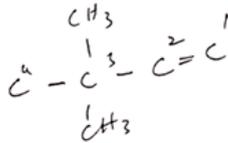
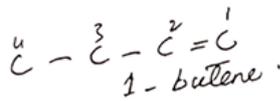


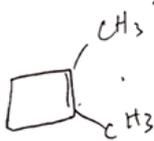
04/11

Nomenclature of alkenes:-

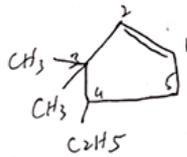
Ending at "ene"



3,3-dimethyl-1-butene



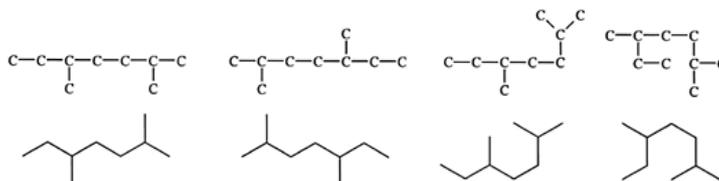
1,2-Dimethyl cyclobutene



4-ethyl-3,3-dimethyl cyclopentene

niceday

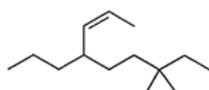
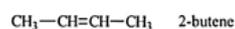
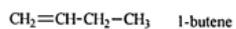
In identifying the longest chain in a molecule, and hence the parent name, do not be deceived by the 2-dimensional representation of the molecule. For instance, 2,5-dimethylheptane could have been drawn in the following ways (and several more).



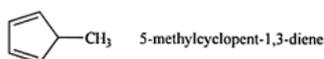
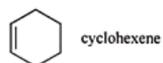
Alkenes

- hydrocarbons having at least one carbon-carbon double bond (C=C).

- Select as the parent structure the longest continuous carbon chain that contains the carbon double bond (C=C). Replace 'ane' with 'ene'.
- Number this chain from the end that will give the C atom starting the double bond the lowest number. Prefix the name with this number.
- Treat side-groups as for alkanes.
- Dienes contain two double bonds, trienes have three, etc.



7,7-dimethyl-4-propylnon-2-ene

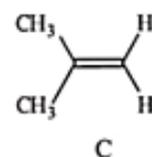
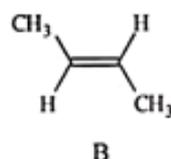
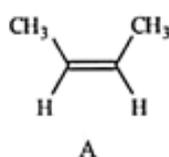


Configurational Isomerism

Structural isomerism deals with the possible different ways in which the carbon atoms are attached to each other. Configurational isomerism deals with the different arrangements in space the atoms can take in one structural isomer.

This type of isomerism shows up in some alkenes and is due to the lack of free rotation about a double bond (or of the cyclic bonds in a cycloalkane).

Consider the compounds



A and B are configurational isomers. In both A and B, the two groups attached to the carbon atom on the left side of the double bond have the same orientation in space (the methyl is up and the hydrogen is down). Now consider the two groups attached to the carbon atom on the right side of the double bond, A has a different arrangement in space than B (in A the methyl is up and in B the methyl is down). A and B are not superimposable on one another.

To name the two isomers, the left side of the double bond is considered first and the two groups are prioritized based on atomic number (**the largest atomic number at the first point of difference has the highest priority**).

Then the two groups on the right side of the double bond are prioritized. If the two highest priority groups (left and right side of double bond) are on the same side of the double bond (top or bottom) then the double bond has the Z configuration (zusammen, German for together) and if they are on opposite sides the configuration is E (entgegen, German for opposite).

A was once called *cis* and B *trans* and this form of nomenclature is still used occasionally for simple compounds.

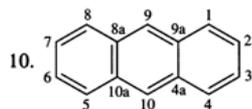
C is a different structural isomer; A and B are the same structural isomer but different configurational isomers.

