Intermolecular Forces, Liquids, Solids

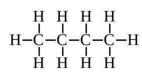
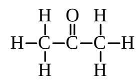
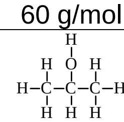
Interactions Between Molecules:

What does it take to separate two (or more) molecules from one another?

-or-

What holds molecules close to one another?

Structure/Property Relationships

Name	**Butane**	**Acetone**	**Isopropyl Alcohol**
Molecular Formula	C_4H_{10}	C_3H_6O	C_3H_8O
Molar Mass	58 g/mol	58 g/mol	60 g/mol
Structure			
Boiling Point	-0.6 ^oC	56 ^oC	82 ^oC

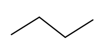
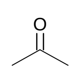
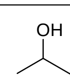
Why is there this discrepancy in boiling point?

INTERMOLECULAR FORCES!

Isopropyl alcohol > acetone > butane

IM Forces and Physical Properties

<u>Why this difference in bp?</u> Let's take a closer look at these molecules:

	Butane	**Acetone**	**Isopropyl Alcohol**
Boiling Point	-0.6 ^oC	56 ^oC	82 ^oC
Structure			
Nonpolar Bonds Present			
Polar Bonds Present			
Molecular Polarity			

Apparently, nonpolar molecules have weaker intermolecular forces. Why?

Electrostatic interactions of molecules

Interactions that result from charges!

- Governed by Coulomb's Law:

$$\text{Force} \propto \frac{(n^{+}e)(n^{-}e)}{d^{2}}$$

- Types of electrostatic "species" possible:
  1. Ions-
  2. Dipoles-
  3. Induced Dipoles-

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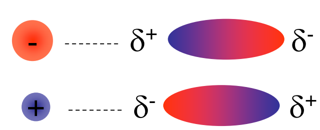
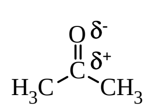
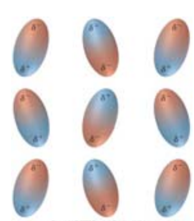
Possible Types of IM Interactions aka "van de Waals forces"

1. **Ion-Dipole Interactions**
   – Remember back to discussion of water as a solvent: Water hydrates an ionic solute.



2. **Dipole-Dipole Interactions**
   Interactions of δ^{+} end of one dipole with the δ^{-} end of another.





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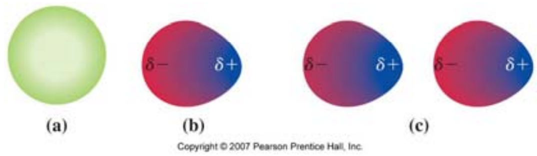
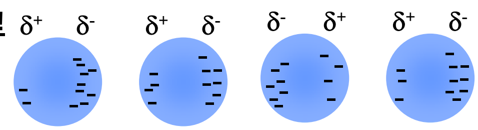
Possible Types of IM Interactions

3. **Dipole-Induced Dipole Interactions**



4. **Induced Dipole-Induced Dipole Interactions**
   – "Dispersion Forces"
   – Aka London Forces
   – **Present in ALL molecules!**



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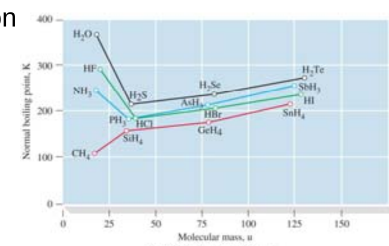
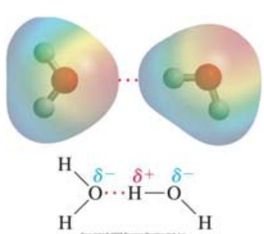
Hydrogen Bonding

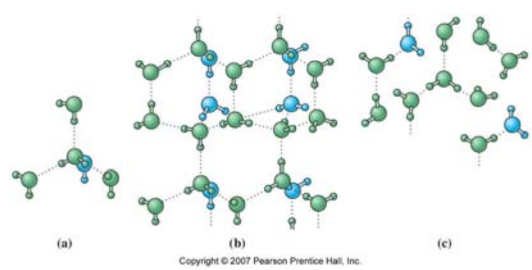
Specialized case of dipole-dipole interaction

- Occurs b/w
  1. H bound to O, N, F
  2. Lone pair of e^- on another N, O, F



- Water forms hydrogen bonded array
  – special!

