NEWSLETTER 1989

IUPAC COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY

Introduction. – The Commission on Nomenclature of Organic Chemistry (CNOC) is the custodian of the language appropriate to the discipline of organic chemistry. The content of this discipline, that is, the number of molecular particles, grows rapidly and often in unexpected directions. A casual reader of any chemical journal will be impressed by the complexity of the terminology and the structures of the chemical compounds under study. When complex structures have to be described among chemists, there is a great temptation to let alphanumeric symbols go and rely only on the picture. However, the resultant 'picture dictionary' would be very difficult to put into any order for searching.

CNOC is mindful of the possibility of constructing giant electronic dictionaries to store the enormous number of chemical compound records (over nine million today), and is encouraging research in that direction. But, for many reasons, social and economic, the day of such dictionaries has not yet come, and in the meantime new compounds have to be described so that they can be identified in listings of various types. Moreover, the molecule or fragments thereof have to be described in running text of learned papers as well as in speech.

Thus, a major task of CNOC is to devise recommendations according to which each structural formula can be unambiguously encoded as alphanumeric symbols. Many circumstances conspire to render this task a daunting one. The recommendations must be friendly to the user, *i.e.* relatively easy to understand and to apply, in order to keep the decoding process convenient. They must respect the guidelines prescribed by those who designed the various systems, in order to protect the patrimony of the existing literature, even though those founding fathers of nomenclature could not have foreseen today's treasure of molecular structure. Finally, the recommendations must be capable of generating unique names, in order to allow an orderly construction of indexes. A second task of CNOC is to keep a mindful eye on the vocabulary of organic chemistry.

The purpose of this and subsequent newsletters is to create a public understanding and tolerance for CNOC in its often unpopular tasks, and to enlist cooperation from chemists throughout the world. A wide variety of points of view from research chemists, information scientists, editors, and publishers, is represented on the Commission, and its recommendations are the result of consultations within itself, with other IUPAC Commissions and Committees, and with the chemical public, insofar as they are willing to provide input.

These newsletters will announce work already completed and describe projects in progress and new problems under consideration. Comments and suggestions are always

welcome and should be sent to any member of the Commission, but preferably to the Secretary[1]).

Collected Recommendations. – A compilation of recommendations from CNOC is found in the 1979 edition of the Nomenclature of Organic Chemistry (The 'Blue Book') [1]:

A. Hydrocarbons (4th edition);
B. Fundamental Heterocyclic Systems (4th edition);
C. Characteristic Groups Containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and/or Tellurium (3rd edition);
D. Organic Compounds Containing Elements that are not Exclusively Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and Tellurium (Provisional Recommendations 1978);
E. Stereochemistry (Recommendations 1974);
F. General Principles for the Naming of Natural Products and Related Compounds (Provisional Recommendations 1976);
H. Isotopically Modified Compounds (Recommendations 1978).

Since the publication of the 1979 edition of the organic nomenclature rules [1], the Commission has been working on refinements and extensions of these recommendations and on comprehensive documentation of recommendations in several areas, as well as preparing the next edition of the 'Blue Book'. Four sets of recommendations have been published to date, as summarized below, and there are a number of others in various stages of preparation.

Recent Publications. – The *Hantzsch-Widman* system, one of the most useful methods in organic nomenclature for naming heteromonocycles with no more than ten ring atoms, evolved over several decades, gradually broadening in scope, resulting in a few inconsistencies and limitations. Exceptions and special treatments for certain heteromonocycles had to be introduced. As a part of a comprehensive study of organic ring nomenclature, recommendations for revision of the *Hantzsch-Widman* system were developed and published: 'Revision of the Extended *Hantzsch-Widman* System of Nomenclature for Heteromonocycles' (Recommendations 1982), *Pure Appl. Chem.* **1983,** *55,* 409–416. There are four important differences in this revision from the recommendations in the 1979 edition of the organic rules [1]. First, for the most part, the distinction between nitrogenous and nonnitrogenous rings has been eliminated. This is most noticeable in the use of '-ane' endings for saturated nitrogenous rings having six through ten

