Chemistry and the Environment

The IUPAC Programme

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Pure and Applied
Chemistry

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Chemistry and the Environment the IUPAC programme

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Chemistry and the Environment

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Recent and ongoing projects
March 1990

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Foreword

Prof. Valentin Koptyug is coordinator of the IUPAC Programme on Chemistry and the Environment. He was IUPAC President from 1987 to 1989. He is also Vice-President of the USSR Academy of Sciences and President of the Siberian branch of the academy.

The continuing need to examine the relationship between man and his environment carefully should be a primary concern throughout the world and therefore a matter of international cooperation. Various United Nations organizations - such as the United Nations Environment Programme (UNEP), World Health Organization (WHO) and Food and Agriculture Organization (FAO), and various international scientific unions and their committees - such as the Scientific Committee on Problems of the Environment (SCOPE) of the International Council of Scientific Unions (ICSU) - are already devoting considerable attention to these problems.

The world community of chemists must also play their part in helping to tackle environmental problems especially since chemical substances are the main indices of the negative effects of industry, energy consumption, transport and intensive agriculture upon natural ecosystems and man. There are a number of areas where chemists need to cooperate with scientists from other disciplines in order to make a positive contribution to the long term protection of life on Earth. These include:

- Development of new environmentally safe chemical products from raw materials.
- Reduction of existing levels of chemical pollutants in the atmosphere, water and land.
- Study of the transformation of anthropogenic chemical substances in the environment.
- Prediction of the impact of chemical substances on ecosystems, man and climate.

To help achieve these humane aims, IUPAC decided in August 1989, at its 35th General Assembly in Lund, Sweden, to concentrate an important part of its efforts in the development and introduction of a programme on 'Chemistry and the Environment.'

The first step in this programme was the preparation of an inventory of recent and ongoing IUPAC projects related to chemistry and the environment. This booklet, which provides summaries of these projects, is the outcome of this first step. Hopefully, this information will reveal areas where IUPAC might fruitfully cooperate with other international organizations concerned with environmental problems.

The second objective of this programme is to stimulate IUPAC working groups, commissions and committees to initiate and develop further projects on chemistry and the environment.

In conclusion, chemical processes are the basis of life and, moreover, chemistry is necessary to promote the evolution of civilization. Chemistry should help to overcome rather than cause environmental problems. I am confident that this new IUPAC initiative will make a significant contribution to the positive application of chemistry to serve mankind and, at the same time, protect our environment.

Prof. Valentin Koptyug
March 1990

A The IUPAC Programme on Chemistry and the Environment

Introduction

Discussions within the IUPAC Bureau and Executive Committee during the period 1987-89 focused on restructuring of the Union, so as to be able to respond more readily and effectively to the changing worldwide needs of chemistry. A main conclusion reached was that there should be in place at any one time at least three 'horizontal' interdisciplinary mission-oriented programmes involving several divisions/commissions.

In February 1989, the President, Vice-President and Secretary General of the Union took an initiative towards the first such horizontal programme - Chemistry and the Environment - by holding preliminary talks in Paris, France with the Scientific Committee on Problems of the Environment (SCOPE), the International Council of Scientific Unions (ICSU) and also with the United Nations Environment Programme (UNEP).

As a basis for more detailed consideration of the collaborative role to be played by IUPAC, the IUPAC Information Officer, Dr Michael Freemantle, was asked to prepare a booklet, with abstracts, of relevant reports issued during the period 1984-89 by IUPAC bodies together with summaries of their current projects. A preliminary compilation was submitted to the IUPAC Executive Committee when it met in Lisbon, Portugal in April 1989. Suggestions put forward by the Executive Committee at and following the Lisbon meeting were incorporated into a second draft which was then submitted to Bureau members at the 35th IUPAC General Assembly held at Lund, Sweden in August 1989.

At this assembly, Bureau approved the formation of four mission-oriented programmes including one on Chemistry and the Environment. Prof. Valentin Koptyug, President of the Union from 1987 to 1989, was appointed overall coordinator of this programme with subcoordinators to have responsibilities for six broad topics:

At the 35th IUPAC General Assembly held in Lund, Sweden in August 1989, Bureau approved the formation of four mission-oriented programmes including one on 'Chemistry and the Environment.'

- Analytical procedures for determination of chemicals in air, water, soil, living organisms, and food (Subcoordinator: Prof. G. den Boef, President, Analytical Chemistry Division).
- Measurement of physicochemical parameters relevant to the environment (Subcoordinators: Prof. G. den Boef and Dr L. E. Coles, President of the Applied Chemistry Division).
- Transfer and transformation of chemicals in the environment (Subcoordinator: Dr L. E. Coles).
- Toxicology of synthetic and natural substances (Subcoordinator: Prof. N. Montalbetti, President, Clinical Chemistry Division).

- Prevention of pollution of the environment (Subcoordinator: Prof. K. I. Zamaraev, Bureau member and immediate Past-President of the Physical Chemistry Division).
- Chemical safety (Subcoordinator: Dr D. Wyrsch, Chairman, Committee on Chemistry and Industry).

The first meeting of the coordinators was held at the IUPAC Secretariat in Oxford, March 1990.

Chemistry and the Environment booklet

The first task of the coordinators was to complete the preparation of, publish and disseminate the *Chemistry and the Environment* booklet. It was agreed that the final version of the booklet should include details of IUPAC's recent and current projects which are closely or indirectly related to environmental chemistry including those initiated at the Lund General Assembly.

This booklet contains abstracts of IUPAC reports on environmental topics published during the six year period ending March 1990. Most of the reports were published in the IUPAC journal *Pure and Applied Chemistry*. Reference is also made to published proceedings of IUPAC sponsored conferences, in particular, the IUPAC programme of conferences on CHEMical Research Applied to World Needs (CHEMRAWN); In addition, the booklet includes details of environmental projects initiated by the Committee on Teaching of Chemistry and articles on chemistry and the environment published

The IUPAC Chemistry and the Environmental Programme encourages interdivisional collaboration in several areas including the use of analytical procedures for determination of chemicals substances in the environment.

in the IUPAC news magazine *Chemistry International.*

Each section contains abstracts of ongoing projects, which are grouped, for convenience, in the six chapters of Section A corresponding to the six topics listed above. The abstracts were extracted from archive material at the IUPAC Secretariat including project initiation proposals and revision sheets. All these projects were ongoing at March 1990.

The following IUPAC divisions, commissions and committees have all contributed reports abstracts of which appear in this booklet:

Physical Chemistry Divisions:
- Commission on Colloid and Surface Chemistry including catalysis

Inorganic Chemistry and Clinical Chemistry Divisions
- Limited Life Time Joint Commission (formerly, Working Party) on Isotope Specific Measurements as References for Toxic/Essential Element Assay

Analytical Chemistry Division:
- Subcommittee on Electroanalytical Methods of Environmental Trace Analysis
- Subcommittee on Environmental Analytical Chemistry (Now a Limited Life Time Commission)
- Commission on Microchemical Techniques and Trace Analysis
- Commission on Analytical Nomenclature
- Commission on Electroanalytical Chemistry
- Commission on Radiochemistry and Nuclear Techniques
- Commission on Solubility Data

Applied Chemistry Division:
- Commission on Food Chemistry
- Commission on Biotechnology
- Commission on Oils, Fats, and Derivatives
- Commission on Atmospheric Chemistry
- Commission on Agrochemicals (formerly Commission on Pesticide Chemistry)
- Commission on Water Chemistry

Clinical Chemistry Division:
- Commission on Toxicology

Committees
- CHEMRAWN Committee
- Committee on Chemistry and Industry
- Committee on Teaching of Chemistry

Prices quoted in this booklet are in one or more of the following currencies:

DEM	Deutsche Mark
GBP	Pound Sterling
USD	US Dollar

1 Determination of chemical substances in air, water, soil, living organisms and food

1.1 General problems

1.1.1 Analytical chemistry in the exploration, mining and processing of materials

This book contains the invited lectures presented at the 2nd International Symposium on Analytical Chemistry in the Exploration, Mining and Processing of Materials held in Pretoria, South Africa, in April 1985.

Analytical chemistry is vital to the mining and mineral industry. To meet the ever increasing demands in the quest for better quality and the more economical exploitation of mineral resources, sophisticated analytical techniques must be developed constantly or existing methods improved.

The aim of the 2nd International Symposium was to highlight the importance of analytical chemistry in the production of materials, from the initial stages of exploration and assessment of ores to their beneficiation, and finally to the refined product.

Edited by L. R. P. Butler. Published by Blackwell Scientific Publications, Oxford, UK, 1986. 264 pages; 150 illustrations. ISBN 0 632 01532 2. Price: GBP 27.60/USD 34.50. Affiliate Members Discount Price: GBP 20.70/USD 25.90.

1.1.2 Acid pressure decomposition in trace element analysis

Wet decomposition procedures within sealed systems (pressure decomposition) provide efficient methods for sample dissolution in trace element analysis. Vessels produced from high-purity materials (PTFE, glassy carbon), contained by compact pressure casings (stainless steel, aluminium alloys) are used in this technique. At temperatures of about 170°C the reaction capacity of acids and oxidizing decomposition agents increases so that inorganic and organic samples of a most widely differing composition are dissolved in a relatively short time.

In this report, an attempt is made to compile the specific advantages of, and the problems posed by, pressure decomposition procedures such as increased reactivity, faster reactions, decrease in blank values, avoidance of trace element losses, easy control of precision and calibration, completeness of sample decomposition, possible formation of explosive products and so on. At the same time, the properties of materials used for vessels, casing and heating systems are discussed.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 56, No. 4, pp. 479-489, 1984.*

1.1.3 Microscale preconcentration techniques for trace analysis

The determination of elemental traces in micro samples, that is, micro-trace analysis can be successfully carried out by combining preconcentration steps with modern instrumental determination methods. In this paper, the problems and their solutions for each analytical stage of micro-trace analysis are presented and briefly discussed.Some typical examples of micro-scale analysis are also reviewed.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 60, No. 9, pp. 1417-1424, 1988.*

1.1.4 Electrochemical analysis of organic pollutants

The electroanalytical techniques of pulse polarography, stripping voltammetry and on-line electrochemical detection have been used for the identification and determination of trace concentrations of a wide variety of environmentally significant organic molecules, usually after the application of sample pretreatment procedures, certain separation techniques and, in some cases, derivatization. Classes of molecules that can be determined using these methodologies are carbonyls, simple aromatics such as nitroaromatics, phenols, polychlorinated aromatics, carboxylic acids, sulphonates, organophosphorus compounds, azomethines, thiols, carbamates and amines.

Analytical Chemistry Division, Commission on Electroanalytical Chemistry, Subcommittee on Electroanalytical Methods of Environmental Trace Analysis: Pure & Appl. Chem., *Vol. 59, No. 2, pp. 245-256, 1987.*

The IUPAC sponsored symposium series on Biological Reference Materials focuses on the production, characterization, and application of these materials in environmental and health related areas.

1.1.5 Voltammetric techniques for complexation measurements in natural aquatic media

The use of voltammetric techniques for the study of complexation between metal ions and synthetic or natural macromolecular ligands is critically reviewed. In particular, attention is paid to the effects of (i) finite rates of association/dissociation of complexes and (ii) the differences between the diffusion coefficients of the various metal species.

The present state of the theory of voltammetry for metal complex systems with unequal diffusion coefficients is reviewed and necessary extensions are indicated. Relevant experimental data from literature are compiled and classified according to the mode of interpretation.

On the basis of the theoretical and experimental results, recommendations are presented for the optimal application of voltammetric methods (both direct and indirect methods) to metal complex studies. These recommendations include the selection of suitable experimental conditions and the required mode of interpretation of the data, as well as their mutual relation. Remaining uncertainties, for example, those dueto distribution of kinetic parameters or by diffusion coefficients, are indicated.

Analytical Chemistry Division, Subcommittee on Environmental Analytical Chemistry: Pure & Appl. Chem., *Vol. 61, No. 2, pp. 255-274, 1989.*

1.1.6 Biological reference materials

The increasing awareness and concern for improving data and measurements of both harmful and beneficial constituents in biological matrices has generated a need and demand for more accurate information from measurement systems that are required to be more sensitve and complex while at the same time more 'routine', fast and economical. Validation of these new methodologies and linking new 'routine' field methods to more definitive, complex and expensive methodology, requires accuracy transfer via use of appropriate reference materials.

The major aim of the IUPAC sponsored symposium series on Biological Reference Materials is to focus efforts in the production, characterization, and application of these reference materials in the environmental, and health related areas. The third in the series of symposium was held in Bayreuth, FRG, May 1988 (see *Fresenius Z. Anal Chem* 332:517,

1988) and the fourth took place in Florida, USA in February 1990.
Clinical Chemistry Division

1.1.7 Water pollution research and control

Published in Chemistry International, *Vol. 10, No. 3, pp. 89-91, 1988.*

1.1.8 Nomenclature for geochemical analysis

The aim of this project is to develop and compile a complete nomenclature for the field of geochemical analysis. At present, no adequate up-to-date compilation exists.
Analytical Chemistry Division, Commission on General Aspects of Analytical Nomenclature: Ongoing Project.

1.1.9 Neutron activation techniques for the determination of trace elements in dusts, ashes and sludges

Fine dusts and fly ashes emitted in the atmosphere or in work rooms can have long residence times and as such be potential hazards for human health and the environment.

Ashes and sludges are disposed of by dumping on landfill or used on agricultural land. Since these procedures may cause contamination of the environment and/or food raw materials, the determination of major, minor and trace components is essential for decisions on the use of thee materials.

At the moment there is a strong tendency to determine as many elements as possible. Elements are determined as indicators of a source, as pollutants or as being important in environmental toxicology.

Therefore, instrumental multi-element techniques like nuclear activation are important tools. Techniques, such as activation with thermal, epithermal and fast neutrons, with protons and with charged particles are being critically examined in this project and recommendations for their application will be given.
Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.1.10 Bioelectroanalysis and biosensors

Current activities in biology have aroused great interest in different fields of analytical chemistry. This has resulted in important achievements in electroanalytical chemistry, among them the development of a wide range of new devices called biosensors and new electroanalytical methods.

The aim of this project is to give a proper definition for the term 'biosensors', to outline the scope of bioelectroanalysis and to summarize systematically the results of the different main streams of developments. Moreover, the project aims to find common measures on the basis of which the different sensors and techniques can be evaluated correctly and compared objectively. An overview of the main application fields will also be given.
Analytical Chemistry Division, Commission on Electroanalytical Chemistry, Ongoing Project.

1.1.11 Determination of trace compounds in biological systems

The application of radioanalysis to the determination of molecular compounds implies (a) separation prior to activation or tagging and (b) the activation or tagging itself.

This project consists of two parts. The first pertains to the realization of an on-line HPLC separation with radioactivity detection. This part has been completed. The tagging by an on-line 'vector' is ongoing. Depending on the specific activity of the radionuclide used, concentration in parts per billion to 10^{-2} parts per billion can be determined.
Analytical Chemistry Division, Commission on Radiochemistry and Nuclear Techniques: Ongoing Project.

1.1.12 Radioanalytical procedures for the determination of trace compounds in biological systems

This project aims to prepare and make available a concise and representative survey of the current possibilities of radioanalysis of molecular trace constituents in biological materials.

The project will cover both the use of radio-labelled compounds and the applications of activation analysis and radiometry. Information is being compiled from systematic literature retrieval, current work in leading laboratories in the field as well as from personal experience in the radiochemical laboratories of commission members.
Analytical Chemistry Division, Commission on Radiochemistry and Nuclear Techniques: Ongoing Project.

1.1.13 Applications of accelerator mass spectrometry

Analytical Chemistry Division, Commission on Radiochemistry and Nuclear Techniques: Ongoing Project.

1.1.14 Study of speciation in the environment by nuclear techniques

This project is a feasibility study of (1) chemistry of ultra-low concentrations; (2) speciation of radionuclides; (3) nuclear methods in speciation and (4) use of radiotracers in speciation work: possibilities and limitations. In each case the study is concerned with applications in environmental research and monitoring.

Analytical Chemistry Division, Commission on Radiochemistry and Nuclear Techniques: Ongoing Project.

1.1.15 Membrane filtration in water analysis

The aim of this project is to identify the major problems which affect 'size' separation of aquatic components by filtration through membranes of various types and porosities. The project will provide recommendations about filtration conditions to obtain reproducible results.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.1.16 Application of voltammetric techniques to low ionic strength solutions

This project has four objectives:

1. To identify the major problems which affect measurements made in low ionic strength solutions.
2. To calculate the relative contributions of different effects at different ionic strengths, and different concentrations of the determinand.
3. To give practical procedures that can be used to verify that low ionic strength is not a problem for the particular solution being measured.
4. To identify how low ionic strength affects different techniques in different ways.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.1.17 Sampling of airborne particulate matter for analysis

In air analysis, as in other branches of analytical chemistry, the sampling step is the most crucial one. The transfer of a representative ambient aerosol sample, containing solid particles and liquid droplets of a wide range of sizes and of different 'reactivity', into anappropriate measurement system may give rise to serious technical problems.

Accordingly, this planned critical review on sampling of airborne particulate matter for analysis will emphasize strengths and weaknesses of current possibilities of extracting and preconcentrating solid particles and liquid droplets from ambient air. The techniques included are based on the following: collision, adhesion, inertia and diffusion in flow fields under the influence of gravitational and/or electrical forces.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.1.18 Single particle characterization through beam techniques

The objective of this project is to describe and discuss various beam techniques applied to the analysis of individual particles in the environment (for example, in aerosols and aqueous suspensions). Techniques include electron-probe X-ray microanalysis, laser microprobe mass analysis, secondary ion mass spectrometry, microbeam proton-induced X-ray emission analysis and laser Raman microprobe analysis.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.1.19 Glossary of terms used in environmental analytical chemistry

This glossary contains definitions of terms frequently used in environmental analytical chemistry. Part I of this glossary includes terms related to environmental analytical methodology. Part 2 is concerned with matrices and materials to be characterized.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.1.20 Evaluation of electron microscopic techniques for characterization of aquatic colloids

The aim of this project is to provide a state of the art evaluation for an IUPAC monograph on particle characterization. The project will focus on technology transfer from the biomedical sciences in conjunction with minimal perturbation technology. The project will presentan optimal blend of analytical chemistry and transmission electron microscopy for characterizing natural particles in surfaces waters and analyzing particle behaviour.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.1.21 Source apportionment of atmospheric particles

The identification and quantification of sources of atmospheric particles directly relates to the terms of reference of this commission, that is its responsibility to assess analytical methodologies for the characterization of the environment, in this case the atmosphere.

