Compiled By

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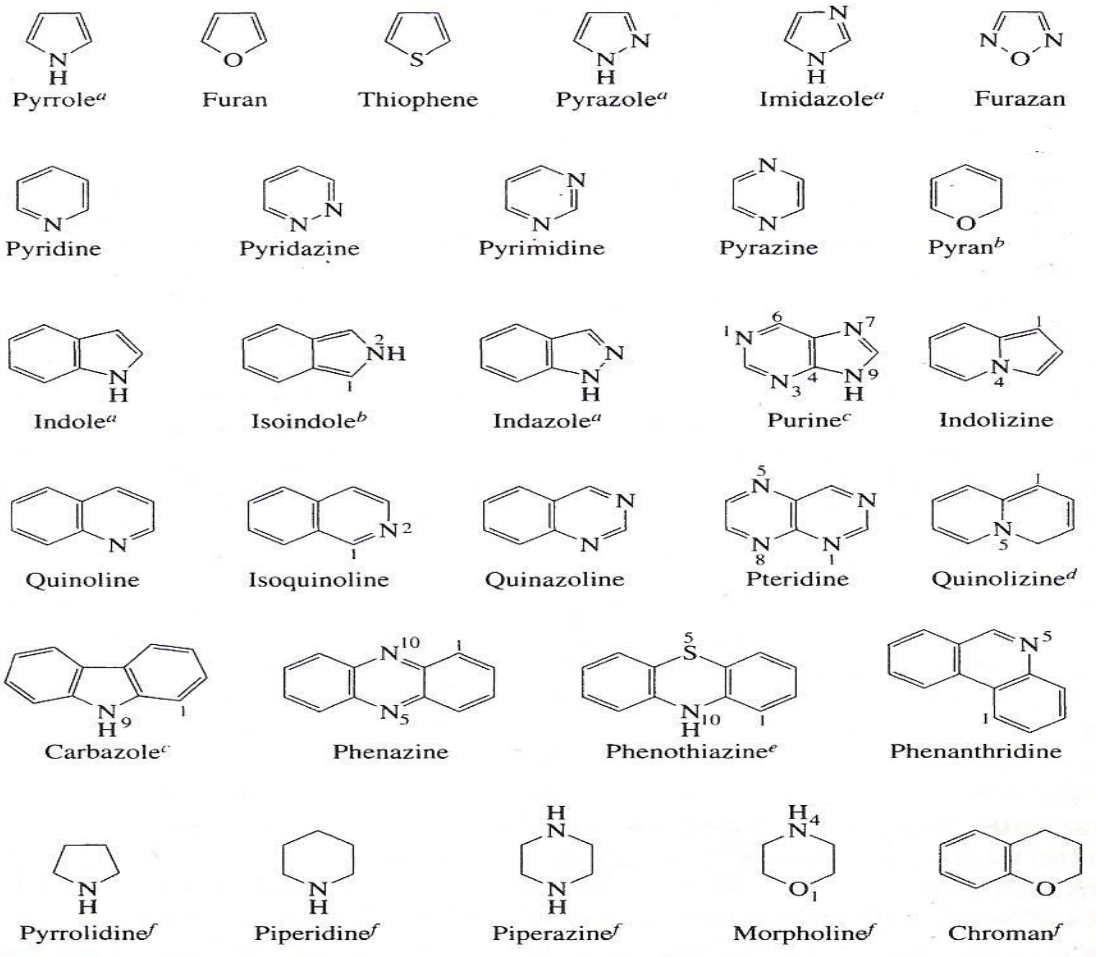
Topic: Heterocyclic Compounds

Nomenclature of Heterocyclic Compounds

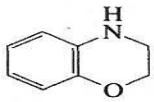
Systematic Nomenclature system: (Hantzsch-Widman System)

Heterocycles with recognized trivial names

Table 11.1 Examples of heterocycles with 'recognized' trivial names



[a] 1*H*-tautomer shown..
[b] 2*H*-tautomer.
[c] 9*H*-tautomer.
[d] 4*H*-tautomer.
[e] 10*H*-tautomer.
[f] Names of these saturated heterocycles are not used in fusion names; for example, compound **X** is 3,4-dihydro-2*H*-1,4-benzoxazine, not benzomorpholine.



X

Naming Heteromonocycles

Prefix (heterotoms, number, positions) + **Stem** (ring size + saturation)

Table 11.2 Hantzsch–Widman system: common prefixes

Element	Valence	Prefix[a]
Oxygen	II	Oxa
Sulfur	II	Thia
Selenium	II	Selena
Tellurium	II	Tellura
Nitrogen	III	Aza
Phosphorus	III	Phospha
Arsenic	III	Arsa
Silicon	IV	Sila
Germanium	IV	Germa
Boron	III	Bora

[a] The final 'a' is dropped when the prefix is followed by a vowel.

Table 11.3 Stems for the Hantzsch–Widman system

Ring size	Unsaturated ring	Saturated ring
3	irene[a]	irane[b]
4	ete	etane[b]
5	ole	olane[b]
6	ine[c]	inane[d]
7	epine	epane
8	ocine	ocane
9	onine	onane
10	ecine	ecane

[a] The stem 'irine' is normally used for three-membered rings which contain nitrogen.
[b] The stems 'iridine', 'etidine' and 'olidine' are preferred for saturated rings containing nitrogen.
[c] The stem 'inine' is used with some phosphorus, arsenic and boron heterocycles: see ref. 5.
[d] The stem 'ane' is used if immediately preceded by the prefixes 'ox', 'thi', 'selen' or 'tellur'.

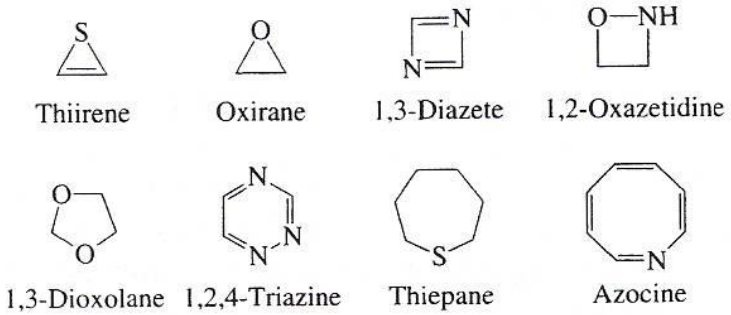
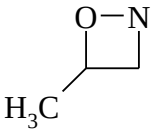
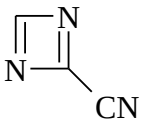
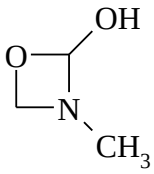


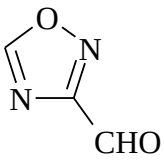
Figure 11.1 Examples of systematically named heterocycles.

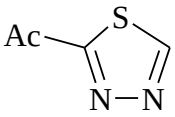
Examples: Name the following compounds

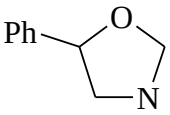


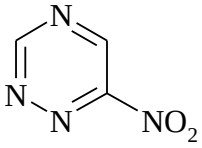


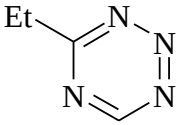


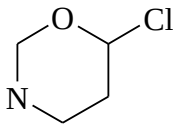


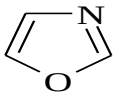




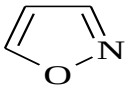




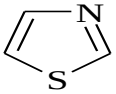




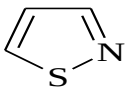
Oxazole



isoxazole



thiazole



isothiazole

Indication of saturated positions

1 position (H)
2 positions (dihydro)
3 positions (dihydro + H)
4 posit ions (tetrahydro)
5 positions (tetrahydro + H)

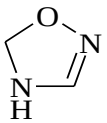
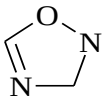
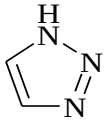
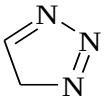
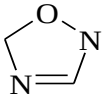
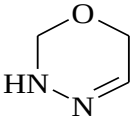
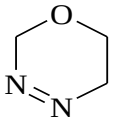
Saturated positions receive the lower number

Examples:

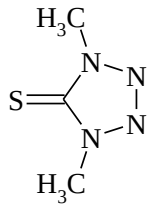




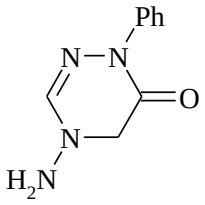


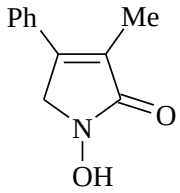
Compounds containing exocyclic C=O and C=S



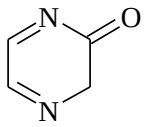
1,4-dihydro-1,4-dimethyl-5H-tetrazol-5-thione



4-amino-6-oxo-1-phenyl-1,4,5,6-tetrahydro-1,2,4-triazine
4-amino-1-phenyl-1,4,5,6-tetrahydro-1,2,4-triazin-6-one



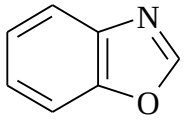
2,5-Dihydro-1-hydroxy-3-methyl-4-phenyl-1H-pyrrole-2-one
2,5-Dihydro-1-hydroxy-3-methyl-4-phenylpyrrole-2-(1H)-one



3H-pyrazin-2-one
Pyrazin-2(3H)-one

Nomenclature of fused ring systems

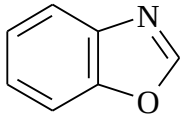
Prefix(O) + Base component



Benzoxazole

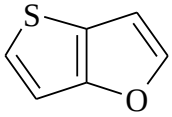
Base Component

1) One ring only contains N, Choose it



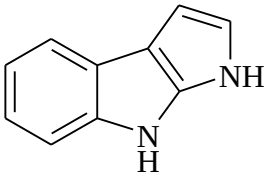
Benzoxazole

2) No, Nitrogen, oxa , thia, aza



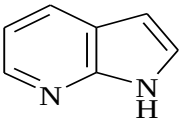
Thieno[ ]furane

3) One consists of two or more rings, choose it



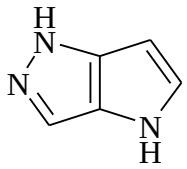
pyrrolo[ ]indole

4) Two rings of different size, choose the larger



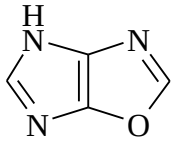
pyrrolo[ ]pyridine

5) Choose the one with more heteroatoms



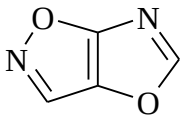
pyrrolo[ ]pyrrazole

6) Same number of heteroatoms, choose oxa > thia > aza

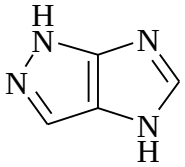


imidazo[ ]oxazole

7) Same number of heteroatoms, same oxa, thia, aza, then choose lower numbering

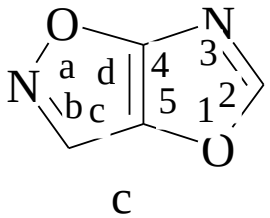


oxazolo[ ]isoxazole



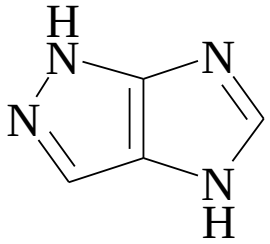
imidazo[ ]pyrrazole

Indicate the fusion by giving letters to the base components and numbers to the prefix (go in the same direction)



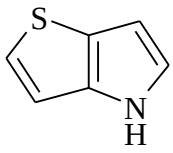
c

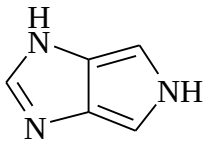
oxazolo[5,4-d]isoxazole

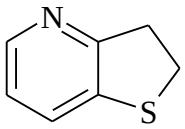


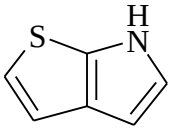
imidazo[ ]pyrrazole

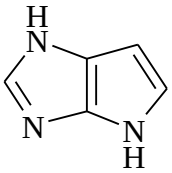
Examples:

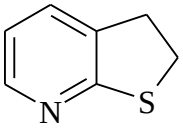


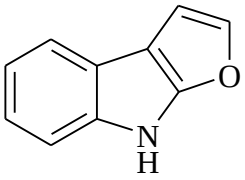


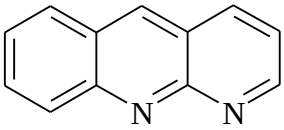


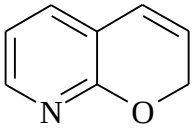


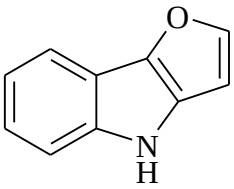


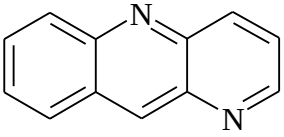


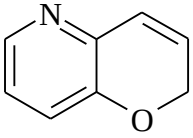




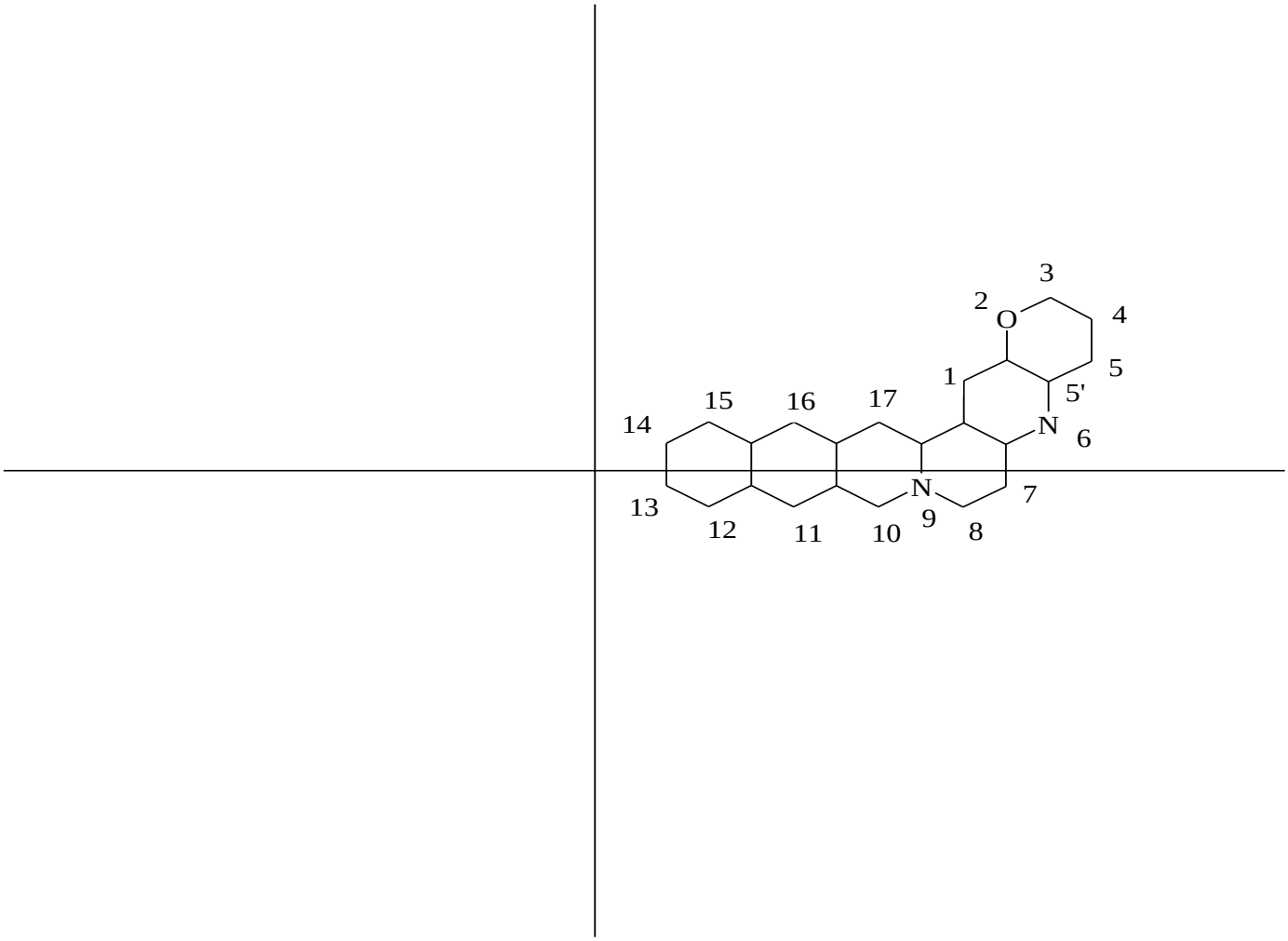








Numbering substituents on fused rings:



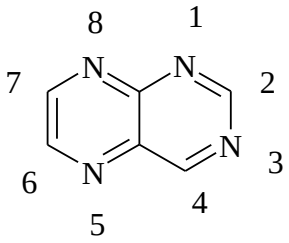
1) **Use rectangular coordinates**
2) **As many rings as possible lie in a horizontal row**
3) **A maximum number of rings are in the upper right quadrant**
4) **The system is numbered in a clockwise direction commencing with that atom which is not engaged in the ring fusion and is furthest to the left:**
    - **in the uppermost ring or**
    - **in the ring furthest to the right in the upper row**
5) **C atoms which belong to more than one ring are omitted**
6) **Heteroatoms in such positions are, however, included**

7) If there are several possible orientations in the coordinate system,

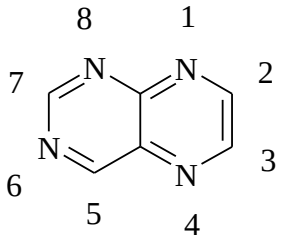
a))) the one in which the heteroatoms bear the lowest locants is valid,,,,,,

b))) or the one in which the C atom that belongs to more than one ring has the lowest locant

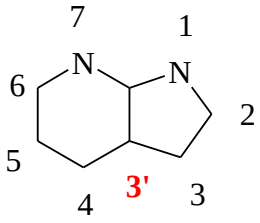
a))))



not



b))))



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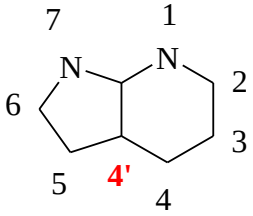

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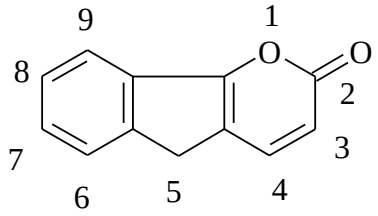

indeno[1,2-b]pyran-2(5H)-one