

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 & Appl. Chem.*

Erratum: IUPAC recommendations on nomenclature and symbols and technical reports from commissions

Commission on Agrochemicals and the Environment (N. K. J. Nfilyamoto, G. D. Paulson, B. Zeeh, M. W. Skidmore, R. M. Hollingworth and H. A. Kuiper) Pesticides Report 37. Chirality in synthetic agrochemicals: Bioactivity and safety consideration (Technical Report) *Pure & Applied Chemistry* 1997, **69**(6), 1335–1348.

Due to a clerical error, Table 1 was omitted from this report. The report is reproduced in its entirety at the end of the September issue of *Pure & Applied Chemistry* 1997, **69**(9), 2007–2025.

Names and symbols of transfermium elements (IUPAC Recommendations 1997)

Synopsis: Revised recommendations for the names and symbols of the transfermium elements (atomic numbers 101–109) are presented along with the reasons for proposing them.

Introduction

The recommendations (ref. 1) of the Commission on Nomenclature of Inorganic Chemistry (CNIC) on the nomenclature of the transfermium elements (101–109, inclusive) were considered by the IUPAC Bureau at Guildford (UK) in September 1995. As a result of the various criticisms of the recommendations and the way

that they had been processed, the Bureau decided to adopt the recommendations as provisional and to circulate them to national/regional nomenclature centres in the normal way, with notices to be published in national/regional chemistry journals and magazines, requesting submission of comments to CNIC. In particular, the National Adhering Organizations (NAOs) were invited to express their views concerning the extant proposals for the names of these elements and the principles and traditions used to derive them. The response from the general chemical community was small, and the bulk of the replies came from nuclear scientists.

Recommendations

The Commission reconsidered all the names at a meeting in Chestertown, Maryland (USA) in August 1996. Although it is accepted that the discoverers of a new element have the right to propose a name and that such suggestions must receive serious consideration, it is also accepted that the final decision in such matters should be taken by CNIC, and ultimately confirmed by the Interdivisional Committee on Nomenclature and Symbols, Bureau, and Council of the Union. At Chestertown, CNIC reiterated its acceptance of the conclusions of the Transfermium Working Group (TWG) as a basis for taking decisions (refs. 2–4). However, it also decided to modify its decision that the name of a living scientist should not be used as the basis for an element name. The responses from the NAOs and the chemical community showed quite clearly that chemists in general do not regard this as an important issue and many thought it irrelevant. The Commission agreed, in keeping with tradition, to the use of appropriate names derived from (a) mythical concepts or characters, (b) place, area or country, (c) a property of the element, and (d) a scientist.

After some discussion CNIC agreed that elements 101, 102 and 103 should retain their commonly accepted names mendeleevium, nobelium, and lawrencium. This is despite the fact that the original Swedish claim to have prepared element 102 was subsequently shown to have been in error by the Dubna laboratory, which finally achieved an undisputed synthesis. The discovery of element 106 by the Berkeley laboratory is uncontested and the name proposed by the discoverers, seaborgium, was accepted. The discoveries of elements 107 jointly by the Darmstadt and Dubna laboratories), and of 108 and 109 (by the Darmstadt laboratories) are also uncontested. The discoverers wished to call these nielsbohrium, hassium, and meitnerium, respectively, and the Commission accepted the last two. However, the proposal for 107 was the subject of vigorous debate. The name nielsbohrium is long and includes the first name of Niels Bohr as well

as his family name. Such an element name is without precedent. Finally it was decided to refer the matter to the Danish NAO. Its preference for bohrium rather than nielsbohrium was ultimately accepted.

The discoveries of elements 104 and 105 are contested by Dubna and Berkeley. Both laboratories appear to have made significant contributions, but what has clearly emerged from the submissions, including those from Berkeley and from Darmstadt, is that the Dubna laboratory has played a key role in developing the experimental strategies used in synthesizing several transfermium elements. The Commission recommended that element 105 should be named dubnium in its honour. The Berkeley laboratory has already been similarly recognized on more than one occasion. Finally, the Commission accepted the name rutherfordium for element 104, to honour the New Zealand nuclear physicist, Ernest Rutherford.