The importance of this objective derives from the potential impact of atmospheric particles on health, visibility and climate. In these respects, the commission is particularly concerned with tropospheric concentrations and sources of toxic compounds (for example, polycyclic aromatic hydrocarbons), sulfate, and graphitic carbon (soot). A primary objective of source apportionment of such species is to delineate the natural and anthropogenic components, since only the latter may be controlled. The scope of the study comprises local, regional and global source apportionment.

The basic approach to particulate source apportionment involves chemical and physical characterization of ambient particles, together with their variations in space and time, plus relevant information on source (emission) composition, atmospheric transport, and chemical transformation. Univariate and multivariate statistical techniques form the link between the observed particle characteristics and the inferred source identification and quantification.

Specific objectives of the project will include consideration of (1) analytical (chemical) particle characterization methods, such as isotopic analysis, elemental and anionic analysis, patterns of homologous series of organic compounds, and individual particle assay; and (2) analytical (mathematical) source apportionment schemes, such as unique tracer regression, enrichment factors, cluster analysis, factor analysis, particle class and chemical mass balance, and wind trajectory analysis. Finally, essential means to control the quality of both the chemical and mathematical phases of analysis will be considered. These derive from source profile databases, representative field experiments, and standard (reference) materials and standard (simulation, multivariate) data.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.1.22 Animal drugs

In order to test methods for measuring residues in animal derived food, it is necessary to transport tissues to laboratories in various countries. Most countries prohibit or limit the import of animal tissues because of the potential for the transfer of diseases.

Two approaches are being taken to solve this problem:

1. The problem has been introduced to the commission for discussion of how extensive the problem is and of possible solutions that others have devised.
2. An experimental approach using freezing drying procedures is being undertaken. Specific animal drugs of interest with available methods are being selected for the study. Tissues containing the physiologically incurred residue are being analysed before and after freeze drying to examine the effect of the procedure on the analyte of interest.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.1.23 Inventory of missing emission data necessary to evaluate global atmospheric changes

Good emission data are available only for industrialized nations, for example USA, Canada and countries in Western Europe. Little or no data are available for socialist and non-developed countries. These data are necessary to understand global atmospheric changes, acid deposition and other environmental problems.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

The Commission on Atmospheric Chemistry is preparing an inventory of emission data in order to evaluate global atmospheric changes

1.1.24 Evaluation and harmonization of current tropospheric sampling networks worldwide

This project aims to evaluate the present state of measurement methodology, sampling techniques, measurement strategy and quality control of network operations. It will also propose measures that ensure harmonization of network results and optimize the possibilities of reaching the objectives of the networks, for example, the average deposition or the detection of trends.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

1.1.25 The use of passive samplers for monitoring atmospheric constituents

Passive samplers are inexpensive devices which collect atmospheric constituents. They are very useful for monitoring these constituents. Many non-developed countries are unable to purchase the expensive equipment used in industrialized countries for this purpose.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

1.1.26 Measurement of contaminants in the workplace

Available analytical methods from a number of typical countries have been collated with reference to chemicals on the United Kingdom list of exposure limits. These methods are not always adequate for the range of workplace contaminants. They are not sufficiently harmonized and are not always cost effective - particularly for developing countries.

This project aims to collate the availability of analytical methods worldwide with the chemical contaminants identified in national and international lists of occupational exposure limit values. The project also aims to obtain the views of national regulatory authorities and other interested parties on the adequacy of available methods, measurement strategies, harmonization and certification of methods and the availability of quality control.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

1.1.27 Workshop on uncertainties in trends in atmospheric chemistry

There exists a wide range of different projections of the future composition of the global atmosphere with respect to the greenhouse effect related to trace compounds, stratospheric ozone and so on. The aim of this workshop is to assess the uncertainties in the assessments of these trends and thereby assess the uncertainties in the formulation of future measures to preserve the environment.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

1.1.28 Leaching tests to assess pollution hazards to ground waters

The objective of this project is to consider critically current procedures for sampling, sample preparation, laboratory leaching procedures and the interpretation of test results for the prediction of potential hazards to ground waters arising from the disposal of waste materials.

Applied Chemistry Division, Commission on Water Chemistry: Ongoing Project.

Recommendations for the determination of pH in sea water and estuarine waters

See Chapter 2 Page 30.

1.2 Determination of inorganic substances

1.2.1 Determination of trace metals in natural waters

Each field of chemistry is confronted with the problem of monitoring water quality and research on trace chemical compounds. This text is designed to meet the needs of the many potential users for reliable guidelines and methods of the analysis of trace elements in natural waters, for example, analytical chemists, hydrologists, oceanographers, toxicologists, ecologists and so on, involved in the quality control of natural waters and the detection of traces.

This project, initiated by the IUPAC Analytical Chemistry Division in 1979, is intended to offer chemists and related scientists a survey of available methods, showing their respective performances, their areas of application and, in general, information that will enable them to apply the data to the resolution of specific problems.

Edited by T. S. West and the late H. W. Nurnberg. Published by Blackwell Scientific Publications, Oxford, UK, 1988. 380 pages, 92 illustrations. ISBN 0 632 02021 0. Price: GBP 60.00/USD 85.00. Affiliate Members Discount Price: GBP 45.00/USD 64.00.

1.2.2 Determination of selenium in biological materials and water

The determination of selenium is of considerable interest because it would appear to be an essential trace element but it is also toxic at relatively low levels. Methods for its determination in biological materials and water are critically evaluated with particular attention given to methods which are widely used in routine analysis.

The method involving the reaction of selenium(IV) with 2,3-diaminonaphthalene to give the strongly fluorescent 4,5-benzopiazselenol is now widely accepted as a satisfactory method for routine work. Reduction of selenium to the hydride for determination by atomic absorption spectroscopy is the basis of another accepted method. A further method which is gaining in popularity involves cathodic stripping voltammetry.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 56, No. 5, pp. 645-651, 1984.*

1.2.3 Trace element analysis in surface waters

A survey is given of methods for the determination of chromium and mercury in various water types, mainly published in the period 1975-80.

Mercury was chosen because in this period there was intensive research of its determination. In the case of chromium, analytical research was in its early stages. Accordingly, there was found to be some agreement on the method to be selected for the determination of mercury. Some attention was given to sample treatment and sampling. There is a severe risk that automation of the end-determination indirectly causes errors.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 56, No. 10, pp. 1477-1498, 1984.*

1.2.4 New type of flotation of ion-association compounds of complexes of multicharged anions with basic dyes

Sparingly soluble ion-association compounds formed between multi-charged anionic complexes (formed from trace amounts of an element to be preconcentrated and determined) and hydrophobic basic dyes, accumulate at the phase boundary after shaking with a solvent of low polarity.

This type of flotation (without surfactant and gas bubbling) depends on the acidity, the dyestuff and the flotation agent. The separated compound can be determined with use of any suitable method. Combination of thisseparation technique with spectrophotometry allows a very sensitive determination, because 2-5 dye cations correspond to one atom of the element in the multicharged anion.

Examples of separation and determination of the six platinum metals prove the effectiveness and precision of the proposed technique.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 57, No. 6, pp. 849-854, 1985.*

1.2.5 Determination of manganese in biological materials

Although the essential nature of manganese in humans has yet to be firmly established, it is clearly an important constituent of a number of enzyme systems, and is clearly implicated in a number of deficiency conditions in animals. The accurate determination of manganese in biological materials is therefore of considerable importance for both metabolic and toxicological studies in humans and animals.

Much of the earlier literature on manganese determinations, in particular in serum and urine, is marred by errors in the analytical procedures due principally to a failure by analytical chemists to fully appreciate the requirements for stringent control of contamination during sampling and sample handling prior to analysis.

The wider availability of electrothermal atomic absorption instruments, particularly those incorporating the most recent advances in technology has brought the determination of manganese in serum and urine within the scope of many routine hospital laboratories. The application of this technique, coupled with the availability of centres providing activation analysis as a reference method, could have a significant impact on our knowledge of the biochemical functions of manganese in the next ten years.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 58, No. 9, pp. 1307-1316, 1986.*

1.2.6 Determination of chromium in biological materials

The determination of chromium in biological materials is of considerable importance because it has been shown to be essential by animal experiments and has potential importance in human medicine. At higher levels it is also toxic and symptoms of chromium toxicity are well established.

Numerous errors have appeared in earlier analytical measurements of chromium because analysts have paid too little attention to potential sources of contamination, and to the stringent requirements of particular instrumental measurements. As a result of recent studies, a clearer understanding of the nutritional requirements of chromium, and of the levels of chromium in the serum and urine of normal subjects is available.

Recent developments in technology have provided analytical techniques with sufficient sensitivity for both these determinations, although serum chromium at the lowest levels is still a difficult determination for routine hospital laboratories without specialized facilities. Recent developments in analytical techniques are reviewed in the light of clinical requirements both now and in the foreseeable future.

Analytical Chemistry Division. Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 58, No. 12, pp. 1707-1720, 1986.*

1.2.7 Determination of aluminium in biological materials by graphite furnace atomic absorption spectrometry (GFAAS)

A survey is given of various methods for the determination of aluminium in biological materials. Graphite furnace atomic absorption spectrometry (GFAAS) is the most widely used technique since it is sufficiently sensitive and simple to operate. The limitations inherent in GFAAS procedures are critically discussed. Reported results for aluminium in blood, serum and tissues differ largely showing that the determination of this element is subjected to large errors due to contamination during sample handling.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 59, No. 2, pp. 221 228, 1987.*

1.2.8 Determination of fluoride in various matrices

Methods for the determination of fluorine in a variety of matrices are reviewed with particular attention to those techniques which are widely adopted as routine methods.

The use of the fluoride ion-sensitive electrode is a very successful potentiometric technique for the determination of fluoride in aqueous solution and it has largely replaced the various colorimetric methods formerly used. However, it is apparent that the rapid development of ion chromatography with its advantage of simultaneous multi-anion determination is introducing a new phase into fluoride analysis.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 59, No. 5, pp. 695-702, 1987.*

1.2.9 Determination of traces of thallium in various matrices

Thallium is a relatively rare element and therefore its application is limited. The determination of traces of thallium, however, is important because of its high toxicity (maximal allowable concentration: 0.1 mg/m3 in air). In addition to the availability of accurate methods for the determination of total thallium, one should consider methods for speciation (at least for the different oxidation states thallium(I) and thallium(III) and for organohalogen compounds such as R_2TlBr).

The determination of thallium is not an easy task as the natural contents in environmental samples are at ng/g levels or less. In discussing analytical methods for thallium, one should pay attention to all relevant parts of the analytical procedure: sampling, digestion, preconcentration and determination.
Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 60, No. 9, pp. 1425-1436, 1988.*

1.2.10 Sample digestion for the determination of elemental traces in matrices of environmental concern

This report summarizes various methods of sample digestion for (wet) chemical element analysis. The digestion method to be chosen for any practical problem depends largely on the element(s) to be determined, their content(s) and the type of matrix. Addition of hydrofluoric acid is necessary in most cases as many organic matrices (for example, plants) contain silicon.

Where the completeness of the digestion is paramount, for example, in voltammetry, perchloric acid should be added, preferably when most of the organic matter is already oxidized. Perchloric acid is also recommended for matrices when $CaSO_4$ (which collects Pb) contain silicon.

Pressurized digestions using strong oxidizing acids and hydrofluoric acid are recommended for many cases; they allow high temperatures during the procedure as well as prolonged durations and are free of contamination, provided that suitable equipment is used.

Microwave heating is also a very powerful technique. Fusion techniques are very powerful in the analysis of ashes and certain rocks, but may be accompanied by high blanks and are time and labour consuming.

Two illustrations of the application of different techniques are given: incinerator ash (high with respect to trace elements, presence of highly resistant alumino-silicates) and milk powder (extremely low in trace elements).

Prior to the application of any digesion technique,

The Commission on Microchemical Techniques and Trace Analysis has published a survey of methods for the determination of chromium and mercury in various water types.

its performance should be carefully studied, using certified reference materials, or in comparisons involving non-destructive techniques.
Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Pure & Appl. Chem., *Vol. 61, No. 6, pp. 1139-1146, 1989.*

1.2.11 Direct polarographic determination of O_2, Fe(II), Mn(II), S(-II) and related species in anoxic waters

Direct polarographic measurements of naturally anoxic waters can readily determine Fe(II), Mn(II), S(-II) and dissolved O_2. Procedures for collecting and handling samples are described and the results from different studies are systematically discussed and evaluated.

The unique capabilities of polarography to distinguish between soluble, colloidal and particulate species have led to the characterization of the time dependent formation of colloidal, complexed and solid phase forms of FeS in natural waters, and to an appreciation of the complicated distribution of various oxidation states of Mn and Fe between particulate and colloidal fractions.
Analytical Chemistry Division, Subcommittee on Environmental Analytical Chemistry: Pure & Appl. Chem., *Vol. 60, No. 10, pp. 1535-1548, 1988.*

1.2.12 Determination of mercury in foodstuffs

This report specifies a reference method for the determination of total mercury in foodstuffs and biological materials. The method is applicable to the determination of the mercury content of all foodstuffs and biological materials to 0.01mg/kg.
Applied Chemistry Division, Commission on Food Chemistry: Pure & Appl. Chem., *Vol. 57, No. 10, pp. 1507-1514, 1985.*

1.2.13 Determination of copper, iron and nickel in oils and fats by direct graphite furnace atomic absorption spectrometry

The pre-oxidant effect of small amounts of metals in edible oils and fats has been known for many years. In particular copper, iron and nickel have a catalytic effect on the mechanism of autoxidation. The metals present in oils and fats may be of natural origin or due to processing actions such as bleaching (Fe), hardening (Ni, Cu) and corrosion of processing equipment (Fe, Ni). In the oils and fat industry a rapid, accurate and standardized method for the determination of these metals is very important for quality control.

Atomic absorption spectrometry (AAS) has been generally accepted for the determination of Cu, Fe and Ni in oils and fats, and a variety of procedures based on AAS are currently used.

In this report, a description is given of the development by collaborative study of a standardized method for the determination of copper, iron and nickel in edible oils and fats by direct graphite furnace atomic absorption spectrometry. The procedure is both rapid and sensitive allowing determination at levels of 0.005-0.20 mg/kg for copper and 0.01-1.00 mg/kg for iron and nickel.
Applied Chemistry Division, Commission on Oils, Fats and Derivatives: Pure & Appl. Chem., *Vol. 60, No. 6, pp. 893-900, 1988.*

1.2.14 A critical survey of hydride generation techniques for trace analysis by atomic absorption spectrometry (AAS)

Hydride generation techniques are widely used in the determination of elements - such as arsenic, selenium, tin, lead and germanium - which readily form hydrides by reaction of their salts with sodium borohydride.

Combined with AAS, hydride generation techniques are capable of giving very low limits of detection. However, the method involving hydride atomization in a heated silica tube is subject to many interferences because decomposition of the hydride is by a radical process at the temperatures normally adopted. This phase of the technique in particular requires careful evaluation.

The review will contain sections on the following topics:

- Formation of the hydride including effect of oxidation state.
- Methods for the concentration of the hydride.
- ecomposition of the hydride and interferences.
- Equipment.
- Specific reference to the various elements.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.15 The determination of trace levels of germanium in various matrices

Germanium is an important element in the natural environment: in water and in plants. It has also been used in a variety of complexes for use as a bacteriocide and fungicide. It is, of course, very important as a trace element in the semiconductor industry. Germanium has a number of biomedical applications although in some forms it is also toxic.

It is, therefore necessary for the analyst in a wide variety of fields to have good, reliable methods for the determination of germanium in a number of different matrices. This report will critically review the methods currently available, including the separation, preconcentration and determination of germanium in various matrices and provide recommendations.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.16 Determination of cadmium and lead in foodstuffs

This is Part XII of a series of papers entitled 'Critical evaluation of analytical methods for the determination of trace elements in various matrices.'

The toxic nature of lead and cadmium and the major contribution made to the total body burden of these elements by food consumption, ensures that these are two of the most important determinations performed by the food analyst.

A wide range of techniques have been adopted of which electrothermal atomization atomic absorption spectrometry (ETA AAS) appears to be the most popular at the present time. In most procedures, some form of pretreatment is required or adopted, including wet and dry ashing, and preconcentration by, for example, solvent extraction. Such preliminary steps must always involve an increased risk of contamination by loss of analyte, and these problems will increase in significance when foodstuffs containing the lowest amounts of the analyte elements are to be analysed.

In order to assess the total dietary intake of lead or cadmium it is necessary to determine these elements at levels as low as 1 ng/g. Most methods in use only reach levels of the order of 10-50 ng/g with convenience, and preconcentration is often adopted to achieve detection capabilities of the order of 1 ng/g. This concentration range is most susceptible to contamination errors.

Germanium is an important element in the natural environment: in water and in plants. The determination of trace levels of this element in the environment is the subject of one of IUPAC's ongoing projects.

It is proposed to prepare a state of the art review of:

1. The requirements for lead and cadmium analysis in foods.
2. The problems of contamination particularly in pretreatment steps when levels of 1 ng/g are to be determined.
3. Evaluation of current methods.

