Heterocyclic compound
Lec 1

Lec. Doctor

Yahya saad yaseen

Heterocyclic compounds are those where one or more atom(s) of the ring are

heteroatoms, for example, N, O, S, P, As, Se, B, and so on (Greek word “heteros”

means different). More than half of the known organic compounds are heterocyclic

compounds. These are widely distributed in nature, and many of them are of fundamental

importance for life processes. For example, nucleic acid bases containing

purines and pyrimidines; hemoglobin and chlorophyll contain ing porphyrin rings;

essential dietary ingredients containing vitamins B1, B2, B3, B6, and ascorbic acid;

the

three essential amino acids, namely, histidine, proline, and tryptophan; almost all the

drugs and pharmaceuticals; and many natural products like alkaloids, carbohydrates,

and plant pigments. All these compounds contain hetero ring(s) in their molecules.

These are the reasons why a great deal of recent research work is concerned with the

methods of synthesis of hetero rings and studying their properties.

Common structural types of heterocycles

The heterocyclic with the structures analogous to that of benzene but with a heteroatom

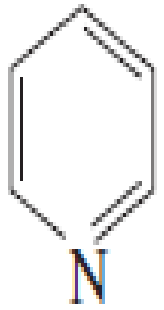
replacing at least one carbon atom of the benzene ring are called aromatic

heterocycles, for example, pyridine. There are other analogous heterocycles where

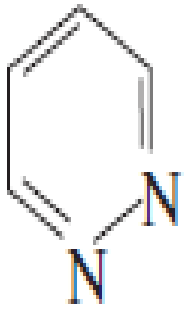
more than one carbon atom of the benzene ring are replaced by heteroatoms, for

example, pyridazine, pyrimidine, pyrazine, 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine,

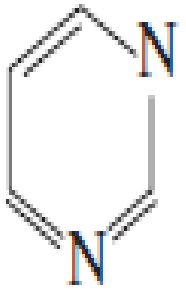
and 1,2,4,5-tetrazine.



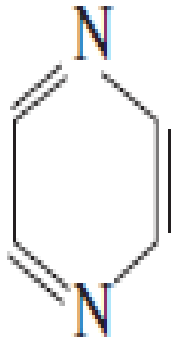
Pyridine



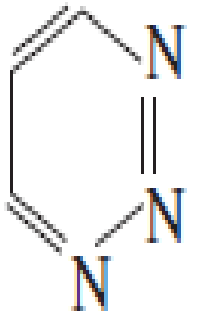
Pyridazine



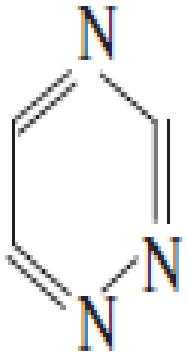
Pyrimidine



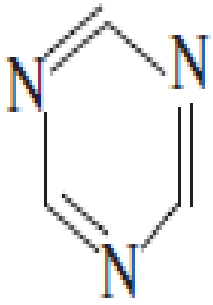
Pyrazine



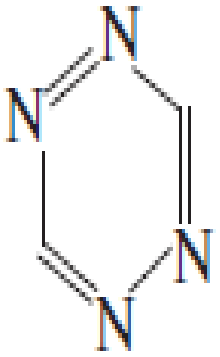
1,2,3-Triazine



1,2,4-Triazine



1,3,5-Triazine



1,2,4,5-Tetrazine

All of the above heterocycles are six-atom, six-pi electron aromatic heterocycles.

There are five-atom, six-pi electron aromatic heterocycles, for example, pyrrole,

furan, and thiophene contain only one heteroatom in the ring system, and oxazole,

thiazole, isothiazole, 1H-pyrazole, 1H-imidazole, and 1H-tetrazole contain two

heteroatoms in the ring.

