

**B.Sc. Semester-IV
Core Course-IX (CC-IX)
Organic Chemistry-III**



III. Heterocyclic Compounds

18. Nomenclature of Fused Heterocyclic Systems



Dr. Rajeev Ranjan
University Department of Chemistry
Dr. Shyama Prasad Mukherjee University, Ranchi

Heterocyclic Compounds

22 Lectures

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis), Structure elucidation of quinoline and isoquinoline, Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner- Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction
Derivatives of furan: Furfural and furoic acid.

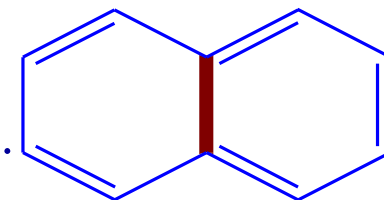
Coverage:

1. Nomenclature of Fused Heterocyclic Systems

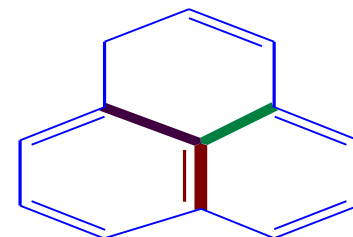
Nomenclature of Fused Heterocyclic Systems

Definitions:

- ❖ **Fusion:** This term is used to describe the process of joining two separate rings with the maximum number of non-cumulative double bonds *via* two atoms and one common bond.
- ❖ **Ortho-fused rings:** are those rings that have only two common atoms and one bond, example; **naphthalene**
- ❖ **Ortho-and peri-fused rings:** are those found in a polycyclic compound with a ring that is *ortho*-fused to different sides of two other rings that are themselves *ortho*-fused together (i.e. there are three common atoms between the first ring and the other two).
 - ❖ *1H*-phenalene is considered as being composed of three benzene rings, each is *ortho*-*peri*-fused to the other two.
- ❖ Polycyclic compounds incorporating one heterocyclic ring or fused heterocyclic system fused to benzene are known benzoheterocycles.
- ❖ Also bicyclic compounds with two fused heterocyclic rings are well known.
- ❖ Both types can be named according to certain rules



Naphthalene



1H-Phenalene

Nomenclature of Fused Heterocyclic Systems

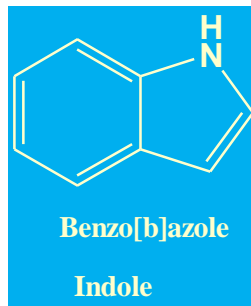
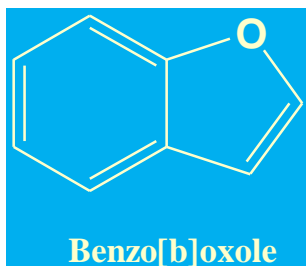
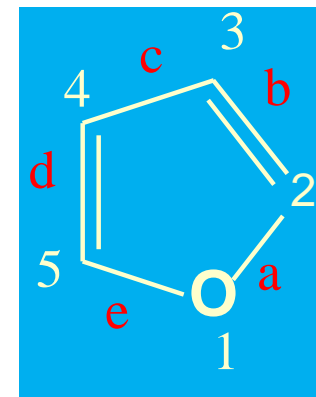
A. Nomenclature of benzofused compounds:

Polycyclic compounds incorporating one heterocyclic ring or fused heterocyclic system fused to benzene are known as benzoheterocycles and are named by:

1. prefix: the word benzo
2. letter in square brackets: indicating the position of fusion
3. name of heterocyclic ring: (common or IUPAC name).

Name= Benzo[letter]name of heterocyclic ring

(the connected bond take letter (a,b,c ...))



Nomenclature of Fused Heterocyclic Systems

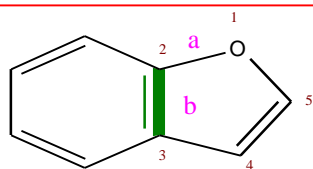
For designating the position of fusion the following rule is followed

1. Numbering the H.C.R

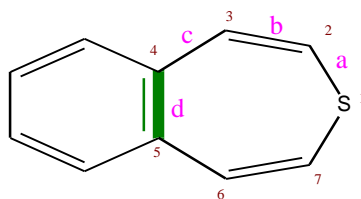
a. When numbering a ring with one heteroatom, the heteroatom is #1 and continues in the direction that is closer to the fused bond.

b. When numbering a ring with more than one heteroatom, the highest priority atom is #1 and continues in the direction that gives the next priority atom the lowest number.

