companies joined the MIACC in three years, an accomplishment that Andersson credits to the Board’s strong team spirit. He became Director of Technical Programmes in 1995. Through the voluntary efforts of a Technical Management Committee, supported by the Board and membership, Roland coordinated the development and implementation of a national programme for the voluntary control of major hazards.

Forming Andersson & Associates in 1997, he has undertaken national and international projects with The Canadian Chemical Producers’ Association (CCPA) on climate change, for Environment Canada on promoting Accelerated Reduction and Elimination of Toxics (ARET) to industry, and for the Intergovernmental Forum on Chemical Safety (IFCS) in the development of an international marketing and funding strategy.

A new name for the International Federation of Clinical Chemistry

The scientific, technological and organizational changes in health care that are taking place in most countries challenged the IFCC Executive Board to consider the advantages of updating the name of the federation. The basis for this proposal arose during the development of the IFCC strategic plan. While the IFCC will continue to strive for excellence in the profession of laboratory analysis—two considerations about the organization’s role have emerged. On the one hand, there is increasing use of techniques of chemical and molecular biology in related fields, which are not strictly subsumed in clinical chemistry. On the other, there is a huge increase in the potential use of laboratory data and diagnostic possibilities in preventive medicine. This requires substantial integration of demographic and clinical-medical information regarding the patient.

These reasons supported the decision of the IFCC Executive Board to ask the national societies affiliated with the IFCC to vote on extending its name to the International Federation of Clinical Chemistry and Laboratory Medicine. A majority of those voting approved this proposal in September 1997.

The Executive Board of the IFCC noted that it must be made clear that this name change in no way implies that laboratory sciences are the exclusive province of medical doctors. While it is clear in all countries that only physicians can provide therapy, diagnostic process today require the integration of skills in biochemistry, physiopathology, chemistry, physics, and so forth. These professional contributions are then used by some physicians for the final diagnosis and by other physicians in prescribing treatment.

Isotope geochemists—Website

Those of you who are interested in the use of stable isotopes in geochemistry should be aware of a website server ISOGEOCHEM at <http://geology.uvm.edu/isogeochem.html>. It is a useful way of getting information on any isotopic problem through its ‘chat-line’, and also provides information on conferences, positions vacant, short courses, student opportunities, suppliers and stable isotope laboratories. A particularly useful aspect is the ‘archive’ link which allows you to search for discussion on any previous item. ISOGEOCHEM has over 1100 subscribers in some 40 countries.

Obituary

Prof. O. Wichterle, the father of soft contact lenses, died on 18 August 1998 in the Czech Republic. Prof. Wichterle was the first President of the Macromolecular Division, 1967–71.

Recent reports

Recent reports published in Pure and Applied Chemistry

pH measurements in non-aqueous and mixed solvents: Predicting pH(PS) of potassium hydrogen phthalate for alcohol–water mixtures (Technical Report)

Synopsis: Predictive equations for estimating pH(PS) (PS = Primary Standard) of the potassium hydrogen phthalate buffer in any aqueous–alcoholic mixture are given as functions of the alcoholic moiety mole fraction, x, in the mixture and of the relative permittivity, ε, and the autoprotolysis constant, pK_{ap} of the pure alcohol at 298.15 K. The two equations, one valid for 298.15 K and the other covering the 263–318 K temperature range, have been optimized by using the experimental data for pH(PS) in aqueous mixtures with the following alcohols: methanol, ethanol, propan-2-ol, ethane-1,2-diol, 2-methoxyethanol (‘methylcellosolve’). The equations, tested on subsets generated from the full set by removing an entire co-solvent at a time, provide predicted pH(PS) values which differ from the ‘true’ ones by less than 0.1 pH over the entire range of co-solvent
composition: \(0 < x < 0.75\). The predictive equations are recommended for calculating pH(PS) only in those aqueous–alcoholic media for which the corresponding experimental values are not available, and not as smoothing equations for water and its mixtures with the above-mentioned solvents.

This report was prepared for publication by: S. Rondinini, P.R. Mussini, T. Mussini and A. Vertova. Department of Physical Chemistry and Electrochemistry, University of Milan, Via Golgi 19, 20133 Milano, Italy. The full details are to be found in Pure Appl. Chem. 1998, 70(7), 1419–1422.

