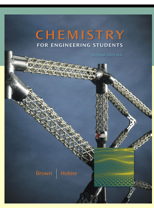

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Chapter 7
Chemical Bonding and Molecular Structure

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Chapter Objectives

- List some factors influencing the biocompatibility of materials and explain how those factors are related to chemical bonding.
- Use electron configurations to explain why metals tend to form cations, whereas nonmetals tend to form anions.
- Describe the energy changes in the formation of an ionic bond.
- Define electronegativity and state how electronegativity varies with position in the periodic table.

Chapter Objectives

- Identify or predict polar, nonpolar, and ionic bonds by comparing electronegativities.
- Write Lewis electron structures for molecules or ions.
- Describe chemical bonding using a model based on the overlap of atomic orbitals and recognize some of the limitations of this simple model.
- Explain how hybridization reconciles observed molecular shapes with the orbital overlap model.

Chapter Objectives

- Predict the geometry of a molecule from its Lewis structure.
- Use models (real or software) to help visualize common molecular shapes.
- Explain the formation of multiple bonds in terms of the overlap of a combination of hybridized and unhybridized atomic orbitals.
- Identify sigma and pi bonds in a molecule and explain the difference between them.

Materials for Biomedical Engineering

- Materials used in the body to replace damaged tissue must have the following properties:
  - Physical properties similar to the tissue they are replacing
    - Strength
    - Durability
    - Polarity: nature of electrical charges on surfaces
  - Biocompatibility: ability of material to interact biologically without triggering an immune response

The Ionic Bond

- An ionic bond is formed by the electrostatic attraction of oppositely charged ions.
  - Ionic compounds form between metals and nonmetals.
  - The greater the difference in metallic/nonmetallic properties (more widely separated in the periodic table), the more likely it is a compound will be ionic.

Formation of Cations

- Metals in the *s* and *p* blocks have low ionization energies and form cations with an np^6 electronic configuration.
  - Large jumps in ionization energy occur when removing an electron from an np^6 electronic configuration.
- Cations are smaller than their corresponding neutral atoms.
  - Losing electrons reduces electron-electron repulsion.
  - Remaining electrons are more tightly bound to the nucleus.

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Formation of Cations

- Transition metals can form cations with more than one possible charge.
  - Transition metals first lose electrons from the *s* subshell.
  - Additional electrons are lost from the partially filled *d* orbitals.
  - A half filled *d* orbital set is a fairly stable arrangement.
  - Fe^{2+} and Fe^{3+} ions are both stable.

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Example Problem 7.1

- Using the data from Table 6.4, predict the ions that magnesium and aluminum are most likely to form.

Table 6.4

The first four ionization energies (all in kJ/mol) for the elements of the first three periods. These ionizations with values shown in shaded cells with bold print involve removing the last electron from a particular shell. Further ionization requires removing an electron from a more stable filled shell, and this leads to a very large increase in ionization energy.

Z	Element	IE_1	IE_2	IE_3	IE_4
1	H	**1312**	—	—	—
2	He	2,372	**5,250**	—	—
3	Li	**520.2**	7,298	11,815	—
4	Be	899.4	**1,757**	14,848	21,007
5	B	800.6	2,427	**3,660**	25,026
6	C	1,086	2,353	4,620	**6,223**
7	N	1,402	2,856	4,578	7,475
8	O	1,314	3,388	5,300	7,469
9	F	1,681	3,374	6,050	8,408
10	Ne	2,081	3,952	6,122	9,370
11	Na	**495.6**	4,562	6,912	9,544
12	Mg	737.7	**1,451**	7,733	10,540
13	Al	577.6	1,817	**2,745**	11,578
14	Si	786.4	1,577	3,232	**4,356**
15	P	1,012	1,908	2,912	4,957
16	S	999.6	2,251	3,357	4,564
17	Cl	1,251	2,297	3,822	5,158
18	Ar	1,520	2,666	3,931	5,771

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Formation of Anions

- Nonmetals have negative electron affinities and generally form anions with an np^6 electronic configuration.
- Anions are larger than their corresponding neutral atoms.
  - Gaining electrons increases electron-electron repulsion.
  - Valence electrons less tightly bound to the nucleus.