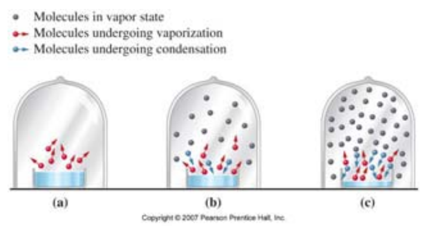




Properties of Liquids:
Try to relate these to IM

Liquid $\underset{\text{Condensation}}{\overset{\text{Vaporization}}{\rightleftarrows}}$ Vapor

1. Heat of Vaporization (ΔH^o_{vap})
2. Vapor Pressure (atm or mm Hg)
3. Boiling Point
   T where v.p. = atmospheric p.
   "Normal boiling point": v.p. = 1 atm
4. Surface Tension
   Cohesive vs **adhesive** forces
5. Viscosity



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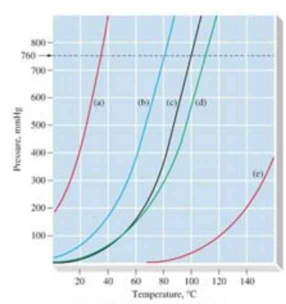
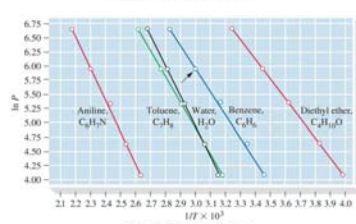
Properties of Liquids:
More on Vapor Pressure

- V.P. depends on
  - Interaction b/w molecules
  - Energy available ("heat")
- Can model V.P. using Clausius-Clapeyron Eqn.

$$\ln\frac{P_2}{P_1} = \frac{\Delta H_{vap}}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$





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Solids: Structure and Properties

Solids are classified based on identity of material and forces that hold solid together. (Table 12.7)

Type of Solid	Forces at Work
Ionic	
Metallic	
Molecular	
Network	
Amorphous	

Describe arrangement of particles in a crystalline solid by describing smallest repeat unit of the solid: **Unit Cell**

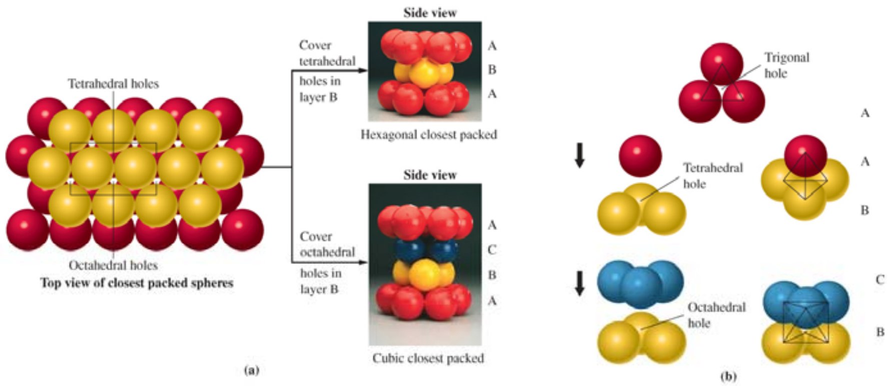
Solids: Structure and Properties

TABLE 12.7 Characteristics of Crystalline Solids

Type	Structural Particles	Intermolecular Forces	Typical Properties	Examples
Metallic	Cations and delocalized electrons	Metallic bonds	Hardness varies from soft to very hard; melting point varies from low to very high; lustrous; ductile; malleable; very good conductors of heat and electricity	Na, Mg, Al, Fe, Sn, Cu, Ag, W
Ionic	Cations and anions	Electrostatic attractions	Hard; moderate to very high melting points; nonconductors as solids, but good electric conductors as liquids; many are soluble in polar solvents like water	NaCl, MgO, $NaNO_3$
Network covalent	Atoms	Covalent bonds	Most are very hard and either sublime or melt at very high temperatures; most are nonconductors of electricity	C (diamond), C (graphite), SiC, AlN, SiO_2
Molecular *Nonpolar*	Atoms or nonpolar molecules	Dispersion forces	Soft; extremely low to moderate melting points (depending on molar mass); sublime in some cases; soluble in some nonpolar solvents	He, Ar, H_2, CO_2, CCl_4, CH_4, I_2
Polar	Polar molecules	Dispersion forces and dipole–dipole attractions	Low to moderate melting points; soluble in some polar and some nonpolar solvents	$(CH_3)_2O$, $CHCl_3$, HCl
Hydrogen-Bonded	Molecules with H bonded to N, O, or F	Hydrogen bonds	Low to moderate melting points; soluble in some hydrogen-bonded solvents and some polar solvents	H_2O, NH_3

