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EXTENSION OF RULES A-1.1 AND A-2.5 CONCERNING NUMERICAL TERMS USED IN ORGANIC CHEMICAL NOMENCLATURE

(Recommendations 1986)

(Supersedes provisional version published 1983)

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Extension of Rules A-1.1 and A-2.5 concerning numerical terms used in organic chemical nomenclature (Recommendations 1986)

Numerical terms are used in chemical names for indicating a number of identical structural features in a compound. Rule A-1.1 of the IUPAC Organic Nomenclature Rules illustrates the numerical terms up through 199 in the names of saturated unbranched acyclic hydrocarbons. The use of these numerical terms for expressing identical simple substituents to a parent structure, and their modifications for use with "complex" substituents, is described in Rule A-2.5.

Recently a desire has been expressed for numerical terms higher than 199. This document provides the necessary guidance, based on principles already established, for generating terms up to 9999 by using the infixes "cta" (for the hundreds digits) and "lia" (for the thousands digits) in a way quite analogous to the use of "conta" now used for the tens digits beyond twenty.

INTRODUCTION

Rule A-1.1 (ref. 1a) uses numerical terms to name saturated unbranched acyclic hydrocarbons containing up to 199 carbon atoms. Until recently, numerical terms higher than 199 have not been required but now, in order to avoid confusion from alternative suggestions, it seems advisable to give a clear method for extending the list.

The number of identical substituents to a parent compound is expressed according to Rule A-2.5 (ref. 1b). For simple substituents, i.e., when not themselves substituted, the multiplying prefixes di-, tri-, and tetra-, are generally used; higher multiplying prefixes are formed by suppressing the ending "-ne" of the name of the corresponding alkane. For substituted substituents, the multiplying prefixes bis-, tris-, and tetrakis-, are used; higher multiplying prefixes are formed by replacing the ending "-ne" of the corresponding alkane by "-kis-".

Multiplying prefixes are used in much the same way to denote other identical structural features of a chemical compound, such as principal characteristic groups, sites of unsaturation, and number of ionic centers. However, the multiplying prefixes "bis-", "tris-", etc., are used instead of "di-", "tri-", etc. when the use of the latter would result in a potential ambiguity; for example, tris(decyl) is used to describe three decyl substituents because tridecyl is the name for a thirteen carbon acyclic substituent.

DISCUSSION

As far as possible, the principles embodied in the present terms have been used to extend the list. The general pattern in which units are cited first, then tens, hundreds, etc., has some disadvantages compared with the natural order of ciphers in arabic numerals, which is used in English and French, but not always in German. Nevertheless, in spite of the difficulties inherent to this "inverted" pattern, it is now so much entrenched in common day practice that any alternative order is out of the question.

Examination of the existing terms shows that names for sets of tens over twenty are formed by adding the ending "-conta-" to the name of the corresponding units, with insertion of an "a" for thirty:

3	tri-	30	triaconta-
4	tetra-	40	tetraconta-
5	penta-	50	pentaconta-, etc.

This appears to be quite a reasonable mnemonic method and if we want to extend the list, we shall need a specific ending for hundreds and for thousands.

The etymology of the prefixes derived from Rule A-1.1 is only loosely based on the corresponding Greek words. Relatively large divergences occur such as octaconta- for 80 instead of ogdoeconta-. In some cases, a Latin root has been preferred, or mixtures of Greek and Latin roots (e.g., nona- for 9, undeca- for 11, nonaconta- for 90).

According to Greek etymology, the ending for hundreds should be "-acosia-" which would lead to terms such as diacosia- for 200, tricosia- for 300, etc. However, these terms happen to be very similar to docosa- for 22, tricosa- for 23, etc. This is why the ending "-cta-", taken from hecta-, was proposed (ref. 2) and is used by Chemical Abstracts in the prefix dicta- for 200 (ref. 3).

For 1000, the term kilia- seems appropriate which suggests that the ending "-lia-" could denote multiplication by 1000.

Example: 2000 dilia (compare with dokilia for 1002)

RECOMMENDATIONS

Rule Nt-1. Numerical terms for simple features.

Nt-1.1 - The fundamental numerical terms for use in hydrocarbon names or as multiplying prefixes for simple features are given in the following list:

1 mono- or hen-*	10 deca-	100 hecta-	1000 kilia-
2 di- or do-*	20 icosa-**	200 dicta-	2000 dilia-
3 tri-	30 triaconta-	300 tricta-	3000 trilia-
4 tetra-	40 tetraconta-	400 tetracta-	4000 tetralia-
5 penta-	50 pentaconta-	500 pentacta-	5000 pentalia-
6 hexa-	60 hexaconta-	600 hexacta-	6000 hexalia-
7 hepta-	70 heptaconta-	700 heptacta-	7000 heptalia-
8 octa-	80 octaconta-	800 octacta-	8000 octalia-
9 nona-	90 nonaconta-	900 nonacta-	9000 nonalia-

Nt-1.2 - Numerical terms for other arabic numbers are formed by combining the fundamental numerical terms given in Nt-1.1, above in an order opposite to that of the constituent digits in the arabic number.

Example: 468 octahexacontatetracta

8 60 400

Nt-1.3 - When alone, the number 1 is represented by "mono-" and 2 by "di-". In association with other numerical terms, the number 1 is represented by "hen-" and 2 by "do-".

Examples:

Compare monochloro with henicosachloro

Compare dichloro with dodecachloro

Nt-1.4 - As an exception to Nt-1.3, the number 11 is represented by undeca- instead of hendeca-.

Rule Nt-2. Numerical terms for complex features.

Nt-2.1 - Numerical terms for use as multiplying prefixes for complex structural features, such as substituted substituents, are formed by adding the ending "-kis-" to the numerical terms defined in Nt-1. However, the ending "-kis-" is not used with "mono-".

Examples: 4 tetrakis-

231 hentriacontadictakis-

Nt-2.2. As exceptions to Nt-2.1, "bis-" is used for the number 2 and "tris-" for 3.

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* See Nt-1.3.

** The initial "i" is elided after a numerical prefix ending with a vowel, e.g., docosa-, tricosa-.

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