Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry*.

Methods for the analysis of transient absorbance data (Technical Report)

Synopsis

Procedures for the generation and collection of transient UV-visible absorbance data are briefly reviewed. Problems associated with signal generation (scattered

light, inhomogeneous distribution of transients, instability of pulsed light sources), signal detection (averaging, filtering) and signal analysis in kinetic and spectrographic flash photolysis are addressed. Methodology for the fitting of model functions to absorbance data that depend on up to three variables (time, wavelength and, e.g. temperature) is discussed.

This report was prepared for publication by Roland Bonneau (LA 348 du CNRS, Université de Bordeaux I, F-33405 Talence Cedex, France), Jakob Wirz (Institut für Physikalische Chemie, Universität Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland) and Andreas D. Zuberbühler (Institut für Anorganizche Chemie, Universität Basel, Spitalstrasse 51, CH-4056 Basel, Switzerland) for the Commission on Photochemistry of the Organic Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 979–992.*

Molecular characterization of commercial polypropylene with narrow and broad distribution of molar mass (Technical Report)

Synopsis

The molar mass and the molar mass distribution of two commercial grades of isotactic polypropylene, Moplen S30S of Himont Srl and Daplen PT55 of PCD Polymere GmbH, were investigated by 16 laboratories. For Moplen S30S M_w = 467 kg/mole ± 6.0% (relative standard deviation), M_n = 83.7 kg/mole ± 9.8% and M_w/M_n = 5.70 ± 10.1% were determined by size exclusion chromatography (31 SEC runs), for Daplen PT55 M_w = 206 kg/mole ± 13.6%, M_n = 61.4 kg/mole ± 13.4% and M_w/M_n = 3.42 ± 17.3% were found (38 SEC runs). Light scattering measurements gave M_w = 445 kg/mole ± 4.1% for Moplen S30S (4 labs) and M_w = 212 kg/mole ± 10% for Daplen PT55 (3 labs). The intrinsic viscosity in 1,2,4-trichlorobenzene at 140 °C of Moplen S30S [η] = 1.87 dl/g ± 5.4% and of Daplen PT55 [η] = 1.12 dl/g ± 6.7% was measured (nine independent measurements). Samples of the respective lots are available from the authors, Moplen S30S from IM, Daplen PT55 from KL.

This report was prepared for publication by K. Lederer (Institut für Chemie der Kunststoffe, Montanuniversität Leoben, A-8700 Leoben, Austria) and I. Mingozzi (Himont Italia, Centro Ricerche G. Natta, I-44100 Ferrara, Italy) for the Working Party on Molecular Characterization of Commercial Polymers, Commission on Polymer Characterization and Properties, Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 993–1006.*

Reference Value Standards and Primary Standards for pH measurements in D_2O and aqueous-organic solvent mixtures: New accessions and assessments (Technical Report)

Synopsis

Recommended Reference Value Standards based on the potassium hydrogen phthalate buffer at various temperatures are reported for pH measurements in various binary solvent mixtures of water with eight organic solvents: methanol, ethanol, 2-propanol, 1,2-ethanediol, 2-methoxyethanol ('methylcellosolve'), acetonitrile, 1,4-dioxane and dimethyl sulfoxide, together with Reference Value Standards based on the potassium deuterium phthalate buffer for pD measurements in D_2O. In addition are reported Primary Standards for pH based on numerous buffers in various binary solvent mixtures of water with methanol, ethanol and dimethyl sulfoxide, together with Primary Standards for pD in D_2O based on the citrate, phosphate and carbonate buffers.

This report was prepared for publication by P. R. Mussini, T Mussini and Sandra Rondinini (Department of Physical Chemistry and Electrochemistry, University of Milan, 20133 Milano, Italy) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1007–1014.*

Properties and units in the clinical laboratory sciences. II: Kinds-of-property (IUPAC Recommendations 1997)

Synopsis

The document circumscribes the concept 'kind-of-property' (property in a general sense) and lists the kinds-of-property mostly used in the clinical laboratory sciences. The concepts are as defined in the 'Compendium of terminology and nomenclature of properties in clinical laboratory sciences', except for a few that are defined intuitively. Each is given a unique code value and is expressed in different languages for use in the assembly of terms representing individual properties.

