

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



III. Heterocyclic Compounds

17. IUPAC Nomenclature in Heterocyclic Compounds : Hantzsch-Widman Method



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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. IUPAC Nomenclature in Heterocyclic Compounds : Hantzsch-Widman Method

Heterocyclic Compounds

Systematic Nomenclature (IUPAC) in Heterocyclic Compounds

A) Hantzsch-Widman Method

- Hantzsch-Widman nomenclature is named after the German chemists Arthur Hantzsch and Oskar Widman, who proposed similar methods for the systematic naming of heterocyclic compounds in 1887 and 1888 respectively.
- According to this system three to ten-membered rings are named by combining the appropriate **prefix (or prefixes)** that denotes the type and position of the heteroatom present in the ring **with suffix** that determines both the ring size (depending on the total number of atoms in the ring) and the degree of unsaturation (**note that fully saturated and fully unsaturated have certain rules for nomenclature while partially unsaturation will be indicated in certain ways**).

In addition, the suffixes distinguish between nitrogen-containing heterocycles and heterocycles that do not contain nitrogen

- IUPAC name = locants + Prefix + suffix

Heterocyclic Compounds

Rules for systematic nomenclature (IUPAC) in heterocyclic compounds:

1- Generally The name consist of tow parts ,

part 1 = prefix = indicate the type of the heteroatom in the ring (N,O,S)

part 2 = suffix = indicate the size (3,4,5,...membered) of ring

1. Name **Prefix-** **Suffix** – **ring size** - **saturation**

			<u>Ring Size</u>	<u>unsaturated</u>	<u>saturated</u>	<u>saturated ring with nitrogen</u>
O	Oxa	O	5	ole	olane	-olidine
S	Thia	S	6	ine	inane (-ane)	?
N	Aza	N				

Heterocyclic Compounds

Rules for systematic nomenclature (IUPAC) in heterocyclic compounds:

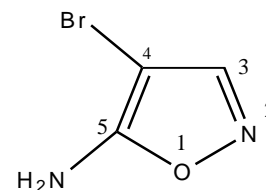
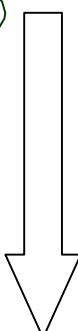
1) Identify the heteroatom present in the ring and choose from (table 1) the corresponding prefix (e.g. thia for sulfur, aza for nitrogen and oxa for oxygen).

O=Oxa; S=Thia; N=Aza

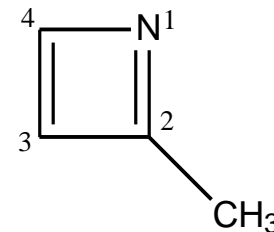
2) The position of a single heteroatom control the numbering in a monocyclic compound. The heteroatom is always assigned position 1 and if substituents present are then counted around the ring in a manner so as to take the lowest possible numbers. **Then they should be listed in alphabetical order.**

Table 1

Atom	Prefix
O	oxa
S	thia
N	aza



5-Amino-4-bromoisoxazole

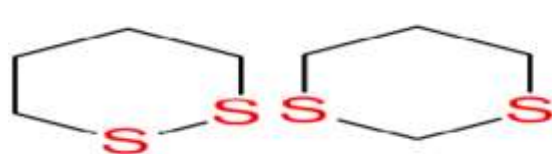


Priority decreases

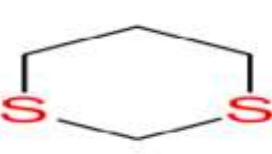
Heterocyclic Compounds

Rules for systematic nomenclature (IUPAC) in heterocyclic compounds:

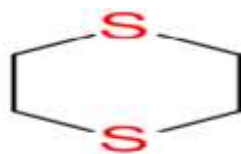
3) A multiplicative prefix (di, tri, ect.) and locants are used when two or more similar heteroatoms contained in the ring(two nitrogen indicated by diaza) and the numbering preferably commenced at a saturated rather than an unsaturated atom, as depicted in the following example: 1,3-diaza....



