

The Nomenclature of Organic Chemistry*

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The current "state of the art" in organic nomenclature is discussed, with emphasis on major problem areas which have emerged during the past 10 to 15 years. The "Organic Nomenclature Guidebook" being prepared by the Division of Organic Chemistry is described.

The purposes of this paper are: (1) to report on the status of activities by committees of the American Chemical Society which are working on various aspects of organic nomenclature, (2) to discuss the rationale of nomenclature review and development, (3) to indicate some of the more important problems which need attention, and (4) to suggest ways in which chemists who are interested in nomenclature can participate in nomenclature work. It is not my purpose to teach the reader how to name organic compounds, but rather to give him an appreciation of the over-all importance and complexity of nomenclature problems. The paper is directed not only to laboratory and literature chemists but also to anyone who is concerned with the written communication of information relating to organic chemistry.

One of the oldest and most important decisions confronting both users and developers of organic nomenclature is the choice between systematic and nonsystematic (trivial) names, and for that very reason this problem will serve appropriately as a first topic for discussion.

Unambiguous, systematic, syllabic designations for the written description of organic compounds will probably always be needed, regardless of ciphers, codes, computer language, etc. Chemists are always creating new compositions of matter, and some of these are novel enough to be unnamable by previous nomenclature principles. This difficulty would have been minimized, though not eliminated, had organic nomenclature been systematic from the beginning and kept pace with the chemist's understanding of structure and bonding in molecules. Unfortunately, this has not been, and probably never will be, the case. The chemist who creates or isolates a new compound does not usually concern himself with its systematic name when he reports the discovery, unless a journal editor or referee insists on it. In many instances, he selects as short and simple a name as possible, which at best is partially systematic; in some cases he coins a nonsystematic trivial name, particularly if the compound is of especially complex structure. This trivial name is very

likely unambiguous, but it is also meaningless to the reader until defined, and perhaps difficult to remember.

In spite of this, there has been an increasing and encouraging trend over the years toward recognition of the need for, and the more widespread use of, systematic organic nomenclature. The main driving force and much of the leadership in this gradual but accelerating change have come from the agencies responsible for publishing, abstracting, and indexing the chemical literature. Among these organizations, Chemical Abstracts Service stands preeminent, though the editors of the *Journal of the Chemical Society (London)*, Beilstein's "Handbuch," and the fundamental American Chemical Society journals have also played important roles. This is not surprising, because as soon as anyone becomes directly involved with the recording and retrieval of chemical information at the publication level, he is immediately confronted with the problem of providing descriptive, unambiguous names for organic chemical compositions which can be readily understood by anyone who has some reasonable knowledge of organic chemistry.

Since, with very few exceptions, organic molecules are inherently complex with respect to (1) the number of atoms comprising them, (2) the nature of the bonding between adjacent atoms, and (3) the spatial arrangement of atoms, systematically formed descriptive names which recite component atoms and groups of atoms are of necessity also complex. Such names tend to be long, highly punctuated, and not well suited for the spoken language. Nevertheless, they are highly useful on the printed page; they convey the required information clearly and accurately with a minimum burden on the memory of the reader, because, generally speaking, the more systematic the nomenclature the fewer the rules which must be memorized. Indeed, if organic nomenclature were completely nonsystematic—i.e., if only trivial names were used—a ridiculous situation would exist wherein the organic chemist's ability to communicate would depend entirely on his memory capacity and that of his colleagues.

Thus, for a good many years, various committees have concerned themselves with studying and trying to improve organic nomenclature rules and practices. As indicated above, such work has proceeded at both the national and international levels. For the most part, the approach has been to revise or "repair" established rules, with atten-

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tion being focused on areas where ambiguities and confusion existed or where the available rules became inadequate owing to new knowledge of organic chemistry arising from laboratory research. Old rules have been rephrased, consolidated, and extended for many classes of compounds, separately and at different times, but a complete review of organic nomenclature has not been undertaken until recent years when the Commission on Organic Nomenclature of the International Union of Pure and Applied Chemistry (IUPAC) addressed itself to this rather overpowering task.

