

## ORGANIC SUBSTANCES AND STRUCTURES, NOMENCLATURE OF ORGANIC COMPOUNDS

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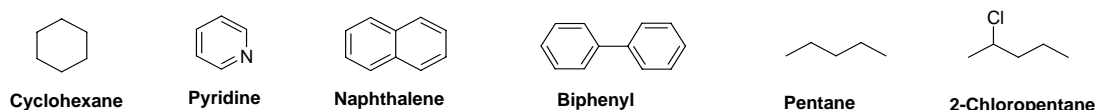
### Summary

Formally, rules established by the International Union of Pure and Applied Chemistry (known as IUPAC nomenclature) are authoritative for the names of organic compounds, but in practice, a number of simply-applied rules can allow one to use and understand the names of many organic compounds. For many compounds, naming can begin by determining the name of the parent hydrocarbon and by identifying any functional groups in the molecule that distinguish it from the parent hydrocarbon. The numbering of the parent alkane is used, as modified, if necessary, by application of the Cahn Ingold Prelog priority rules in the case that ambiguity remains after consideration of the structure of the parent hydrocarbon alone. The name of the parent hydrocarbon is modified by the application of the highest-priority functional group suffix, with the remaining functional groups indicated by numbered prefixes, appearing in the name in alphabetical order from first to last. We will present herein the basic of the organic nomenclature. In contrast to such systematic names, there are traditional names, semisystematic or trivial, which are widely used for a core group of common compounds (e.g.: acetic acid, toluene, adenosine, alanine, porphyrin, phenol). For a deep knowledge, readers are suggested to visit the above mentioned references website for nomenclatures.

- A Guide to IUPAC Nomenclature of Organic Compounds, 1993, Blackwell Scientific Publications
- Chemical Abstracts Service
- Beilstein Institute
- Explore IUPAC and CAS Nomenclature tools, such as Free IUPAC name generation and professional ACD/Name Software

## 1. Type(s) of Nomenclature Operations

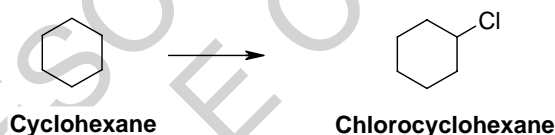
Systematic naming of an organic compound generally requires the identification and naming of a parent structure. This name may then be modified by prefixes, infixes, and, in the case of a parent hydride, suffixes, which convey precisely the structural changes required to generate the actual compound from the parent structure. Rules for naming parent hydrides are given below; in addition, a special class of parent structures termed functional parents, for example, phosphinic acid, is considered.



In order to generate the parent structure from a molecule to be named, various formal operations must be carried out.

### 1.1. Substitutive Operation



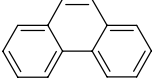
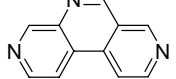
The substitutive operation is the operation most extensively used in organic nomenclature. Indeed, the comprehensive nomenclature system based largely on the application of this operation to parent structures is, for convenience, termed "substitutive nomenclature", although this system also involves many of the other types of operations. The substitutive operation involves the exchange of one or more hydrogen atoms for another atom or group. This process is expressed by a prefix or suffix denoting the atom or group being introduced.



### 1.2. Replacement Operation

The replacement operation can be used for naming organic compounds in which skeletal atoms of a parent structure are replaced by other skeletal atoms, or in which oxygen atom and/or hydroxy groups of characteristic groups are replaced by other atoms or groups. The replacement operation involves the exchange of one group of atom or a single non hydrogen atom for another. This can be expressed in several ways as follow:

- **By use of "a" prefixes representing the element(s) being introduced**, usually signifying replacement of carbon.

|   |   |  |
|---|---|--|
| <br>Cyclohexane  | → | <br>Silacyclohexane<br>(replacement prefix = sila)         |
| <br>Phenanthrene | → | <br>2,7,9-Triazaphenanthrene<br>(replacement prefix = aza) |

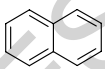
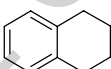
- **By use prefixes or infixes signifying replacement of oxygen atoms or oxygen-containing group.** These affixes represent the group(s) being introduced.

|   |   |   |
|---|---|---|
| $(\text{CH}_3)_2\text{P}(\text{O})(\text{OCH}_3)$<br>Methyl dimethylphosphinate | → | $(\text{CH}_3)_2\text{P}(\text{NH})(\text{OCH}_3)$<br>Methyl <i>P,P</i> -dimethylphosphinimidate<br>(replacement infix = imid(o)) |
| $\text{C}_6\text{H}_5\text{P}(\text{O})(\text{OH})_2$<br>Phenylphosphonic acid  | → | $\text{C}_6\text{H}_5\text{P}(\text{N})(\text{OH})$<br>Phenylphosphonitridic acid<br>(replacement infix = nitrid(o))              |