These three compounds are named: A: (Z)-2-butene, B: (E)-2-butene, C: 2-methyl-1-propene

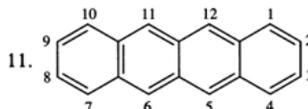


CHAPTER 4

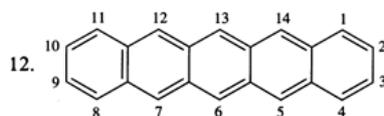
Examples



anthracene



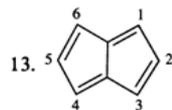
tetracene



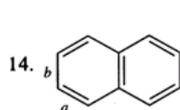
pentacene

When a system does not have a retained name or a name that can be composed systematically as above, and when *ortho*- and *ortho-peri*-fusion are possible, it is named using fusion nomenclature, i.e. by combining the names of the two or more systems that are fused. One system is adjudged to be the senior according to criteria described elsewhere and is taken as a parent hydride, and the other is denoted in the name by a non-detachable prefix. The junction of the two systems is indicated in a specific manner. Instead of numerical locants, italic letters 'a', 'b', 'c', etc. are used to identify bonds in the parent hydride. The final letter 'o' and normal locants are characteristic of the prefix. The examples below illustrate the fusion operation and the resulting fusion name.

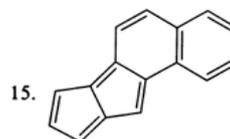
Examples



pentalene



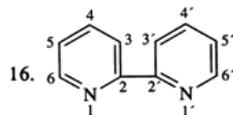
naphthalene



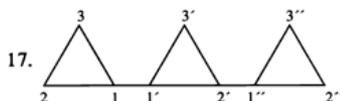
pentaleno[2,1-a]naphthalene

• Assemblies of identical rings are named by using a unique set of multiplicative prefixes, bi-, ter-, quater-, etc., to indicate the number of rings. The name phenyl is used instead of benzene for the aromatic C₆ ring.

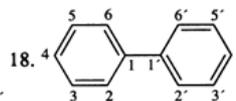
Examples



2,2'-bipyridine



tercyclopropane



biphenyl



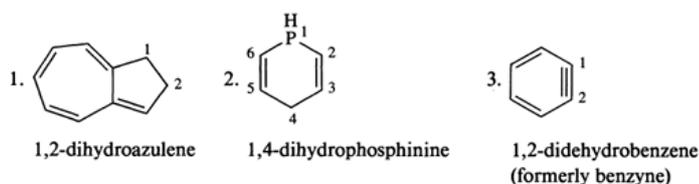
NAMING OF SUBSTANCES

4.5.4 Names for substances with various degrees of saturation

4.5.4.1 *General.* Two methods are used to indicate the degree of saturation in a compound, depending on the nature of the parent hydride.

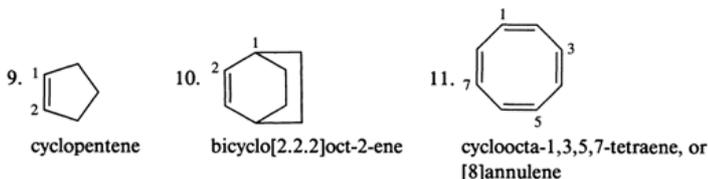
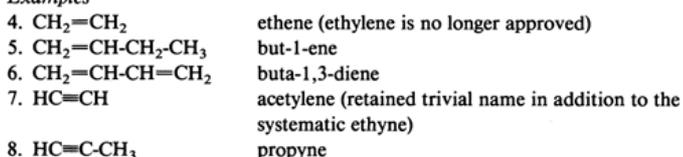
In one method, the non-detachable prefixes hydro- and dehydro- (in the case of mancudes only) can be used to indicate the addition or subtraction of one hydrogen atom. As even numbers of hydrogen atoms are involved when a carbon-carbon single bond becomes a double or triple bond, the multiplicative prefixes di-, tetra-, etc., as well as the appropriate locants, are used. The prefix dehydro- is always used to indicate the subtraction of hydrogen atoms from saturated heterocycles having Hantzsch-Widman names.

