

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*.

Nomenclature and terminology of fullerenes: a preliminary survey

Synopsis

Some difficult problems are encountered with fullerene molecules, in particular with regard to numbering, the description of isomers having the same symmetry, the question of describing ring systems attached to the fullerene structure, and indeed how to define a fullerene adequately in the first place. A set of proposals is presented for naming the principal fullerene structures and some of their derivatives, using IUPAC nomenclature principles and practices insofar as they can be taken to apply, together with usages developed by the Chemical Abstracts Service (CAS), cited wherever such comparison has been considered useful.

This Report was prepared for publication by E.W. Godly (10 Lawrence Avenue, New Malden, Surrey KT3 5LY, UK) and R. Taylor (Chemistry Laboratory, CPES Building, University of Sussex, Falmer, Brighton BN1 9QJ, UK). The full details are to be found in Pure Appl. Chem. 1997, 69, 1411–1434.

Nomenclature, symbols, units and their usage in spectrochemical analysis—XVI. Laser-based molecular spectroscopy for chemical analysis—luminescence (IUPAC Recommendations 1997)

Synopsis

This report is the 16th in a series on spectrochemical methods of analysis issued by IUPAC Commission V.4. It is concerned with the use of lasers in molecular spectroscopy dealing with luminescence.

This Report was prepared for publication by T. Vo-Dinh (Health Sciences Research Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6101, USA), N.H. Velthorst (Department of Analytical Chemistry, Free University, 1081 HV Amsterdam, the Netherlands), D.S. Moore (Chemical and Laser Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA) and B. Schrader (Institut für Physikalische und Theoretische Chemie, Universität-GH-Essen, D-

45117, Essen, Germany) for the Commission on Spectrochemical and Other Optical Procedures for Analysis of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1435–1449.

Nomenclature symbols, units and their usage in spectrochemical analysis—XVIII. Laser-based molecular spectroscopy for chemical analysis: Raman scattering processes (IUPAC Recommendations 1997)

Synopsis

This report is 18th in a series on spectrochemical methods of analysis issued by IUPAC Commission V.4. It is concerned with Raman scattering processes, usually induced by lasers, covering the UV, visible, and near infrared spectral regions. Raman scattering can be divided into linear and non linear processes. Due to their importance for chemical analysis, mainly the linear Raman effects are treated.

This Report was prepared for publication by B. Schrader (Institut für Physikalische und Theoretische Chemie, Universität-GH-Essen, D-45117 Essen, Germany) and D.S. Moore (Chemical Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA) for the Commission on Spectrochemical and Other Optical Procedures for Analysis of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1451–1468.

Analytical chiral separation methods (IUPAC Recommendations 1997)

Synopsis

In recent years there has been considerable interest in the synthesis and separation of enantiomers of organic compounds especially because of their importance in the biochemistry and pharmaceutical industry. Frequently the methods used for the separations, for monitoring the progress of an asymmetric synthesis or optical purity of the products are chromatographic with liquids, gases or supercritical fluids as the mobile phase. More recently capillary electrophoresis has

been added as an analytical chiral separation method. These applications have led to a number of terms and expressions in addition to those commonly used or recently recommended for the chemistry and physical properties of chiral compounds. This Nomenclature provides the descriptions and definitions for additional terms particularly related to analytical separation methods, and to the formation and enantiomeric purity of chiral products.

This Report was prepared for publication by Vadim A. Davankov (Nesmeyanov-Institute of Organo-Element Compounds, Russian Academy of Sciences, Moscow 117813, Russia) for the Commission on Separation Methods in Analytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1469–1474.

Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology (IUPAC Recommendations 1997)

Synopsis

A wide range of stationary phases and column packing materials have been developed over the years for liquid chromatography and these need to be described accurately and unambiguously. The present paper, which is the first of a series planned for this area, recommends terms for the description of the stationary phase materials and their properties and expands the list of terms given in Nomenclature of Chromatography (*Pure Appl. Chem.* 1993, **65**, 819–872). It concentrates on the chemical properties and chromatographic role of the materials. Many of the terms to describe their physical properties as particles have been discussed in a recent paper on the characterization of porous solids (*Pure Appl. Chem.* 1994, **66**, 1739–1758).