IUPAC Reports on Pesticides(40)

Bound xenobiotic residues in food commodities of plant and animal origin (Technical Report)

Synopsis: In order to assess the dietary risk resulting from the use of pesticides or veterinary drugs, the nature of the chemical residues on food commodities needs to be determined. Elucidation of the nature of the chemical residue is carried out using radiolabelled studies, where the radiolabelled xenobiotic is applied or dosed in a manner which reflects its conditions of use. Food commodities are exhaustively extracted to remove the individual components of the residue. Once extracted, the identity and toxicological significance of the components can be assessed and, where appropriate, analytical methods developed to quantitatively determine the amount of the components in food items.

Depending on the characteristics of the components of the residue, the extraction regime may not remove all the chemical residue from the sample matrix. These residues are frequently characterized as being ‘bound’, however, the amount and nature of this residue will be highly dependent on the extraction regime used. To provide guidance and standardization, a definition of the term ‘bound residues’ is recommended. This definition builds on a previous IUPAC definition, but takes account of the current availability of enzyme systems, which effectively solubilize the entire matrix rather than extracting the residue. It is also recommended that where the extraction falls short of the full definition, then the residues should be termed as ‘unextractable’ and the conditions of the extraction should also be defined.

Where residues are bound, the assessment of dietary risk cannot be directly assessed, thus raising issues relating to the significance of the bound residue. The overall toxicological significance of a bound residue will depend primarily on its bioavailability and the level of exposure. In order to determine the bioavailability, study design is crucial in order to perform a critical safety assessment.

This report was prepared for publication by: M.W. Skidmore¹, G.D. Paulson², H.A. Kuiper³, B. Ohlin⁴ and S. Reynolds⁵. ¹Zeneca Agrochemicals, Jealotts Hill, Bracknell, UK. ²State Institute for Quality Control of Agricultural Products, Wageningen, Netherlands. ³US Department of Agriculture, ARS, Fargo, ND 58105, USA. ⁴National Food Administration, Uppsala, Sweden. ⁵Central Science Laboratories, York, UK. The full details are to be found in Pure Appl. Chem. 1998, 70(7), 1423–1447.

Critically evaluated propagation rate coefficients in free radical polymerizations—II. Alkyl methacrylates (Technical Report)

Synopsis: Propagation rate coefficients, \(k_p\), with confidence ellipses of the Arrhenius parameters, are reported for bulk free-radical homopolymerizations of \(n\)-butyl and \(n\)-dodecyl methacrylate at ambient pressure and low conversion. The data, which are from independent experiments in two laboratories, were obtained by the pulsed-laser polymerization/size-exclusion chromatography method. They obey the consistency criteria established for this technique. Plotting the \(n\)-butyl and \(n\)-dodecyl methacrylate \(k_p\) data, together with the benchmark \(k_p\) values for methyl methacrylate and recent data for four other linear and branched alkyl methacrylates, clearly shows a pronounced family type behaviour of alkyl methacrylate \(k_p\).

This report was prepared for publication by: Sabine Beuermann and Michael Buback, Institut für Physikalische Chemie der Universität Göttingen, Tammannstr. 6, D-37077 Göttingen, Germany. The full details are to be found in Pure & Appl. Chem. 1998, 70(7), 1415–1418.


Synopsis: In this technical paper a summary of the available in situ spectroelectrochemical methods, their basic principles, their typical applications, and their limitations is given. With respect to the names of the methods and usual abbreviations, the paper follows the literature as far as possible, but tries to point out inconsistencies. An introductory section gives a summary of the basic equations and introduces the IUPAC recommendations for quantities and symbols.

This report was prepared for publication by: W. Plieth¹, G.S. Wilson² and C. Gutiérrez de la Fe³. ¹Institut für Physikalische Chemie und Elektrochemie, Technische Universität Dresden, Bergstr. 66b, D-01062 Dresden, Germany. ²Department of Chemistry, University of
Analytical aspects of chemically modified electrodes: classification, critical evaluation and recommendations (IUPAC Recommendations 1998)

Synopsis: Analytical aspects of chemically modified electrodes (CMEs) are critically reviewed. Effects of analyte and/or reagent accumulation, chemical transformation, electrocatalysis, permeability, ionic equilibria, controlled release and change of mass, as well as combinations of these effects are evaluated and classified. In addition, relevant definitions are provided and recommendations formulated for the most effective CME operation.