The agreed list of recommendations is as follows:

Element	Name	Symbol
101	mendelevium	Md
102	nobelium	No
103	lawrencium	Lr
104	rutherfordium	Rf
105	dubnium	Db
106	seaborgium	Sg
107	bohrium	Bh
108	hassium	Hs
109	meitnerium	Mt

The Commission benefited from the presence of a representative of the International Union of Pure and Applied Physics (IUPAP) at its meeting in Chestertown. It is to be hoped that such a person will always be available if needed, and the Commission believes that it will be important to revive a joint IUPAC–IUPAP Working Group to confirm the discovery of new elements and to adjudicate on competing claims for priority of discovery. The Commission hopes that the present collection of names will be accepted as a fair compromise between the various claims and suggestions. It recognizes important experimental and theoretical contributions to the discovery of new elements and also the international nature of our science.

References

1. *Pure Appl. Chem.* 1994, **66**, 2419–2421.
2. *Pure Appl. Chem.* 1991, **63**, 879–886.
3. *Pure Appl. Chem.* 1993, **65**, 1757–1763.
4. *Pure Appl. Chem.* 1993, **65**, 1764–1814.

This report was prepared for publication by the Commission on Nomenclature of Inorganic Chemistry, Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 2471–2473.

Nomenclature of glycolipids (IUPAC Recommendations 1997)

Contents

GL-1. General considerations

GL-2. Generic terms

- 2.1. Glycolipid,
- 2.2. Glycoglycerolipid
- 2.3. Glycosphingolipid
- 2.4. Glycophosphatidylinositol
- 2.5. Psychosine
- 2.6. Other names

GL-3. Principles of nomenclature

- 3.1. Number of monosaccharide residues
- 3.2. Naming of monosaccharide residues
- 3.3. Use of symbols for defining oligosaccharide structures
- 3.4. Ring size and conformation

GL-4. Classification of glycolipids based on their lipid moieties

- 4.1. Glycoglycerolipids
- 4.2. Glycophosphatidylinositols
- 4.3. Glycosphingolipids

GL-5. Neutral glycosphingolipids

- 5.1. Monoglycosylceramides
- 5.2. Diosylceramides
- 5.3. Neutral glycosphingolipids with oligosaccharide chains

GL-6. Acidic glycosphingolipids

- 6.1. Gangliosides
- 6.2. Glycuronoglycosphingolipids
- 6.3. Sulfatoglycosphingolipids
- 6.4. Phosphoglycosphingolipids
- 6.5. Phosphonoglycosphingolipids

GL-7. Short abbreviations

- 7.1. Recommended abbreviations
- 7.2. The Svennerholm abbreviations for brain gangliosides

GL-8. References

GL-1. General considerations

Glycolipids are glycosyl derivatives of lipids such as acylglycerols, ceramides and prenols. They are collectively part of a larger family of substances known as glycoconjugates. The major types of glycoconjugates are glycoproteins, glycopeptides, peptidoglycans, proteoglycans, glycolipids, and lipopolysaccharides. The structures of glycolipids are often complex and difficult to reproduce in the text of articles and certainly cannot be referred to in oral discussions without a nomenclature that implies specific chemical structural features.

The 1976 recommendations on lipid nomenclature

contained a section (Lip-3) on glycolipids, with symbols and abbreviations as well as trivial names for some of the most commonly occurring glycolipids. Since then, more than 300 new glycolipids have been isolated and characterised some having carbohydrate chains with more than twenty monosaccharide residues and others with structural features such as inositol phosphate. The nomenclature needs to be convenient and practical, as well as extensible, to accommodate newly discovered structures. It should also be consistent with the nomenclature of glycoproteins, glycopeptides and peptidoglycans, oligosaccharides, and carbohydrates in general.

This document supersedes the glycolipid section in the 1976 Recommendations on lipid nomenclature.

This report was prepared for publication by M. Alan Chester (Blood Centre, University Hospital, S-221 85 Lund, Sweden), for the Joint Commission on Biochemical Nomenclature. The full details are to be found in Pure Appl. Chem. 1997, 69, 2475–2487.

