

NSF-RANN  
Trace  
Contaminants  
Abstracts

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OAK RIDGE NATIONAL LABORATORY

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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

Date Published: April 1977

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Oak Ridge, Tennessee 37830  
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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. Ross 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 MC7 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: APC, 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, Hoornwijkherhout, The Netherlands. Write: George L. Baughman, Environmental Research Laboratory, U.S. Environmental Protection Agency, College Station Road, Athens, Georgia 30601 (404)546-3145.

**C12**  
Optically Pumped Superluminescent  $\text{Ba}^2$  Molecular Laser

Benesch, R.A.; Berist, F.L.; Pyat, J.L.

Exxon Research Laboratory, U.S. Research Laboratories of Physics, Stanford University, Stanford, CA 94305

PHONE NO: (415) 697-6224 (Pyat)

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

OPTICAL PUMPING; SCIENCE; QUANTITATIVE MEASUREMENTS; LASERS; ELECTRICAL DISCHARGE DEVICES; FLASH-LAMP PUMPING METHODS; PUMP ABSORPTION; BUFFER GAS; SATURATION INTENSITY; QUENCHING; SUPERLUMINESCENCE; E-X-BAND TRANSITIONS; LASER OSCILLATION; A-X-BAND TRANSITIONS; PUMP SATURATION; LASER GAIN; LASER SATURATION INTENSITY; ALKALI DIPOLE SYSTEMS; BIBLIOGRAPHY REFERENCES; 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 optical 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  $\text{Ba}^2$  molecule is optically pumped at 0.673 and 0.659 micrometers, a superluminescent laser emission on a series of green and yellow molecular E-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.  $\text{Ba}^2$  is representative of the other alkali dioptric systems which have molecular emission bands extending from the visible into the infrared.

**C13**  
Identification of the SF6 Transitions Pumped by a CO<sub>2</sub> Laser

McBowell, R.S.; Galbraith, R.W.; Stacha, R.J.; Costrell, C.D.; Bishley, T.E.

Ics Alamos Scientific Laboratory, Los Alamos, NM 87545; RTI Lincoln Laboratory, Lexington, MA 02171

PHONE NO: (617) 662-0660 (Bishley)

Ext. Comm., 17(2), 176-181; 1976

SULFUR REAFLUOCIDE; LASERS; MOULTEP ABSORBERS; SULFUR ISOTOPES; ROTATIONAL STATES; RESONANCE; LASER LINES; J-VALUES; OCTAHEDRAL SYMMETRY TYPES; TRANSITIONS; VIBRATIONAL GROUND STATE; POLYCYCLIC-TCP MOLECULES; DICE-LOCERS; SATURABLE ABSORBERS; REAFLUOCIDES; BIBLIOGRAPHY METHOD; FUTURE DEVELOPMENT; ANALYSIS

Sulfur hexafluoride (SF<sub>6</sub>) is of interest to the

laser community as a nonlinear absorber of 10.6 micrometer CO<sub>2</sub> 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 SF<sub>6</sub> 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 SF<sub>6</sub> that lie within plus or minus 1.5 GHz (0.05 cm<sup>-1</sup>) of the 12C 1602 P(10), P(19), and P(20) laser lines is presented. The SF<sub>6</sub> absorptions nearest these three laser frequencies are P(20)A(2)(20), P(5)A(2)(17), and an F(2) component of P(19) or P(20), respectively. An improved set of molecular constants also allows a more accurate estimate of the J-values of the SF<sub>6</sub> absorptions in the vicinity of other CO<sub>2</sub> laser lines. This method is also applicable to other spherical-top molecules (such as CS<sub>2</sub>) used as passive mode-locked or saturable absorbers and to other hexafluorides.

**C14**  
Particle Size Distribution and Chemical Composition of Coal-tar Fumes

Hittle, G.C.; Stakel, J.J.

U.S. Army Construction Engineering Research Laboratory, Champaign, IL 61020; University of Illinois, Urbana, IL 61801

PHONE NO: (217) 333-6961 (Stakel)

Ext. Ind. Eng. Assoc. J., 37(4), 193-200; 1976, April

PARTICULATES; COAL; COAL-TAR FUMES; SIZE DISTRIBUTION; CHEMICAL COMPOSITION; PHYSICAL CHARACTERISTICS; DROPLETS; CRYSTALLINE PARTICLES; FLUORESCENCE; POLYCYCLIC AROMATIC HYDROCARBONS; PYROLYSIS; AUTOXIDATION; 3,6-BENZPYRENE; 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 compound 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. Naphthalene polycyclic aromatic hydrocarbons were also found. 3,6-Benzpyrene was not present in the fumes.

**(4)**  
**Long-Path Monitoring with Tunable Lasers**

Pinkley, R.E.; Ho, F.T.

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

PHONE NO: (617) 432-2600

Presented at the 6th Materials Research Symposium - Methods and Standards for Environmental Measurement, Gaithersburg, MD, September 20-24, 1976

TUNABLE LASER; SIGNAL REFLECTION; DIFFERENTIAL ABSORPTION; QUANTITATIVE ANALYSIS; BIFURCATED CAVITY; BIFURCATED LASER; SULFUR DIOXIDE; CADMIUM DIOXIDE; BICARBONATE; FIELD STUDIES; IR-SALT LASER; BIMODAL; INFRARED 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 BC, SO<sub>2</sub>, SO<sub>3</sub>, CO, and Cl, have already been monitored by this technique. Tunable lasers in the ultraviolet, visible, and infrared regions of the electrooacoustic spectrum have been employed. The laser source is a Ft-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 over-range to a remote retroreflector which reflects it back towards the parabolic mirror, which refocuses it onto the infrared detector situated behind a calibration 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 ITC meter test range in Bedford, PA 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.

**(5)**  
**Inhibition of Cork and Sunflower Photosynthesis by Lead**

Bazzaz, F.A.; Carlson, D.M.; Wolfe, G.L.

