Chemical Bonding and Reactivity

- Chemical reactivity is driven largely by an atom's **valence electrons**
  - Leads to *similar* reactivity among groups on the periodic table
- Spontaneous reactions lead to lower energy (aka more "stable") situations.
  - Often by producing "filled" valence shells for atoms

Table 4.1 Lewis Symbols for Selected Main Group Elements

Group 1A	Group 2A	Group 3A	Group 4A	Group 5A	Group 6A	Group 7A	Noble Gases
H·							He:
Li·	·Be·	·B·	·C·	:N·	:O·	:F·	:Ne:
Na·	·Mg·	·Al·	·Si·	:P·	:S·	:Cl·	:Ar:
K·	·Ca·				:Se·	:Br·	:Kr:
Rb·	·Sr·				:Te·	:I·	:Xe:
Cs·	·Ba·						

Naming Chemical Compounds

Many, many rules exist depending on the type of compound. (IUPAC)

Binary Ionic Compounds

- Metal and nonmetal
  - How do I know??
- Metal typically becomes cation, nonmetal becomes anion
- Name metal first using element name, name nonmetal second with an –ide suffix.
- NaCl, MgS…

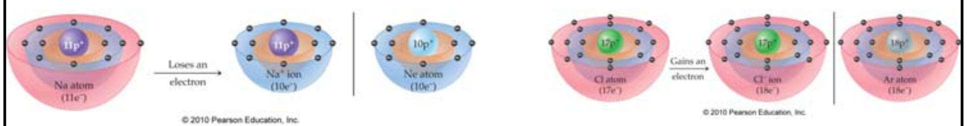
Table 4.3 Prefixes That Indicate the Number of Atoms of an Element in a Covalent Compound

Prefix	Number of Atoms
Mono-	1
Di-	2
Tri-	3
Tetra-	4
Penta-	5
Hexa-	6
Hepta-	7
Octa-	8
Nona-	9
Deca-	10

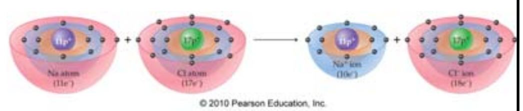
Some compounds have common names: water, ammonia…

Ion formation

- Goal for main group elements: achieve noble gas configuration
  - Where/what are noble gases?
  - Can lose or gain electrons:
    - Loss of electrons: <u>Oxidation</u>, leads to +charge: **Cation**
    - Gain of electrons: <u>Reduction</u>, leads to –charge: **Anion**



- Ionic compounds form because of electrostatic interaction: **Ionic Bond**



Ions and Ionic Compounds

- Ionic compounds are neutral!
  - Total positive charge = total negative charge
- Transition metals often have more than one **<u>oxidation state</u>**.
  - Specify this in compound name
- Working with **<u>polyatomic ions</u>**

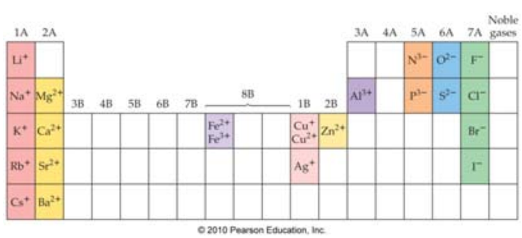


Fig 4.4

Table 4.4 Some Common Polyatomic Ions

Charge	Name	Formula
1+	Ammonium ion	NH_4^+
	Hydronium ion	H_3O^+
1−	Hydrogen carbonate (bicarbonate) ion	HCO_3^-
	Hydrogen sulfate (bisulfate) ion	HSO_4^-
	Acetate ion	$CH_3CO_2^-$ (or $C_2H_3O_2^-$)
	Nitrite ion	NO_2^-
	Nitrate ion	NO_3^-
	Cyanide ion	CN^-
	Hydroxide ion	OH^-
	Dihydrogen phosphate ion	$H_2PO_4^-$
	Permanganate ion	MnO_4^-
2−	Carbonate ion	CO_3^{2-}
	Sulfate ion	SO_4^{2-}
	Chromate ion	CrO_4^{2-}
	Monohydrogen phosphate ion	HPO_4^{2-}
	Oxalate ion	$C_2O_4^{2-}$
	Dichromate ion	$Cr_2O_7^{2-}$
3−	Phosphate ion	PO_4^{3-}

Covalent Bonds and Covalent Compounds

- Desire to achieve noble gas configuration still holds
  - Want filled shells
- In covalent bonds, electrons are shared to fill shells
  - typically 8 e^-, “octet”
- What is a covalent bond?
  - Shared electrons
  - Electrons typically in pairs
    - Species with unpaired electrons tend to be fairly reactive
  - May be multiple pairs of electrons shared between the same pair of elements
    - Single, double, triple bonds and strength
  - Sharing not necessarily equal
    - Polar bonds
    - What makes a bond polar (or not)

Covalent Bonding…Endless Possibilities

- Wide variety of bonding characteristics for atoms
  - Types of bonds
  - Numbers of bonds
- Leads to the possibilities for forming a huge number of unique compounds
  - Ultimately, the types of elements, bonds, and orientation control properties.

