1.1 Atomic Structure

- Structure of an atom
  - Positively charged nucleus (very dense, protons and neutrons) and small (10^-15 m)
  - Negatively charged electrons are in a cloud (10^-10 m) around nucleus
- Diameter is about 2 \times 10^{-10} m (200 picometers (pm)) [the unit angstrom (Å) is 10^{-10} m = 100 pm]

![](image)

1.2 Atomic Structure: Orbitals

- Quantum mechanics: describes electron energies and locations by a wave equation
  - Wave function solution of wave equation
  - Each Wave function is an orbital, \( \psi \)
- A plot of \( \psi^2 \) describes where electron most likely to be
- Electron cloud has no specific boundary so we show most probable area
Atomic Orbitals

- Each orbital has a principle quantum number, \( n \), 1, 2, 3, etc., shell
- Second quantum number, \( l \), 0, 1, 2, 3, \( n-1 \), whose value gives the orbital shape
- Orbital shape is predicted mathematically by a probability function
- Orbitals are commonly known by letters, s, p, d, f

Orbital Characteristics

- S orbitals are spherical, are lowest in energy, and hold two electrons
- P orbitals are dumbbell shaped and each major energy shell has three
- All p orbitals in an energy level are of equal energy or degenerate
- P orbitals are oriented at right angles to each other
- Areas of low probability of finding an electron are called nodes
Electron Configurations

- **Aufbau Principle**
  - Places electrons in lowest energy orbitals first
  - Periodic table is assembled on this principle
- **Pauli Exclusion Principle**
  - Each orbital can hold two spin-paired electrons
- **Hund’s Rule**
  - When degenerate or equal energy orbitals exist, electrons are added to each orbital unpaired
- **Valence Electrons**
  - Electrons in outermost or highest energy level
  - Electrons involved in bonding and reactions

Ground-State Electron Configuration

- What is the ground-state electron configuration of carbon?
- 1s²2s²2p²
- How many valence electrons does carbon have?

<table>
<thead>
<tr>
<th>Element</th>
<th>Atomic number</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>1</td>
<td>1s²</td>
</tr>
<tr>
<td>Carbon</td>
<td>6</td>
<td>1s²2s²2p²</td>
</tr>
<tr>
<td>Sulfur</td>
<td>16</td>
<td>1s²2s²2p⁶3s²3p⁴</td>
</tr>
</tbody>
</table>

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<tr>
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</thead>
<tbody>
<tr>
<td>Lithium</td>
<td>3</td>
<td>1s²</td>
</tr>
<tr>
<td>Neon</td>
<td>10</td>
<td>1s²2s²2p⁶3s²3p⁶</td>
</tr>
</tbody>
</table>
Bond Formation

- **Octet Rule**
  - Electrons are either transferred or shared in a bond
  - In this way, bonded atoms can achieve a complete octet
  - There are some elements that do not need an octet
- **Ionic Bonds**
  - Usually occur between metals and non-metals
  - Metals usually lose electrons and non-metals usually gain electrons
- **Covalent Bonds**
  - Usually occur between two non-metals
  - Typical type of bond found in most organic molecules

Lewis Structures

- Atom with highest bonding requirement is in center
- In organic molecules, carbon is usually in the center
- Consider CH₃NH₂
- Calculate electrons each atom needs to be stable
  - \( C (8) + H \times 5(2) + N (8) = 26 \)
- Calculate the number of available electrons (valence)
  - \( C (4) + H \times 5(1) + N (5) = 14 \)
- Calculate the difference or number to be shared
  - \( 26-14 = 12 \) electrons or 6 pairs between 7 atoms

- Draw the Lewis Structure for Methane, CH₄
Theories of Bonding

• Three theories of bonding
  - Lewis Models
  - Hybridization
  - Molecular Orbital Theory

• Hybridization
  - Enhances the Lewis structure
  - Helps distinguish between different types of atoms, electrons, and bonds
  - Predicts molecular shape and bond angle

• Molecular Orbital Theory
  - Provides insight into structure and reactivity
  - Predicts areas of electron density

1.6 Valence Bond Theory

• Covalent bond forms when two atoms approach each other closely so that a singly occupied orbital on one atom overlaps a singly occupied orbital on the other atom

• Electrons are paired in the overlapping orbitals and are attracted to nuclei of both atoms
  - H–H bond results from the overlap of two singly occupied hydrogen 1s orbitals
  - H–H bond is cylindrically symmetrical, sigma (σ) bond

• Cannot account for Carbon’s ability to make 4 equivalent bonds.

Hybridization

• Hybridization theory resulted from refining valence bond theory (VBT)
  - VBT could not account for carbon’s ability to make 4 bonds

• Ground state carbon configuration is 1s²2s²2pₓ, 2pᵧ, 2pᵦ

• 1930’s Linus Pauling proposes electron promotion so now, 1s²2s²2pₓ, 2pᵧ, 2pᵦ

• But, orbitals must be of equal energy to allow 4 bonds

• Four new orbitals are formed by hybridizing or mixing the 2s and 2pₓᵧᵦ

• Four sp³ hybrid orbitals are created
**Sp³ Hybridization**

![Diagram of Sp³ hybridization]

**Methane, CH₄**

![Diagram of methane molecule]

**Tetrahedral Geometry**

![Diagram of a regular tetrahedron and a tetrahedral carbon atom]
1.9 Hybridization: $sp^2$ Orbitals and the Structure of Ethylene

- $sp^2$ hybrid orbitals: 2s orbital combines with two $2p$ orbitals, giving 3 orbitals ($sp = sp^2$)
- $sp^2$ orbitals are in a plane with 120° angles
- Remaining $p$ orbital is perpendicular to the plane
1.10 Hybridization: sp Orbitals and the Structure of Acetylene

- C-C a triple bond sharing six electrons
- Carbon 2s orbital hybridizes with a single p orbital giving two sp hybrids
  - two p orbitals remain unchanged
- sp orbitals are linear, 180° apart on x-axis
- Two p orbitals are perpendicular on the y-axis and the z-axis
Ethyne (acetylene)

Non-carbon sp hybridized atoms

Problem

What is the hybridization of each of the indicated atoms in this molecule?
1.12 Molecular Orbital Theory

- A molecular orbital (MO): where electrons are most likely to be found (specific energy and general shape) in a molecule
- Additive combination (bonding) MO is lower in energy
- Subtractive combination (antibonding) forms MO is higher

Contrast with Valence Bond Theory

- Results in one bonding orbital rather than two overlapping atomic orbitals.
- Don’t confuse with hybridization of atomic orbitals on each atom of molecule in valence theory.