[1]) The current Titular Members of CNOC are: Prof. *P. A. S. Smith* (Chairman), Department of Chemistry, The University of Michigan, Ann Arbor, Michigan 48109, USA; Prof. *J. C. Richer* (Vice-chairman), Département de Chimie, Université de Montréal, BP 6128, Succursale A, Montréal, Quebec H3C 3J7, CANADA; Dr. *W. H. Powell* (Secretary), Chemical Abstracts Service, 2540 Olentangy River Road, P.O. Box 3012, Columbus, Ohio 43210, USA; Prof. *H. J. T. Bos,* Afdeling Organisch Chemische Synthese, Vakgroep Organische Chemie, Rijksuniversiteit Utrecht, Padualaan 8, NL–3584CH Utrecht, NETHERLANDS; Dr. *J. R. Bull,* Department of Organic Chemistry, University of Capetown, Rondebosch 7700, REPUBLIC OF SOUTH AFRICA; Mr. *E. W. Godly,* Laboratory of the Government Chemist, DTI, Cornwall House, Waterloo Road, London SE1 8XY, UNITED KINGDOM; Prof. *R. Panico,* Attaché à la Direction des Études, École Supérieure de Physique et de Chemie Industrielles, 10, rue Vauquelin, F–75231 Paris Cédex 05, FRANCE; Dr. *O. Weissbach,* Beilstein Institut für Literatur der Organischen Chemie, Carl-Bosch-Haus, Varrentrappstrasse 40–42, D–6000 Frankfurt (Main) 90, FEDERAL REPUBLIC OF GERMANY.

ring members. For example, the name azepane describes a saturated seven-membered monocyclic ring with one nitrogen ring atom; the name hexahydro-1*H*-azepine was used previously. Second, the special terminations '-etine', '-etene', '-oline', and '-olene' for four- and five-membered rings with one double bond (when more than one double bond is possible) are no longer recommended. Third, the stems '-inine' and '-inane' for six-membered rings, where the stems '-ine' and '-ane' would be ambiguous, have been introduced. For example, the names phosphinine and phosphinane describe unsaturated and saturated, respectively, six-membered monocyclic rings with one phosphorus ring atom (the names phosphine and phosphane cannot be used because they describe the mononuclear parent hydride PH_3). Fourth, the halogen elements have been added to the system so that heteromonocycles with cationic halogen atoms and halogen atoms in nonstandard valency states, can be included in the system; for example, 1,1,1-trifluoro-1λ^5-iodinane for $\underline{CH_2-[CH_2]_4-}IF_3$ and 1λ^3-brominan-1-ylium for $\underline{CH_2-[CH_2]_3-}Br^+$. It should be emphasized that, just as in the previous rules, it is not the intention of the Commission to recommend replacement of commonly used trivial names, such as thiophene, pyran, pyridine, piperidine, *etc.*

The λ-Convention. In order to use substitutive nomenclature for naming organic compounds containing heteroatoms that can occur in more than one bonding state, a method for distinguishing between these bonding states is needed. A variety of methods have been used for this purpose, none of which is completely satisfactory over a broad range of compounds. In 1984, CNOC published recommendations for treating such variable-valence situations in organic nomenclature, called, for convenience, the 'λ-convention', *Pure Appl. Chem.* **1984,** *56,* 769–778. This convention provides a single, general method for indicating nonstandard, classical valence states of formally neutral, nonradical skeletal atoms of parent structures. It is consistent with basic principles of substitutive nomenclature and directly applicable for naming organic derivatives of inorganic parent hydrides. The convention consists of a symbol λ^n, where '*n*' is the classical bonding number defined as the sum of the total number of classical valence bonds to adjacent skeletal atoms, if any, and the number of hydrogen atoms; for example, the name λ^4-sulfane describes the parent hydride SH_4. If needed, the λ^n symbol is attached to a locant of the skeletal atom in the parent structure, for example, 2λ^4-benzothiopyran. This method is equally useful for designating bonding states higher or lower than the standard one.

