

Hetrocyclic compoud

B.Sc.-III Chemistry(H/S)

Organic chemistry

Paper- VII

Lecture-04

By

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Key points:

- ❖ Heterocyclic compounds are cyclic compounds with the ring containing carbon and other element, such as oxygen, nitrogen and sulfur.
- ❖ Heterocyclic compounds have one or more hetero atoms in their structure
- ❖ These five membered ring contains single heteroatoms.
- ❖ They may be cyclic or non cyclic in nature.
- ❖ The simple five membered heterocyclic compounds are pyrrole, furan and thiophene

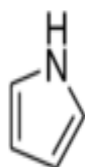
Note: The name of the heterocyclic ring is chosen as the parent compound and the name of the fused ring is attached as a prefix. The prefix in such names has the ending 'o', i.e., benzo, naphtho and so on.



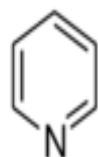
Furan



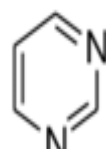
Thiophene



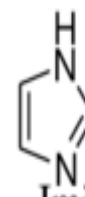
Pyrrole



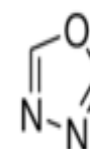
Pyridine



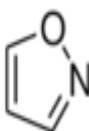
Pyrimidine



Imidazole



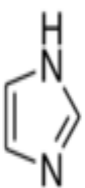
Oxadiazole



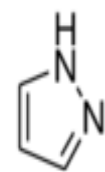
Isoxazole



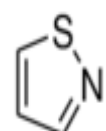
Oxazole



Imidazole



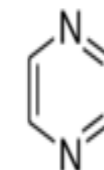
Pyrazole



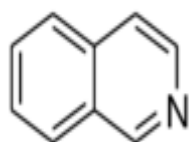
Isothiazole



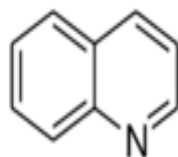
Thiazole



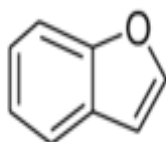
Pyrazine



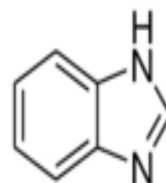
Isoquinoline



Quinoline



Benzofuran



Benzimidazole

Example of heterocyclic ring

Furan

Chemical Formula: C_4H_4O

Boiling point: 31.3 °C

Molar mass: 68.07 g/mol

Density: 936 kg/m³

Melting point: -85.6 °C

Point group: C_{2v}

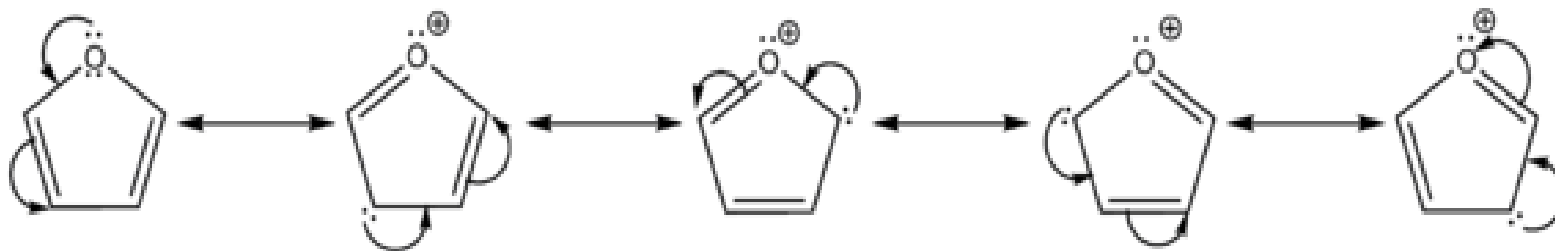
- ❖ **Furan** is a heterocyclic organic compound, consisting of a five-membered aromatic ring with four carbon atoms and one oxygen
- ❖ Furan is a colorless aromatic ring
- ❖ It is Flammable in nature
- ❖ It is highly volatile liquid and its boiling point is very close to room temperature.
- ❖ It is soluble in common organic solvents, including alcohol, ether and acetone
- ❖ It is slightly soluble in water.
- ❖ Its odor is "strong, ethereal; chloroform-like".
- ❖ It is toxic and may be carcinogenic in humans.