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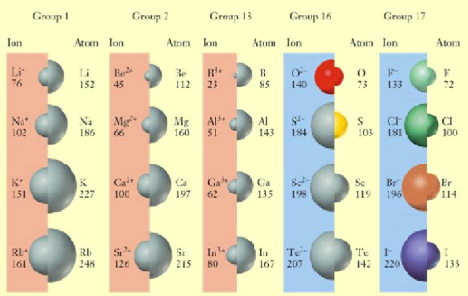
Formation of Ions



- Sizes of ions compared to corresponding neutral atoms.

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Formation of Ions

- Cations decrease in size from left to right across the periodic table.
  - Cations in a period have the same electronic configuration.
- Anions decrease in size from left to right across the periodic table.
  - Anions in a period have the same electronic configuration.
- Number of protons increases from left to right across a period.
- Electrons are held more tightly from left to right across a period, resulting in smaller ions.

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Formation of Ions

- Forming an ionic bond between a metal and nonmetal usually requires energy to form the ion pair.
  - Ionization energies are positive.
  - Electron affinities for nonmetals are negative.
  - Energy input to form the cation is not offset by energy released by forming the anion.

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Formation of Ions

- Once an ion pair is formed, electrostatic force of attraction between the ions significantly lowers overall energy.
  - F is force of attraction, q_1 and q_2 are the charges, and r is the distance between the nuclei of the two ions.

$$F \propto \frac{q_1 q_2}{r^2}$$

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Formation of Ions

- The potential energy, V, for the ion pair can be calculated.
  - $k = 1.389 \times 10^5$ kJ pm/mol

$$V = k\frac{q_1 q_2}{r}$$

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Formation of Ions

- The energy released in forming NaF can be calculated.
  - First the ion pair must be formed. (496 – 328 = +168 kJ/mol)
    - The ionization energy for Na is 496 kJ/mol.
    - The electron affinity for F is -328 kJ/mol.
  - Second the potential energy from coulombic attraction is calculated. Use the ionic radii to calculate V.
    - V = -591 kJ/mol.
- The energy released from the coulombic attraction is much greater than the energy required to form the NaF ion pair.
  - The formation of the NaF ionic bond releases energy.

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Formation of Ions

- In ionic solids, the ions are arranged in a crystal lattice.
  - Ions experience attractive and repulsive interactions in three dimensions.
  - Strength of interaction decreases with distance.

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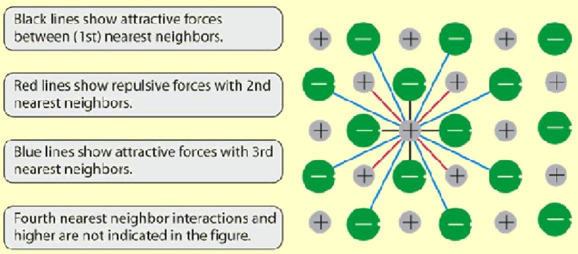
Formation of Ions



- In a solid lattice, any given ion experiences a large number of attractive and repulsive interactions.

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Formation of Ions

- The lattice energy is the overall result of the attractive and repulsive forces a crystal contains.
  - Small ions with large charges form ionic compounds with large lattice energies.
  - Large ions with small charges form ionic compounds with small lattice energies.

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Example Problem 7.2

- In each of the following pairs of ionic solids, the ions are arranged into similar lattices. Which one has the largest lattice energy?
  - CaO or KF
  - NaF or CsI

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The Covalent Bond

- A covalent bond is based on the sharing of pairs of electrons between two atoms.
- Driving force behind bond formation is lowering of overall energy.
  - Ionic bonding lowers energy by transferring electrons between a metal and a nonmetal.
  - Covalent bonding lowers energy by sharing electrons between two nonmetals.