This Report was prepared for publication by Roger M. Smith (Department of Chemistry, Loughborough University, Loughborough, Leics. LE11 3TU, UK) and Aurél Marton (Department of Analytical Chemistry, University of Veszprém, PO Box 158, H-8201, Veszprém, Hungary) for the Commission on Separation Methods in Analytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1475–1480.

Classification and characterization of stationary phases for liquid chromatography: Part II. Characterization of ion exchange chromatographic stationary phases (IUPAC Recommendations 1997)

Synopsis

In order to characterize ion exchange chromatographic stationary phases, the thermodynamic exchange constant and the free energy interaction parameters are recommended. These parameters are calculated from the experimentally available corrected selectivity coefficient vs. exchanger phase composition functions. The equations used for the calculations have been obtained by introducing the Friedman equation (developed for the calculation of the excess free energy change) into the thermodynamic derivation. The suggested parameters also make possible the estimation of the value of the selectivity coefficient at an arbitrary exchanger phase composition. The characteristic parameters of the ion exchange resins and the equations in a directly suitable form for the estimation of the selectivity coefficient are calculated and presented for several systems.

This Report was prepared for publication by Aurél Marton (Department of Analytical Chemistry, University of Veszprém, PO Box 158, H-8201, Veszprém, Hungary) for the Commission on Separation Methods in Analytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1481–1487.

Critical survey of stability constants of complexes of thiocyanate ion (Technical Report)

Synopsis

Presented is a review of the stability constants for metal complexes with thiocyanate ion. The literature data presented are critically discussed and recommended values, where warranted, listed from the many studies cited.

This Report was prepared for publication by Abraha Bahta (Department of Chemistry & Biochemistry, University of California-Los Angeles, Los Angeles, CA 90024-1569, USA), Gordon A. Parker (Department of Natural Sciences, University of Michigan-Dearborn, Dearborn, MI 48128-1491, USA) and Dennis G. Tuck (Department of Chemistry & Biochemistry, University of Windsor, Windsor, Ontario, Canada) for the Commission on Equilibrium Data of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1489–1548.

Critical survey of stability constants of metal-imidazole and metal-histamine systems (Technical Report)

Synopsis

Thermodynamic data for the proton and metal ion complexation equilibria of imidazole (1,3-diazole, glyoxaline) and histamine (4-imidoazoethylamine, 4-(2'-aminoethyl)imidazole) have been collected and critically evaluated. The literature search has been performed by using IUPAC's 'Stability Constants Database' and covers the literature until 1992. Important criteria for acceptance comprise specification of the essential reaction conditions, the correctness of calibration techniques and appropriate equilibrium analysis of experimental data. Recommended values with respect to proton-ligand and metal ion-ligand equilibria have been tabulated. Furthermore, the medium dependence of these reactions has been evaluated using an extended Debye-Hückel expression.

This Report was prepared for publication by Staffan Sjöberg (Department of Inorganic Chemistry, Umeå University, S-90187 Umeå, Sweden) for the Commission on Equilibrium Data of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1549-1570.

The importance of natural organic material for environmental processes in waters and soils (Technical Report)

Synopsis

The role and function of natural organic material (NOM) for the terrestrial and aquatic environment is strongly related to nutrient availability for plants, relevant for crop production, as well as to be a source of energy for macro- and microorganisms, to influence physico-chemical conditions of soil and sediments and to buffering and exchange capacity, relevant for the immobilization and mobilization of environmental pollutants. This article reviews the available information about the importance of natural organic material for environmental processes in water and soil. After explaining general terms regarding natural organic material and its chemical structure and presenting the actual state of analytical methods, interactions between environmental variables and the natural organic material as regards its formation and behaviour, as well as interactions between natural organic material and the fate of pollutants in the terrestrial and aquatic environment are discussed emphasizing some relevant processes such as sorption, mobility and bioavailability. Finally some aspects on modelling such processes are presented.