Guidelines for presentation of methodological choices in the publication of computational results. A. Ab initio electronic structure calculations (IUPAC Recommendations)

Synopsis: Guidelines are presented to assist authors in preparing manuscripts that describe the results of ab initio computation. These guidelines are not intended to recommend how ab initio calculations should be done, but rather to ensure that the reader can have a clear understanding of what was actually carried out. They are written in a form to facilitate reprinting in original research journals and as information sheets that can be distributed to authors and reviewers.


Synopsis: This IUPAC nomenclature document has been prepared to establish a uniform and meaningful approach to terminology, notation and formulation for calibration in analytical chemistry. In this first part, the general fundamentals of calibration are presented, namely for both relationships of qualitative and quantitative variables (relations between variables characterizing certain types of analytes and measured signals in certain positions of a measured function on the one hand and between variables characterizing the amount or concentration of the chemical species and the intensities of the measured signals, on the other hand). On this basis, the fundamentals of the common single component calibration which models the relationships
\( y = f(x) \) between the signal intensities \( y \) and the amounts or concentration are represented. Additional papers will be prepared dealing with extensive relationships between several signal intensities and analyte contents, namely with multivariate calibration and with optimization and experimental design.

This report was prepared for publication by: K. Danzer and L. A. Currie, The full details are to be found in Pure Appl. Chem. 1998, 70(4), 993–1014.

Definitions of terms relating to the non-ultimate mechanical properties of polymers (IUPAC Recommendations 1998)

Synopsis: The document gives definitions of terms related to the nonultimate mechanical behaviour of polymeric materials, in particular bulk polymers and concentrated solutions and their elastic and viscoelastic properties. The terms which have been selected are those met in the conventional mechanical characterization of isotropic polymeric materials. They have additionally been limited to those which can be defined precisely and with mathematical rigour. They are arranged in sections dealing with basic definitions of stress and strain, deformations used experimentally, stresses observed experimentally, quantities relating stress and deformation, linear viscoelastic behaviour and oscillatory deformations and stresses used experimentally for solids. An index, an alphabetical list of terms and a glossary of symbols are included for ease of reference.

This report was prepared for publication by: A. Kaye (UK), R.F.T. Stepto (UK), W. J. Work (USA), J. V. Alemán (Spain), A. Ya. Malkin (Russia). The full details are to be found in Pure Appl. Chem. 1998, 70(3), 701–754.


Synopsis: This report is the 14th in a series on Spectrochemical Methods of Analysis issued by IUPAC Commission V.4. Because of the complexity and the lack of uniformity of the present nomenclature (e.g. ‘2 step excited resonance fluorescence’, ‘resonance enhanced multiphoton ionization’, etc.) a new way is needed to describe these transitions. The aim of this document is therefore to present a new notation, the IUPAC Notation, to describe the various processes involved in atomic laser spectroscopy. Using a few assumptions, this notation has the advantage of being simple and systematic. States and processes can be described in a general way irrespective of the type of laser spectrometry.

This report was prepared for publication by: N. Omenetto, J.-M. Mermet, G.C. Turk, and D. S. Moore.

History of the recommended atomic-weight values form 1882 to 1997: A comparison of differences from current values to the estimated uncertainties of earlier values (Technical Report)

Synopsis: International commissions and national committees for atomic weights (mean relative atomic masses) have recommended regularly updated, best values for these atomic weights as applicable to terrestrial sources of the chemical elements. Presented here is a historically complete listing starting with the values in F.W. Clarke’s 1882 recalculation, followed by the recommended values in the annual reports of the American Chemical Society’s Atomic Weights Commission. From 1903, an International Commission published such reports and its values (scaled to an atomic weight of 16 for oxygen) are used here in preference to those of national committees of the UK, Germany, Spain, Switzerland and the USA. We have, however, made scaling adjustments from Ar(16O) to Ar(12C) where not negligible.