Examples



In the other method, the ending -ane is changed to -ene or -yne to indicate the presence of a double or triple bond. This is used for alkanes and mono- and polycyclic alkane parent hydrides. In alkanes and cycloalkanes, the change of the -ane ending to -ene or -yne indicates the presence of one double or triple bond. Multiplicative prefixes di-, tri-, tetra-, etc. are used to signal the multiplicity of unsaturated bonds. Locants placed immediately in front of the endings -ene and -yne are used as needed.

Examples



If double and triple bonds are present in a structure, they are considered together when assigning lowest locants. Only when this does not allow a resolution do double

bonds receive the lowest locants. In a name, the ending -ene is cited before -yne, but with elision of the final 'e'.

Examples

12. $\text{HC}\equiv\text{C}-\text{CH}=\text{CH}-\text{CH}_3$ pent-3-en-1-yne
 13. $\text{HC}\equiv\text{C}-\text{CH}=\text{CH}_2$ but-1-en-3-yne

4.5.4.2 *Unsaturated and divalent substituents.* Unsaturated monovalent substituents are named systematically by attaching the suffixes -yl to the stem of the parent name that carries the ending -ene or -yne. Retained trivial names include vinyl for $-\text{CH}=\text{CH}_2$, allyl for $-\text{CH}_2-\text{CH}=\text{CH}_2$ and isopropenyl for $-\text{C}(\text{CH}_3)=\text{CH}_2$, but only when it is unsubstituted.

Examples

1. $-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}_3$ pent-3-en-1-yl
 2. $-\text{CH}_2-\text{C}\equiv\text{CH}$ prop-2-yn-1-yl

Note that the position of the free valence is always given the locant 1.

Divalent substituents of the type $\text{R}-\text{CH}=\text{}$ or $\text{R}_2\text{C}=\text{}$ are named by appending the suffix -ylidene to an appropriate stem. When the two free valencies are on different atoms or of the type $\text{R}-\text{CH}<$ or $\text{R}_2\text{C}<$ and not involved in the same double bond, the composite suffix -diyl (di- + -yl) is used. Retained names include methylene for $-\text{CH}_2-$, ethylene for $-\text{CH}_2-\text{CH}_2-$ and isopropylidene for $=\text{C}(\text{CH}_3)_2$, but only when it is unsubstituted.

Examples

3. methylydene $=\text{CH}_2$
 4. ethylydene $=\text{CH}-\text{CH}_3$
 5. ethane-1,1-diyl $>\text{CH}-\text{CH}_3$
 6. propane-1,3-diyl $-\text{CH}_2-\text{CH}_2-\text{CH}_2-$

4.5.4.3 *Selection of the principal chain in unsaturated branched acyclic hydrocarbons.* A principal chain must be chosen upon which to base the name of branched unsaturated acyclic hydrocarbons. The general criteria listed in Table 4.10 are applied. Those that are specifically relevant to polyenes and polyynes are: criterion (b), which is the maximum number of double and triple bonds considered together; criterion (c), which is the maximum length; criteria (d), (f) and (g); criterion (h), which is the maximum number of substituents cited as prefixes; and criteria (i) and (j).

Examples

1. $\begin{array}{c} \text{H}_2\text{C}=\text{CH}-\text{C}=\text{CH}_2 \\ | \\ \text{C}_6\text{H}_{13} \end{array}$ 2. $\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_3 \\ | \\ \text{C}_2\text{H}_5 \end{array}$
 2-hexylbuta-1,3-diene 2-ethylhex-1-ene
 (criterion b) (criteria b and c)

CHAPTER 4

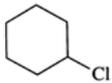
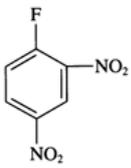
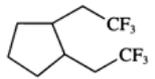
4.5.6.2 *Names of characteristic groups always cited as prefixes.* The names of the two polyhalogenated ethanes, a and b, are a good illustration of the application of the rule of lowest locants and of the alphabetical order to assign lowest locants.