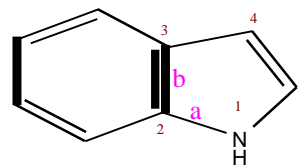
2. The bonds of the heterocyclic ring are assigned by alphabetical letters starting with the 1,2-bond



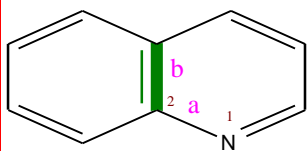
Benzo[b]furan



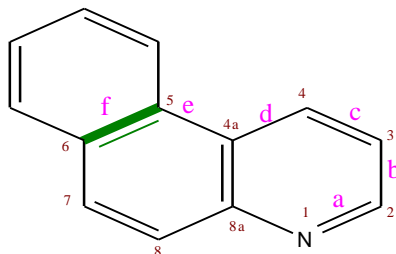
Benzo[d]thiophene



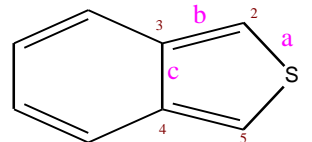
Benzo[b]pyrrole
Indole



Benzo[b]pyridine
Quinoline



Benzo[f]quinoxaline



Benzo[c]thiophene

Nomenclature of Fused Heterocyclic Systems

B. Nomenclature of fused heterocyclic compounds:

Naming a fused heterocyclic systems composed of two monoheterocyclic units or benzoheterocycles (e.g. chromene) fused with another heterocycle ring is based upon considering one system as the parent (base) and the second is considered as substituent

The name is formed of :

name of substituent ring (minor ring)[number, number-letter] name of base ring (major ring)

❖ The name of the minor ring is derived by writing a contracted prefix for the substituent ring present

| | | |
|------------|------|------------|
| Furo | from | Furan |
| Imidazo | from | Imidazole |
| pyrido | from | Pyridine |
| Pyrimido | from | Pyrimidine |
| Thieno | from | Thiophene |
| Pyridazino | from | pyridazine |
| Pyrazino | from | pyrazine |
| Chromeno | from | chromene |

Nomenclature of Fused Heterocyclic Systems

- ❖ The numbers indicate which atoms in the minor ring are common to the major ring (fusion sites in minor ring).
- ❖ The order of the numbers indicates which atom of the minor ring is encountered closest to atom 1 in the major numbering system (i.e. these numbers may be written in ascending or descending order e.g.2,3 or 3,2)
- ❖ The letter defines the position of attachment of the minor ring to the major ring (fusion sites in base component)
- ❖ Finally a suffix indicate the name of the base ring is written.
- ❖ The numbering system for the whole fused system is not the same as the numbers in the square brackets (i.e. there are three numbering systems; one for minor ring, one for major ring and the third is for the system as a whole)

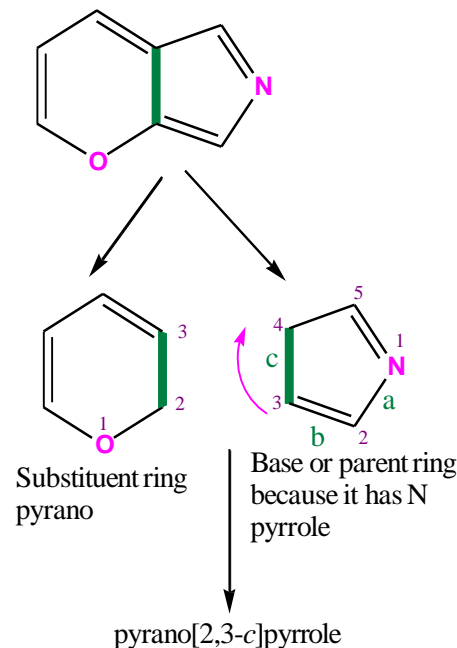
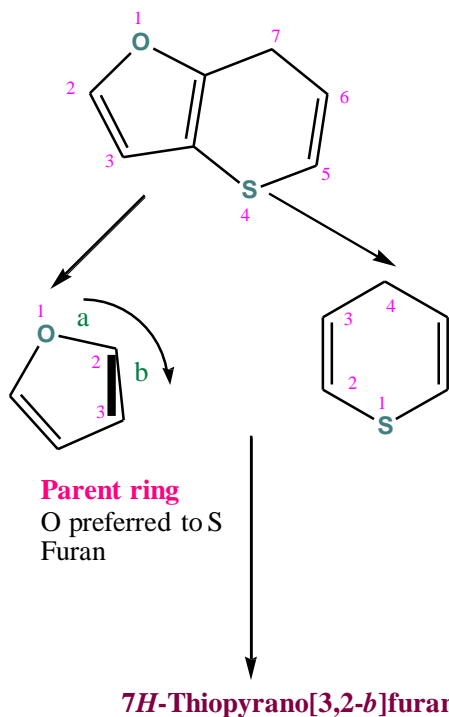
Nomenclature of Fused Heterocyclic Systems