This Report was prepared for publication by W. Kördel (Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, Auf dem Aberg 1, Graftschaff, D-57392 Schmallingenberg, Germany), M. Dassenakis (Department of Chemistry, Section III, University of Athens, 15 Athens, Greece), J. Lintemann (Institut für Ökologische Chemie, GSF Forschungszentrum für Umwelt und Gesundheit GmbH, Postfach 1129, 85758 Oberschleissheim, Germany) and S. Padberg (Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, Auf dem Aberg 1, Graftschaff, D-57392 Schmallingenberg, Germany) for the Commission on Soil and Water Chemistry of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1571-1600.

Calculation and application of coverage intervals for biological reference values: a supplement to the approved IFCC recommendation (1987) on the theory of reference values (Technical Report)

Synopsis

The costs of sampling and analysis of samples are sometimes too high to obtain 120 or more reference values as recommended by the International Federation of Clinical Chemistry (IFCC). Here coverage intervals should be used to give a statistically well defined measure of the uncertainty of the interval. Additionally, when many reference values are available, the coverage interval may provide useful information on the distribution. Hence, extending the IFCC recommendation, the calculation and presentation of the 0.95 coverage interval is recommended, together with information on its coverage uncertainty with a probability of at least 0.95. Non-parametric coverage intervals can be calculated regardless of the distribution of reference values, and parametric coverage intervals can be calculated if transformation of the distribution of reference values to a normal distribution is feasible. The Report gives guidance in calculating both types of intervals. However, in agreement with IFCC, the non-parametric intervals are recommended, thus avoiding the transformation step. A numerical example concerning coverage intervals for blood lead concentration is presented.

This Report was prepared for publication by O.M. Poulsen, E. Holst and J.M. Christensen (National Institute of Occupational Health, Denmark, Lersøe Parkallé 105, DK-2100 Copenhagen, Denmark) for the Commission on Toxicology of the Clinical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1601-1611.

Biotransformations of non-natural compounds: state of the art and future development

Synopsis

The transformation of non-natural compounds by enzymes—generally referred to as ‘biocatalysis’—has evolved as a trend-section of organic synthesis during the mid-1980s. As a consequence, a remarkable number of reliable biochemical techniques have been developed during the last decade, which constitute powerful tools for modern organic synthesis. In this report, the state of the art of biotransformations as well as future developments are critically reviewed with respect to strengths and weaknesses of the existing methods.

This Report was prepared for publication by Kurt Faber (Institute of Organic Chemistry, Graz University of Technology, Stremayrgasse 16, A-8010 Graz, Austria) for the Commission on Biotechnology. The full details are to be found in Pure Appl. Chem. 1997, 69, 1613–1632.

Notations and conventions in molecular spectroscopy: Part 1. General spectroscopic notation (IUPAC Recommendations 1997)

Synopsis

The field of molecular spectroscopy was surveyed in order to determine a set of conventions and symbols which are in common use in the spectroscopic literature. This document, which is Part 1 in a series, establishes the notations and conventions used for general spectroscopic notations and deals with quantum mechanics, quantum numbers (vibrational states, angular momentum and energy levels), spectroscopic transitions and miscellaneous notations (e.g. spectroscopic terms).

This Report was prepared for publication by C.J.H. Schutte (University of South Africa, PO Box 392, Pretoria 0001, South Africa), J.E. Bertie (Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2), P.R. Bunker (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada), J.T. Hougen (Molecular Physics Division, National Institute for Standards and Technology, Gaithersburg, Maryland 20899, USA), I.M. Mills (Department of Chemistry, University of Reading, Whiteknights, Reading RG6 2AD, UK), J.K.G. Watson (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada) and B.P. Winnewisser (Justus Liebig Universität, Physikalisch-Chemisches Institut, Heinrich-Buff-Ring

58, D-6300 Giessen, Germany) for the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1633–1639.

