTERFERENCE; ISOTOPE ZEEMAN ATOMIC ABSORPTION; ZEEMAN COMPONENTS; MAGNETIC FIELD; ANALYSIS

The use of background-corrected atomic absorption spectrometric techniques allows the analysis of a broad range of samples with complex matrices. These techniques eliminate the interference arising from molecular absorption and particulate light scattering by the matrix constituents. In conjunction with standard addition methods, very low levels of analyte can be determined in complex samples with a minimum of sample preparation and a high degree of accuracy. Two methods of background-correction are generally utilized. The two-line method requires that the analyte have a close, non-absorbing line available. Any signal measured at this line will be from the background and can be subtracted from the resonance line absorption signal. Not all elements have close non-absorbing lines, e.g., Zn. Conventional background correctors available on many AA units utilize a second source of continuum radiation to operate in the background-corrected mode. The analyte continuum atomic absorption is assumed to be negligible, and the signal from the second channel arises solely from the background. This requires increasing the spectral bandpass of the monochromator. Hollow cathode continuum sources have a limited range of intensity so that some elements cannot be analyzed in this manner, e.g., Cu. There is a possibility of self-correction. This is due to matrix atomic absorption which can become significant with increased spectral bandpasses. Methods have been developed which more adequately compensate for background interference. The isotope Zeeman atomic absorption (IZA) technique places the light source in a magnetic field so that the resonance line is split into its Zeeman components. The outer components are used to monitor the background close to the absorption line. Atomic absorption using a continuum source and a wavelength-modulated echelle monochromator (CEMA) takes advantage of the high resolution of the echelle to eliminate matrix absorption lines and of the background discrimination capability of a wavelength modulated detection system to compensate for molecular absorption and scatter.

411
A Laboratory Biosay Using Daphnia Sp. for
Refinery Effluent Toxicity Testing

Parsons, R.L.; Lee, J.C.; Cairns, J.

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Studies, Virginia Polytechnic Institute and State
University, Blacksburg, VA 24061

PHOTO NO: (017) 562-5500, EXT. 411

Appl. Opt., 1979, 18-661, 1979, April

RESEARCH: INVENTORIES; ZINC; AMBIENT EFFLUENT;
COPPER; AMMONIA; CHLORINE; COPPER; ZINC;
AMBIENT; AMBIENT; AMBIENT; AMBIENT; AMBIENT;
AMBIENT; AMBIENT; AMBIENT; AMBIENT; AMBIENT;
AMBIENT; AMBIENT; AMBIENT; AMBIENT; AMBIENT;
AMBIENT; AMBIENT; AMBIENT; AMBIENT; AMBIENT;
AMBIENT; AMBIENT; AMBIENT; AMBIENT; AMBIENT;
AMBIENT; AMBIENT; AMBIENT; AMBIENT; AMBIENT;

A simple method using unsophisticated equipment
is suggested for on-site toxicity testing of
refinery effluents. This test provides an
immediate means of identifying critical
materials and establishing priorities for coping
with these materials. An arbitrary reference
culture, containing six known constituents of
refinery wastewater, is used for static toxicity
tests of 15 species of freshwater invertebrates
and a species of fish. Daphnia Sp. has been
selected for further testing because it is the
most sensitive of the animals tested, relatively
inexpensive and easy to maintain, and a potential
fish-feeding organism. If the reference culture is
representative of a refinery effluent, the
Daphnia bioassay would be sufficiently sensitive
to give reliable results within 48 hr, whereas a
fish bioassay would show no toxicity even after
96 hr. To assess the suitability of the Daphnia
bioassay, tests have been conducted by personnel
at six petroleum refineries. Duplicate tests are
in progress. Results of tests using actual
refinery effluents ranged from no toxicity after
96 hr to a mean lethal concentration of 1.7%
effluent after 48 hr. The data presented show
that the method is reproducible and that refinery
wastewater can be used to confirm the bioassay.
Potential problems and advantages of the method
are discussed.

PARSONS, R.L.; LEE, J.C.; CAIRNS, J.

412
Long-Path Monitoring of Atmospheric Carbon
Monoxide with a Tunable Diode Laser System

Ho, P.T.; Pickley, P.E.; Sample, J.C.

Lincoln Laboratory, Massachusetts Institute of
Technology, Lexington, MA 02173

PHOTO NO: (017) 562-5500, EXT. 412

Appl. Opt., 1979, 18-661, 1979, April

LONG-PATH MONITORING; ATMOSPHERIC CHEMISTRY;
ATMOSPHERIC CARBON MONOXIDE; TUNABLE DIODE LASER
SYSTEM; RESONANCE ABSORPTION; BASIC FREQUENCY
MODULATION; ATMOSPHERIC TOBACCO; DETECTION
LIMITS; COMPUTED TRAFFIC; AMBIENT CO; ANALYSIS

Long-path measurements of carbon monoxide in the

atmosphere are described. The technique of
resonance absorption, in which the wavelength of
radiation from a $125(0.42)5(0.16)$ semiconductor
diode laser was tuned into coincidence with an
absorption line of CO in its fundamental band
around 4.7 microns, was used. By employing
rapid frequency modulation of the laser emission
to overcome atmospheric turbulence effects, it
was possible to achieve a minimum detectable
concentration of 5 parts per billion over a
0.41-km path. Continuous monitoring was also
performed and this permitted increases in the
ambient CO level due to commuter traffic to be
observed.

413

Field-Measured Nitrogen Guide Concentrations,
Soil Potentials, Oxygen Diffusion Rates, and
Oxygen Partial Pressures in Relation to
Denitrification

Fishler, M.; Ardakani, M.S.; Szaszewicz, T.L.;
Stolzy, L.W.

University of California, Riverside, CA 92502;
University of California, Berkeley, CA 94720

PHOTO NO: (017) 767-5112 (Stolzy)

Soil Sci., 122(2), 107-116, 1976

ROOT GROWTH; DENITRIFICATION; SOIL AERATION;
ANEROBIC MICROBES; FIELD SOIL; AERATION
MEASUREMENTS; GASEOUS CONCENTRATIONS; SOIL
ATMOSPHERE; OXYGEN DIFFUSION RATES; REDOX
POTENTIALS; FIELD EXPERIMENTS; SUDAN GRASS;
HANFORD SANDY LOAM; IRRIGATION WATER;
FERTILIZERS; NITRATES; NITRATES; NITRATES;
AERATION CONDITIONS; SOIL SOILS; SOIL FACTORS
INTERACTIONS; OXYGEN DIFFUSION RATES; OXYGEN
PARTIAL PRESSURE; ANALYSIS; SOIL CHEMISTRY

Under conditions critical for root growth or
favorable for denitrification the pattern of soil
aeration is very heterogeneous. There is no
method available to measure directly the amount
and the sites of anaerobic microsites in a field
soil. Aeration measurements such as jarvis
concentrations in the soil atmosphere, oxygen
diffusion rates, or redox potentials are indirect
expressions of this aspect of soil aeration. In
order to quantify the soil aeration status in the
critical range mentioned above, a large number of
measurements is needed and hence a considerable
investment of time and money is involved. In
this paper different methods of measuring soil
aeration with respect to denitrification are
compared. A field experiment was carried out on
two Sudan grass covered plots or a Hanford sandy
loam. The irrigation water contained fertilizer,
with nitrate for one plot, without nitrate for
the other. Different aeration measurements were
made during three drainage periods following
irrigations. Nitrous oxide, a gaseous product of
an anaerobic process, was a good indicator to
differentiate the aeration conditions of
relatively wet soils. Redox potential is an
efficient and sensitive measurement to determine
soil aeration in a wet soil range but
interpretation of results is difficult because of
the multiple interactions between different soil
factors. Oxygen diffusion rates and oxygen
partial pressure were less satisfactory for the
Hanford sandy loam.