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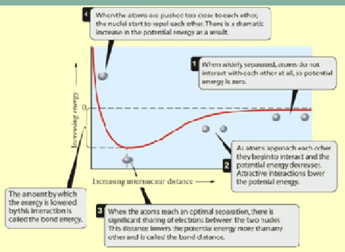
Chemical Bonds and Energy



- Potential energy between two atoms.
  - Electrons on each atom are attracted to the nucleus of the other atom.
  - Nuclei of the bonding atoms repel each other, as do the bonding electrons.
  - A covalent bond forms where the attractive and repulsive forces balance each other and energy is at a minimum.

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Chemical Bonds and Energy

- Bond energy - energy released when isolated atoms form a covalent bond.
- Bond length - the distance between the nuclei of the bonding atoms where the potential energy is a minimum.
- Electron density distribution is different for isolated atoms and covalently bonded atoms.
  - Isolated atoms have spherical electron density around the nucleus.
  - Covalently bonded atoms have a build up of electron density between bonded atoms.

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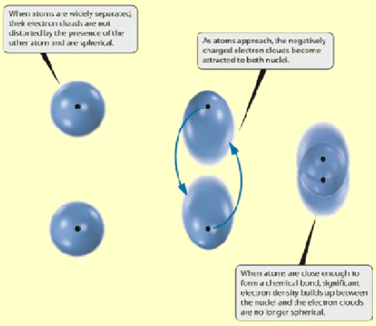
Chemical Bonds and Energy



- When two atoms approach one another, the negatively charged electron clouds are attracted to the other atom's positively charged nucleus.
- The diagram represents electron density during bond formation.

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Chemical Bonds and Energy

- Formation of bonds always releases energy.
  - Once a bond is formed, the same amount of energy, the bond energy, is needed to break the bond apart.
  - Bond energies vary depending on the bonding atoms involved.
- Chemical reactions involve rearranging bonds, turning reactants into products.
  - Reactions are energetically favored if the energy required to break reactant bonds is less than energy released making product bonds.

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Chemical Bonds and Reactions

Table 7.1

Bond energies of some types of bonds important in the combustion of hydrocarbons and fluorocarbons

Type of Bond	Bond Energy (kJ/mol)
C—F	485
C—H	415
O—F	190
C—H	460

- Bond energies for covalent bond types in Teflon.
- For the combustion of Teflon, the weak O–F bonds of OF_2 compared to the strong C-F bonds in Teflon accounts for Teflon's resistance to burning.

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Chemical Bonds and the Structure of Molecules

- During ionic bond formation, the cations and anions achieve np^6 electronic configurations (noble gas configuration).
  - Metals lose electrons.
  - Nonmetals gain electrons.
- During covalent bond formation, electrons are shared between two atoms.
  - Shared electrons are available to both bonding atoms.
  - Sharing leads to 8 valence electrons around each atom.

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Chemical Bonds and the Structure of Molecules

- Octet rule - an atom will form covalent bonds to achieve a complement of eight valence electrons.
  - The valence shell electronic configuration is ns^2np^6 for a total of eight electrons.
  - For the n = 1 shell, hydrogen violates the octet rule and shares only 2 electrons.

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Chemical Bonds and the Structure of Molecules

- Lewis dot symbols keep track of valence electrons, especially for main group elements, allowing prediction of bonding in molecules.
  - To draw a Lewis dot symbol, the valence electrons are represented by dots and are placed around the element symbol.
  - The first four dots are placed singly.
  - Starting with the fifth dot, they are paired.
  - The second period Lewis symbols are shown below:

·Li ·Be· ·B· ·C· ·N· ·O· :F· :Ne:

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Chemical Bonds and the Structure of Molecules

Group	1	2	13	14	15	16	17	18
Number of electrons in valence shell	1	2	3	4	5	6	7	8 (except He)
Period 1	H·							He
Period 2	Li·	·Be·	·B·	·C·	·N·	·O·	:F·	:Ne:
Period 3	Na·	·Mg·	·Al·	·Si·	·P·	·S·	:Cl·	:Ar:
Period 4	K·	·Ca·	·Ga·	·Ge·	·As·	·Se·	:Br·	:Kr:
Period 5	Rb·	·Sr·	·In·	·Sn·	·Sb·	·Te·	:I·	:Xe:
Period 6	Cs·	·Ba·	·Tl·	·Pb·	·Bi·	·Po·	:At·	:Rn:
Period 7	Fr·	·Ra·						

- Lewis dot symbols for main group elements.
  - Elements within a group have the same number of valence electrons and identical Lewis dot symbols.