Priority order of component ring systems:

- ❖ Selection of a parent or base ring is based on the following rules which are applied in order

Rule 1: A heterocyclic ring containing the heteroatom occurring earliest in the order **N, O, S**,

(i.e. ring containing N preferred to the rings does not contain N or containing O, or S)

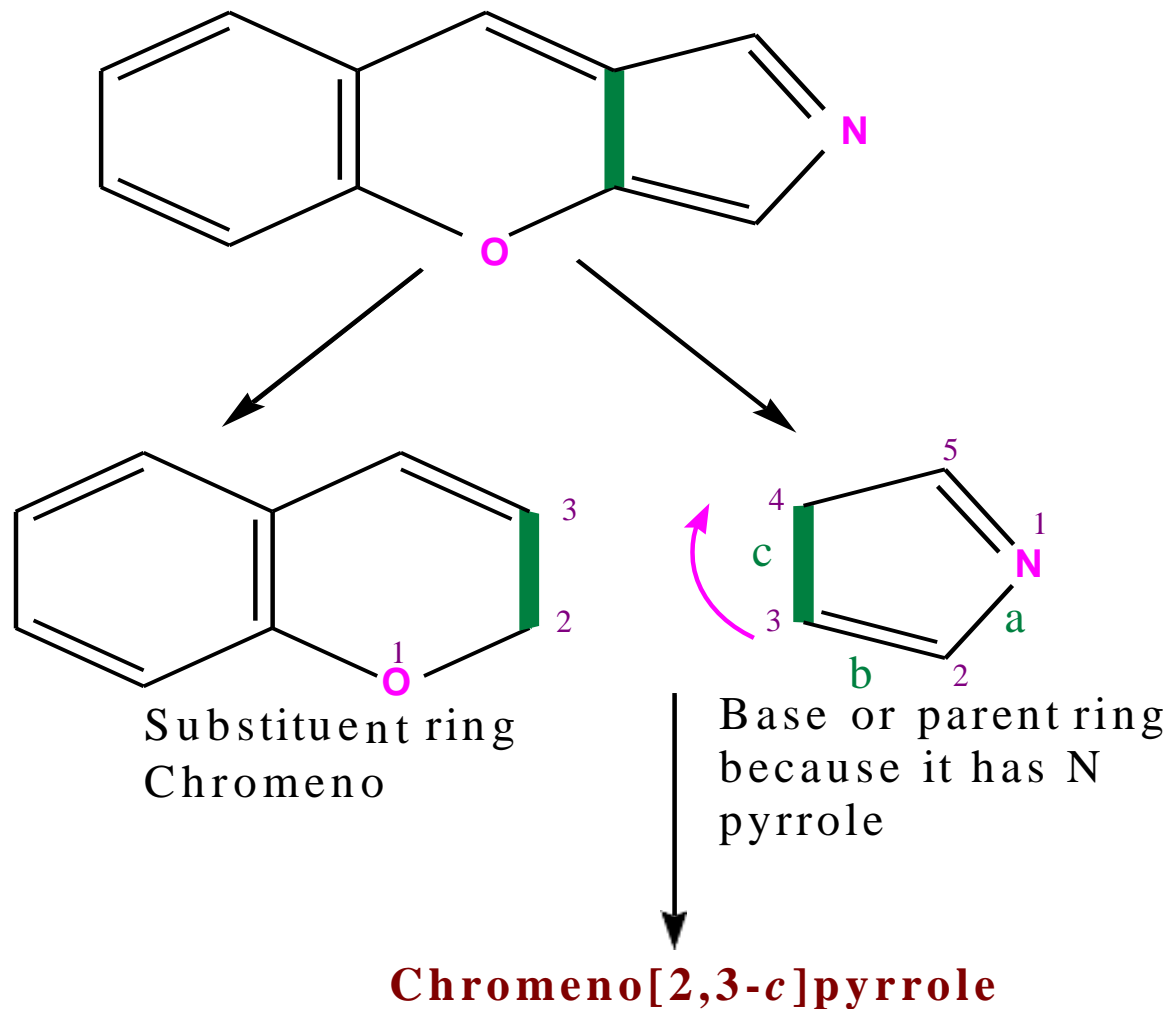


Note: The numbering system for the whole fused system is not the same as the numbers in the square brackets (i.e. there are three numbering systems; one for parent ring, one for substituent ring and the third is for the system as a whole)