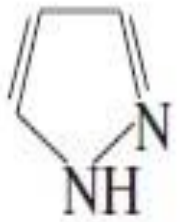
Pyrrole

Furan

Thiophene

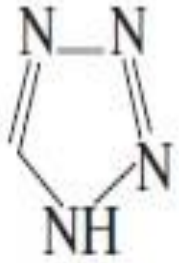
Oxazole

Thiazole



1H-pyrazole

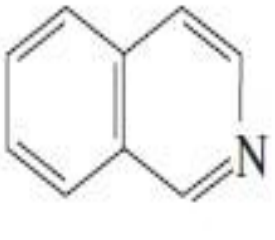
1H-imidazole



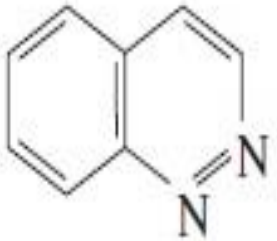
1H-tetrazole

There are fused-ring system aromatic heterocycles. For example, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, phthalazine, indole, isoindole, and benzimidazole.

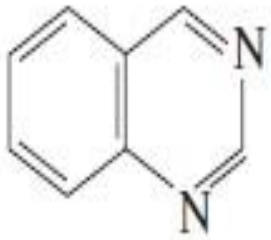
Quinoline



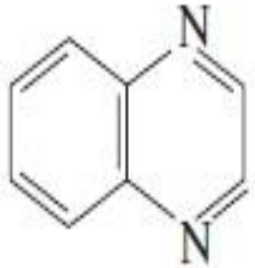
Isoquinoline



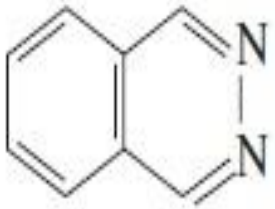
Cinnoline



Quinazoline



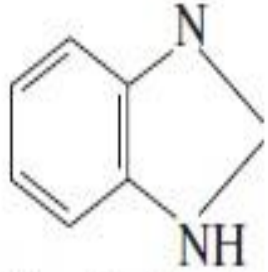
Quinoxaline



Phthalazine

Indole

Isoindole



Benzimidazole

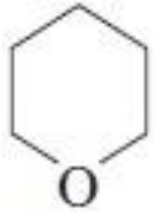
Besides the above fully unsaturated aromatic heterocycles, there are other nonaromatic small-ring heterocyclic compounds that may be either partially or fully saturated. In these heterocyclic compounds, there is no possibility of cyclic delocalization of *p*-electrons for which they lack any aromatic character

These small-ring heterocycles suffer from considerable angle strain. For example, pyrrolidine, tetrahydrofuran, thiolan, pyran, aziridine, oxiran, azetidine, oxetan, and so on, are fully saturated heterocycles and dihydropyrrole, azirine, oxetene, and so on, are partially saturated heterocycles.

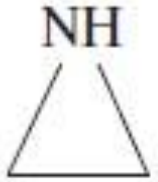
Pyrrolidine

Tetrahydrofuran

Thiolan

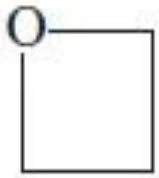


Pyran



Aziridine

Oxiran

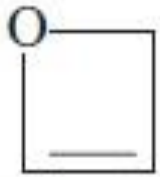


Oxetan

Fully saturated nonaromatic heterocycles

Dihydropyrrole

Azirine



Oxetene

Partially saturated nonaromatic heterocycles

Nomenclature of heterocyclic compounds

Monocyclic compounds are named by prefixing the name that indicates the nature of the heteroatom. For example, nitrogen n aza, sulfur n thia, oxygen n oxa, silicon n sila, phosphorus n phospha, and boron n bora.

The size of the ring of monocyclic compounds is indicated by appropriate suffixing for each ring size.

The suffixing depends on the nature of the heteroatom—nitrogen-containing heterocycles and heterocycles without nitrogen are suffixed in different but distinct

ways. The suffixing of aromatic (fully unsaturated) and nonaromatic (fully or partially

sat urated) heterocycles have different but related suffixes.

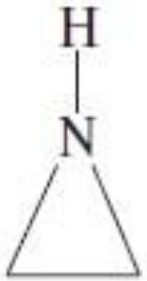
An example will help to understand the method of naming a heterocyclic compound.