Application:

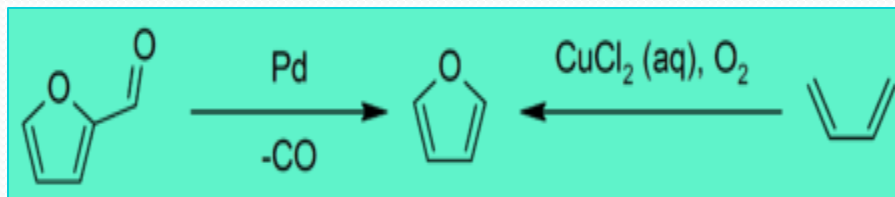
- ❖ Heterocyclic compounds have a wide range of application.
- ❖ They are predominantly used as **pharmaceuticals**, as **agrochemicals** and as **veterinary product**
- ❖ Furan is used as a starting point for other chemicals.

Resonating structure of furan

The resonating structure shows the increased electron density of the ring, leading to increased rates of electrophilic substitution in many chemical reaction.



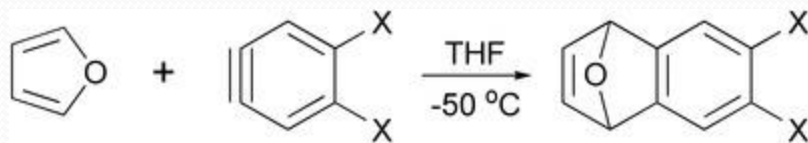
Furan is manufactured by the palladium-catalyzed decarbonylation of furfural, or by the copper-catalyzed oxidation of 1,3-butadiene



Reaction of furan

Diels-Alder reaction of furan

When furan reacts with arynes then it give corresponding derivatives of **dihydronaphthalenes**, which are useful intermediates in synthesis of other polycyclic aromatic compounds.



Hydrogenation

Hydrogenation of furans sequentially affords **dihydrofurans** and **tetrahydrofurans**.

Chemistry of Furan

- ❖ Furan is aromatic because one of the lone pairs of electrons on the oxygen atom is delocalized into the ring
- ❖ It follows Huckel's rule ($4n + 2$) aromatic system similar to benzene.
- ❖ Due to this aromaticity, the molecule is flat and lacks discrete double bonds.
- ❖ The other lone pair of electrons of the oxygen atom extends in the plane of the flat ring system.
- ❖ Due to sp^2 hybridization, one of the lone pairs of oxygen is reside in a p orbital and thus allow it to interact within the π system.
- ❖ Due to its aromaticity, furan's behavior is quite different to that of heterocyclic tetrahydrofuran.
- ❖ Furan is significantly more reactive than benzene in electrophilic substitution reactions because of the increased electron density of the ring.
- ❖ Due to the electron-donating effects of the oxygen heteroatom, rate of electrophilic substitution is increased.

Synthesis of Furan in the laboratory,

- Furan can be prepared from **furfural** by oxidation to **2-furoic acid**, followed by decarboxylation
- It can also be prepared directly by thermal decomposition of pentose-containing materials, and cellulosic solids, especially pine wood.

Reactivity

- Thiophene is considered to be aromatic, but theoretical calculations suggest that the degree of aromaticity is less than that of benzene.
- The “Lone pairs” on sulfur are significantly delocalized in the pi electron system. As a result of this , thiophene does not show the properties which is seen in conventional sulfides.

For example, the sulfur atom resists alkylation and oxidation.



Problem for Practice:

Q1. why is furan aromatic?

Q2. what is furan used for?