



**SEMMELWEIS  
UNIVERSITY**



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**Development of Complex Curricula for Molecular Bionics and Infobionics Programs within a consortial\* framework\*\***

Consortium leader

**PETER PAZMANY CATHOLIC UNIVERSITY**

Consortium members

**SEMMELWEIS UNIVERSITY, DIALOG CAMPUS PUBLISHER**

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# World of Molecules

(Molekulák Világa )

## Organic compounds and nomenclature: why 'organic', conventions and rules

(Szerves vegyületek és elnevezésük: miért 'szerves', konvenciók, szabályok)

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**with contribution by dr. Gábor Krajsovszky**  
**Formatted by dr. Balázs Balogh**



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# IUPAC Nomenclature of Organic Compounds

According to the recommendation of the Commission on Nomenclature of Organic Chemistry 1993  
(IUPAC: *International Union of Pure and Applied Chemistry*)



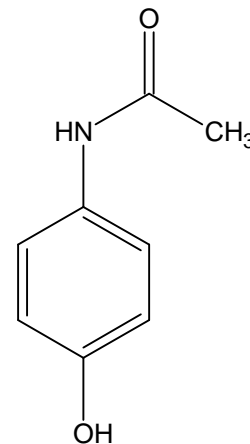
## Purpose of naming:

clear identification, e.g., one compound must have one name, or one name must correspond to one structure

## Problems:

Many types of naming do exist

Chemical names (IUPAC) are complicated, too long  
systematic – semi-trivial – trivial names



## Artificial names:

1. Generic name: made by the abbreviation of the full chemical name  
e.g., *p*-acetylamino-phenol → paracetamol
2. International registered names : a) proposed name  
b) recommended name
3. Registered / trade names: in many cases, these are fantasy names e.g., Panadol<sup>®</sup>
4. Names used in Pharmacopoeias



## Name Construction of organic compounds

- 1. Determining** the type(s) of **nomenclature operations** to be used – depending on the type of compounds
  - most frequently: by *substitutive nomenclature*
- 2. Determining the principal group:**
  - a *principal group* is a characteristic group, which should be named as **suffix** at the end of the name of the principal chain (only one kind of the functional groups must be cited as suffix, with the highest ranking)
- 3. The principal chain or ring** (system) as well as the prefixes:
  - the *principal chain or ring (system)* is such a *linear chain without branching or cyclic structure*, or such an *acyclic or cyclic structure* with a hemisystematic or trivial name, which has only hydrogen atoms attached and does not contain any characteristic groups



- *principal chain, preferred ring or ring system*: the one with the highest ranking among many possible chains or ring systems
  - *non-detachable prefixes*: such an atom or group that substitutes one or more hydrogen atoms of a principal chain
  - *detachable prefixes*: indicates modification(s) of the skeleton of the principal chain; to be listed immediately before the name of the principal chain
4. Numbering of the **principal chain, preferred ring or ring system**:
- in regarding to the *principal group, prefixes, etc.,...*
5. Composition of the whole **name**:
- list prefixes in alphabetic order, with multiplying prefixes if these are to be applied



## NOMENCLATURE SYSTEMS

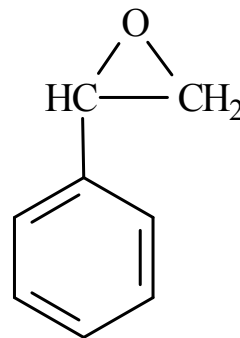
1. **ADDITIVE** name
2. **RADICOFUNCTIONAL** name
3. **FUSION** name
4. **HANTZSCH-WIDMAN** name
5. **REPLACEMENT** name
6. **CONJUNCTIVE** name
7. **MULTIPLYING** name
8. *SUBSTITUTIVE* name
9. **SUBTRACTIVE** name



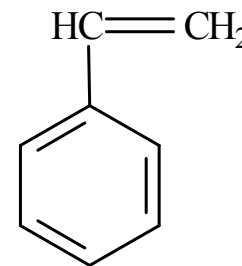


## ADDITIVE names:

a) The name of the compound is made by formal attachments of the name of the components, without loss of atoms or groups



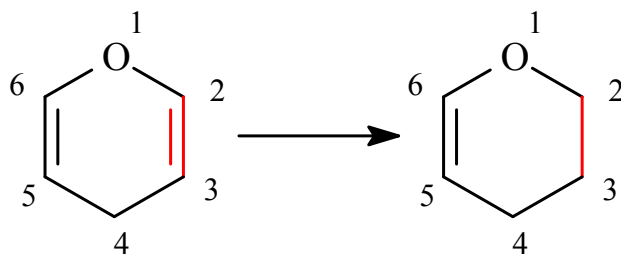
styrene oxyde



styrene

b) Marking addition or insertion of atoms or groups:

*Hydro prefix*

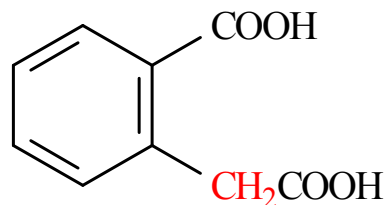


pyrane

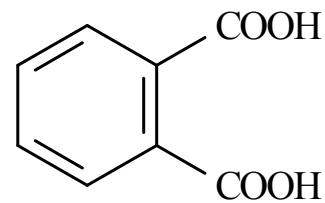
2,3-dihydropyrane



## *Homo prefix (skeleton modifying name)*

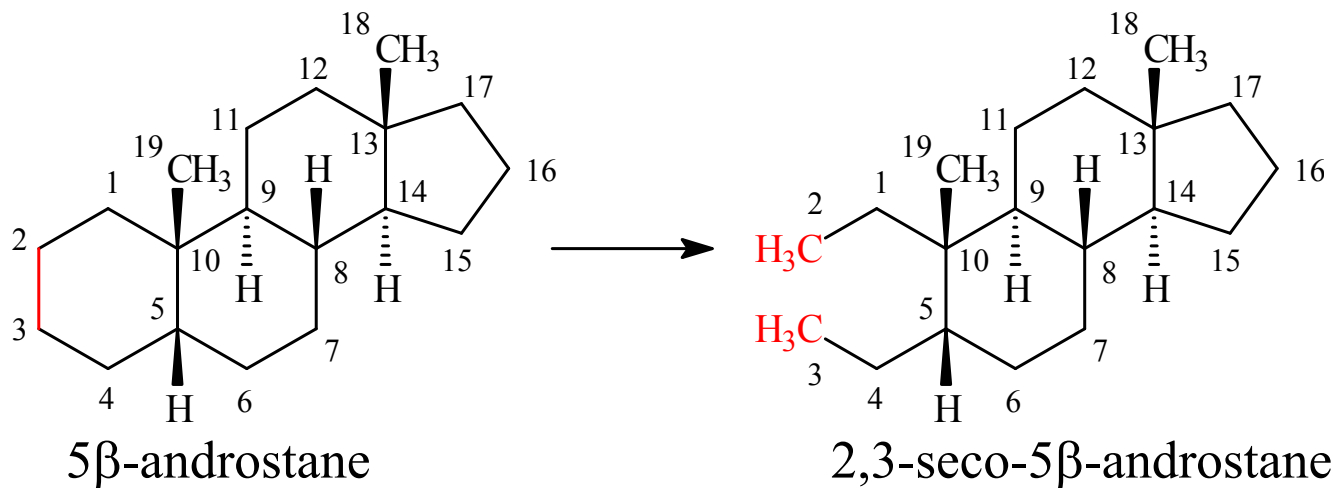


homophthalic acid



phthalic acid

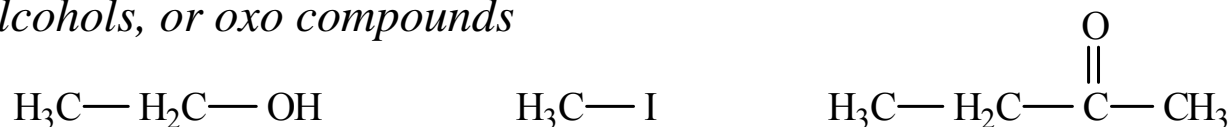
## *Seco prefix (skeleton modifying name)*





## RADICOFUNCTIONAL name

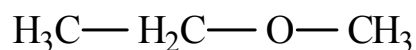
- Expresses a characteristic group as a class term written as a separate word following the name of a parent structure or a name derived from a parent structure
- *applied only for simple, acyclic compounds with halogen, or pseudohalogen groups, or for ethers, alcohols, or oxo compounds*



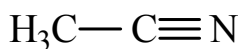
ethyl alcohol

methyl iodide

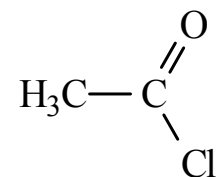
ethyl methyl ketone



ethyl methyl ether

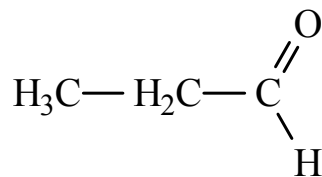


methyl cyanide

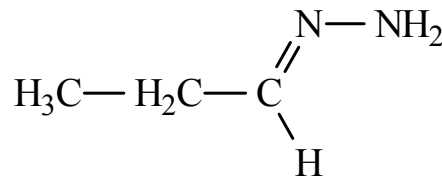


acetyl chloride

- *Indicating the modification of a functional group*



propanal



propanal hydrazone



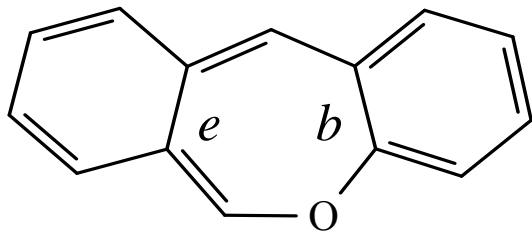
- The *functional group* with the highest priority would be the principal group expressed by a suffix, the others might be mentioned in the name as prefixes
- **Decreasing order of seniority of functional groups:**

Functional group	Radicofunctional name
$-\text{C}\equiv\text{N}$ , $-\text{NC}$	cyanide, isocyanide
$-\text{S}-\text{C}\equiv\text{N}$ , $-\text{N}=\text{C}=\text{S}$	thiocyanate, isothiocyanate
$>\text{C}=\text{O}$	ketone
$-\text{OH}$	alcohol
$-\text{SH}$	hydrosulfide
$-\text{O}-\text{OH}$	hydroperoxide
$>\text{O}$	ether, oxide
$>\text{SO}_2$ , $>\text{SO}$ , $>\text{S}$	sulfone, sulfoxide, sulfide
$-\text{F}$ , $-\text{Cl}$ , $-\text{Br}$ , $-\text{I}$ , $-\text{N}_3$	fluoride, chloride, bromide, iodide, azide



## FUSION name

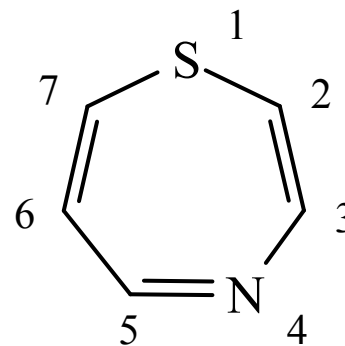
- A composite name having the maximum number of noncumulative double bonds and at least one *ortho* fusion.
- Dissection of the structure into contiguous component having recognized trivial or semisystematic names, one of which is selected as the base component. Attachment of the other component(s) is described by prefix(es).



dibenzo[*b,e*]oxepine

## HANTZSCH-WIDMAN name

- For heteromonocyclic parent structure having no more than 10 ring members
- one or more heteroatoms



1,4-thiazepine

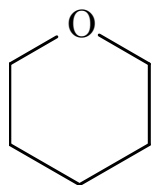


## **REPLACEMENT name:**

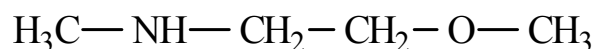
Replacement of one atom or group of a parent structure by another atom or group.

