



Nomenclature of Heterocyclic Compounds Part 1



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Recommended Textbook:

Heterocyclic Chemistry, 5th Edition, J. A. Joule, K. Mills, **2010**, Wiley

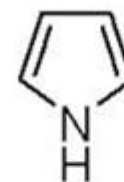
Nomenclature of Heterocyclic Compounds

- Early discovered heterocycles were received **common/trivial names**
- With millions of compounds to deal with, convenient, generally accepted systems must be available for the naming of the compounds
- Highly versatile system was created by **A. Hantzsch** in 1887 and independently by **O. Widman** in 1888 for the naming of 5- and 6-membered rings containing nitrogen
- The system was later applied to different ring sizes and to rings with other heteroatoms; it is now known as the **Hantzsch–Widman system**
- For instance; these 3 heterocyclics have common/trivial name in **bold** and systematic names beneath in *italic*



furan

oxzole



1H-pyrrole

azole

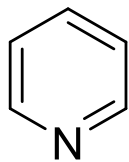


thiophene

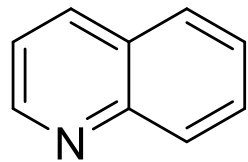
thiole

Common Names of Heterocyclic Compounds

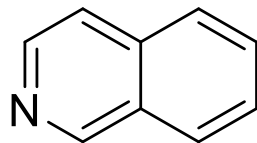
Lecture 4



pyridine

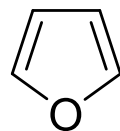


quinoline

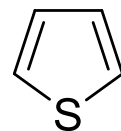


isoquinoline

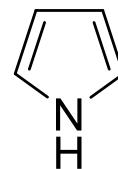
Lecture 5



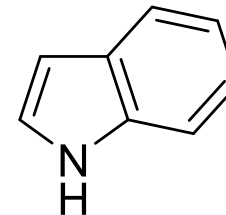
furan



thiophene

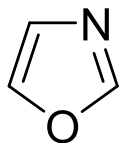


pyrrole

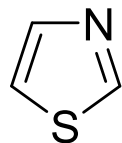


indole

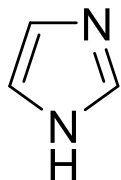
Lecture 6



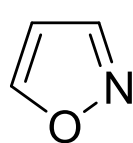
oxazole



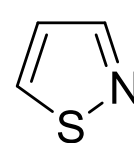
thiazole



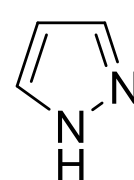
imidazole



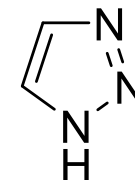
isoxazole



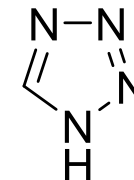
isothiazole



pyrazole



triazole



tetrazole

2nd half of the course



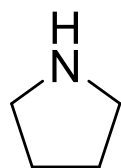
oxirane



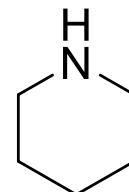
thiirane



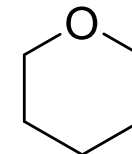
aziridine



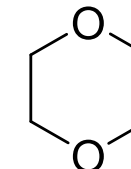
pyrrolidine



piperidine



tetrahydropyran



dioxane

Systematic Naming of Monocyclic Compounds

The systematic names from the **Hantzsch–Widman naming system** can be derived using the following **four rules**:

Rule #1 The **heteroatom** is given a name and is used as a **prefix**

Element	oxygen	sulfur	selenium	nitrogen	phosphorous	silicon	boron
Valence	II	II	II	III	III	IV	III
Prefix	Oxa	Thia	Selena	Aza	Phospha	Sila	Bora

- If there are more than one heteroatoms in a ring, the **priority order** is from left to right in the table
- The “a” ending is dropped if the next syllable starts with a **vowel**
example: “**aza-irine**” is properly written “**azirine**”

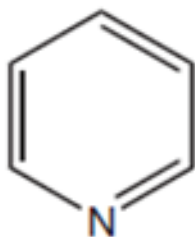
Systematic Naming of Monocyclic Compounds

Rule #2: Ring size is designated by **stems** that follow the prefix:

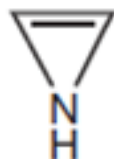
Ring Size	3	4	5	6	7	8	9
Stems	-ir-	-et-	-ol-	-in-	-ep-	-oc-	-on-

Rule #3 If the ring is **fully unsaturated**, the name is concluded with a **suffix** for ring size:

- 3 atoms, **-ene** (except **-ine** for **N**)
- 4, 5, and 6 atoms, **-e**
- 7, 8, and 9 atoms, **-ine**



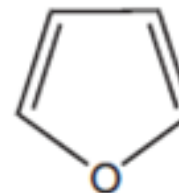
azine



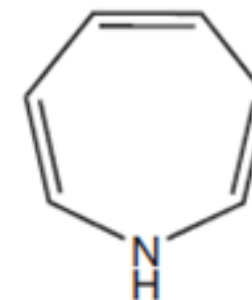
azirine



thiete



oxole



azepine

Systematic Naming of Monocyclic Compounds

Rule #4:

If **fully saturated**, the name is concluded with a **suffix** for ring size:

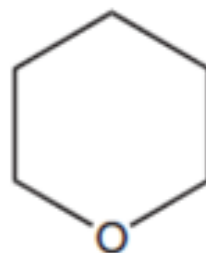
- the suffix is **-ane** for all ring sizes,
- except for **N** which uses **-idine** for rings of **3, 4, or 5** atoms, and for **6** atoms, a prefix of **hexahydro-** is used.
- the name oxane, not oxinane, is used for the 6-membered ring with O present



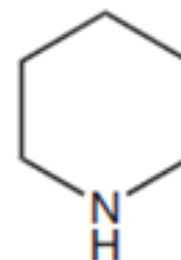
oxirane



azetidine



oxane



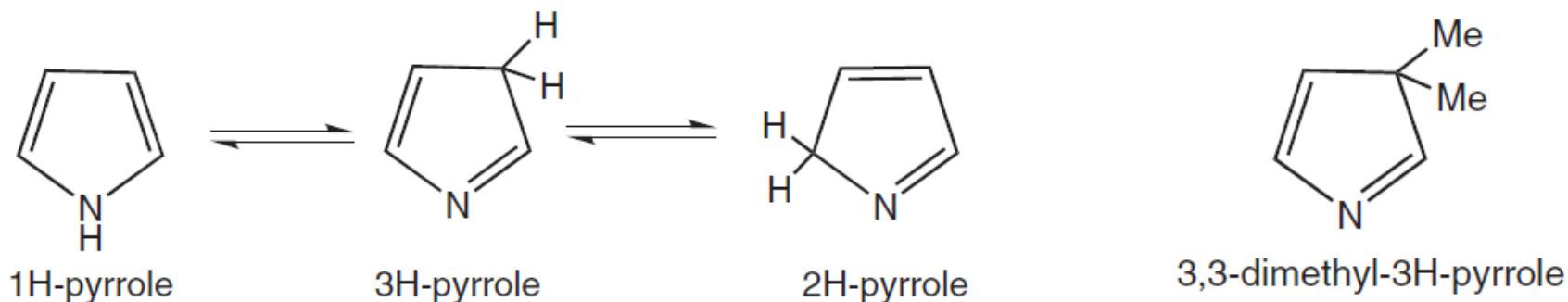
hexahydropyridine

Exceptions: there are several exceptions and modifications to accommodate conflicts with prior usage!

Systematic Naming of Monocyclic Compounds

The Extra Hydrogen

- There is a special problem resulting from **isomerism** in certain heterocyclic systems that requires clarification in the name
- simply adding a prefix that indicates the number of the ring atom that possesses the hydrogen, thus, **1H**, **2H**, and **3H**
- Consider the case of **pyrrole**: There are actually two additional isomeric forms that result from apparent 1,3-shifts of hydrogen

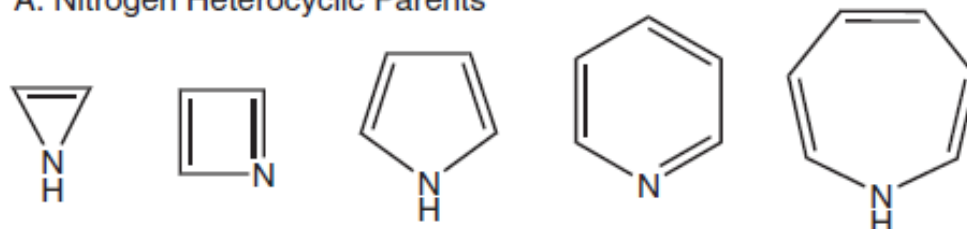


- The extra-hydrogen problem can occur in any ring system of **nitrogen** containing an **odd** number of ring atoms or **oxygen** containing **even** number of ring atoms

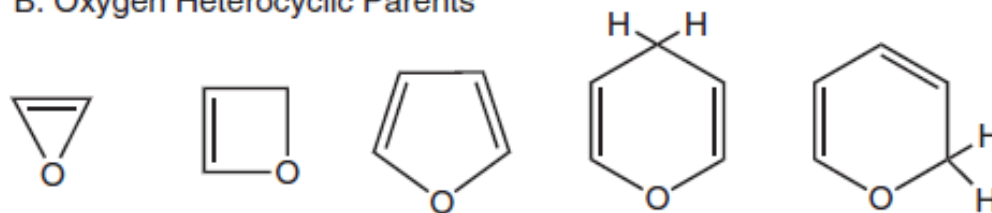
Systematic Naming of Monocyclic Compounds

Examples

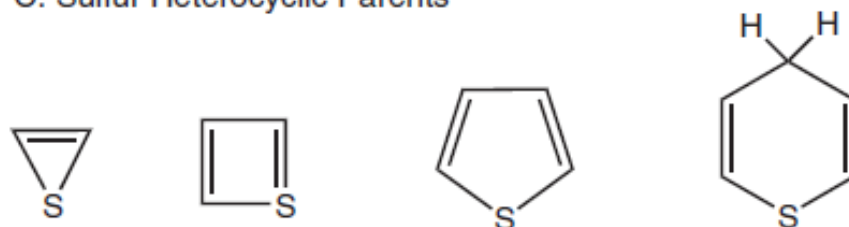
A. Nitrogen Heterocyclic Parents



B. Oxygen Heterocyclic Parents



C. Sulfur Heterocyclic Parents



D. Some Saturated Rings