Parameters and symbols for use in nuclear magnetic resonance (IUPAC Recommendations 1997)

Synopsis: NMR is now frequently the technique of choice for the determination of chemical structure in solution. Its uses also span structure in solids and mobility at the molecular level in all phases. The research literature in the subject is vast and ever-increasing. Unfortunately, many articles do not contain sufficient information for experiments to be repeated elsewhere, and there are many variations in the usage of symbols for the same physical quantity. It is the aim of the present recommendations to provide simple check-lists that will enable such problems to be minimised in a way that is consistent with general IUPAC formulation. The area of medical NMR and imaging is not specifically addressed in these recommendations, which are principally aimed at the mainstream use of NMR by chemists (of all sub-disciplines) and by many physicists, biologists, materials scientists and geologists etc. working with NMR.

The document presents recommended notation for use in journal publications involving a significant contribution of nuclear magnetic resonance (NMR) spectroscopy. The recommendations are in two parts:

A. Experimental parameters which should be listed so that the work in question can be repeated elsewhere.

B. A list of symbols (using Roman or Greek characters) to be used for quantities relevant to NMR.

This report was prepared for publication by Robin K. Harris¹, Jozef Kowalewski² and Sonia Cabral De Menezes³ (¹Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, UK; ²Division of Physical Chemistry, Arrhenius Laboratory, Stockholm University, S-10691 Stockholm, Sweden; ³PETROBRAS/CENPES, Divisão de Química, Ilha do Fundão, Quadra 7, Cidade Universitária, 21949 900 Rio de Janeiro, R.J., Brazil), of the Commission on Molecular Structure and Spectroscopy, Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 2489–2495.

Compilation and critical evaluation of structure–reactivity parameters and equations: Part 2. Extension of the Hammett σ scale through data for the ionization of substituted benzoic acids in aqueous organic solvents at 25 °C (Technical Report)

Synopsis: Data have been compiled for the pK values in certain aqueous organic solvents at 25 °C of about 70 *meta*- or *para*-substituted benzoic acids, with a view to proposing values of Hammett constants, σ , in the case of substituents for which values cannot be based on the ionization of substituted benzoic acids in water (Part 1). The emphasis of the work is on the use of data for the apparent pK values of the acids in 1:1-EtOH-H₂O, i.e. a solvent made up of equal volumes of ethanol and water. A calibration equation is derived relating substituent effects measured in this solvent to those measured in water. On the basis of this equation σ values are proposed for 25 substituents, although some of the values are subject to *caveats*, and several further substituents are also discussed.

This report was prepared for publication by: John Shorter (School of Chemistry, University of Hull, Hull HU6 7RX, UK), for the Working Party on Structure–Reactivity Parameters and Equations of the Commission on Physical Organic Chemistry, Organic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 2497–2510.

Source-based nomenclature for non-linear macromolecules and macromolecular assemblies (IUPAC Recommendations 1997)

Synopsis: A source-based nomenclature for non-linear macromolecules and macromolecular assemblies is proposed. Source-based or structure-based names for linear regular (single-strand and double-strand) and irregular macromolecules can be derived using rules published previously. In contrast, the present document deals with the source-based naming of non-linear macromolecules and assemblies of macromolecules. The former comprise branched, graft, comb, star, cyclic and network macromolecules; the latter comprise polymer blends, interpenetrating polymer networks and polymer-polymer complexes. The names of non-linear macromolecules are formed by citing source-based name(s) of the constituent linear chains(s) and denoting their mode(s) of combination by prefixes and connectives. Specification of molecular weight, composition or branch-point functionality(ies) of the macromolecule or its constituents may be given, in parentheses.

Contents

- Abstract
- Introduction
- 1 Definitions
- 2 General principles
- 3 Non-linear homopolymer molecules
- 4 Non-linear copolymer. molecules
 - 4.1 Copolymer molecules comprising a single species of linear chain...
 - 4.2 Copolymer molecules comprising a variety of species of chains...
- 5 Macromolecular assemblies
- 6 Quantitative specifications
- 7 References

This report was prepared for publication by: J. Kahovec (Czech Republic), P. Kratochvíl (Czech Republic), A. D. Jenkins (UK), I. Mita (Japan), I. M. Papisov (Russia), L. H. Sperling (USA) and R. F. T. Stepto (UK). For the Commission on Macromolecular Nomenclature, Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 2511–2521.