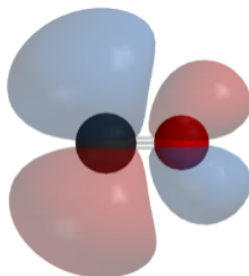


2.1: Prelude to Molecular Orbital Theory

Valence bond (VB) theory gave us a qualitative picture of chemical bonding, which was useful for predicting the shapes of molecules, bond strengths, etc. It fails to describe some bonding situations accurately because it ignores the wave nature of the electrons. Molecular orbital (MO) theory has the potential to be more quantitative. With it we can also get a picture of where the electrons are in the molecule, as shown in the image at the right. This can help us understand patterns of bonding and reactivity that are otherwise difficult to explain.

Although MO theory in principle gives us a way to calculate the energies and wavefunctions of electrons in molecules very precisely, usually we settle for simplified models here too. These simple models do not give very accurate orbital and bond energies, but they do explain concepts such as resonance (e.g., in the ferrocene molecule) that are hard to represent otherwise. We can get more accurate energies from MO theory by computational "number crunching." While MO theory is more correct than VB theory and can be very accurate in predicting the properties of molecules, it is also rather complicated even for fairly simple molecules. For example, you should have no trouble drawing the VB pictures for CO, NH₃, and benzene, but we will find that these are increasingly challenging with MO theory.



The lowest unoccupied molecular orbital of the carbon monoxide molecule is a π antibonding orbital that derives from the 2p orbitals of carbon (left) and oxygen (right)

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