The IUPAC Commission has elected, wisely, to codify rather than create rules of organic nomenclature, taking into account not only problems of ambiguity, inconsistency, and inadequacy, but international language difficulties as well. Publication by the commission of its Definitive Rules for Hydrocarbons and Heterocyclic Systems in 1957 (1) and for Functional Classes (alcohols, amines, acids, etc.) in 1965 (2) represents a major contribution to the written communication of chemical information the world over.

In its Definitive Rules, the IUPAC Commission does not attempt in all instances to specify a single "correct" name for each organic compound. Although emphasis is on systematic names, deference is made to usage by presentation of alternative rules and by limited recognition of trivial names. Occasionally, where the Commission was unable to agree on a preferred rule or type of nomenclature and two approaches were deemed to have equal merit, two types of systematic name have been accorded equal status. The rules are stated concisely, with explanation where needed, and liberal use is made of examples. It is to be hoped that continuing use of the Definitive Rules as an authoritative reference will be made by all those who originate and publish the chemical literature.

Until publication of the IUPAC Definitive Rules in 1957 and 1965, the only official rules of organic nomenclature readily available to American chemists were those published by the International Union of Chemistry (IUC) in 1930 (3). However, the IUC Rules were far from complete in their coverage of compounds and served mainly as a stepping stone toward later nomenclature work by Chemical Abstracts Service and the Division of Organic Chemistry of the American Chemical Society.

With the IUC Rules of 1930 as the only published official standard available to the chemist, it is extremely fortunate that *Chemical Abstracts*, and in particular Dr. Austin M. Patterson, assumed leadership in the development of systematic nomenclature in the United States during the 1930's and 40's. By publishing a description of the rules and practices used in naming organic compounds in its Subject Indexes, *Chemical Abstracts* has provided us with a sound and comprehensive semisystematic organic nomenclature over the past 30 years. Since 1945, "The Naming and Indexing of Chemical Compounds from Chemical Abstracts," which was originally published in conjunction with the Subject Indexes, has been separately available from Chemical Abstracts Service in paperback form, and many thousands of copies have been sold.

It must be remembered, however, that the organic nomenclature used by *Chemical Abstracts*: (1) is not entirely systematic, (2) is designed to provide a single preferred index name for each compound, (3) is in an

inverted form needed to achieve a degree of classification in a word index, and (4) makes rather liberal use of trivial names. These characteristics of *Chemical Abstracts* nomenclature combine to make it useful but not always satisfactory to chemical authors, particularly to those who have no intrinsic personal interest in nomenclature and find it burdensome to learn and remember the many rules, conventions, and exceptions which are required in formulating *Chemical Abstracts* index names. In spite of these limitations (until publication of the 1957 and 1965 IUPAC Definitive Rules), *Chemical Abstracts* nomenclature has been the best all-round official source of guidance to American chemists publishing in American Chemical Society journals; in recent years the Society's fundamental journals have adopted a policy of requesting authors to use this nomenclature when and wherever possible. This has had a salutary effect and has helped the Chemical Abstracts Service staff in its task of abstracting and indexing articles appearing in these journals.

In 1946 the Division of Organic Chemistry of ACS, recognizing the need for an improved general purpose organic nomenclature, established a Nomenclature Committee reporting to the Executive Board of the Division. The first chairman of the Committee was Dr. Howard S. Nutting of the Dow Chemical Co. In 1952, Miss Mary Alexander of Universal Oil Products Co. became chairman and continued in that capacity until her untimely death in 1955. The present chairman (the author) was appointed in 1957.

During the two decades since its inception the Committee has maintained a healthy balance in membership between industry-employed chemists and those affiliated with universities, government laboratories, and research institutes. From the beginning, *Chemical Abstracts* has been represented on the Committee by at least two members.

At the first meeting of the Nomenclature Committee in April 1946 the differing needs of the chemist-author on the one hand and the abstractor-indexer on the other were pointed out. Preparation of an official nomenclature guidebook for chemists was suggested, and the need for encouraging authors to use systematic nomenclature was recognized. Ever since that initial discussion, the work of the Committee has continued toward these goals, sometimes slowly and with difficulty, but never with lack of enthusiasm.