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Chemical Bonds and the Structure of Molecules

- Lewis dot structures show how electrons are shared in a molecule.
  - A pair of shared electrons between two atoms is a bonding pair.
  - Bonding pairs represented by a line between two atomic symbols.
  - Pairs of electrons associated with one atom are nonbonding or lone pair electrons.

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Chemical Bonds and the Structure of Molecules

$$\text{H}\cdot + \cdot\text{H} \longrightarrow \text{H}:\text{H} \quad \text{or} \quad \text{H}-\text{H}$$

- By sharing an electron from each atom, two hydrogen atoms can form a covalent bond.
  - Hydrogen violates the octet rule by sharing only two electrons.

$$:\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}\cdot + \cdot\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}: \longrightarrow :\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}:\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}: \quad \text{or} \quad :\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}-\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}:$$

- When two fluorine atoms combine, they form a stable covalent bond.
  - By sharing a pair of electrons, each atom is surrounded by eight valence electrons.

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Chemical Bonds and the Structure of Molecules

- Bonding atoms in molecules can share more than one bonding pair of electrons.
  - A double bond results when two bonding pairs are shared.
  - A triple bond results when three bonding pairs are shared.
  - Strength of the covalent bond increases as the number of bonding pairs increases.

Type of Bond	Bond Energy (kJ /mol)
C—C	346
C═C	602
C≡C	835

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Electronegativity and Bond Polarity

- Bonding between the two ends of the bonding continuum, ionic and covalent bonding, is described using electronegativity and bond polarity.
- Electronegativity is the attraction of an atom for the shared electrons in a covalent bond.
  - Electronegativities are not measured quantities.
  - Electronegativities are assigned based on factors such as atomic size, electron affinity, and ionization energy.
  - The higher the electronegativity value, the more likely an element will attract extra electron density during compound formation.

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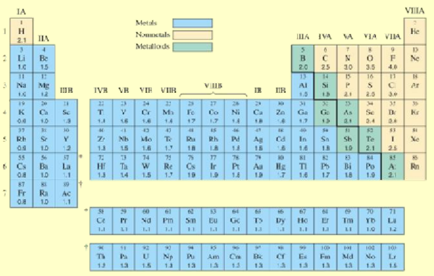
Electronegativity



- Electronegativities increase from left to right across a period and from bottom to top for a group.
- Fluorine is the most electronegative element, with an electronegativity of 4.0.

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Bond Polarity

- Electron density is not shared equally when elements with different electronegativities bond.
  - More than half of the electron density is associated with the more electronegative element.
  - The more electronegative element experiences an increase in electron density and attains a partial negative charge.
  - The less electronegative element experiences a decrease in electron density and attains a partial positive charge.
  - The two points of positive and negative charge constitute a dipole.
  - The bond has an electric field associated with it.

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Bond Polarity

- A bond along which a dipole exists is a polar bond.
  - Also referred to as a polar covalent bond since electrons are still being shared.
- The greater the electronegativity difference, the more polar the bond.
- When the electronegativity difference is zero, the bond is classified as nonpolar covalent.
- When the electronegativity difference exceeds 2.0, the bond is classified as ionic.

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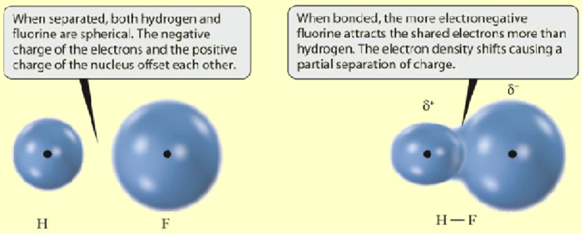
Bond Polarity



- The formation of the polar covalent HF bond.
  - The more electronegative F has a partial negative charge.
  - The less electronegative H has a partial positive charge.

