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NAMING ORGANIC COMPOUNDS

a systematic instruction manual

E. W. Godly

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YELLOW PAGES:

Seniority of ring-systems, chains and ring-with-chain systems

Author's note

In 1981 I was asked if it would be possible to write an instruction manual on systematic organic chemical nomenclature—capable of covering 90% or so of all new compounds of interest in international trade—to be useful to readers with some knowledge of chemistry but little or none of the IUPAC Rules of Organic Nomenclature. It would not have been in any way reprehensible to have given a negative answer and only time and usage will show whether a simple 'NO' will prove ultimately to have been the correct response.

However, my feeling was that IUPAC systematic names are constructed according to rational and logically consistent principles which ought to be capable of explanation in terms comprehensible to the general reader and so I undertook the task despite the fact that no such 'stand-alone' work had to my knowledge been successfully produced.

At that time, my division of the Laboratory of the Government Chemist had been very active in producing a Euro-list of trade chemicals classified under their respective headings of the Common Customs Tariff. This list, now incorporated into the 'European Customs Inventory of Chemicals', EEC, Luxembourg, 1988, contained over 16 000 entries and its compilation had compelled us to supplement the IUPAC rules with in-house sub-rules and rationales aimed at consistent treatment of analogues. Armed with this body of experience, I felt that the task should not prove too onerous. That proved to be over-optimistic. However, trials on an earlier attempt gave a 70% success-rate and this 1988 revision has plugged a number of gaps, removed errors and inconsistencies and remedied inadequacies.

Mercifully, an instruction manual leaves no room for argument and non-preferred methods of naming, however valid, are omitted from consideration. Names produced by following these instructions should prove consistent with those of the Euro-Customs Inventory, Nos. 10001–26591.

For best results, readers should beware of using their own knowledge of the subject to modify specific instructions. These should be read carefully and applied faithfully.

Not every conceivable molecular structure is covered by the book; some rarely encountered species have been omitted, for to aim close to 100% success would require a very much thicker volume even than this. However, it is hoped that it will prove effective in most cases.

If this is found not to be so, or if a reader experiences any difficulty in obtaining such a result, enquiries should be directed to the Chemical Nomenclature Advisory Service, at the Laboratory of the Government Chemist, Teddington.

I am indebted to my colleague Mr Ivor Cohen for valuable advice and help in the preparation of this revised version.

E.W.G.

1 Introduction

This work was undertaken in the context of the application of Council Directive 79/831/EEC; of 18th September 1979, amending for the sixth time Directive 67/548/EEC on the approximation of the laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances.

1.1 AIMS AND FUNCTIONS

This book is in no way intended to replace the IUPAC Rules of Organic Chemical Nomenclature, to which serious students of the subject are directed,† but rather to provide a programme or recipe for devising an acceptable name for a new chemical under those Rules, in the form of a set of procedures not requiring the skills of a nomenclature-specialist. Some knowledge of basic chemistry is, however, assumed on the part of the reader. The names so generated will, it is hoped, provide unambiguous names in an internationally acceptable style, namely that of the IUPAC Rules.

These rules have been the basis of our naming rationales because the above-cited directive requires notification of new chemical substances before they are placed on the Community market, defined in these notifications by an IUPAC name. This approach has been adopted because the IUPAC philosophy for naming chemicals offers the following practical advantages for normal communication in international trade-contexts over more highly systematized methods:

(1) they incorporate a body of useful, established trivial names, which must continue to be the obvious first-choice names in all manner of practical industrial as well as legislative and regulatory contexts,
(2) their rules are translated into several languages and are continuing to expand their international acceptance,

† *Nomenclature of Organic Chemistry*, Sections A–F & H, 1979, Pergamon.

(3) their usages and conventions tend more often than not to result in names which are comparatively neat, succinct and readily intelligible to the chemical community,
(4) the IUPAC Rules have remained very largely the same for the last 30 years.

Against all that it must be admitted that, because of their traditional function of codifying various 'respectable' current nomenclature-practices, IUPAC Rules frequently allow more than one name for a given chemical. Accordingly, with a view to harmonizing the designation of new chemicals for the application of Directive 79/831/EEC, the methodology leading to a single, preferred IUPAC name had to be developed. To this end, *ad hoc* sub-rules devised for the purpose of obtaining consistency in the selection of preferred names for trade-chemicals in '*Classification of Chemicals in the Customs Tariff of the European Communities*'† have been used—with some amplification—in this book also.

In view of limitations on size and convenient handling, such a treatment could not hope to cover all possible structures, including those not yet conceived. Accordingly deliberate omissions of rarely seen structure-elements have been made and no treatment has been attempted for sections of the rules which are particularly complicated. It is, however, hoped that 90–95% of naming problems likely to be encountered will be found to be covered adequately by following the detailed instructions provided. Questions on naming arising either from the 5–10% area not covered, or for any other reason should be directed to the

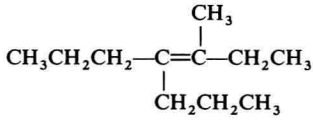
Chemical Nomenclature Advisory Service (CNAS),
Laboratory of the Government Chemist,
Department of Trade and Industry,
Queens Road, Teddington,
Middlesex, TW11 0LY, UK

1.2 HOW TO USE THE BOOK

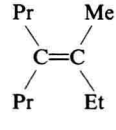
It is advisable to read Appendix D before attempting to name any but the simplest structures. Having done that, proceed as follows:

Unfold the **flow-diagram** at the back of the book and, commencing at the starting-point on the left, follow the track by addressing each question to the known structure of the single chemical under consideration, following the path according to the answer at each stage. To do this effectively, it may be necessary to rotate the structural formula about any of the three Cartesian axes for purposes of comparison with the structures printed in the book. Moreover, there are a number of ways to depict the same molecular situation and non-chemists may fail to appreciate that they are, in fact, identical. As an example, the following methods of depicting 3-methyl-4-propylhept-3-ene by no means exhaust all the possibilities:

(a)



(b)



(c)

$Pr_2C{=}C(Me)(Et)$

† Ed. by Forcheri, S. and de Rijk, J. R., EEC, Brussels, 1981.