Through the years, the size of the Nomenclature Committee of the Division of Organic Chemistry has varied, probably never exceeding 25, including ex officio members. Development work has been carried out by assigning specific problems to subcommittees or by establishing advisory committees, sometimes in cooperation with some other nomenclature committee. Because participation in subcommittee work is not restricted to members of the main committee, we have a means of enlisting the temporary services of experts in specialized areas of organic chemistry.

Currently, members of the main committee are appointed to three-year terms, approximately one-third of the total committee being reappointed or replaced each year. As with many other kinds of continuing activity where a group of individuals must work as a unit to be effective, we have found that continuity of membership

is of prime importance, but that judicious selection and addition of new members is the best insurance against the development of ingrown and stereotyped thinking. Through appointment of ex officio members to the Organic Division Committee and through interlocking membership with nomenclature committees of other Divisions and of the parent Society, cooperation and communications with these groups and with the IUPAC Commission are assured.

Inevitably, the very nature of the over-all chemical nomenclature problem engenders wide diversity of thinking, not only among individuals but among groups representing different fields of specialization. This means that unless a continuing free exchange of information is maintained among all of the committees officially engaged in nomenclature development work, both at the national and international levels, the over-all result may be a multiplicity of nomenclature systems, each with its own set of rules, whereas what is really needed is a simple integrated system applicable to all types of chemical compounds. Fortunately for the chemical profession, tremendous strides have been made in the latter direction during the past two decades.

To illustrate, it is appropriate to explain how proposals for the revision of organic nomenclature rules and introduction of new rules are handled within the American Chemical Society. Development of an official proposal (usually called a report) is carried out by the Nomenclature Committee of the Division of Organic Chemistry, usually with the assistance of a subcommittee or advisory committee. In advance of final approval by the Organic Committee, copies of the report are distributed to the nomenclature committees of other divisions, to the National Research Council (NRC) Subcommittee on Organic Nomenclature, and to the IUPAC Commission on the Nomenclature of Organic Chemistry for informal review and comment.

In its final version the report is submitted to the Society's Committee on Nomenclature (a standing committee of the Council) for official review and approval. If approved, the report then goes to the Council for official adoption on behalf of the Society. Customarily, the Council approves the rules of nomenclature recommended in the report on a tentative basis for one year to allow publication and opportunity for comment or criticism from Society members. If no serious objections are raised during that year, the Council takes action to make the new nomenclature rules official. Official transmission and recommendation of the report to the IUPAC Commission may be made at any time by the NRC Committee on Nomenclature, acting on the advice of its Subcommittee on Organic Nomenclature.

Individuals interested in organic nomenclature who wish to make proposals for change or additions to rules should contact the Nomenclature Committee of the Organic Division. Suggestions so received are always given careful consideration by the Committee and in some cases lead to official recommendations, with full credit given to the originator. This procedure is much preferred to the premature publication of nomenclature proposals, which usually results in confusion among readers as to what has been officially accepted as good nomenclature practice. For this reason, most editors of ACS journals consult the appropriate nomenclature committee before accepting papers proposing new or revised rules of nomenclature.

During the past several years, the Nomenclature Committee of the Organic Division has devoted its attention to the preparation of a nomenclature guidebook for use by practicing chemists and students. As mentioned earlier, the need for such a volume had been recognized 20 years ago at the time the committee began its work, but partly because of the lack of published rules for functional classes of compounds, initiation of the guidebook project was delayed. We now hope to go to press in 1967.

The Organic Nomenclature Guidebook, although designed primarily as a reference for those who wish to follow good, up-to-date nomenclature practice, is arranged so that it may be used as a teaching aid in chemical literature courses. Rather than quoting rules, the Guidebook offers recommendations for naming organic compounds based mainly on the latest IUPAC Definitive Rules and *Chemical Abstracts* practice. Systematic nomenclature is emphasized and given preference, although many common and well-established trivial names are recognized as acceptable. Liberal use is made of specific examples illustrating the principles presented.