From 1920, this International Commission constituted itself under the International Union of Pure and Applied Chemistry (IUPAC). Since then, IUPAC has published reports (mostly biennially) listing the recommended atomic weights, which are reproduced here. Since 1979, these values have been called the ‘standard atomic weights’ and, since 1969, all values have been published with their estimated uncertainties. Few of the earlier values were published with uncertainties. Nevertheless, we assessed such uncertainties on the basis of our understanding of the likely contemporary judgement of the values’ reliability. While neglecting remaining uncertainties of 1997 values, we derive ‘differences’ and a retrospective index of reliability of atomic-weight values in relation to assessments of uncertainties at the time of their publication. A striking improvement in reliability appears to have been achieved since the commissions have imposed upon themselves the rule of recording
Isotopic compositions of the elements 1997 (Technical Report)

Synopsis: The Commission’s Subcommittee for the Isotopic Composition of the Elements (SIAM) has carried out its biennial review of isotopic compositions, as determined by mass spectrometry and other relevant methods. This involves a critical evaluation of the published literature, element by element, and forms the basis of the table of isotopic compositions of the elements as determined by mass spectrometry presented here. New guidelines have been used to arrive at the uncertainties on the isotopic abundances and there are numerous changes to the table since it was last published in 1991. Atomic weights calculated from this table are consistent with Ar(E) values listed in the Table of Standard Atomic Weights 1997.

This report was prepared for publication by: K.J.R. Rosman1 and P.D.P. Taylor2. 1Department of Applied Physics, Curtin University of Technology, GPO Box U1987, Perth 6001, Australia. 2Institute for Reference Materials and Measurements, European Commission-JRC, B-2440 Geel, Belgium. The full details are to be found in Pure Appl. Chem. 1998, 70(1), 217–235.

Nomenclature of fused and bridged fused ring systems (IUPAC Recommendations)

Synopsis: These recommendations constitute a comprehensive documentation for naming fused ring systems and bridged fused ring systems. It expands and extends the recommendations given in rules A-21, A-22, A-23, A-34, B-3 of the IUPAC Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 and rule R-2.4.1 of A Guide to IUPAC Nomenclature of Organic Compounds, 1993. Any ring system with two or more rings ortho- or ortho- and peri-fused together may be named by these recommendations. Two rings which are ortho-fused together have only two atoms and one bond in common. The nomenclature of spiro systems and von Baeyer nomenclature will be considered in separate recommendations.

This report was prepared for publication by: G.P. Moss. Department of Chemistry, Queen Mary and Westfield College, Mile End Road, London, E1 4NS, UK. The full details are to be found in Pure Appl. Chem. 1998, 70(1), 117–142.

Recommendations for the presentation of NMR structures of proteins and nucleic acids (IUPAC Recommendations 1998)

Synopsis: The recommendations presented here are designed to support the easier communication of NMR data and NMR structures of proteins and nucleic acids through unified nomenclature and reporting standards. Much of this document pertains to the reporting of data in journal articles; however, in the interest of the future development of structural biology, it is desirable that the bulk of the reported information be stored in computer-accessible form and be freely accessible to the scientific community in standardized formats for data exchange. These recommendations stem from an IUPAC-IUBMB-IUPAB interunion venture with the direct involvement of ICSU and CODATA. The Task Group has reviewed previous formal recommendations and has extended them in the light of more recent developments in the field of biomolecular NMR spectroscopy. Drafts of the recommendations presented here have been examined critically by more than 50 specialists in the field and have gone through two rounds of extensive modification to incorporate suggestions and criticisms.

This report was prepared for publication by: John L. Markley1, Ad Bax2, Yoji Arata3, C.W. Hilbers4, Robert Kaptein5, Brian D. Sykes6, Peter E. Wright7 and Kurt Wüthrich8. 1Department of Biochemistry, University of Wisconsin-Madison, Madison, WI, USA. 2Laboratory of Chemical Physics, NIDDK, National Institutes of Health, Bethesda, MD, USA. 3Water Research Institute, Tsukuba, Japan. 4Laboratory of Biophysical Chemistry, University of Nijmegen, the Netherlands. 5Department of Chemistry, University of Utrecht, the Netherlands. 6Department of Biochemistry, University of Alberta, Edmonton, Alberta, Canada. 7Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, USA. 8Institut für Molekularbiologie und Biophysik, ETH Hönggerberg, Zürich, Switzerland (convenor of the task group to whom correspondence should be addressed). The full details are to be found in Pure Appl. Chem. 1998, 70(1), 117–142.