



NOMENCLATURE OF
ORGANIC CHEMISTRY

1957



**INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY**

NOMENCLATURE OF ORGANIC CHEMISTRY

**DEFINITIVE RULES FOR
SECTION A. HYDROCARBONS
SECTION B. FUNDAMENTAL HETEROCYCLIC SYSTEMS**

*issued by the Commission on
the Nomenclature of Organic Chemistry*

**DEFINITIVE RULES FOR
NOMENCLATURE OF STEROIDS**

*issued by the Commissions on
the Nomenclature of Organic Chemistry
and the Nomenclature of Biological Chemistry*

**TENTATIVE RULES FOR
NOMENCLATURE IN THE VITAMIN B₁₂ FIELD**

*issued by the Commission on
the Nomenclature of Organic Chemistry*

JULY 1957

**LONDON
BUTTERWORTHS SCIENTIFIC PUBLICATIONS**

1958

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International Union of Pure and Applied Chemistry
1958

MADE AND PRINTED IN GREAT BRITAIN
AT THE CHAPEL RIVER PRESS
ANDOVER, HANTS

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DEFINITIVE RULES* FOR
NOMENCLATURE OF ORGANIC CHEMISTRY
SECTION A. HYDROCARBONS
SECTION B. FUNDAMENTAL HETEROCYCLIC SYSTEMS

*issued by the Commission on
the Nomenclature of Organic Chemistry
of the
International Union of Pure and Applied Chemistry*

July, 1957

*These Rules shall be known as the I.U.P.A.C. 1957 Rules

INTRODUCTION

The first international proposals on the nomenclature of organic chemistry, made at Geneva in 1892, were revised and extended by the Definitive Report of the Commission for the Reform of Nomenclature in Organic Chemistry of the International Union of Chemistry (I.U.C.) which appeared after the meeting at Liège in 1930 (Liège Rules), and was supplemented by less extensive reports from the meetings at Lucerne in 1936 and at Rome in 1938. Although these proposals rendered great service, it was apparent at the meeting of the International Union of Pure and Applied Chemistry at London in 1947 that, in some matters, extension and revision of the nomenclature rules for organic chemistry were required. Those who have served on the Commission on Nomenclature of Organic Chemistry for varying periods, from 1947 to date (1957) are: M. Betti*, R. S. Cahn, L. T. Capell, G. Dupont, G. M. Dyson, C. S. Gibson*, G. Kersaint, N. Lozac'h, R. Marquis*, A. D. Mitchell, H. S. Nutting, A. M. Patterson*, V. Prelog, F. Richter, S. Veibel, P. E. Verkade and E. Votocek*.

The Commission's progress in the period 1947 to 1955, inclusive, has been reported in successive issues of the *Comptes Rendus* of the Conferences of the Union. Relevant parts of those reports are included, with a few revisions, in the rules which form the body of this publication.

GENERAL PRINCIPLES

The Commission believes that differences in nomenclature frequently hinder the accurate and intelligible conveyance of information from one chemist to another, so tending to hamper understanding and progress. The Commission urges conformity with internationally agreed nomenclature even when this nomenclature may not seem the best possible from the point of view of the chemists of a particular nation or group.

The rules now presented are intended to be suitable for textbooks, journals and patents, for lexicons and similar compilations, and for indexes, even if not always wholly so for conversation or lectures. The rules will be issued in parts, as they become approved by the Union. They constitute recommendations for the naming of types of compounds and of individual compounds. They are not exhaustive, except in specified cases. Where, for various reasons, limitation to a single method of nomenclature appears undesirable or impossible, alternatives are given; but the Commission hopes that elimination of alternatives may become acceptable as the merits of one method become more generally recognized. The Commission hopes also that each nation will try to reduce the variations in nomenclature with regard to spelling, the position of numbers, punctuation, italicizing, abbreviations, elision of vowels, certain terminations, and so forth; the present rules are not to be held as making recommendations in these matters; the rules are written in accord with the conventions of *Chemical Abstracts* (except where specifically stated otherwise), but solely for uniformity from one rule to another.

* Deceased.