1,2-dithiane



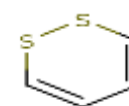
1,3-dithiane



1,4-dioxine



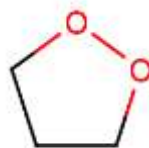
1,4-dithiine



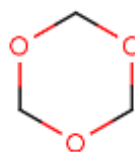
1,2-dithiine



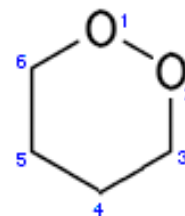
1,4-dioxane



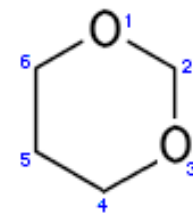
1,2-dioxolane



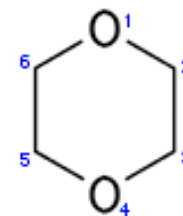
1,3,5-trioxane



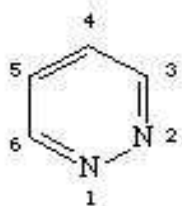
1,2-dioxane
o-dioxane



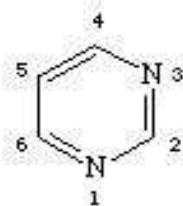
1,3-dioxane
m-dioxane



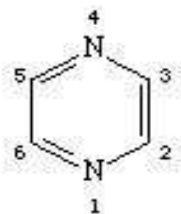
1,4-dioxane
p-dioxane



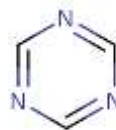
pyridazine



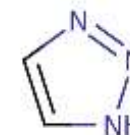
pyrimidine



pyrazine



1,3,5-Triazine



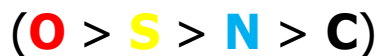
1,2,3-triazole

Heterocyclic Compounds

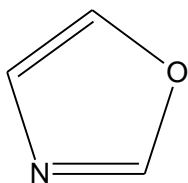
Rules for systematic nomenclature (IUPAC) in heterocyclic compounds:

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.

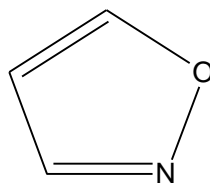
Atom prefixes have a strict order of priority (preference) in which they are to be listed. For example, "Oxa" (for oxygen) always comes before "aza" (for nitrogen) in a name (see table 1).



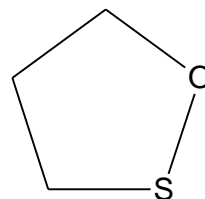
When combining the prefixes (e.g. oxa and aza) two vowels may end up together, therefore the vowel on the end of the first part should be omitted (oxaza).



IUPAC name: 1,3-oxazole
Common name: oxazole

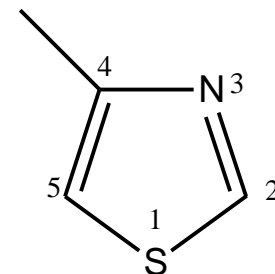


IUPAC name: 1,2-oxazole
Common name: isoxazole



1,2-oxathiolane

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).



4-Methyl-1,3-Thiaza....





Heterocyclic Compounds

Rules for systematic nomenclature (IUPAC) in heterocyclic compounds:

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 double bonds

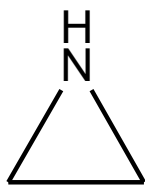
Table 2

(Ring size)

	ete	etidine	irene	sat
	ole	olidine	etane	irane
	ine	a	ole	etane
	epine	a	in	olane
			epin	ane
				epane

a: means use the prefix perhydro followed by the fully unsaturated name

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



This ring contains (N) → Prefix is **aza**

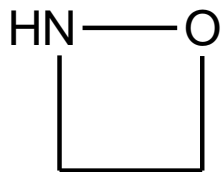
The ring is 3-membered and fully saturated → suffix is **iridine**

