

8-0

University Chemistry I
Chemistry 120, Section A
Chapter 8—Bonding

Thomas J. Wiese, Ph.D.
Professor of Chemistry
Fort Hays State University

8-previous

Valence e⁻ in Yellow

H	1s ¹		
He	1s ²	full	Noble gas
Li	1s ² ,2s ¹		
Be	1s ² ,2s ²		
B	1s ² ,2s ² p ¹		
C	1s ² ,2s ² p ²		
N	1s ² ,2s ² p ³		
O	1s ² ,2s ² p ⁴		
F	1s ² ,2s ² p ⁵		
Ne	1s ² ,2s ² p ⁶	full	Noble gas

8-1

The Octet Rule

Octet Rule- atoms will lose, gain, or share e⁻ to achieve the e⁻ configuration of the nearest noble gas in the periodic table (8 valence e⁻).

Special Case- He has only two e⁻ (First principle energy level full) and thus H is "happy" just having two e⁻.

8-2

Valence e⁻ Are Used to Form Bonds

- 3 types bonds
 - Ionic: metal-nonmetal
 - Covalent: nonmetal-nonmetal
 - Metallic: metal-metal
- Covalent are actually not all the same

8-3

Bonds

- Forces that hold groups of atoms together and make them function as a unit.

8-4

Bond Energy

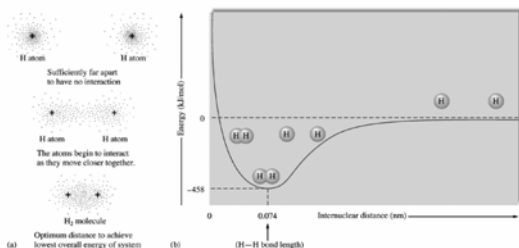
- It is the energy required to break a bond.
- It gives us information about the strength of a bonding interaction.

8-5

Bond Length

Fig. 8.9 Zumdahl and Zumdahl, 6th Ed.

- The distance where the system energy is a minimum.



8-6

Ionic Bonds: Transferring e⁻

Ionization Energy- the amount of energy it takes to remove an e⁻ from an atom.

Electronegativity- how strongly an atom pulls on another atom's e⁻.

Ions- atoms that have either lost (cations) or gained (anions) e⁻.

Ionic Compounds- form when a reaction takes place between two atoms with widely different ionization energies (metal and nonmetal).

8-7

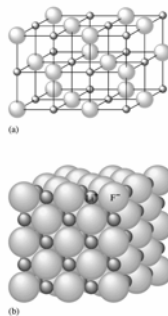
Ionic Bonds are *Electrostatic Bonds*

Fig. 8.9 Zumdahl and Zumdahl, 6th Ed.

+ charge is attracted to - charge

A *crystal lattice* will form to spread out the charge.

Crystal lattice- large, regular shaped structure which forms when ions interact to form an electrically neutral structure.



8-8

Formulas



Formula unit is used since a crystal of NaCl is too big

Formula unit- the simplest whole-number ratio which will describe an ionic crystal

Use "criss-cross" method to determine formula (demonstrated on board).

8-9

Ionic Bonds

$$E = 2.31 \times 10^{-19} \text{ J nm} \frac{Q_1 Q_2}{r}$$

Where E = energy of interaction
 Q_1 and Q_2 = numerical ion charges
 r = distance between ion centers (in nm)

8-10

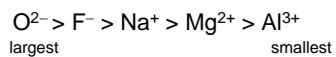
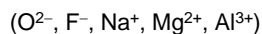
Achieving Noble Gas Electron Configurations (NGEC)

- A nonmetal and a representative group metal react (ionic compound): The valence orbitals of the metal are emptied to achieve NGEC. The valence electron configuration of the nonmetal achieves NGEC.
- Two nonmetals react: They share electrons to achieve NGEC.

8-11

Isoelectronic Ions

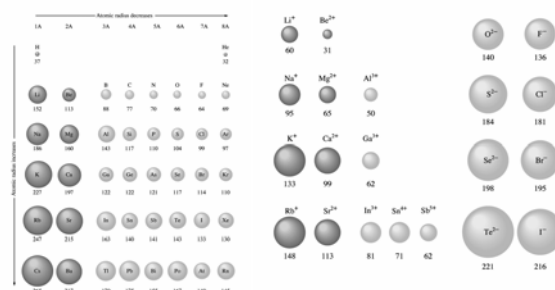
Different ions containing the the same number of electrons



8-12

Size (Radii) of Atoms and Ions (in pm)

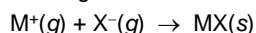
Fig. 7.35 (left), 8.7 (right) Zumdahl and Zumdahl, 6th Ed.



8-13

Lattice Energy

- The change in energy when separated gaseous ions are packed together to form an ionic solid.



- Lattice energy is negative (exothermic) from the point of view of the system.