This report was prepared for publication by Desmond Kenny (Our Lady's Hospital for Sick Children, Crumlin, Dublin 12, Ireland) and Henrik Olesen (Department of Clinical Pharmacology, Copenhagen University Hospital, Copenhagen, Denmark) for the Committee on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1015–1042.*

Properties and units in the clinical laboratory sciences. V: Properties and units in thrombosis and haemostasis (Technical Report)

Synopsis

For historical reasons, the elements of properties (terms) used in the nomenclature for properties in thrombosis and haemostasis differ according to 'school' of thought. This hampers communication. In collaboration, the Scientific and Standardization Committee of the International Society on Thrombosis and Haemostasis and the Commission (Committee) of Nomenclature, Properties and Units, previously 'Quantities and Units', have prepared a set of recommended systematic names for properties in that domain. For use in electronic transmission each property has been given a code value. The prefix to the code values has been changed from 'QU' to 'NPU' because of the change of name of the Commission (Committee).

This report was prepared for publication by M. Blombäck (Department of Clinical Chemistry and Blood Coagulation, Karolinska Hospital, Stockholm, Sweden), R. Dybkaer (Department of Clinical Chemistry, Frederiksberg Hospital, Copenhagen, Denmark), K. Jørgensen (Department of Clinical Biochemistry KB 3011, Copenhagen University Hospital, Copenhagen, Denmark), H. Olesen (Department of Clinical Pharmacology Q 7642, Copenhagen University Hospital, Copenhagen, Denmark) and S. Thorsen (Department of Clinical Biochemistry KB 3011, Copenhagen University Hospital, Copenhagen, Denmark) for the Commission on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division (in collaboration with the Scientific and Standardization Committee of the International Society on Thrombosis and Haemostasis). The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1043–1079.*

Properties and units in the clinical laboratory sciences. VI: Properties and units in IOC prohibited drugs (Technical Report)

Synopsis

The term designating a substance being an active ingredient of a drug may be a generic name, a non-proprietary name, a registered trade name, a fantasy name or other. This causes difficulties in the transmission of request and report on such substances to and from the clinical laboratories, and in the collating of this information from different sources. The document comprises a list of properties of drugs of abuse in biological fluids as defined by the International Olympic Committee Medical Code for use in electronic transmission systems. Standard systematic names are presented with a code value for each. The coding schemes thus prepared are accessible on the Internet from the Commission on Nomenclature, Properties and Units' Home Page address: http://inet.uni-c.dk/~qukb7642.

This report was prepared for publication by H. Olesen (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark), D. Cowan (Drug Control Centre, London University, King's College, London, UK), I. Bruunshuus (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark), K. Klempel (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark) and G. Hill (Department of Clinical Chemistry, Hospital for Sick Children, Toronto, Ontario, Canada) for the Commission on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1081–1136.*

Glossary of terms used in computational drug design (IUPAC Recommendations 1997)

Synopsis

Computational drug design is a rapidly growing field which is now a very important component in the discipline of medicinal chemistry. At the same time many medicinal chemists lack significant formal training in this field and may not have a clear understanding of some of the terminology used but need to grasp concepts, follow research results, define problems for, and utilize findings of, computational drug design. In this context the IUPAC Medicinal Chemistry Section Committee felt it would be useful to develop a glossary of terms used in computational drug design for easy reference purposes. Also there is the possibility that in different countries certain terms may not have the same meaning and in such a case there would be value in trying to establish an international definition standard. Accordingly a Working Party of seven experts in the field was assembled who constructed a glossary of some 100 terms. Concise but sufficiently explanatory definitions have been formulated based on a variety of literature sources and selected key references provided.