Notations and conventions in molecular spectroscopy: Part 2. Symmetry notation (IUPAC Recommendations 1997)

Synopsis

The field of molecular spectroscopy was surveyed in order to determine a set of conventions and symbols which are in common use in the spectroscopic literature. This document, which is Part 2 in a series, establishes the notations and conventions used for the description of symmetry in rigid molecules, using the Schoenflies notation. It deals firstly with the symmetry operators of the molecular point groups (also drawing attention to the difference between symmetry operators and elements). The conventions and notations of the molecular point groups are then established, followed by those of the representations of these groups as used in molecular spectroscopy.

This Report was prepared for publication by C.J.H. Schutte (University of South Africa, PO Box 392, Pretoria 0001, South Africa), J.E. Bertie (Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2), P.R. Bunker (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada), J.T. Hougen (Molecular Physics Division, National Institute for Standards and Technology, Gaithersburg, Maryland 20899, USA), I.M. Mills (Department of Chemistry, University of Reading, Whiteknights, Reading RG6 2AD, UK), J.K.G. Watson (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada) and B.P. Winnewisser (Justus Liebig Universität, Physikalisch-Chemisches Institut, Heinrich-Buff-Ring 58, D-6300 Giessen, Germany) for the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1641–1649.

Notations and conventions in molecular spectroscopy: Part 3. Permutation and permutation–inversion symmetry notation (IUPAC Recommendations 1997)

Synopsis

The field of molecular spectroscopy was surveyed in order to determine a set of conventions and symbols which are in common use in the spectroscopic literature. This document, which is Part 3 in a series, deals with

symmetry notation referring to groups that involve nuclear permutations and the inversion operation.

*This Report was prepared for publication by P.R. Bunker (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada), C.J.H. Schutte (University of South Africa, PO Box 392, Pretoria 0001, South Africa), J.T. Hougen (Molecular Physics Division, National Institute for Standards and Technology, Gaithersburg, Maryland 20899, USA), I.M. Mills (Department of Chemistry, University of Reading, Whiteknights, Reading RG6 2AD, UK), J.K.G. Watson (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada) and B.P. Winnewisser (Justus Liebig Universität, Physikalisch-Chemisches Institut, Heinrich-Buff-Ring 58, D-6300 Giessen, Germany) for the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1651–1657.*

Nomenclature of inorganic chains and ring compounds (IUPAC Recommendations 1997)

Synopsis

A systematic, additive approach to name inorganic chain and cyclic compounds is introduced. The method does not require any prior knowledge about the nature of bonds between the atoms. Though the method can be applied to all compounds, its use is mainly intended for inorganic compounds which are mainly composed of atoms other than carbon. In the case of neutral chain frameworks the compound is called 'catena' preceded by a multiplicative prefix 'di-', 'tri-', etc., to indicate the number of branches in the molecule. Likewise cyclic compounds are called 'cycle' preceded by the appropriate multiplicative prefix. A mixed chain and ring compound is named as 'catenacycle'. In the case of charged species the names are modified by the suffixes '-ium' and '-ate'. The connectivity in the framework is indicated by a nodal descriptor which is placed in square brackets immediately before the terms 'catena', 'cycle' or 'catenacycle'. In simple chain and ring compounds it is permissible to replace the nodal descriptor with a numeric indicator [*n*] when *n* is the number of atoms in the principal chain or ring. The atoms are numbered according to the general nodal nomenclature regardless of their chemical identity. Only in the case of ambiguity is the chemical nature of the atoms taken into consideration. The atoms forming the nodal skeleton are listed in alphabetical order complete with their locants and are named by modifying the element radical names in Table VII of 'Nomenclature of Inorganic Chemistry' by substi-

tuting '-y' for the terminal '-io'. Atoms and groups of atoms which are not a part of the nodal framework are named as ligands and are cited in alphabetical order together with their locants before the cited sequence of the atoms constituting the nodal framework.

