

HIV-Protease

- HIV-protease is a protein synthesized by the human immunodeficiency virus (HIV).
- This particular protein is crucial to the virus's ability to multiply and cause AIDS.
- Pharmaceutical companies designed molecules that would disable HIV-protease by sticking to the molecule's active site—**protease inhibitors**.
- To design such a molecule, researchers used **bonding theories** to *simulate* the shape of potential drug molecules and how they would interact with the protease molecule.

Bonding Theories

- Explain how and why atoms attach together to form molecules
- Explain why some combinations of atoms are stable and others are not
 - Why is water H_2O , not HO or H_3O ?
- Can be used to predict the shapes of molecules
- Can be used to predict the chemical and physical properties of compounds

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Lewis Model

- One of the simplest bonding theories is called **Lewis theory**.
- Lewis theory emphasizes valence electrons to explain bonding.
- Using Lewis theory, we can draw models, called Lewis structures.
 - Also known as electron dot structures
- Lewis structures allow us to predict many properties of molecules.
 - Molecular stability, shape, size, and polarity



Why Do Atoms Bond?

- Chemical bonds form because they lower the potential energy between the charged particles that compose atoms.
- A chemical bond forms when the potential energy of the bonded atoms is less than the potential energy of the separate atoms.
- To calculate this potential energy, you need to consider the following interactions:
 - Nucleus-to-nucleus repulsions
 - Electron-to-electron repulsions
 - Nucleus-to-electron attractions

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Types of Bonds · We can classify bonds based on the kinds of atoms that are bonded together. **Types of Atoms Type of Bond Characteristic of Bond** Metal and nonmetal Ionic Electrons transferred Nonmetal and nonmetal Covalent Electrons shared Metal and metal Metallic Electrons pooled © 2017 Pearson Education. Inc.



Ionic Bonds When a metal atom loses electrons it becomes a cation. Metals have low ionization energy, making it *relatively* easy to remove electrons from them. When a nonmetal atom gains electrons it becomes an anion. Nonmetals have high electron affinities, making it advantageous to add electrons to these atoms. The oppositely charged ions are then attracted to each other, resulting in an ionic bond.















Lewis Bonding Theory

- Atoms bond because bonding results in a more stable electron configuration.
 - More stable = lower potential energy
- Atoms bond together by either transferring or sharing electrons.
- Usually, this results in all atoms obtaining an outer shell with eight electrons.
 - Octet rule
 - There are some exceptions to this rule: The key to remember is to try to get an electron configuration like a noble gas.





Lewis Theory Predictions for Ionic Bonding

- Lewis theory predicts the number of electrons a metal atom should lose or a nonmetal atom should gain in order to attain a stable electron arrangement.
 - The octet rule
- This allows us to predict the formulas of ionic compounds that result.
- It also allows us to predict the relative strengths of the resulting ionic bonds from Coulomb's law.

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Ionic Bonding and the Crystal LatticeThe extra energy that is released comes from the formation of a structure, called a **crystal lattice**, in which every cation is surrounded by anions, and vice versa. The crystal lattice is held together by the electrostatic attraction of the cations for all the surrounding anions. The crystal lattice maximizes the attractions between cations and anions, leading to the most stable arrangement.



Lattice Energy

- The extra stability that accompanies the formation of the crystal lattice is measured as the **lattice energy**.
- The lattice energy is the energy released when the solid crystal forms from separate ions in the gas state.
 - Always exothermic
 - Hard to measure directly, but can be calculated from knowledge of other processes
- Lattice energy depends directly on the size of charges and inversely on distance between ions.































































Bond Polarity

- Most bonds have some degree of sharing and some degree of ion formation to them.
- Bonds are classified as covalent if the amount of electron transfer is insufficient for the material to display the classic properties of ionic compounds.
- If the sharing is unequal enough to produce a dipole in the bond, the bond is classified as polar covalent.







Effect of Electronegativity Difference on Bond Type					
TABLE 9.1 The Effect of Electronegativity Difference on Bond Type					
lectronegativity Difference (Δ EN)	Bond Type	Example			
Small (0–0.4)	Covalent	Cl ₂			
ntermediate (0.4–2.0)	Polar covalent	HCI			
arda (2.04)	Ionic	NaCl			





TABLE 9.2 Dipole Moments of SeveralMolecules in the Gas Phase				
Molecule	ΔEN	Dipole Moment (D		
Cl ₂	0	0		
CIF	1.0	0.88		
ΗF	1.9	1.82		
_iF	3.0	6.33		

Percent Ionic Character

- The **percent ionic character** is the percentage of a bond's measured dipole moment compared to what it would be if the electrons were completely transferred.
- The percent ionic character indicates the degree to which the electron is transferred.



Writing Lewis Structures of Molecules

- 1. Write the correct skeletal structure for the molecule.
 - Hydrogen atoms are always terminal.
 - The more electronegative atoms are placed in terminal positions.
- 2. Calculate the total number of electrons for the Lewis structure by summing the valence electrons of each atom in the molecule.
- 3. Distribute the electrons among the atoms, giving octets (or duets in the case of hydrogen) to as many atoms as possible.
- 4. If any atoms lack an octet, form double or triple bonds as necessary to give them octets.