During preparation of the Guidebook, in which all members of the Committee have participated, there was often diversity of opinion on the degree of emphasis given to systematic names at the expense of their trivial and partially systematic counterparts. This was to have been expected, particularly in cases where the latter are still used as the preferred entries in the Subject Indexes of *Chemical Abstracts*. Nevertheless, the international trend toward systematic chemical nomenclature as evidenced by the 1957 and 1965 IUPAC Definitive Rules, and the continuing changes being made by *Chemical Abstracts* provides ample support for the forward-looking attitude of the guidebook.

Chemists may ask: Why, long before this, have we not redesigned organic nomenclature to make it thoroughly systematic, at least for purposes of formal writing and publication? Actually, such attempts have been started on various occasions, the earliest and best known being the Geneva Rules in 1892, but no group or individual has done a complete job. As a result, although we have achieved a partially systematic nomenclature which is becoming more systematic year by year, it appears unlikely (1) that the present rules will ever become thoroughly systematic, or (2) that a new, entirely systematic fiducial nomenclature will be introduced.

There are several factors which weigh heavily against the adoption of a completely new fiducial nomenclature. First, there is no practical way to revise and republish the tremendous existing chemical literature, hence chemists would have to learn both old and new nomenclature. Second, the task of converting to a fiducial nomenclature by *Chemical Abstracts* and other chemical information processing agencies, both public and private, would be time consuming and costly. Third, unless adopted by *Chemical Abstracts* for its Subject Indexes, an entirely new organic nomenclature would probably not be widely accepted and used by the chemical profession. Fourth, for specialized information storage-retrieval operations, where conventional publication is not involved, chemical codes and computer language are required, and syllabic nomenclature is not directly applicable.

On the other hand, the possibility of developing a revised version of our present semisystematic organic nomen-

clature, which would be for all intents and purposes thoroughly systematic, is real, and the accomplishment of such an objective is not to be ruled out. Such a systematic nomenclature would retain as much as possible of present organic rules and principles and would add new rules only where present rules are inadequate or overcomplex. Admittedly, it would lead to many names strange to us, but it would have the advantages of maximum simplicity of rules and minimum burden on memory, particularly for chemists of coming generations. The technical feasibility of developing a thoroughly systematic syllabic organic nomenclature by reconstructing established rules and adding new rules where needed was demonstrated by the proposals of Dyson (4) and Taylor (5) and by extensive experimentation at the American Cyanamid Co. a number of years ago. However, among the questions which must be answered before official work along these lines by the American Chemical Society or by IUPAC can be justified are: (1) Would an extensively modified systematic nomenclature be considered for adoption by *Chemical Abstracts*? and (2) What would be its chances for eventual use by chemists in reports and publications? Attempts to answer these questions will provide the basis for much discussion and debate by the many parties involved, when and if

serious consideration is given to the development and introduction of a fully systematic organic nomenclature.

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Inorganic Nomenclature in 1966: Progress and Problems*

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A brief discussion of the history and current status of inorganic nomenclature is presented along with a discussion of the relationship between the American Chemical Society's work in inorganic nomenclature and that of the International Union of Pure and Applied Chemistry. Problem areas, especially those in the nomenclature of boron compounds, inorganic polymers, and cluster compounds are discussed.

The standardization of nomenclature practice is always a slow and halting process. Different workers in the same country have different nomenclature needs arising from different approaches to the same problem; in particular, workers from different language backgrounds have an increased problem in finding a uniformly acceptable nomenclature. The first definitive report of the Inorganic Nomenclature Commission of the International Union for Pure and Applied Chemistry (IUPAC) appeared in 1940

(1) and the second in 1957 (2). Currently the commission is taking steps to update and strengthen the 1957 report with a view toward publication of a tentative report in 1967 and a new definitive report in 1968. Since coordination nomenclature seems to be capable of unifying nearly all types of inorganic nomenclature, changes which appear to the writer to be most significant are in this area and include:

1. adoption of alphabetical order for ligands;
2. acceptance of the Ewens and Bassett system as an alternate to Stock numbers;
3. acceptance of the McDonnell and Pasternack system for designation of stereoisomerism.

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