<14>

Relative Rate Constants for the Reactions of OH Radicals with Isopropyl Alcohol, Diethyl and Di-n-propyl Ether at 305 plus or minus 2 Degrees K

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EPRI NO: (714) 787-8586 (Pitts)

Chem. Phys. Lett., 42(2), 205-208; 1976, September

RATE CONSTANTS; HYDROXYL RADICALS; ISOPROPYL ALCOHOL; DIETHYL ETHER; DI-N-PROPYL ETHER; ENVIRONMENTAL CHAMBER STUDIES; FOTOCHEMICAL; HYDROCARBONS; NITROGEN OXIDES; ISOCYANIDE; ATMOSPHERIC CHEMISTRY; ANALYSIS

Relative rate constants have been obtained for the reaction of the hydroxyl radical (OH) with isopropyl alcohol and diethyl and di-n-propyl ether in environmental chamber photoxidation studies employing hydrocarbon-NO(x) mixtures in air at 1 atmosphere and 305 plus or minus 2 degrees K. These results were obtained from measurements of the relative rates of disappearance of these compounds on the previously validated basis that OH radicals are dominantly responsible for their disappearance in the initial stages of reaction under the experimental conditions employed. Absolute rate constants, obtained by using the published rate constant for OH plus isobutene of 3.05×10^{10} (E-10) 1 mole (E-1), s(E-1) are (k $\pm$ 10(E-9) 1 mole(E-1)s(E-1)): isopropyl alcohol, 4.3 plus or minus 1.3; diethyl ether, 5.6 plus or minus 1.1; and di-n-propyl ether, 10.4 plus or minus 2.1. No previous determinations of these rate constants have been reported.

<15>

The Effect of Latitude on the Potential for Formation of Photochemical Smog

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Atmos. Environ., 10, 731-734; 1976

LATITUDE; SMOG POTENTIAL; PHOTOCHEMICAL SMOG; SUMMER SOLSTICE; SUNLIGHT INTENSITY; POLLUTANT EMISSION INVENTORY; OZONE; FAD; EMISSIONS; PHOTOLOGICAL CONDITIONS; ATMOSPHERIC CHEMISTRY; ANALYSIS

The effect of latitude on the potential for the formation of photochemical smog has been assessed. Calculations suggest that at the

summer solstice, the integrated sunlight intensity at Rotterdam or Fairbanks (Alaska) is very similar to that in Los Angeles. Computations carried out, assessing the same pollutant emission inventory for the three locations, showed that ozone and PAN dosages depend more on the integrated light intensity than on the nature of the light density distribution with time. Therefore, if factors such as emissions and meteorological conditions are equal, the potential for significant photochemical smog formation during the summer months is similar for Los Angeles (34 degrees N) and northern cities such as Rotterdam (52 degrees N) and Nome or Fairbanks, Alaska (65 degrees N).

GEOGRAPHICAL DESCRIPTION: US, Alaska, Nome, Fairbanks; US, California, Los Angeles; The Netherlands, Rotterdam

<16>

Water Quality Control in Mine Spoils - Upper Colorado River Basin

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EPRI-670/2-75-048, 54 p.; PB-242-908; 1975, June

COAL MINES; STRIP MINING; WASTE DISPOSAL; DRAINAGE; MINE WATERS; WATER QUALITY; GROUND WATER; WATER CHEMISTRY; SALINITY; SOIL CHEMISTRY; TAILINGS; RUNOFF; PERCOLATION; MINE SPOILS; SALTS; HEAVY METALS; COPPER; LEAD; ZINC; HYDROLOGY; MONITORING; LEACHING; ALUMINUM; CALCIUM; CHLORIDE; IRON; POTASSIUM; MAGNESIUM; MANGANESE; SODIUM; SULFATE; NITRATES; ANALYSIS

The purpose of this study was to identify potential water quality problems associated with runoff and percolation through mine spoils at selected sites in the Upper Colorado River Basin. The results show that the production of soluble salts from mine spoils into receiving waters is probably the most significant water quality problem that can be expected. No significant release of heavy metals was observed in the coal mine spoils studied. Some significant heavy metal concentrations were observed in the stream below the tailings disposal area from a copper-lead-zinc mill. A portion of these metals are contributed by the tailings, but a variety of old mines and mine dumps also make a contribution. The quality of percolate and runoff from spoils was found to correspond to the constituents of extracts prepared from saturated pastes of the spoil material. A method of estimating salt production into receiving waters was derived and found to agree very well with measured salt pickup at one coal site. The minimum quantities of salts that will eventually be released from the spoils studied are estimated.

GEOGRAPHICAL DESCRIPTION: US(W), Colorado River Basin

<17>
Evidence for Alkyl Radical Isomerization in
Photooxidations of C(4)-C(6) Alkanes under
Simulated Atmospheric Conditions

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Chem. Phys. Lett., 42(1), 22-27; 1976, August

RATE CONSTANTS; ALKYL RADICALS; HYDROGEN SHIFTS;
ISOMERIZATIONS; PHOTOCHEMISTRY; ALKANES; ALKYL
RADICALS; ALKYLPEROXYRADICALS; PHOTOCHEMICAL
SMOG; APPARENT AID; N-BUTANE; N-PENTANE; N-HEXANE;
HYDROGEN OXIDES; PENTANONE; FREE RADICALS;
CHEMISTRY; ATMOSPHERIC CHEMISTRY; ANALYSIS

We have calculated approximate room temperature
rate constants for intramolecular hydrogen shift
isomerizations of alkyl, alkyl and alkylperoxy
radical intermediates in photochemical smog and
found that alkyl radicals with delta hydrogens
appear to undergo 1,5 hydrogen shifts at ambient
conditions. Product distributions observed
during irradiations of alkanes (n-butane,
n-pentane and n-hexane)-N(2)-air systems in two
quite different approximately 6000-liter
environmental chambers were found to be
consistent with this prediction. For example, in
the n-pentane-N(2)-air system the observed large
yields of 3-pentanone relative to 2-pentanone
were consistent with room temperature rate
constants which we have estimated for the
corresponding hydrogen shift isomerizations.
While such isomerizations have been well
recognized in studies of free radicals and high
temperature hydrocarbon oxidations, they are not
taken into account in current kinetic mechanisms
for alkane oxidation under ambient atmospheric
conditions. This has implications for the
construction of computer models of photochemical
smog formation.