Nomenclature of Fused Heterocyclic Systems

Priority order of component ring systems:

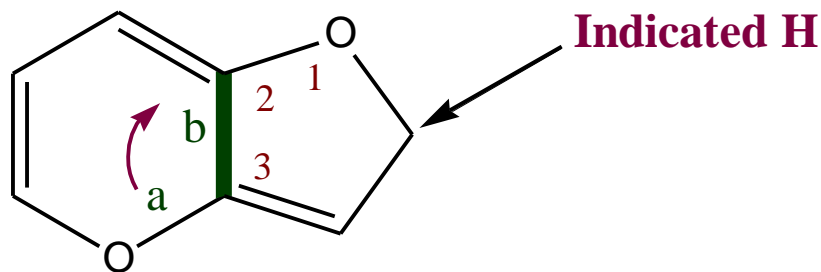
Rule 1: more example



Nomenclature of Fused Heterocyclic Systems

Priority order of component ring systems:

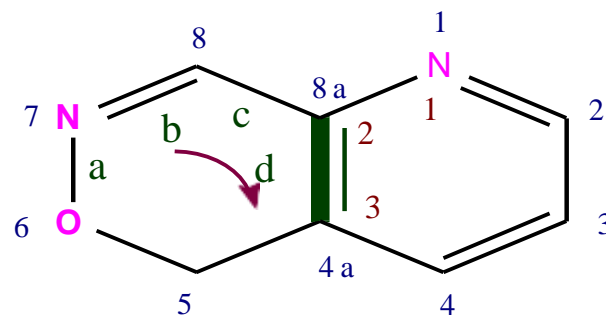
Rule 2: A heterocyclic component containing the largest possible individual ring



2H-Furo[3,2-*b*]pyran
(pyran [6] preferred to furan [5])

Numbering the whole system is started from O in furan ring to give the two heteroatoms 1,4 while starting from O in pyran ring gives them 1,5, thus the indicated H takes 2

Rule 3: A heterocyclic component containing the greater number of heteroatom of any kind



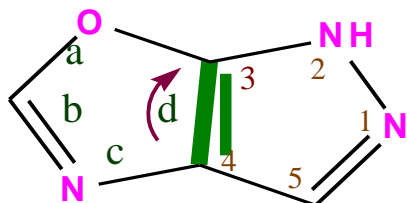
5H-Pyrido[2,3-*d*][1,2]oxazine
(Oxazine preferred to pyridine)

Note: The whole molecule is numbered starting from pyridine ring to give the three heteroatom the lowest possible number (1,6,7), however, starting from oxazine ring will give them (2,3,5) or (2,3,8).

Nomenclature of Fused Heterocyclic Systems

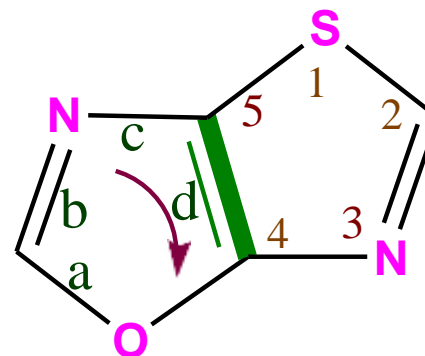
Priority order of component ring systems:

Rule 4: A heterocyclic component containing the greater variety of heteroatom



1H-Pyrazolo[4,3-*d*]oxazole
(O & N preferred to N only)

Rule 5: A heterocyclic component containing the greater number of heteroatoms most preferred when considered in order O, S, N,



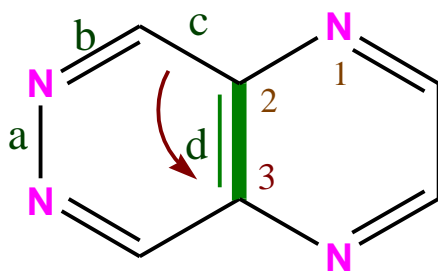
[1,3]Thiazolo[5,4-*d*][1,3]oxazole
(N & O preferred to N & S)

Note: The whole molecule is numbered starting from pyrazole ring to give the four heteroatom the lowest possible number (1,2,4,6). While starting from oxazole ring give them (1,3,4,5) or (1,3,5,6).