INTRODUCTION

Owing to the very extensive nomenclature which has come into being since the last revision, the Commission has, in the main, confined its efforts to codifying sound practices which already existed, rather than to originating new nomenclature—the latter may form a later stage of the Commission's activities.

In so doing, the Commission had in mind the following main principles: (a) as few changes as possible should be made in existing nomenclature, though utility is more important than priority; (b) rules and names should be unequivocal and unique, but simple and concise; (c) records in journals, abstracts, compendia, and industry should be used to assess the relative extent of past use of various alternatives; (d) rules should be consistent with one another, yet aid expression in the particular field of chemistry involved and be capable of extension with the progress of science; (e) trivial names, and names having only a very small systematic component, cannot be eliminated when in very common use, but those of less value should be replaced by systematic (or at least more systematic) ones, and the creation of new trivial names should be discouraged by provision of extensible systematic nomenclature; (f) names should be adaptable to different languages. The Commission is aware that acceptance of its recommendations depends in large measure on the success which has attended its attempts to assess, for each particular case, the relative merits of these often conflicting claims.

GLOSSARY

The Commission considered it unnecessary to define chemical terms in common use. However, certain terms which have special meaning in nomenclature merit brief description; namely:

Parent name: that part of the name from which a particular name is derived by a prescribed variation; *e.g.*, ethane giving rise to ethanol. Names often have more than one parent; *e.g.*, (chloromethyl)cyclohexane has methylcyclohexane as parent, which in turn has cyclohexane as its parent.

Systematic name: a name composed wholly of specially coined or selected syllables, with or without numerical prefixes; *e.g.*, pentane, oxazole.

Trivial name: a name no part of which is used in a systematic sense; *e.g.*, xanthophyll.

Semi-systematic name or semi-trivial name: a name of which only a part is used in a systematic sense; *e.g.*, methane (-ane), butene (-ene), calciferol (-ol). (Most names in organic chemistry belong to this class.)

Substitutive name: a name involving replacement of hydrogen by a group or by another element; *e.g.*, 1-methylnaphthalene, 1-pentanol.

Replacement name: an "a" name, where C, CH, or CH₂ is replaced by a hetero-atom; *e.g.*, 2,7,9-triazaphenanthrene. Also, certain names involving thio- (also seleno- or telluro-) to indicate replacement of oxygen by sulfur (or selenium or tellurium, respectively); *e.g.*, thiopyran.

Subtractive name: a name involving removal of specified atoms; *e.g.*, in the aliphatic series names ending in -ene or -yne. Also names involving anhydro-, dehydro-, deoxy-, *etc.*, or nor-.

INTRODUCTION

Radicalfunctional name: a name formed from the name of a radical and the name of a functional class; *e.g.*, acetyl chloride, ethyl alcohol.

Additive name: a name signifying addition between molecules and/or atoms; *e.g.*, styrene oxide.

Conjunctive name: a name formed by placing together the names of two molecules, it being understood that the two molecules are linked by loss of one hydrogen atom from each; *e.g.*, naphthaleneacetic acid.

Fusion name: a name for a cyclic system formed by use of a linking "o" between the names of two ring systems, denoting that the two systems are fused by two or more common atoms; *e.g.*, benzofuran.

Hantzsch-Widman name: a name for a heterocyclic system, as devised by Hantzsch and Widman, from a prefix or prefixes (to denote a hetero-atom or atoms) and a suffix -ole or -ine (to denote a five- or a six-membered ring, respectively); *e.g.*, triazole, thiazole.

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A. HYDROCARBONS

ACYCLIC HYDROCARBONS

Rule A-1

1.1—The first four saturated unbranched acyclic hydrocarbons are called methane, ethane, propane and butane. Names of the higher members of this series consist of a numerical prefix and the termination “-ane”. Examples of these numerical prefixes are shown in the table below. The generic name of saturated acyclic hydrocarbons (branched or unbranched) is “alkane”.