Numerical terms are used in chemical names for indicating a multiplicity of identical structural features in a structure. *Rule A-1.1* of the organic nomenclature rules [1] illustrates the numerical terms through 199 in names of saturated unbranched acyclic hydrocarbons. The use of these terms for expressing identical simple substituents to a parent structure, and their modification for use with 'complex' substituents, is described in *Rule A-2.5.* In response to expressed desires for numerical terms higher than 199, CNOC developed and published recommendations for extending *Rules A-1.1* and *A-2.5, Pure Appl. Chem.* **1986,** *58,* 1693–1696. These recommendations provide the necessary guidance, based on principles already established, for generating numerical terms through 9999. The infixes 'cta' (for the hundreds digits) and 'lia' (for the thousands digits) are used in a way that is quite analogous to the use of 'conta' for the tens digits beyond twenty. Thus, the numerical term for 231 is hentriacontadicta.

The δ-Convention. Organic substitutive nomenclature requires that the number of hydrogen atoms, if any, on each skeletal atom of a parent structure be known unam-

biguously. Trivial or semisystematic names are used to denote many rings and ring systems containing the maximum number of noncumulative double bonds. In order to use substitutive nomenclature and the same skeletal name when formal cumulative double bonds, actual or theoretical, are present in a ring or ring system that otherwise has the maximum number of noncumulative double bonds, a method for indicating the location of a cumulative double bond system is required. Techniques that have been used are either quite cumbersome or tend to use established techniques in ways other than those for which they were designed. The δ-convention for specifying nonstandard valency states of skeletal atoms in parent hydrides, described above, although useful, is not, by itself, sufficient for this purpose. Thus, CNOC developed and published recommendations for such situations, called, for convenience, the 'δ-convention', *Pure Appl. Chem.* **1988,** *60,* 1395–1401. When combined with the λ-convention, where necessary, the δ-convention defines the number of hydrogen atoms available for substitution on each skeletal atoms in a ring or ring system unambiguously.

The δ-convention is fully consistent with the fundamental principles of substitutive nomenclature, which is based on formalized bonding in structural diagrams, and is applicable to organic derivatives of inorganic rings. It involves the use of a symbol, δ^c, where *'c'* is an arabic number representing the number of double bonds attached to the skeletal atom indicated by the preceding locant. A nonstandard valence of the skeletal atom is given by the λ-convention, where necessary. For example, the name 6*H*-1λ^4,δ^2,3λ^4,5,7,2,4,6,8-tetrathiatetrazocine describes an eight-membered ring consisting of alternating sulfur and nitrogen atoms, two sulfur atoms of which are in a bonding state of four, one with two formal skeletal double bonds attached to it and the other with only one.

Projects in Progress. – *The Next Edition of the 'Blue Book'.* For several years, CNOC has been working toward a major reorganization and updating of the 1979 edition of its nomenclature recommendations [1]. The new edition should be more logical in its presentation, combining similar principles that are scattered about in the 1979 edition. At the time of this writing, it is planned to produce the new edition in two parts, the first of which will describe in general terms the techniques for generating an unambiguous, though not necessarily unique, name. A more comprehensive treatment of various aspects fo organic nomenclature and rules necessary to derive a unique IUPAC name is planned for the second part. *Part I* is in an advanced stage of development and should be ready for public review soon; *Part II* is in a very early stage of development, although comprehensive documentation in three areas as noted below is well advanced.

Radicals, Ions, and Radical Ions. A comprehensive codification of recommendations for naming radicals, ions, radical ions, and related substances in substitutive nomenclature based on the principles in *Subsection C-0.8* of the 1979 edition of the organic rules [1] *is in* an advanced stage of development and should be ready for public review soon.

