Atomic Structure

- Atoms consist of protons, neutrons, and electrons
- Protons have a plus charge, electrons a negative charge, and neutrons have no charge
- Protons and neutrons are found in the nucleus, electrons are outside
- Protons and neutrons account for most of the atom’s mass
- Electrons participate in bonding and reactions

 Atomic Orbitals

- Electrons reside in distinct regions called orbitals
- Orbitals represent the area of highest probability of electron location
- Each orbital has a principle quantum number, n, 1,2,3, etc. and a 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

cloud of electrons
nucleus
(protons and neutrons)
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
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 atoms to be stable
  - C (8) + H 5x(2) + N (8) = 26
- Calculate the number of available electrons (valence)
  - C (4) + H 5x(1) + N (5) = 14
- Calculate the difference or number to be shared
  - 26-14 = 12 electrons or 6 pairs between 7 atoms

<table>
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<tr>
<th>Element</th>
<th>Atomic number</th>
<th>Configuration</th>
<th>Element</th>
<th>Atomic number</th>
<th>Configuration</th>
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<tbody>
<tr>
<td>Hydrogen</td>
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<td>H</td>
<td>Lithium</td>
<td>3</td>
<td>Li</td>
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<tr>
<td>Carbon</td>
<td>6</td>
<td>1H</td>
<td>Neon</td>
<td>10</td>
<td>He</td>
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<td>16</td>
<td>1S</td>
<td>Argon</td>
<td>18</td>
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\[
\begin{align*}
\text{CN} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\end{align*}
\]
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

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 $1s^22s^22p_x^12p_y^12p_z^0$
- 1930’s Linus Pauling proposes electron promotion so now, $1s^22s^12p_x^22p_y^22p_z^1$
- But, orbitals must be of equal energy to allow 4 bonds
- Four new orbitals are formed by hybridizing or mixing the 2s and 2p_x,y,z
- Four sp$^3$ hybrid orbitals are created

Sp$^3$ Hybridization
Methane, CH₄

Tetrahedral Geometry

Ethane

sp³ carbon  sp² carbon  sp³–sp² σ bond
Ethylene

Non-carbon sp$^2$ hybridized atoms

C$\equiv$N
sp$^2$ hybridized N

C$\equiv$O
sp$^2$ hybridized O

π bond
Sp Hybridization

One sp hybrid

Another sp hybrid

Ethyne

π bond

Non-carbon sp hybridized atoms

π bond

H\(_3\)C\(-C\equiv N\): sp hybridized N
Problem

What is the hybridization of each of the indicated atoms in this molecule?