**a) Skeletal replacement name:** the replacement of skeletal atoms and their associated hydrogen atoms of a parent hydride by other atoms with the appropriate number of hydrogen atoms is indicated by nondetachable prefixes.

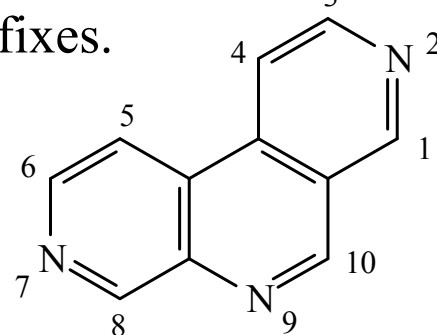
Proper number -O- oxa; -S- thia; -NH- aza, respectively:



oxacyclohexane

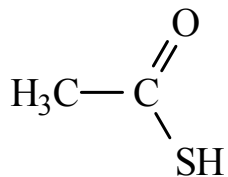


2-oxa-5-azahexane

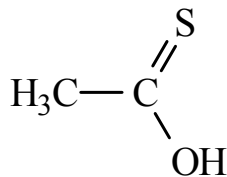


2,7,9-triazaphenanthrene

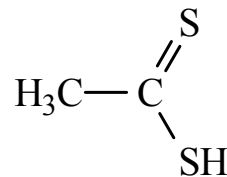
**b) Functional replacement name:** replacement of an oxygen atom or hydroxy group by another atom or group:



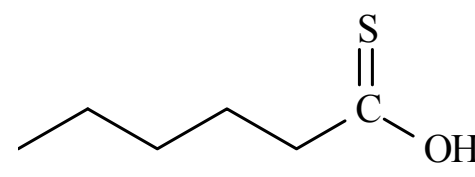
thioacetic-S-acid



thioacetic-O-acid



dithioacetic acid



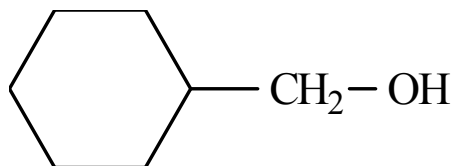
hexanethio-O-acid



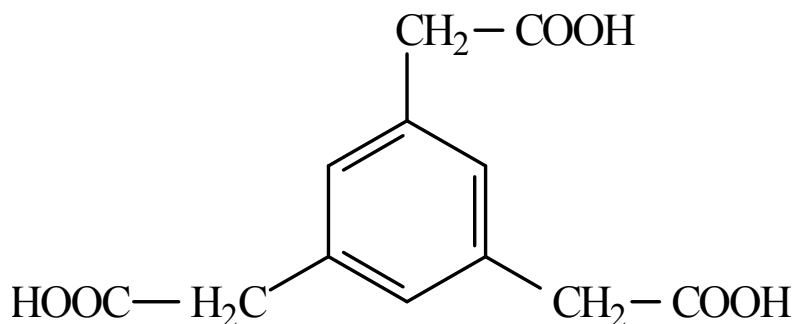
## **CONJUNCTIVE name:**

Assembling cyclic systems with acyclic side chain.

Implying the loss of an appropriate number of hydrogen atoms from each.



cyclohexanemethanol

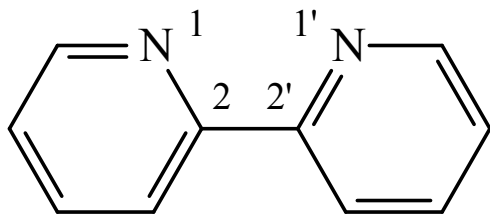


benzene-1,3,5-triacetic acid

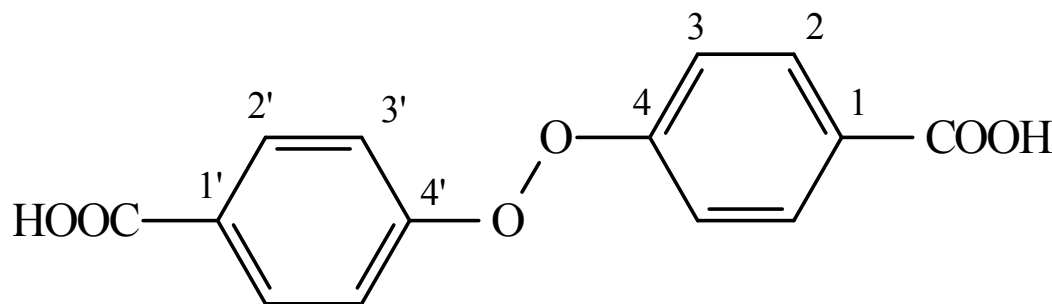


## MULTIPLYING name:

Expresses multiple occurrence of identical parent structures skeletons. These are attached symmetrically, or the same rings are attached.



2,2'-bipyridine



4,4'-peroxydibenzoic acid





**SUBSTITUTIVE name** (details of this nomenclature system see in advance part of nomenclature):

The **most important names**, that are recommended by IUPAC.

Substitutive name indicates the exchange of one or more hydrogen atoms attached to a skeletal atom of a parent structure, which may be expressed by a **suffix** or by **prefixes**.

The *parent chain or ring (system)* is such a *linear chain without branching* or *cyclic structure*, or such an *acyclic* or *cyclic structure* with a semisystematic or trivial name, which has only hydrogen atoms attached and does not contain any functional groups.

If the main skeleton is linear, than this should be chosen as *parent chain*, if it is cyclic, then the ring of the highest priority would make the *parent ring*.