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Example Problem 7.3

- Which bond is the most polar: C–H, O–H, or H–Cl? For each of these bonds, determine which atom has a partial positive charge.

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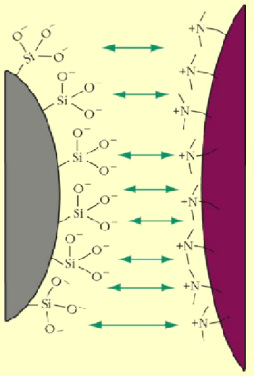
Bond Polarity

- Bond polarity is important in biocompatibility.
  - Cells often have polar bonds on their surfaces that interact with water.
  - Substances such as amorphous silica can interact strongly with cell surfaces, such as the red blood cell, and damage them.



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Keeping Track of Bonding: Lewis Structures

- Lewis structures indicate how many bonds are formed and between which elements in a compound.
- **Step 1** - Count the total valence electrons in the molecule or ion.
  - Sum the number of valence electrons for each element in a molecule.
  - For ions, add or subtract valence electrons to account for the charge.

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Keeping Track of Bonding: Lewis Structures

- For the compound OF_2, the number of valence electrons is 20.

F	2 x 7	= 14
O	1 x 6	= 6
	Total	= 20

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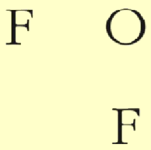
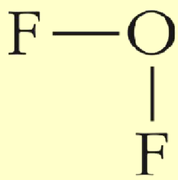
Keeping Track of Bonding: Lewis Structures

- **Step 2** - Draw the "skeletal structure" of the molecule.
  - The element written first in the formula is usually the central atom, unless it is hydrogen.
  - Usually, the central atom is the least electronegative.



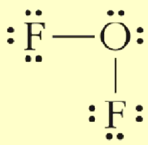
Keeping Track of Bonding: Lewis Structures

- **Step 3** - Place single bonds between all connected atoms in the structure by drawing lines between them.
  - A single line represents a bonding pair.
  - Four electrons are placed in bonds.
  - Sixteen electrons are left to place.



Keeping Track of Bonding: Lewis Structures

- **Step 4** - Place the remaining valence electrons not accounted for on individual atoms until the octet rule is satisfied. Place electrons as lone pairs whenever possible.
  - Place electrons first on outer atoms, then on central atoms.
    - Six electrons are placed as lone pairs on each F satisfies the octet rule for each F.
    - The four remaining electrons are placed on the O to satisfy the octet rule for each O.



Keeping Track of Bonding: Lewis Structures

- **Step 5** - Create multiple bonds by shifting lone pairs into bonding positions as needed for any atoms that do not have a full octet of valence electrons.
  - Correctly choosing which atoms to form multiple bonds between comes from experience.
  - Multiple bonds are not required for OF_2, as the octet rule is satisfied for each atom.

Example Problem 7.4

- Calcium phosphate is an important precursor for the formation of bioceramic coatings. Draw the Lewis structure of the phosphate ion, PO_4^{3-}.

Example Problem 7.5

- Poly(vinyl alcohol) is used in several biomaterials applications, including surgical sutures. Draw the Lewis structure of vinyl alcohol, CH_2CHOH, the monomer from which poly(vinyl alcohol) is made.

Resonance

- Resonance structures can be drawn when the choice of multiple bond location is arbitrary.
  - The position of all atoms are identical; only the positions of the electrons are different.
  - The actual structure is a hybrid, an average of the contributing structures, and NOT a mixture of them.

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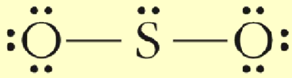
Resonance



- SO_2 has a total of 18 valence electrons.
- S is the least electronegative element and the central atom.
  - Octet not satisfied for S.
  - A double bond can be made to satisfy the octet rule, but from which side?

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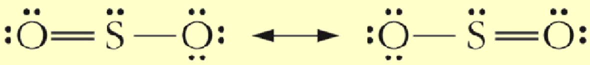
Resonance



- The two resonance structures for SO_2.
  - The "real" structure is a hybrid of the two structures.
  - The double arrow indicates the structures are resonance structures.