<18>
Development and Application of a Hydrocarbon
Reactivity Scale Based on Reaction with the
Hydroxyl Radical

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PMCAE NO: (714) 787-4584 (Pitts)

Presented at the 69th Annual Air Pollution
Control Association Meeting, Portland, OR, June
27-July 1, 1976, 15 p.; 1976

RATE CONSTANTS; HYDROXYL RADICAL; HYDROCARBONS;
DIFFUSION CHAMBER; N-BUTANE; ISOPENTANE;
ELEMENTARY REACTION MEASUREMENTS; PHOTOCHEMICAL
SMOG; REACTIVITY SCALES; ALKANES; ALKANES;
AROMATICS; OXYGENATES; N-HEXANE; OZONE;
PHOTOCHEMICAL SMOG; ATMOSPHERIC CHEMISTRY;
ANALYSIS

Measurements of the relative rate constants for
the reaction of the hydroxyl radical (OH) with
some 35 atmospherically important hydrocarbons
have been made in the SAPHIR 6000 liter glass
irradiation chamber. These rate constants were
placed on an absolute basis using literature
values for either n-butane or isobutene and have
been augmented with OH rate data obtained by
elementary reaction measurements and other

appropriate data, such as that from
photooxidation studies, from which relative and
absolute OH rate constants could be calculated.
Utilizing these data, a reactivity scale for some
80 compounds, including alkenes, alkanes,
aromatics, oxygenates, and naturally occurring
hydrocarbons, has been formulated based on the
removal of the hydrocarbons by reaction with OH.
The resulting scale is an ordering of the
reactivities of the hydrocarbons relative to
methane. The scale can be divided into an
arbitrary number of classes for purposes of
application to control strategies or comparison
with other reactivity scales. Some comparisons
of the present scale with proposed EPA and APO
reactivity scales are made, and the implications
of the present scale for the role of alkanes and
a number of aromatic hydrocarbons in the
formation of ozone in regions downwind of urban
centers is analyzed.

<19>
The Concentration, Size Distribution and Modes of
Formation of Particulate Nitrate, Sulfate and
Ammonium Compounds in the Eastern Part of the Los
Angeles Basin

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PMCAE NO: (714) 787-4584 (Pitts)

Presented at the 69th Air Pollution Control
Association Annual Meeting, Portland, OR, June
17-July 1, 1976, 10 p.; 1976

PARTICULATES; NITRATE; AMMONIA;
AEROSOLS; METEOROLOGICAL CHANGES; PHOTOCHEMICAL
SMOG; SECONDARY POLLUTANTS; VISIBILITY; ANALYSIS;
ATMOSPHERIC CHEMISTRY

Particulate sulfate, nitrate and ammonium
concentrations were measured daily during a six
month period (May-October 1975) in the eastern
part of the Los Angeles Air Basin. Gas phase
pollutants, meteorological variables,
condensation nuclei and aerosol size distribution
and light scattering were monitored continuously.
In addition to the 24 samples, 2 hr size
resolved samples were collected during
photochemical smog episodes and analyzed for SO₄,
NO₃, and NH₄ ions. As a result of gas to
particle conversion during transport from the
western part of the basin, high sulfate and
nitrate levels (up to 48.7 and 70.2 ug m⁻³)
were observed during the six month study, with
gas-particle distribution factors as high as 77%
and 49%, respectively. Six month-averaged SO₄
and NO₃ ion concentrations, calculated from 176,
24 hr measurements, were 16.3 and 23.7 ug m⁻³.
Both sulfate and nitrate levels increase
markedly with photochemical activity. Sulfate
and nitrate aerosols accumulate in the submicron
range, and are produced below 0.6 u at rates
exceeding 10 ug m⁻³ hr⁻¹ during
photochemical episodes. Although secondary
pollutant concentrations were found in the order:
NO₃ ion was greater than SO₄ ion was
approximately equal to organic carbon,
statistical treatment of 159, 24 hr measurements
of light scattering, NO₃ ion, SO₄ ion, carbon and
other aerosol constituents (total aerosol - SO₄
ion plus NO₃ ion plus C) indicated sulfate
aerosols as the major species responsible for
visibility reduction in the eastern part of the
Los Angeles Air Basin.

GEOGRAPHICAL DESCRIPTION: US, California, Los
Angeles Basin

<24>

Atmospheric Water Vapor Measurements with an Infrared (10-um) Differential-Absorption Lidar System

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Appl. Phys. Lett., 26(9), 542-543; 1976, May

DIFFERENTIAL ABSORPTION LIDAR SYSTEM: GASEOUS SPECIES; ATMOSPHERIC; CHATING-TUNED CO₂ TEA LASER; INFRARED DETECTORS; ANALYTICAL METHODS; METHOD DEVELOPMENT; ANALYSIS; ATMOSPHERIC CHEMISTRY; WATER; OZONE; SULFUR DIOXIDE; AMMONIA; FREON 11; FREON 12; FREON 113; VINYL CHLORIDE; ETHYLENE; METHANE; ABSORPTION COEFFICIENTS

The design, construction, and operation of the first infrared differential-absorption lidar system for remote range-resolved sensing of gaseous species is described. The target gas in these experiments was water vapor, which was measured using several CO₂ laser lines near 10.um. Feasibility of such a scattering system depends on the magnitude of the backscatter from naturally occurring aerosols and on the magnitude of the absorption coefficients of pollutant species. The present system performance indicates a backscatter coefficient sufficient to attain a range of 12 km with commercially available components. O₃, SO₂, NH₃, Freon 11, Freon 12, Freon 113, vinyl chloride, ethylene, and methanol could probably be monitored with this system.

<25>

Generation of Standard Metal Oxide Particulates in the Respirable Range

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Anal. Chim. Acta, 85, 399-402; 1976

METALS; METAL PARTICULATES; ANALYTICAL METHOD DEVELOPMENT; ANALYSIS; ATMOSPHERIC CHEMISTRY; SAMPLE STANDARDS; PARTICULATE GENERATION; RESPIRABLE PARTICULATES; TOXICOLOGY; LEAD; ZINC; COPPER

A method which is a modification of the method of Charnarajan and West for the generation of reliable standards of metal oxide particulates of copper, lead, and zinc is presented. More than 94% of the particles generated are in the respirable range, the maximum concentration being in the 1.1 to 2.1 um range. In addition to being useful for generation of standards for air pollution analyses, this method is potentially useful in the toxicological and industrial hygiene studies of complex mixtures of metal particulates.

<26>

Organic and Conventional Crop Production in the Corn Belt: A Comparison of Economic Performance and Energy Use for Selected Years

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NSF/BA-760004, 42 p.; CENS-AR-7; PB-255-458; 1976, June

ORGANIC FARMS; CONVENTIONAL FARMS; CROPS; LIVESTOCK; PESTICIDES; YIELDS; PRODUCTION COSTS; ENERGY CONSUMPTION; CROP PRODUCTION; MARKET VALUE; LABOR; PHOSPHORUS; POTASSIUM; NUTRIENT BALANCE; NUTRIENTS; CROPS; SOYBEANS; UREAS; HARROW; TINE; TILLAGE; CULTIVATION; PLANTING; HAY; OATS; SILAGE; SOILS; ANALYSIS

A two year study of fourteen pairs of crop-livestock farms in the Corn Belt, in which one member of each pair used only organic fertilization methods and no pesticides, while the other used conventional fertilizers and pesticides is described. Data are presented on the yields, production costs, and energy consumption for crop production in 1976 and 1975. The organic group has an overall production level an average of 10% below that of the conventional group in terms of market value of output per acre of cropland. Their operating costs are also lower, so that returns to crop production are equal for the two groups. The conventional group is 1.3 times more energy intensive, primarily because of the energy needed to produce conventional fertilizers. The organic group requires 12% more labor per unit of market value of crops produced. Whereas the input and removal of P and K were in balance on the conventionally managed cropland, the organic farmers were drawing somewhat on pre-existing reservoirs of these nutrients.