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

PHONE NO: (217) 293-6177

Physiol. Plant., 30, 326-329; 1974

CORK; SUNFLOWERS; LEAD CHLORIDE; TRANSPERSION STREAM; PHOTOSYNTHESIS; LEAD; LEAF UPTAKE; TRANSPERSION RATES; STOMATAL RESISTANCE; CARBON DIOXIDE; WATER VAPOR EXCHANGE; ANALYSIS

Detached cork and sunflower leaves supplied with PbCl<sub>2</sub> 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 CO<sub>2</sub> and water vapor exchange are discussed in relation to the effects of Pb on photosynthesis and transpiration.

TRANSPORT: ZEA MAYS L., WEIPIVTHUS ANNUS L.

**(6)**  
**Application of the Unified Transport Model to the Movement of Pb, Cd, Zn, Cu, and S Through the Crooked Creek Watershed**

Panero, J.R.; Lassonde, P.J.; Begovich, C.L.; Diaz, E.P.; Larson, A.F.; Patterson, T.B.; Jackson, L.R.

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

PHONE NO: (615) 580-8611, Ext. 3-6266

OWR-HSP-ETMC/4, 92 p.; 1976, September

MODELS; MODELING; TRANSPORT MODELS; HEAVY METALS; LEAD; CADMIUM; ZINC; COPPER; SULFUR; WATERSHEDS; SOIL; HEAVY METAL ACCUMULATION; STREAMS; PLANT UPTAKE; HYDROLOGY; STREAMFLOW; COMPUTER 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.<sup>2</sup> (3.4 km<sup>2</sup>) forested headwaters area adjacent to a Pb mine and smelter in southeast Missouri. The Wisconsin Hydrologic Transport Model (WHTM) 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: US, Missouri, Ozark Mountains, Crooked Creek Watershed

(7)  
Laser Spectroscopic Instrumentation and Techniques: Long-Path Monitoring by Resonance Absorption

Finsley, F.E.

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

EECEP SC: (617) 452-1600

CPL. Quat. Electron., 7, 145-167; 1976

TELESCOPIC LASER SPECTROSCOPY; LONG-PATH SCATTERING; RESONANCE ABSORPTION SPECTROSCOPY; RATE MEASURE CALIBRATION; TUNABLE INFRARED LASERS; AIR POLLUTION MONITORING; LONG-PATH MONITORING; APPARENT GASES; RESONANCE ABSORPTION; ANALYTICAL SPECTROLOGY; REVIEW

Tunable laser spectroscopy has necessitated 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 monitoring of ambient gases in the atmosphere by resonance absorption. The results of these measurements are discussed. Table I is a summary of the laser methodology used for detection of low molecular weight gases, replicated in air pollution. The spectra obtained range from the simple diatomic structure of HCl and CO to complex spectra associated with molecules such as SO<sub>2</sub>.

(8)  
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, D.J.; Wetterran, A.C.; Black, J.A.

University of Kentucky, Water Resources Research Institute, Lexington, KY 40506

EECEP SC: (606) 252-5500

University of Kentucky Water Resources Research Institute Report No. 41, 27 p; PP-140-000; 1975

FISH EGGS; INFECTED EGGS; FRYESES; LARVAL STAGES; BIOINDICATOR ORGANISMS; WATER QUALITY; FILTER WATER; STREAM WATER; FISCHER CIVILLETTI; FISCHER DENSITY; EGG HATCHABILITY; 200-FUEL TIEFEBRUG; GRAY TREEFROG; RAINBOW TROUT; EGG DEVELOPMENT; WATER QUALITY INDEX; INFRARED HEMATOLOGY; FISH TERATOGENIC EFFECTS; MERCURY; TRACE METALS; EGG HATCHABILITY; ANALYSIS; LARGEMOUTH FISH; GOBLIFISH; CRABBL CATFISH; BIG EYE; BIG-SPOOTED TROUT; HABDOMENOTUS TROUT

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 9 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. Incubating data for all 9 animal species, egg hatchability (embryonic survival) ranged from 0% for the most contaminated water to 96% for uncontaminated water found to support a healthy somatic flora. Eggs of the squirrel treefrog and gray treefrog were the most sensitive of 5 amphibian species tested, and of 4 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 40% of the embryos which survived to complete the hatching process. Defective survivors were rare in cultures where egg hatchability exceeded 90%. The selected water resources were analyzed for mercury and other trace metals. Appreciable levels of mercuric 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 ppm or more.

GEOPGRAPHICAL DESCRIPTION: US, Kentucky, Case Run, Tom Branch, Wolf Run, East Hickory Creek, West Hickory Creek, Gainesway Branch, Hickory Creek, Smoky Branch, Kentucky River, Elkhorn Creek, Steele's Run

FAUNA: RICHTERUS SALMOIDES; CARASSIUS BARBATUS; ICTHALUS PUNCTATUS; SALMO GAIRDNERI; CASTORPHYREUS CAROLINENSIS; DUFO PUNCTATUS; BARBOTYLIC; SYLA CYPHOCEPHALA; RYASQUINELLA

(4)  
A Comparison of Factors Affecting Accuracy in  
Graphite Furnace and Atomic Absorption  
Spectroscopy Using a Graphite Furnace for Trace  
Metal Analysis in Water

Fryman, R.S.; Bailes, T.C.; O'Naver, 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

SPCR 8C: (30) 470-2610 (O'Naver)

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

Sensitivity; Trace Metals; Atomic Absorption;  
Graphite Furnace; Flame Techniques;  
Molecular 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  
corrections 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 (GFAES) 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.