Examples

- | | |
|---------------------------------|---|
| 1. $\text{ClF}_2\text{C-CHBrI}$ | a 2-bromo-1-chloro-1,1-difluoro-2-iodoethane |
| 2. $\text{BrF}_2\text{C-CClFI}$ | b 1-bromo-2-chloro-1,1,2-trifluoro-2-iodoethane |

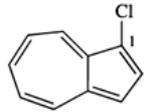
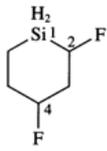
In monocyclic hydrocarbons, the locant '1' is omitted, but it is necessary in polysubstituted compounds.

Examples

- | | |
|--|---|
| 3.  | chlorocyclohexane |
| 4.  | 1-fluoro-2,4-dinitrobenzene |
| 5.  | 1,2-bis(2,2,2-trifluoroethyl)cyclopentane |

When the numbering is predetermined by the nature of the parent hydride, as in polycyclic hydrocarbons and in heterocyclic compounds, lowest locants are still the rule.

Examples

- | | |
|--|----------------------|
| 6.  | 1-chloroazulene |
| 7.  | 2,4-difluorosilinane |

CHAPTER 4

4.5.6.3 *Names of characteristic groups cited as suffixes or prefixes.* In substitutive nomenclature, a suffix must be used whenever possible for the preferred functional group. Prefixes are used to name all characteristic groups except principal functional groups. Lowest locants and multiplicative prefixes di-, tri-, tetra-, etc. are used following the general rules stated in Section 4.5.2 (p. 70). Suffixes and prefixes are listed in Tables 4.11 and 4.12. Monofunctional compounds are named as follows:

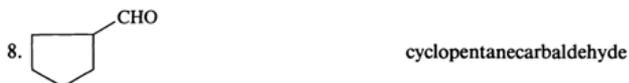
- | | |
|---|-----------------|
| 1. $\text{CH}_3\text{-CH}_2\text{-CH}_2\text{OH}$ | propan-1-ol |
| 2. $\text{CH}_3\text{-CO-CH}_2\text{-CH}_2\text{-CH}_3$ | pentan-2-one |
| 3. $\text{CH}_3\text{-CH(OH)-CH(OH)-CH}_3$ | butane-2,3-diol |



The suffixes -oic acid, -al, -amide and -nitrile are used to name acyclic compounds having one or two characteristic groups. Locants are not necessary, as these groups must be at the end of a chain. The suffixes -carboxylic acid, -carbaldehyde, -carboxamide and -carbonitrile are used when more than two groups are attached to chains or one or more groups are attached to cycles.

Examples

- | | |
|---|----------------------------------|
| 5. $\text{CH}_3\text{-CH}_2\text{-COOH}$ | propanoic acid |
| 6. $\text{OHC-CH}_2\text{-CH}_2\text{-CHO}$ | butanedial |
| 7. $\text{CH}_2(\text{COOH})\text{-CH}(\text{COOH})\text{-CH}_2(\text{COOH})$ | propane-1,2,3-tricarboxylic acid |



- | | |
|---|-----------------|
| 9. $\text{CH}_3\text{-(CH}_2\text{)}_3\text{-CONH}_2$ | pentanamide |
| 10. $\text{NC-(CH}_2\text{)}_4\text{-CN}$ | hexanedinitrile |



Suffixes and prefixes are necessary to name structures with discontinuities, for instance when characteristic groups are situated on side-chains, or when the carbon skeleton is composed of rings and chains. A principal component, ring or chain, must be chosen. The principal chain is chosen in accordance with the selection criteria listed in Table 4.10 and is the chain supporting the greatest number of