<27>

Environmental Pollution in the Lead Belt, RARE Utilization Experience, Case Study No. 2

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NSF/PA-6-75-030, 23 p.; PB-247-246; 1975

LEAD MINING; FORESTS; HEAVY METALS; LEAD SMELTING; LEAD; ZINC; COPPER; CADMIUM; MILLING; UTILIZATION PLANNING; EFFLUENTS; ANALYSIS; PROJECT COORDINATION

The rapid development of the lead mining industry in the "New Lead Belt" of southeastern Missouri caused serious concern as to the effects of lead mining activities on the surrounding virgin forest ecosystems. The objectives of this research are to examine the extent and causes and effects of heavy metal contamination from lead mining and smelting on the surrounding forest, and to develop information for state and federal agencies so that appropriate corrective action could be taken. This project is a good example of a well-utilized research program having significant value to industry, government, and to the public. The project study team served as a catalyst, bringing together industry and regulatory agencies in a cooperative effort to understand and solve a potentially serious problem.

GEOGRAPHICAL DESCRIPTION: US, Missouri, Ozark Mountains, New Lead Belt

<28>

The Effect of pH, Salt Concentration, and Nature of Electrolyte on the Charge Characteristics of Brazilian Tropical Soils

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Soil Sci. Soc. Amer. J., 40(4), 521-527; 1976

JB; SALT CONCENTRATION; ELECTROLYTES; CHARGE CHARACTERISTICS; ION DETENTION; ELECTROCHEMICAL BEHAVIOR; SOILS; NITROGEN ION; NITRATE ION; EQUILIBRIUM SOLUTIONS; MAGNESIUM SULFATE; POTASSIUM SULFATE; POTASSIUM CHLORIDE; MAGNESIUM CHLORIDE; COUNTER-IONS; FIELD IN; SURFACE HORIZONS; SUBSURFACE HORIZONS; ANION ABSORPTION; ZERO POINT OF CHARGE; ANALYSIS

A study of the distribution of electric charges in the A and B horizons of some Oxisols, Ultisols, and Alfisols from Brazil was made by direct measurement of retention of ions in the presence of varying electrolyte concentrations. Soil samples were collected from the Amazonian Jungle and from the principal cocoa-producing zone of the country, the southern part of Bahia State. The electrochemical behavior of these soils was found to be similar to that of the constant potential systems in which the surface potential is determined by H and Cl ions in the equilibrium solution, hence charge distribution varied substantially with pH and electrolyte concentration. Direct measurement of adsorption of ions from solutions of H_2SO_4 , H_2SO_4 , HCl , and $HgCl_2$ showed that the nature and valence of the counter-ions also influenced the magnitude of the electric charges on the soil particles. The pH at the zero point of charge (ZPC) of the soils varied from 1.2 to 3.4 in the A horizons and from 4.0 to 6.7 in the B horizons. At or near their field pH the surface horizons were, in general, net negatively charged, while the subsurface horizons were either isoelectric or positively charged. This fact was found to be related to differences in organic matter contents of the horizons.

GEOGRAPHICAL DESCRIPTION: Brazil, Amazonian Jungle, Bahia State

<29>

Airborne Pb, Cd, Zn and Cu Concentration by Particle Size Near a Pb Smelter

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Atmos. Environ., 10, 443-446; 1976

LEAD; CADMIUM; ZINC; COPPER; PARTICLE SIZE; LEAD SMELTER; ATMOSPHERIC CHEMISTRY TEST FARMS; LEAD EXCRETION; AIR SAMPLES; SEASONAL SAMPLING; ATOMIC ABSORPTION SPECTROPHOTOMETRY; RESPIRABLE PARTICLES; ANALYSIS; DUSTFALL; SOIL;

METEOROLOGICAL DATA; AIRBORNE PARTICLES

A study of airborne Pb, Cd, Zn and Cu was conducted on 2 farms: a test farm exposed to a lead smelter and associated sources of lead contamination in the New Lead Belt of southeast Missouri, and a control farm outside the lead production area. An Andersen eight-stage impactor sampler was used on both farms to collect air samples during winter, spring and summer seasons. The trace element concentrations were measured by atomic absorption spectrometry. The concentrations of all four elements were higher on the test farm than on the control farm in all of the three seasons. Approximately 66% of the Pb, 88% of the Cd, 73% of the Zn, and 54% of the Cu was composed of particles smaller than 4.7 μ m the upper practical limit of respirable size.

GEOGRAPHICAL DESCRIPTION: US, Missouri, Ozark Mountains, New Lead Belt

<30>

Nitrogen Balance in the Southern San Joaquin Valley

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J. Environ. Qual., 5(3), 274-278; 1976

NITROGEN BALANCE; AREA; AGRICULTURAL FUNCTION; NITROGEN INPUT; FLOW DIAGRAM; NITROGEN POOLS; NITROGEN USE; NITROGEN FLUXES; NITROGEN OUTPUT; PLANTS; SOIL; NITRATE; LAND SURFACE; SUBSTRATA; WATER; ANALYSIS

A nitrogen balance for the southern San Joaquin Valley of California has been calculated, using techniques and methodology developed for the Upper Santa Ana River Basin of southern California. The two areas differed considerably in both size (the latter being much smaller) and agricultural function. Data were compiled on N inputs, use, and outputs for many sources within the study area. Such data enabled construction of a flow diagram depicting best estimates of N pools and fluxes within the San Joaquin Valley Basin. Results show N inputs into the study area from various sources were somewhat greater than output to the atmosphere and by plant removal. Inputs to the soil N pool were about 9 kg/ha more in 1971 than 1961. Since the soil N pool was estimated to be about 11 metric tons/ha, this represented an increase of about 0.1%. However, since the increases of N are not evenly distributed over the study area, high N concentrations can develop in some local areas.

GEOGRAPHICAL DESCRIPTION: US, California, San Joaquin Valley; Tulare Lake Basin

C21)

Variable Nature of Chemical Composition of Sewage Sludges

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J. Environ. Qual., 5(3), 302-306; 1976

SEWAGE SLUDGE; CARBON; NITROGEN; PHOSPHORUS; POTASSIUM; CALCIUM; MAGNESIUM; IRON; CUPRUM; ZINC; COPPER; NICKEL; LEAD; ORGANIC MATTER; HEAVY METALS; PLANT NUTRIENTS; INORGANIC NITROGEN; INORGANIC CARBON; ORGANIC NITROGEN; ORGANIC PHOSPHORUS; INORGANIC PHOSPHORUS; ANALYSIS

Sewage sludge samples were collected over a 2-year period from eight Indiana cities and analyzed for C, N, P, S, Ca, Mg, Fe, Cd, Zn, Cu, Ni, and Pb. The sludges contained approximately 50% organic matter and 1-4% inorganic C. Organic and inorganic C, organic N, inorganic P, and Ca and Mg were found to be present in a given sludge at a relatively constant concentration with respect to sampling time. Inorganic N, organic P, S, and all metals were found to be quite variable with time for sewage sludge produced by a given city. In general, organic P and inorganic P constituted the majority of total P and S, respectively, in sludges. The largest deviations between the mean and median were found for Cd, Zn, Cu, Ni, and Pb. Variable nature of inorganic P and metal contents of sludges indicates that a sound sampling and analysis program is essential prior to formulating recommendations for rates of sewage sludge applications on soils used for crop production.