The paper will highlight methods suitable for reaching the lowest levels required for total diet analysis, the precautions necessary to use them, and the need for regular checks on accuracy with acceptable criteria.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.17 Determination of vanadium in biological materials

The metabolism and biological functions of vanadium are not well established. The main reason for this appears to be the relatively low levels of the element in the blood and urine of normal subjects, and the consequent difficulty in developing reliable analytical methods (particularly atomic absorption spectrometry methods).

Despite this problem, there is considerable increst in the biochemical role of vanadium at low levels, and there is evidence which indicates involvement of the element in the regulation of the membrane pump system. As with chromium and manganese, the older literature shows many erroneous values.

Recent work has confirmed normal mean levels of vanadium in blood serum but also indicates a wide range of values in normal subjects. There is, however, considerable controversy between two groups one of which believes that the normal mean levels of vanadium in serum are approximately one order higher. Since both groups use neutron activation analysis, the argument currently revolves round the sensitivity available in specific reactors and the chemical procedures adopted.

Occupational exposure to vanadium is fairly common - in both the chemical industry where V_2O_5 is used widely as a catalyst and in the metal industry. Monitoring of urinary vanadium at higher levels in exposed subjects is more convenient using electrothermal atomization (ETA).

Within this series, it is timely for IUPAC to produce a state of the art review discussing the requirements for vanadium determinations, appropriate levels, problems of sampling and contamination, and a critical evaluation of past literature and methods. The paper will highlight weaknesses and strengths of published methods, and suggest areas for improvement and research.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.18 Determination of molybdenum in biological materials

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.19 Determination of arsenic species in environmental and biological samples

The aim of this project is to review work on the identification and determination of chemical species of arsenic in environmental and biological samples. Through a critical evaluation of the literature, it will recommend a reference analytical procedure for specific arsenic species, including arsenobetaine and arseno-sugars and suggest analytical methods to be developed in the near future.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.20 Determination of trace elements bound to soil and sediment fractions

This project aims to provide a critical evaluation of operationally defined analytical procedures applied to soils and sediments with the aim of assessing critical metal pools. This will lead to a better understanding of element pathways through ecocompartments such as water and sediment. The current diversity of methods renders an interpretation of results and a comparison of conclusions obtained in various analytical institutes very difficult if not impossible.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.21 Determination of mercury species in environmental and biological samples

The aim of this project is to review work on the identification and determination of chemical species of mercury in environmental and biological samples. Through a critical evaluation of the literature, it will recommend a standard procedure for specific mercury species including methyl mercury, phenyl mercury and inorganic mercury in a variety of matrices.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.22 Determination of tin species in biological and environmental samples

The objective of this project is to review methods of identifying and characterizing chemical species of tin in environmental and biological samples. It aims to recommend procedures for the determination of organic species of tin, especially butyl tin and phenyl derivatives resulting from, for example, industrial wastes and use of special paints.

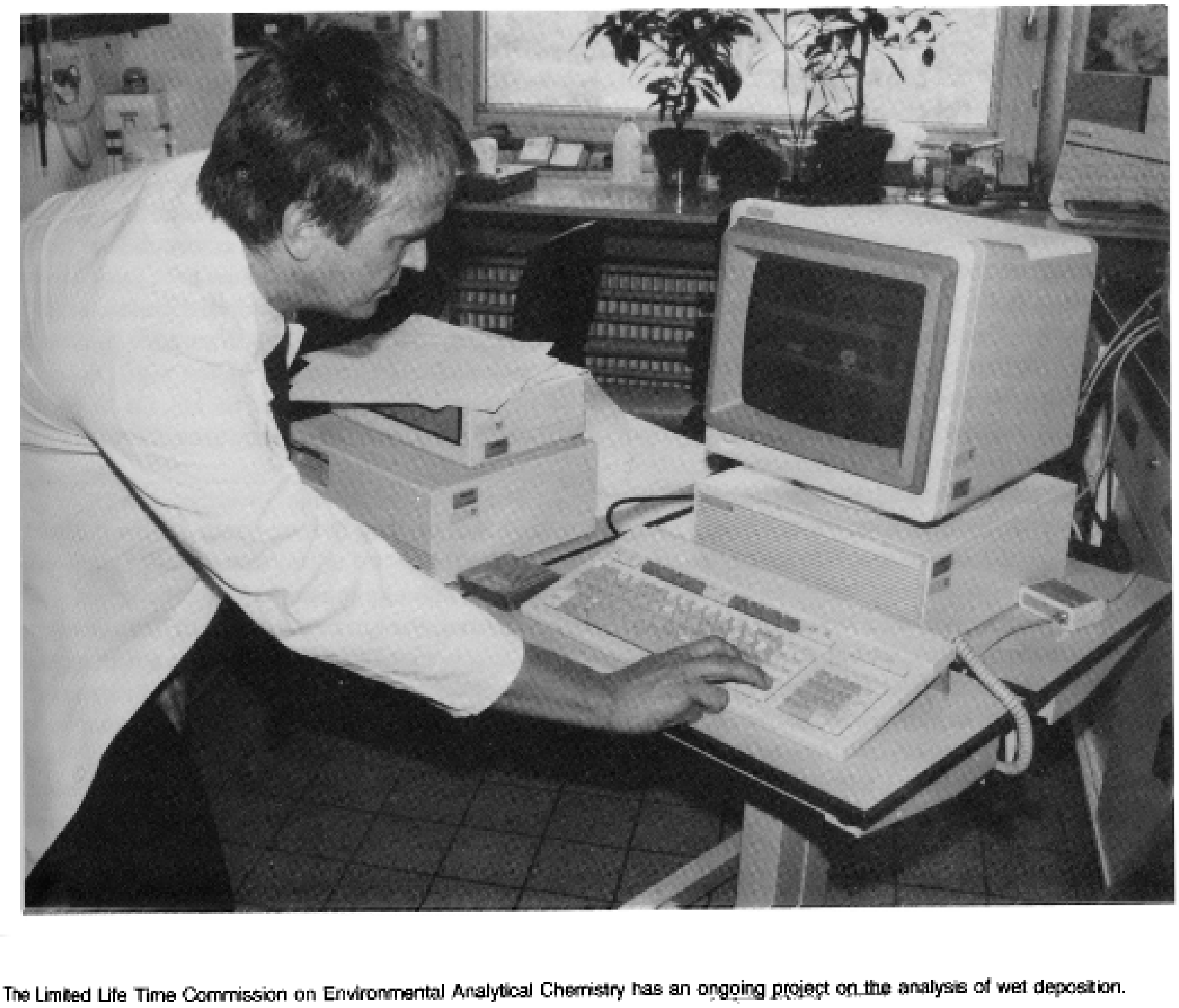
Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.23 Determination of lead species in biological and environmental samples

The purpose of this project is to present a critical overview of trace speciation methods for lead. The speciation of lead is not only important in view of the use of lead petrol but also to understand bio-alkylation processes in waste dumps and sediments for example. Most results of investigations are worthless because inadequate analytical methods are used. Based on experience and a critical method evaluation, some harmonized well-suited methods will be proposed.
Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.2.24 Analysis of wet deposition: Determination of anionic constituents by ion chromatography

The project will define all aspects of the analytical procedure needed for the determination of Cl^-, NO_3^-, and SO_4^{2-} in wet deposition (rain water, snow, sleet, hail and dew). This project will report on sampling methods, container materials, calibration standards, as well as ion chromatographic and conductimetric detector conditions and characteristics.
Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.



The Limited Life Time Commission on Environmental Analytical Chemistry has an ongoing project on the analysis of wet deposition.

1.2.25 Characterization of the Cr(III)/Cr(VI) ratio in aerosols

Chromium behaves as a redox chameleon. However, the occurrence of highly toxic Cr(VI) species in Cr-containing aerosols is still questioned, not least because of analytical difficulties of measuring very small quantities of Cr(VI) in the presence of relatively large amounts of Cr(III) under controlled redox conditions.

In this project, the analytical route from aerosol sampling to the determination of Cr(VI) species is being evaluated, considering thermodynamic, kinetic and mechanistic aspects with respect to the Cr(III)/Cr(VI) ratio and physico-chemical aspects with respect to the sampled particles at every stage of the analysis.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.2.26 Application of adsorptive cathodic stripping voltammetry to the measurement of trace elements in natural waters including sea water

Until a few years ago, anodic stripping voltammetry was the only voltammetric technique of practical use to the determination of trace elements in natural waters, and then only for Cu, Pb, Cd and sometimes Zn.

Recent developments have made a new voltammetric technique, adsorptive cathodic stripping voltammetry applicable to the determination of a growing number (presently 15) of elements, including Cu, Fe, V, U, Cr, Ni, Co, As and Pt. This technique uses the adsorption of complexes of the trace elements with certain added complexing ligands on a hanging mercury drop electrode to form a monomolecular layer on the electrode. The reduction current of either the elements or the ligands in the adsorbed layer is then used to quantify the solution concentration.

The technique is not affected by non-specific matrix components (for example, the major ions in sea water) and is therefore applicable to saline waters.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

1.2.27 Aluminium in foods

This project aims to prepare an inventory and evaluate the present status and performance of methodologies for the determination of aluminium in foods.

Depending on the outcome of this study, the collaborative trial of a suitable method of analysis willbe considered. The study will help to clarify the role of aluminium methodologies in the discrepancies found in literature on the aluminium dietary intake and levels in food.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.2.28 Evaluation and development of human reference material for quality assurance and harmonization of trace element determination

The aim of this project is to organize interlaboratory surveys, evaluate methodology and analytical methods to establish human materials as analytical control materials useful in clinical chemistry and toxicology.

Interlaboratory cooperative studies have been conducted on human materials such as lyophilized serum, whole blood and urine developed for these studies. Selenium concentrations in batches of serum and urine have been established as well as some preliminary results for other elements.

Whole blood material is distributed world-wide to expert laboratories for Se, Pb, Cd and Hg deerminations. In addition, the project will focus on the following elements: Al, As, Cr, Mn, Co, Ni, Sb, F, Tl, Bi, V, Be, Sn and other more general clinical trace elements.

Clinical Chemistry Division, Commission on Toxicology: Ongoing Project.

1.2.29 Health significance of metal concentrations in body fluids and tissues

The purpose of the project is to suggest guidelines for interpreting results obtained by analysis of metals in human tissues and body fluids, that is, biological monitoring.

The IUPAC Commission on Toxicology has devised several reference methods and field methods, in particular for monitoring trace metals in body fluids and tissues. Valid results obtained by these methods must be interpreted according to the toxicological data available.

In the past, permissible limits of various kinds have served as a simple guideline for interpretation, although technical and economic considerations have in some cases been taken into consideration. A more detailed evaluation must taken into regard the sampling time, analytical quality, dose-response and dose-effect relationships, existence of risk groups and individual susceptibility.

The project therefore aims at defining, in appropriate detail, relevant reference levels for metals in body tissues and fluids and at proposing appropriate decision rules for abnormal metal concentrations. *Clinical Chemistry Division, Commission on Toxicology: Ongoing Project.*

1.2.30 Standardization of a method for the determination of cadmium in urine

Determination of cadmium in urine is routinely performed by electrothermal atomization atomic absorption spectrometry in occupational and environmental health.

Two previous intercomparison studies have made clear the situation on the accuracy and precision of these methods. The studies revealed that a simple dilution with nitric acid is the favoured method. This project is developing a standardized procedure for this method which should lead to a determination protocol. *Clinical Chemistry Division, Commission on Toxicology: Ongoing Project.*

1.3 Determination of organic substances

1.3.1 Extraction, clean-up and group separation techniques in organochlorine trace analysis

This paper critically reviews and gives recommendations for the isolation/extraction and subsequent clean-up stages of analysis of persistent halogenated hydrocarbons, related pesticides and biocides which occur in the environment at the trace level.

Many analytical schemes currently in use for the determination of these compounds have been developed from specific methods of analysis for individual or related pesticide, herbicide and fungicide residues and are well documented.

Many of these separation and clean-up protocols are well established and have now been applied to many areas of trace organic analysis. This has broadened the scope of this field in terms of the number and type of compounds to be determined, and the range of concentration and limits of detection. These protocols have been incorporated in Master Analytical Schemes for the analysis of priority pollutants.

The development of the Master Analytical Scheme approach has led, in some degree, to compromise the optimum analytical conditions for the determination of the individual compounds. This has produced the 'Black Box' syndrome where compounds having some chemical similarities are treated in a uniform manner. Such multi-residue schemes are understandable on economic grounds, but the chemist should always be aware of the level of compromise. It is essential for any specific determination to optimise the method for the particular analyte, or group of analytes of interest, for example, chlorobiphenyl congeners. *Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis:* Pure & Appl. Chem., *Vol. 60, No. 9, pp. 1437-1448, 1988.*

1.3.2 Recommended method for the gas chromatographic profile analysis of polycyclic aromatic hydrocarbons in smoked food

Results are reported of a collaborative study on the determination of polycyclic aromatic hydrocarbons (PAH) including benz(a)anthracene, chrysene, benzofluoranthenes (b+j+k), benzo(a)pyrene, benzo(e)pyrene, and indeno(1,2,3-cd)pyrene in smoked meat.

After calibration of the instrument with a standard solution, four samples of smoked meat (two of each were identical samples, respectively) were analysed. Variation coefficients for the above PAH were found to be 19.5-57.5% with the exception of indeno-(1,2,3-cd)pyrene for which a coefficient of 105.5-126.9% was found due to an external impurity which interferes with this PAH in gas chromatography. *Applied Chemistry Division, Commission on Food Chemistry:* Pure & Appl. Chem., *Vol. 59, No.12, pp. 1729-1734, 1987.*

1.3.3 Recommended method for a thin layer chromatographic screening method for the determination of benzo(a)pyrene in smoked food

Results are reported of a collaborative study on the determination of benzo(a)pyrene in smoked meat. To this end, four meat samples were analysed.

Polycyclic aromatic hydrocarbons (PAH) are a well known class of environmental carcinogens and in the past benzo(a)pyrene (BaP) often has been used as an indicator for their presence and even as a numerical parameter for the carcinogenic potency of environmental matter, although numerous other PAH also exhibit comparable biological activity in various systems.

This has lead to national regulations in some countries. For instance, in FRG; an upper concentration limit has been set for BaP in smoked meat. Accordingly, a rapid method is required to check smoked food for its benzo(a)pyrene concentration. A method for the determination of BaP, based on thin layer chromatographic comparison of BaP of a meat extract with authentic BaP concentrations, has been optimized and applied in an international exercise by several laboratories.
Applied Chemistry Division, Commission on Food Chemistry: Pure & Appl. Chem., *Vol. 59, No.12, pp. 1735-1738, 1987.*

1.3.4 Improved cost-effective approaches to pesticide residues analysis

Sample collection and preparation stages are time consuming and labour intensive. However, there are few obvious savings to be made in this area. It is necessary to collect an appropriately large sample and to reduce the sample size by well-tested procedures.

The only important savings can be made by extracting a small final sample. Improvements can be made in the clean-up of the extract prior to final determination. This stage can be speeded up by reducing the sample size or by taking an aliquot of the extract through the clean-up procedure. Reduction of scale is possible with conventional equipment but, for true miniaturization, specially designed laboratory equipment is needed.

For many analyses, especially when methods are miniaturized, the use of internal standard (IS) can be valuable. The IS must behave in an identical way and be a compound of very similar chemicl structure to the test compound. The IS should be added at the extraction stage and carried through each stage of the analysis.

The usefulness of IS in pesticide residue analysis has become accepted and their use should be encouraged. Recovery data for the IS and for the compound to be determined, as well as relative response factors, should be published together with the results.

In recent years, a variety of laboratory procedures have been automated. Fully automated GLC and HPLC procedures are available for the determination of pesticide residues at the subnanogram level. The latest developments in automation and miniaturization of the extraction and the clean-up have shown that this difficult and costly part of the analysis can be automated and hopefully integrated with the well-developed step of determination by gas and liquid chromatography.

For many years now, a number of IUPAC projects have been concerned with the analysis of pesticide residues.

A more radical alternative to improving residue anlysis is by adopting immunochemical techniques. Immunochemical techniques especially the ELISA method offers great potential and exploration of this area by residue chemists should be encouraged.
Applied Chemistry Division, Commission on Pesticide Chemistry: Pure & Appl. Chem., *Vol. 56, No. 8, pp. 1131-1152, 1984.*

1.3.5 Application of multiresidue procedures in pesticides residues analysis

The fields of application of multiresidue procedures and the proper selection of compounds and samples to be analysed are discussed. The various processes of well established multiresidue procedures are reviewed and critically assessed in order to give guidance for the analysis of compounds being not included in current methods and to help laboratories to improve their own methodology.
Applied Chemistry Division, Commission on Pesticide Chemistry: Pure & Appl. Chem., *Vol. 58, No. 7, pp. 1035-1062, 1986.*

1.3.6 Mass spectrometric determination of pesticide residues

This is No.25 in the series IUPAC Reports on Pesticides.

A review is made of current approaches to mass spectrometry (MS) of pesticides, pesticide metabolites and related compounds such as PCBs and polychlorinated dibenzo-dioxins. Basic relationships between instrument sensitivity and detection limits in various operating modes are outlined.

Recent developments in instrumentation are introduced such as 'bench top' GC-MS, LC-MS, MS-MS and surface ionization techniques. Objective criteria are developed for interpretation of MS data for identification and quantitation of residues. The advantages of isotopically labelled internal standards to ultra trace analysis are highlighted. The recent literature on applications of MS to various pesticide classes are summarized.

The conclusions are that requirements for detailed residue data on crop protection and environmentally significant chemicals will increasingly rely on MS techniques as detection limits are lowered and the number of chemicals grows. MS applications are increasingly becoming polarized between routine confirmation of identity and sophisticated structural elucidation or ultra trace analysis.
Applied Chemistry Division, Commission on Agrochemicals, Pure & Appl. Chem., *Vol. 62, No. 2, pp. 317-336, 1990.*

1.3.7 Analytical methods for halogenated phenols

With the exception of a few compounds, most halogenated phenols are of anthropogenic origin. They have been used extensively as biocides in many applications including agricultural treatments, timber preservation and additives in drilling muds. In addition, phenoxyacids have been used extensively as herbicides and a complex series of chlorinated phenolics are formed and discharged from pulp and paper processing plants.