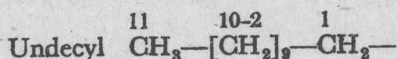
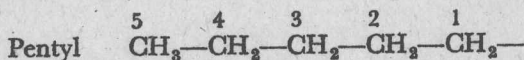
Examples:

(n = total number of carbon atoms)

n		n		n	
1	Methane	15	Pentadecane	29	Nonacosane
2	Ethane	16	Hexadecane	30	triacontane
3	Propane	17	Heptadecane	31	Hentriacontane
4	Butane	18	Octadecane	32	Dotriacontane
5	Pentane	19	Nonadecane	33	Tritriacontane
6	Hexane	20	Eicosane	40	Tetracontane
7	Heptane	21	Heneicosane	50	Pentacontane
8	Octane	22	Docosane	60	Hexacontane
9	Nonane	23	Tricosane	70	Heptacontane
10	Decane	24	Tetracosane	80	Octacontane
11	Undecane	25	Pentacosane	90	Nonacontane
12	Dodecane	26	Hexacosane	100	Hectane
13	Tridecane	27	Heptacosane	132	Dotriacontahectane
14	Tetradecane	28	Octacosane		

1.2—Univalent radicals derived from saturated unbranched acyclic hydrocarbons by removal of hydrogen from a terminal carbon atom are named by replacing the ending “-ane” of the name of the hydrocarbon by “-yl”. The carbon atom with the free valence is numbered as 1. As a class, these radicals are called normal, or unbranched chain, alkyls.

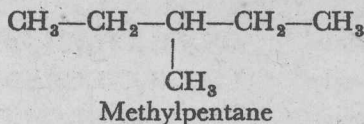
Examples:



Rule A-2

2.1—A saturated branched acyclic hydrocarbon is named by prefixing the designations of the side chains to the name of the longest chain present in the formula.

Example:

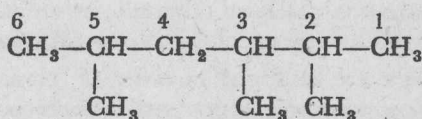
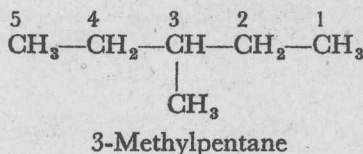


The following names are retained for unsubstituted hydrocarbons only:

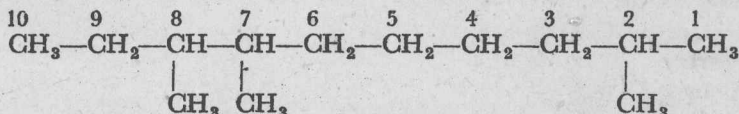
Isobutane	$(\text{CH}_3)_2\text{CH}-\text{CH}_3$
Isopentane	$(\text{CH}_3)_2\text{CH}-\text{CH}_2-\text{CH}_3$
Neopentane	$(\text{CH}_3)_4\text{C}$
Isohexane	$(\text{CH}_3)_2\text{CH}-\text{CH}_2-\text{CH}_2-\text{CH}_3$

2.2—The longest chain is numbered from one end to the other by arabic numerals, the direction being so chosen as to give the lowest numbers possible to the side chains. When series of locants containing the same number of terms are compared term by term, that series is "lowest" which contains the lowest number on the occasion of the first difference. This principle is applied irrespective of the nature of the substituents.

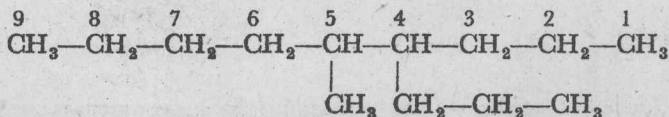
Examples:



2,3,5-Trimethylhexane (not 2,4,5-Trimethylhexane)



2,7,8-Trimethyldecane (not 3,4,9-Trimethyldecane)

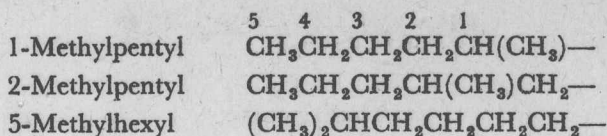


5-Methyl-4-propylnonane

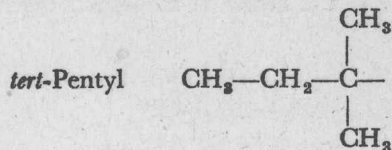
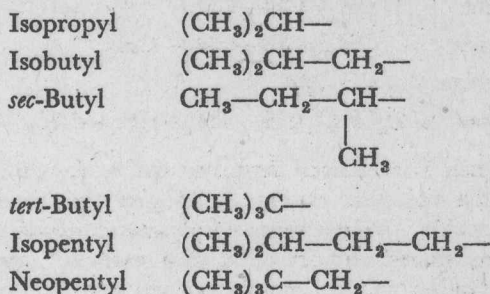
(not 5-Methyl-6-propylnonane because 4,5 is lower than 5,6)

2.25—Univalent branched radicals derived from alkanes are named by prefixing the designation of the side chains to the name of the unbranched alkyl radical possessing the longest possible chain starting from the carbon atom with the free valence, the said atom being numbered as 1.