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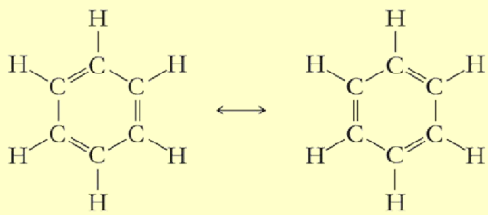
Resonance



- The two resonance structures for benzene.
  - Indicates the two ways to distribute 3 double bonds among 6 carbon atoms.
  - The true structure is an average of the two resonance structures.

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Orbital Overlap and Chemical Bonding

- Lewis dot structures provide insight into a molecule's bonding, but does not tell how a covalent bond is formed.
  - Electrons are modeled as waves.
  - When two waves occupy the same space, they interfere with each other.
  - Constructive and destructive interference are possible.

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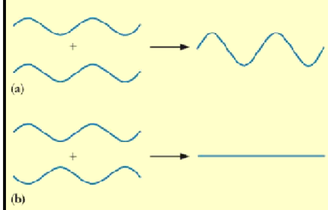
Orbital Overlap and Chemical Bonding



- Two sine waves illustrate interference.
  - Two in phase sine waves add together with constructive interference; new amplitude is twice the original
  - Two out of phase sine waves add together with destructive interference; they cancel out

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Orbital Overlap and Chemical Bonding

- Formation of chemical bonds is an example of constructive interference between electron waves.
  - For interference to occur, electron waves must occupy the same space.
  - Valence orbitals of one atom must be positioned to overlap with the valence orbitals of the other atom.

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Orbital Overlap and Chemical Bonding

- Valence bond model of chemical bonding - all chemical bonds are the result of overlap between atomic orbitals.
- For H_2, each H atom has a single valence electron in a 1*s* orbital.
  - The 1*s* orbitals overlap to form the covalent bond.
  - *s* orbitals are spherical, there is no preferred direction of approach.

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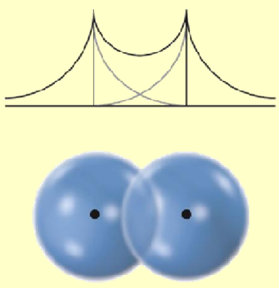
Orbital Overlap and Chemical Bonding



H — H

- Overlap of the 1*s* orbitals for the covalent bond in molecular hydrogen.
  - Top: Overlap shown by plotting the wave functions for the 1*s* orbitals.
  - Bottom: Shading to represent the buildup of electron density.

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Orbital Overlap and Chemical Bonding

- For N_2, the Lewis structure shows a total of 6 electrons shared.

$$:\mathrm{N}\equiv\mathrm{N}:$$

  - Each N atom has a single valence electron in each 2*p* orbital.
  - The 2*p* orbital set can overlap in different orientations due to their shapes.
  - A 2*p* orbital on one N overlaps end-to-end with a 2*p* orbital on the second N forming a sigma, σ, bond.
  - A sigma bond is the result of constructive interference for end-to-end overlap, where electron density lies along a line between the bonding atoms.

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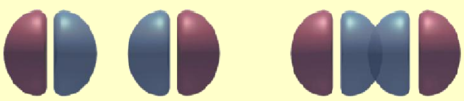
Orbital Overlap and Chemical Bonding



- Formation of a sigma bond by the end-to-end overlap of two *p* orbitals.
  - Two *p* orbitals approach each other along the *x*, *y*, or *z* axis.
  - All *p* orbitals are described as lying along the *x*, *y* or *z* axis.

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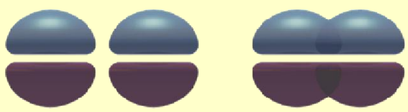
Orbital Overlap and Chemical Bonding

- The remaining two 2*p* orbitals on each N overlap side-to-side forming pi, π, bonds.
  - A pi bond is the result of constructive interference for side-to-side overlap, where electron density lies above and below, or in front and in back of a line between the bonding atoms.
  - Two pi bonds can form between the two nuclei.