Nomenclature of Fused Heterocyclic Systems

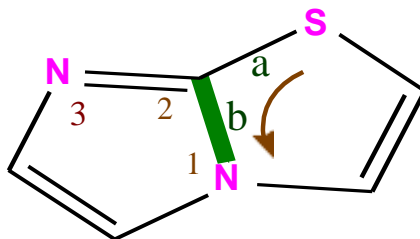
Priority order of component ring systems:

Rule 6: A heterocyclic component with the lower possible number for heteroatoms



Pyrazino[2,3-*d*]pyridazine
(pyridazine [2N-1,2] preferred to pyrazine [2N-1,4])

Rule 7: If a position of fusion is occupied by a heteroatom the name of the component rings to be used are so chosen as both to contain the heteroatom.



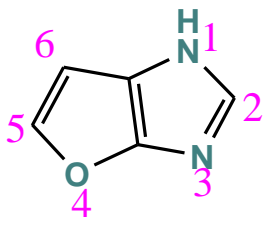
Imidazo[2,1-*b*]thiazole

Nomenclature of Fused Heterocyclic Systems

Order of preference between alternative numbering system of the whole molecule

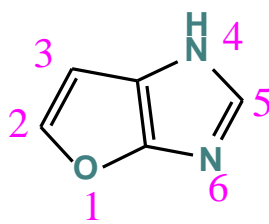
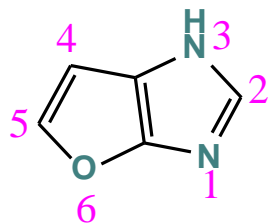
Numbering the whole fused system should start from the first atom after fusion in any direction to fulfill the following rules in order:

a) Give low numbers for the heteroatoms as a set

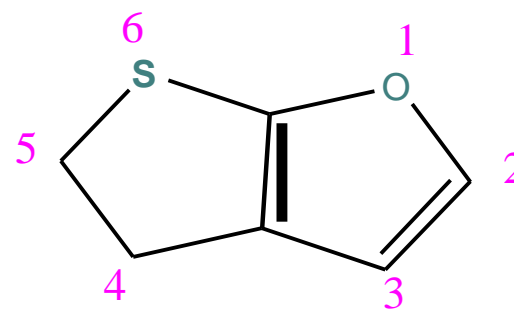


1H-Furo[2,3-d]imidazole

(heteroatoms 1,3,4 is preferred to 1,3,6 or 1,4,6)

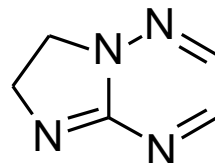
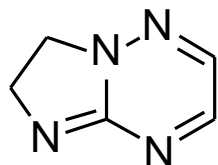
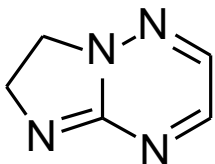


b) Give low numbers for heteroatoms of higher priority O, S, N



4,5-Dihydro-thieno[2,3-b]furan

c) Give low numbers to fusion carbon atom

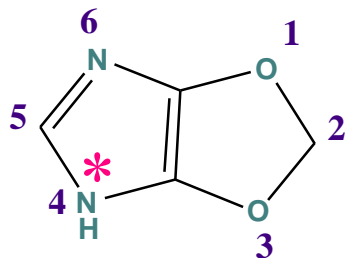


6,7-dihydroimidazo[1,2-b][1,2,4]triazine

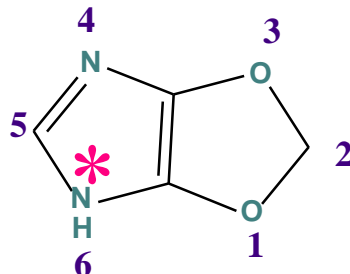
Fusion carbon 4a is preferred to 7a

Nomenclature of Fused Heterocyclic Systems

D) Give low numbers to indicate hydrogen atom



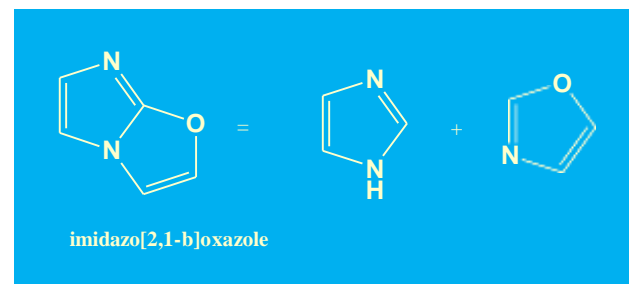
Not



4*H*-[1,3]dioxolo[4,5-*d*]imidazole

B)- If there is a heteroatom at the position of the fusion ...)

divide the components such that the common heteroatom is a member of both component parts



Thank You



Dr. Rajeev Ranjan
University Department of Chemistry
Dr. Shyama Prasad Mukherjee University, Ranchi