By combining the prefix and suffix, two vowels ended up together (**azairidine**), therefore the vowel on the end of the first part should be dropped. This gives **the correct name:**

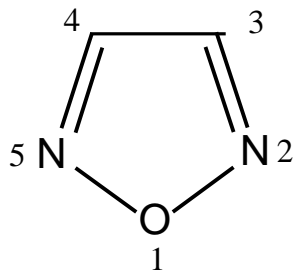
Aziridine

Heterocyclic Compounds

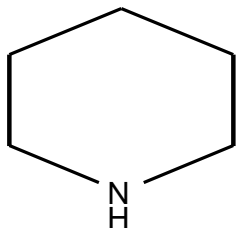
Rules for systematic nomenclature (IUPAC) in heterocyclic compounds:



- This ring contains (O ,N) and (o) has higher priority than (N) and by starting numbering the ring at (O) → Prefix is 1,2-Oxaaza, but the first vowel must be omitted to give
1,2-Oxaza
- The ring is 4-membered and fully saturated → suffix is **etidine**
- By combining the prefix and suffix, two vowels ended up together (**1,2-oaxazaetidine**), therefore the vowel on the end of the first part should be dropped. This gives the correct name: **1,2-oxazetidine**



- This ring contains (O) → prefix1 (oxa), and two (N) → prefix2 diaza
Locants, since (O) is higher priority than (N) so it is in position 1 by default and the two (N) are therefore at positions 2 and 5, this gives the combined prefixes as **1,2,5-oxadiaz** (note that the **a** in oxa is not dropped)
It is 5-membered, fully unsaturated ring with (N) → the suffix is **ole**
By combining the prefixes and the suffix and dropping the appropriate vowels we get the correct name as : **1,2,5-Oxadiazole**



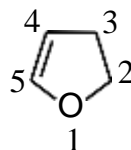
The ring is 6-membered, fully saturated with N → Prefix perhydro followed by the name of fully unsaturated 6-membered ring with nitrogen → **azine**
Thus the full name is **perhydroazine**

Heterocyclic Compounds

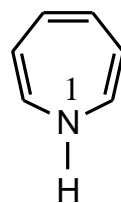
Rules for systematic nomenclature (IUPAC) in heterocyclic compounds:

Partial unsaturation in heterocyclic compounds can be indicated by one of the following methods:

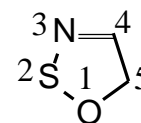
1) The position of nitrogen or carbon atoms which bear extra hydrogen atoms must be indicated by numbers and italic capital H (e.g. *1H*, *2H*, etc.) followed by the name of maximally unsaturated ring.



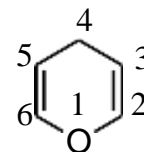
2H, 3H-Oxole



1H-Azepine

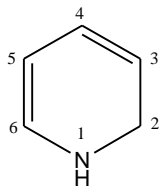


5H-1,2,3-Oxathiazole

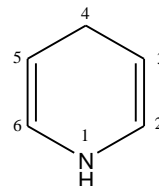


4H-Oxin

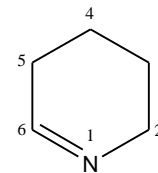
2) The words **dihydro**, or **trihydro**, or **tetrahydro** are used if two or three or four atoms are saturated. These words are preceded by numbers indicate the position of saturated atoms as low as possible and followed by the corresponding fully unsaturated Hantzsch-Widman name