GEOGRAPHICAL DESCRIPTION: US, Indiana, Anderson, Crawfordville, Elletts, Lebanon, Peru, Logansport, Noblesville, Tipton

C22)

Movement of Heavy Metal below Sewage Disposal Ponds

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J. Environ. Qual., 5(3), 330-334; 1976

SOILS; SLUDGE; EFFLUENTS; DISPOSAL PONDS; SEWAGE TREATMENT PLANTS; ZINC; CALCIUM; COPPER; CHROMIUM; NICKEL; HEAVY METALS; ACID-EXTRACTABLE METALS; METAL MOBILITY; AERATION CONDITIONS; SATURATION EXTRACTS; CHEMICAL OXYGEN DEMANDS; METAL MOVEMENT; METAL-ORGANIC COMPLEXES; ANALYSIS

Coarse-textured soils below sludge and effluent disposal ponds at the sewage treatment plants were studied. The concentrations of Zn, Cd, Cu,

Cr, and Ni in the soils at various depths were determined to investigate the downward movement of these heavy metals below the two types of disposal ponds. Concentrations of acid-extractable metals (AN HNO₃) were greater under disposal ponds than effluent control sites at both treatment plants. Metal enrichment was evident to depths as great as 1 m under some ponds. The depth and degree of metal enrichment depended on the specific pond type and the treatment plant. Metal concentrations were greater under anaerobically digested sludge-holding ponds than effluent ponds. Concentrations of the metals in saturation extracts of soils beneath the ponds were much greater than those typically found for California soils. The distributions of metals with depth were closely related to the changes in chemical oxygen demands of soil samples with depth. This suggests that the metals have moved as soluble metal-organic complexes.

C33)

A Rapid Method for the Determination of Methylmercury Chloride in Water Samples by Gas Chromatography with a Microwave Emission Spectrometric Detector.

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Anal. Chim. Acta, 85, 263-268; 1976

ANALYTICAL METHODS; METHOD DEVELOPMENT; TESTIARY AMIDES; METHYL MERCURY CHLORIDE; GAS CHROMATOGRAPHY; MICROWAVE EMISSION DETECTOR; WATER; METHYL MERCURY CHLORIDE-AMINE COMPLEX; ANALYSIS

A method is described in which tertiary amines preferably extract methylmercury(II) chloride. With 0.5% solutions of tertiary amine in 1-methyl-2-pyrrolidone, a quantitative (95% plus or minus 3%) extraction of methylmercury(II) chloride, as a CH₃HgCl-amine complex, can be achieved for aqueous solvent volume ratios as high as 400. After the extraction, aliquots (1-10 µl) of the benzene layer are injected into the g.c. column. In the injection port, which is held at 200 degrees C, the CH₃HgCl-amine complex is instantly cleaved to release the volatile methylmercury(II) chloride which is then separated by the g.c. column in exactly the same manner as pure methylmercury(II) chloride. When this technique is used, traces of methylmercury chloride as low as 1 ng/l can be determined in various water samples with an accuracy and precision of 10-15%. The excellent sensitivity and relative simplicity of this technique should be of interest to environmentalists concerned with the mechanisms of alkylmercury accumulation in various biological systems.

<20>

Importance of NO₂ + NO in Alkyl Nitrate Formation from C₄-C₆ Alkane Photooxidations under Simulated Atmospheric Conditions

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J. Phys. Chem., 80(17), 1982-1990; 1976

NITROGEN MASS BALANCE; ALKYL NITRATES; METHYL NITRATE; ETHYL NITRATE; BUTYL NITRATES; PENTYL NITRATES; HEXYL NITRATES; ALKYL NITRATES; FACTORIAL; ALKANE; NITROGEN CHEMISTRY; ATMOSPHERIC CHEMISTRY; ALKANE; ANALYSIS; MODELING

Evidence that alkyl nitrates are formed from precursors other than alkyl radicals and that nitrate formation is independent of NO or NO₂ levels, provided that some NO_x remains in the n-alkane-NO_x-air photooxidation reaction system, is presented. The amount of alkyl nitrate formed and the amount of hydrocarbon reacted both increase with reaction time, but their ratio is relatively independent of reaction time until either all the hydrocarbon or the NO_x has been consumed. These ratios increase with the size of the reacting alkane. It is concluded that the mechanism of reaction depends on the nature of the alkane.

<21>

External Cavity CO₂ - Pump InSb Spin-Flip Laser

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IEEE, J. Quant. Electron., 12(1)-12(2); 1976, March

LASERS; EXTERNAL CAVITY SPIN-FLIP LASER; AXIAL MODES; TRANSVERSE MODES; PUMP-POWER MODES; OUTPUT COUPLER; MAGNETIC FIELD; FREQUENCY COUPLING; ANALYTICAL METHOD; ANALYSIS; INSTRUMENTATION

The use of an external cavity spin-flip laser is described in which the axial and transverse modes are carefully controlled to provide a device that is useful for spectroscopic and photochemical applications. The CO₂-pumped spin-flip laser is operated such that the output frequency of the spin-flip laser is governed to a large extent by the Fabry-Pérot (FP) modes of a resonant output coupler. By tuning this output coupler in tandem with the magnetic field, essentially complete frequency coverage with single-mode operation can be obtained and should enhance the usefulness of the spin-flip laser for many applications. An output spectral width of 0.027 plus or minus 0.003 cm⁻¹ has been attained.

<22>

CERES - A Model of Forest Stand Biomass Dynamics for Predicting Trace Contaminant, Nutrient, and Water Effects

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ORNL-RSP-RATC-25, 102 p.; 1976, October

FORESTS; FOREST GROWTH; MODELS; MODELING; SOIL TRANSPORT; SOIL CHEMISTRY; SOLUTE UPTAKE; WATER STATUS; PLANT GROWTH; BIOMASS; LITTER; LEAVES; STEM; ROOTS; FRUITS; SEEDS; LEAD; DRYFALL; DRYFALL; DECOMPOSITION RATE; LITTER MASS; ANALYSIS

CERES is a forest stand growth model which incorporates sugar transport in order to predict both short-term effects and long-term accumulation of trace contaminants and/or nutrients when coupled with the soil chemistry model (SCHEM), and models of solute uptake (DIPHAS and DUTAS) of the Unified Transport Model, UTM. An important feature of CERES is its ability to interface with the soil-plant-atmosphere water model (PROSPER) as a means of both predicting and studying the effects of plant water status on growth and solute transport. CERES considers the biomass dynamics of plants, standing dead and litter with plants divided into leaves, stems, roots, and fruits. The plant parts are divided further into sugar substrate, storage, and in the case of stems and roots, heartwood components. Several applications of the model are described. Simulation results for ten days in May illustrate the hourly patterns of photosynthesis, leaf sugar levels and translocation. The second application of CERES is a one-year simulation, showing seasonal dynamics of biomass fluxes in plants and litter. Results from a six-year simulation with the complete set of coupled models illustrate toxic metal effects on litter decomposition and slight reduction of root growth with the parameters chosen. Heavy metal pollutants from a lead mine and smelter complex were introduced to the ecosystem as wetfall and dryfall. The CERES and DIPHAS models calculated the heavy metal uptake by the vegetation and accumulation in litter. During the six-year period, the steady annual input of plant litter and the reduced decomposition rate resulted in an increase in litter mass of nearly 50%. Input data were chosen to represent the oak forest characteristics of the Crooked Creek watershed in southeastern Missouri.