Examples:



The following names are retained for the unsubstituted radicals only:

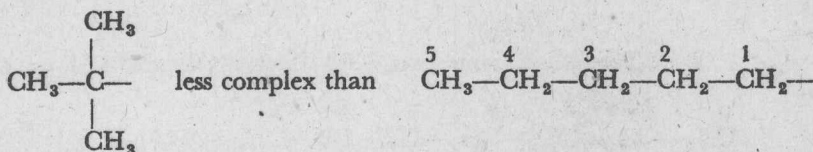


2.3—If two or more side chains of different nature are present, they may be cited (a) in order of increasing complexity or (b) in alphabetical order.

(a) The side chains are arranged in order of increasing complexity by applying the following criteria in series until a decision is reached:

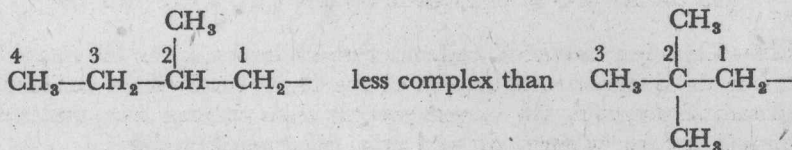
(i) The less complex is that containing the smaller total number of carbon atoms.

Example:



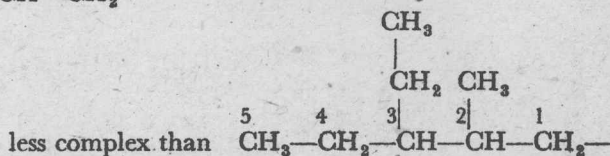
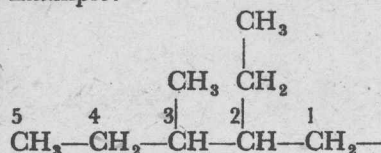
(ii) The less complex is that containing the longer straight chain.

Example:



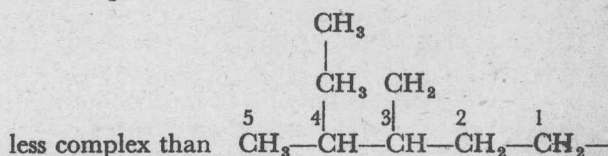
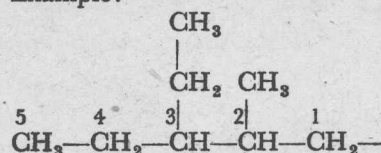
(iii) The less complex is that whose longest substituent has the lower locant.

Example:



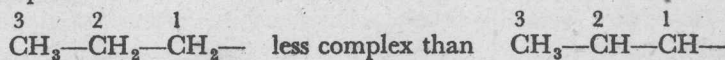
(iv) The less complex is that whose next longest substituent has the lower locant.

Example:



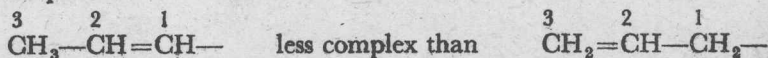
(v) The less complex is that which is the more saturated.

Example:



(vi) The less complex is that whose multiple linkage has the lower locant.

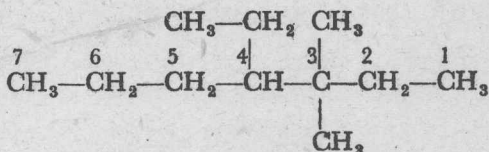
Example:



(b) The alphabetical order is decided as follows:

(i) The names of simple radicals are first alphabetized and the multiplying prefixes are then inserted.