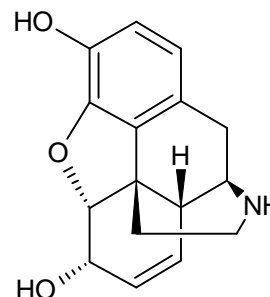
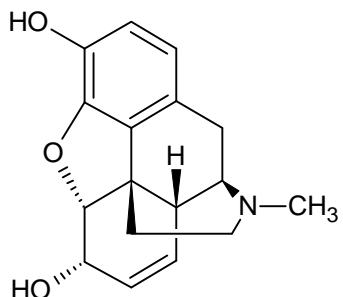


## **SUBTRACTIVE name:**

Made by removal of atoms or groups from the parent structure, shown by prefixes and/or suffixes. The added hydrogens are also indicated in the names.

a) *By prefix:* methyl group → hydrogen: *demethyl*

morphine

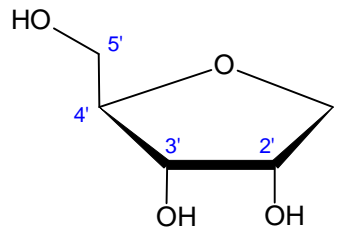
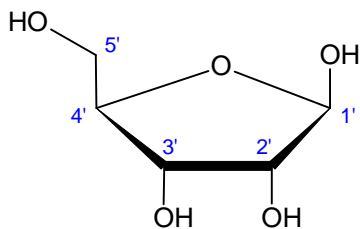


N-demethyl-  
morphine

hydroxyl group →

hydrogen: *deoxy*

ribose

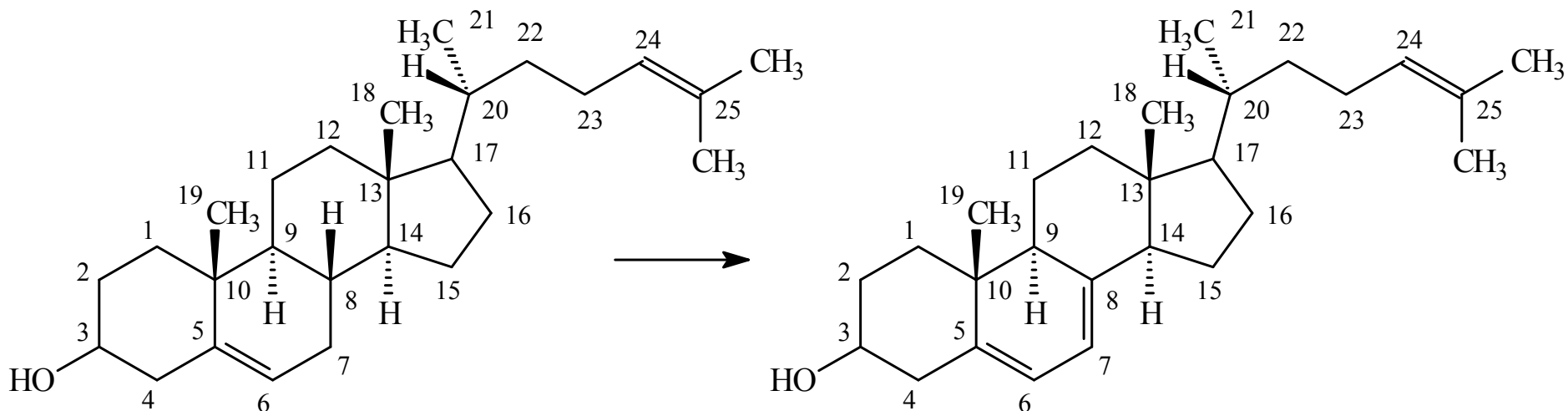


deoxyribose



## Increasing unsaturation:

*didehydro*



cholesterol

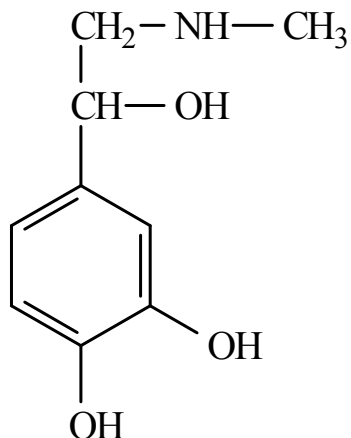
7,8-didehydrocholesterol



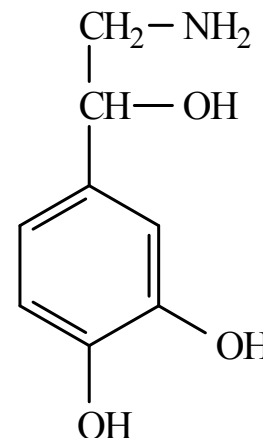
## removal of a methyl group:

*nor*

adrenaline



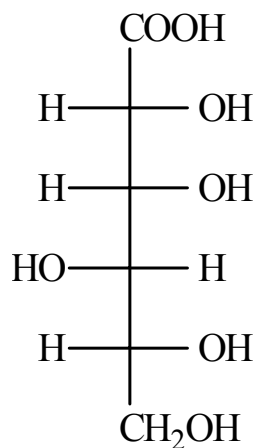
noradrenaline



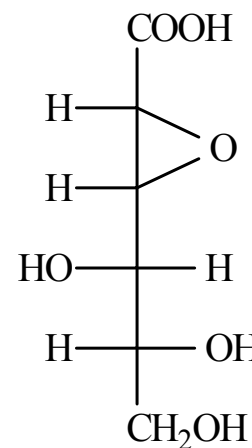
## removal of water from two hydroxyl groups:

*anhydro*

ascorbic acid



anhydroascorbic acid



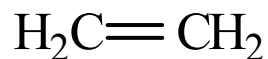


**b) By suffix:** removal of two or four hydrogen atoms:

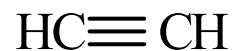
*-ene / -yne*



ethane



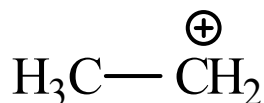
ethene



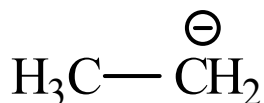
ethyne

Loss of a hydrid anion, a proton, a hydrogen radical:

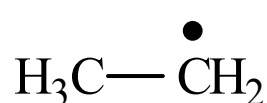
*-ilium / -ide / -yl*



ethylium



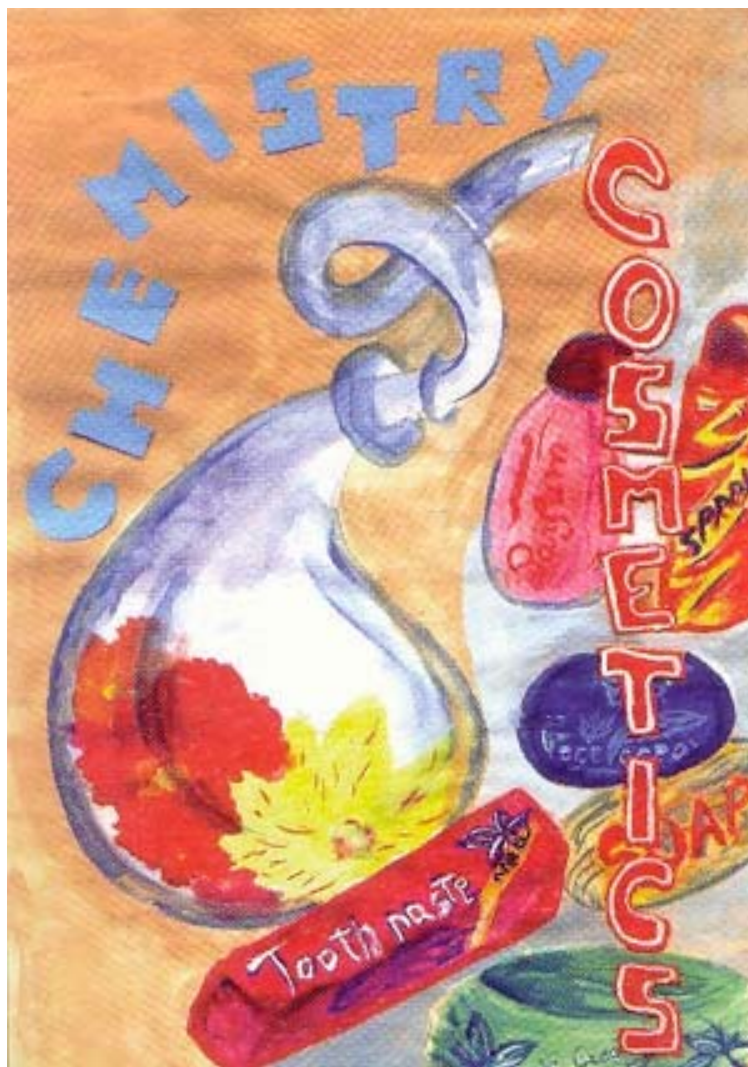
ethanide



ethyl

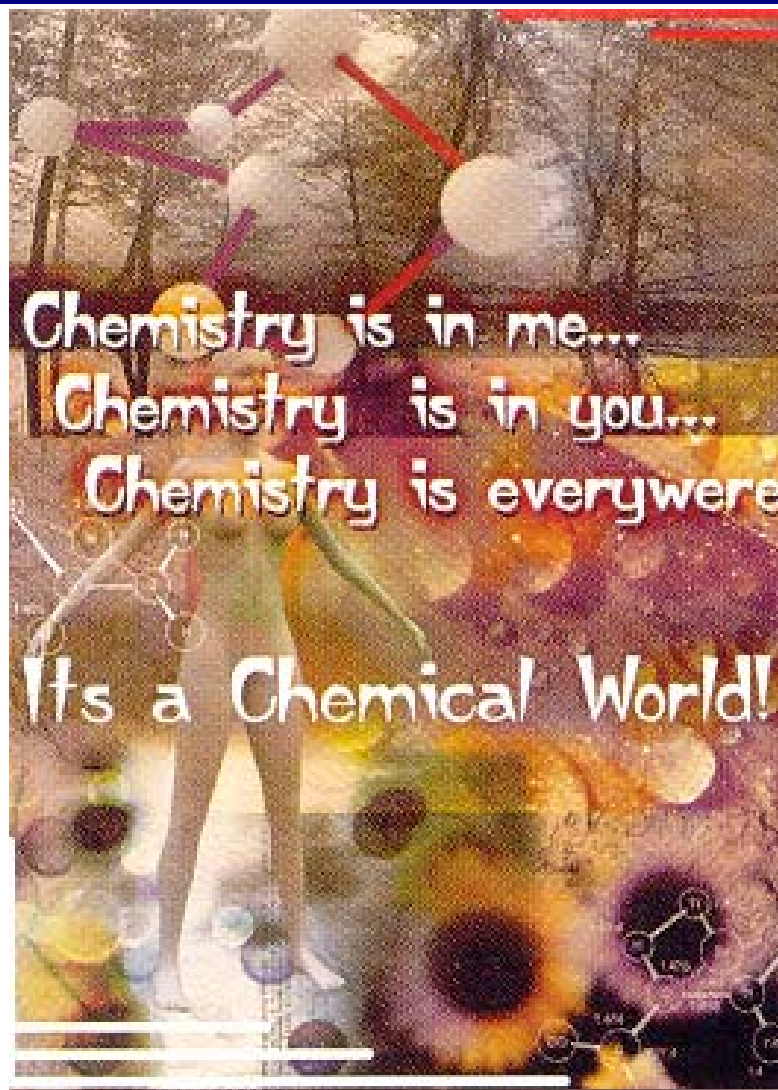