GEOGRAPHICAL DESCRIPTION: US, Missouri, Crooked Creek Watershed

<37>

ERTABS and BIFBAS, Fortran Models for
Investigating Solute Uptake and Incorporation
into Vegetation and Litter

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CSBI-WSP-PATC-26, 122p.; 1976, October

DETAILS: MODELING; SOLUTE MOVEMENT; SOIL; SOIL
SCOLUTIONS; ROOTS; PLANT TISSUES; LITTER;
ECCUMULATION; FOLIAR UPTAKE; TERRESTRIAL
ECOSYSTEMS; LEAF PERMEABILITY; ROOT CONDUCTIVITY;
ROOT SAFETY; BIOMASS PATTERNS; DECOMPOSITION
RATES; MINERALIZATION LOSSES; ANALYSIS: SULFUR
CICLONE

The concepts and FORTRAN algorithms of a model describing solute movement from bulk soil solution into roots (BIFBAS) and a mode of solute dynamics and accumulation in plant tissues and litter (ERTABS) are presented. Foliar uptake of solutes and gases are included in the ERTABS code. These models form components in a coupled system of models having hourly resolution of carbon, water, and solute dynamics in terrestrial ecosystems. The input data requirements of the solute models and the methods of coupling these codes with the other component models are given in detail as a guide to users. Applications showing successive hourly, monthly, and annual results illustrate the utility of the models. The ERTABS model sensitivity to both leaf solute permeability and root solute conductivity parameters suggest the importance of careful experimental determination of these plant properties. The tissues of solute entry (leaves, roots) initially accumulate solutes in a fixed form in preference to the more reactive tissues (stems, fruits). Model application results suggest that root sagwood is the first major site of trace contaminant accumulation from soil borne pollutants. The algorithm describing solute movement along a concentration gradient in phloem and as mass flow in the xylem transpiration stream result in high mobility of solutes in vegetation. The simulated diurnal pattern of root solute uptake showed that more than 85% of solutes are taken up during the daylight hours. The simulations further showed that contaminants had the greatest effect on the litter system. Toxic effects of contaminants on decomposition resulted in lower mineralization losses and higher accumulations of contaminant in litter with continuing deposition.

<38>

Corrected South Coast Air Basin Oxidant Data:
Some Conclusions and Implications

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Environ. Sci. Technol., 10(8), 798-801; 1976,
August

CRITICAL AIR QUALITY; AIR QUALITY DATA;
ATMOSPHERIC CHEMISTRY; SCALED DATA; OXIDANTS;
ANALYSIS

The rationale for and the results obtained by

scaling existing oxidant air quality data for Los Angeles County (LAC) air monitoring stations by a factor of 1.1 and existing air quality data for non-LAC stations by a factor of 0.9 are presented. Thus, an internally consistent set of oxidant data for the California South Coast Air Basin is generated. The scaled oxidant data show that, contrary to the indications of the data as reported, cities such as Azusa and Pasadena in LAC have yearly total oxidant levels than cities in the easternmost portion of the Basin. The scaled data also show that non-LAC oxidant dosages are substantially lower than was previously believed. Furthermore, if non-LAC oxidant data and any oxidant episode levels dependent on data referenced to neutral buffered KI are both scaled downward by 0.9, the new dosage calculated using the scaled standard and scaled data is lower than the old dosage by 70%.

<39>

Long-Path Infrared Spectroscopic Investigation at
Ambient Concentrations of the 2% Neutral Buffered
Potassium Iodide Method for Determination of Ozone

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Environ. Sci. Technol., 10(8), 787-793; 1976,
August

OZONE; CALIBRATION PROCEDURES; INFRARED
SPECTROMETRY; AMBIENT AIR; POTASSIUM IODIDE;
ENVIRONMENTAL CHANGES; HUMIDITY; LIQUID
REFRACTION ANALYSIS; ANALYTICAL METHODS;
ANALYSIS; ATMOSPHERIC CHEMISTRY

Following disclosure by the California Air Resources Board (ARB) and the Los Angeles Air Pollution Control District (LAAPCD) of a significant discrepancy (approx. 30%) between their respective ozone calibration procedures, we investigated the stoichiometry of the 2% neutral buffered potassium iodide (NBKI) method for ozone (ARB method). An environmental chamber with an in-situ long-path optical system was employed to simultaneously obtain infrared (IR) spectra and 2% NBKI impinger samples over a range of ozone concentrations (0.1-1.2 ppm) encompassing ambient levels at several relative humidities (RH). Absolute ozone concentrations were calculated from the well-resolved 9.00 μ B-branch absorption of ozone using an absorptivity of 4.23×10^4 (E-8) ppm(E-1) m(E-1) BTP which was experimentally determined by two independent methods. Linear regression analyses of the 2% NBKI and IR ozone concentrations yielded:
 $((O_3)KI) = 1.10((O_3)IR) + 0.013$ for 1% RH, $((O_3)KI) = 1.12((O_3)IR) + 0.001$ for approximately 10% RH, $((O_3)KI) = 1.23((O_3)IR) + 0.001$ for 50% RH. Although the dependence on RH is not understood, these results indicate that the 2% NBKI method yields ozone concentrations 12-10% higher than the absolute spectroscopic determinations at low RH, and 23-25% higher at high RH. In the course of this investigation, a collaborative study with U.S. Bureau demonstrated excellent agreement between simultaneous measurements of ozone samples by IR and UV spectroscopies where the absorptivities employed were 4.23×10^4 (E-8) ppm(E-1) m(E-1) and 135 cm(E-1) at λ (E-1), respectively.

<83>

Chemical Ionization Mass Spectrum of Peroxyacetyl Nitrate

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Org. Mass Spectrom., 11, 552-555; 1976

IONIZATION: MASS SPECTROSCOPY;
PEROXYACETYL NITRATE; PHOTOCHEMICAL SMOG;
TOXICITY; HAP; PLANTS; METABOLISM; ISOTOPES;
SIMULATED ATMOSPHERES; ANALYSIS;
ANALYTICAL METHODS

The chemical ionization mass spectrum of peroxyacetyl nitrate, a major component of photochemical smog highly toxic to man and plants, was obtained using both methane and isobutane as reagent gas. The spectrum contains a ($M + 1$) positive ion at m/e 122, intense fragment ions at m/e 43 ((CH_3CO) positive ion) and m/e 46 ((OC_2) positive ion), and less intense ions at m/e 61 ((CH_3CO_2) positive ion), m/e 77 ((CH_3CO_2) positive ion) and m/e 88 positive ion ($CH_3CO_2O_2$) formed by internal rearrangements. These results confirm the commonly accepted structure for peroxyacetyl nitrate, $CH_3(CO)OONO_2$.