### 1.3. Additive Operation

The additive operation involves the formal assembly of a structure from its component parts without loss of any atoms or groups. This can be expressed in various ways as follows:

- **By use of an additive prefix**

|  |   |  |
|--|---|--|
| <br>Naphthalene | → | <br>1,2,3,4-Tetrahydronaphthalene<br>(hydro = addition of one H atom) |
|--|---|--|

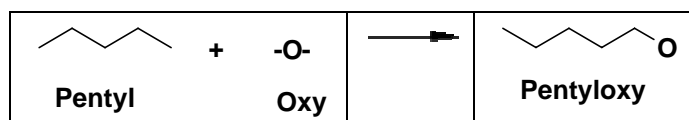
- **By use of an additive suffix**

|   |   |   |
|---|---|---|
| <br>Pyridine | → | <br>Pyridinium<br>(-ium = addition of one H <sup>+</sup> ) |
|---|---|---|

- **By use of a separate word**

|  |   |  |
|--|---|--|
| $\text{C}_6\text{H}_5\text{—CH=CH}_2$<br>Styrene     | → | $\text{C}_6\text{H}_5\text{—CH}_2\text{—CH}_2\text{—O}$<br>Styrene oxide |
| $\text{H}_3\text{C—} + \text{HO—}$<br>Methyl Alcohol | → | $\text{H}_3\text{C—OH}$<br>Methanol                                      |

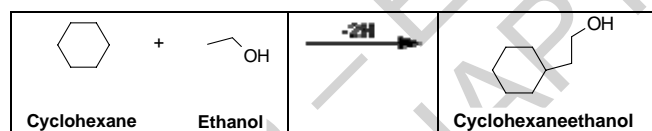
- **By juxtaposition or multiplication of substituent prefix terms**



#### 1.4. Conjunctive Operation

The conjunctive operation involves the formal construction of the name of a compound from those of its components with abstraction of the same number of hydrogen atoms from each component at each site of conjunction. This operation may be expressed:

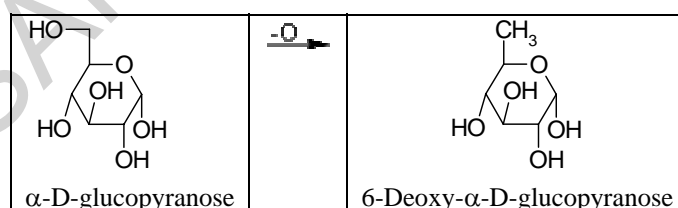
**By juxtaposition of component names.** This method is most commonly used when the two components to be joined are: (a) a ring or a ring system; and (b) a carbon chain (or chains) substituted by a principal characteristic group. In this method, both the principal characteristic group and the ring or ring system must terminate the chain; the rest of the structure attached to the chain, if any, is described by substituent prefixes, the location of which is indicated by Greek letter locants,  $\alpha, \beta, \dots$  (designating the atom next to the principal characteristic group).



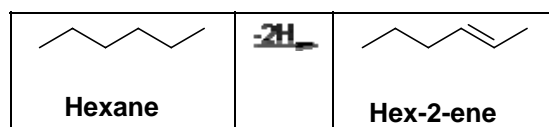
#### 1.5. Subtractive Operation

The subtractive operation involves the removal of an atom, ion, or group implicit in a name. This can occur with no other change, with exchange for hydrogen, with introduction of unsaturation, or with bond scission and reformation. The elimination of the elements of water with concomitant bond formation can also be regarded as a subtractive operation. Subtraction can be expressed in the following ways:

- **By use of a prefix**

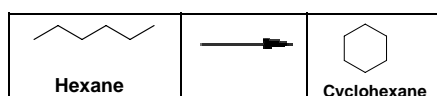


- **By a change in ending or addition of a suffix**



#### 1.6. Ring Formation or Cleavage

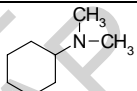
- **The prefix cyclo-**. The formation of a ring by means of a direct link between any two atoms of a parent structure, with loss of one hydrogen atom from each, is indicated by the prefix "cyclo-" followed by the name of the parent structure; when appropriate, this prefix is preceded by the locants of the positions joined by the new bond and by the Greek letter ( $\alpha, \beta, \gamma$ ) denoting the configurations at the ends of the new bond. (See R-2.3.1.1 and Section F of the 1979 edition of the IUPAC *Nomenclature of Organic Chemistry*).