Fused-Ring Nomenclature. The 1979 edition of the organic rules [1] contains fundamental principles for naming fused and bridged-fused polycyclic ring systems *(cf. Rules A-21, 22, 23, 34,* and *B-2, 3, 4, 6, 14).* These recommendations have been modified very little, since they were first published in the 1957 Rules [2], but the CAS files now contain over 70,000 rings and ring systems, a six-fold increase over the number in 1960. Roughly two-thirds of these rings and ring systems are fused and bridged-fused systems, many of which are complex systems requiring extensions and additions to the documented fundamental principles.

CNOC is preparing a comprehensive documentation of procedures for naming fused and bridged-fused polycyclic ring systems based on the fundamental principles given in the 1979 organic rules [1]. Extensive consultation with CAS and *Beilstein Institut* will allow this documentation to be more broadly based and to be as close as possible to the current procedures used by these institutions. Although this is a very large and difficult task, CNOC hopes to have these recommendations ready for review within the next year or so.

Natural Products. The provisional recommendations of general principles for naming natural products contained in *Section F* of the organic rules [1] are being revised and expanded into a comprehensive set of recommendations. This is a very arduous task, given the breadth of structure types and local nomenclature practices that must be considered. Nevertheless, a draft is well advanced and will soon be ready for review by specialists in various natural product fields.

Phane Nomenclature. For a long time, CNOC has been studying the proposals for naming cyclophane structures (and their acyclic analogs) that began appearing in the literature nearly twenty years ago. Although the Commission would prefer a more general numbering scheme than offered by these proposals, their codification, relying on the experience of the *Beilstein Institut* in their use, is at last well advanced. (CAS does not use a 'cyclophane nomenclature'; such structures are named by the usual rules for polycyclic ring systems.)

Class Name Glossary. CNOC, with assistance from the Commission on Physical Chemistry (CPOC), is preparing an extensive glossary of structure-based class names used in organic chemistry. It is in the first review stage.

Stereochemical Terminology. The Commission plans to revise and substantially extend the stereochemical nomenclature recommendations contained now in *Section E* of the 1979 organic rules [1]. Concurrently, and in cooperation with the IUPAC Commissions on Physical Organic Chemistry (CPOC), Nomenclature of Inorganic Chemistry (CNIC), and Macromolecular Nomenclature, CNOC is developing a glossary of stereochemical terminology. It is nearly ready for the first review stage.

To conclude this first newsletter, it should be noted that, as part of an international public service organization, *i.e.* IUPAC (International Union of Pure and Applied Chemistry), CNOC consists of volunteer chemists from various countries around the world trying to meet the nomenclatural needs and requirements of a wide variety of chemists, organizations, and governmental agencies. This is not an easy task. Therefore, as well as your problems and complaints, we solicit your ideas and opinions, without which our task becomes much more difficult. Chemical nomenclature is often a personal matter and must serve a wide variety of purposes. It is our job to meet as many needs as we can.

REFERENCES

[1] International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F,* and *H,* 1979 edition, Pergamon Press, Oxford, 1979, 559 pp.

[2] International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, *Nomenclature of Organic Chemistry, Definitive Rules for Sections A. Hydrocarbons; Section B. Fundamental Heterocyclic Systems,* July 1957, Butterworths Scientific Publications, London, 1958, 92 pp.

Schweizerische Chemische Gesellschaft SCG

Frühjahrsversammlung in Zürich

Freitag, den 17. März 1989

Paul Karrer Centennial Symposium

Universität Zürich-Irchel, Hörsaal G 45, Winterthurerstr. 190

09.15 h Geschäftlicher Teil

09.45 h Einführung

10.15 h **C. Weissmann,** Universität Zürich: 'Molekulare Ökologie'

11.15 h Pause

11.30 h **T. R. Cech,** University of Colorado, Boulder: 'Catalytic Activity of Ribonucleic Acids'

12.30 h Ehrungen der Schweizerischen Chemischen Gesellschaft:
Übergabe des *Werner-Preises*
Verleihung von *Ehrenmitgliedschaften* der SCG

12.45 h Mittagspause

14.30 h **A. R. Fersht,** University of Cambridge: 'Factors Responsible for Enzyme Catalysis and Stability'