<84>

Economic Analysis of Irrigated Farming with Diminishing Ground Water Reserves

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WEE/PA-760605, 5C p.; COME-AR-0; FE-255-033;
1976, 84y

CCBB; ECONOMIC ANALYSIS; IRRIGATION; FARMING;
GROUND WATER; WATER TABLE; CROP YIELDS; PLANT
GROWTH; WATER REQUIREMENTS; HYDROLOGY; MODELS;
MODELING; WATER RESOURCES; ANALYSIS; FERTILIZATION

With the rapid expansion of irrigated farming in the Great Plains, irrigation from ground water reserves has caused water tables to fall in many areas in the last few decades. As the saturated thickness of an aquifer declines, net returns to irrigated farming are vulnerable from two sources: the increased cost of pumping water and the decrease in expected crop yields. The latter source of decreased net returns is the more important of the two. An economic evaluation of irrigation from ground water requires careful specification of the production function for a crop. Crop yields, for example, are highly sensitive to the availability of water in certain critical periods in the stages of plant growth making neo-classical production functions unsuitable for an economic analysis when well capacities are inadequate to meet water requirements in critical periods. A method of economic analysis is proposed that rests on a production function that incorporates the availability of water in critical periods of plant growth and its effect on yields. Hypothetical, but plausible, examples of corn under center pivot irrigation with declining water tables are used to demonstrate the usefulness of the approach.

<85>

Relative Rate Constants for the Reaction of the Hydroxyl Radical with Selected Ketones, Chloroethenes, and Monoterpene Hydrocarbons

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J. Phys. Chem., 80(14), 1635-1649; 1976

MONOTERPENE HYDROCARBONS; CHLOROETHENES;
ALIPHATIC KETONES; ENVIRONMENTAL CHEMISTRY;
SIMULATED ATMOSPHERES; RELATIVE RATE CONSTANTS;
ABSOLUTE RATE CONSTANTS; HYDROXYL RADICALS;
HYDROCARBONS; ISOPRENE; ALPHA-PINENE;
BETA-PINENE; DELTA-LINOLENE; METHYL ETHYL KETONE;
METHYL ISOBUTYL KETONE; DIISOBUTYL KETONE;
TRICHLOROETHENE; TETRACHLOROETHENE; ANALYSIS;
ATMOSPHERIC CHEMISTRY

The relative rates of disappearance of three monoterpene hydrocarbons, two chloroethenes, and three aliphatic ketones were measured in an environmental chamber under simulated atmospheric conditions at 305 plus or minus 2 degrees K. The observed rates of disappearance were used to derive relative rates of reaction of these organic compounds with the hydroxyl radical (OH) on the previously validated basis that OH is the species predominantly responsible for α -hydrocarbon disappearance under the experimental conditions employed. Absolute rate constants, obtained from the relative values using the published rate constant for $OH + isobutene$ ($3.05 \times 10^{10}(E-1)5(E-1)$), are ($k \times 10^{10}(E-1)5(E-1)$): alpha-pinene, 3.5 plus or minus 0.5; beta-pinene, 4.1 plus or minus 0.6; delta-limonene, 9.0 plus or minus 1.4; methyl ethyl ketone, 0.20 plus or minus 0.06; methyl isobutyl ketone, 0.9 plus or minus 0.3; diisobutyl ketone, 1.5 plus or minus 0.5; trichloroethene, 0.27 plus or minus 0.08; tetrachloroethene, 0.13 plus or minus 0.04. No previous determinations of these rate constants have been found in the literature. Rate constants for an additional nine monoterpene hydrocarbons have been derived from data recently published by Grimmer, Westberg, and Patai.

<83>

Microwave Plasma Emission Spectroscopy

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Anal. Chem., 48(7), 611A-612A, 614A, 616A, 618A, 620A; 1976

PLASMAS; MICROWAVE FREQUENCY ELECTRICAL FIELDS; GASES; SPECTRAL EXCITATION SOURCES; MICROWAVE COUPLED PLASMAS; PLASMA CONFIGURATIONS; SPECTROSCOPIC APPLICATIONS; ANALYTICAL METHODS; ANALYSIS

Plasmas produced by the interaction of microwave frequency (usually 2450 MHz) electrical fields with gases show considerable potential as spectral excitation sources. The purpose of the present report is to discuss methods that have been used to produce microwave coupled plasmas, examine the operational characteristics of various plasma configurations, summarize their present status in terms of spectrometric applications, and project directions of future development.

<84>

Potential Carcinogens in Water: GC/MS Analysis

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Presented at the 8th Materials Research Symposium - Methods and Standards for Environmental Measurement, Gaithersburg, MD, September 20-24, 1976; 1976

WATER; RIVER WATER; WASTEWATER; RECEIVING WATERS; SEDIMENTS; INDUSTRIAL PLANTS; MASS SPECTROMETRY; GAS CHROMATOGRAPHY; ORGANIC COMPOUNDS; SOLUBILITY; SOLVENTS; BIOLOGICAL SOURCE; CHEMICAL INTERACTIONS; ANALYSIS; REPLICATION; EFFLUENT CONTROL; ANALYSIS

Analysis of wastewater, receiving waters and sediments of several industrial plants by mass spectrometric and gas chromatographic techniques has indicated that organic compounds which are actually water insoluble can be accommodated in wastewater by interaction with high concentrations of dissolved and suspended organic materials such as solvents and biological sludge. The concentration of these organic compounds in the river water may be only a few parts per billion but in the river sediments concentration may reach very high levels (up to 0.5% for 2-(2'-hydroxy-5'-ethylphenyl)-2H-tetrazole). The presence of these organic compounds in sediments may be a source of continual repollution even after effluent control measures have been implemented.

<85>

Tunable Lasers in the Infrared

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Laser Focus, 47-51; 1976, April

TUNABLE LASERS; RESOLUTION; INFRARED FINGERPRINTS; MOLECULAR VIBRATION-ROTATION LINES; TUNING RANGE; TUNABLE INFRARED LASERS; SEMICONDUCTOR DIODE LASERS; CRYOGENIC COOLING; SPIN FLIP-RAMAN LASERS; NONLINEAR DEVICES; LASER INSTRUMENTATION; GAS LASERS; ANALYSIS

Development of tunable lasers with emission between 1 and 20 microns has provided spectroscopists with much higher resolution than has been possible in this infrared "fingerprint" region, rich in characteristic molecular vibration-rotation lines. The major problem with lasers has been their limited continuous tuning range. This paper reviews the capabilities and present limitations of some of the tunable infrared lasers being developed. Semiconductor diode lasers are the simplest of the tunable lasers, providing modest continuous-wave power with narrow linewidth and good frequency stability, and tunable over a wide spectral range. They require cryogenic cooling and do not generally have the controllable mode qualities of other, more complex lasers. Spinflip-raman lasers can provide high-power cw or pulsed tunable radiation having high spatial-mode quality; spectral coverage is somewhat limited, good frequency stability being difficult to achieve. The apparatus is rather complex and cryogenic temperatures are required. Several important tunable infrared sources are based on frequency mixing in materials with nonlinear indices of refraction. Operation at room temperature makes these nonlinear devices more convenient than spinflip or diode lasers; however nonlinear devices generally have limited spectral coverage with relatively poor resolution. The instrumentation is also complex. Zeeman-tuned gas lasers and high pressure CO₂ and gas lasers are also discussed.