There are many sources and indiscriminate discharges of these materials to a wide number of environmental compartments have been identified as hazardous contaminants.

Although some analytical protocols for a few phenolics do exist, it is timely to critically review these older and the newer methods available for the isolation, separation and determination of this class of compounds, their metabolites and breakdown products and to make recommendations on the current and most reliable analytical schemes.
Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.3.8 Extraction and preconcentration of some environmental trace pollutants by supercritical fluid extraction

The objective of this project is to review the field of supercritical fluid extraction - also known as dense gas extraction. The focus is on analytical applications, particularly on extraction and preconcentration in trace organic analysis.
Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.3.9 Analytical techniques for trace organic compounds VI. Application of LC/MS to trace organic analysis to polar and thermally labile compounds

This project is a continuation of the series on analytical techniques for trace analysis which will be an expansion of the brief treatment of LC/MS which was presented in paper I of the series. The objective of the project is to provide some basic information on and critical evaluation of LC/MS techniques such as thermospray and particle beam interfacing. The report will provide some advice to the analyst and guidelines for the application of LC/MS techniques to organic trace analysis in areas including environmental and biomedical analyses.

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis: Ongoing Project.

1.3.10 Ethyl carbamate in foods and alcoholic beverages

Recently, high levels of ethyl carbamate, a potential human carcinogen, have been found in certain alcoholic beverages. This has spurred considerable scientific international activity in this area. A compilation of achievements was thought to be appropriate.

The project offers the possibility of achieving significantly lower ethyl carbamate levels in food, thus lowering human exposure to this potentially hazardous compound.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

A survey of laboratories developing methods for animal drug residues in food is one of the ongoing projects of the Commission on Food Chemistry.

1.3.11 Chromatographic separation of chlorinated dibenzo-p-dioxin and -furan isomers

Chromatographic behaviour of all 136 PCDDs and PCDFs containing 4 to 8 chlorines now has been studied on 10 capillary columns with different stationary phases. Phases included were of low, medium and high polarity, polar cyanopropyl phases and a liquid crystalline phase (smectic column). All data generated are now being prepared for publication.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.12 Evaluation of PCB quantitation in food and other biological samples

Part of this project is a check sample program which has been completed. Participants from 18 laboratories analysed 4 ampouled solutions: one PCB's test solution, two solutions of Aroclors 1242 and 1254 and one human milk extract.

No correlations were observed between results and a number of capillary gas chromatography parameters. Most 'outliers' were found in laboratories using 15 m columns. the experimental is completed: results are now being prepared for publication.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.13 Survey of laboratories developing methods for animal drug residues in food

Numerous laboratories throughout the world are involved in the development of methods for animal drugs. Those laboratories involved in method development will be polled to determine the veterinary drug residue projects that they are currently working on and their future interest.

Each laboratory will be asked to describe their rationale for their projects and their approach to solving a particular veterinary drug residue problem. This information will be compiled and distributed to the participating laboratories to involve them in IUPAC activities as far as possible.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.14 Reliability study of immunoassay based methods for detecting drug residues in food

Numerous immunoassay based tests have been developed and made commercially available for measuring drug residues in animal derived food. These tests have several characteristics that make them potentially very useful in a regulatory program:

1. They are inexpensive.
2. They are rapid.
3. They are simple enough for field use.

However, there is insufficient experience with these tests to base a regulatory action without additional chemical analysis of the samples that test positive. There is a need to study the reliability of these tests in several laboratories using unknown samples.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.15 Reliability study of immunoassay based methods for detecting residues in food

A report discussing the potential use of biochemical assays for residue analyses has been completed. Key issues addressed include validation of these types of methods, quality specifications of reagents, assay sensitivity, matrix effects, and components of validation studies. The goal is the preparation of immunoassay guidelines.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.16 Non-volatile N-nitrosamines in foods

Phase I of this project involved the preparation of an inventory and the critical evaluation of current methodologies. Phase II was concerned with the occurrence of these compounds in foods and involved a collaborative study of a selected method.

Phase I, a review of methodologies, was published in 1987. One of the conclusions was that existing methods need further improvement and simplification. At the moment no method is available which is suitable for collaborative testing. Therefore, first a review on the occurrence of non-volatile nitrosamines will be carried out and then a collaborative trial will be reconsidered.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.17 Collaborative study of three methods of analysis for the determination of N-nitrosoproline, N-nitrosothioproline and N-nitrososarcosine in urine

The three most frequently used methods of analysis for nitrosamino acids will be studied in a collaborative trial. The main objective of the project is to establish the analytical performance of the determination of N-nitrosoproline, N-nitrosothioproline and N-nitroso-sarcosine in urine.

Most hopefully, the data collected also will provide a basis to select a reference method for these compounds.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.18 Determination of the water soluble fraction of the total N-nitroso compounds

This project is concerned with method development and validation of the determination of the water soluble fraction of the total N-nitroso compounds. However, experimental progress was considerably delayed due to a number of technical difficulties in the method development.

A new method for total N-nitroso compounds has recently been presented and a pilot interlaboratory study is to be organized and, based on the outcome, a collaborative study will be considered.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.19 Collaborative study of a solvent efficient thin layer chromatographic (TLC) method for aflatoxins in corn and peanut products

The aim of this project is to carry out a collaborative study to evaluate the performance characteristics of the solvent efficient TLC method for the determination of aflatoxin B_1, B_2, G_1 and G_2 in corn, and raw and roasted peanuts.

The validated method will be used in aflatoxin monitoring and quality control programs in industrial and regulatory operations.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.20 Collaborative study of an enzyme linked immunosorbent screening assay for aflatoxin B1 in corn, peanut and cottonseed products and mixed feed

The objective of this project is to carry out a collaborative study to evaluate the performance characteristics of an enzyme linked immunosorbent screening assay for the determination of aflatoxin B1 in corn, raw and roasted peanuts, whole cottonseed, cottonseed meal, ammoniated cottonseed meal and mixed feed.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.21 Check sample program for polychlorinated dibenzo-dioxins (PCDDs) and -furans (PCDFs) in foods

A recent study demonstrated that all 136 PCDDs and PCDFs with 4 upto 8 chlorines can be separated by capillary gas chromatography on two or at most three appropriate stationary phases. A check sample program, using standard solutions and food sample extracts is being carried out to demonstrate that these separations and identifications can be repeated in other laboratories. The quality of the PCDD and PCDF standards and the semi-quantitative aspects of the determination of these compounds are also being assessed.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.22 Check sample survey on N-nitroso compounds - 1989

This project consists of the preparation of an inventory of the state of the art of the determination of some N-nitroso compounds in various foods. The project includes the determination of N-nitroso dimethylamine (NDMA), N-nitrosopyrrolidine (NPY) and particularly N-Nitrosoproline (NPRO) in beer and malt samples; each laboratory is applying its own method of analysis. The results of this cooperative study should enable laboratories to improve their method performance and reliability and eventually stimulate them to develop quality assurance programmes.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.3.23 Evaluation of a rapid method for the determination of benzo(a)pyrene in oils and fats

A ring test for the rapid determination of benzo(a)pyrene in oils and fats has been carried out in the company of the coordinator and found satisfactory. This project will enable oils and fats producing companies to check that the level of one of the most carcinogenic polycyclic hydrocarbons is below a harmful level.

Applied Chemistry Division, Commission on Oils, Fats and Derivatives: Ongoing Project.

1.3.24 Contamination of edible oils shipped in bulk

This project has been initiated by the Commission on Oils, Fats and Derivatives at the request of the International Federation of Oilseeds and Fats Association. The project is investigating the contamination of edible oils shipped in bulk by chemical substances remaining in tanks from previous cargoes.

Applied Chemistry Division, Commission on Oils, Fats and Derivatives: Ongoing Project.

1.3.25 Determination of residual hydrocarbons in edible oils

A report by the International Olive Oil Council has indicated that the determination of residual hydrocarbons in edible oils warrants further study. Contamination of olive oil, and solvents derived from ink on packaging materials, are serious problems.

Applied Chemistry Division, Commission on Oils, Fats and Derivatives: Ongoing Project.

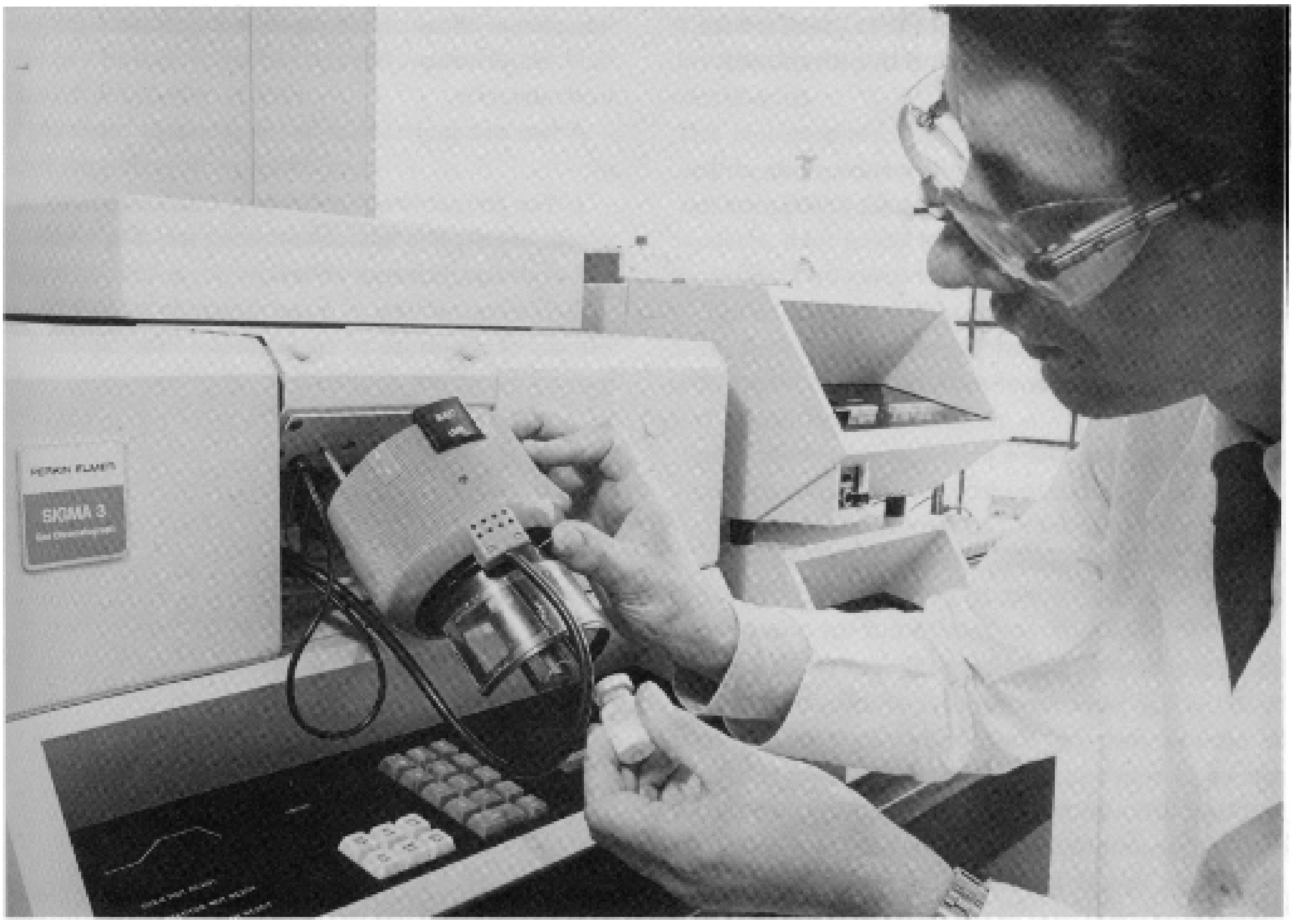
1.3.26 Pesticide residues problems involving common moieties

The project will identify the problems that arise for the residues analyst and the regulatory authorities when groups of related pesticides may be analysed by the determination of a common moiety. The report will give relevant examples and recommend an approach to the problems that occur.

Applied Chemistry Division, Commission on Pesticide Chemistry: Ongoing Project.

Toxicology of synthetic and natural compounds

See Chapter 4 for summaries of IUPAC projects on this topic.



IUPAC, through its Commission on Oils, Fats and Derivatives, is investigating the contamination of edible oils.

1.4 Determination of natural toxins

1.4.1 Check sample survey for mycotoxins

The aim of this project is to allow laboratories around the world engaged in mycotoxin analysis of various foodstuffs to compare their results with those of other laboratories and to improve and adapt their methodology if required or appropriate.

This project should lead to improvement of analytical quality control of products potentially contaminated by mycotoxins.

In 1987, 203 laboratories from 50 countries participated in the check sample program for aflatoxins B_1, B_2, G_1 and G_2 and 125 laboratories from 38 countries in the aflatoxin M_1 in milk program.

About one third of the laboratories used high performance liquid chromatography (HPLC) methods for aflatoxin analyses, 5% immunoassay methods and the large majority thin layer chromatography (TLC) methods. A report describing and evaluating the results is in preparation.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.2 Collaborative study of a TLC and HPLC method for ochratoxin A in barley, corn and tissue

Difficulties with ochratoxin A stability in samples have been overcome. Meanwhile, the revised method has been finalized and is being prepared in a suitable format for collaborative testing. The collaborative method was presented at the 8th IUPAC International Symposium on Mycotoxins and Phycotoxins held in Tokyo, Japan, 16-19 August, 1988.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.3 Collaborative study of a HPLC method for the determination of aflatoxins in groundnuts and cereal grains

The experimental part of this project has been completed. The report of the collaborative study of the HPLC method for aflatoxins B_1, B_2, G_1 and G_2 has been finalized and is under review.
Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.4 Spectro-analytical parameters of fusarium toxins

Nineteen toxins have been identified to be studied. So far, spectro-analytical data have been obtained on nine. Supplies of seven toxins have to be located.
Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.5 Natural toxicants in foods

Phase I of this project concerns current knowledge and the status of analytical methodology. Preparation of a monograph is in progress: three chapters have been completed and another four are nearing completion.
Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.6 Limits and regulations for mycotoxins in food and feeds

A report outlining the actions and rationale of the US authorities for regulating aflatoxin decontamination has been prepared for publication. Another report on limits and regulations will be expanded to include data on how tolerances were established by various countries.
Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.7 Aquatic biotoxin analyses

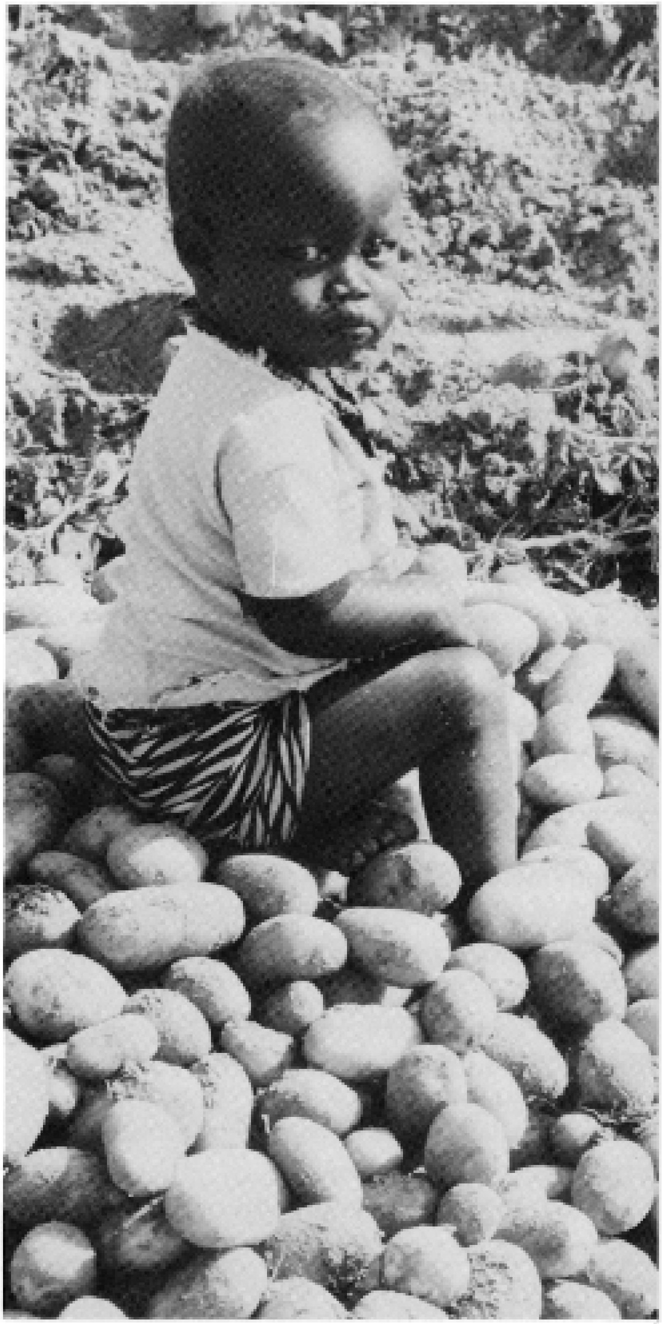
Episodes of aquatic biotoxin contamination of marine foods have been noted more and more frequently all over the world during the last decade. Consequently, occurrence of PSP (paralytic shellfish poisons) and DSP (diarrheic shellfish poisons) has been reported from many new areas and countries. This often was associated with outbreaks of human diseases and had adverse economic effects on seafood industry.

Health authorities are therefore trying to develop surveillance programs in order to control the problem. So far, this has been hampered because of lack of information on which laboratories are active in this field and the state of the art of their analytical methodologies.

A two step project therefore is proposed consisting of:

1. The preparation of a directory of laboratories conducting aquatic biotoxin analyses which specifies and evaluates their procedures.