*This Report was prepared for publication by E.O. Fluck (Gremlin-Institut für Anorganische Chemie und Grenzgebiete der Max-Planck-Gesellschaft, Carl Bosch Haus, Varrentrappstrasse 40–42, D-60486, Frankfurt, Germany) and R.S. Laitinen (Department of Chemistry, University of Oulu, Linnanmaa, FIN-90570 Oulu, Finland) for the Commission on Nomenclature of Inorganic Chemistry of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1659–1692.*

Characterization of finite length composites: Part I. Introductory paper (Technical Report)

Synopsis

A project representing a sizeable effort of IUPAC Working Party 4.2.1 on two thermoplastic matrices reinforced with three different fibre types and involving two different injection techniques is introduced in terms of its objectives, adopted strategy, materials, main variables, outcome reporting and participating laboratories. The paper outlines details (constituents, composites, injection moulding, mould cavity) common to all undertaken studies. At the same time it summarizes the major outcome in terms of moulding anisotropy and heterogeneity as both controlled by the constituting materials—matrix and fibre and processing conditions used for moulding preparation. More detailed information which is contained in publications dedicated to individual areas under investigation, namely to: (1) mechanical performance of injected moulded composites, (2) studies on thin sections extracted from mouldings (wafers), (3) determination of structural aspects of composites, (4) modelling of stiffness and (5) rheological studies, is referred to in appropriate places.

*This Report was prepared for publication by A. Cervenka (Shell Research BV, Koninklijke/Shell Laboratorium Amsterdam, the Netherlands) and P.S. Allan (Brunel University, The Wolfson Centre for Materials Processing, Uxbridge, Middlesex, UK) for the Working Party on Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1693–1705.*

Characterization of finite length fibre composites. Part II. Mechanical performance of injection moulded composites (Technical Report)

Synopsis

An overview is given of the mechanical performance (stiffness, strength, toughness, creep...) of finite fibre length reinforced thermoplastics based on polypropylene and polyamide as the matrices and glass, carbon and Kevlar as the reinforcement. Different degrees of fibre orientation distribution and fibre attrition as produced by classical injection moulding and multiple-live feed moulding were evaluated. It was found that the simple test geometry used (injection moulded plaques) resembled more a complicated structure than a material. The properties measured therefore were more the complex response of a strongly anisotropic structure than simple material properties. Increased alignment of the fibres in a given direction affected all the mechanical properties, but the effect was largest for the tensile stiffness. A higher degree of fibre orientation was not accompanied by an increase in properties related to failure (ultimate stress). The modelling of ultimate stress showed that this could be explained by the more severe fibre attrition which resulted from the forces applied to orient the fibres.

This Report was prepared for publication by L. Glas (Shell Research SA, Chemical Research Centre Shell, Louvain-la-Neuve, Belgium), P.S. Allan (Brunel University, The Wolfson Centre for Materials Processing, Uxbridge, Middlesex, UK), T Vu-Khanh (Université de Sherbrooke, Faculté des Sciences Appliquées, Département de Génie Mécanique Sherbrooke (Quebec), Canada) and A. Cervenka (Shell Research BV, Koninklijke/Shell Laboratorium Amsterdam, the Netherlands) for the Working Party on Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1707-1723.