This report was prepared for publication by H. van de Waterbeemd, Chairman (F. Hoffmann-La Roche, Pharma Research New Technologies, CH-4070 Basel, Switzerland), R.E. Carter (Astra Hässle AB, Computational Chemistry, S-43183 Mölndal, Sweden), G. Grassy (Centre de Biochimie Structurale, Faculté de

Pharmacie, F-34060 Montpellier, France), H. Kubinyi (BASF AG, ZHB/W A30, D-67056 Ludwigshafen, Germany), Y.C. Martin (Abbott Laboratories, Computer-Assisted Molecular Design, Abbott Park, IL 60064-3500, USA), M.S. Tute (University of Canterbury, Kent CT2 7NH, UK) and P. Willett (University of Sheffield, Department of Information Studies, Sheffield S10 2TN, UK) for the Medicinal Chemistry Section of the Chemistry and Human Health Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1137–1152.*

Intrinsic characterization of continuous carbon fibre thermoplastic composites. 3: Fatigue crack growth (Technical Report)

Synopsis

This paper reports some fatigue crack growth results obtained on unidirectional laminates of AS4/PEEK. Crack growth is intralaminar and the study has included the influence of laminate thickness, method of consolidation and level of applied stress level. Presentation of data is by a Paris Law type approach, where crack growth per cycle is plotted against a stress field intensity factor. The measurements have involved four different laboratories and therefore it has been possible to attempt to embrace the likely scatter involved in the collection of fatigue data commensurate when several laboratories conduct seemingly similar measurements.

This report was prepared for publication by D.R. Moore (ICI plc, Wilton, Middlesbrough, Cleveland, UK) and J.C. Seferis (Polymeric Composites Laboratory, University of Washington, Seattle, USA) for the IUPAC Working Party IV.2.1: Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1153–1161.*

Guidelines for publication of equations of state. I: Pure fluids (Technical Report)

Synopsis

During recent decades equations of state have become a major tool for the correlation and prediction of thermodynamic properties of fluids. Equations of state can be applied to pure substances as well as to mixtures, and therefore a very large number of publications deal with the development or improvement of equations of state. In order to give authors, editors and reviewers of publications on new equations of state some guidelines and to ensure that future publications will be more profitable for the reader, some criteria for pure fluids are given that ought to be fulfilled by a good manuscript.

This report was prepared for publication by U.K. Deiters (Institut für Physikalische Chemie, Universität zu Köln, D-50939 Köln, Germany) and K.M. de Reuck (Chemical Engineering Department, Imperial College of Science, Technology & Medicine, London SW7 2BY, UK) for the Commission on Thermodynamics of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1237–1249.*

Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997)

Synopsis

The glossary contains definitions and (where needed) explanatory notes for about 400 terms used in the multidisciplinary field of bioinorganic chemistry. A need has been recognized for globally acceptable definitions of terms in this field and this glossary was compiled with the objective of fulfilling this need. It is by no means a comprehensive dictionary. The terms selected were those considered essential and/or widely used. The definitions given reflect current usage and complement IUPAC guidelines. Abbreviations and acronyms, frequently used in bioinorganic chemistry, are included.

This report was prepared for publication by M.W.G. de Bolster (Vakgroep Organische en Anorganische Chemie, Faculteit der Scheikunde, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands) for the Working Party on IUPAC Glossary of Terms Used in Bioinorganic Chemistry of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1251–1303.*

Characterization of SiC powders and the influence of powder properties on sintering (Technical Report)

Synopsis

This report summarizes the characteristics of SiC powders which influence the ability to obtain fully dense (non-porous) ceramics, with good mechanical properties, via the sintering process. Methods for characterizing powder properties, such as particle size, morphology, bulk and surface chemistry, are outlined and specific examples are referenced. The characteristics of typical commercial SiC powders are tabulated.