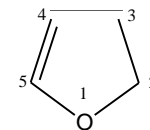
1,2-Dihydroazepine



1,4-Dihydroazepine



2,3,4,5-Tetrahydroazepine



2,3-Dihydrooxole

Isomers have the same M.F.
but differ in the position of
the double bond

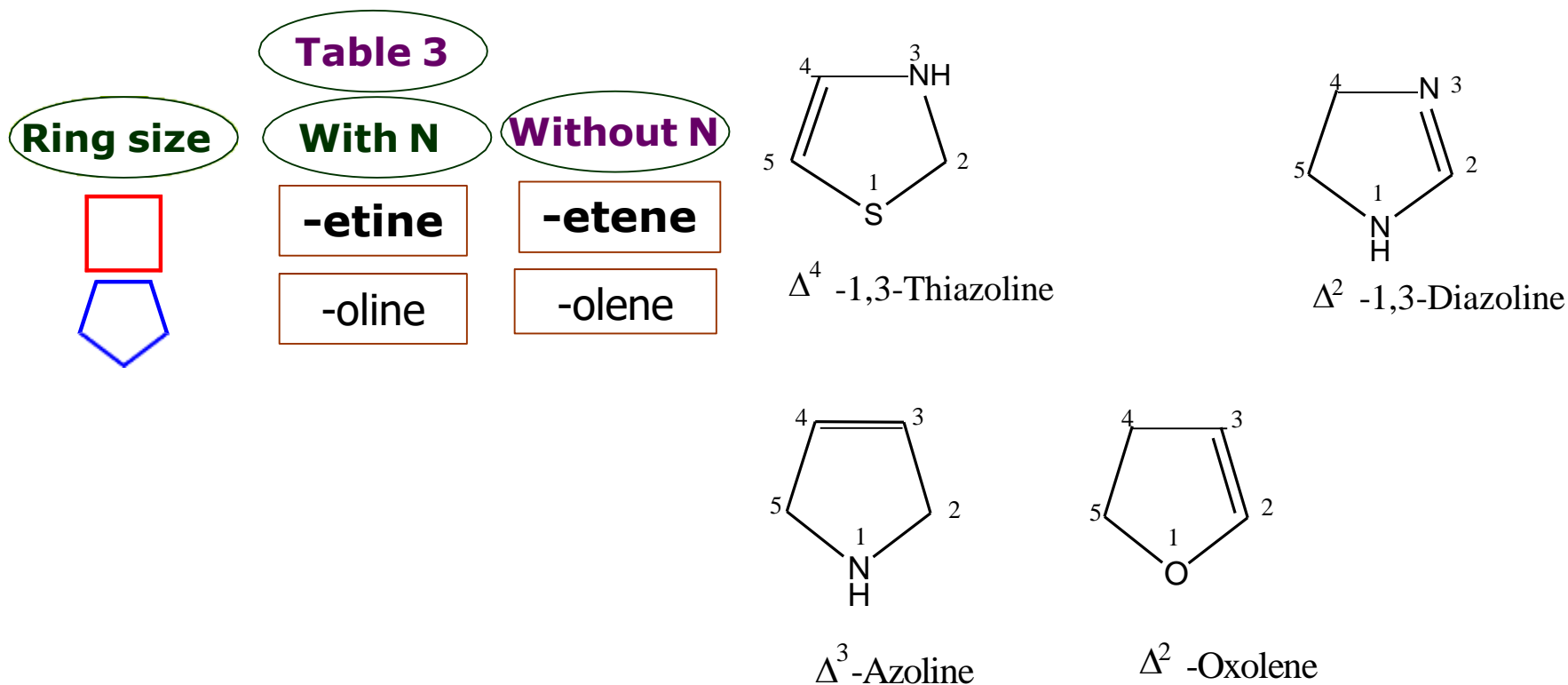
Heterocyclic Compounds

Rules for systematic nomenclature (IUPAC) in heterocyclic compounds:

3) Alternatively, the **partially unsaturated 4 and 5 rings** (i.e. rings contain one double bond) are given special Hantzsch-Widman suffixes as in **table 3** and the double bond is specified as Δ^1 , Δ^2 , Δ^3 , etc.. Which indicates 1 and ; 2 and 3; 3 and 4 atoms respectively have a double bond

(i.e. Name : Δ^x + Prefix + special suffix)

(x= locant of the double bond)



Thank You



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