2. The organization of a check sample study using extracts of contaminated shellfish as a first step in



The project on 'Solanine and chaconine in potatoes' will provide a reliable method for the judgement and assessment of new potato cultivars.

mapping analytical performance on a world-wide basis.
Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.8 Agaritine in mushrooms

The objective of this project is to establish an internationally recognized method of analysis for the natural constituent 'agaritine' in the common mushroom Agaricus bisporus.

Agaritine has been suspected of causing cancer in laboratory animals being fed raw mushrooms over a prolonged period. The project offers the possibility of monitoring mushrooms with respect to their agaritine content and selecting as food those varieties with the lowest concentration.
Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.9 Solanine and chaconine in potatoes

The aim of this project is to establish an internationally accepted method of analysis for the glycoalkaloids solanine and chaconine in potato tubers.

The project will provide a reliable tool for the judgement and assessment of new potato (and tomato) cultivars.
Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

1.4.10 Survey of data on the incidence and levels of ochratoxin A in food and animal feed world-wide

This project aims to gather information on the occurrence (incidence and levels) of ochratoxin A in various types of food and animal feed (grains, dairy products, meat products), and other biological materials.

The information will be used along with new toxicological information to assess the human health safety concerns resulting from contamination of food and animal feed by ochratoxin A.
Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

Collection, processing and storage of specimens for the biological monitoring of occupational exposure to toxic chemicals

See Chapter 4 Page 41 for summaries of IUPAC projects on this topic.

Isotope specific measurements as references for toxic/essential element assay

See Chapter 4 Page 41 for summaries of IUPAC projects on this topic.

2 Measurement of physico-chemical parameters related to the environment

2.1 Solubility data series - Hydrocarbons with water and seawater, Part I: Hydrocarbons C5 to C7; Part II: Hydrocarbons C8 to C36.

These are volumes 37 and 38 respectively of the IUPAC *Solubility Data Series.* They present compilations of all published solubility data for binary systems involving the title compounds as one component, and water, heavy water or seawater as the other.

Comparison and critical evaluation of the data result in recommended values; for each critical evaluation of a particular system, the closing date for literature searching is given, so users are assured that virtually all relevant published data have been assessed.

Special difficulties can arise as a result of the variable composition of seawater and through colloidal effects, but care has been taken to make the user aware of this. The volumes are comprehensively indexed.

Edited by D. G. Shaw. Published by Pergamon Press, Oxford, UK, 1989. Volume 37: 548 pages; 30 illustrations; 400 lit. refs. ISBN 0 08 029215 1. Volume 38: 582 pages; 25 illustrations; 320 lit. refs. ISBN 0 08 030737 X. Price per volume: USD 85.00.

2.2 Solubility of hydrogen sulfide and hydrogen selenide in aqueous and non-aqueous systems

Volume 32 of the *Solubility Data Series* Contains data published prior to January 1987 on the solubility of hydrogen sulfide, deuterium sulfide and hydrogen selenide in pure water, in aqueous solutions containing other components and in organic solvents.

Published solubilities of these gases have been tabulated and evaluated and the recommended data are indicated. Where appropriate recommended expressions giving mole fraction solubities at a partial pressure of 1.013 bar as a function of temperature are given.

The bulk of the volume is devoted to hydrogen sulfide because very little data for deuterium sulfide and for hydrogen selenide have been published. Many of the solvents for which data are given are used to remove hydrogen sulfide in industrial desulfurization processes. Dissolution of hydrogen sulfide in some solvents has been studied under elevated pressure and all the available high pressure solubility data are tabulated.

The book has special relevance to the control of pollution.

Edited by P. G. T. Fogg and C. L. Young and published by Pergamon Press, Oxford, UK, 1989. xvi + 352 pages; ISBN 0 08 0324819. Price USD 85.00.

2.3 Carbon monoxide

Carbon monoxide, which is Volume 43 of the *Solubility Data Series*, contains tabulated collections and critical evaluations of orginal data for the solubility of carbon monoxide in a variety of liquid solvents. Most of these solubilities were measured at temperatures around ambient, and for partial pressures of carbon monoxide around 101.3 kPa. Some data, however, are for temperatures as low as 93 K and as high as 573 K, and for pressures up to 101 MPa.

Within the volume, material is arranged according to solvent class, with solubility data for low pressures and high pressures collected together. The solvents include water, aqueous an non-aqueous salt solutions, a variety of hydrocarbons, a variety of oxygen containing, halogen containing, sulphur containing, and nitrogen containing organic compounds, and also some biological fluids with which carbon monoxide has an important interaction.

The data were gathered from a search of the world's chemical literature through to the end of 1988, and make up a unique and valuable historical survey of the solubility of carbon monoxide. Their publication is timely in view of current concern about carbon monoxide as an atmospheric pollutant, and in view of the role which carbon monoxide as an atmospheric pollutant, and in view of the role which carbon monoxide is likely to play in the future, as chemical feedstocks may have to change in response to supply and demand patterns, and as alternative energy sources are developed, especially coal gasification technology. For all these applications, and for numerous others, this volume of well documented and critically evaluated gas solubility data will be of tremendous benefit.

Edited by R. W. Cargill and published by Pergamon Press, Oxford, UK, 1990. xxi + 330 pp. ISBN 0 08 0307337 (H). Price USD 85.00.

2.4 Recommendations for the determination of pH in low ionic strength fresh waters

This project reviews the problems of measuring the operational pH in low ionic strength media such as fresh waters and recommends a method by which reproducible values can be obtained.

Analytical Chemistry Division, Commission on Electroanalytical Chemistry: Pure & Appl. Chem., *Vol. 57, No. 6, pp. 877-886, 1985.*

2.5 Recommendations for the determination of pH in sea water and estuarine waters

This project reviews problems of the measurement of the operational pH in sea water and variable ionic strength media estuarine waters and recommends methods by which reproducible values can be obtained.

Analytical Chemistry Division, Commission on Electroanalytical Chemistry: Pure & Appl. Chem., *Vol. 60, No. 6, pp. 865-870, 1988.*

2.6 Determination of pH in highly saline waters

The problem of the measurement of the operational pH in natural and artificial highly saline waters (salinity greater than in ocean water) is discussed, and

The Commission on Electroanalytical Chemistry has published recommendations for the determination of pH in sea water and estuarine waters.

tentative recommendations by which reproducible and meaningful results can be obtained are presented.
Analytical Chemistry Division, Subcommittee on Environmental Analytical Chemistry: Pure & Appl. Chem., *Vol. 61, No. 6, pp. 1133-1138, 1989.*

2.7 Inventory of current tropospheric sampling programmes

The problems of network design and operation are such that harmonization and standardization of networks is called for. The value of the results obtained by networks is dependent on the quality control measures. At present comparison of results obtained by different networks is hampered by a lack of consistent quality control measures.

The design of many networks is not optimized in line with their objectives.

Sampling procedures are the most important source of errors. The available analytical methods for mesurement of SO_2, NO_x, O_3, CO, CO_2, in air and of so-called bulk elements in precipation are generally adequate for monitoring purposes. For other components the situation is less satisfactory.
Applied Chemistry Division, Commission on Atmospheric Chemistry: Pure & Appl. Chem., *Vol. 62, No. 1, pp. 163-176, 1990.*

2.8 Evaluation of facilities for the determination of very low levels of radioactivity

Evaluation of underground facilities for the determination of very low level radiation (neutron, muon, proton decay) or very low radioactivity (neutrino induced radioactivity in Cl-37, Ga-71 and so on; double decay nuclides such as Ge-76; cosmogenic nuclides; environmental radioactivity) are made.

Sixteen facilities in the world are listed. Background problems are discussed with respect to the decrease of radon levels in a Japanese facility. Other practical applications of these facilities are also considered.
Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

2.9 Critical evaluation of techniques and methodologies for studying metal equilibria in seawater

This project involves a critical assessment of the wide variety of techniques which are currently used or are of potential use, in examining metal equilibria in seawater.

In addition to a general assessment of techniques and methodologies, the comparative utiity of techniques which can be used in seawater investigations are being examined on a metal-by-metal basis. For those techniques judged to be of primary importance in seawater investigations, proper experimental protocols will be evaluated and described in detail.
Analytical Chemistry Division, Commission on Equilibrium Data: Ongoing Project.

2.10 Equilibrium constants for solid-liquid adsorption equilibria

The concept of adsorption of cationic trace elements by solid hydrous oxides can be applied to natural solids. The adsorption process can thus be understood in terms of classical complexation leading to the formation of surface (heterogeneous) ligand complexes, with competition between cations (including H+) for surface sites. This can lead to adsorption constants and extension to speciation calculations of the aqueous phase at the solid-liquid interface.

This concept will be applied to freshwater, estuarine and marine environments.
Analytical Chemistry Division, Commission on Equilibrium Data: Ongoing Project.

2.11 Recommendations for the determination of the pH of acid rain

Acid rain is a very important environmental problem. Solutions can be found only by comparing the data obtained over very large geographic regions since emission and precipitation locations may be widely separated from each other.

There is therefore an urgent need to get comparable data, irrespective of the institution or country in which they are obtained. Hence it will be useful to recommend generally acceptable procedures in this field. This project aims to recommend appropriate electroanalytical methods for the determination of pH

using a glass electrode in natural precipitation, that is, acid rain and snow.
Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

2.12 Surface characterization of airborne particulate matter

This project involves a compilation of methods and results of surface characterization of airborne particulate matter with the following topics:

- Characterization of deposited particulate matter by: Leaching techniques; SIMS; LAMMA (thermodesorption mode); ESCA; Auger spectroscopy; Solid state NMR.
- 'In situ' aerosol characterization by: gas/particle interaction kinetics; aerosol photoemission; laser-induced aerosol fluorescence; photoacoustic spectroscopy; epiphaniometer; condensation properties; optothermal interaction.

Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

2.13 Acid-base equilibria on particles and gases in the atmosphere

The aim of this project is to describe the state of knowledge of the formation, neutralization and gas-particle acid-base equilibria which are believed to determine the amounts of acids and bases which are available for removal from the atmosphere by dry and wet deposition processes.
Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

2.14 Dynamic aspects of metal speciation in aquatic colloidal systems

To a considerable extent, the properties of metal ions in aquatic systems are determined by their interaction with dispersed particles. Little attention has been given so far to the dynamic aspects of the ion-particle interaction. More often than not, slow ion adsorption/desorption processes are known to occur and to affect the analytical and physical chemistry of the natural system.

The purpose of this project is to (i) survey the existing literature data on relevant ion adsorption/desorption rates; (ii) outline the impact of dynamic factors on various analysis procedures; (iii) indicate the implications of dynamic factors for the properties of natural aquatic colloidal systems.
Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

2.15 Characterization of particle surface charge

This project will result in a critical review of experimental methods used currently to determine the charge on the surfaces of heterogeneous particles in soils and sediments. Methods for 'reference' particles as well as natural particles will be reviewed and compared. This will include effects of aqueous solution composition on particle charge.
Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

2.16 *In situ* determination of sorption in natural waters

Sorption processes are thought to play a prominent role in the biogeochemistry of trace elements in aquatic systems. Laboratory studies have determined the adsorption characteristics of many well defined solids. Some of these solid phases (for example, iron and manganese oxyhydroxides; humic material; algae) are constituents of the natural suspended or bottom sediments.

Research on the sorption of trace elements on natural particles is an increasingly important field. The commission will review methods used to investigate sorption of trace elements on natural particles present in rivers, lakes and oceans, and the information gained.
Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

2.17 Ion binding in heterogeneous particles

Ion adsorption on natural particles is an important phenomenon in environmental sciences. Natural particles are, in general, chemically heterogeneous and characterized by a variable charge or potential. Both these aspects are of prime importance for the description of ion adsorption. The role of these aspects for the adsorption behaviour will be reviewed and discussed.

For the description of the adsorption in practice, the heterogeneity of the sorbent should be known. In the 'simple' and often used heterogeneity analysis, electrostatic effects show up as an apparent heterogeneity on top of the intrinsic heterogeneity.

In principle however, elimination of the electrostatic contribution to the adsorption free energy is possible, so that with the heterogeneity analysis the more informative intrinsic affinity distribution can be obtained. The possibilities of the elimination of the electrostatic effects will be discussed and a critical review will be given of the assessment of the (intrinsic) heterogeneity. With respect to the heterogeneity analysis, specific attention will be paid to the effect of experimental error and the fact that often only a data set is available over a limited range (window) of ion concentrations.
Analytical Chemistry Division, Limited Life Time Commission on Environmental Analytical Chemistry: Ongoing Project.

2.18 Glossary of terms in atmospheric chemistry

About 600 terms in common use by atmospheric scientists are detailed in this document. The unambiguous definition of terms and units employed by the international research community in atmospheric chemistry is essential to the achievement of reliable communications between all parties.

The diversified nature of the scientists involved in research in atmospheric chemistry (chemists, engineers, meteorologists, physicists, biologists etc) points to the very special need for harmonization of terms employed by each specialization.
Applied Chemistry Division, Commission on Atmopsheric Chemistry: Ongoing Project.

2.19 Compendium of agencies, institutes and ongoing activities in the field of atmospheric chemistry

An internal survey by the IUPAC Commission on Atmospheric Chemistry has indicated that it is very difficult, especially for developing countries, to locate specific information regarding agencies, institutes or recent developments in atmospheric chemistry. This compendium will contain this information.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

The Commission on Atmospheric Chemistry has a project concerned with the distribution of information on atmospheric chemistry to chemists, other scientists and research organizations throughout the world.

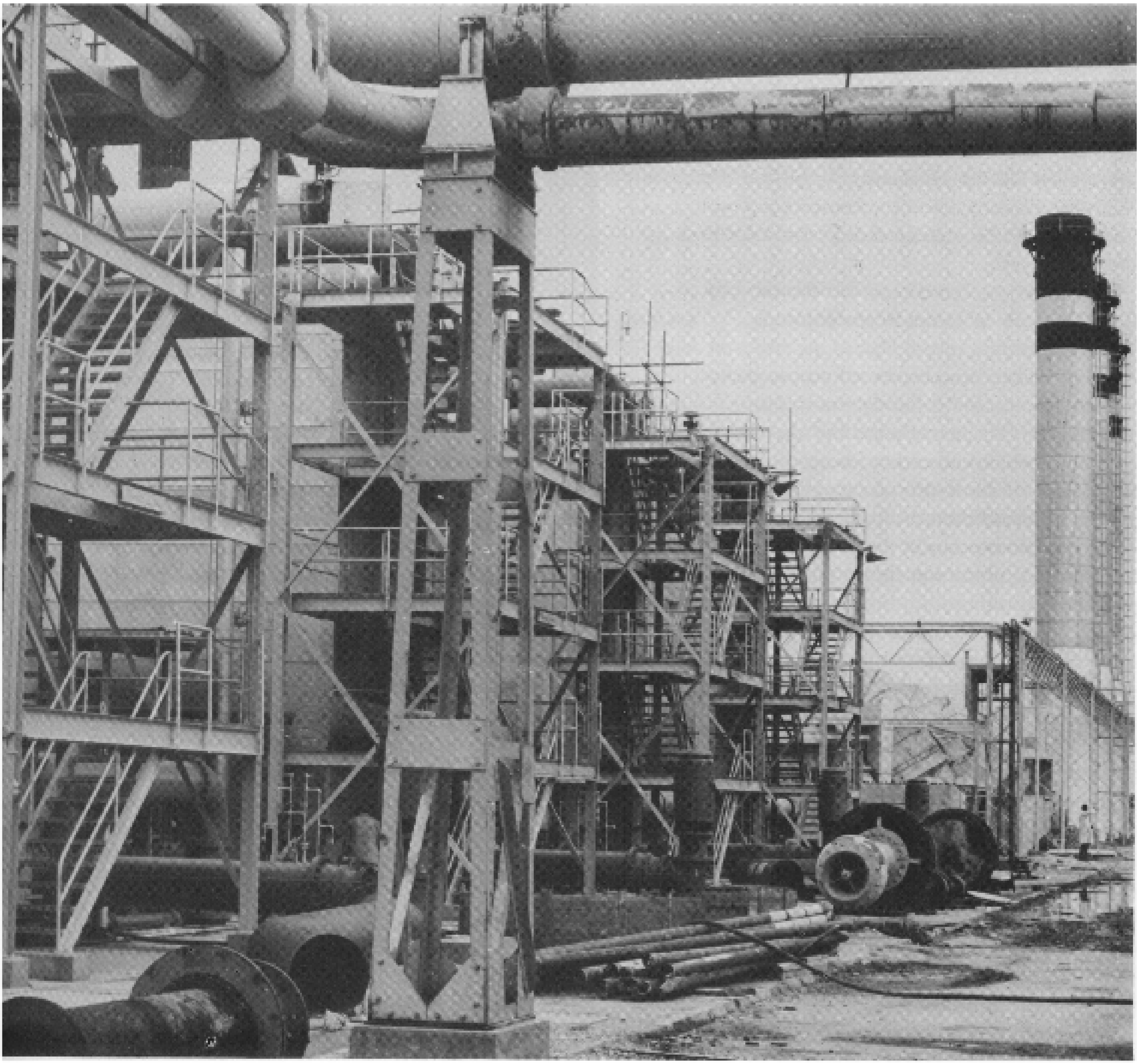
2.20 Major concerns and research needs for our understanding of the chemistry of the atmosphere

Through the input from recognized leaders in atmospheric chemistry from throughout the world, a working party of the IUPAC Commission on Atmospheric Chemistry will identify the perceived major concerns and research needs for an improved understanding of the chemistry of the atmosphere.

This important information will be organized and summarized for wide distribution among chemists and other scientists and research organizations throughout the world. The purpose of this project is to stimulate research efforts which focus on the solutions to identified major problems.
Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

2.21 Determination of chemical substances in air, water, soil, living organisms and food

See Chapter 1 for summaries of IUPAC projects on this topic.