(19)  
Improved Accuracy in Background-Corrected Atomic  
Absorption Spectroscopy

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College Park, MD 20742

SPCR 8C: (30) 470-2610 (O'Naver)

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

BACKGROUND-CORRECTED ATOMIC ABSORPTION  
SPECTROSCOPY; MOLECULAR ABSORPTION; PARTICULATE  
LIGHT SCATTERING; FLAMELESS METHODS; TWO-LINE  
METHOD; BACKGROUND CORRECTION METHODS;  
WIS-CORRECTION; ISOTOPIC ATOMIC ABSORPTION;  
BACKGROUND INTERFERENCE; ISOTOPIC 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 all 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. Compensation background correctors available  
on some ICP units utilize a second source of  
continuous radiation to operate in the  
background-corrected mode. The analyte continuous  
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. Below cathode continuous sources  
have a limited range of intensity so that some  
elements cannot be analyzed in this manner, e.g.,  
Ca. There is a possibility of wiz-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 (IZAA) 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 continuous source and a  
wavelength-modulated echelle monochromator  
(CWEM) 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.

**A CONVERGENCE INDEX FOR PREDICTED SPHERICAL BIFOCALS AND INTRINSIC SPHERICAL LENSCHING WITH PRESCRIBED**

Journal of the American Statistical Association, 3-

OPERATION ROLLING MEET, Center for Transnational  
Studies, The George Washington Institute and State  
University, Washington, DC 20052

J. Geol., 1941, 49(3), 116-122; 1942

A simple method using unsophisticated equipment is suggested for crude toxicity testing of refinery effluents. This set "includes an inexpensive device for identifying cyclical materials and establishing priorities for repeat with these materials. An arbitrary reference mixture, containing six known constituents of refinery wastewater, is used for static toxicity tests on 11 species of freshwater invertebrates and 1 species of fish. Daphnia pulex has been selected for further testing because it is the most sensitive of the animals tested, relatively cheap-to-use and easy to maintain, and a potential fish-food cleaner. If the reference mixture is representative of a refinery effluent, the Daphnia bioassay would be sufficiently sensitive to give reliable results within 48 h, whereas a fish bioassay would show no toxicity even after 96 h. To assess the suitability of the Daphnia bioassay, tests have been conducted by personnel at six petrochemical refineries. Duplicate tests are in agreement. Results of tests using actual refinery effluents suggest that no toxicity after 48 h to a mean initial concentration of 1.26 effluent after 48 h. The data presented show that the method is reproducible and that refinery personnel can use it to select the bioassay-priority priorities are advantages of the method are discussed.

TRICERATOPS PREHENSILE TAIL: DIAPHRAGMUS

## LCPD-PART 2: Characterizing of Heterophotonic Carbon Carbonyls with a Tunable "Ridge" Laser System

Ho, S.-T.; Pickley, R.F.; Sample, J.C.

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

FPCB# REC: (117) 562-150G, Ext. 2358

B.R.L. Oct., 1970, 650-661; 1974, April

## ICRQ-DARK BISULFATE OF CARBON DIOXIDE IN THE

atmosphere are concluded. The technique of resonance absorption, in which the wavelength of radiation from a  $\text{He-}(\text{O}_2)$  or  $\text{O}_3$  (1.66) semiconductor diode laser was tuned into coincidence with an absorption line of  $\text{C}$  in its fundamental band around 6.7 micrometers, was used. By employing rapid frequency oscillation of the laser gas source to overcome atmospheric turbulence effects, it was possible to achieve a minimum detectable concentration of 1 part per billion over a 0.61-cm path. Continuous monitoring was also performed and this permitted increases in the ambient CO level due to commuter traffic to be observed.

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Field-Measured *Sarcina* Spore Concentrations, Biotix Potentials, Oxygen Diffusion Rates, and Oxygen Partial Pressures in Relation to Denitrification.

Fischler, M.; Erdoszak, S.S.; Szuszkevics, T.E.;  
Stolzy, L.W.

**University of California, Riverside, CA 92330**  
**University of California, Berkeley, CA 94720**

PROB# 40: 17143767-4112 (540129)

Soil Sci., 122(2), 307-318, 1976

BUDGETS; DEBTIFICATION; SOIL ABSTRACTION;  
AEROBIC MICROBES; FIXED SCALE; ABSTRACTION  
REASSESSMENTS; GASEOUS CONCENTRATIONS; SOIL  
ATMOSPHERE; OXYGEN DIFFUSION RATES; DRY  
POTENTIALS; FIXED EXPERTISE; SUDAN (PLANT);  
RAMPED CRAB LICE; IRRIGATION WATER;  
FERTILIZERS; BITRITES; BITRITES; BITRITES; CRIDES;  
ABSTRACTION CONDITIONS; OPT SOILS; SOIL PARTS  
INTERACTIONS; CAGED DIFFUSION RATES; CYCLEN  
PARTIAL PRESSURE; ANALYSIS; SOIL CHEMISTY

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 sizes of anaerobic microsites in a field soil. Aeration measurements such as gaseous 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 on a Ranford 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. Nitrogen dioxide, 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 Ranford sandy loam.

&lt;10&gt;

**(10)**  
**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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ERCPF NO: (714) 787-4560 (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; PHOTOCHLORINATION; POLYCARBONS; NITROGEN OXIDES; ISOPROPYL; 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 photokinetics studies employing hydrocarbons-NO<sub>x</sub>(s) 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 CH<sub>3</sub> plus isobutene of 3.05 x 10 (10<sup>-10</sup>) 1 mole (L<sup>-1</sup>s<sup>1/2</sup>) are (k + 10<sup>10</sup>) 1 mole(L<sup>-1</sup>s<sup>1/2</sup>): 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.