<46>

Transient Infrared Antisymmetric Spin-Flip Laser

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Opt. Commun., 10(1), 15-16, 1976

TRANSIENT RESPONSE; INFRARED ANTISYMMETRIC SPIN-FLIP LASER; PULSED CO₂ LASER; TEMPORAL BEHAVIOR; OSCILLATIONS; SPIN-RELAXATION TIME; SPECTROSCOPIC APPLICATIONS; PHOTOCHEMICAL APPLICATIONS; ANALYTICAL METHODS; REMOTE SENSING; ANALYSIS

The transient response of an InSb spin-flip Raman laser has been investigated for the first time using a pulsed CO₂ laser. The spin-flip laser output power does not simply saturate as the CO₂ pump power is increased, but rather shows a complex temporal behavior that cannot be explained by existing theories. Part of the temporal behavior is due to oscillations analogous to those obtained in solid state lasers. These relaxation oscillations provide a direct measurement of the spin-relaxation time T₁ in InSb. Only indirect measurements of T₁ have been reported previously with values ranging from 1-600 ns. The spin-relaxation time (at $\lambda = 1.2 \times 10^{16}$ cm⁻², $\nu = 60$ K, τ approximately 20K) is determined to be 75 plus or minus 20 ns. By using 200 ns duration input pulses to study the effects of carrier heating, it is found that the system recovery time did not increase substantially indicating that the energy relaxation time are somewhat faster than the spin-relaxation time. In addition to measurement of T₁, the multiple pulse technique can provide a means to efficiently extract larger output energies and high average power in a low order mode from a CO₂ laser excited spin-flip laser. This can enhance its usefulness for spectroscopic and photochemical applications.

<47>

Rate Constants for the Reaction of OH Radicals with 2-Methyl-2-Butene over the Temperature Range 297-425 K

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Chem. Phys. Lett., 38(3), 607-610, 1976, March

HYDROXYL RADICAL; INTERMEDIATES; ATMOSPHERIC CHEMISTRY; RATE CONSTANTS; CLEFINS; CHEMICAL KINETIC MODELS; URBAN ATMOSPHERES; ABSOLUTE RATE CONSTANTS; 2-METHYL-2-BUTENE; FLASH PHOTOLYSIS-RESONANCE FLUORESCENCE TECHNIQUES; APPARENTLY SUPPRESSIONS; ANALYSIS

The hydroxyl radical has been shown to be a

reactive intermediate of importance in combustion processes and in atmospheric chemistry. Consequently, the rate constants for the reaction of OH radicals with olefins are of fundamental interest and are a necessary input into chemical kinetic models of polluted urban atmospheres. Absolute rate constants, k₂, for the reaction of OH radicals with 2-methyl-2-butene have been determined over the temperature range 297-425 degrees K using a flash photolysis-resonance fluorescence technique. The Arrhenius expression obtained was $k_2 = 3.6 \times 10^{-11} \exp(14500 \pm 1000 / RT)$ cm³ molecule⁻¹ sec⁻¹.

<48>

Nitrate-Nitrogen Movement Through Soil As Affected by Soil Profile Characteristics

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J. Environ. Qual., 5(3), 283-288, 1976

GROUND WATERS; SURFACE WATERS; NITROGEN; SOIL PROFILE CHARACTERISTICS; SOIL SOLUTION SAMPLES; NITRATES; NITRATE-NITROGEN; MANGANESE; CHLORIDE; ELECTRICAL CONDUCTIVITY; REDOX POTENTIALS; TENSIONMETERS; HYDRAULIC GRADIENTS; TILE SYSTEMS; DENITRIFICATION POTENTIAL; WATER MOVEMENT; LEACHING; CLAY CONTENT; EUTROPHICATION; DENITRIFICATION; ANALYSIS

The contribution of agricultural practices to pollution of ground and surface waters by nitrogen is not completely known. Six tile systems installed on commercial farms with differing soil profile characteristics were selected for investigation. Soil solution samples were extracted from 61-, 91-, 122-, and 183-cm depths and analyzed for nitrate-nitrogen, manganese and chloride concentrations, and electrical conductivity. Redox potential measurements were made at 91- and 183-cm depths. Tensionmeters were installed at 61-, 91-, and 122-cm depths to measure hydraulic gradients. Tile effluent samples were also collected and analyzed. Data on redox potential, manganese concentrations, and nitrate-nitrogen concentrations indicated that there was very low denitrification potential in coarse-textured profiles and that the nitrate-nitrogen concentration and movement were dependent on water movement and amounts of nitrate available for leaching. Irrigation management to provide low leaching fractions resulted in relatively higher nitrate-nitrogen concentration in the tile effluent but smaller amounts of total nitrate lost as compared to irrigation management for high leaching fractions. Redox potential and the chloride to nitrate-nitrogen ratios indicated that subsurface layers of high clay content promote denitrification. With one exception, a smaller fraction of the applied nitrogen was lost in the tile effluent from profiles containing layers of high clay content as compared to the coarse-textured profiles. The one exception was a profile having high clay content throughout which was recently brought under cultivation. Extremely high residual nitrate-nitrogen was found in this profile which would account for the high concentrations in the tile effluent.

(49)

Rate Constants for the Reaction of C(3P) Atoms with CH₂CH₂, CH₂CHCl, and CH₂(CH₂)CH₂ at 290 Plus or Minus 2 Degrees K

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Int. J. Chem. Kinet., 8(3), 475-480; 1976

RATE CONSTANTS; ABSOLUTE RATE CONSTANTS; OZONE; VINYL FLUORIDE; VINYL CHLORIDE; VINYL BROMIDE; DISCHARGE FLOW TECHNIQUES; RELATIVE RATE MEASUREMENTS; MODULATION PHASE SHIFT TECHNIQUES; ATOMIC SPECTROSCOPY; ANALYSIS

Absolute rate constants for the reaction of O(3P) atoms with CH₂CH₂, CH₂CHCl, and CH₂CHBr have been obtained at 290 plus or minus 2 degrees K using a modulation phase shift technique. The rate constants (k₂ x 10¹⁰ (l./mole sec) obtained are: CH₂CH₂ (1.61 plus or minus 0.20), CH₂CHCl (2.54 plus or minus 0.26), and CH₂CHBr (2.85 plus or minus 0.25). These rate constants are lower than those determined by discharge flow techniques, but that for CH₂CH₂ is in good agreement with relative rate measurements.

(50)

Effect of Microorganisms on the Sorption and Fate of Sulfur Dioxide and Nitrogen Dioxide in Soil

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J. Environ. Qual., 5(3), 227-230; 1976

SULFUR DIOXIDE; GAS PHASE; NONSTERILE SOIL; STERILE SOIL; MICROORGANISMS; ATOMOSPHERE-SOIL INTERFACES; SULFATE; NITROGEN DIOXIDE; NITRITE; NITRATE; NITRIFICATION; ANALYSIS; SOIL SORPTION; SOILS; ANALYSIS

Sulfur dioxide was rapidly removed from the gas phase in contact with both nonsterile and sterile soil so that viable microorganisms are not directly involved in removal of this pollutant from the atmosphere. Sulfate was formed from the SO₂ in nonsterile and sterile soil. About one-fourth of the sulfur from the SO₂ introduced was not recovered in inorganic form, but the recovery was quantitative if the soil was first ignited to destroy organic matter. Nitrogen dioxide was also readily lost from the gas phase in contact with nonsterile and sterile soil, and both nitrite and nitrate were generated. The role of microorganisms in the fate of this pollutant is in the conversion of the nitrite to nitrate.

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