3 Transfer and transformation of chemical substances in the environment

3.1 Pesticide metabolism: Extrapolation from animals to man

One of the most difficult areas of toxicology is the extrapolation of results obtained with experimental animals to man. The common occurrence of species differences in a number of biological processes confounds this extrapolation.

The metabolism of pesticides, drugs and other foreign compounds is a very important determinant of their toxicological effects. An understanding of species differences in metabolism and the ability to predict or to study directly the metabolic fate of a pesticide in man therefore are of great value in the validation of animal models for man.

This review is concerned with the factors affecting species differences in the metabolism of foreign compounds in experimental animals and man. Additionally, specific examples of the metabolism of pesticides, drugs and industrial chemicals in man are assessed and the approaches to the execution of metabolism studies in humans proposed.

Edited by J. Miyamoto, H. Kaneo, D. H. Hutson, H. O. Esser, S. Gorbach and E. Dorn. Published by Blackwell Scientific Publications, Oxford, UK, 1988. 128 pages; 63 illustrations. ISBN 0 632 02256 6. Price GBP 12.50/USD 22.50. Affiliate Members Discount Price: GBP 9.50/USD 16.50.

3.2 Pesticide science and biotechnology

This report on the 6th International Congress of Pesticide Chemistry held in August 1986, in Ottawa, Canada, under the auspices of IUPAC, constitutes a comprehensive review of the current understanding of this topical subject.

The major theme of the conference was the use of biotechnology to provide new approaches to pest control These published proceedings contain papers on subjects such as synthesis, mode of action, analysis of residue and environmental factors.

The book is an essential reference work for researchers and chemists in the agrochemical industry, pesticide science, weed research and biotechnology.

Edited by R. Greenhalgh and T. R. Roberts. Published by Blackwell Scientific Publications, Oxford, UK, 1987. 618 pages; 272 illustrations. ISBN 0 632 01618 3. Price GBP 79.90/USD 100.00. Affiliate Members Discount Price: GBP 59.90/USD 75.00.

3.3 Microbial adaptation to pesticides

Edaphic and genetic processes influence the rate of microbial adaptation to pesticides and subsequent metabolism of these pesticides in soils. Availability of the degradable molecule to soil microorganisms is determined by a number of competing sorption reactions with soil colloids.

Kinetic studies on readily biodegradable herbicides exhibit an initial lag phase followed by a rapid decline in concentration. A number of genetic alterations can occur in bacteria responsible for degradative enzyme synthesis during the lag phase. In addition to specific internal DNA sequence changes and recombinations, external DNA additions can occur via plasmids between various soil bacteria.

Degradative plasmids for the herbicides 2,4-D and dalapon have been isolated and characterized. There are interesting parallels between the development of antibiotic resistance in the clinical environment and enhanced pesticide metabolism in problem soils.

Applied Chemistry Division, Commission on Pesticide Chemistry: Pure & Appl. Chem., *Vol. 57, No. 2, pp. 389-403, 1985.*

3.4 Critical evaluation of model ecosystems

This report critically evaluates terrestrial, aquatic and mixed laboratory and outdoor model ecosystems with respect to their use and limitations in studying the fate of pesticides in the environment.

Despite the difficulties of comparing the environmental relevance of the different models in use, an attempt has been made to appraise the reported systems in sequence from the point of view of effort involved and their prediction potential.

The review concentrates on describing the concepts of the models, typical results which have been obtained and emphasises reliability and prediction potential.

Applied Chemistry Division, Commission on Pesticide Chemistry: Pure & Appl. Chem., *Vol. 57, No. 10, pp. 1523-1536, 1985.*

3.5 Potential contamination of ground water by pesticides

The objectives of this review are to summarize existing information on the occurrence of pesticides in groundwater and processes resulting in their detection; to identify existing technologies, and to describe missing information needed to make assessments and predictions.

Validated data on the occurrence of pesticides in groundwater are still limited. Pesticides can reach groundwater following normal agricultural usage and improper disposal and handling. Three frequently detected pesticides, aldicarb, atrazine and DBCP, are considered in detail, while other reported occurrences are summarized.

Transformation processes include microbial metabolism and chemical reactions. While these processes are well researched for the root zone, less data are available on the subsoil and saturated zone. Other factors influencing the rate and amount of pesticide infiltration include the soil-subsoil-groundwater structure, depth of groundwater, macropore flow, and rainfall or water management practices.

An attempt is made to quantify the pesticide properties and field conditions to predict their potential for leaching. Experimental and mathematical models are described and the importance of well designed field studies is emphasized.

Applied Chemistry Division, Commission on Pesticide Chemistry: Pure & Appl. Chem., *Vol. 59, No. 10, pp. 1419-1446, 1987.*

3.6 Recommended approach to the evaluation of the environmental behaviour of pesticides

Concepts and experimental approaches are proposed which lead to a rational testing of the fate of pesticides in soil, water, air, plants and animals.

The stepwise test programme presented is flexible, cost effective and ensures that all aspects of a pesticide's environmental fate are studied in sufficient detail. It also indicates, at different stages of testing, the results which are of relevance to the estimation of exposure to this pesticide, an essential element of the hazard assessment process concerning producers, applicators, consumers and the environment.

Applied Chemistry Division, Commission on Agrochemicals: Pure & Appl. Chem., *Vol. 60, No. 6, pp. 901-932, 1988.*

3.7 The role and limitations of microorganisms in the conversion of xenobiotics

This is No.27 in the series IUPAC Reports on Pesticides.

The role of microorganisms in the detoxification of pesticides is described. Basic processes of microbial conversion of pesticides are considered with characterization of the enzymes that bring about these bioconversions. Special attention is paid to the processes of microbial transformations of pesticides that lead to more recalcitrant and toxic intermediates compared to their parent compounds.

Microorganisms prove to be responsible for both enhanced degradation of pesticides and formation of soil-bound pesticide residues and, conversely, their release. a few examples of such transformations are considered and causes underlying them are discussed. A separate section is devoted to the use of biotechnology in agriculture and to prospects of practical application of microorganisms for degradation of pesticides.

Applied Chemistry Division, Commission on Agrochemicals, Pure & Appl. Chem., *Vol. 62, No. 2, pp. 351-364, 1990.*

3.8 Atmospheric chemistry: kinetic and photochemical data

This 216 page report of work carried out under the auspices of the IUPAC Subcommittee on Gas Phase Kinetic Data Evaluation for Atmospheric Chemistry updates and extends previous critical evaluations of the kinetics and photochemistry of gas phase chemical reactions of neutral species involved in atmospheric chemistry.

Data sheets were prepared for 360 thermal and photochemical reactions, containing summaries of the available experimental data with notes giving details of the experimental procedures. For each reaction, a preferred value of the rate coefficient at 298 K is given together with a temperature dependence where possible.

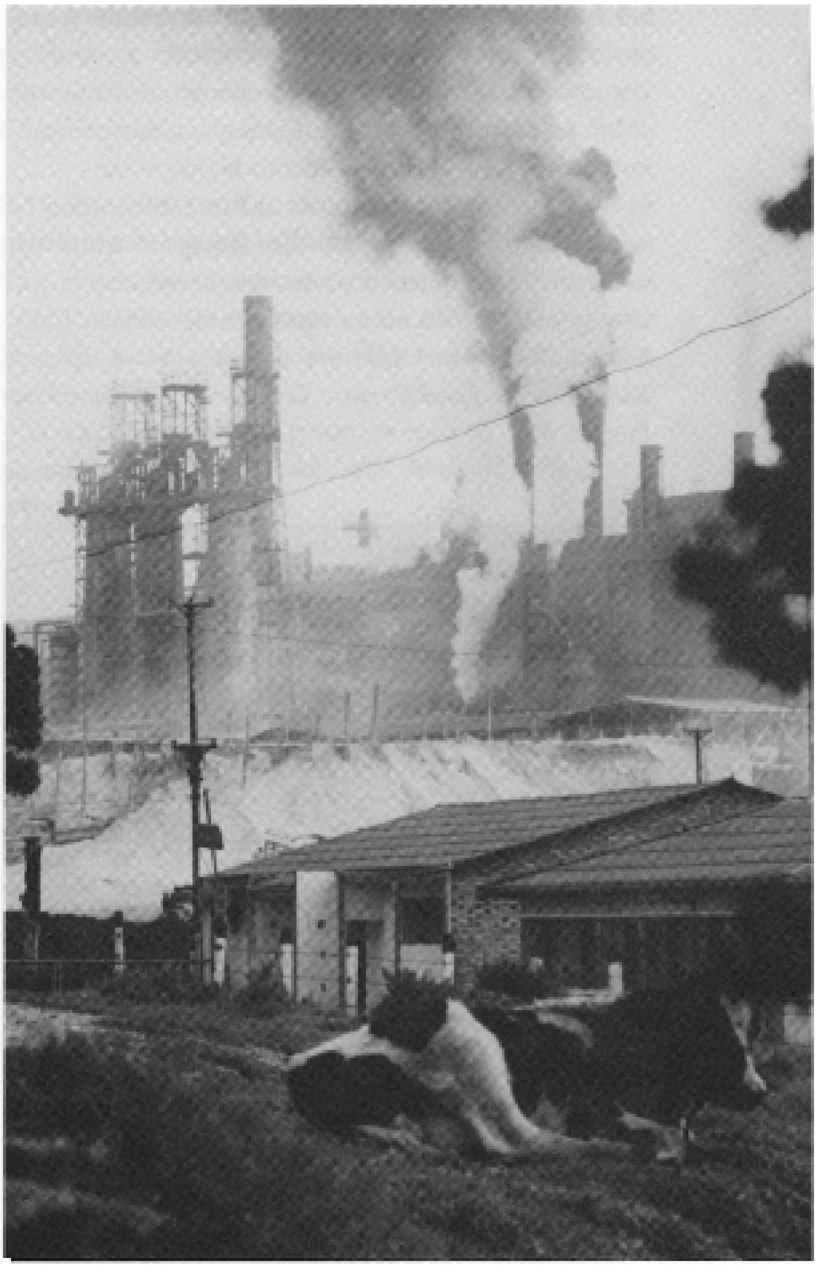
The selection of the preferred value is discussed; and estimates of the accuracies of the rate coefficients and temperature coefficients have been made for each reaction. The data sheets are intended to provide the basic physical chemical data needed as input for calculations which model atmospheric chemistry. A table summarizing the preferred rate data is provided, together with an appendix listing the available data on enthalpies of formation of the reactant and product species.

The paper, entitled "Evaluated kinetic and photochemical data for atmospheric chemistry: Supplement III" was published in *Journal of Physical and Chemical Reference Data*, Volume 18, No. 2, pp. 881-1087, 1989.

It is the third supplement to the original set of critically evaluated kinetic and photochemical rate parameters for atmospheric chemistry, published by the International Council of Scientific Unions (ICSU) Committee on Data for Science and Technology (CODATA) Task Group on Gas phase Phase Chemical Kinetics in 1980 and subsequently updated by the first supplement in 1982 and the second supplement in 1984. The original evaluation and the first two supplements were primarily intended to furnish a kinetic data base for modeling middle atmospheric chemistry (10-55 km altitude).

With the publication of the present evaluation, this database has been updated and extended to include reactions involved in tropospheric chemistry. It is not possible to cope with all of the very large number of chemical reactions involved in tropospheric chemistry at this stage. A start has been made by selecting those organic reactions for which kinetic or photochemical data exist for species containing up to three carbon atoms. Future evaluations will add to this list.

A copy of this supplement (Reprint No. 366, Journal of Physical and Chemical Reference Data, *Vol. 18, No. 2, pp. 881-1097, 1989) may be ordered from the American Chemical Society, Distribution Office, 1155 Sixteenth Street, N. W., Washington, DC 20036-9976, USA. Price USD 18.00 plus (for foreign orders) USD 2.50 for postage and handling. Orders must be prepaid and checks made payable to the American Chemical Society.*



In 1989, the IUPAC Subcommittee on Gas Phase Kinetic Data Evaluation for Atmospheric published a 216 page report on 'Atmospheric chemistry: kinetic and photochemical data.'

3.9 Radionuclide migration in groundwaters review of the behaviour of actinides

The objective of the project is to give the current state of the art concerning actinide (plutonium, americium and mainly neptunium) in order to highlight the various aspects of the question, and to point out the needs required to bridge the existing gaps in terms of research and compilation works, that have either already been carried out or should be developed.

Analytical Chemistry Division, Commission on Radiochemistry and Nuclear Techniques: Ongoing Project.

3.10 Bioavailability of pesticides and metabolites

The properties of an individual chemical, such as lipophilicity, and molecular size and weight, influence its bioavailability in various systems. As this is a broad topic, the IUPAC Commission on Pesticide Chemistry felt that a short project to evaluate factors governing bioavailability would be appropriate. A definition of 'bioavailability' is also needed.

Applied Chemistry Division, Commission on Pesticide Chemistry: Ongoing Project.

The Commission on Water Chemistry has an ongoing project concerned with the treatment of waste-water.

3.11 Occurrence and fate of pesticides in surface waters

Pesticides can reach surface water by various routes, the major ones being run-off, spray drift, and in selected cases, direct application (aquatic herbicides). With increasing legislation on allowable concentrations of pesticides in drinking water, the objective of this project is to review monitoring studies and consider factors affecting the fate of pesticides in water in order to put the situation in perspective.

Applied Chemistry Division, Commission on Pesticide Chemistry: Ongoing Project.

3.12 Current recognised environmental problems and related research efforts

The aim of this project is to organize a symposium to discuss the current recognized environmental problems and the research efforts on national and international levels.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

3.13 Waste-water treatability tests

A review of world literature indicates the need for screening test procedures, especially biodegradation tests, of waste waters in order to predict the performance of biological treatment plants.

Applied Chemistry Division, Commission on Water Chemistry: Ongoing Project.

3.14 The effects of processing and storage on pesticide residues in food

This project has four aims:

1. To review the literature on the effects of processing of raw food commodities on pesticde residues.
2. To summarize unit processes used in food preparation (both commercial and domestic cooking) which can affect residues.
3. To make predictions on the fate of residues in food based on physico-chemical parameters.
4. To review existing approaches to regulation of residues in processed food and make recommendations.

Applied Chemistry Division, Commission on Water Chemistry: Ongoing Project.

Toxicology of synthetic and natural compounds

See Chapter 4 for summaries of IUPAC projects on this topic.


PYREX

4 Toxicology of synthetic and natural chemical substances

4.1 Progress in nickel toxicology

The 3rd International Conference on Nickel Toxicology was held in Paris, France, September 1984 under the joint sponsorship of IUPAC, the Association of Clinical Scientists and the Nickel Producers Environmental Research Association. This volume contains synopses of the scientific papers presented at the conference.

Edited by S. S. Brown and F. W. Sunderman, Jr. Published by Blackwell Scientific Publications, Oxford, UK. 1985. 270 pages, 67 illustrations. ISBN 0 632 01355 9. Price: GBP 33.90/USD 36.80. Affiliate Members Discount Price: GBP 25.40/USD 27.60.

4.2 Occupational and environmental chemical hazards

This book is subtitled: Cellular and biochemical indices for monitoring toxicity. It has six parts:

1. Biological indicators of dose and effects: general concepts.
2. Biochemical indices of liver toxicity: enzyme induction, lipid peroxidation and other indices relevant to liver function changes.
3. Biochemical indices of liver toxicity: porphyrin metabolism.
4. Biochemicals and cellular indices of renal changes induced by exogenous chemicals.
5. Biological indices for assessment of human genotoxicity induced by exogenous chemicals.
6. Biochemical indices of nervous tissue toxicity and exposure to neurotoxicants.

Edited by V. Foa, E. A. Emmet, M. Moroni and A. Colombi. Published by Ellis Horwood, Chichester, UK. 1986. 544 pages. ISBN 0-7458-0088-2. Price: GBP 59.50.

4.3 Toxicology of metals

Even the trace elements which are essential to life may exert toxic effects, depending upon chemical form, dose, adsorption, route and so on. Other biologically non-essential metals are important to industry, but their use has been associated with adverse effects upon the environmental and health problems.

This volume places itself at the frontiers of research in strategic areas of metal toxicology, reflecting its relevance to the environment as well as the workplace. Covering subjects of world-wide importance, internationally recognized authors deal in the first section with some general aspects of the roles of trace metals in health and disease under three main headings: essentiality and toxicity, interactions and monitoring and analysis.

The second section of the work probes chemical and experimental studies of specific metals which are considered under four main headings: aluminium and light elements; lead, cadmium and heavy elements; chromium, nickel and transition elements; and platinum and gold, noble elements.

The book stems from an IUPAC symposium organized jointly with the University of Occupational and Environmental Health, Japan. The symposium reflected the interdisciplinary nature of metal toxicology by providing selected aspects of the chemical, biochemical, environmental and clinical toxicology of trace metals and metalloids.

Edited by S. S. Brown and Yasushi Kodama. Published by Ellis Horwood Limited, Chichester, UK. 1987. 448 pages. ISBN 0-7458-0016-5. Price: GBP 50.00/USD 79.95.

4.4 Cadmium - Environmental toxin series

The *Environmental Toxin Series* is dedicated to the publication of comprehensive reviews and monographs on compounds of classes of chemicals which are of importance in environmental toxicology. The series is designed to serve as a background of information for scientific investigations as well as risk analysis and political decision making.

The main aim of the series is to describe in as complete a way as possible all potentially hazardous chemicals from the point of view of chemistry, ecology, toxicology, risk analysis and regulatory implications.

Volume 2 of the series is entitled Cadmium. It contains 18 of the 22 contributions to the 3rd IUPAC Cadmium Workshop held in Juelich, FRG, August 1985. The volume is divided into four sections:

1. Toxicity, carcinogenicity, animal experiments.
2. Epidemiology.
3. Cadmium in the environment.
4. Methodology and quality assessment.

Edited by M. Stoeppler and M. Piscator. Publisher by Springer-Verlag, Berlin, FRG. 1988. 237 pages. ISBN 3 540 15551 1. Price: DEM 148.00.