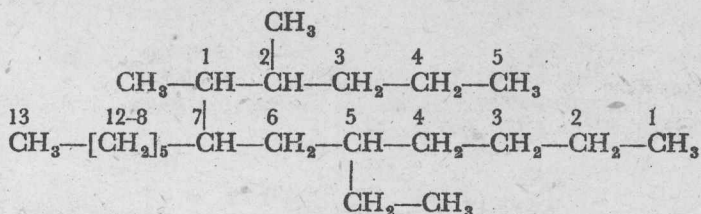
Example:



ethyl is cited before methyl, thus 4-Ethyl-3,3-dimethylheptane

(ii) The name of a complex radical is considered to begin with the first letter of its complete name.

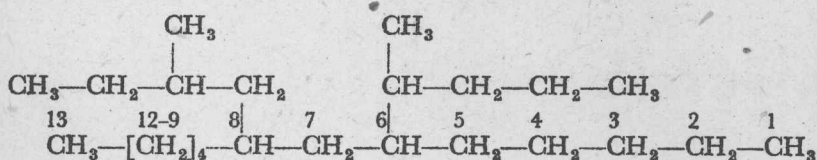
Example:



dimethylpentyl (as a complete single substituent) is alphabetized under "d", thus 7-(1,2-Dimethylpentyl)-5-ethyltridecane

(iii) In cases where complex radicals are composed of identical words, priority for citation is given to that radical which contains the lowest locant at the first cited point of difference in the radical.

Example:

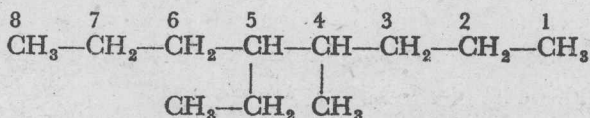


6-(1-Methylbutyl)-8-(2-methylbutyl)tridecane

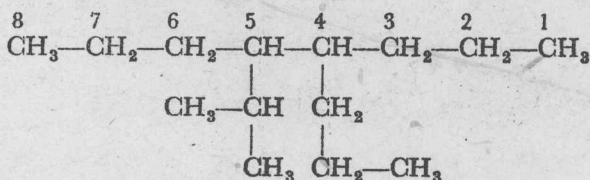
2.4—If two or more side chains are in equivalent positions, the one to be assigned the lower number is that cited first in the name, whether the order of citation is based on complexity or on the alphabetical order.

Examples:

(a) Order based on complexity:

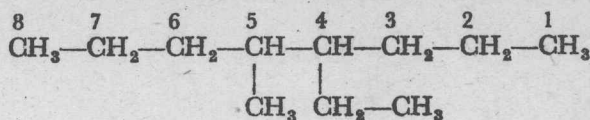


4-Methyl-5-ethyloctane

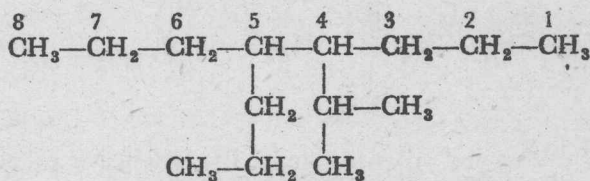


4-Propyl-5-isopropyloctane

(b) Alphabetical order:



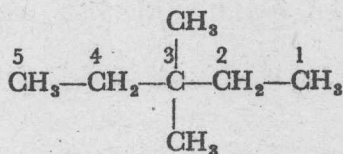
4-Ethyl-5-methyloctane



4-Isopropyl-5-propyloctane

2.5—The presence of identical unsubstituted radicals is indicated by the appropriate multiplying prefix di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, deca-, undeca-, etc.

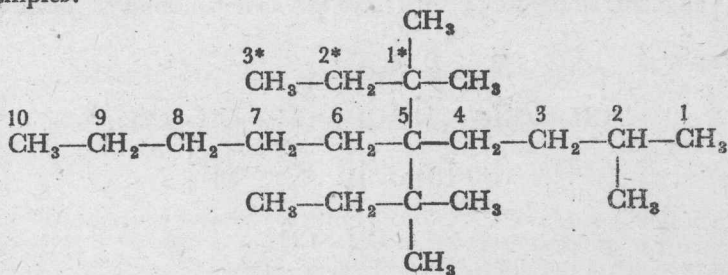
Example:



3,3-Dimethylpentane

The presence of identical radicals each substituted in the same way may be indicated by the appropriate multiplying prefix bis-, tris-, tetrakis-, pentakis-, etc. The complete expression denoting a side chain may be enclosed in parentheses or the carbon atoms in side chains may be indicated by primed numbers.