This report was prepared for publication by G. Schwier and I. Teusel (H.C. Starck GmbH & Co. KG, D-38642 Goslar, Germany) and M.H. Lewis (Centre for Advanced Materials, University of Warwick, Coventry CV4

7AL, UK) for the Commission on High Temperature Materials and Solid State Chemistry of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1305–1316.*

Chemically modified electrodes: Recommended terminology and definitions (IUPAC Recommendations 1997)

Synopsis

Chemically modified electrodes (CMEs) comprise a relatively modern approach to electrode systems that finds utility in (1) a wide spectrum of basic electrochemical investigations, including the relationship of heterogeneous electron transfer and chemical reactivity to electrode surface chemistry, electrostatic phenomena at electrode surfaces and electron and ionic transport phenomena in polymers, and (2) the design of electrochemical devices and systems for applications in chemical sensing, energy conversion and storage, molecular electronics, electrochromic displays, corrosion protection and electro-organic syntheses. Compared with other electrode concepts in electrochemistry, the distinguishing feature of a CME is that a generally thin film of a selected chemical is bonded or coated onto the electrode surface to endow the electrode with the chemical, electrochemical, optical, electrical, transport and other desirable properties of the film in a rational, chemically designed manner. In this report, the authors have attempted to identify and define the most widely used terminology in the growing field of CMEs and to recommend a particular term in cases where a multiplicity of terms has arisen over the past several years or where previously defined terms have taken on broadened meanings for the special cases of CMEs.

This report was prepared for publication by R.A. Durst (Analytical Chemistry Laboratories, Cornell University, Geneva, NY 14456, USA), A.J. Bäumner (Institute for Technical Biochemistry, University of Stuttgart, D-70569 Stuttgart, Germany), R.W. Murray and R.P. Buck (Department of Chemistry, University of North Carolina, Chapel Hill, NC 27514, USA) and C.P. Andrieux (Laboratoire d'Électrochimie Moléculaire, Université de Paris 7, 75251 Paris Cedex 05, France) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1317–1323.*

Consistency of pH standard values with the corresponding thermodynamic acid dissociation constants (Technical Report)

Synopsis

With the simplest possible assumptions on the ion activity coefficients, namely a Debye–Hückel approach, pH values of eleven standard buffer solutions have been calculated from the corresponding thermodynamic acidity constants, $K_{(I\to 0)}$, and compared to the electrometrically assigned pH(S) values (by Harned cell method). Agreement is within ± 0.01 in the temperature range 10–40 °C for all standards, except carbonate. The results for the phthalate, acetate, phosphate and carbonate systems at 25 °C indicate that this consistency is improved if specific ion interactions are taken into account, according to the Pitzer theory.

This report was prepared for publication by M. Filomena Camoes and M.J. Guiomar Lito (Centro de Electroquímica e Cinética da Universidade de Lisboa, 1294 Lisboa Codex, Portugal), M. Isabel A. Ferra (Universidade da Beira Interior, 6200 Covilhã, Portugal) and Arthur K. Covington (Department of Chemistry, University of Newcastle, Newcastle-upon-Tyne, NE1 7RU, UK) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1325–1333.*

Chirality in synthetic agrochemicals: Bioactivity and safety consideration (Technical Report)

Synopsis

Most synthetic agrochemicals with chiral structures are marketed as racemates even though the desired biological activity may be derived from only one enantiopure isomer. However, some synthetic agrochemicals such as pyrethroid insecticides, aryloxypropanoate herbicides and triazole fungicides are marketed as the most biologically active enantiopure isomer. Numerous reports describing the relative biological activities, preparations and analyses of enantiopure agrochemicals are available. Some examples of how different enantiomers in racemates are selectively metabolized have also been reported. When agrochemicals have chiral structures, efforts should be made to define the mode of action, elucidate metabolic pathways and to define the human and environmental toxicity of each enantiopure isomer. If there are large differences in the biological activities of individual enantiomers in racemates, it is desirable to develop and use only the enantiopure isomer with the highest

sought-after biological activities.