4.5 Collection, processing and storage of specimens for the biological monitoring of occupational exposure to toxic chemicals

Biological monitoring of workers exposed to toxic chemicals has gained increasing attention as a means of assessing the hazard to health. Biological monitoring is primarily an activity where repetitive measurement of toxic chemicals in biological specimens is used to assess the exposure levels of individual workers and of groups of workers.

Toxicology of synthetic and natural chemical substances were amongst the topics discussed by commissions of the Clinical Chemistry Division at the 35th IUPAC General Assembly held in Lund, Sweden in August 1989.

More recently, attempts have been made to use this kind of information to produce limit levels which could ensure that no relevant ill health would ensue from the exposure.

In some instances an effect of the toxic compound on certain physiological or biochemical functions has also been measured as a part of biological monitoring. The current report is limited to measurement of toxic chemicals or their metabolites. Due to developments in analytical chemistry, a wide variety of toxic compounds, at least 100 chemicals or their metabolites may be analysed in human specimens.

At present the main obstacle in broadening the application of biological monitoring is not the problem of analysis, but lack of information on toxicology and toxicokinetics of the chemicals in questions.

This document briefly reviews sources of error in the procedures of measurement and pitfalls in the interpretation of results of biological monitoring. Analytical errors are not considered. Various aspects of sources of error in biological monitoring of exposure to chemicals have been reviewed. This document is complemented by practical guidelines for specific chemicals. The first of these guidelines is in preparation.

Clinical Chemistry Division, Commission on Toxicology: Pure & Appl. Chem., *Vol. 56, No. 4, pp. 549-566, 1984.*

4.6 Beta-2 microglobulin and other urinary proteins as an index of cadmium-nephrotoxicity

One of the most detrimental effects of cadmium exposure pertains to the renal function. The tubular and/or the glomerular function will be affected resulting in an elevated excretion of low molecular mass and/or high molecular mass proteins respectively. Of these proteins, a few have been selected from each group.

The relationships between protein concentration and cadmium concentration in kidney tissue, liver tissue and urine are discussed. Critical concentration values for each parameter are given. A preferred analytical method for the determination of the low molecular

One of the projects of the Commission on Pesticide Chemistry is concerned with the relevance of impurities in technical grade pesticides.

mass proteins is described and a recommendation is made as to which protein(s) should be determined.
Clinical Chemistry Division, Commission on Toxicology: Pure & Appl. Chem., *Vol. 56, No. 7, pp. 957-965, 1984.*

4.7 Recommended approach to the appraisal of risks to consumers from pesticide residues in crops and food commodities

In order to assess potential health problems from pesticide residues in food the extent to which dietary intakes approach or exceed an estimated no-toxicological-effect level should be determined. Retrospective intake data may be obtained from dietary studies.

The 'best estimate' of prospective intake may be made from a knowledge of the use of a pesticide, its residue on a crop at harvest and the subsequent fate of those residues, including the effects of cooking and processing. A stepwise approach which contrasts the 'best estimate' of consumer dietary intake with an estimate of theoretical maximum dietary intake is recommended to government agencies and to the pesticide industry.
Applied Chemistry Division, Commission on Pesticide Chemistry: Pure & Appl. Chem., *Vol. 59, No. 4, pp. 611-624, 1987.*

4.8 Global significance of mycotoxins

By C. W. Hesseltine. Published in Chemistry International, *Vol. 8. No. 6, pp. 9-15, 1986.*

4.9 Congress of pesticide chemistry

Published in Chemistry International, *Vol. 9. No. 1, pp. 12-21, 1986.*

4.10 Removal of aflatoxin from animal feeds by ammoniation: current status and regulation

Ammoniation of animal feeds is currently permitted in Arizona and California for cottonseed, North Carolina and Georgia for corn (all in USA), and France, Senegal and Sudan for peanut cakes/meal.

Extensive studies have been carried out on the use of ammonia to decontaminate aflatoxin contaminated feed. The scope of these studies includes the efficacy of the method to reduce aflatoxin levels, identification of aflatoxins ammonia reaction products, effect of process of nutritive value and acceptability of the product, and the formation and significance of toxic residues.

The objective of this project is to summarize these studies as well as to outline current applications and regulatory status of ammonia for reducing aflatoxin levels in animal feeds.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

4.11 Laboratory safety: Detoxification of some mycotoxins

This project aims to develop and validate laboratory methods on decontamination and detoxification of the mycotoxins ochratoxin A, citrinin, patulin and sterigmatocystin. The project is being carried out in two phases:

1. Development of procedures which will enable efficient degradation of the compounds followed by mutagenicity testing of the residues.
2. Validation of the method by means of a collaborative study.

The number of laboratories active in the biological and analytical research of mycotoxins other than aflatoxins is rapidly increasing. Several of these compounds are known mutagens, carcinogens or co-carcinogens. Therefore, guidelines on the safe handling of waste and detoxification of these compounds in the laboratory are urgently required.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

4.12 Relevance of impurities in technical grade pesticides

Formation of impurities cannot be prevented during the production process of pesticides. Their identification and potential contribution to the toxicity of the tested and produced manufactured product has to be considered during the development of a new pesticide. The project will cover all aspects of the relevance of impurities resulting in defined recommendations on how to proceed during all stages of pesticide development.

Applied Chemistry Division, Commission on Pesticide Chemistry: Ongoing Project.

4.13 Glossary of terms in toxicology and ecotoxicology

The aim of this project is to produce an internationally acceptable glossary of terms in toxicology and ecotoxicology starting from existing glossaries.

This glossary will facilitate communication and thus collaboration in the advancement of toxicology. Once an English glossary is available, further glossaries in other languages could be prepared and stored in terminological computer data banks to facilitate translation of essential literature.

Clinical Chemistry Division, Commission on Toxicology: Ongoing Project.

4.14 Isotope specific measurements as references for toxic/essential element assay

It is the opinion that isotope-specific methods have now matured to the stage that, if they are correctly applied under rigorous control an based on highly skilled expertise, they can provide "reference values" against which laboratories can then evaluate their routine performance in regular interlaboratory measurement evaluation programmes.

Joint Inorganic Chemistry Division/Clinical Chemistry Division Limited Life Time Commission Isotope Specific Measurements as References for Toxic/Essential Element Assay: Ongoing Project.

4.15 Development of criteria and guidelines for collection, storage and transport of body fluids for element analysis

Contamination of biological specimens during collection, storage and transport is still a serious problem in element analysis. A need for general guidelines (criteria) exists as well as that for protocols that take into account the ideosyncrasies of individual elements.

Clinical Chemistry Division, Commission on Toxicology: Ongoing Project.

The Commission on Toxicology is assessing data on reference levels for nickel and mercury in human body fluids of well-defined populations.

4.16 Recommendations for collection, storage and transport of body fluids for nickel analysis

Clinical Chemistry Division, Subcommittee on Environmental and Occupational Toxicology of Body Fluids for Nickel Analysis: Ongoing Project.

4.17 Guidelines for the preparation and characterization of nickel compounds used in toxicological research

Clinical Chemistry Division, Subcommittee on Environmental and Occupational Toxicology of Body Fluids for Nickel Analysis: Ongoing Project.

4.18 Reference intervals for nickel in body fluids

The objective of this project is to review the literature of published values of nickel in human body fluids employing strict methodological and epidemiological (demographic) criteria to assess, respectively, the reliability of such data and to establish normal reference intervals for well-defined populations.
Clinical Chemistry Division, Commission on Toxicology: Ongoing Project.

4.19 Reference levels for mercury in human body fluids

Clinical Chemistry Division, Commission on Toxicology: Ongoing Project.

Application of multiresidue procedures in pesticides residues analysis

See Section 1.3 Page 19 for summaries of IUPAC projects on this topic.

Critical evaluation of model ecosystems

See Chapter 3 Page 35 for summaries of IUPAC projects.

Determination of natural toxins

See Section 1.4 Page 25 for summaries of IUPAC projects on this topic.

5 Environmental legislation and standards

5.1 The prediction of pesticide residues in crops by the optimum use of existing data

This is No.26 in the series IUPAC Reports on Pesticides.

The commitment of large resources to the provision and evaluation of data on pesticide residues in/on crops makes it vital to optimize the value of existing extensive information. Variations in the many (sometimes uncontrollable) factors which determine pesticide deposits on crops and their subsequent dilution and disappearance make the consideration of pesticide residues and the estimation of maximum residues levels an inexact subject

A knowledge of these factors and their variability can reduce, or at least modify, the current regulatory requirements for expensive formal residues trials, which often have considerable limitations, both in their execution and in their interpretation. Information required for the successful prediction of pesticide deposits and residues at harvest is discussed and summarized in a recommended stepwise approach to the consideration of pesticide residues in crops.

Applied Chemistry Division, Commission on Agrochemicals, Pure & Appl. Chem., *Vol. 62, No. 2, pp. 337-350, 1990.*

5.2 Code of conduct on the distribution and use of pesticides

Published in Chemistry International, *Vol. 7, No. 1, pp. 26-27, 1985.*

5.3 Occupational hazards present risk to future generations

Published in Chemistry International, *Vol. 9, No. 3, pp. 97-998, 1987.*

5.4 Worldwide limits and regulations on plant toxins and phycotoxins

The aim of this project is to collect data on limits and regulations for plant toxins and phycotoxins in foodstuffs and animal feedstuffs. These data will be summarized and published. The project will also involve a critical evaluation of the compiled data by national representatives and affiliate members of the Commission on Food Chemistry.

Applied Chemistry Division, Commission on Food Chemistry: Ongoing Project.

5.5 Inventory of regulations for emissions and standards on ambient and workplace atmospheres

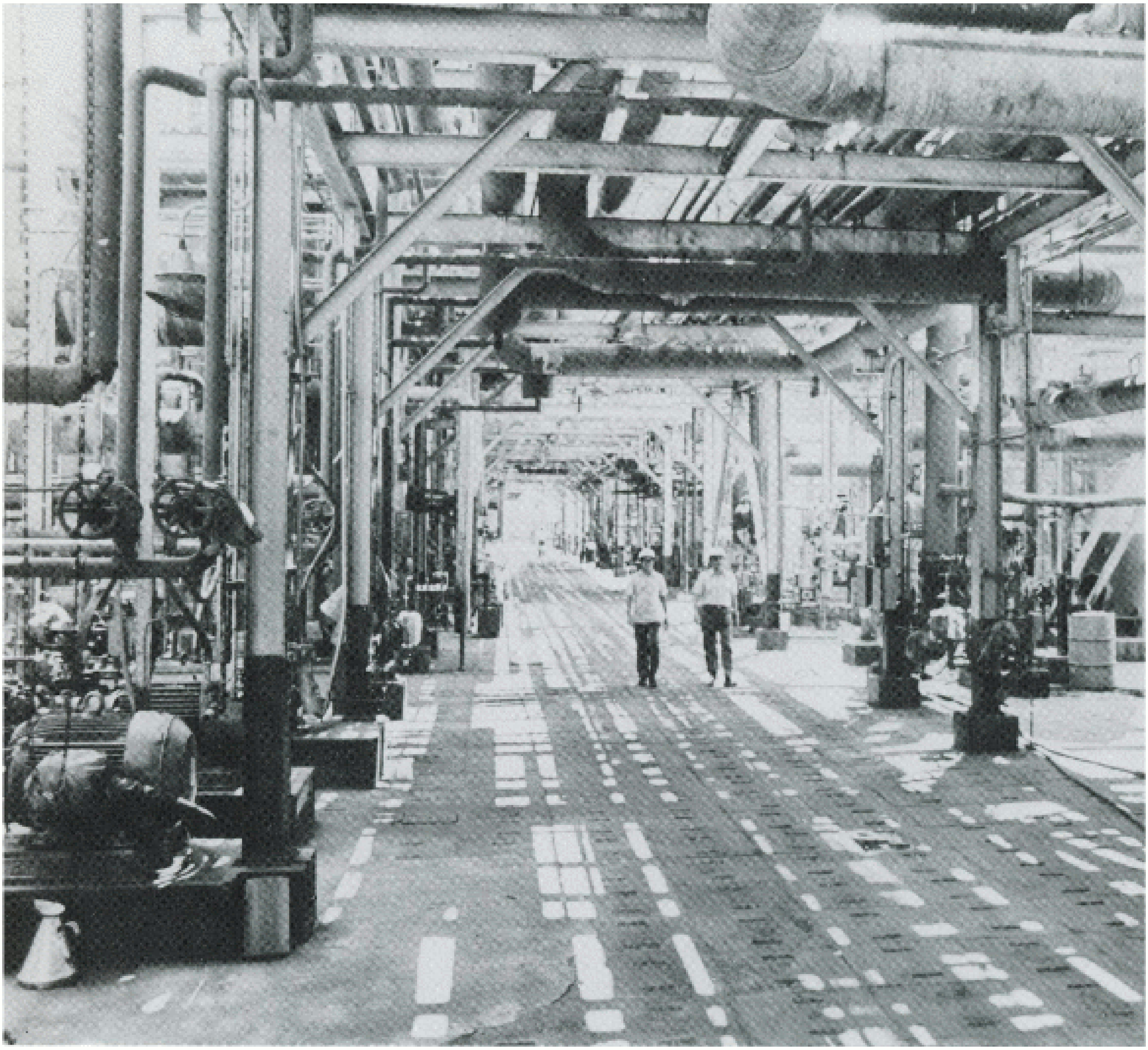
The aim of this feasibility study is to make an inventory of the existing regulations and standards regarding emissions, ambient levels and workplace atmospheres of different countries.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

5.6 Advantages of the use of molar concentration in setting water quality standards

Water quality standards are generally expressed in mass per volume units and water chemists in general tend to use these units for a variety of determinands. This project will consider the advantages and disadvantages of using the more widely accepted mole per volume units for the generally measured water quality parameters.

Applied Chemistry Division, Commission on Water Chemistry: Ongoing Project.



6 Prevention of environmental pollution using chemical and biochemical methods

6.1 Recommended methods for characterization of agricultural residues and feed products derived through bioconversion

This set of guidelines has been put forth with the objective of providing a frame of reference which could be used to evaluate microbial biomass products grown on agro-industrial raw materials. They should be taken in a new perspective and should complement the previous guidelines prepared for SCP grown on synthetic raw materials.

The guidelines make reference to important agro-industrial raw materials like animal waste, lignocellulosic crop residues and their mixtures.

Applied Chemistry Division, Commission on Biotechnology: Pure & Appl. Chem., *Vol. 59, No.5, pp. 723-730, 1987.*

6.2 SCOPE for solving problems of the environment

Report on the Scientific Committee of the Environment (SCOPE) of the International Council of Scientific Unions (ICSU).

Published in Chemistry International, *Vol. 7. No. 6, pp. 31-35, 1985.*

6.3 Safeguarding our tomorrows

This article examines these changes and outlines the efforts of UNESCO's Man and Biosphere Programme to help man better adapt to his changing situation.

Published in Chemistry International, *Vol.11. No. 4, pp. 145-147, 1989.*

6.4 SCOPE 1989-1991

Report on the Scientific Committee of the Environment (SCOPE) of the International Council of Scientific Unions (ICSU).

Published in Chemistry International, *Vol. 11: No. 5, pp. 192-194, 1989.*

6.5 IUPAC Workshops on Safety in Chemical Production

These workshops will be concerned with safety in chemical production: risk assessment, risk reduction, implications on eduction. The first workshop will be held in Basle, Switzerland in September 1990.

Committee on Chemistry and Industry: Ongoing Project.

6.6 The role of surface and colloid chemistry (including catalysis) in environmental protection

The objectives of this feasibility study are: (1) to define the problems of pollution control which involve surface and colloid science; (2) to specify those areas in which the Commission on Colloid and Surface Chemistry (including Catalysis) should become involved; and (3) To recommend appropriate action by the commission.

Physical Chemistry Division, Commission on Colloid and Surface Chemistry including Catalysis: Ongoing Project.

6.7 A study of the chemical interactions in the disinfection of potable waters, between the disinfectants, existing trace pollutants, and reaction products

There is a great deal of research currently being undertaken in many countries on the identification of chemicals formed during water disinfection. Much of this concern is motivated by concern about potential toxicants that can be formed, for example, mutagens produced by chlorination.

This project aims to collect and collate information in this area, to assist with further studies and to identify areas receiving too little attention.

Applied Chemistry Division, Commission on Water Chemistry: Ongoing Project.

B CHEMical Research Applied to World Needs, education and other IUPAC activities related to the environment

1 CHEMRAWN: The IUPAC Programme on CHEMical Research Applied to World Needs

CHEMical Research Applied to World Needs: CHEMRAWN
Published in Chemistry International, *Vol. 10. No. 5, pp. 175-176, 1988.*

CHEMRAWN I:
Future sources of organic raw materials
IUPAC's initial enterprise in the CHEMRAWN programme was to convene the first "World Conference on Future Sources of Organic Raw Materiales". This international conference, held in Toronto, Canada, July 1978, attempted to define and set in perspective those factors that will ultimately determine the sources of organic raw materials necessary to support world chemical industries at the end of the century. The various sessions not only dealt with the future life-blood of some of our major industries but inspired anhd stimulated vast and fertile new fields for those working in the more basic, exploratory areas. These proceedings are essential reading for policy makers in both government and industry, and for scientists concerned with the need to plan for the future resources.
Edited by L. E. St-Pierre and G. R. Brown. Published by Pergamon Press, Oxford, UK, 1980. 612 pages, ISBN 0 08 022390 7. Price: USD 56.00.

Resources of organic matter for the future — Perspectives and recommendations
Edited by L. E. St-Pierre. Published by Multiscience Publications Ltd., Montreal, Quebec, Canada, 1979. ISBN 0 919868 06 1

CHEMRAWN II:
Chemistry and world food supplies: The new frontiers
Proceedings of the CHEMRAWN II conference held in Manila, Philippines, 6-10 December 1982.
Edited by L. W. Shemilt. Published by Pergamon Press, Oxford, UK, 1983. 600 pages, ISBN 0 08 029243 7 (hardcover); ISBN 0 08 029242 9 (flexicover). Price: USD 132.80 (hardcover); USD 75.00 (flexicover).