## 2. General Rules

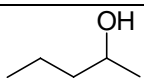

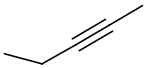
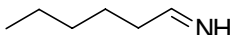
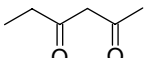
### 2.1. Capitalized and Italic

The capitalized italic letters such as O-, N-, P-, S-, are used to indicate a substituent on those heteroatoms:

| Name                        | Structure   |
|-----------------------------|---|
| N,N-Dimethylcyclohexylamine |  |

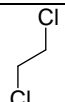
### 2.2. Numbers of Position

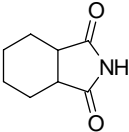
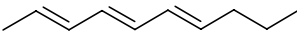

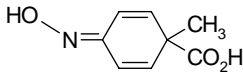
The number dealing with the position of a substituent or a functional group is located before (and not after) the function referred:

| Name            | Structure  |
|-----------------|--|
| Pentan-2-ol     |  |
| Hex-2-ene       |  |
| Pent-2-yne      |  |
| Hexan-1-imine   |  |
| Hexan-2,4-dione |  |




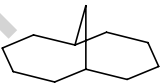
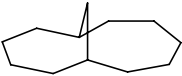
### 2.3. Punctuation

- The comma is used to separate various successive numbers:

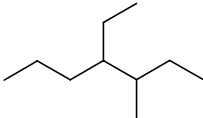
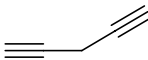
| Name               | Structure  |
|--------------------|--|
| 1,2-Dichloroethane |  |

|   |   |
|---|---|
| Hexahydro-isoindole-1,3-dione                                 |   |
| Deca-2,4,6-triene   |   |
| Cyclohexa-1,4-diene   |  |
| 4-Hydroxyimino-1-methyl-cyclohexa-2,5-diene-1-carboxylic acid |   |

- The point is used to separate numbers which indicate the number of atoms and not their positions:

| Name                   | Structure  |
|------------------------|--|
| Bicyclo[2.2.1]heptane  |    |
| Bicyclo[3.2.2]nonane   |    |
| Bicyclo[3.3.2]decane   |  |
| Bicyclo[4.4.1]undecane |  |
| Bicyclo[5.4.1]dodecane |  |

- The dash is used to separate numbers from letters, and the name of the last group or radical is joined to the base name as a continuous word. The groups may be given in alphabetical order or in the order of decreasing complexity.

| Name                    | Structure  |
|-------------------------|--|
| 4-Ethyl-3-methylheptane |  |
| Penta-1,4-diyne         |  |

### 3. Parent Name

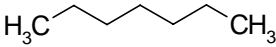
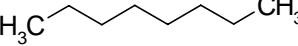
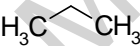
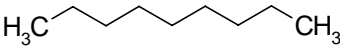
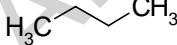
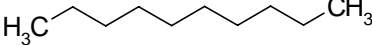
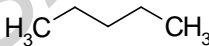
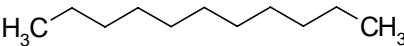
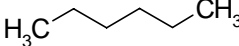
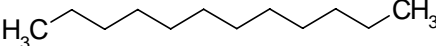
A "parent hydride" is the structure which is named before the addition of affixes denoting substituents to yield the name of a specific compound. Its name is understood to signify a definite population of hydrogen atoms attached to a skeletal structure. Acyclic parent hydrides are always unbranched (for instance pentane) although a few trivial names for branched acyclic hydrocarbons are retained, their use for naming substitutive derivatives is not recommended. Cyclic parent hydrides are usually either fully saturated, for example, cyclopentane, cyclotrisiloxane, azepane, bicyclo[2.2.2]octane, and spiro[4.5]decane, or fully unsaturated, i.e., they contain the maximum number of non cumulative double bonds, for example, pyridine, 1,3-oxazole, 1*H*-phenalene, phenanthroline, and benzo[*a*]anthracene.

#### 3.1. Alkanes

Alkanes or saturated hydrocarbons are compounds containing only carbon and hydrogen. Alkanes may be divided into (1) normal alkanes, whose carbon chains are straight or unbranched and (2) branched alkanes.

