**2**

**Nomenclature**

**Nomenclature (2)**

 Many of the important heterocyclic ring systems has been identified since the earliest day of chemistry, and many of the compounds were named unsystematically and given names related to their origin, color, or the person who discovered them. These trivial (common) names are still in use and it is impractical to ignore them. Some of the most common heterocyclic compounds with their common names are given at the end of this section.

 Now, heterocyclic compounds are named systematically by the International Union of Pure and Applied Chemistry (IUPAC). One of these IUPAC systems of nomenclature is called **Hantzsch-Widman** method and is used for simple, one-ring heterocylces, and is summarized by the following rules:

1- The name is constructed by combining prefixes that indicate the heteroatoms present with suffixes that indicate the ring size and the degree of unsaturation.

2- The prefixes for the heteroatoms are: oxa (O), thia (S), and aza (N).

3- The letter **a** in the prefix is omitted when the prefix is followed by a vowel (the first letter in the suffix).

4- The suffixes used are listed in the table below.

***Name suffixes (determines ring size and degree of Unsaturation).***

|  |  |  |
| --- | --- | --- |
|  | Nitrogen present | Nitrogen absent |
| Unsat. | Partial | Sat. | Unsat. | Partial | Sat. |
| 3 | irine | ---- | iridine | Irene | ---- | irane |
| 4 | ete | etine | etidine | ete | etene | etane |
| 5 | ole | oline | olidine | ole | olene | olane |
| 6 | ine | ---- | ine | in | ---- | ane |
| 7 | epine | ---- | epine | epin | ---- | epane |

5- When a ring system with the maximum number of double bonds still has a saturated atom in the ring, the position of this atom is numerically indicated, together with the prefix *H* (italic) as a part of the name of the ring system.

6- Partial unsaturation for six or seven membered ring structures is indicated by the prefix dihydro or tetrahydro.

7- Fully saturated six or seven membered ring structures containing nitrogen is indicated by the prefix perhydro.

8- When two or more different heteroatoms are present, prefixes are listed in order of priority and numbering starts at the highest priority atom as follows.

O > S > N.

9- Two or more heteroatoms of the same kind are indicated by the prefix di, tri, .etc.

10- Substitutions on the heterocyclic ring are named as prefixes and arranged alphabetically. Some substituents are always named as prefixes such as the halogens ( named as flouro, chloro, bromo and iodo ), nitroso ( NO ), nitro ( NO2 ), alkyloxy ( RO- ), alkylthio ( RS- ), and those that can be named as either prefixes or suffixes. The following is a list of some functional groups and their names as prefixes, and suffixes: -COOH ( carboxy ; oic acid or carboxylic acid ), -COOR ( alkyloxycarbonyl ; oate or carboxylate ), -COCl ( chlorocarbonyl ; oyl chloride or carbonyl chloride ), -CONH2( carbamoyl ; amide or carboxamide ), -CN (cyano ; nitrile or carbonitrile ), -CHO (formyl or oxo ; al or carbaldehyde ), C=O ( oxo ; one ), -OH ( hydroxyl ; ol), -SH ( mercapto; thiol), NH2( amino ; amine )

11- Fused–polyheterocyclics have non systematic names, and numbering is similar to the analogous non heterocyclic compound.



**Few examples as an application of the Hantzsch-Widman method are given below.**

|  |  |  |  |  |
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**Replacement nomenclature**

Another method of nomenclature, and is summarized by the following rules:

1. The name of heteroatoms, their sequence and numbering is the same as in Hantzsch – Widman method.

2. When there is a choice, priority in numbering is given to the heteroatom, then un-saturations, then to substituents in alphabetical order.

3. The position and prefix for each heteroatom is written in front of the name of the corresponding hydrocarbon, which represents the parent name.

4. In fused heterocycles, numbering of the corresponding hydrocarbon is retained, irrespective of the position of the heteroatom, except when there is a choice, low numbers are assigned to the heteroatoms.

Few examples as an application of the replacement method of nomenclature are given below.





**Common Names( Trivial ) of Some Heterocyclic Compounds ( Monocyclic ).**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |
| **Aziridine** | **Azetidine** | **Pyrrolidine** | **Piperidine** | **Piperazine** | **Morpholine** |
|  |  |  |  |  |  |
| **Pyrrole** | **Thiophene** | **Furan** | **Pyrazole** | **Imidazole** |  |
|  |  |  |  |  |  |
| **Thiazole** | **Oxazole** | **Isoxazole** | **Isothiazole** | **Furazan** |  |
|  |  |  |  |  |  |
| **Pyridine**  | **Pyrazine**  | **Pyrimidine**  | **Pyridazine** | **2*H*-Pyran** |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |

**Common Names( Trivial ) of Some Fused- Heterocyclic Compounds.**



|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |
|  |  |  |  |  |  |



**Common Names ( Trivial ) of Some Polycyclic Hydrocarbons .**



**Nomenclature of Bridged structures ( von Baeyer system ).**

 1. The number of rings determined by the minimum number of bond scissions required to convert the skeleton into a monocyclic hydrocarbon.

2. The name consists of a prefix indicating the number of cycles ( bicyclo, tricyclo, tetracyclo, …etc ), followed by a square brackets containing in decreasing order the numbers indicating the number of carbon atoms in the two branches of the main ring, the main bridge, then secondary bridges, and a suffix taken from the name of the open chain hydrocarbon containing the same total number of carbon atoms.

3. The main ring must contain as many carbon atoms as possible, two of which must serve as bridgeheads for the main bridge which must be as large as possible.

4. Numbering starts from one of the bridgeheads, proceeding by the longest possible path to the second bridgehead, numbering is then continued from this atom back to the first atom by the longer path back to the first bridgehead and is completed by the shortest path. Secondary bridges are considered in decreasing order starting from the highest numbered bridgehead.

5. The location of secondary bridges is shown by superscripts following the number indicating the number of carbon atoms in that bridge and must be as small as possible.

6. When there is a choice in numbering, un-saturations is given the lowest number.

7. Heterocycles are named by straight forward application of the replacement rules.

8. When there is a choice heteroatoms are given priority in numbering, and heteroatoms are preferred over un-saturations.

**Examples on the nomenclature of polycyclic compounds.**

**1. Carbocyclic.**



**1. Heterocyclic.**





**Nomenclature of spiro compounds.**

A single atom ( spiro atom ) is common member of two rings.

1. The number of carbon atoms linked to the spiro atom in each ring is indicated in ascending order in brackets placed after the prefix spiro followed by the suffix

( the hydrocarbon name ), which is the name of the n-alkane hydrocarbon of the same total number of carbon atoms.

2. The carbon atoms are numbered starting with ring atom next to the spiro atom, first through the spiro atom and around the second ring.

3. When there is a choice, unsaturations are given the smallest number possible and the same numbering system is maintained.

4. Polyspiro compounds are named by placing dispiro, trispiro, tetraspiro, etc, before the name of the n-alkane hydrocarbon.

- The number of carbon atoms linked to the spiro atoms in each ring are indicated in brackets in the same order as the numbering proceeds about the ring.

- Numbering starts with the ring atom next to a terminal spiro atom and proceeds in such a way as to give the spiro atoms as low number as possible.

5- Heterocycle analouges are named by the replacement principles and when there is a choice, heteroatoms are given the lowest number possible and preferred over unsaturations.

**Examples on spiro compounds.**