# World of Molecules: Organic compounds and nomenclature



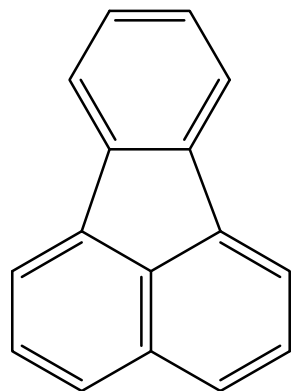


# World of Molecules: Organic compounds and nomenclature

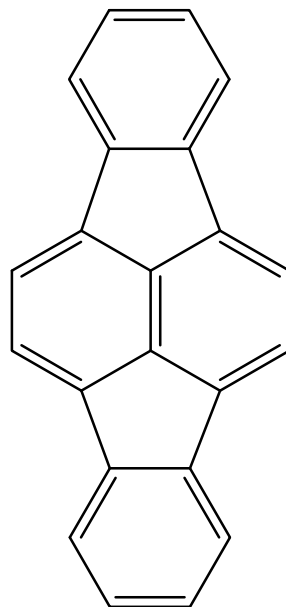




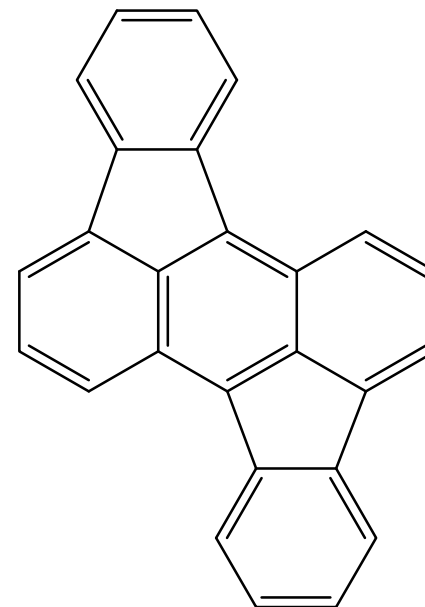
# World of Molecules: Organic compounds and nomenclature



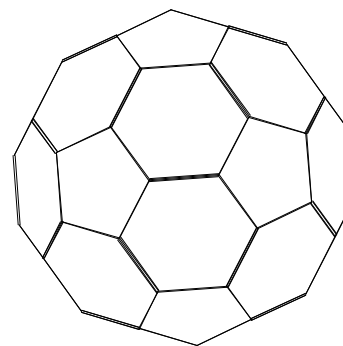
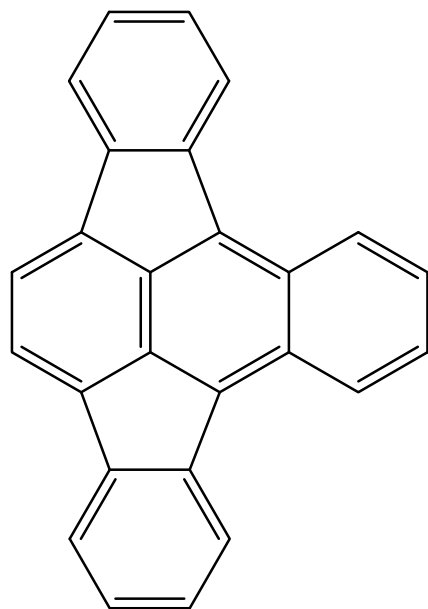
1



2



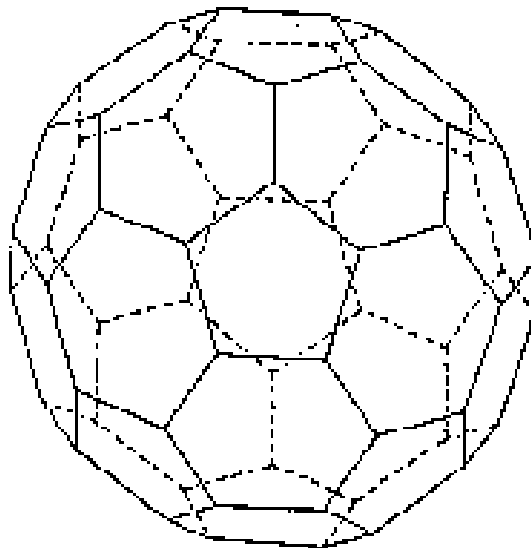
3







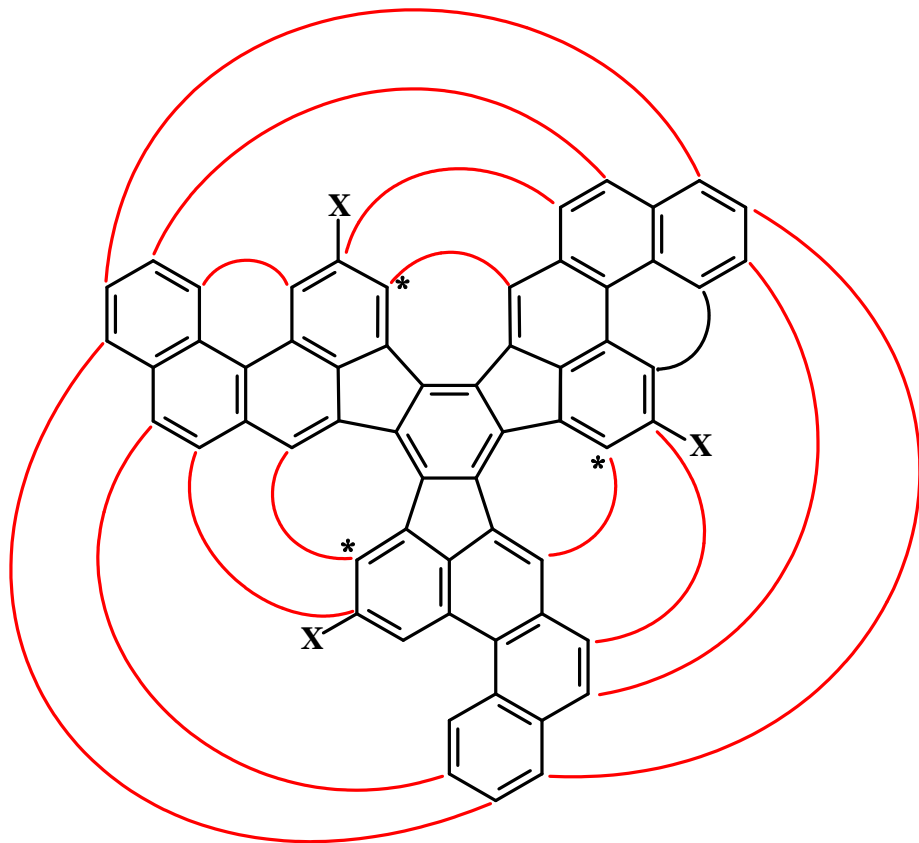
### A Rational Chemical Synthesis of $C_{60}$ , the smallest stable fullarene.



A molecular polycyclic aromatic precursor bearing chlorine substituents at key positions forms  $C_{60}$  when subjected to flash vacuum pyrolysis at  $1100^{\circ}\text{C}$ .

Scott L. T. et al.: Science 295, 1500 (2002)





1 X = H

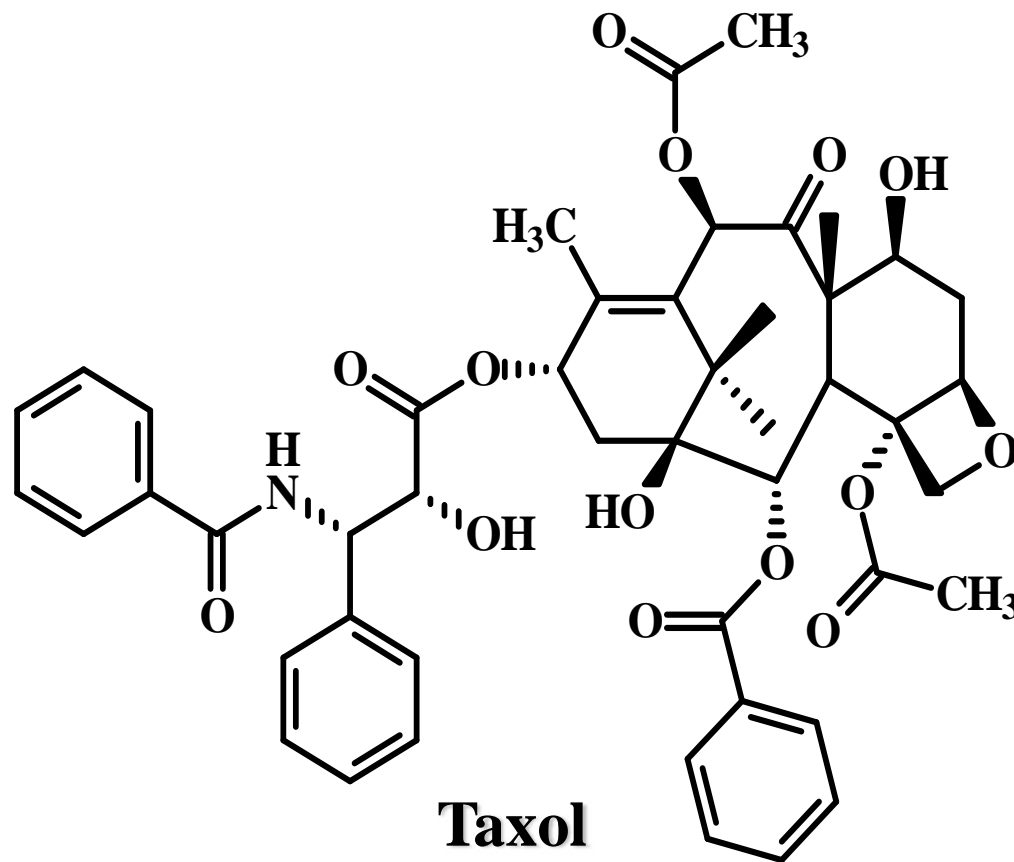
2 X = Cl

Final step in the synthesis of C<sub>60</sub>.  
Curved lines indicate where the  
new bonds are formed in the  
molecular precursor 2 (C<sub>60</sub>H<sub>27</sub>Cl<sub>3</sub>).

Scott L. T. et al.: Science 295, 1500 (2002)



The best-selling anticancer drug ever.



Isolated from the pacific yew tree, total synthesis



## Chemistry

### Chemical substance:

Nuclei + electrons

### Types

According to the type of interaction

- Atomic                      single nucleus + electrons

- Molecular                      nuclei + electrons
---

- Macromolecular    many nuclei + electrons

### Chemical particles:

- Molecules
- Ions
- Radicals





## Subject of Organic Chemistry

- vis vitalis; 1824, Wöhler (Synthesis of an organic compound from an inorganic compound)
- **Organic Chemistry = Chemistry of Carbon Compounds**

(except for the simplest carbon compounds,  
e.g., carbon dioxide, hydrogen cyanide)

C, H, N, O, halogens, S, P (*C + organogenic elements*)

*C + other elements*                       $\longrightarrow$  *'Organoelement' Chemistry*

> 14 Millions

$\longrightarrow$  Deals with structures and reactions of organic molecules

---



## Topics of Organic Chemistry

### Chemical bond

- MO
- Hybridization
- Resonance theory
- Lewis
- Ionic bond

### Stability - reactivity

---



**Structure** → **core structure** („molecule structure’’)  
→ **electronic structure**

- **Molecular formula**
- **2D** description by classic structural formula
- **3D** (stereochemistry)