This report was prepared for publication by N. Kurihara (Radioisotope Research Center, Kyoto University, Kyoto 606-01, Japan), J. Miyamoto (Sumitomo Chemical Co. Ltd, Osaka 541, Japan), G.D. Paulson (US Department of Agriculture, ARS, Fargo, ND 58105, USA), B. Zeeh (BASF AG, Agricultural Research Station, D-67114 Limburgerhof, Germany), M.W. Skidmore (Zeneca Agrochemicals, Jealotts Hill, Bracknell, Berks., RG42 6EY, UK), R.M. Hollingworth (Pesticide Research Center, Michigan State University, East Lansing, MI 48824, USA) and H.A. Kuiper (State University for Quality Control of Agricultural Products, Rikult-Dlo Wageningen, The Netherlands) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1335–1348.*

Pesticide fate in tropical soils (Technical Report)

Synopsis

Pesticide use is an important component of agricultural and non-agricultural pest control in tropical areas. However, the fate of pesticides in tropical soils is not as well understood as that for soils from temperate regions. Tropical soils defy easy generalizations, but they are typically very old soils characterized by year-round uniformity of temperature regime. Although only a few studies have directly compared pesticide fate in tropical and temperate soils, there is no evidence that pesticides degrade more slowly under tropical conditions. Laboratory studies in which soils have been held under standardized conditions reveal that pesticide degradation rate and pathway are comparable between tropical and temperate soils. However, field investigations of tropical pesticide soil fate indicate that dissipation occurs more rapidly, in some cases much more rapidly, than for pesticides used under similar temperate conditions. The most prominent mechanisms for this acceleration in pesticide dissipation appear to be related to the effect of tropical climates, and would include increased volatility and enhanced chemical and microbial degradation rates on an annualized basis.

This report was prepared for publication by K.D. Racke (DowElanco, Indianapolis, IN, USA), M.W. Skidmore (Zeneca Agrochemicals, Bracknell, Berkshire, UK), D.J. Hamilton (Resources Sciences Centre, Indooroopilly, Queensland 4068, Australia), J.B. Unsworth (Rhône-Poulenc, Ongar, Essex, UK), J. Miyamoto (Sumitomo Chemical Company, Osaka 541, Japan) and S.Z. Cohen (Environmental and Turf Services, Wheaton, MD, USA) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1349–1371.*

Optimum use of available residue data in the estimation of dietary intake of pesticides (Technical Report)

Synopsis

Prediction of pesticide residue intake in human diets is vital for approving the use of pesticides and for gaining official acceptance of pesticide residue levels which occur in food commodities in international trade. Estimates for pesticide residue levels likely to be present in food as consumed are derived from supervised pesticide residue trials, residue monitoring, pesticide metabolism and food processing studies. The results of properly conducted total diet studies should generally displace other estimates, but they do not cover all pesticides and, in particular, are not available for a pesticide at its initial registration. Information was compiled on the range of residues occurring in a set of supervised residue trials with identical application rate, number of applications and pre-harvest interval, but at different sites with various crop varieties, operators, equipment and cultural practices. Eighteen recommendations are provided for estimating the level of pesticide residues likely to be present in food as consumed.

This report was prepared for publication by D.J. Hamilton (Resources Sciences Centre, Indooroopilly, Queensland 4068, Australia), P.T. Holland (Horticulture and Food Research Institute of New Zealand Ltd, Hamilton, New Zealand), B. Ohlin (National Food Administration, Uppsala, Sweden), W.J. Murray (Pest Management Regulatory Agency, Health Canada, Ottawa, Canada), A. Ambrus (Plant Health and Soil Conservation Centre, Budapest, Hungary), G.C. de Baptista (Departmento de Entomologia, Universidade de São Paulo, Brazil) and J. Kovacicová (Institute of Preventive and Clinical Medicine, Bratislava, Slovakia) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1373–1410.*