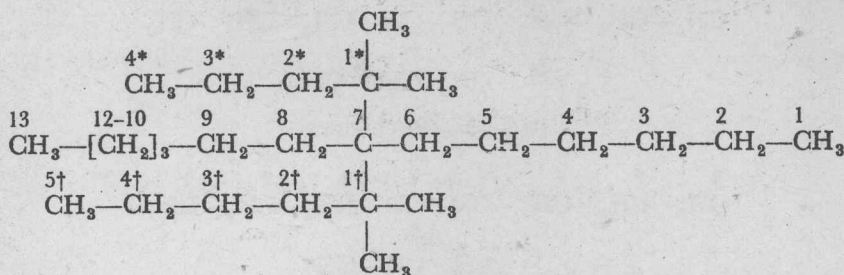
Examples:



(a) Use of primes and order of complexity, * indicates primed numbers:
2-Methyl-5,5-bis-1',1'-dimethylpropyldecane.

(b) Use of parentheses and alphabetical order, * indicates unprimed numbers:
5,5-Bis(1,1-dimethylpropyl)-2-methyldecane.

- (c) Use of primes and alphabetical order, * indicates primed numbers:
5,5-Bis-1',1'-dimethylpropyl-2-methyldecane.

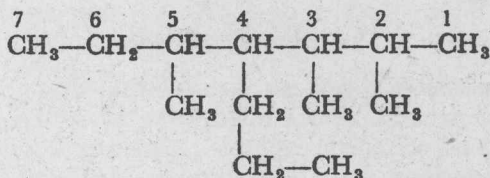


- (a) Use of primes and order of complexity, * indicates primed numbers, † indicates doubly primed numbers:
7-1', 1'-Dimethylbutyl-7-1'', 1''-dimethylpentyltridecane.
- (b) Use of parentheses and alphabetical order, * and † indicate unprimed numbers:
7-(1,1-Dimethylbutyl)-7-(1,1-dimethylpentyl)tridecane.

2.6—If chains of equal length are competing for selection as main chain in a saturated branched acyclic hydrocarbon, then the choice goes in series to:¹

- (a) The chain which has the greatest number of side chains.

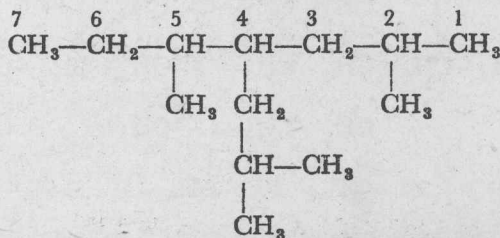
Example:



2,3,5-Trimethyl-4-propylheptane

- (b) The chain whose side chains have the lowest-numbered locants.

Example:

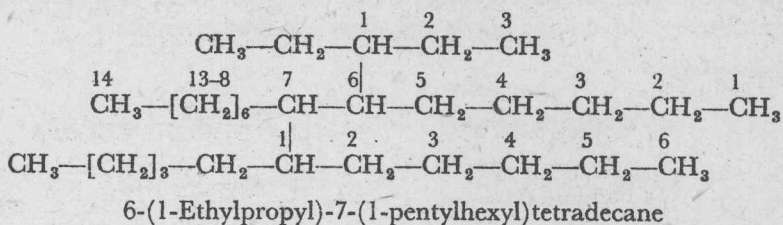


4-Isobutyl-2,5-dimethylheptane

- (c) The chain having the greatest number of carbon atoms in the smaller side chains.