**(11)**  
**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; SUBLIGHT INTENSITY; POLLUTANT EMISSION INVENTORY; OZONE; PAN; EMISSIONS; PHOTOCHLORIC 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 (36 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**

**(12)**  
**Water Quality Control in Mine Spoils - Upper Colorado River Basin**

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ERCPF NO: (303) 491-6226

EPA-670/2-75-04E, 59 p.; PB-262-908; 1975, June

**COAL SITES; 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 Alkoxy Radical Isomerization in Photooxidations of C(4)-C(6) Alkanes under Simulated Atmospheric Conditions**

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PROBE NO: (710)787-0568 (Pitts)

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

**PARTICULARS:** ALKOXY RADICALS; HYDROGEN SHIFTS; ISOMERIZATIONS; PHOTOCHEMISTRY; ALKenes; ALKYL RADICALS; ALKYLPEROXO RADICALS; PHOTOCHEMICAL SPOCs; APPARENT AIR;  $\delta$ -HETABDE;  $\eta$ -PENTANE;  $\eta$ -HEXANE; NITROGEN OXIDES; PESTICIDES; FREE RADICALS; QUENCHERS; ATMOSPHERIC CHEMISTRY; ANALYSIS

We have calculated approximate room temperature rate constants for intramolecular hydrogen shift isomerizations of alkyl, alkoxy and alkylperoxy radical intermediates in photochemical smog and found that alkoxy radicals with delta hydrogens appear to undergo 1,5 hydrogen shifts at ambient conditions. Product distributions observed during irradiations of alkanes ( $\eta$ -hexane,  $\eta$ -pentane and  $\eta$ -hexane)-NO<sub>2</sub>-air systems in two quite different approximately 6000-liter environmental chambers were found to be consistent with this prediction. For example, in the  $\eta$ -pentane-NO<sub>2</sub>-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 hydroxative 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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PROBE NO: (710)787-0568 (Pitts)

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

**PARTICULARS:** HYDROXYL RADICAL; HYDROCARBONS; IRRADIATION CHAMBER;  $\eta$ -BUTANE; ISOPENTENE; ELEMENTARY REACTION MEASUREMENTS; PHOTOXIDATION STUDIES; REACTIVITY SCALES; ALKENES; ALKATES; ALKATICS; OXYGENATES; METHANE; 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 SAPFC 6400 liter glass irradiation chamber. These rate constants were placed on an absolute basis using literature values for either  $\eta$ -hexane 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 50 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 ARB reactivity scales are made, and the implications of the present scale for the role of alkenes 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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PROBE NO: (710)787-0568 (Pitts)

Presented at the 69th Air Pollution Control Association Annual Meeting, Portland, OR, June 27-July 1, 1976, 16 p.; 1976

**PARTICULARS:** CONCENTRATION; PARTICLES; 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 SO<sub>4</sub>, NO<sub>3</sub>, and NH<sub>4</sub> 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 46.7 and 70.2  $\mu\text{g m}^{-3}$ ) were observed during the six month study, with gas-particle distribution factors as high as 77% and 49%, respectively. Six month-averaged SO<sub>4</sub> and NO<sub>3</sub> ion concentrations, calculated from 176, 24 hr measurements, were 16.3 and 23.7  $\mu\text{g m}^{-3}$ . 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  $\mu\text{m}$  at rates exceeding 10  $\mu\text{g m}^{-3} \text{ hr}^{-1}$  during photochemical episodes. Although secondary pollutant concentrations were found in the order: NO<sub>3</sub> ion was greater than SO<sub>4</sub> ion was approximately equal to organic carbon, statistical treatment of 159, 24 hr measurements of light scattering, NO<sub>3</sub> ion, SO<sub>4</sub> ion, carbon and other aerosol constituents (total aerosol - SO<sub>4</sub> ion plus NO<sub>3</sub> 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

<20>

**<20> Behavior Changes as End Points in Health Impact Assessment**

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TECBIE RC: (716) 275-2791

Fact of Impact of Energy Products on Human  
Health, An Evaluation of Beans for Assessment.  
EPA Symposium Series 39, p 85-96; 1976

BEHAVIORAL CHANGES; BEHAVIORAL TOXICOLOGY;  
BIOASSAY; PSYCHOCHEMICAL COMPLAINTS; LEAD  
TOXICITY; METAL-INDUCED INTEGRITY;  
ESTIMATES; ATMOSPHERIC POLLUTANTS; MICROWAVE  
EXPOSURE; PIGMENTS; ESTIMATES; CHROM DISULFIDE;  
DIOXINS OXIDES; CARBON MONOXIDE; SPECIES; MAGNETIC  
FIELDS; ANALYSIS

Behavioral toxicology is beginning to make a significant impact on evaluations of the health effects of environmental agents. Its role is based on three considerations: the fact that many agents act directly on the nervous system, that psychological complaints precede overt signs of many intoxications, and that behavior represents an integrated functional assessment of the whole organism. Among the issues that involve behavioral variables are the following: the significance of elevated lead body burdens without overt poisoning, early signs of methylmercury intoxication, effects of chronic exposure to pesticides, solvent abuse, performance impairment by atmospheric pollutants, and standards for microwave exposure.

**<21> The Fate of Chlordane and Toxaphene in a Terrestrial-Aquatic Model Ecosystem**

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Environ. Entomol., 5(3), 533-538; 1976

CHLORDANE; TOXAPHENE; MOREL ECOSTATE; ALGAE;  
BOSCQUETTES; FISH; BIOACCUMULATION; PESTICIDES;  
SNAILS; WATER; ANALYSIS

The fate of C<sub>10</sub>-chlordane and toxaphene have been investigated in a terrestrial-aquatic-model ecosystem. The alga, snail, mosquito, and fish accumulated C<sub>10</sub>-chlordane 98,306, 112,113, 1132, and 2258X, respectively, the concentration of C<sub>10</sub>-chlordane in the water. In comparison, C<sub>10</sub>-toxaphene was accumulated by the alga, snail, mosquito, and fish 6962, 9600, 890, and 8287X, respectively, the bioconcentration of C<sub>10</sub>-toxaphene in the water. In parallel studies using unlabeled chlordane and toxaphene and gas chromatographic analysis it was established that the accumulation values for these unlabeled compounds closely approximated the values obtained for the experiments with the labeled compounds.

**<22> Adsorption Characteristics of Traces of Barium, Beryllium, Cadmium, Manganese, Lead and Zinc on Selected Surfaces**

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Anal. Chim. Acta, 64, 409-417; 1976

ADSORPTION CHARACTERISTICS; BARIUM; BERYLLIUM;  
CADMIUM; MANGANESE; LEAD; ZINC; PYRE GLASS;  
FLINT GLASS; POLYTHENE; LIGAND SYSTEMS; WATER  
SAMPLE STABILIZERS; AMMONIUM  
PYRROLIDINEDITHIOCARBONATE; ETHYL  
ISOBUTYL KETONE; ANALYTICAL METROD DEVELOPMENT;  
ANALYSIS; TRACE METALS; METAL-LIGAND COMPLEXES

The adsorption characteristics of Ba, Be, Cd, Mn, Pb, and Zn on Pyrex, flint glass and polyethylene surfaces during storage under different conditions are described. It is concluded that the method of stabilization of water samples recommended by EPA, i.e. addition of 5 ml of 16 N HNO<sub>3</sub> per liter, is satisfactory. Stabilization and concentration with a mixed ligand system is recommended, except for Mn and Be which are not extracted quantitatively. Extraction with ammonium pyrrolidinedithiocarbonate (APDC) and methyl isobutyl ketone (MIBK) is unsatisfactory for storage purposes.

**<23> Differential Susceptibility of Potato Cultivars to Four Herbicides**

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Amer. Potato J., 53(6), 211-219; 1976

GREENHOUSE STUDIES; FIELD STUDIES; POTATOES;  
HERBICIDES; CULTIVARS; METRIBUZIN; LINDBOR; SOIL  
TEXTURE; SEED PIECE SIZE; LC50s; FOLIAR WEIGHT;  
PHOTOTOXICITY; BETOBORBURON; OTADIYAZON; ANALYSIS

Greenhouse and field studies were conducted to evaluate the susceptibility of six potato (*SOLANUM TUBEROSUM* L.) cultivars to injury by four herbicides. The White Rose cultivar was the most susceptible to injury, especially from metribuzin (4-amino-6-tert-butyl-3-(methylthio)-s-triazin-5-yl) one, and lisurazone (3-(3,4-dichlorophenoxy)-1-methoxy-1-methylurea). Injury was attenuated by decreasing the rate of herbicide in the range of 0.5 to 0.5 kg/ha (0 to 0.5 lb/ha) and by increasing the seed piece size. Injury seemed to be associated with soil texture and was greater in a sandy loam than in a sandy clay loam soil. Greenhouse studies provided valuable leads on cultivar susceptibility to herbicides but reductions in foliar weight of 15 to 20% are required to justify any suspicion that field injury will occur.

TAXONOMY: *SOLANUM TUBEROSUM* L.

**<26>**  
Atmospheric Water Vapor Measurements with an Infrared (10-μm) Differential-Absorption Lidar System

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Appl. Phys. Lett., 29(9), 502-503; 1976, Ray

DIFFERENTIAL ABSORPTION LIDAR SYSTEM; GASEOUS SPECIES; AEROSOLS; CRYSTAL-TUBE CO2 TEA LASER; INFRARED DETECTORS; ANALYTICAL METHODS; METHOD DEVELOPMENT; ANALYSIS; ATMOSPHERIC CHEMISTRY; GASES; OZONE; SULFUR DIOXIDE; AMMONIA; FREON 11; FREON 12; FREON 113; VINYL CHLORIDE; ETHYLENE; REFRACTANCE; 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 CO<sub>2</sub> laser lines near 10.3 μm. 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 gaseous species. The present system performance indicates a backscatter coefficient sufficient to attain a range of 12 km with commercially available components. O<sub>3</sub>, SO<sub>2</sub>, NH<sub>3</sub>, Freon 11, Freon 12, Freon 113, vinyl chloride, ethylene, and methanol could probably be monitored with this system.

**<27>**  
Generation of Standard Metal Oxide Particulates in the Respirable Range

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FRCB UC: (504) 388-2270

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

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

A method which is a modification of the method of Charukajan and West for the generation of reliable standards of metal oxide particulates of copper, lead, and zinc is presented. More than 95% of the particles generated are in the respirable range, the maximum concentration being in the 1.1 to 2.1 μm range. In addition to being useful for generation of standards for air particulates analyses, this method is potentially useful in the toxicological and industrial hygiene studies of complex mixtures of metal particulates.

**<28>**  
Organic and Conventional Crop Production in the Corn Belt: A Comparison of Economic Performance and Energy Use for Selected Yields

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FSP/PA-760008, 22 p.; CRHS-AE-7; PB-255-058; 1976, June

ORGANIC FARMS; CONVENTIONAL FARMS; CROPS; LIVESTOCK; PESTICIDES; YIELDS; PRODUCTS; COSTS; ENERGY CONSUMPTION; CROP PRODUCTION; MARKET VALUE; LABOR; PHOSPHORUS; POTASSIUM; NUTRIENT BALANCE; NUTRIENTS; CCBP; SOYBEANS; WHEAT; BARLEY; 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 1974 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 2.3 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.

**<29>**  
Environmental Pollution in the Lead Belt, RARE Utilization Experience, Case Study No. 2

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FSP/PA-6-75-030, 23 p.; PB-267-246; 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

&lt;28&gt;

**<28>**  
**The Effect of pH, Salt Concentrations, and Nature of Electrolytes on the Charge Characteristics of Brazilian Tropical Soils**

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

**PB: SALT CONCENTRATION; ELECTROLYSES; CHARGE CHARACTERISTICS; ION RETENTION; ELECTROCHEMICAL BEHAVIOR; SOILS; HYDROXYL ION; HYDRATION SOLVENTS; MAGNESIUM SULFATE; POTASSIUM SULFATE; POTASSIUM CHLORIDE; MAGNESIUM CHLORIDE; CATIONIC-ICHS; FIELD PT; SURFACE HORIZONS; SUBSURFACE HORIZONS; ATOMIC ABSORPTION; ZEROP 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 cacao-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 K and Ca ions in the equilibrium solution, hence charge distribution varied substantially with pH and electrolyte concentration. Direct measurement of adsorption of ions from solutions of MgSO<sub>4</sub>, K<sub>2</sub>SO<sub>4</sub>, KCl, and MgCl<sub>2</sub> 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 3.2 to 3.6 in the A horizons and from 4.0 to 5.1 in the B horizons. At pH near their field pH the surface horizons were, in general, net negatively charged, while the subsurface horizons were either isolectric 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 Pt Smelter**

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Atmos. Environ., 10, 883-886; 1976

**LEAD; CADMIUM; ZINC; COPPER; PARTICLE SIZE; LEAD SMOKE; ATMOSPHERIC CHEMISTRY; TEST FARMS; LEAD EMISSIONS; AIR SAMPLES; SEASONAL SAMPLING; ATOMIC ABSORPTION SPECTROPHOTOMETRY; RESPIRABLE PARTICLES; ANALYSIS; EUSTEALL; SOIL;**

#### HYDROLOGICAL 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 6.7  $\mu$ 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; SUBSTRATE; 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 4 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

<31>  
Variable Nature of Chemical Composition of Sewage Sludges

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

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

Sewage sludge samples were collected over a 2-year period from eight Indiana cities and analyzed for C, N, P, K, Ca, Mg, Fe, Cd, Zn, Cu, Bi, and Pb. The sludges contained approximately 55% 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, N, 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 P, respectively, in sludges. The largest deviations between the mean and median were found for Cd, Zn, Cu, Bi, and Pt. 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.

GEOPGRAPHICAL DESCRIPTION: US, Indiana, Anderson, Crawfordsville, Elkhart, Indianapolis, Peru, Logansport, Noblesville, Tippecanoe

<32>  
Movement of Heavy Metal below Sewage Disposal Ponds

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J. Enviro. Qual., 5(3), 330-336; 1976

SOILS; SLUDGE; EFFLUENTS; DISPOSAL PONDS; SEWAGE TREATMENT PLANTS; ZINC; CALCIUM; COPPER; CALCIUM; NICKEL; HEAVY METALS; ACID-EXTRACTABLE METALS; METAL ENRICHMENT; ANAEROBIC CONDITIONS; SATURATED EXTRACTS; CHEMICAL OXYGEN DEMANDS; METAL MOVEMENT; METAL-CARBONIC 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 (as MnO<sub>2</sub>) were greater under disposal ponds than offplant control sites at both treatment plants. Metal enrichment was evident to depths as great as 3 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.

<33>  
A Rapid Method for the Determination of Methylmercury Chloride in Water Samples by Gas Chromatography with a Negative Emission Spectrometric Detector.

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

ANALYTICAL METHODS; METHOD DEVELOPMENT; TERTIARY AMINES; METHYL MERCURY CHLORIDE; GAS CHROMATOGRAPHY; HYDROGEN EMISSION DETECTOR; WATER; METHYLMERCURY CHLORIDE-AMINE COMPLEX; ANALYSIS

A method is described in which tertiary amines preferably extract methyl-mercury(II) chloride. With 0.5% solutions of tertiary amine in *t*-butane, a quantitative (95 plus or minus 3%) extraction of methylmercury(II) chloride, as a CH<sub>3</sub>NgCl-amine complex, can be achieved for aqueous solvent volume ratios as high as 400. After the extraction, aliquots (1-10  $\mu$ l) of the benzene layer are injected into the g.c. column. In the injection port, which is held at 200 degrees C, the CH<sub>3</sub>NgCl-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.

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**<34>**  
**Importance of NO<sub>2</sub> + RO in Alkyl Nitrate Formation from C<sub>4</sub>-C<sub>6</sub> Alkanes Photooxidations under Simulated Atmospheric Conditions**

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J. Phys. Chem., 80(17), 1948-1950; 1976

NITROGEN BASS BALANCE; ALKYL NITRATES; METHYL NITRATE; ETHYL NITRATE; BUTYL NITRATES; PENTYL NITRATES; HEPTYL NITRATES; ALKYL SPECIEIS; PHOTOXIDATION; ALKANES; NITROGEN CHIDES; ATMOSPHERIC CHEMISTRY; ALKANES; ANALYSIS; MODELING

Evidence that alkyl nitrates are formed from precursors other than alkyl radicals and that nitrate formation is independent of NO or NO<sub>2</sub> levels, provided that some NO<sub>x</sub> remains in the alkane-NO<sub>x</sub> photoxidation reaction system, is presented. The amount of alkyl nitrate formed and the amount of hydrocarbons reacted both increase with reaction time, but their ratio is relatively independent of reaction time until either all the hydrocarbon or the NO<sub>x</sub> has been consumed. These ratios decrease with the size of the reacting alkane. It is concluded that the mechanism of reaction depends on the nature of the alkane.

**<35>**  
**External Cavity CO<sub>2</sub> - Pump Infrared Spin-Flip Laser**

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FRCR NC: (617) 862-5500, Ext 100

IEEE, J. Quant. Electron., 22-202; 1976, March

LASERS; EXTERNAL CAVITY SPIN-FLIP LASER; AXIAL BEAMS; TRANSVERSE BEAMS; FABRY-PEROT MODES; OUTPUT COUPLED; MAGNETIC FIELD; FREQUENCY COVERAGE; ANALYTICAL METHODS; 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 CO<sub>2</sub>-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-Perot (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 GHz or finesse 6,003 (2-1) has been attained.

**<36>**  
**CEDS - A Model of Forest Stand Biomass Dynamics for Predicting Trace Contaminant, Nutrient, and Water Effects**

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OAKR-BSP-FATC-25, 162 p.; 1976, October

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

CEDS 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 (DIFMAS and DIFMAS) of the Unified Transport Model, UTM. An important feature of CEDS 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. CEDS 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 CEDS 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 choices. Heavy metal pollutants free a lead zinc and smelter complex were introduced to the ecosystem as rainfall and dryfall. The CEDS and DIFMAS 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>  
**EFYDAS and EYFADS, Fortran Models for Investigating Solute Uptake and Incorporation into Vegetation and Litter**

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CBRI-BST-PATC-26, 132p.; 1976, October

**REFELS; MODELING; SOLUTE movement; SOIL; SOIL SORPTIONS; ROOTS; PLANT TISSUES; LITTER; ACCUMULATIONS; FLUXES; TERRESTRIAL ECOSYSTEMS; LEAF PERMEABILITY; ROOT CONDUCTIVITY; ROOT SURFACE; DIURNAL PATTERNS; DECOMPOSITION RATES; MINERALIZATION LOSSES; OXIDATION CYCLIDE**

The concepts and FORTRAN algorithms of a model describing solute movement from bulk soil solution into roots (EFYDAS) and a mode of solute dynamics and accumulation in plant tissues and litter (EYFADS) are presented. Plant uptake of solutes and gases are included in the EYFADS 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 EYFADS 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 absorption is the first major site of trace contaminant accumulations from soil borne pollutants. The electrophoresis describing solute movement along a concentration gradient in plumes 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), 798-807; 1976, August

**CORRECTED AIR QUALITY; AIR QUALITY DATA; INFRASPECTRIC CHEMISTRY; SEALED 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 Aluma and Pasadena in LAC have yearly total oxidant levels than cities in the eastern 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 ST 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 20%.

<39>  
**Long-Path Infrared Spectroscopic Investigation at Ambient Concentrations of the 25 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 CHAMBERS; HUMIDITY; LINEAR REGRESSION 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 25 neutral buffered potassium iodide (NPKI) method for ozone (ARB method). An environmental chamber with an in-situ long-path optical system was employed to simultaneously obtain infrared (IP) spectra and 25 NPKI 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-known 9.49 nm R-trough absorption of ozone using an absorptivity of  $0.13 \times 10^{12} \text{ cm}^2 \text{ mol}^{-1}$  at 254 nm which was experimentally determined by the independent methods. Linear regression analyses of the 25 NPKI and IP ozone concentrations yielded:

$$\begin{aligned} ((O_3)_{\text{NPKI}}) &= 1.10((\text{C}_3)\text{IP}) + 0.013 \text{ for } 3\% \text{ RH}, \quad ((O_3)_{\text{NPKI}}) \\ &= 1.12((\text{C}_3)\text{IP}) + 0.001 \text{ for approximately } 10\% \text{ RH}, \\ ((O_3)_{\text{NPKI}}) &= 1.23((\text{C}_3)\text{IP}) + 0.001 \text{ for } 50\% \text{ RH}. \end{aligned}$$

Although the dependence on RH is not understood, these results indicate that the 25 NPKI method yields ozone concentrations 12-14% 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. Boron demonstrated excellent agreement between simultaneous measurements of ozone samples by IP and UV spectrometry where the absorptivities employed were  $0.23 \times 10^{12} \text{ cm}^2 \text{ mol}^{-1}$  at 254 nm and 135 nm at 254 nm, respectively.

&lt;80&gt;

**(80)**  
**Chemical Ionization Mass Spectrum of Peroxyacetyl Nitrate**

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Cir. Mass Spectro., 11, 552-555; 1976

ICUBIZATION; MASS SPECTROSCOPY;  
 PEROXYACETYL NITRATE; PHOTOCHEMICAL SMOG;  
 TOXICITY; RAD; PLANTS; METABOL; ISOCYANIDE;  
 REAGENT GASES; FRAGMENTATION; 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/e 119 positive ion at m/e 121, intense fragment ions at m/e 43 (KCNCO) positive ion and m/e 66 (HCNCO) positive ion, and less intense ions at m/e 61 (KCN3NO2) positive ion, m/e 77 (KCN3NO2C2) positive ion and m/e 88 positive ion (C2C2N3O2) formed by internal rearrangements. These results confirm the currently accepted structure for peroxyacetyl nitrate,  $\text{C}_3\text{H}_5\text{NO}_2$ .

**(81)**  
**Economic Analysis of Irrigated Farming with Diminishing Ground Water Reserves**

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BSE/PA-366(C05, SC p.; COHS-8E-6; FF-255-433;  
 1976, Gay

CCB; ECONOMIC ANALYSIS; IRRIGATION; FARMING;  
 GROWTH RATES; WATER TABLE; CROP YIELDS; PLANT  
 GROWTH; WATER REQUIREMENTS; HYDROLOGY; MODELS;  
 SCHEDULING; WATER SUBSETS; 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. Corn yields, for example, are highly sensitive to the availability of water in certain critical periods in the stages of plant growth making non-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.

**(82)**  
**Relative Rate Constants for the Reactions of the Hydroxyl Radical with Selected Ketones, Chlorophenols, and Monoterpene Hydrocarbons**

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

MONOTERPENE HYDROCARBONS; CHLOROPHENOLS; ALIPHATIC KETONES; ENVIRONMENTAL CHAMBER; SIMULATED ATMOSPHERES; RELATIVE RATE CONSTANTS; ABSOLUTE RATE CONSTANTS; HYDROXYL RADICALS; HYDROCARBONS; ISOCYANIDE; ALPHA-PINENE; BETA-PINENE; DELTA-LINOLENE; BIS(2-METHYL KETONE); METHYL ISOBUTYL KETONE; DIISOBUTYL KETONE; TRICHLOROETHENE; TETRACHLOROETHENE; ANALYSIS; ATMOSPHERIC CHEMISTRY

The relative rates of disappearance of three monoterpene hydrocarbons, two chlorophenols, 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  $\sim$  hydrocarbon disappearance under the experimental conditions employed. Absolute rate constants, obtained from the relative values using the published rate constant for OH + isobutene ( $3.05 \times 10^{10} \text{ M}^{-1} \text{s}^{-1}$ ), are ( $k \pm 10\% \pm 1\%$ ): alpha-pinene,  $3.5$  plus or minus  $0.5$ ; beta-pinene,  $4.1$  plus or minus  $0.6$ ; delta-linoleic,  $9.0$  plus or minus  $1.4$ ; methyl ethyl ketone,  $0.20$  plus or minus  $0.06$ ; methyl isobutyl ketone,  $0.9$  plus or minus  $0.1$ ; 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 Grinrud, Bentberg, and Passusen.

<83>  
**Microwave Plasma Emission Spectroscopy**

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Anal. Chem., 48(7), 611A-612A, 613A, 616A, 618A, 620A; 1976

PIASMAS; MICROWAVE FREQUENCY ELECTRICAL FIELDS; GASES; SPECTRAL EXCITATION SOURCES; MICROWAVE COUPLED PLASMAS; PLASMA CONFIGURATIONS; SPECTROQUANTITATIVE 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 spectroanalytical 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 Symposia - Methods and Standards for Environmental Measurement, Gaithersburg, MD, September 20-24, 1976; 1976

WATER; RIVER WATER; WASTEWATER; RECEIVING WATERS; SPECIEMS; INDUSTRIAL PLANTS; MASS SPECTROMETRY; GAS CHROMATOGRAPHY; CHROMATOGRAPHS; SOLVENTS; SOLVENTS; BIOLOGICAL SLUDGE; CHEMICAL INTERACTIONS; ANALYSIS; REPLICATIVES; EFFLUENT CONTROL; ANALYSIS

Analysis of wastewaters, receiving waters and sediments of several industrial plants by mass spectrometric and gas chromatographic techniques has indicated that organic compounds which are scarcely 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 1-(2'-hydroxy-5'-methylphenyl)-2-terzotriazole). The presence of these organic compounds in sediments may be a source of continual regeneration 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 micrometers has provided spectroscopists with much higher resolutions 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 continuouswave 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-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. Coarse-tuned gas lasers and high pressure CO<sub>2</sub> and gas lasers are also discussed.

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**(46)**  
**Transient Indium Antimonide Spin-Flip Laser**

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Cpt. Commun., 18(1), 15-16; 1976

**TRANSIENT RESPONSE; INDIUM ANTIMONIDE SPIN-FLIP LASER; PULSED CO<sub>2</sub> LASER; TEMPORAL BEHAVIOR; OSCILLATIONS; SPIN-RELAXATION TIME; SPECTROSCOPIC APPLICATIONS; PHOTOCHEMICAL APPLICATIONS; ANALYTICAL METHODS; METHOD DEVELOPMENT; ANALYSIS**

The transient response of an InSb spin-flip laser has been investigated for the first time using a pulsed CO<sub>2</sub> laser. The spin-flip laser output power does not simply saturate as the CO<sub>2</sub> 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  $T_1$  in InSb. Only indirect measurements of  $T_1$  have been reported previously with values ranging from 1-600 ns. The spin-relaxation time (at  $n = 1.2 \times 10^{16}$  cm<sup>-3</sup>,  $V = 60$  kc,  $T$  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  $T_1$ , the multiple pulse technique can provide a means to efficiently extract larger output energies at high average power in a less order mode from a CO<sub>2</sub> 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., 39(3), 607-610; 1976, March

**HYDROXYL RADICALS; INTERMEDIATES; ATMOSPHERIC CHEMISTRY; RATE CONSTANTS; CLEAVAGE; CHEMICAL KINETIC MODELS; URBAN ATMOSPHERES; ABSOLUTE RATE CONSTANTS; 2-METHYL-2-BUTENE; FLASH PYROLYSIS-RESORANCE FLUORESCENCE TECHNIQUES; APPENDIXES; EXPRESSIONS; 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,  $k_2$ , 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  $k_2 = 3.6 \times 10^{12} \text{ L} \cdot \text{mol}^{-1} \text{ sec}^{-1}$  plus or minus 400/RT  $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ .

**(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; NITRATE 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. Tensionometers 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 potentials 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 could account for the high concentrations in the tile effluent.

<69>  
Rate Constants for the Reaction of O(3P) Atoms  
with CH<sub>2</sub>ClF, CH<sub>2</sub>ClCl, and CH<sub>2</sub>(2)CHCl at 298 Plus  
or Minus 2 Degrees K

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RATE CONSTANTS; ABSOLUTE RATE CONSTANTS; OZONE;  
VINYL FLUORIDE; VINYL CHLORIDE; VINYL CHLORIDE;  
DISCHARGE FLOW TECHNIQUES; RELATIVE RATE  
MEASUREMENTS; MODULATION PHASE SHIFT TECHNIQUES;  
ATMOSPHERIC CHEMISTRY; ANALYSIS

Absolute rate constants for the reaction of O(3P) atoms with CH<sub>2</sub>ClF, CH<sub>2</sub>ClCl, and CH<sub>2</sub>(2)CHCl have been obtained at 298 plus or minus 2 degrees K using a modulator phase shift technique. The rate constants ( $k_2 \times 10^{12} \text{ P-0.5 mole sec}$ ) obtained are: CH<sub>2</sub>ClF (1.61 plus or minus 0.20, CH<sub>2</sub>ClCl (2.54 plus or minus 0.26), and CH<sub>2</sub>(2)CHCl (2.05 plus or minus 0.25). These rate constants are lower than those determined by discharge flow techniques, but that for CH<sub>2</sub>ClF is in good agreement with relative rate measurements.

<69>  
Effect of Microorganisms on the Scraption and Fate  
of Sulfur Dioxide and Nitrogen Tioxide in Soil

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SULFUR DIOXIDE; GAS PHASE; MONSTERILE SOIL;  
STERILE SOIL; MICROORGANISMS; ATMOSPHERE-SOIL  
INTERACTIONS; SULFATE; NITROGEN DIOXIDE; NITRITE;  
NITRATE; BIOTRIPICATION; ANALYSIS; SOIL SODIUM;  
SCILS; DIALYSIS

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 SO<sub>2</sub> in nonsterile and sterile soil. About one-fourth of the sulfur from the SO<sub>2</sub> 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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