8-14

Formation of an Ionic Solid

- Sublimation of the solid metal

$$\text{M}(\text{s}) \rightarrow \text{M}(\text{g}) \quad [\text{endothermic}]$$
- Ionization of the metal atoms

$$\text{M}(\text{g}) \rightarrow \text{M}^{+}(\text{g}) + \text{e}^{-} \quad [\text{endothermic}]$$
- Dissociation of the nonmetal

$$\frac{1}{2} \text{X}_2(\text{g}) \rightarrow \text{X}(\text{g}) \quad [\text{endothermic}]$$
- Formation of X^{-} ions in the gas phase:

$$\text{X}(\text{g}) + \text{e}^{-} \rightarrow \text{X}^{-}(\text{g}) \quad [\text{exothermic}]$$
- Formation of the solid MX

$$\text{M}^{+}(\text{g}) + \text{X}^{-}(\text{g}) \rightarrow \text{MX}(\text{s}) \quad [\text{quite exothermic}]$$

8-15

Lattice Energy

$$\text{Lattice Energy} = k \frac{Q_1 Q_2}{r}$$

Where Q_1, Q_2 = charges on the ions
 r = shortest distance between centers of the cations and anions
 k = proportionality constant that depends on shape of solid and electron configuration

8-16

Models and Their Fundamental Properties

Models- attempts to explain how nature operates on the microscopic level based on experiences in the macroscopic world.

- A model does not equal reality.
- Models are oversimplifications, and are therefore often wrong.
- Models become more complicated as they age.
- We must understand the underlying assumptions in a model so that we don't misuse it.

8-17

Electronegativity

- The ability of an atom in a molecule to attract shared electrons to itself.
- $\Delta = (H - X)_{\text{actual}} - (H - X)_{\text{expected}}$

Chart I. Electronegativities of Selected Elements

H											He		
2.21											—		
Li	Be							B	C	N	O	F	Ne
0.98	1.57							2.04	2.55	3	3.44	3.98	—
Na	Mg							Al	Si	P	S	Cl	Ar
0.93	1.31							1.61	1.90	2.19	2.58	3.16	—
K	Ca							Ga	Ge	As	Se	Br	Kr
0.82	1.00							1.81	2.01	2.18	2.55	2.96	—
Rb	Sr							In	Sn	Sb	Te	I	Xe
0.82	0.95							1.78	1.96	2.05	2.10	2.66	—
Cs	Ba							Tl	Pb	Bi	Po	At	Rn
0.79	0.89							2.04	2.33	2.02	2.0	2.2	—

8-18

Polarity

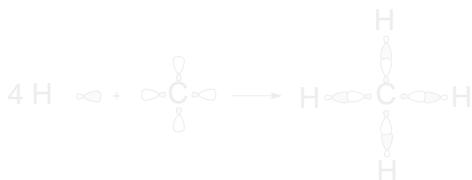
- A molecule, such as HF, that has a center of positive charge and a center of negative charge is said to be polar, or to have a dipole moment.

The arrowhead, or δ^- end, is the element with highest electronegativity.

8-19

Localized Electron Model

- A molecule is composed of atoms that are bound together by sharing pairs of electrons using the atomic orbitals of the bound atoms.



8-20

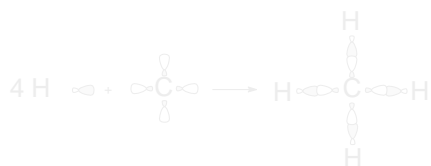
Localized Electron Model

- Description of valence electron arrangement (Lewis structure).
- Prediction of geometry (VSEPR model).
- Description of atomic orbital types used to share electrons or hold long pairs. (Very important later: *hybridized atomic orbitals*)

8-21

Lewis Structure

- Shows how valence electrons are arranged among atoms in a molecule.
- Reflects central idea that stability of a compound relates to noble gas electron configuration.



8-22

Lewis Electron Dot Structures

- Add the number of valence electrons from each atom in the formula.
- Join atoms with covalent bonds.
- For each bond, subtract 2 from the total electrons to account for. Use the leftover electrons to give each atom 8 electrons (except H).
- Repeat as necessary.

8-23

Some of the Ways Molecules Trick Us

Multiple Covalent Bonds- double and triple bonds can form between two atoms



8-24

Some of the Ways Molecules Trick Us

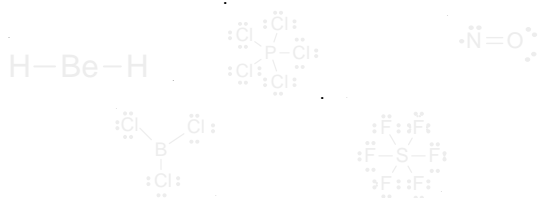
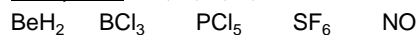
Coordinate Covalent Bond- one atom contributes both electrons to a bond



8-25

Some of the Ways Molecules Trick Us

Exceptions- Be, B, P, S, N



8-26

Comments About the Octet Rule

- 2nd period elements C, N, O, F observe the octet rule.
- 2nd period elements B and Be often have fewer than 8 electrons around themselves - they are very reactive.
- 3rd period and heavier elements CAN exceed the octet rule using empty valence d orbitals.
- When writing Lewis structures, satisfy octets first, then place electrons around elements having available d orbitals.

