

Unit –V

Heterocyclic Compounds

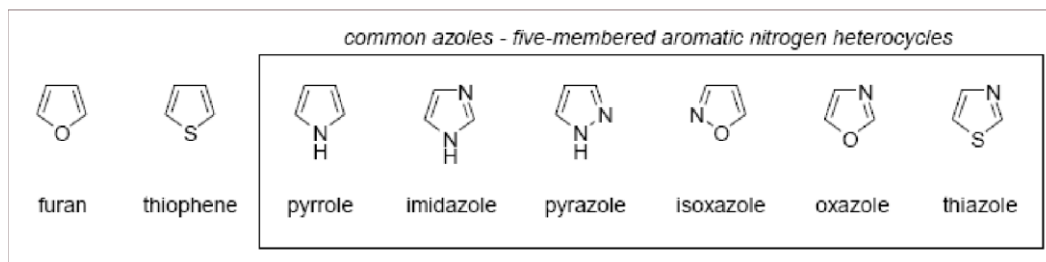
1) Two type of compounds:

- Homocyclic (cyclopropane, cyclobutane)
- Heterocyclic (containing N, S, O etc.)

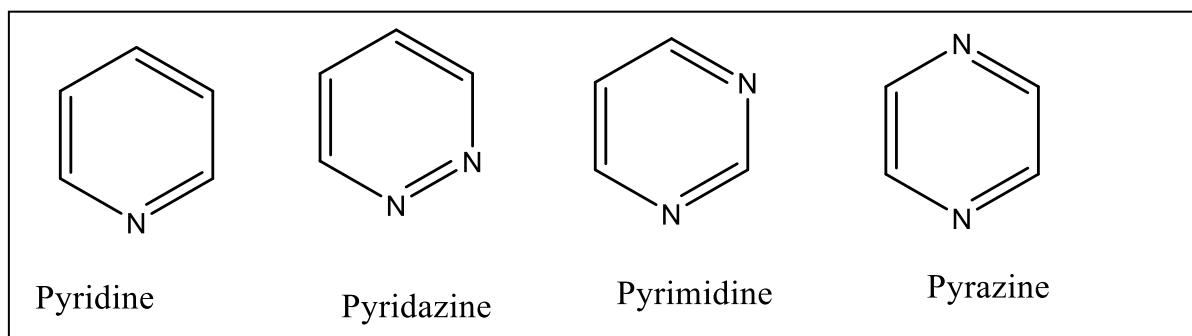
Aromatic stable cyclic compounds having at least one heteroatom (N, O, S etc.)

Types of Heterocycles:

1) 5-membered heterocycles with one or two heteroatoms

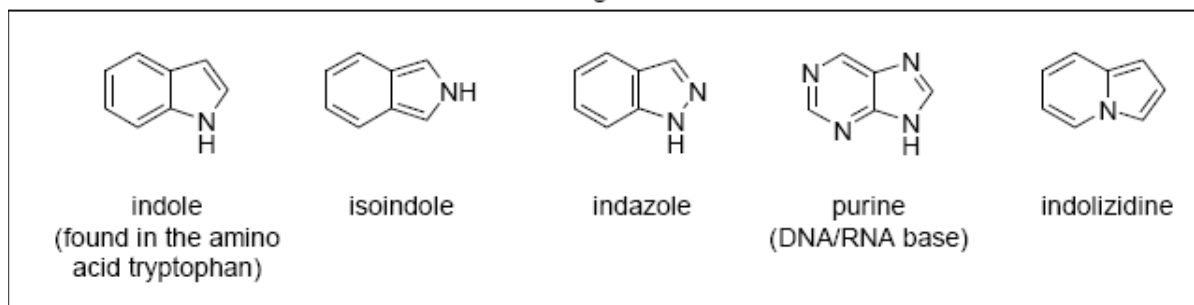


2) 6-membered heterocycles with one or two heteroatom

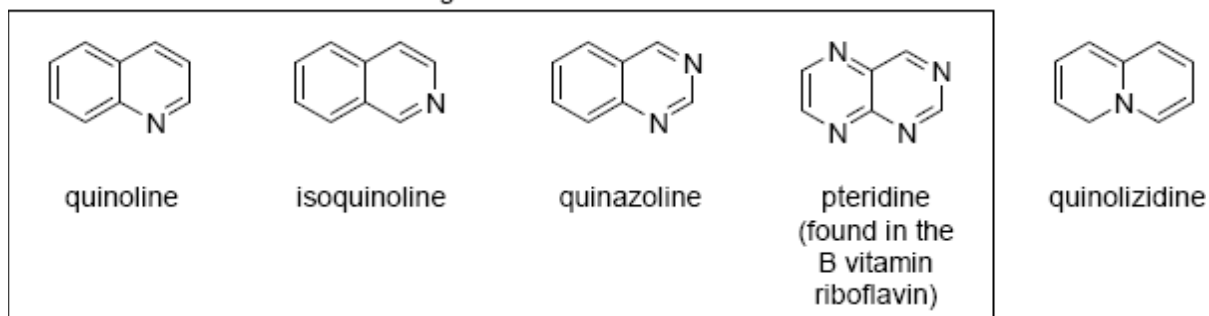


3) Fused Heterocycles:

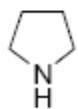
common ring-fused azoles



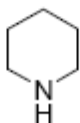
common ring-fused azines



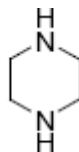
4) Saturated Heterocycles



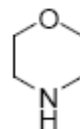
pyrrolidine



piperidine



piperazine



morpholine

The IUPAC rules allow three nomenclatures.