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Hybrid Orbitals

- Orbital Hybridization reconciles the notion of orbital overlap with observations of molecular shapes and structures.
  - Bond angle predicted by orbital overlap of *p* and *s* orbitals in H_2O is 90º.
  - Bond angle in H_2O actually larger than 90º.

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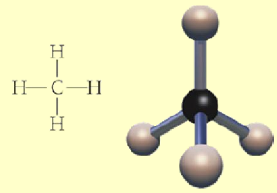
Hybrid Orbitals

- During orbital hybridization the repulsion between electrons in bonding atoms can be strong enough to reshape the orbitals of the atoms.
  - The angles between the reshaped orbitals must match observed bond angles.



- CH_4 is the simplest binary compound of C and H.
  - All four bond angles are 109.5º.
  - Four identical orbitals with angles of 109.5º between them are needed on C.

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Hybrid Orbitals

- Hybrid orbitals are created by a linear combination of atomic orbitals, producing an equal number of hybrid orbitals.
  - Orbitals are mathematical in nature.
  - Two atomic orbitals combine, two hybrid orbitals are generated.

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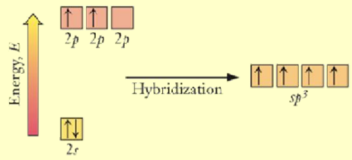
Hybrid Orbitals



- Hybridization of the *s* and *p* orbitals on carbon.
  - The four sp^3 hybrid orbitals have equal energy.
  - The four valence electrons are distributed evenly across the sp^3 hybrid orbitals.
  - The angle between the sp^3 hybrid orbitals is 109.5º.

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Hybrid Orbitals

Table 7.2

The five common orbital hybridization schemes are shown. The names for these hybrid orbitals are derived from the type and number of orbitals that combine to form them. Thus sp^2 hybrids result from combining an *s* orbital with a pair of *p* orbitals. The orbital geometries shown in the left-hand column give rise to the common molecular shapes described in the next section.

Orbitals Combined	Hybridization	Orbital Geometry	Orbitals Combined	Hybridization	Orbital Geometry
s, p	sp		s, p, p, p	sp^3	
s, p, p	sp^2		s, p, p, p, d	sp^3d	
			s, p, p, p, d, d	sp^3d^2	

- Hybrid orbital name comes from the type and number of atomic orbitals combined (e.g., sp^3)
- The indicated orbital geometry gives rise to common molecular shapes.

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Shapes of Molecules

- Molecular shape - the way bonded atoms arrange themselves in three dimensions.
  - Molecular shape affects molecular properties, including reactivity.
- Valence Shell Electron Pair Repulsion (VSEPR) theory - molecules assume a shape that allows them to minimize the repulsions between electron pairs in the valence shell of the central atom.
  - Electron pairs include both lone pair electrons and bonding pair electrons.

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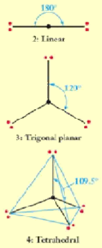
Shapes of Molecules

Table 7.3

Each of the geometrical arrangements shown in the table minimizes the electron pair repulsions for the indicated number of electron pairs. To visualize the shapes of molecules, it is essential that you have a sound mental picture of each of these geometries.

Number of Electron Pairs	Geometric Name	Bond Angles	Diagram
2	Linear	180°	2: Linear
3	Trigonal planar	120°	3: Trigonal planar
4	Tetrahedral	109.5°	4: Tetrahedral



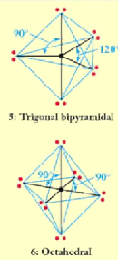
- Bond angles and shapes are predicted by electron pair repulsion between valence electron pairs.

Shapes of Molecules

Table 7.3

Each of the geometrical arrangements shown in the table minimizes the electron pair repulsions for the indicated number of electron pairs. To visualize the shapes of molecules, it is essential that you have a sound mental picture of each of these geometries.