8-27

Lewis Dot Structures of Polyatomic Ions



Sulfate
32 e⁻ instead of 30

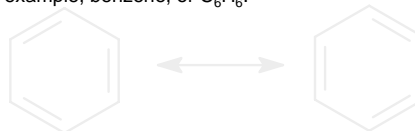


carbonate
24 e⁻ instead of 22

8-28

Resonance

- Occurs when more than one valid Lewis structure can be written for a particular molecule.
- For example, benzene, or C₆H₆.



- These are resonance structures. The actual structure is an average of the resonance structures.
Bond length 1.39 Å and Table 8.5

8-29

Formal Charge

- The difference between the number of valence electrons on the free atom and the number assigned to the atom in the molecule.
- Must calculate formal charge *of each atom*
- We need the number of valence e⁻ "belonging" to the atom in the molecule
 - Lone pairs belong to the atom on which they reside
 - ½ of bonding pairs belong to each atom bonded
- FC = group # - "owned" e⁻

8-30

Formal Charge



Not as good



Better

8-31

VSEPR Model

- The structure around a given atom is determined principally by minimizing electron pair repulsions.

8-32

Predicting a VSEPR Structure

- Draw Lewis structure.
- Put pairs as far apart as possible.
- Determine positions of atoms from the way electron pairs are shared.
- Determine the name of molecular structure from positions of the atoms.

8-33

Example Molecules in Two and Three Dimensions

- | | |
|--------------------------------|----------------------|
| • O ₂ | Linear |
| • H ₂ O | Bent, or angular |
| • NH ₃ | Pyramidal |
| • CH ₄ | Tetrahedral |
| • NH ₄ ⁺ | Tetrahedral |
| • PCl ₅ | Trigonal bipyramidal |
| • SF ₆ | Octahedral |
- Above list not all-inclusive: square pyramidal, e.g. ?What would cause this shape?
 - Above list not all-inclusive: square pyramidal, trigonal planar, etc. ?What would cause these shapes?

8-34

Sample Test Questions

What is the molecular shape of the following compound, for which the correct Lewis dot structure is given?



- What is the molecular shape of PF₃?
- What is the molecular shape of dinitrogen tetroxide?

8-35

Bond Energies

- Bond breaking requires energy (endothermic).
- Bond formation releases energy (exothermic).

$$\Delta H = \underbrace{\sum D(\text{bonds broken})}_{\text{energy required}} - \underbrace{\sum D(\text{bonds formed})}_{\text{energy released}}$$

8-36

Polarity of Bonds

- Using chart I, indicate whether the following bonds are polar or nonpolar

Chart I. Electronegativities of Selected Elements

H								He
2.21								—
Li	Be		B	C	N	O	F	Ne
0.98	1.57		2.04	2.55	3.04	3.44	3.98	—
Na	Mg		Al	Si	P	S	Cl	Ar
0.93	1.31		1.61	1.90	2.19	2.58	3.16	—
K	Ca		Ga	Ge	As	Se	Br	Kr
0.82	1.00		1.81	2.01	2.18	2.55	2.96	—
Rb	Sr		In	Sn	Sb	Te	I	Xe
0.82	0.95		1.78	1.96	2.05	2.10	2.66	—
Cs	Ba		Tl	Pb	Bi	Po	At	Rn
0.79	0.89		2.04	2.33	2.02	2.0	2.2	—

- C-H
- C-O
- C-Cl
- C-N

8-37

Polarity of Molecules

- Using chart I, indicate whether the following molecules are polar or nonpolar

Chart I. Electronegativities of Selected Elements

H								He
2.21								—
Li	Be		B	C	N	O	F	Ne
0.98	1.57		2.04	2.55	3.04	3.44	3.98	—
Na	Mg		Al	Si	P	S	Cl	Ar
0.93	1.31		1.61	1.90	2.19	2.58	3.16	—
K	Ca		Ga	Ge	As	Se	Br	Kr
0.82	1.00		1.81	2.01	2.18	2.55	2.96	—
Rb	Sr		In	Sn	Sb	Te	I	Xe
0.82	0.95		1.78	1.96	2.05	2.10	2.66	—
Cs	Ba		Tl	Pb	Bi	Po	At	Rn
0.79	0.89		2.04	2.33	2.02	2.0	2.2	—

- CH₄
- CO
- CO₂
- CHCl₃
- C-N