**Chemical reactivity**  
**biological reactivity**  
**other properties** } are dependent on the structure

**Purpose: planning and prediction of the properties**

## **Chemical reactions – mechanism**

- **synthesis**
- **transformation: preparation of derivatives**





## Classification of organic compounds

- characteristic groups
- carbon skeleton

- Acyclic (aliphatic)
- Cyclic

carbocyclic and heterocyclic compounds

monocycles

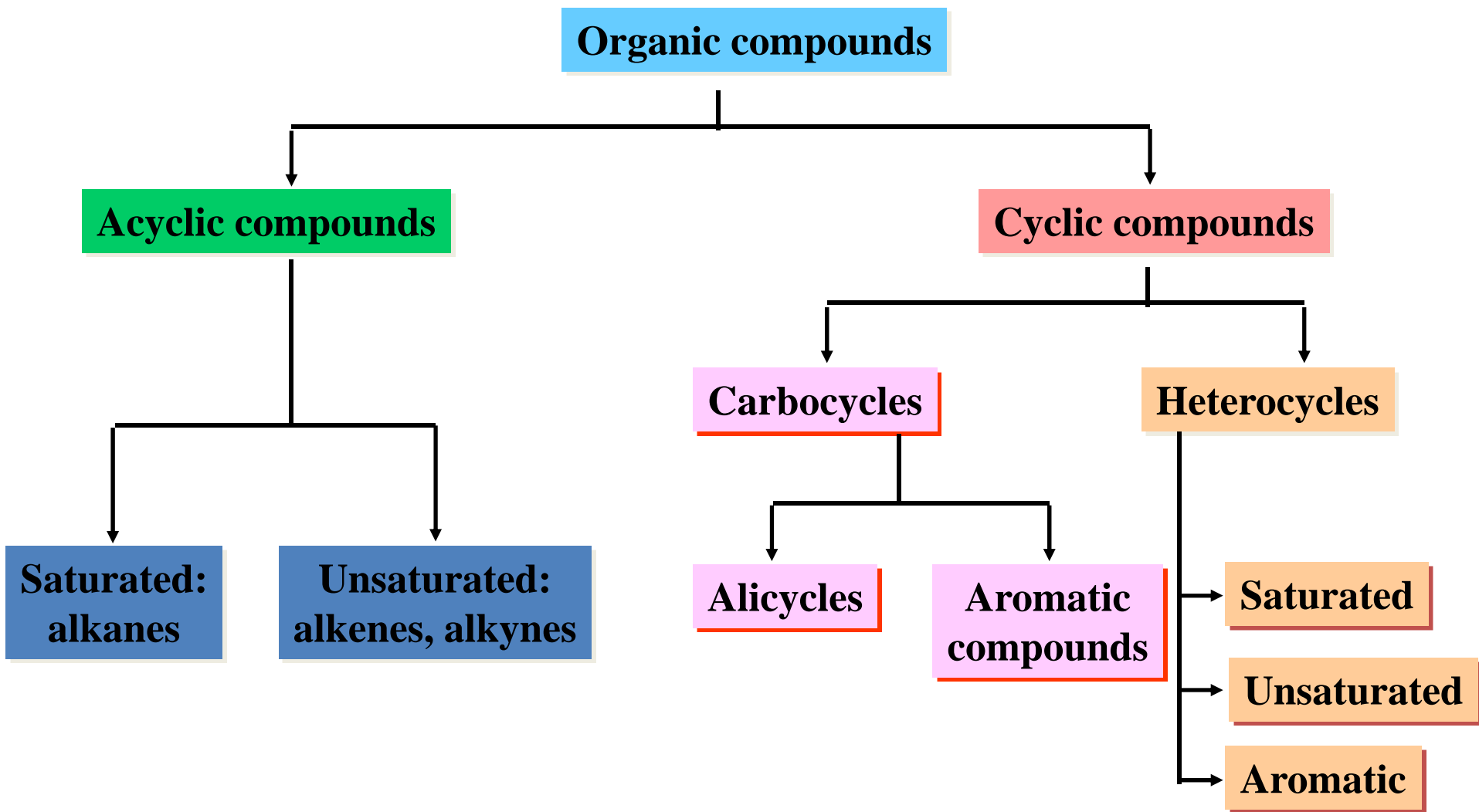
polycycles

- isolated polycycles
- spirocycles (1 bridgehead atom)
- condensed (2 bridgehead atoms)
- bridged (more than 2 bridgehead atoms)

- Hydrocarbons
- Substituted derivatives of hydrocarbons

Heterocyclic compounds







## Unsaturated compounds

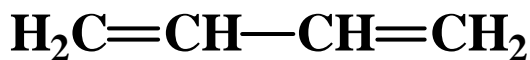
Containing C=C  
double bonds

Alkenes

Polyenes



propene



buta-1,3-diene

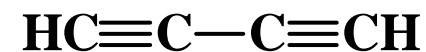
Containing C≡C  
triple bonds

Alkynes

Polyynes



ethyne

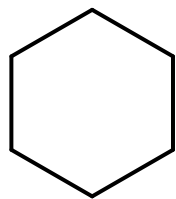


buta-1,3-diyne



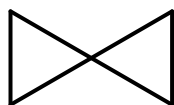
## Alicyclic compounds

Cycloalkanes



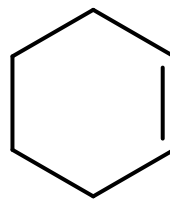
cyclohexane

Polycyclic  
alkanes



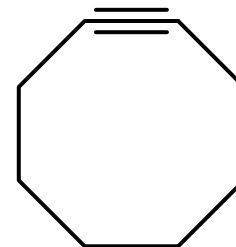
spiro[3.3]heptane

Cycloalkenes



cyclohexene

Cycloalkynes



cyclooctyne