$$\begin{array}{ccccccc}
 & \text{CH}_3 & & \text{CH}_3 & & \text{CH}_3 & & \text{CH}_2-\text{CH}_3 \\
 & | & & | & & | & & | \\
 \text{CH}_3\text{CH}_2\text{CH}-\text{CH}_2-\text{CH}-\text{CH}_2 & & & & & & & \text{CH}_2-\text{CH}-\text{CH}_2-\text{CH}-\text{CH}_2\text{CH}_3 \\
 13 & 12 & 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\
 & & & & & & \text{C} & & & & & & \\
 & & & & & & / \quad \backslash & & & & & & \\
 \text{CH}_3\text{CH}_2\text{CH}-\text{CH}_2-\text{CH}-\text{CH}_2 & & & & & & \text{CH}_2-\text{CH}-\text{CH}_2-\text{CH}-\text{CH}_2\text{CH}_3 \\
 & | & & | & & & | & & | \\
 & \text{CH}_3 & & \text{CH}_3 & & & \text{CH}_2 & & \text{CH}_3
 \end{array}$$

(d) The chain having the least branched side chains.



3.1—Unsaturated unbranched acyclic hydrocarbons having one double bond are named by replacing the ending “-ane” of the name of the corresponding saturated hydrocarbon with the ending “-ene”. If there are two or more double bonds, the ending will be “-adiene”, “-atriene”, *etc.* The generic names of these hydrocarbons (branched or unbranched) are “alkene”, “alkadiene”, “alkatriene”, *etc.* The chain is so numbered as to give the lowest possible numbers to the double bonds.

$$\begin{array}{l} \text{2-Hexene} \qquad \qquad \qquad \begin{array}{cccccc} 6 & 5 & 4 & 3 & 2 & 1 \\ \text{CH}_3 & -\text{CH}_2 & -\text{CH}_2 & -\text{CH} & =\text{CH} & -\text{CH}_3 \end{array} \\ \text{1,4-Hexadiene} \qquad \qquad \begin{array}{cccccc} 6 & 5 & 4 & 3 & 2 & 1 \\ \text{CH}_3 & -\text{CH} & =\text{CH} & -\text{CH}_2 & -\text{CH} & =\text{CH}_2 \end{array} \end{array}$$

Ethylene $\text{CH}_2=\text{CH}_2$ Allene $\text{CH}_2=\text{C}=\text{CH}_2$

first choice	1, 1, 1, 2, 8, 8
second choice	1, 1, 1, 1, 8, 9

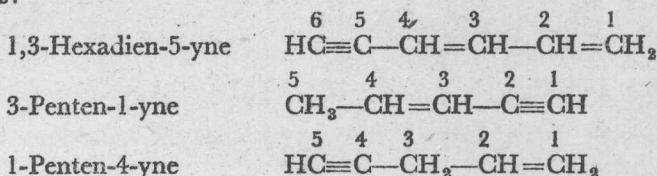
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3.2—Unsaturated unbranched acyclic hydrocarbons having one triple bond are named by replacing the ending “-ane” of the name of the corresponding saturated hydrocarbon with the ending “-yne”. If there are two or more triple bonds, the ending will be “-adiyne”, “-atriyne”, *etc.* The generic names of these hydrocarbons (branched or unbranched) are “alkyne”, “alkadiyne”, “alkatriyne”, *etc.* The chain is so numbered as to give the lowest possible numbers to the triple bonds.

The name “acetylene” for $\text{HC}\equiv\text{CH}$ is retained.

3.3—Unsaturated unbranched acyclic hydrocarbons having both double and triple bonds are named by replacing the ending “-ane” of the name of the corresponding saturated hydrocarbon with the ending “-enyne”, “-adienyne”, “-atrienyne”, “-enediyne”, *etc.* Numbers as low as possible are given to double and triple bonds even though this may at times give “-yne” a lower number than “-ene”. When there is a choice in numbering, the double bonds are given the lowest numbers.

Examples:



3.4—Unsaturated branched acyclic hydrocarbons are named as derivatives of the unbranched hydrocarbons which contain the maximum number of double and triple bonds. If there are two or more chains competing for selection as the chain with the maximum number of unsaturated bonds, then the choice goes to (1) that one with the greatest number of carbon atoms; (2) the number of carbon atoms being equal, the one containing the maximum number of double bonds. In other respects, the same principles apply as for naming saturated branched acyclic hydrocarbons. The chain is so numbered as to give the lowest possible numbers to double and triple bonds in accordance with Rule A-3.3.

Examples:

