Nomenclature of Heterocyclic Compounds

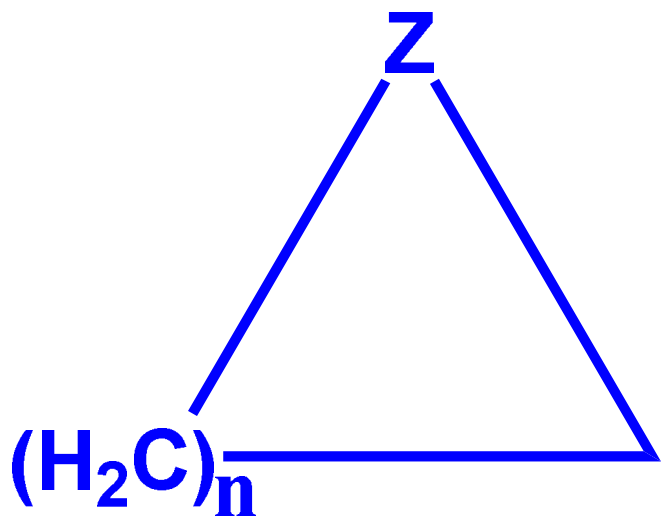
The IUPAC rules allow three nomenclatures.

I. The Hantzsch-Widman Nomenclature.

II. Common Names

III. The Replacement Nomenclature

I. Hantzsch-Widman Nomenclature



n = 1,2,3, ...

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 hetreroatoms:

Hetreroatom	Prefix
O	Oxa
N	Aza
S	Thia
P	Phospha

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	
7	-epane	-epine	
8	-ocane	-ocine	
9	-onane	-onine	
10	-ecane	-ecine	

According to this system heterocyles are named by combining appropriate prefix/prefixes with a stem from Table II. The letter “a” in the prefix is omitted where necessary.

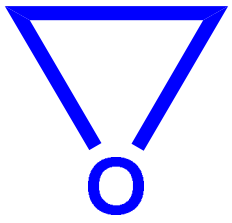
Each suffix consists of a ring size root and an ending intended to designate the degree of unsaturation in the ring.

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 non-cumulated double bonds.

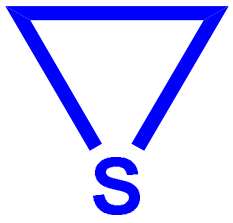
Systems having a lesser degree of unsaturation require an appropriate prefix, such as "dihydro"or "tetrahydro".

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

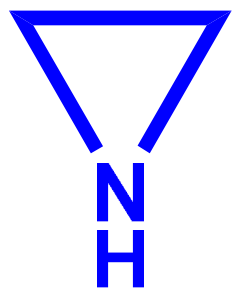
Examples



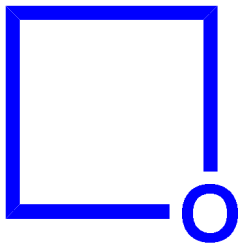
Oxa+irane= Oxirane



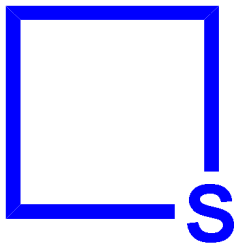
Thia+irane= Thiirane



Aza+iridine= Aziridine

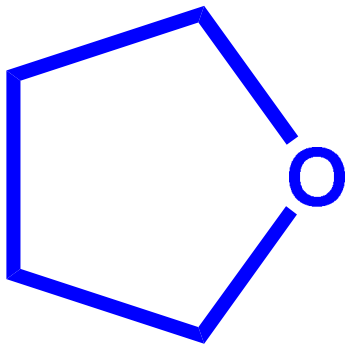


Oxa+etane=Oxetane

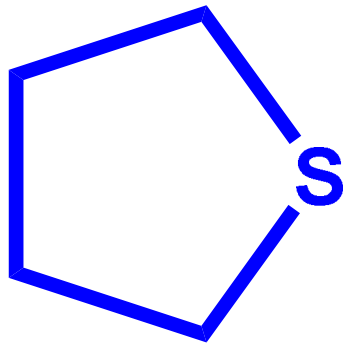


Thia+etane=Thietane

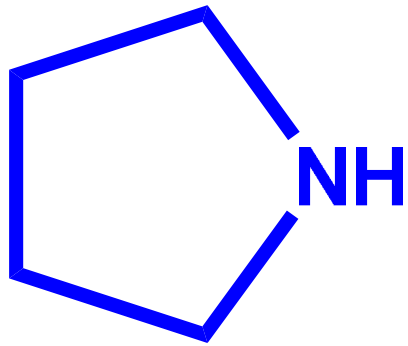
Aza+etidine=Azetidine



Oxa+olane= Oxolane

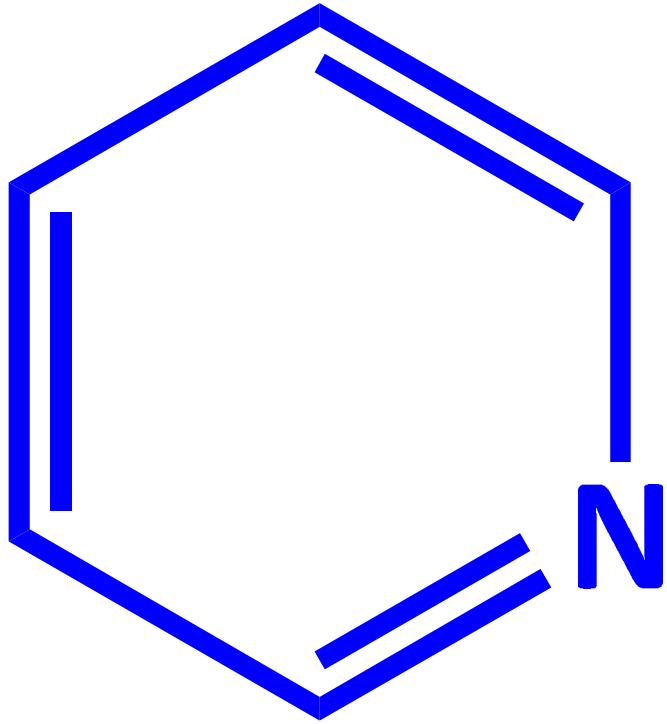


Thia+olane= Thiolane



Aza+olidine= Azolidine

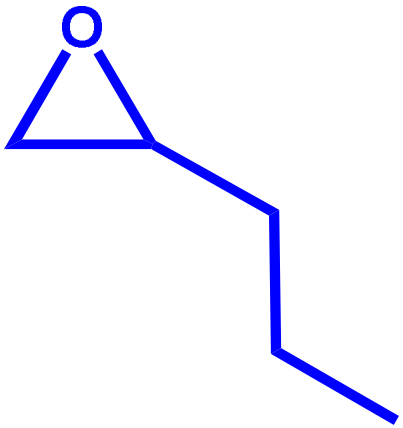
Azinane



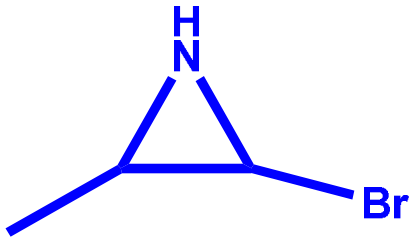
Azine

Pyridine

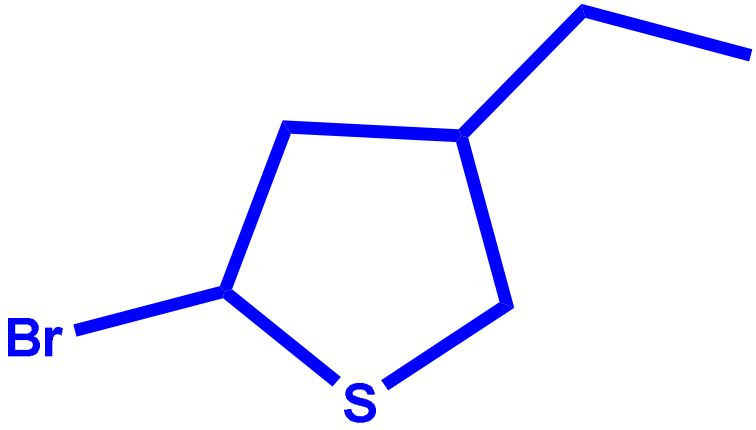
In case of substituents, the heteroatom is designated number 1, and the substituents around the chain are numbered so as to have the lowest number for the substituents.



2-Propyloxirane

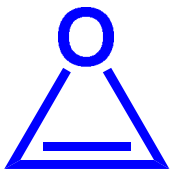


2-Bromo-3-methylaziridine

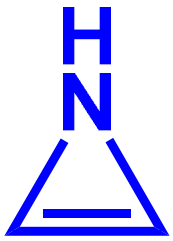


2-Bromo-4-ethylthiolane

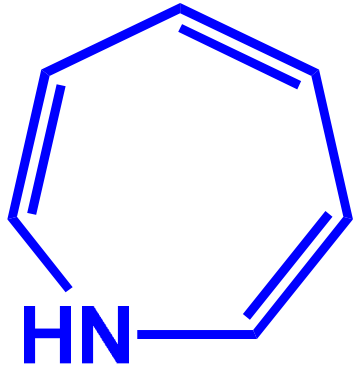
The compound with the maximum number of noncumulative double bonds is regarded as the parent compound of the monocyclic systems of a given ring size.



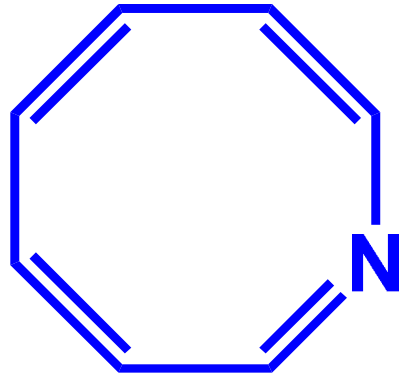
Oxirine



Azirine



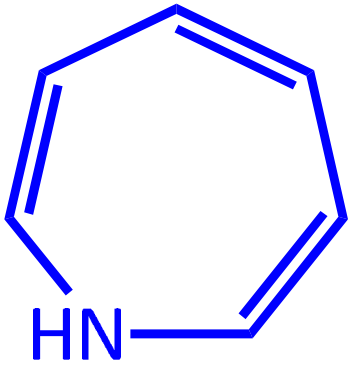
Azepine



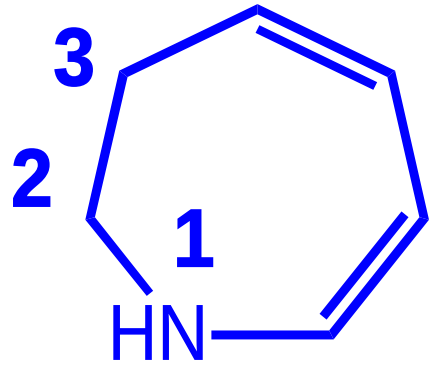
Azocine

Partial Unsaturation

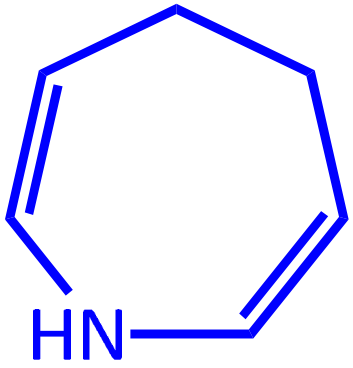
Use fully unsaturated name with dihydro, tetrahydro, etc



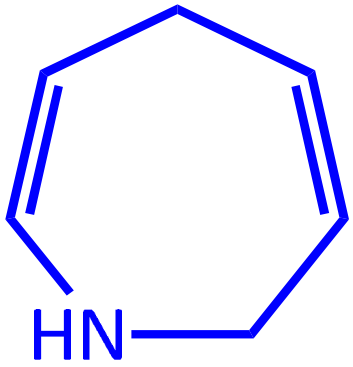
Azepine



2,3-Dihydroazepine

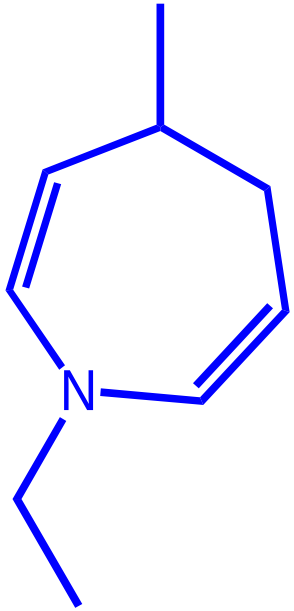


4,5-Dihydroazepine

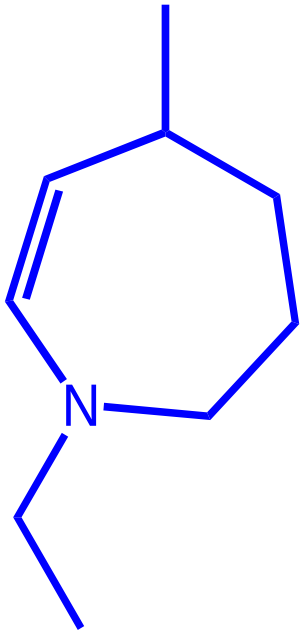


2,5-Dihydroazepine

When numbering give priority to saturated atoms.

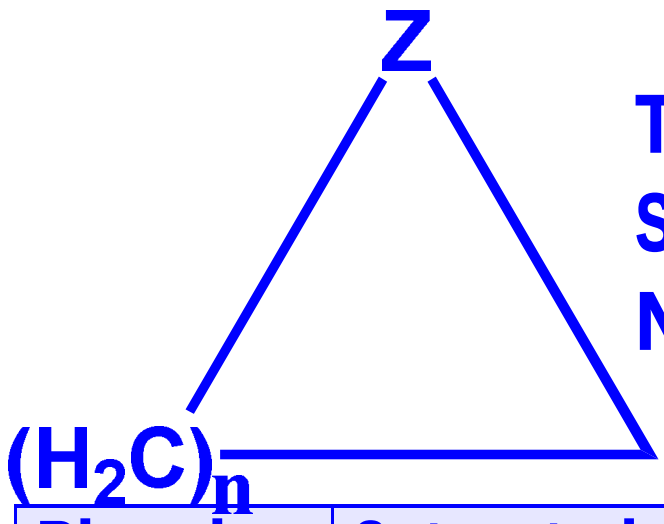


1-Ethyl-4-methyl-4,5-dihydroazepine



1-Ethyl-5-methyl-2,3,4,5-tetrahydroazepine

Revision



Type (Z) - Prefix

Size (n) - Suffix

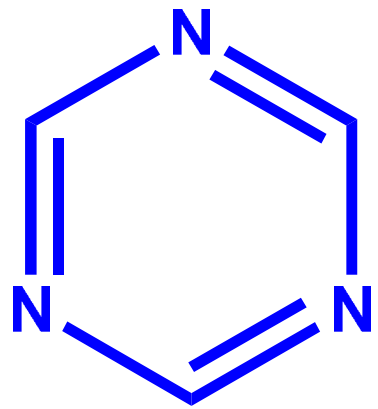
Nature of ring - Ending

Hetreroatom	Prefix
O	Oxa
N	Aza
S	Thia
P	Phospha

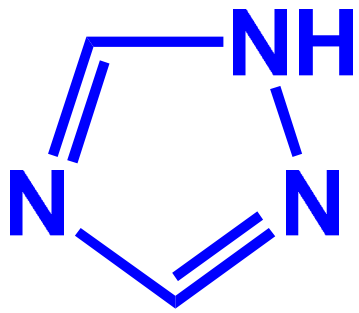
Ring size	Saturated	Unsaturated	Saturated (With Nitrogen)
3	-irane	-irine	-iridine
4	-etane	-ete	-etidine
5	-olane	-ole	-olidine
6	-inane	-ine	
7	-epane	-epine	
8	-ocane	-ocine	
9	-onane	-onine	
10	-ecane	-ecine	

Rings With More Than One Heteroatom

Two or more similar atoms contained in a ring are indicated by the prefixes '*di-*', '*tri*', *etc.*

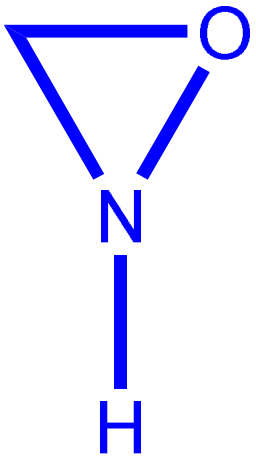


1,3,5-Triazine

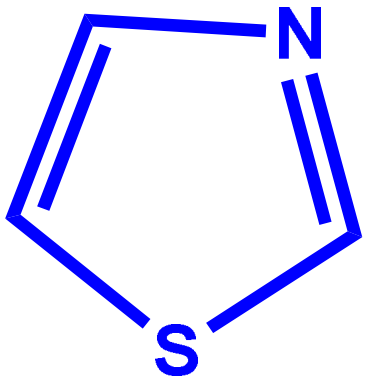


1,2,4 - Triazole

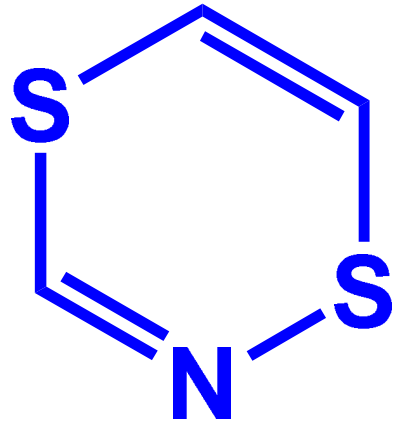
If more than one hetero atom occur in the ring, then the heterocycle is named by combining the appropriate prefixes with the ending in Table I in order of their preference, O > S > N.



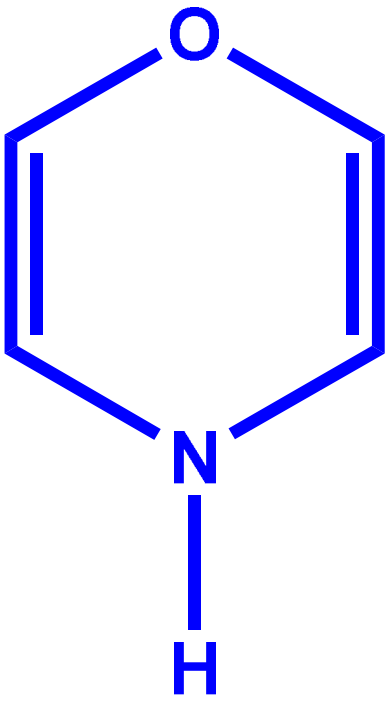
Oxaziridine



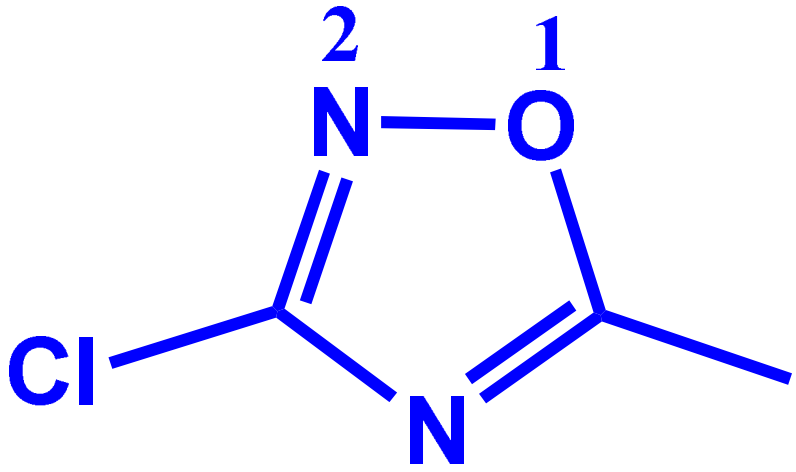
1,3-Thiazole
(Thiazole)



1,4,2 - Dithiazine

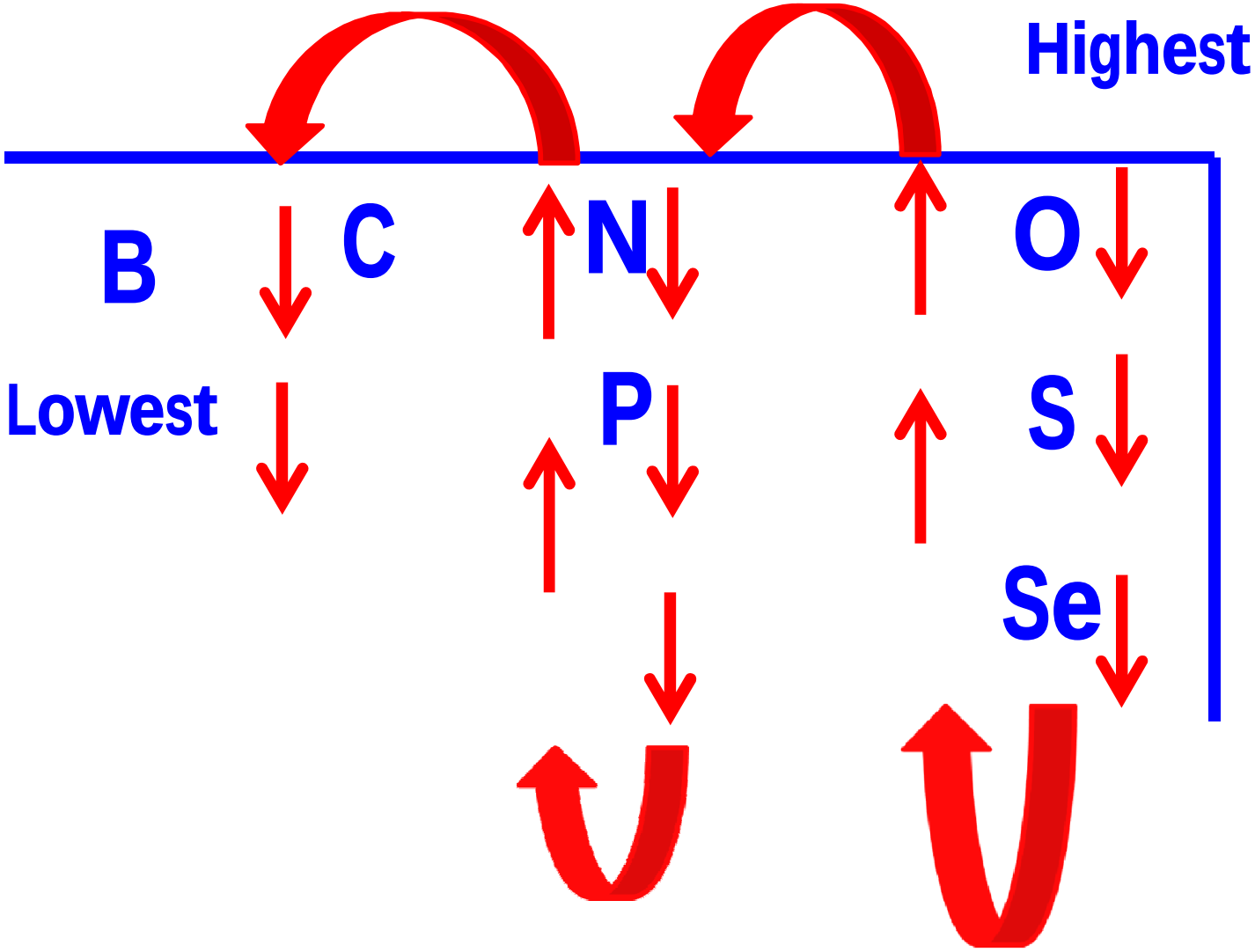


1,4-Oxazine

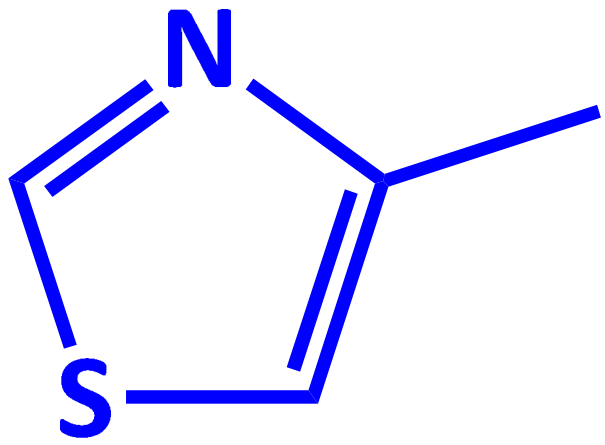


3-chloro-5-methyl-1,2,4-oxadiazole

Priority of heteroatoms for numbering purposes:



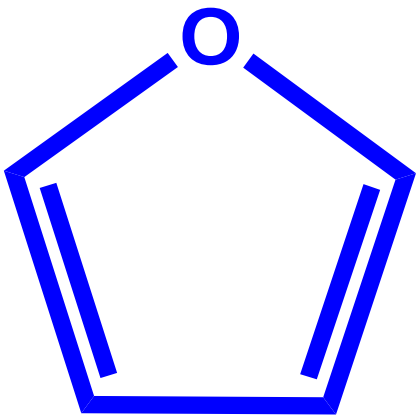
The ring is numbered from the atom of preference in such a way so as to give the smallest possible number to the other hetero atoms in the ring. As a result the position of the substituent plays no part in determining how the ring is numbered in such compounds.



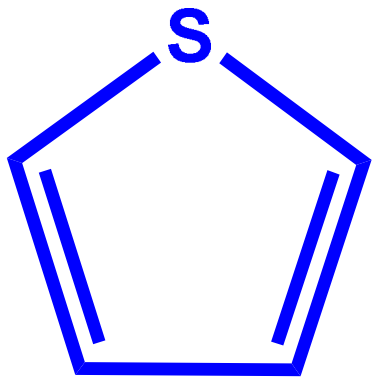
4-Methyl-1,3-thiazole

II. Common Names

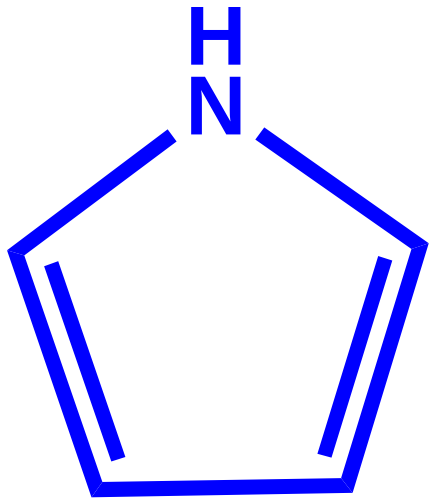
There are a large number of important ring systems which are named widely known with their non-systematic or common names.



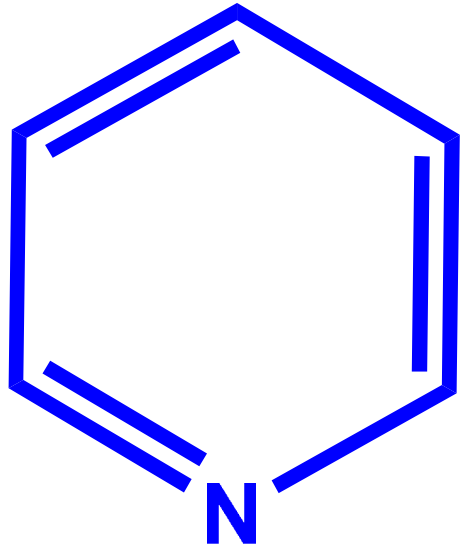
Furan



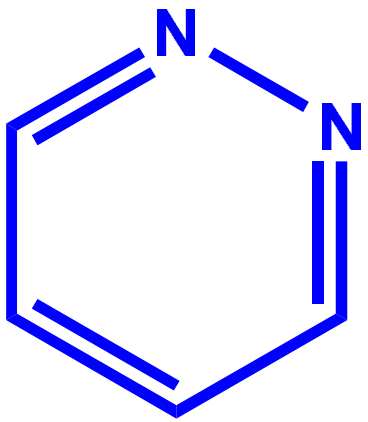
Thiophene



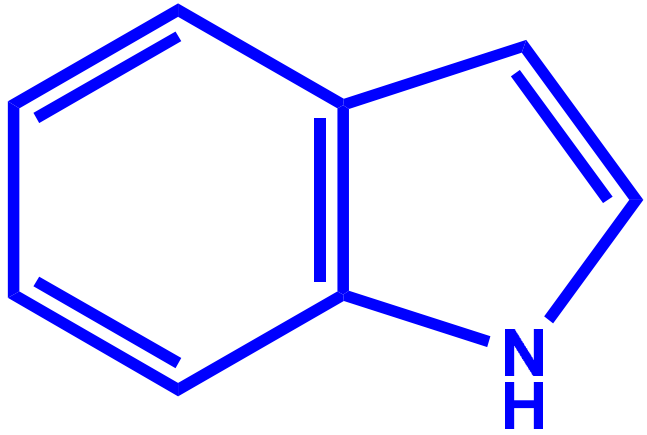
Pyrrole



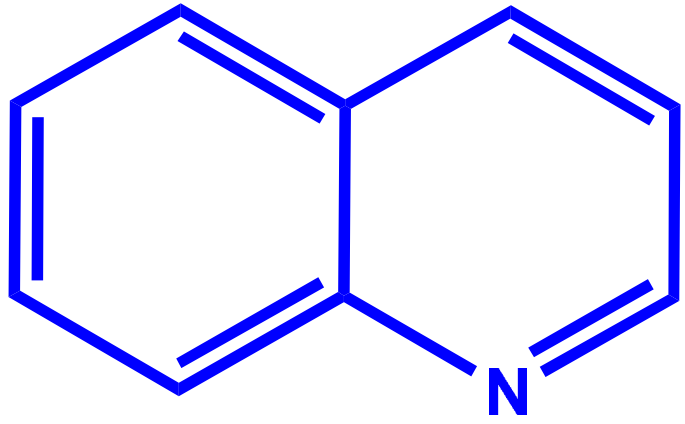
Pyridine



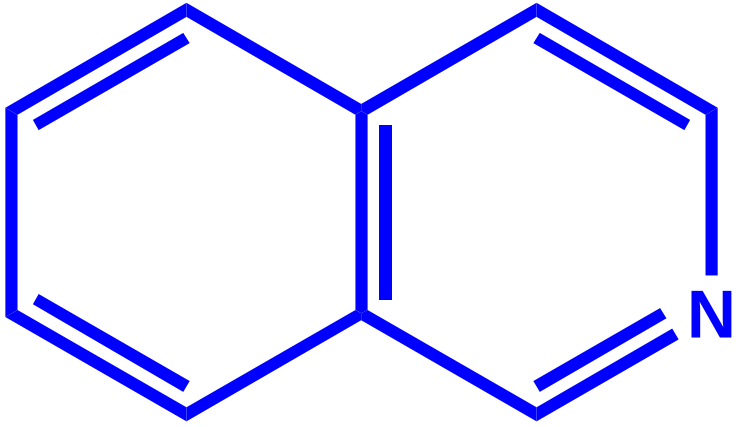
Pyridazine



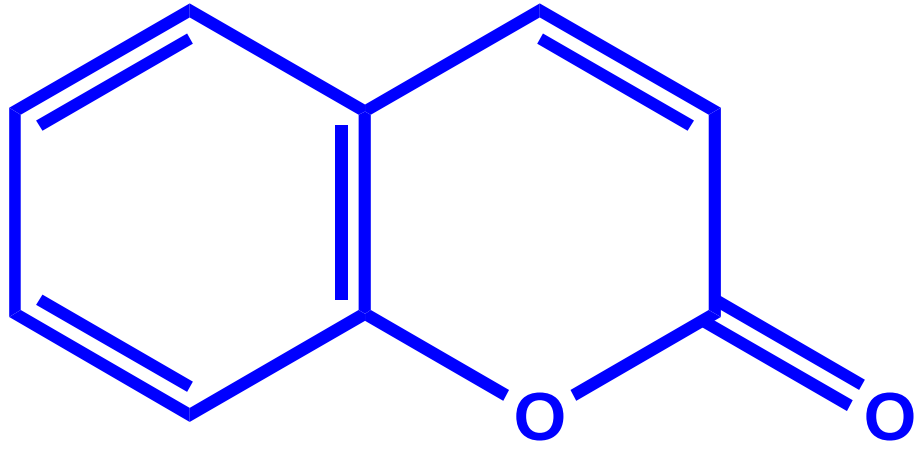
Indole



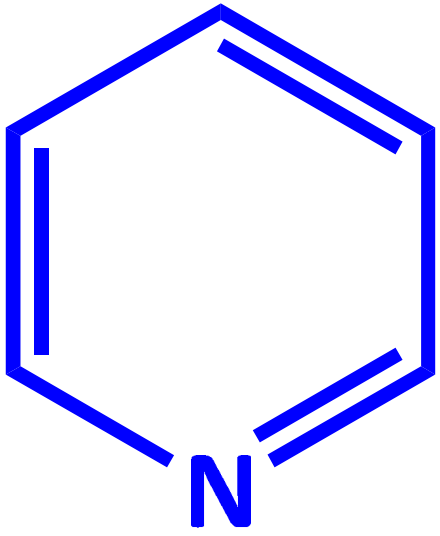
Quinoline



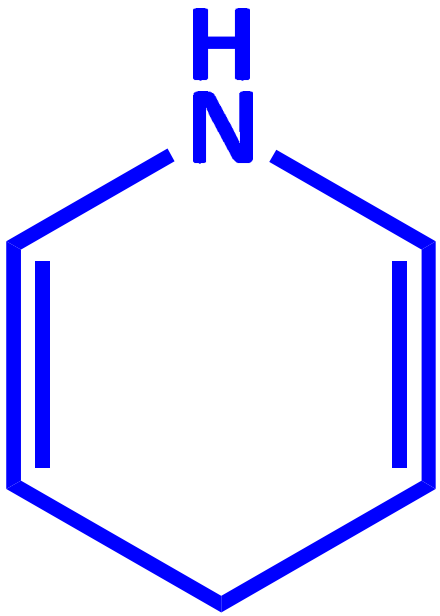
Isoquinoline



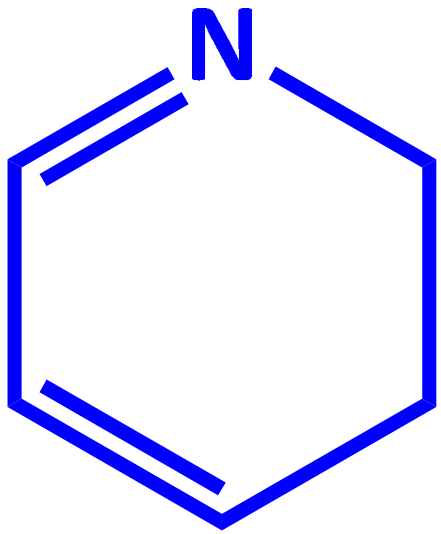
Coumarin



Pyridine



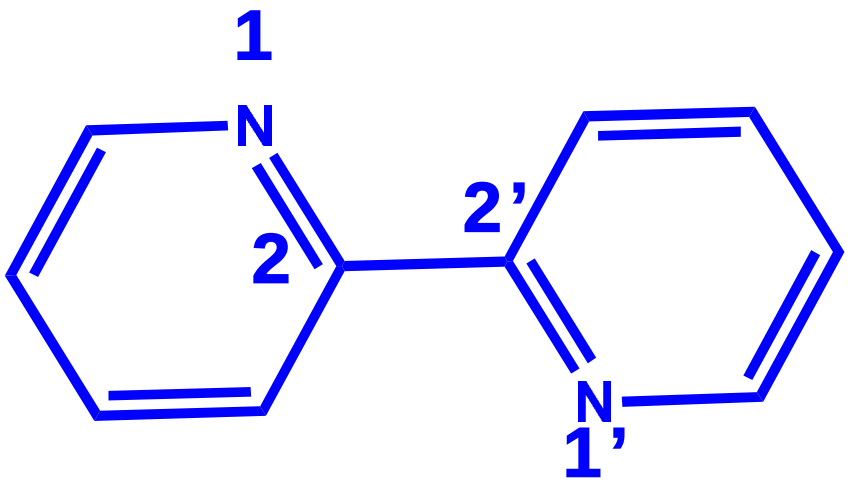
1,4-Dihydropyridine



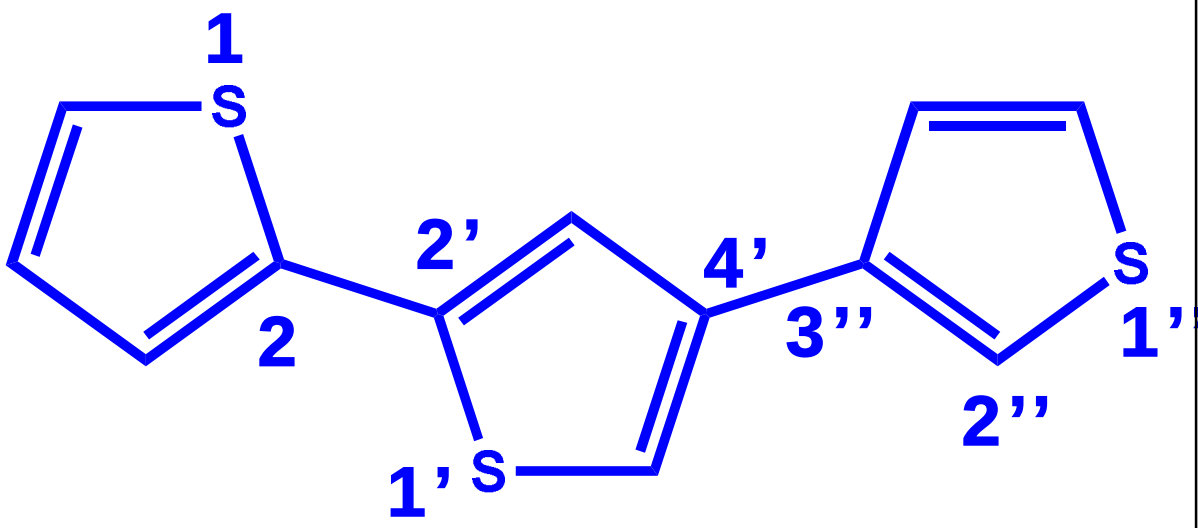
2,3-Dihydropyridine

Identical systems connected by a single bond

Such compounds are defined by the prefixes bi-, tert-, quater-, etc., according to the number of systems, and the bonding is indicated as follows:



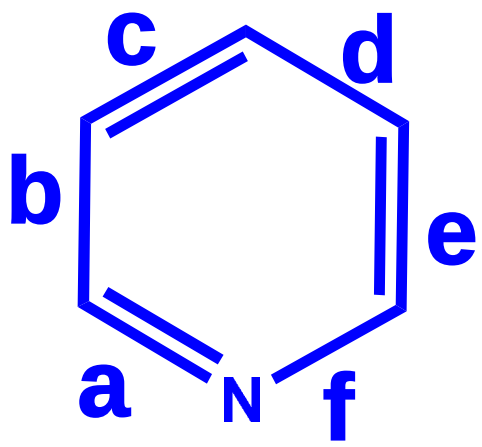
2,2' - Bipyridine



2,2': 4',3'' - Terthiophene

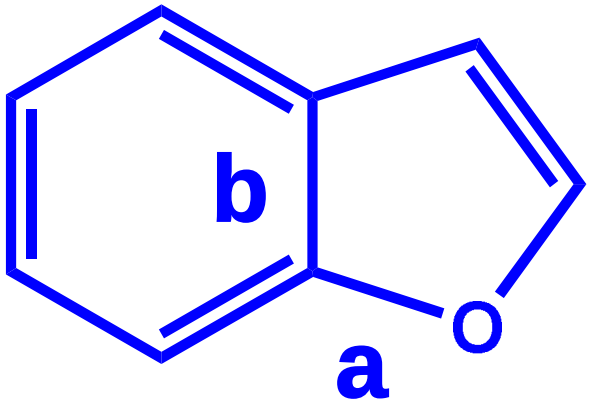
Naming Hetrocycles with fused rings

When naming such compounds the side of the heterocyclic ring is labeled by the letters a, b, c, etc., starting from the atom numbered 1. Therefore side *'a' being between atoms 1 and 2, side 'b' between atoms 2 and* 3, and so on as shown below for pyridine.

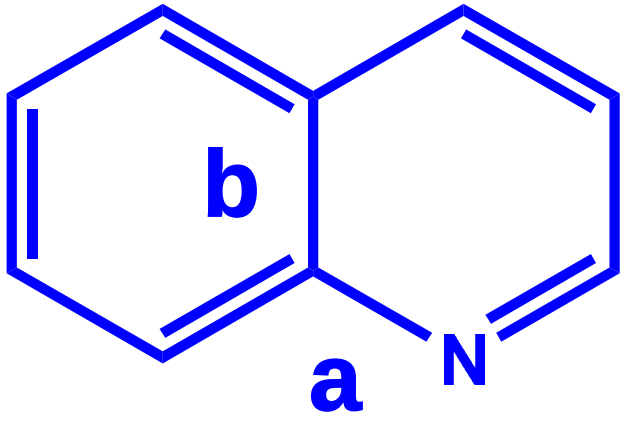


Pyridine

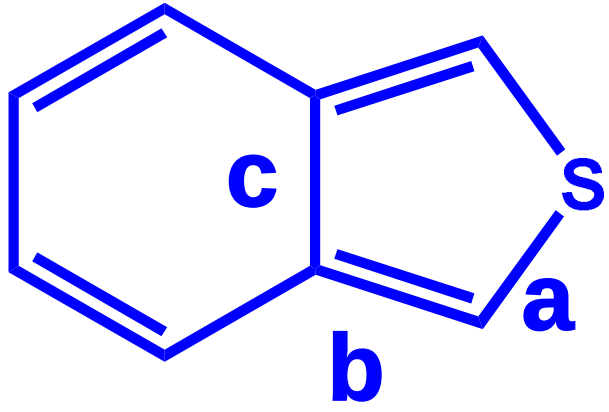
The name of the heterocyclic ring is chosen as the parent compound and the name of the fused ring is attached as a prefix. The prefix in such names has the ending *'o', i.e., benzo, naphtho and so on.*



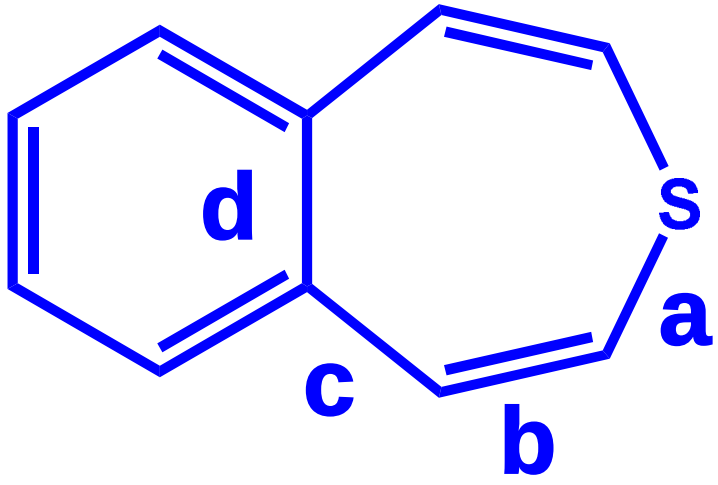
Benzo [b] furan



Benzo [b] pyridine

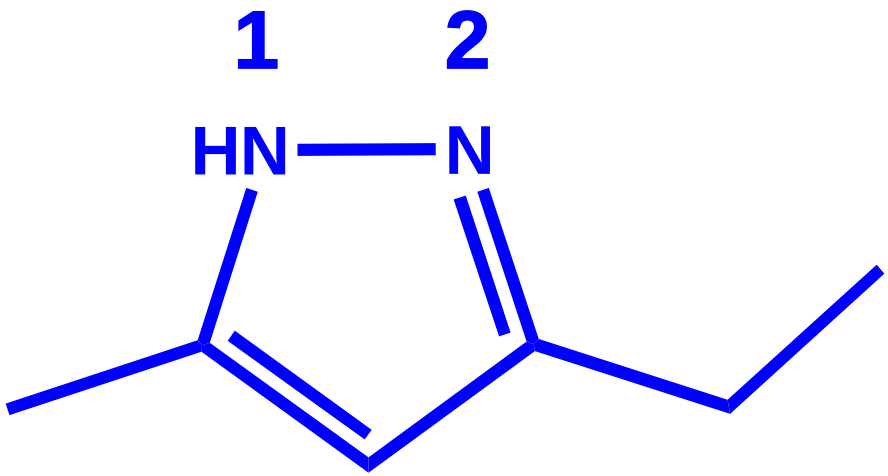


Benzo [c] thiophene

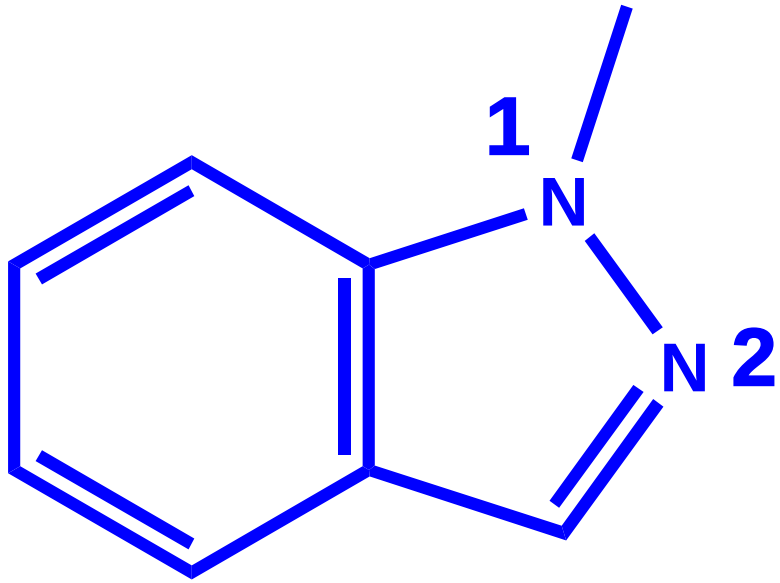


Benzo [d] thiepine

In a heterocyclic ring, other things being equal, numbering preferably commences at a saturated rather than at an unsaturated hetero atom.



3-Ethyl-5-methylpyrazole



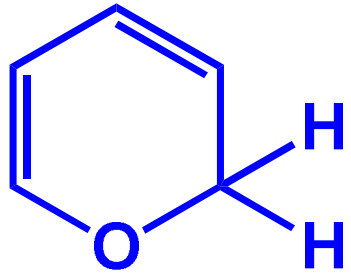
1-Methylindazole

Handling the “Extra Hydrogen”

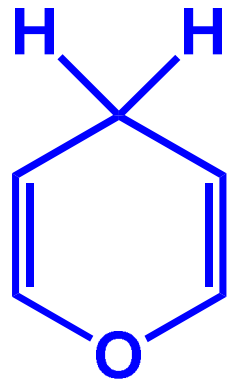
Heterocycles with maximum number of double bonds which can be arranged in more than one way.

Examples

Pyrans



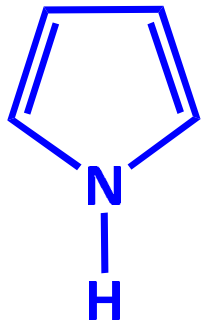
Double bonds @ 2 and 4

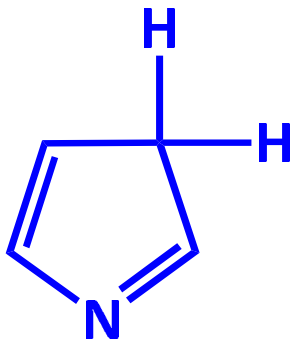


Double bonds @ 2 and 5

Pyrroles

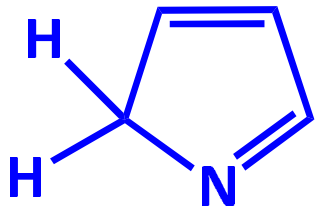
Double bonds @ 2 and 4





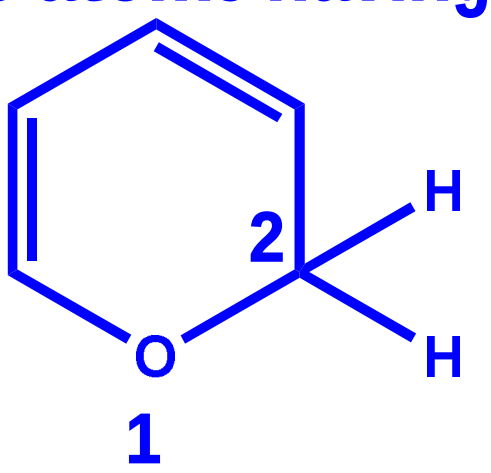
Double bonds @ 1 and 4

Double bonds @ 1 and 3

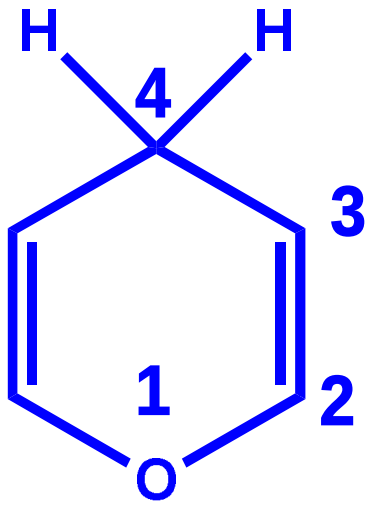


Therefore, should have different names.

This is a special problem resulting from isomerism in the position of the double bonds which is sometimes referred to as "extra-hydrogen" and this can be addressed by simply adding a prefix that indicates the number of the ring atom that possesses the hydrogen using *italic capital '1H' '2H' '3H', etc. The* numerals indicate the position of these atoms having the extra hydrogen atom.

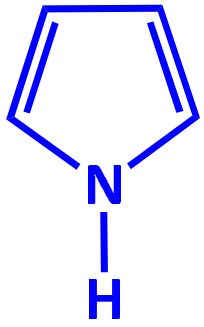


2*H*-Pyran

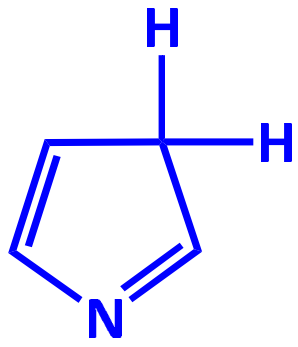


4*H*-Pyran

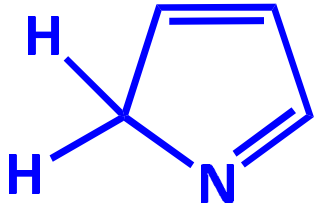
The saturated position takes priority in numbering.



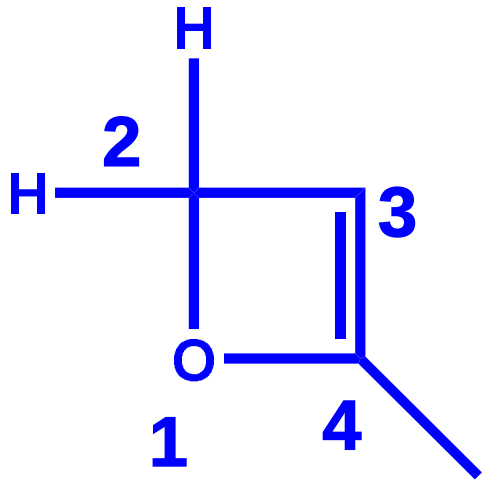
1*H*-Pyrrole (Pyrrole)



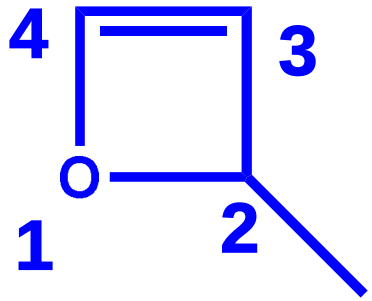
3*H*-Pyrrole



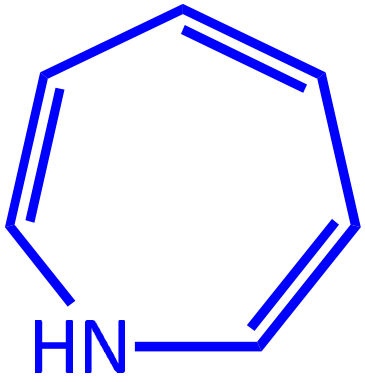
2*H*-Pyrrole



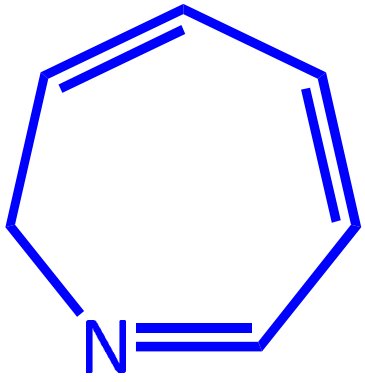
4-Methyl-*2H*-oxete



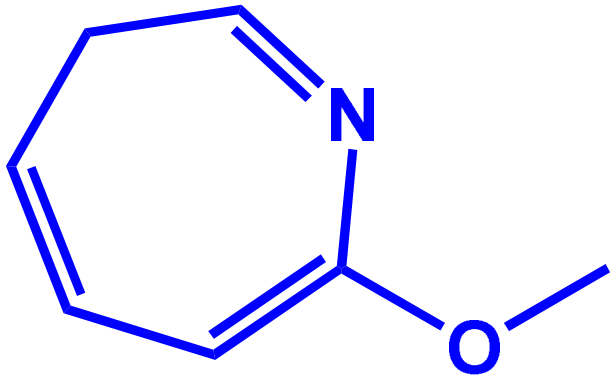
2-Methyl-*2H*-oxete



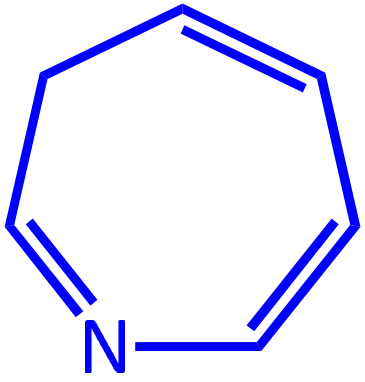
Azepine



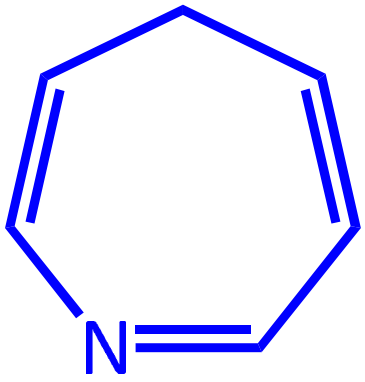
2*H*-Azepine



7-Methoxy-3*H*-azepine



3*H*-Azepine



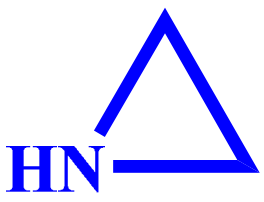
4*H*-Azepine

III. The Replacement Nomenclature

In replacement nomenclature, the heterocycle's name is composed of the carbocycle's name and a prefix that denotes the heteroatom.

Thus, "aza", "oxa", and "thia" are prefixes for a nitrogen ring atom, an oxygen ring atom, and a sulfur ring atom, respectively.

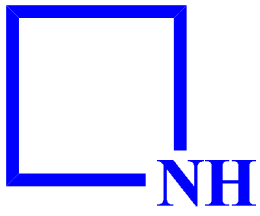
Notice that heterocyclic rings are numbered so that the heteroatom has the lowest possible number.



Azacyclopropane

or

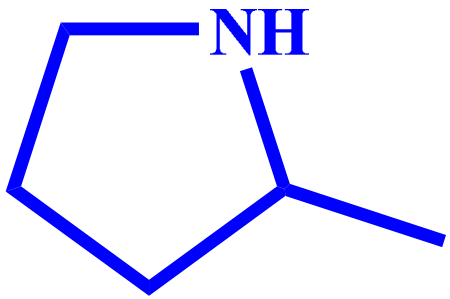
Aziridine



Azacyclobutane

or

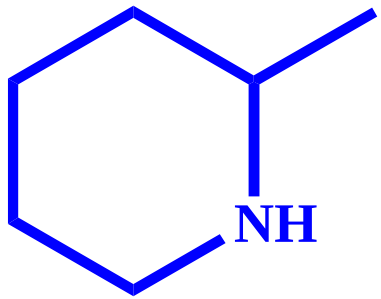
Azetidine



2-Methylazolidine

or

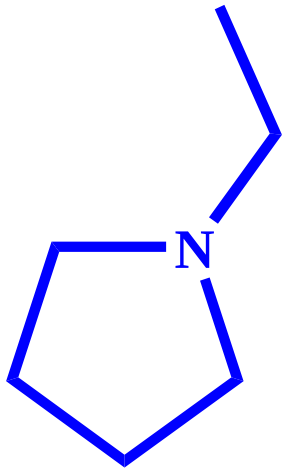
2-Methylazacyclopentane



2-Methylazacyclohexane

or

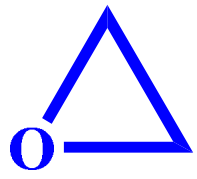
2-Methylpiperidine



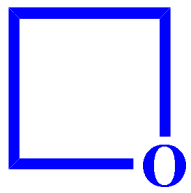
N-Ethylazacyclopentane

or

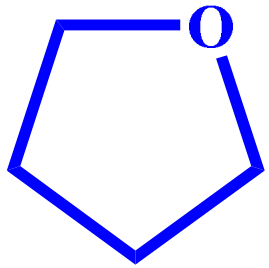
N-Ethylpyrrolidine



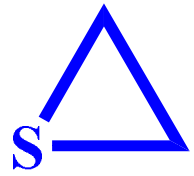
Oxacyclopropane
or
Oxirane
or
Ethyleneoxide



Oxacyclobutane
or
oxetane



Oxacyclopentane
or
Tetrahydrofuran



Thiacyclopropane
or
Thiirane