Packing of Spheres

- Closest packed vs. non-closest packed
- Unit cells that result



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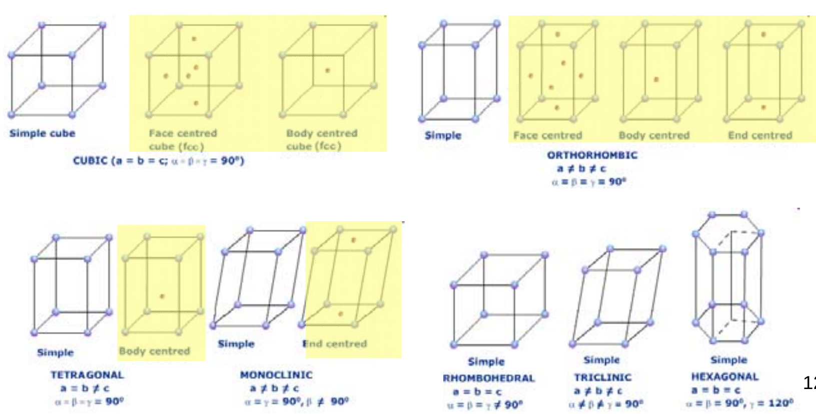
Crystalline Unit Cells

Seven different "simple" unit cells (crystal systems)

- Defined by distance and angles between lattice points.
- We'll focus on **<u>cubic unit cells</u>** - if you understand how cubic works, you can extend to the other six!



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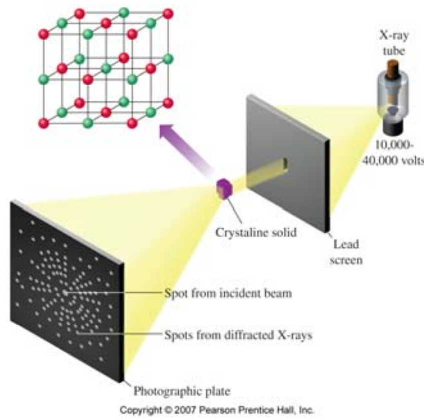
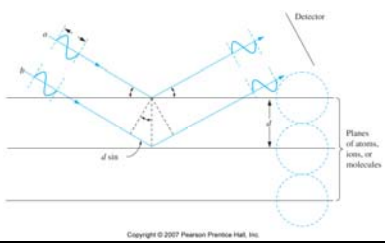
Adapted from: http://www.tutorvista.com/content/chemistry/chemistry-iv/solid-state/unit-cells-types.php

X-Ray Diffraction

- As x-rays impinge on crystal planes, they are scattered…*difracted*
- Angle of scatter depends on spacing in the crystal

  Bragg Equation: $n\lambda = 2d\sin\theta$
- Changing orientation allows 3-D structure to be calculated.





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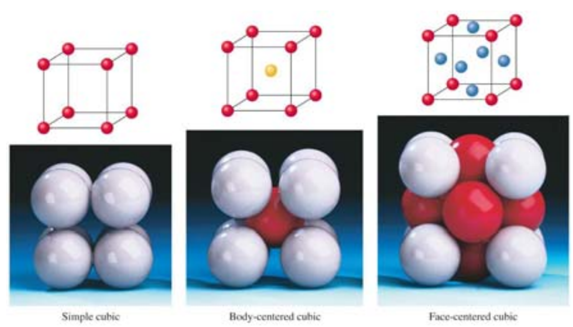
Cubic Cells

- Three symmetries: simple, bcc, fcc
- Counting atoms in the unit cell:
  - Corners
  - Faces
  - Edges



- Determination of atomic/ionic radii and cell dimensions: 2 keys
  1. Know simple, fcc, bcc
  2. Remember right triangle math!