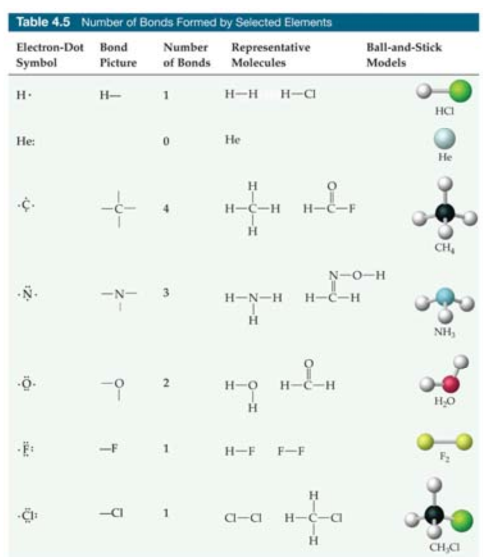


Table 4.5 Number of Bonds Formed by Selected Elements

Electron-Dot Symbol	Bond Picture	Number of Bonds	Representative Molecules	Ball-and-Stick Models
H·	H—	1	H—H H—Cl	HCl
He:		0	He	He
·C·	—C—	4	H–C(H)(H)–H H–C(=O)–F	CH_4
·N·	—N—	3	H–N(H)–H H–C(=N–O–H)–H	NH_3
·O·	—O	2	H–O–H H–C(=O)–H	H_2O
·F:	—F	1	H—F F—F	F_2
·Cl:	—Cl	1	Cl—Cl H–C(H)(H)–Cl	CH_3Cl

Bond Polarity

- ***Electronegativity*** is a measure of an atom's attraction for the electrons in a bond.
  - More electronegative atom, the greater the "tug" in the bond
  - Fluorine is the most electronegative atom

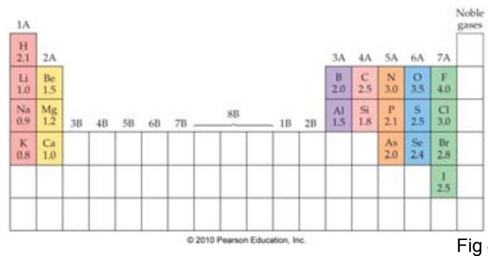


Fig 4.5

- Consider HCl
  - Chlorine is more elctronagative, pulls on the electrons more
  - Result is a bond *dipole* or a **polar covalent bond**.
  - "Size" of dipole depends on electronegativity difference between atoms.

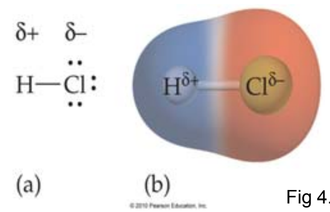


Fig 4.6

Modeling Bonding: Lewis Dot Structures

- Very simple model, not universal but works for several compounds
  - Electron bookkeeping based on the "Octet Rule"
- Drawing Lewis Structures (Examples: CCl_4, NH_3, H_2O, CO_2)
  - Least electronegative atom in the middle (if necessary)
  - Count **valence** electrons
  - Draw single bonds between central atom and each peripheral atom
  - Distribute remaining e^- as lone pairs around peripheral atoms until all have an octet
  - Add multiple bonds to central atom if necessary until all atoms have filled octets
  - Double-check that all e^- have been used and all atoms have filled octets!
- Ultimately, the structure we draw must agree with real life!
  - If it doesn't, our approach is incorrect and we need to modify our model
    - Resonance and Ozone

Predicting Molecular Shape

- 3D Shape can be critical in reactivity (enzymes)
- Various shapes depending on electron-pair geometry
  - Things want to be as far apart in space as possible
  - Valence Shell Electron Pair Repulsion theory (VSEPR)