Number of Electron Pairs	Geometric Name	Bond Angles	Diagram
5	Trigonal bipyramidal	120°, 90°	5: Trigonal bipyramidal
6	Octahedral	90°, 180°	6: Octahedral



Shapes of Molecules

- Molecular geometries are predicted systematically.
  - Draw the Lewis dot structure.
  - Count the number of bonding and nonbonding electron pairs around the central atom.
    - Double and triple bonds count as one bonding pair.
  - For zero nonbonding pairs on central atom, molecular shape matches shape predicted by VSEPR.
  - For nonbonding pairs on central atom, a base geometry predicted by VSEPR theory is used.

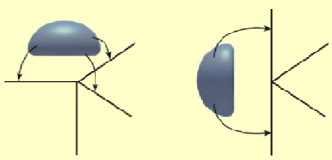
Shapes of Molecules

- Nonbonding electrons on central atom influence molecular geometry.
- Actual molecular geometry based on what base geometry would look like if nonbonding electron positions were “empty”.
- If more than one shape is possible, choose the shape that minimizes overall repulsion of electron pairs.
- The order of repulsive interactions is lone pair–lone pair > lone pair– bond pair > bond pair–bond pair.
- Lone pair electrons occupy more space than bonding pair electrons since they are not localized between two nuclei.

Example Problem 7.6

- Determine the shape of each of the following species:
  - PO_4^{3-}
  - PCl_5

Shapes of Molecules



- Lone pair electrons occupy more space than bonding electrons.
  - For 4 bonding electron pairs and a lone pair, the lone pair occupies the less repulsive equatorial position.

Shapes of Molecules

Table 7.4

The molecular shapes resulting from various combinations of the total number of electron pairs around the central atom and the number of lone pairs

Number of Electron Pairs	Number of Lone Pairs	Shape	Ball and Stick Model	Number of Electron Pairs	Number of Lone Pairs	Shape	Ball and Stick Model
3	0	Trigonal planar		4	1	Trigonal pyramidal	
3	1	Bent (120°)		4	2	Bent (109.5°)	
4	0	Tetrahedral		5	0	Trigonal bipyramidal	

(continues)

- Molecular shapes for various combinations of bonding and nonbonding electron pairs.

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Shapes of Molecules

Table 7.4 (continued)

The molecular shapes resulting from various combinations of the total number of electron pairs around the central atom and the number of lone pairs

Number of Electron Pairs	Number of Lone Pairs	Shape	Ball and Stick Model	Number of Electron Pairs	Number of Lone Pairs	Shape	Ball and Stick Model
5	1	Seesaw		6	1	Square pyramidal	
5	2	T-shape		6	2	Square planar	
5	3	Linear		6	3	T-shape	
6	0	Octahedral		6	4	Linear	

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Example Problem 7.7

- Determine the shape of the following molecules using VSEPR theory:
  - SF_4
  - BrF_5

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Example Problem 7.8

- Use VSEPR theory to determine the shape of the NOF molecule.

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Shapes of Molecules

- Molecular geometry for larger molecules is possible.
  - Geometry is assigned for each central atom.
  - Hybridization on each central atom assists in determination of overall geometry.

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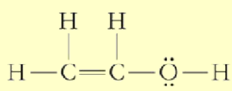
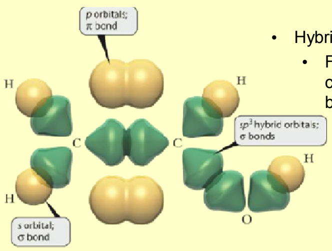
Shapes of Molecules





- For vinyl alcohol, each carbon has 3 bonded atoms and no lone pairs.
  - Each carbon has trigonal planar geometry.
- Hybridization on each carbon is sp^2.
  - Formation of pi bond between carbon atoms forces molecule to be planar.

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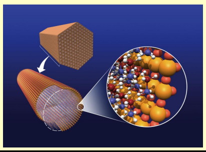
Molecular Scale Engineering for Drug Delivery

- Mesoporous silica nanoparticles (MSN) may offer a promising route for drug delivery, since they can deliver drugs to a targeted location and thus avoid side effects from affecting non-targeted organs.
  - One gram has about the same surface area as a football field.
  - Pores can be used to store drug molecules.
  - Different from amorphous silica; honeycomb structure and small size prevents cell damage



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