Chemical Bonding and Molecular Structure

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4.1 Kössel-Lewis Approach to Chemical Bonding

- Electrons occupy specific energy levels within an atom.
- Atoms aim to attain a stable octet or electronic configuration of eight electrons in their valence shell (for elements in period 2).
- Metals tend to lose electrons and form positively charged ions, while non-metals tend to gain electrons and form negatively charged ions.
- The attraction between oppositely charged ions forms an ionic bond.

4.2 Ionic or Electrovalent Bond

- A chemical bond formed by the complete transfer of valence electrons from a metal atom to a non-metal atom.
- The metal atom becomes a positively charged metal ion, and the non-metal atom becomes a negatively charged non-metal ion.
- The electrostatic attraction between these ions holds the compound together.
- Examples:
  - Sodium chloride (NaCl): Sodium atom loses an electron to Chlorine atom, forming Na^+ and Cl^- ions.
  - Potassium oxide (K_2O): Potassium atom loses an electron to Oxygen atom, forming K^+ and O^{2-} ions.

4.3 Bond Parameters

- **Bond Length:** The distance between the nuclei of two bonded atoms. Shorter bond lengths indicate stronger bonds.
- **Bond Strength:** The energy required to break a bond. Stronger bonds correspond to higher bond energies.
- **Bond Order:** The number of shared electron pairs between two atoms. Higher bond orders indicate stronger bonds.
- **Bond Enthalpy:** The change in enthalpy when a bond is formed. Negative values indicate exothermic bond formation, while positive values indicate endothermic bond formation.

4.4 The Valence Shell Electron Pair Repulsion (VSEPR) Theory

- VSEPR theory predicts the molecular geometry of a molecule based on the number of valence electron pairs surrounding the central atom.
- Valence electron pairs repel each other, leading to a geometry that minimizes repulsion.
- The basic shapes predicted by VSEPR theory are:
  - **Linear:** 2 pairs
  - **Trigonal planar:** 3 pairs
  - **Tetrahedral:** 4 pairs
  - **Trigonal pyramidal:** 5 pairs
  - **Octahedral:** 6 pairs

4.5 Valence Bond Theory

- Explains the formation of covalent bonds by the overlap of atomic orbitals
- Overlap of orbitals results in the formation of sigma bonds, pi bonds, and lone pairs of electrons
- Sigma bonds are formed by head-to-head overlap of atomic orbitals & pi bonds are formed by lateral overlap of p-orbitals
- The strength of a covalent bond depends on the extent of orbital overlap
- Hybridisation of atomic orbitals can lead to stronger covalent bonds

4.6 Hybridisation

- Mixing of atomic orbitals to form new orbitals with different shapes and energies
- Hybridisation occurs when atomic orbitals overlap to form covalent bonds
- The type of hybridisation depends on the number and type of atomic orbitals involved
- Common types of hybridisation include:
  - sp^3 hybridisation: mixing of one s and three p orbitals, resulting in four equivalent hybrid orbitals with tetrahedral geometry (e.g., CH_4)
  - sp^2 hybridisation: mixing of one s and two p orbitals, resulting in three equivalent hybrid orbitals with trigonal planar geometry (e.g., C_2H_4)
  - sp hybridisation: mixing of one s and one p orbital, resulting in two equivalent hybrid orbitals with linear geometry (e.g., $BeCl_2$)
- Hybridisation helps to explain the geometry and bonding of molecules

4.7 Molecular Orbital Theory

- Molecular orbital theory (MOT) describes the electronic structure of molecules using the concept of molecular orbitals (MOs).
- MOs are mathematical functions that describe the wave-like behavior of electrons in molecules.
- Each MO represents a region of space where the probability of finding an electron is high.
- MOs are formed by the combination of atomic orbitals of the constituent atoms.
- The combination of atomic orbitals can lead to the formation of both bonding and antibonding molecular orbitals.
- Bonding MOs have lower energy than the individual atomic orbitals and result in a stabilization of the molecule.
- Antibonding MOs have higher energy than the atomic orbitals and result in a destabilization of the molecule.

4.8 Bonding in Some Homonuclear Diatomic Molecules

- **Homonuclear diatomic molecules** are molecules that consist of two identical atoms.
- **Bond order** is a measure of the strength of a chemical bond and is calculated as half the difference between the number of bonding and antibonding electrons.
- **Hydrogen (H2)**:
  - Has a bond order of 1 and is formed by the overlap of two 1s orbitals.
  - The molecular orbital diagram consists of a bonding σ1s MO and an antibonding σ1s* MO.

- **Helium (He_2)**:
  - Has a bond order of 0 and is not stable as a molecule.
  - The molecular orbital diagram consists of a bonding σ1s MO and an antibonding σ1s* MO that are degenerate (equal in energy).
- **Lithium (Li_2)**:
  - Has a bond order of 1 and is formed by the overlap of two 2s orbitals.
  - The molecular orbital diagram consists of a bonding σ2s MO and an antibonding σ2s* MO.
- **Nitrogen (N_2)**:
  - Has a bond order of 3 and is formed by the overlap of two 2p orbitals.
  - The molecular orbital diagram consists of a bonding σ2p MO, two nonbonding π2p MOs, and an antibonding σ2p* MO.
- **Oxygen (O_2)**:
  - Has a bond order of 2 and is formed by the overlap of two 2p orbitals.
  - The molecular orbital diagram consists of a bonding σ2p MO, two nonbonding π2p MOs, an antibonding σ2p MO, and two antibonding π2p MOs.

4.9 Hydrogen Bonding

Hydrogen bonding is a special type of dipole-dipole interaction that occurs between a hydrogen atom covalently bonded to a highly electronegative atom (such as O, N, or F) and another electronegative atom. It is a relatively strong intermolecular force that can have a significant impact on the physical and chemical properties of substances.

- **Characteristics of Hydrogen Bonding:**
  - Involves a hydrogen atom covalently bonded to F, O, or N
  - Forms when a hydrogen atom donates a partial positive charge (δ+) to an electronegative acceptor atom (δ-)
  - Results in a strong electrostatic attraction between the partially charged atoms
- **Types of Hydrogen Bonding:**
  - **Intermolecular Hydrogen Bonding:** Occurs between molecules, such as water molecules or hydrogen fluoride molecules
  - **Intramolecular Hydrogen Bonding:** Occurs within a single molecule, usually forming a ring structure
- **Examples of Hydrogen Bonding:**
  - **Water:** The intermolecular hydrogen bonding between water molecules is responsible for its high boiling point and surface tension
  - **DNA:** The base pairs in DNA are held together by hydrogen bonds between adenine and thymine, and guanine and cytosine
  - **Proteins:** The folding and stability of proteins are influenced by hydrogen bonding between amino acid side chains
- **Effects of Hydrogen Bonding:**
  - **Physical Properties:** Hydrogen bonding affects melting points, boiling points, solubility, and viscosity of substances
  - **Chemical Properties:** Hydrogen bonding can influence reaction rates, equilibrium constants, and molecular structures