Characterization of finite length composites: Part III. Studies on thin sections extracted from mouldings (wafers) (Technical Report)

Synopsis

Through-thickness aspects of composites are studied by means of structural investigations and mechanical testing of thin 'wafers' machined from moulded specimens. Two injection moulding regimes, namely the Dynamic and Static mode, have been used to induce different fibre orientations in polypropylene (PP) rein-

forced with glass (g) and polyamide (PA) reinforced with carbon (c). Novel experimental techniques such as the 'rebound technique', uniaxial compressive yield and flexural testing of circular discs have been used for evaluation of longitudinal and transverse properties. A strong anisotropy of properties in composite mouldings is governed by the spatial fibre orientation. This depends on both the matrix and the processing conditions used with the system PP/g being more regularly structured (skin/core morphology) than PA/c. A satisfactory agreement in the area (a) structure/performance and (b) experiment/theory has been achieved.

This Report was prepared for publication by A. Cervenka (Shell Research BV, Koninklijke/Shell Laboratorium Amsterdam, the Netherlands) and P.S. Allan (Brunel University, The Wolfson Centre for Materials Processing, Uxbridge, Middlesex, UK) for the Working Party on Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1725-1740.

Characterization of finite length composites: Part V. Modelling of stiffness (Technical Report)

Synopsis

This characterization of a range of glass and carbon fibre reinforced polypropylene and polyamide injection mouldings forms part of a wider IUPAC Working Party 4.2.1 study of these materials. In this part of the work we summarize observations of stiffness and microstructural characterization with the aim of linking these features via a micromechanical model. The model makes a number of simplifying assumptions in order to be tractable and is based on calculating the stiffness of a number of 'imaginary' layers through the thickness of the moulding, with each layer having a singular fibre orientation. The stiffness of the moulding is then determined by an appropriate summation of the stiffness of these layers. The agreement between observed and 'modelled' stiffness is reasonable within the context of the assumptions necessary for tractability.

This Report was prepared for publication by P.S. Allan (Brunel University, The Wolfson Centre for Materials Processing, Uxbridge, Middlesex, UK), A. Cervenka (Shell Research BV, Koninklijke/Shell Laboratorium Amsterdam, the Netherlands) and D.R. Moore (ICI plc, Wilton, Middlesbrough, Cleveland, UK) for the Working Party on Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1741-1751.

Critical evaluation of the use and analysis of stable isotopes (Technical Report)

Synopsis

The methodology of isotopic analysis is discussed. In the first instance because a choice of analytical methods often conditions the success of research carried out with stable isotopes. The methodology of use is treated in two different chapters according to their resting or not on measurements of isotope effects. In the second case, stable isotopes are specially useful for isotope dilution analysis, studies of transport phenomena, medical diagnoses. Advantages and drawbacks of their use with respect to that of radioactive isotopes are described and examples are given. Usage of isotope effects is a specificity of stable isotope work. Methods of measuring equilibrium and kinetic effects are explained. A discussion is given of tenets of applications in research in pharmacology, geochemical processes, and of kinetic effects in studies of reaction mechanisms, especially in biology. Utilization of nuclear properties, particularly in medicine, are mentioned. This report does not cover techniques of isotope separation, preparation of labelled compounds, uses of isotopes in dating methods or in nuclear industries.

This Report was prepared for publication by Etienne Roth (CEA, SPAM, CE Saclay, 103 rue Brancas, 92310,

Sèvres, France) for the Commission on Radiochemistry and Nuclear Techniques of the Analytical Chemical Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1753–1828.

The determination of trans unsaturated fatty acids in edible oils and fats by capillary gas–liquid chromatography (Technical Report)

Synopsis

Collaborative studies on the application of capillary gas–liquid chromatography for the determination of *trans* unsaturated fatty acids are described. The method investigated involves preparation of methyl esters with methanolic potassium hydroxide followed by analysis of fatty acid methyl esters by gas–liquid chromatography on polar capillary columns. Care has to be taken in selecting working conditions to obtain the best obtainable resolution of signals necessary for reliable identification and determination of *trans* unsaturated fatty acids.

This Report was prepared for publication by A. Dieffenbacher and P. Dysseler for the Commission on Oils, Fats and Derivatives of the Environmental Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1829–1837.