1 Introduction

What should you know already ?

From first year chemistry courses you should have a basic appreciation of some of the simpler models for bonding in molecules - these ideas and concepts are also covered in the following excellent book:

Chemical Bonding , by Mark J. Winter (Oxford Chemistry Primer 15)
Oxford Science Publications ISBN 0 19 855694 2

If you have not taken an introductory course in *Chemical Bonding* (and perhaps even if you have) then you are strongly advised to obtain a copy of the above book and to carefully read through it.

Localized and Non-localized Approaches to Bonding

There are two main ways of trying to explain how the electrons of a molecule are involved in bonding.

1. *Localized bond approach* (also known as the *valence bond theory*) : involves regarding all bonds as localized interactions involving two electrons shared between two atoms. In polyatomic molecules this leads to the use of orbital *hybridization* as a convenient mathematical (and pictorial) procedure of manipulating the atomic orbitals to permit the bonding to be described in terms of a collection of simple two-centre, two-electron bonds.

2. *Molecular orbital approach* (also known as *MO theory*) : involves the assignment of electrons to molecular orbitals which are, in general, delocalized over the whole molecule.

Which approach is better ?

There is no straightforward answer to this question - neither approach is exact.

- In some instances, such as in the description of bonding in diatomic molecules, the two approaches give essentially identical results.
- The valence bond approach is the approach with which you will be most familiar - it is conceptually simpler and is widely used in organic chemistry, but it fails to adequately explain the bonding in certain classes of molecules, including aromatic compounds.
- The MO approach is generally harder to implement but better explains the bonding in those molecules where the valence bond approach fails, and is generally more consistent with the results of spectroscopic measurements.

This course will provide an introduction to the molecular orbital approach.