(fully unsaturated
nitrogen-containing
three-membered heterocycle)

Azirine
Prefix: az-
Suffix: -irine

(fully unsaturated three-membered heterocycle without a nitrogen atom)

Oxiren
Prefix: ox-
Suffix: -iren

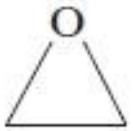
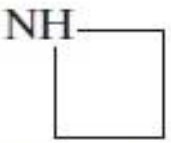
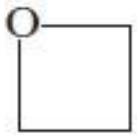
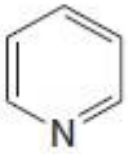
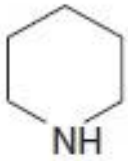
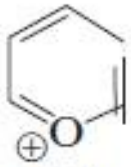
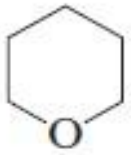


(fully saturated nitrogen containing three-membered heterocycle)

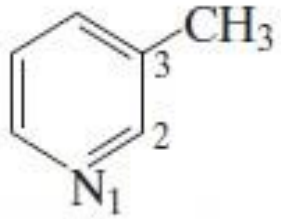
Aziridine
Prefix: az-
Suffix: -iridine

(fully saturated three-membered heterocycle without a nitrogen atom)

Oxiran
Prefix: ox-
Suffix: -iran

Number of ring members	Nitrogen present: Fully unsaturated (suffix)	Nitrogen present: Fully saturated (suffix)	Nitrogen absent: Fully unsaturated (suffix)	Nitrogen absent: Fully saturated (suffix)
3	-irine	-iridine	-iren	-iran
	 Azirine	 Aziridine	 Oxiren	 Oxiran
4	-ete	-etidine	-et	-etan
	 Azete	 Azetidine	 Oxet	 Oxetan
5	-ole	-olidine	-ole	-olan
	 Azole	 Azolidine	 Thiole	 Thiolan
6	-ine	-perhydro.....ine	-in	-ane
	 Azine	 Perhydroazine	 Oxin	 Oxane

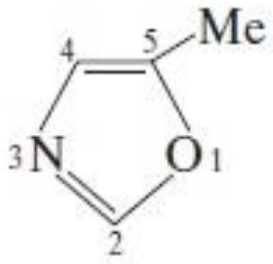
In a monocyclic compound, numbering starts from the heteroatom and moves in the direction where the substituent gets lower location. For example,



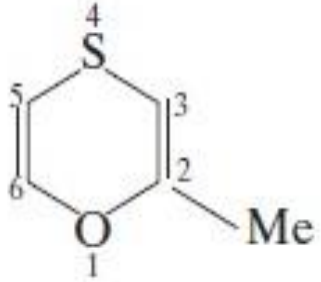
3-Methylazine

For monocyclic compounds having more than one heteroatom, the priority of the heteroatoms is decided as follows:

1. If the group number of the heteroatoms are different, the atom of the higher group number gets higher preference, for example, O (Gr. vi) > N (Gr. v)
2. If the group number of the heteroatoms are same, then the lighter atom is preferred, for example, O (atomic mass 16) > S (atomic mass 32)



5-Methyl-1,3-oxazole



2-Methyl-1,4-thiaoxin

For fused-ring heterocycles, the heterocyclic ring having maximum number of rings

with a simple name is chosen. If more than one heterorings are present, then the

nitrogen containing ring is given preference. For heterorings having no nitrogen, the

order of preference is decided by the above mentioned two rules (1) and (2). When

the parent heteroring is chosen, its name is prefixed by the name of the ring fused

with it, for example, benzo-, naphtho-.

The structure is now written with the greatest number of rings in horizontal

position, and the other nonhorizontal rings are written at the right of the horizontal

row and above it.