15.30 h **D. Oesterhelt,** Max-Planck-Institut für Biochemie, München: 'Die Photoisomerisierung des Retinals als Basis seiner biologischen Funktion'

16.30 h Pause

16.45 h Verleihung der *Paul-Karrer-Medaille* durch den Präsidenten des Kuratoriums der Stiftung für die Paul-Karrer-Vorlesung, Rektor Prof. H. H. Schmid
23. Paul-Karrer-Vorlesung
D. Arigoni, ETH Zürich: 'Zur Biogenese von Naturstoffen'

18.00 h Schluss der Versammlung

Information/Kontakt:
Dr. E. Zass, Sekretär SCG, ETH Zürich, Universitätstr. 16, CH–8092 Zürich

Royal Society of Chemistry

Annual Chemical Congress
Hull, April 4–7, 1989

9th International Meeting on NMR Spectroscopy
Warwick, July 10–14, 1989

9th European Symposium on Fluorine Chemistry
Leicester, September 4–8, 1989

5th Boc Priestley Conference on Separation of Gases
Birmingham, September 19–21, 1989

Autumn Meeting
Loughborough, September 26–28, 1989

Faraday Division

General Discussion on Catalysis by Well Characterised Materials
Liverpool, April 11–13, 1989

General Discussion on Charge Transfer in Polymeric Systems
Oxford, September 11–13, 1989

Symposium on Large Gas Phase Clusters
Warwick, December 12–14, 1989

Dalton Division

International Conference on Chemistry of the Early Transition Metals
Sussex, July 10–14, 1989

Perkin Division

International Symposium on Molecular Mechanisms in Bioorganic Processes
Newcastle upon Tyne, July 17–20, 1989

11th International Symposium on Synthesis in Organic Chemistry
Oxford, July 24–27, 1989

Analytical Division SAC 89

Analytical Chemistry
Cambridge, July 30 – August 5, 1989

Dalton/Perkin Division

International Symposium on Synthetic Applications of Transition Metals
St Andrews, September 11–14, 1989

Further information: Dr. John F. Gibson, The Royal Society of Chemistry, Burlington House, London W1V 0BN, England

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Symposium on Transmembrane Signalling, Intracellular Messengers and Implications for Drug Development

Royal Institution, London, April 17/18, 1989

Further information: Administrative Secretary: Yvonne Haseldine, Department of Pharmacology, School of Pharmacy, 29/39 Brunswick Square, London WC1N 1AX, England

Société Française de Chimie
Gesellschaft Deutscher Chemiker

1st Franco-German Chemistry Days
Contribution of Chemistry to Human Society
Strasbourg, April 27/28, 1989

Further information: Franco-German Chemistry Days, Secretariat, E.H.I.C.S., 1, rue Blaise Pascal, F–67008 Strasbourg Cedex, France, Telephone: (33) 88 41 68 66

9th National Quantum Electronics Conference

University of Oxford, Oxford, September 18–22, 1989

Further information: Mrs. Marjorie Sherwen, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, England

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Société Française de Chimie

International Symposium on Chemistry of Organobrominated Compounds and their Uses
Mulhouse-Thann, October 3–6, 1989

Further information: J. Klapuch, Société Française de Chimie, ENSCMU, 3, rue Alfred Werner, F–68093 Mulhouse Cedex, France

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10th IUPAC Meeting on Physical Organic Chemistry

Haifa, Israel, August 5–10, 1990

Further information: Prof. Y. Apeloig, Department of Cemistry, Technion – Israel Institute of Technology, Technion City, Haifa 32000, Israel

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Bei der Redaktion eingelaufene Bücher

(Die Redaktion verpflichtet sich nicht zur Besprechung eingelaufener Bücher.)

Livres reçus par la rédaction

(La rédaction ne s'engage pas à publier des œuvres, qui lui sont soumis.)

Studies in Natural Products Chemistry, Vol. 2: Structure Elucidation (Part A), ed. by Atta-ur-Rahman, Elsevier, Amsterdam–Oxford–New York–Tokyo, 1988, pp. 469, $ 155.25.