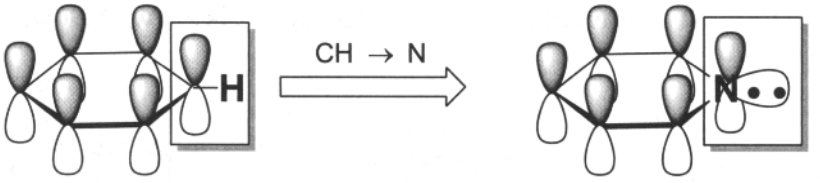
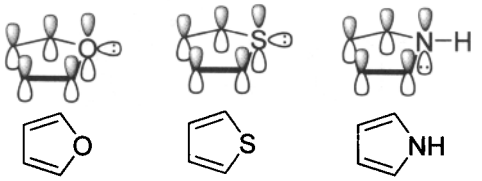
1.2 Aromaticity of Heterocycles



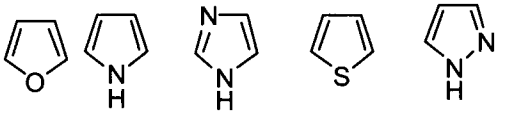
benzene pyridine

The major thrust of this book is aromatic heterocycles. According to Hückel's rule of aromaticity, a cyclic ring molecule is aromatic when the number of its π-electrons equals 4n + 2, where n is zero or any positive integer. The most common aromatic compound is benzene, which has 4 + 2 = 6 π-electrons. Pyridine, an electron-deficient aromatic heterocycle, also has 6 π-electrons. In comparison with benzene, pyridine has an additional lone pair of electrons at the nitrogen atom after it contributes a pair of two electrons to make up the 6 π-electrons for aromaticity. These lone pair electrons are responsible for much of pyridine's unique physical and chemical properties. On the other hand, furan, an electron-excessive aromatic heterocycle also with 6 π-electrons, is different from both benzene and pyridine. The oxygen atom has two lone pairs of electrons, one of which contributes to the 6 π-electrons to achieve the aromaticity. The second pair of electrons is located in an sp^2 hybrid orbital in the plane of the furan ring. Thiophene is similar to furan in its aromaticity although thiophene is more "aromatic" because the S atom is larger than the O atom.



furan thiophene pyrrole

The relative aromaticity of common heterocycles is shown below:



furan	pyrrole	imidazole	thiophene	pyrazole
12	31	43	45	61