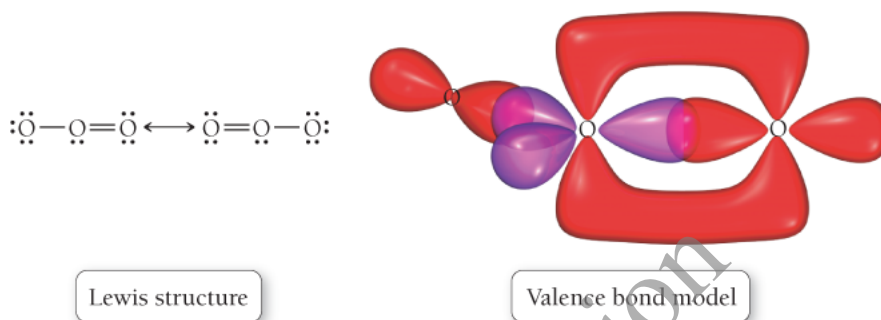
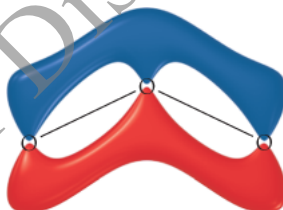


6.5: Molecular Orbital Theory: Polyatomic Molecules

With the aid of computers, we can apply molecular orbital theory to polyatomic molecules and ions, yielding results that correlate very well with experimental measurements. These applications are beyond the scope of this text. However, the delocalization of electrons over an entire molecule is an important contribution of molecular orbital theory to our basic understanding of chemical bonding. For example, consider the Lewis structure and valence bond diagram of ozone:

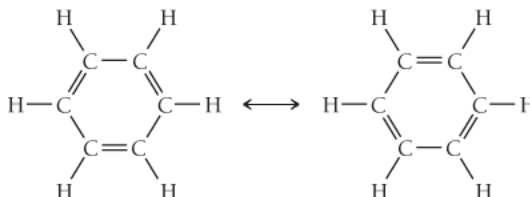


In the Lewis model, we use resonance forms to represent the two equivalent bonds. In valence bond theory, it appears that the two oxygen–oxygen bonds differ from each other. Molecular orbital theory, however, indicates that the π molecular orbitals in ozone form from a linear combination of the three oxygen 2p orbitals and are delocalized over the entire molecule. The lowest energy π bonding molecular orbital in ozone is shown here:



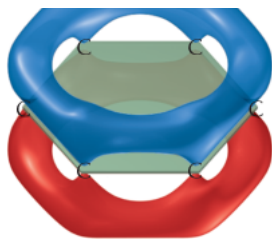
When we examine ozone in nature, we indeed find two equivalent bonds.

A similar situation occurs with benzene (C_6H_6). In the Lewis model, we represent the structure with two resonance forms:



In molecular orbital theory, the π molecular orbitals in benzene form from a linear combination of the six carbon 2p orbitals and delocalize over the entire molecule. The lowest energy π bonding molecular orbital is shown here:





Benzene is in fact a highly symmetric molecule with six identical carbon–carbon bonds. The most accurate picture of the π electrons in benzene is one in which the electrons occupy roughly circular-shaped orbitals above and below the plane of the molecule in accordance with the molecular orbital theory approach.

Conceptual Connection 6.4 What Is a Chemical Bond? Part II

Interactive

Not for Distribution