##### • Unbranched alkanes

The saturated unbranched acyclic hydrocarbons from C<sub>1</sub> to C<sub>4</sub> are named methane, ethane, propane, and butane. Systematic names of the higher members of this series consist of a numerical term, followed by "-ane" with elision of a terminal 'a' from the basic numerical term. The generic name for saturated acyclic hydrocarbons (branched or unbranched) is "alkane". The chain is numbered from one end to the other with Arabic numerals.

| Name    | Structure   | Name            | Structure  |
|---------|---|-----------------|--|
| Methane | CH <sub>4</sub>   | Heptane         |  |
| Ethane  | H <sub>3</sub> C-CH <sub>3</sub>  | Octane          |  |
| Propane |  | Nonane          |  |
| Butane  |  | Decane          |  |
| Pentane |  | Undecane        |  |
| Hexane  |  | <i>Dodecane</i> |  |

##### • Branched alkanes

To name members of a branched series, the longest straight chain becomes the "base" name. On that chain are located various alkyl radicals.

Alkyl radicals represent alkanes with a terminal hydrogen missing and end with -yl.

| Alkane  | Structure                        | Alkyl Radical | Structure                        |
|---------|----------------------------------|---------------|----------------------------------|
| Methane | CH <sub>4</sub>                  | Methyl        | CH <sub>3</sub>                  |
| Ethane  | H <sub>3</sub> C-CH <sub>3</sub> | Ethyl         | H <sub>3</sub> C-CH <sub>2</sub> |
| Propane |                                  | Propyl        |                                  |
| Butane  |                                  | Butyl         |                                  |
| Pentane |                                  | Pentyl        |                                  |
| Hexane  |                                  | Hexyl         |                                  |

The location of an alkyl radical is indicated by numbering the carbon atoms in the basic straight chain and assigning the lower number to the alkyl radical. In general, numbers may proceed from either direction of the molecule, but one must strive to have the lowest numbers possible.

| Name   | Structure |
|--|-----------|
| 2-Methylpentane<br>(and not 4-methylpentane) |           |
| 3-Methylpentane<br>(and not 2-ethylbutane)   |           |

When similar groups are present in a compound, then prefixes are used to indicate their numbers.

- **Prefixes used in naming organic compounds**

| Prefix | Number of groups |
|--------|------------------|
| mono-  | 1                |
| di-    | 2                |
| tri-   | 3                |
| tetra- | 4                |
| penta- | 5                |
| hexa-  | 6                |
| hepta- | 7                |
| octa-  | 8                |
| nona-  | 9                |
| deca-  | 10               |









One number must be used to indicate the position of each group. That is, there must be a number for each group even if the groups are attached to the same carbon atom.

| Name                | Structure |
|---------------------|-----------|
| 2,3-Dimethylpentane |           |
| 2,2-Dimethylbutane  |           |

- **Cycloalkanes**



The names of saturated monocyclic hydrocarbons are formed by attaching the prefix "cyclo-" to the name of the acyclic saturated unbranched hydrocarbon with the same number of carbon atoms. The generic name of monocyclic hydrocarbons is "cycloalkane". Numbering proceeds sequentially round the ring.

| Name         | Structure   | Name         | Structure   |
|--------------|---|--------------|---|
| Cyclopropane |  | Cycloheptane |  |
| Cyclobutane  |  | Cyclooctane  |  |
| Cyclopentane |  | Cyclononane  |  |
| Cyclohexane  |  | Cyclodecane  |  |

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### **Biographical Sketches**

**Luigi A. Agrofoglio**, born in Antibes, France (1965), received his B.S. (1987) and Ph.D. (1993) degrees in chemistry from the University of Nice Sophia-Antipolis (Fr) working on the synthesis of carbocyclic analogues of nucleosides. Dr. Agrofoglio has held two postdoctoral appointments, first at the University of Alabama at Birmingham, USA, working with Professor J.-P. Sommadossi, then at the University of Georgia at Athens (UGA) within the laboratory of Professor C.K. Chu. He joined the Institute of Organic and Analytical Chemistry (ICOA), a CNRS research laboratory associated with the University of Orléans (Fr), as Assistant Professor in 1995; he assumed now his current position as full Professor at the same institution. His main areas of expertise and interest deal with organic chemistry, molecular imprinted polymers as well as bioanalysis of nucleosides.

**Patrick Rollin**, born in Fontainebleau, France, received his chemical education from Professor P. Sinaÿ. After joining in Orleans Professor G. Guillaumet to create a new laboratory in organic chemistry, he became full Professor in 1991 and Director of the IUP Applied Chemistry School (1991-2004). He is now currently PRCE at the ICOA with the following major research interests: thiochemistry of sugars and chemistry of thio-sugars, use of thio-functions in stereo controlled synthesis, brassicale chemistry (glucosinolates and their metabolites), and green chemistry (integrated valorization of renewable resources and bioproducts).