9-1

Valence e⁻ in Yellow and Lewis Dot Structures of Atoms

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

9-2

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 (more later)

9-3

Valence e⁻ in Yellow (all four methods are acceptable)

H	$1s^1$		
He	$1s^2$	full	Noble gas
Li	$1s^2,2s^1$		
Be	$1s^22s^2$		
B	$1s^2,2s^2p^1$		
C	$1s^2,2s^22p^2$		
N	$1s^22s^22p^3$		
O	$1s^22s^22p^4$		
F	$1s^22s^22p^5$		
Ne	$1s^22s^22p^6$	full	Noble gas

9-4

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^-.

9-5

Bonds

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

9-6

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 atoms e^- (or shared 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).

9-7

Formulas

$Na_{5,956,000}Cl_{5,956,000}$

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).

9-8

Strength of Ionic Bonds

$$E = 2.31 \times 10^{-19} \text{ J nm } \frac{Q_1Q_2}{r}$$

Where E = energy of interaction

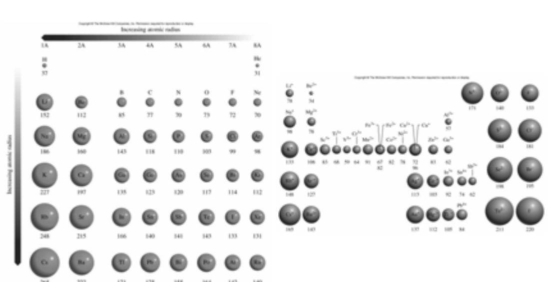
Q_1 and Q_2 = numerical ion charges

r = distance between ion centers (in nm)

9-9

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

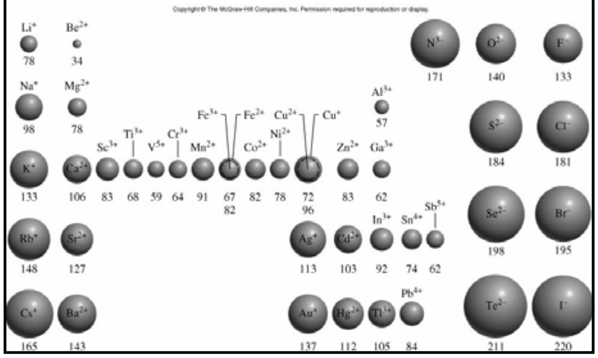
Fig. 8.5 (left), 8.9 (right) Chang, 9th Ed.



9-10

Size (Radii) of Ions (in pm)

Fig. 8.9 (right) Chang, 9th Ed.



9-11

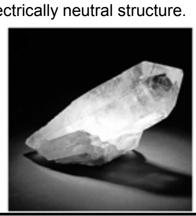
Ionic Bonds are *Electrostatic Bonds*

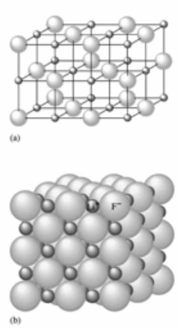
Fig. 8.9 Zumdahl and Zumdahl, 6th Ed.

+ 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.





9-12

Lattice Energy

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

  $M^+(g) + X^-(g) \rightarrow MX(s)$

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

9-13

Formation of an Ionic Solid

1. Sublimation of the solid metal
   $M(s) \rightarrow M(g)$ [endothermic]
2. Ionization of the metal atoms
   $M(g) \rightarrow M^+(g) + e^-$ [endothermic]
3. Dissociation of the nonmetal
   $\frac{1}{2} X_2(g) \rightarrow X(g)$ [endothermic]
4. Formation of X^- ions in the gas phase:
   $X(g) + e^- \rightarrow X^-(g)$ [exothermic]
5. Formation of the solid MX
   $M^+(g) + X^-(g) \rightarrow MX(s)$ [quite exothermic]

9-14

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

9-15

Isoelectronic Ions

Different ions containing the the same number of electrons

(O^{2-}, F^-, Na^+, Mg^{2+}, Al^{3+})

$O^{2-} > F^- > Na^+ > Mg^{2+} > Al^{3+}$
largest smallest

9-16

Bond Energy

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

9-17

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.

9-18

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.

9-19

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.

9-20

Localized Electron Model

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

9-21

Lewis Structure

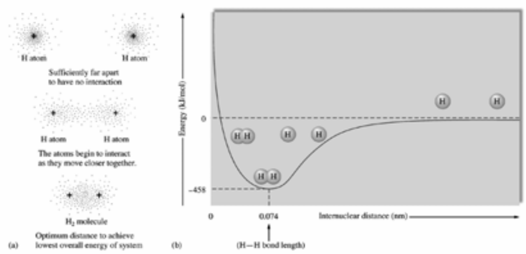
- Shows how valence electrons are arranged among atoms in a molecule.
- Reflects central idea that stability of a compound relates to noble gas electron configuration.

9-22

Bond Length

Fig. 8.9 Zumdahl and Zumdahl, 6th Ed.

- The distance where the system energy is a minimum.



9-23

Lewis Electron Dot Structures

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

9-24

Some of the Ways Molecules Trick Us

<u>Multiple Covalent Bonds</u>- double and triple bonds can form between two atoms

CO_2 N_2

9-25

Some of the Ways Molecules Trick Us

<u>Coordinate Covalent Bond</u>- one atom contributes both electrons to a bond

9-26

Some of the Ways Molecules Trick Us

<u>Exceptions</u>- Be, B, P, S, N

BeH_2 BCl_3 PCl_5 SF_6 NO

9-27

Generalizations 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.

9-28

Lewis Dot Structures of Polyatomic Ions

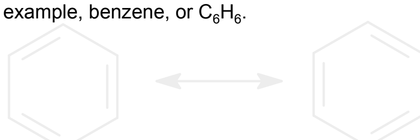
Sulfate
32 e⁻ instead of 30

carbonate
24 e⁻ instead of 22

9-29

Resonance

- Occurs when more than one valid Lewis structure can be written for a particular molecule.
- For example, benzene, or C_6H_6.



- These are resonance structures. The actual structure is an average of the resonance structures.

Bond length 1.39 Å and Table 9.2 on page 368

9-30

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⁻

9-31

Formal Charge

Not as good — Better

How about that BCl_3 molecule?

9-32

Electronegativity

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

Chart I. Electronegativities of Selected Elements

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

9-33

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 $\delta-$ end, is the element with highest electronegativity.

9-34

Polarity of *Bonds*

- Using chart I, indicate whether the following *bonds* are polar or nonpolar
- C-H
- C-O
- C-Cl
- C-N

Chart I. Electronegativities of Selected Elements

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

9-35

Polarity of *Molecules*

- Using chart I, indicate whether the following *molecules* are polar or nonpolar
- CH_4
- CO
- CO_2
- $CHCl_3$
- H_2S
- BCl_3

Chart I. Electronegativities of Selected Elements

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

9-36

Bond Energies

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

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

9-37

STQ

- Use bond energies (attached table) to predict ΔH for the following properly balanced equation: (5 points)

$$2\ C_2H_6 + 7\ O_2 \rightarrow 4\ CO_2 + 6\ H_2O$$