I. The Hantzsch-Widman Nomenclature.

II. Common Names

III. The Replacement Nomenclature

The Hantzsch-Widman nomenclature is based on the type (Z) of the heteroatom; the ring size (n) and nature of the ring, whether it is saturated or unsaturated .

This system of nomenclature applies to monocyclic three-to-ten-membered ring heterocycles.

I. Type of the heteroatom

The type of heteroatom is indicated by a prefix as shown below for common heteroatoms:

Heteroatom	Prefix
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O	Oxa
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N	Aza
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S	Thia
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P	Phospha
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O>S>N>P>Si (priority in case of heteroatoms)

II. Ring size (n)

The ring size is indicated by a suffix according to Table I below. Some of the syllables are derived from Latin numerals, namely ir from tri, et from tetra, ep from hepta, oc from octa, on from nona, ec from deca.

Table I: Stems to indicate the ring size of heterocycles

Ring Size	Suffix	Ring Size	Suffix
3	ir	7	ep
4	et	8	oc

5	ol	9	on
6	in	10	ec

The endings indicate the size and degree of unsaturation of the ring.

Table II: Stems to indicate the ring size and degree of unsaturation of heterocycles

Ring size	Saturated	Unsaturated	Saturated (With Nitrogen)
3	irane	irine	iridine

4	etane	ete	etidine
5	olane	ole	olidine
6	inane	ine	inidine
7	epane	epine	
8	ocane	ocine	
9	onane	onine	

Each suffix consists of a ring size root and an ending intended to designate the degree of unsaturation in the ring.

It is important to recognize that the saturated suffix applies only to completely saturated ring systems, and the unsaturated suffix applies to

rings incorporating the maximum number of noncumulated double bonds.

According to this system heterocycles are named by combining appropriate prefix/prefixes with a stem from Table II.

The letter “a” in the prefix is omitted where necessary.

Saturated 3, 4 & 5-membered nitrogen heterocycles should use respectively the traditional "iridine", "etidine" & "olidine" suffix.

Systems having a lesser degree of unsaturation require an appropriate prefix, such as "dihydro" or "tetrahydro".

Examples

Oxa+irane= Oxirane

Aza+iridine= Aziridine

Oxa+etane=Oxetane

Aza+etidine=Azetidine

Oxa+olane= Oxolane

Aza+olidine= Azolidine

Thia+irane= Thiirane

Thia+etane=Thietane

Thia+olane= Thiolane

Rules

- 1) Identify the heteroatom present in the ring and choose from (table 1) the corresponding prefix.
- 2) The position of a single heteroatom controls the numbering in a monocyclic compound. The heteroatom is always assigned position 1 and if substituents present are then counted around the ring in a manner so as to take the lowest possible numbers.
- 3) A multiplicative prefix (di, tri) and locants are used when two or more similar heteroatoms are contained in the ring (two nitrogen indicated by diaza) and the numbering preferably commenced at a saturated rather than an unsaturated atom.

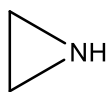
4) If more than one type of heteroatoms present in the ring the name will include more than one prefix with locants to indicate the relative position of the heteroatoms.

- When combining the prefixes (e.g. oxadiazole) two vowels may end up together, therefore the vowel on the end of the first part should be omitted (oxadiazole).
- The numbering is started from the heteroatom of the highest priority in such a way so as to give the smallest possible numbers to the other heteroatoms in the ring (the substituents are irrelevant).

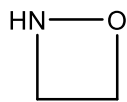
5) Choose the appropriate suffix from (table 2) depending on whether or not nitrogen atom is present in the ring, the size of the ring and presence or absence of any doublebonds

6) Combine the prefix(s) and suffix together and drop the first vowel if two vowels came together.

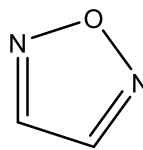
Examples:



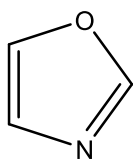
aziridine



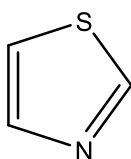
1,2-oxazetidine



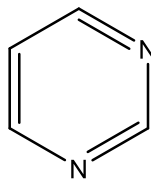
1,2,5-oxadiazole



1,3-oxazole



1,3-Thiazole



1,3-diazine