EXAMPLE: Gold is a face-centered cubic unit cell. The density of the solid is 19.32 g/cm^3. Calculate the radius of a gold atom.

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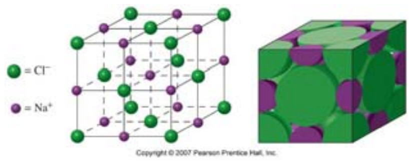
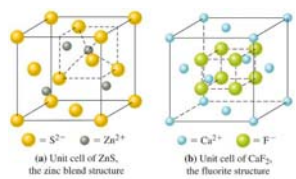
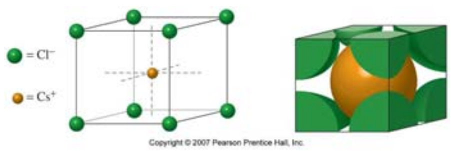
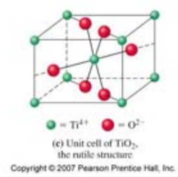
Ionic Crystals

- Typically anions are closest packed and cations fit into "holes"
  - 3 Types: Trigonal, Tetrahedral*, Octahedral*
- * most common
  - Relative size of hole and cation drives structure.
    - Maximize M-X, minimize X-X









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Properties of Solids

$$\text{Solid} \underset{\text{Freezing}}{\overset{\text{Melting}}{\rightleftharpoons}} \text{Liquid}$$

- Enthalpy of Fusion (ΔH^o_{fusion}):
- Freezing point/melting point:
  - "normal" m.p.

$$\text{Solid} \underset{\text{Deposition}}{\overset{\text{Sublimation}}{\rightleftharpoons}} \text{Vapor}$$

- Enthalpy of Sublimation ($\Delta H^o_{sublimation}$):

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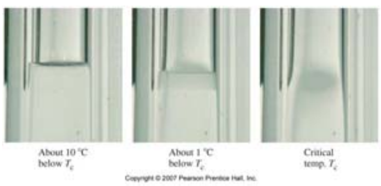
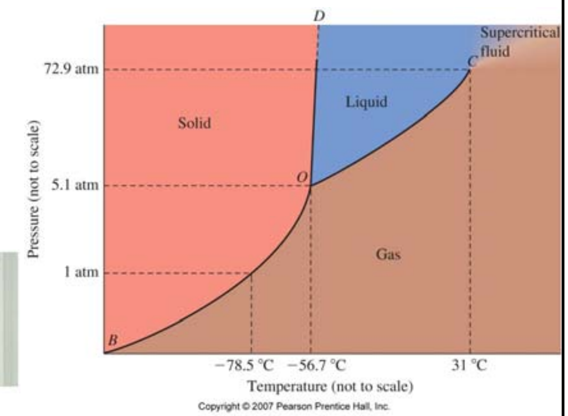
Phase Diagrams

Map out temperature/pressure/phase relationships for materials.

- Shapes differ as physical properties differ.
- What occurs at each boundary?
- Triple Point:
- Critical Point and supercritical fluids

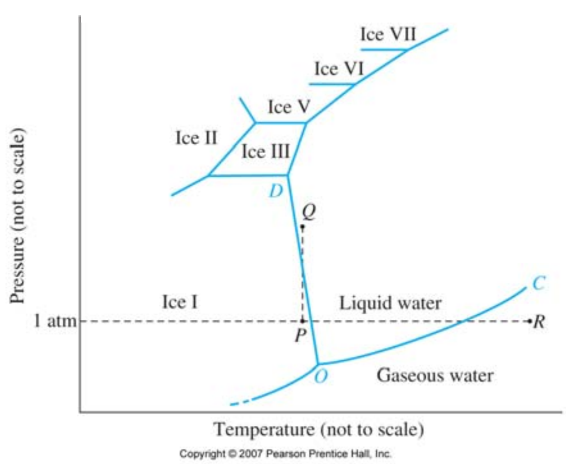




Water: Sorta Weird, Sorta Not!

Triple point: 0.00098^{o}C, 4.58 Torr; Critical point: 374.1^{o}C, 218.2 atm

- Behavior of s-l line
- Polymorphism



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