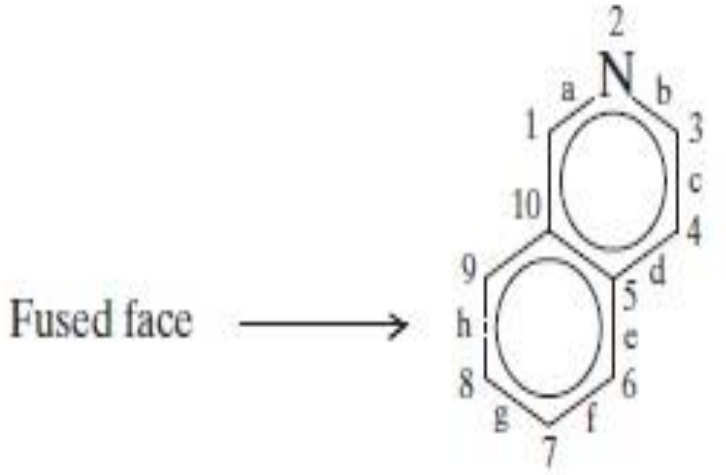
To distinguish isomers, the peripheral sides of the parent compound are lettered

as a, b, c . . . , and so on, beginning with “a” for the side C1—C2, “b” for C2—C3 . . . , and

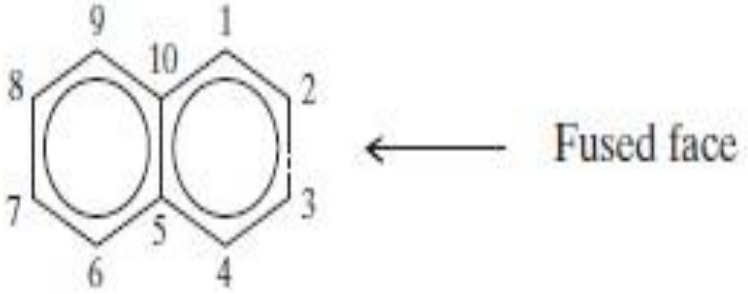
so on. The numbering of the parent ring is done in such a way that the side undergoing

fusion gets the *lowest alphabet*. For example heterocycle isoquinoline ring should

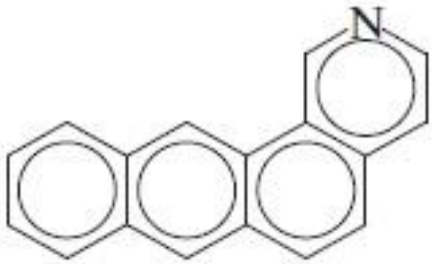
be numbered as follows:



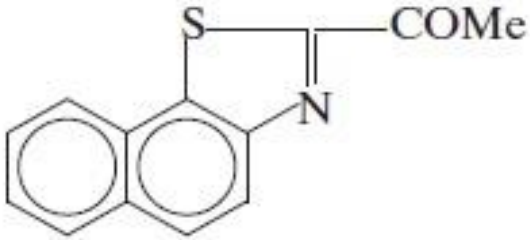
The naphthalene ring is numbered as follows:



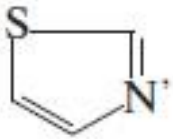
Therefore, the name of the isomer



is naphtho[3,2-h]isoquinoline. Another example is given below.



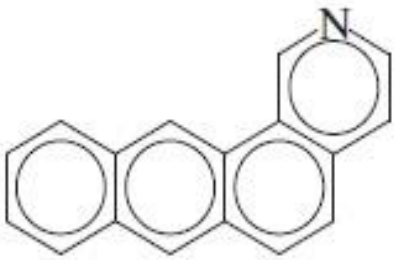
In the above compound, the heteroring is



which is called 1,3-Thiazole.

The compound is, therefore, naphthothiazole. To identify the fused side, the lettering is done as follows:

Therefore, the name of the isomer



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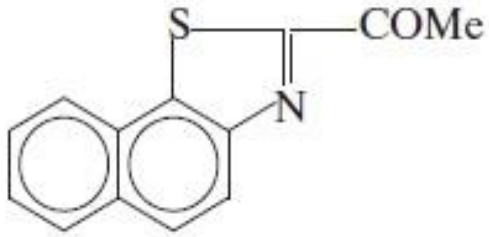

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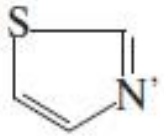

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THANK YOU

IN JAPANESE

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