Chemistry and world food supplies: The new frontiers — Perspectives and recommendations
Edited by G. Bixler and L. W. Shemilt Published 1983 - Available from American Chemical Society, Washington, DC, USA or International Rice Research Institute, Manila, Philippines. 169 pages. ISBN 971 104 105 7

CHEMRAWN III:
World conference on resource material conversion: (Bio-) Chemical process bridges to meet future needs
Proceedings of the CHEMRAWN III conference held in The Hague, The Netherlands, June 25-29, 1984. This volume contains the conference working papers in loose leaf form in a ring binder. Plenary sessions were on the following topics: resources; world needs; and chemical processes. There were also parallel sessions on: resources; resource to base chemicals; base chemicals to end products; resubstitution; and loss prevention, environment and safety.
Published by QLT Convention Services, Amsterdam, Netherlands 1985.

The CHEMRAWN V Conference on Contributions of Chemistry to Health was held in Heidelberg, FRG in 1986. The conference attracted distinguished scientists from all over the world.

CHEMRAWN IV:
Modern Chemistry and Chemical Technology Applied to the Ocean and Its Resources

Proceedings of the CHEMRAWN IV conference held at Keystone, Colorado, USA, 4-9 October 1987.
Published as a special issue of Applied Geochemistry *(Vol. 3, No. 1, January/February 1988).*

Ocean chemistry: CHEMRAWN IV

Published in Chemistry International, *Vol. 10. No. 5, pp. 177-180, 1988.*

CHEMRAWN V:
Contributions of chemistry to health

Volume 1: Perspectives and recommendations compiled at the CHEMRAWN V conference, Heidelberg, FRG, 1986.
Edited by H. Machleidt, H Meyer and P. Tanswell. Published by VCH Verlagsgesellschaft mbH, Weinheim, FRG, 1987. 54 pages. ISBN 3 527 267174. Price: DEM 28.00.

Volume 2: Proceedings of the CHEMRAWN V conference.
Edited by H. Machleidt. Published by VCH Verlagsgesellschaft mbH, Weinheim, FRG, 1987. 403 pages, ISBN 3 527 26618 6. Price: DEM 145.00.

CHEMRAWN VI:
World conference on advanced materials for innovations in energy, transportation and communications

Invited papers and posters from the CHEMRAWN VI conference held in Tokyo, Japan. May 17-22, 1987.

World conference on advanced materials for innovations in energy, transportation and communications - Perspectives and recommendations
Copies of CHEMRAWN VI publications may be ordered from The Chemical Society of Japan, 1-5 Kanda-Surugadai, Chiyoda-ku, Tokyo 101, Japan.

CHEMRAWN VII:
Chemistry of the atmosphere: Its impact on global change

This conference will be held in Baltimore, Maryland, USA from 2-6 December 1991.
Ongoing Project.

Second International Conference on Chemistry and World Food Supplies: The New Frontiers

This 'tentative' CHEMRAWN conference is a follow up to CHEMRAWN II (see above). The meeting is planned to be held in India, possibly Delhi or Bangalore, in either 1991 or 1992.
Ongoing Project.

Waste as a raw material for industry

Proposed CHEMRAWN Conference on Waste as a Raw Material for Chemical Industry to be held in 1991 or later.
Ongoing Project.

CHEMRAWN I:
Future sources of organic raw materials

Toronto, Canada, 1978.

CHEMRAWN II :
Chemistry and world food supplies: The new frontiers

Manila, Philippines, 1982.

CHEMRAWN III :
Resources material conversion

The Hague, Netherlands, 1984.

CHEMRAWN IV :
Modern chemistry and chemical technology applied to the ocean and its resources

Keystone, Colorado, USA, 1987.

CHEMRAWN V:
Current and future contributions of chemistry to health

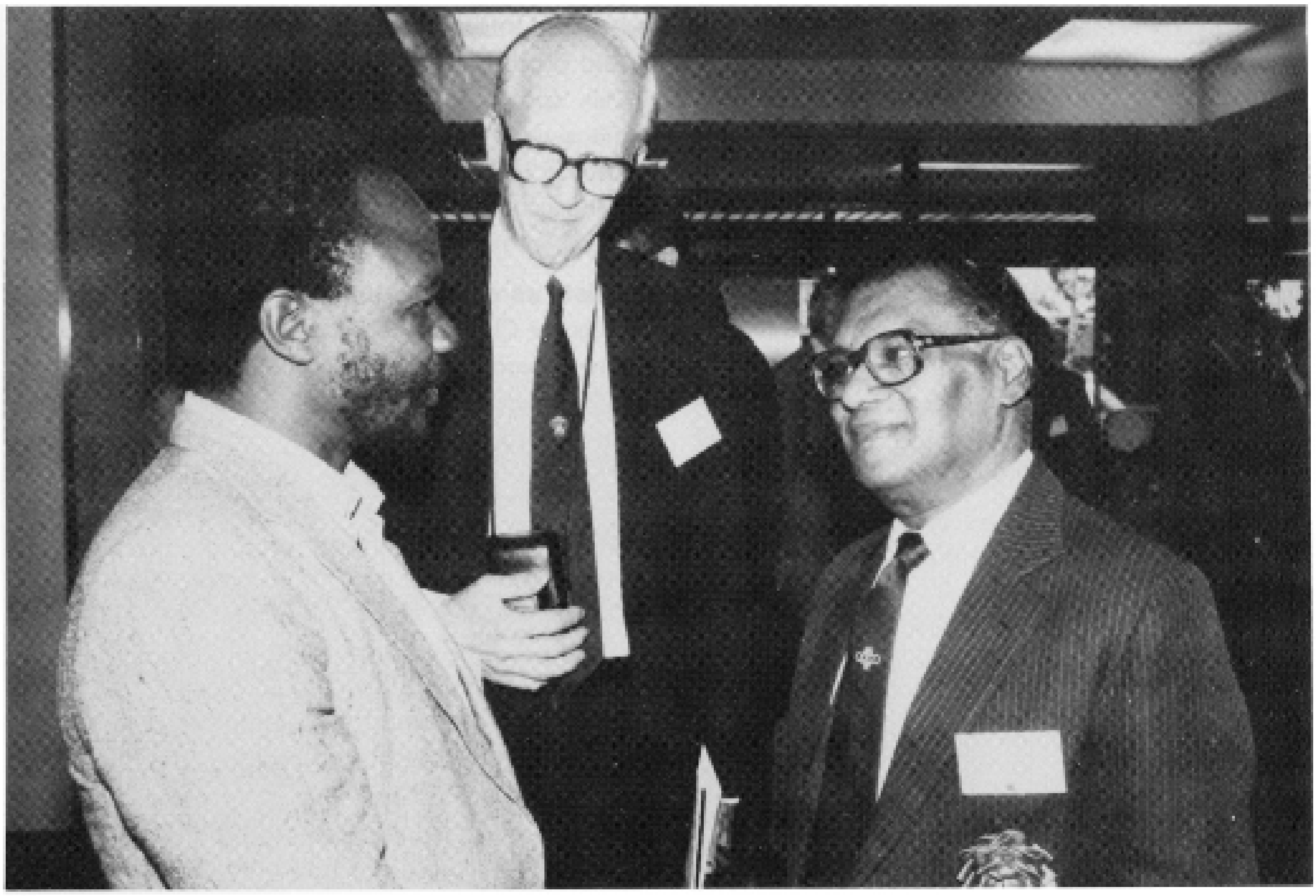
Heidelberg, FRG, 1986.

CHEMRAWN VI:
Advanced materials for innovation in energy, transportation and communications

Tokyo, Japan, 1987.

CHEMRAWN VII:
Chemistry of the atmosphere: Its impact on global change

Baltimore, USA, 1991.



The Commission on Atmospheric Chemistry is promoting the exchange of information on local environmental problems in different countries.

2 Education and other IUPAC activities related to the environment

Global change: The education program of the International Geosphere Biosphere project

This proposed international curriculum development project will be developed in parallel with the research project of the International Council of Scientific Unions (ICSU) entitled International Geosphere Biosphere Project (IGBP).

Committee on Teaching of Chemistry: Ongoing Project.

Experiments in environmental chemistry

This project is concerned with the design of experiments in environmental chemistry which can be carried out using low cost equipment.

Committee on Teaching of Chemistry: Ongoing Project.

Energy and the environment as related to chemistry teaching

An international workshop/seminar on energy and the environment is planned.

Committee on Teaching of Chemistry: Ongoing Project.

International Symposium on Environment and Chemistry

An international symposium to be held in Moscow, USSR.

Committee on Teaching of Chemistry: Ongoing Project.

International Symposium on Biotechnology and the Environment

Applied Chemistry Division, Commission on Biotechnology: Ongoing Project.

Education in atmospheric chemistry

Information is being collected on the extent of atmospheric chemistry teaching throughout the world. Suggestions will be made on the formulation of material suitable for teaching at levels ranging from schools to universities.

Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

Environmental problems in different countries

The exchange of information regarding local environmental problems in different countries is of interest to the general public and also helps scientists in the field of environmental research to define properly the problems in his or her own country. The outcome of this project will be a series on short articles, to be published in Chemistry International, on these local problems.

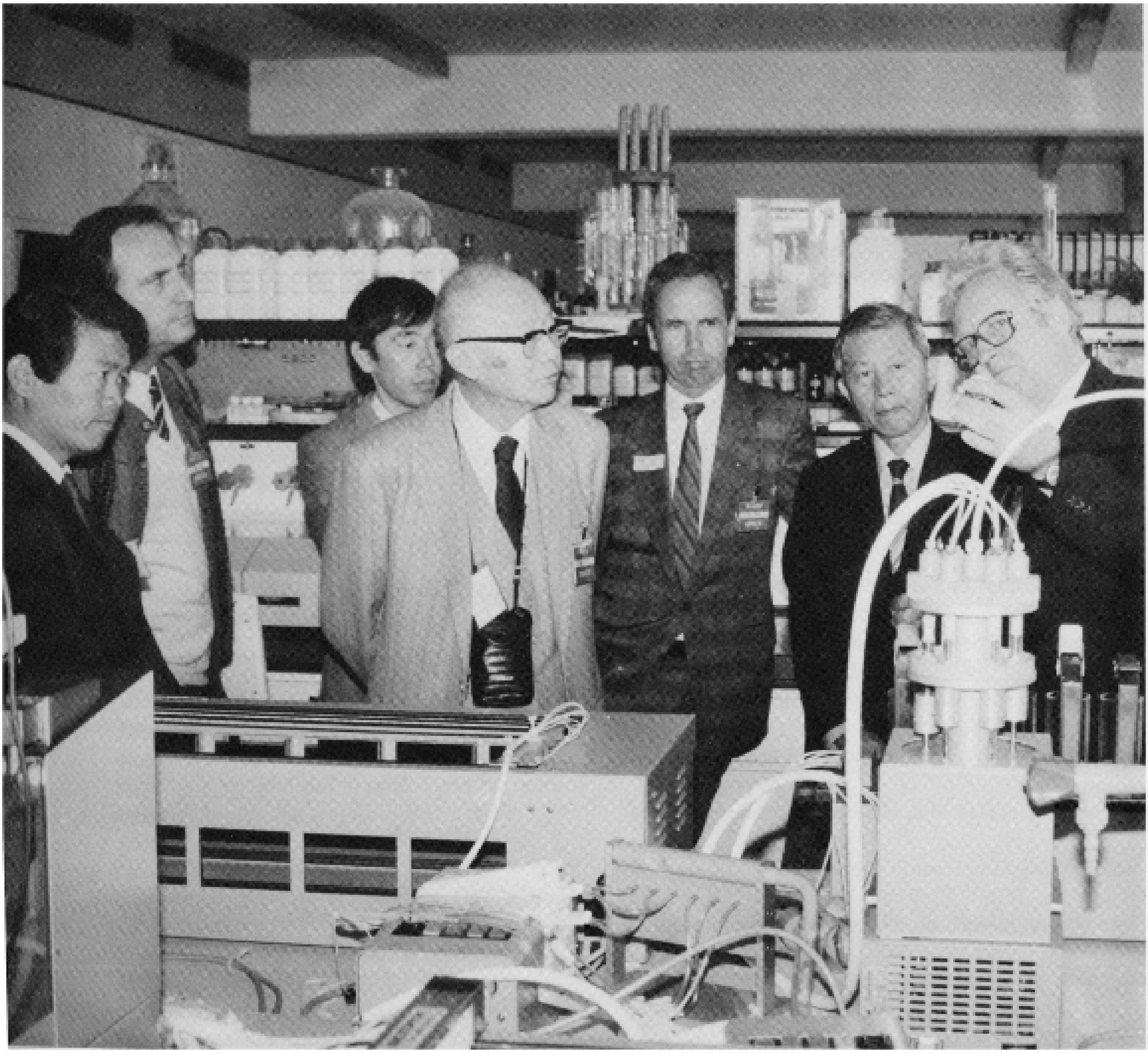
Applied Chemistry Division, Commission on Atmospheric Chemistry: Ongoing Project.

Chemistry's cornucopia

By Sir George Porter. Published in Chemistry International, *Vol. 8. No. 1, pp. 17-23, 1986.*

Global change and nuclear war

Published in Chemistry International, *Vol. 9. No. 2, pp. 54-62, 1987.*



C International Union of Pure and Applied Chemistry

What is IUPAC?

Formed in 1919, IUPAC is a voluntary, non-governmental, non-profit association of 45 organizations known as national adhering organizations (NAOs). An NAO represents the chemists of a member country.

Some eleven other countries, known as Observer Countries, are also linked to IUPAC.

IUPAC is the recognized world authority on chemical nomenclature, terminology, symbols, units, atomic weights and related topics.

IUPAC provides advice on chemical matters to international agencies such as the United Nations World Health Organization (WHO), United Nations Environment Programme (UNEP), United Nations Food and Agricultural Organization (FAO), United Nations Education, Scientific and Cultural Organization (UNESCO), International Organization for Legal Metrology (OIML) and International Organization for Standardization (ISO). IUPAC is a member of the International Council of Scientific Unions (ICSU) and has close links with the ICSU Scientific Committee on Problems of the Environment (SCOPE).

IUPAC has formal links with 34 regional and international organizations - Associated Organizations - concerned with chemistry and applications.

Divisions, Commissions and Committees

Some 1500 chemists throughout the world are engaged in the scientific work of IUPAC on a voluntary basis. These chemists work on IUPAC's commissions and committees. IUPAC has 34 commissions and these are grouped into seven divisions:

I Physical
II Inorganic
III Organic
IV Macromolecular
V Analytical
VI Applied
VII Clinical

There is also a section on Medicinal Chemistry.

At the 35th IUPAC General Assembly held in Lund, Sweden, August 1989, Council approved the formation of six Limited Life Time Commissions (LLTCs). These included a Division V LLTC on Environmental Analytical Chemistry and a joint Division II and Division VII LLTC on Isotope Specific Measurements as References for Toxic/Bioessential Element Assays.

IUPAC also has a number of standing committees, for example: Committee on Chemistry and Industry (COCI); Committee on Teaching of Chemistry; Committee on Chemical Research Applied to World Needs (CHEMRAWN); and Committee on Chemical Databases.

IUPAC Company Associate Scheme

The IUPAC Company Associate Scheme provides an opportunity for chemical companies - at relatively low cost - to play a leading role in the representative body for chemistry at international level. Through the scheme, companies can speak as an international voice and thereby influence the way chemistry is preceived by the community at large and the scientific community in particular on matters such as: the image of chemistry, safety, pollution, energy conversion, and the environment.

About 175 chemical companies - large and small - from about 25 countries have already joined the scheme. When there are two or more Company Associates in a particular country or region, they may form a National Company Associates Group to discuss

IUPAC sponsors about 30 conferences each year and publishes conference proceedings, the scientific journal *Pure and Applied Chemistry* and the IUPAC news magazine *Chemistry International*. Many conferences include poster sessions.

IUPAC matters and provide an input to the Union via COCI.

Company Associates receive the IUPAC news magazine *Chemistry International*, the biennial *IUPAC Handbook* and advance information on IUPAC-sponsored conferences. They may also subscribe to the IUPAC journal *Pure and Applied Chemistry* at a discount of 25%. This journal contains IUPAC recommendations on nomenclature, symbols and other technical reports plus plenary lectures from sponsored symposia.

Affiliate Membership Programme

The IUPAC Affiliate Membership Programme was launched in 1986 in order to maximize the participation of chemists throughout the world in the affairs of IUPAC and also to disseminate information about its activities to a much wider audience.

At present there about 8000 affiliates from some 80 countries. These include 800 chemists from Third World countries, many of whom are sponsored by IUPAC grants.

Affiliates receive *Chemistry International*. A number of other benefits are also available to them. For example, they are entitled to reductions in conference registration fees and the prices of most IUPAC publications and they may also purchase IUPAC ties or scarves.

Conferences and Publications

IUPAC sponsors about 30 conferences throughout the world each year. Amongst the most successful are the CHEMRAWN conferences. The IUPAC Safety in Chemical Production Workshops are a recent initiative of the COCI.

The Union publishes conference proceedings, definitive volumes of chemical data and compendia on nomenclature, quantities, symbols and units (the famous Green, Red, Blue and Orange Books). Its scientific journal *Pure and Applied Chemistry* cuts across disciplinary boundaries to present major research in all areas of chemistry. It includes the main invited lectures from IUPAC-sponsored conferences and also the recommendations of its commissions on nomenclature, symbols and units and technical reports on standardization, recommended procedures, collaborative studies an data compilations.

News about IUPAC, its chemists, its Affiliate Membership Programme, its publications, its recommendations, its conferences and its commission and committee meetings appears regularly in the IUPAC news magazine *Chemistry International*.

WINDECK

International Union of Pure and Applied Chemistry (IUPAC)

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary, non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 45 countries, each represented by a national organization, such as an academy of science or research council.

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