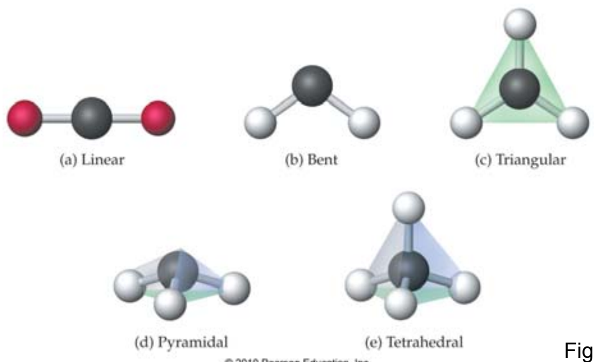


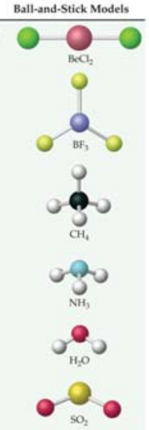
Fig 4.8

Predicting Molecular Shape

- Electron pair geometry versus molecular geometry

Table 4.6 Bonding and the Shape of Molecules

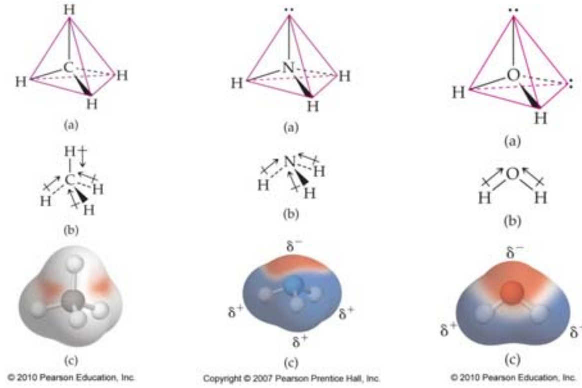
Number of Bonded Atoms	Number of LP*	Number of Sets	Molecular Shape	Examples	Ball-and-Stick Models
2	0	2	Linear	$BeCl_2$ $HgCl_2$ CO_2 HCN	$BeCl_2$
3	0	3	Triangular	BF_3 $AlBr_3$ CH_2O	BF_3
4	0	4	Tetrahedral	CH_4 CBr_4 $SiCl_4$	CH_4
3	1	4	Pyramidal	NH_3 PCl_3	NH_3
2	2	4	Bent	H_2O H_2S SCl_2	H_2O
2	1	3	Bent	SO_2 O_3	SO_2



*LP: Lone pair(s) of electrons.

Molecular Polarity

- Individual bond dipoles can reinforce or cancel one another
  - May produce a "molecular dipole"
  - Contributes dramatically to properties

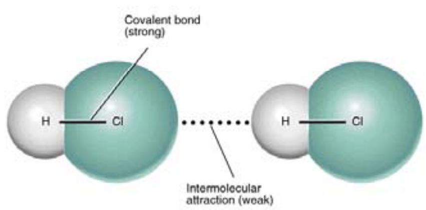


Figs 4.9-4.11

Intermolecular Forces: Structure and Properties

- Consider the boiling points for methane (-161.6 °C), ammonia (−33.34 °C) and water (100.0 °C). Why are they so different?

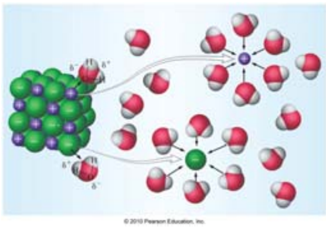
- Much of the difference is due to interactions between molucules
  - Intermolecular forces (between molecules)
  - Intramolecular forces (within molecules, aka "bonds")
  - Figure 6.1



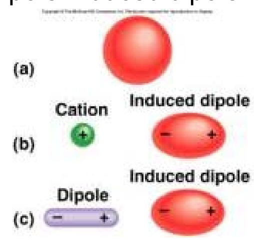
Types of IM Forces

Depends on the two species interacting

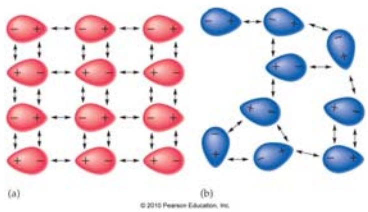
1. Ion-dipole



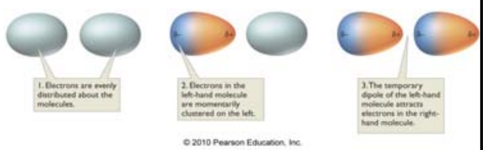
3. Dipole-induced dipole



2. Dipole-dipole



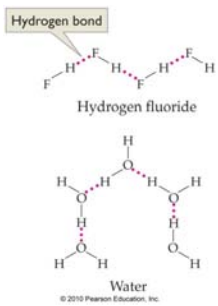
4. Dispersion

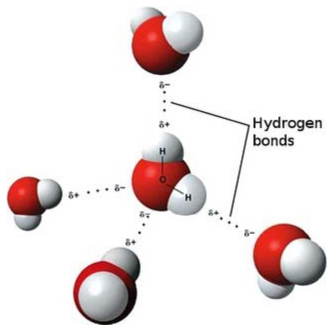


Figs 6.4, 6.5, 6.9

Hydrogen Bonding Interactions

- Special case of dipole-dipole interactions
- Requirements: Hydrogen covalently bound to an electronegative atom (like O, N, F) AND unshared electrons on the electronegative atom.





- Leads to very unique properties for some compounds…like water!
- http://www.edinformatics.com/interactive_molecules/ice.htm

Predicting IM forces

- Back to methane, ammonia, and water