Resonance

- Lewis theory localizes the electrons between the atoms that are bonding together.
- Extensions of Lewis theory suggest that there is some degree of delocalization of the electrons; we call this concept **resonance**.
- Delocalization of charge helps to stabilize the molecule.





Formal Charge is a fictitious charge assigned to each atom in a Lewis structure that helps us to distinguish among competing Lewis structures. In a Lewis structure, we calculate an atom's formal charge, which indicates the charge it would have if all bonding electrons were shared equally between the bonded atom. FC = # valence e⁻ - [nonbonding e⁻ + ½ bonding e⁻] Sum of all the formal charges in a molecule = 0. In an ion, total equals the charge.

	Structure A		Structure B			
	н -	— C =	= N:	H	— N ≡	C:
number of valence e ⁻	1	4	5	1	5	4
-number of nonbonding e^-	-0	-0	-2	-0	-0	-2
$-\frac{1}{2}$ (number of bonding e ⁻)	$-\frac{1}{2}(2)$	$-\frac{1}{2}(8)$	$-\frac{1}{2}(6)$	$-\frac{1}{2}(2)$	$-\frac{1}{2}(8)$	$-\frac{1}{2}(6$
Formal charge	0	0	0	0	+1	-1

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Exceptions to the Octet Rule

- Odd number electron species (e.g., NO)
 - Will have one unpaired electron
 - Free-radical
 - Very reactive
- Incomplete octets
 - B, Al
- Expanded octets
 - Elements with empty *d* orbitals can have more than eight electrons.

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Bond Energies

- The amount of energy it takes to break one mole of a bond in a compound is called the **bond** energy, or bond enthalpy.
 - In the gas state
 - Homolytically—each atom gets half of the bonding electrons
 - Always positive, endothermic
- Chemical reactions involve breaking bonds in reactant molecules and making new bonds to create the products.
- The ∆H°_{reaction} can be estimated by comparing the cost of breaking old bonds to the income from making new bonds.

Trends in Bond Energies

- In general, the more electrons two atoms share, the stronger the covalent bond.
 - Must be comparing bonds between like atoms
 - C≡C (837 kJ) > C=C (611 kJ) > C−−C (347 kJ)
 - C≡N (891 kJ) > C = N (615 kJ) > C—N (305 kJ)
- In general, the shorter the covalent bond, the stronger the bond.
 - Must be comparing similar types of bonds
 - Br—F (237 kJ) > Br—Cl (218 kJ) > Br—Br (193 kJ)
 - Bonds get weaker down the column.
 - Bonds get stronger across the period.

TABLE 9.3 Average Bond Energies						
Bond	Bond Energy (kJ/mol)	Bond	Bond Energy (kJ/mol)	Bond	Bond Energy (kJ/mol)	
н—н	436	N-N	163	Br—F	237	
н-с	414	N=N	418	Br-Cl	218	
H-N	389	N=N	946	Br—Br	193	
н-о	464	N-0	222	I-CI	208	
H-S	368	N=0	590	I—Br	175	
H-F	565	N-F	272	1-1	151	
H-CI	431	N-CI	200	Si-H	323	
H-Br	364	N-Br	243	Si-Si	226	
н—і	297	N-1	159	Si-C	301	
c-c	347	0-0	142	s-0	265	
C = C	611	0=0	498	Si=0	368	
c = c	837	0-F	190	s=0	523	
C-N	305	0-CI	203	Si-Cl	464	
C = N	615	0-1	234	s=s	418	
$C \equiv N$	891	F-F	159	S-F	327	
c-0	360	CI-F	253	s-ci	253	
C=0	736*	CI-CI	243	S—Br	218	
C≡0	1072			s—s	266	
C-CI	339					









TABLE 9.4 Average Bond Lengths							
Bond	Bond Length (pm)	Bond	Bond Length (pm)	Bond	Bond Length (pm)		
н—н	74	c-c	154	N-N	145		
н-с	110	c=c	134	N=N	123		
H—N	100	C≡C	120	N=N	110		
н—о	97	C-N	147	N-0	136		
H—S	132	C = N	128	N=O	120		
H—F	92	C≡N	116	0-0	145		
н—сі	127	c-0	143	0=0	121		
H—Br	141	C=0	120	F-F	143		
-11	161	c-ci	178	ci-ci	199		
				Br—Br	228		
				1—1	266		

Metallic Bonds

- The low ionization energy of metals allows them to lose electrons easily.
- The simplest theory of metallic bonding involves the metal atoms releasing their valence electrons to be shared by all atoms/ions in the metal.
 - An organization of metal cation islands in a sea of electrons
 - Electrons delocalized throughout the metal structure
- Bonding results from attraction of the cations for the delocalized electrons.



