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

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Comments on these recommendations are welcome and should be sent within 8 months from September 1983 to the Secretary of the Commission:

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Comments from the viewpoint of languages other than English are especially encouraged. These may have special significance regarding the publication in various countries of translations of the nomenclature eventually approved by IUPAC.

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

Numerical terms are used in chemical names for indicating a number of identical structural units in a compound. Rule A-1.1 of the IUPAC Organic Nomenclature Rules illustrates the numerical terms up to 199 in the names of saturated unbranched acyclic hydrocarbons. The use of these numerical terms for expressing identical 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 numerical 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-" for the tens digits beyond twenty.

INTRODUCTION

The number of identical chemical entities substituted in a parent compound is expressed according to Rule A-2.5 (ref. 1a). If these entities are unsubstituted, the multiplying prefixes di-, tri-, tetra-, penta-, etc., are used. If these entities are more complex (e.g., substituted radicals), the multiplying prefixes bis-, tris-, tetrakis-, pentakis-, etc., are used. Higher multiplying prefixes for simple entities are formed by suppressing the "-ne" of the name of the corresponding alkane; higher multiplying prefixes for complex entities are formed by replacing the "-ne" of the corresponding alkane with "-kis-".

Rule A-1.1 (ref. 1b) explains how 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.

GENERAL PRINCIPLES

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 numbers, 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 multiples of tens beyond 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- (200), triacosia- (300), etc. However, these terms happen to be very similar to docosa- (22), tricosa- (23), etc. This is why the ending "-cta-", taken from hecta-, was proposed (ref. 2) and has been adopted by Chemical Abstracts for 200 (dicta-).

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

Example:

2000 dilia- (compare 1002 dokilia-)

PROPOSED RULES FOR NUMERICAL TERMS

Rule NT-1

NT-1.1 - Numerical terms for use in hydrocarbon names or as multiplying prefixes for simple entities 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 - Composite numerical terms are built up by citing the basic terms from Rule NT-1.1 in the order opposite to that of the constituent Arabic numerals.

Example:

468 octahexacontatetracta-

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* See Rule NT-1.3.

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

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 henicosane

Compare dichloro with dodecane

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

Rule NT-2

NT-2.1 - Numerical terms for use as multiplying prefixes for complex entities, such as substituted substituents, are obtained by adding the ending "-kis-" to the numerical terms defined in Rule NT-1. However, the ending "-kis-" is not used with "mono-" or "hen-".

Examples:

4	tetrakis-
231	hentriacontadictakis-

NT-2.2 - As exceptions to Rule NT-2.1, bis- is used for 2 and tris- for 3.

REFERENCES

1. International Union of Pure and Applied Chemistry, Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H, 1979 edition, Pergamon Press, Oxford, 1979: [a] p. 7; [b] p. 5.

2. N. Lozac'h, La Nomenclature en Chimie Organique, Masson Editeurs, Paris, 1967, p. 32.