AP Chemistry Midterm Study Guide

Chapter 1: Matter and Measurement

- <u>Chemistry</u>: the science that seeks to understand the behavior of matter by studying the behavior of atoms and molecules
- Scientific method:
 - <u>Hypothesis</u>: a tentative interpretation or explanation of observations; should be falsifiable
 - <u>Experiment</u>: a controlled procedure to generate observations to support or refute a hypothesis
 - <u>Scientific law</u>: a statement that explains past observations that can be used to predict future ones
 - e.g., <u>law of conservation of mass</u>: matter neither created nor destroyed in chemical reaction
 - <u>Scientific theory</u>: a model to help explain nature and made up of multiple well-established hypotheses, laws, and/or other theories
 - e.g., <u>atomic theory</u>: explains law of conservation of mass and proposed that atoms were small, indestructible particles
- Classification of matter:
 - <u>Matter</u>: something that occupies space and has mass
 - <u>Substance</u>: a specific instance of matter, classified by state and composition
 - <u>Pure substance</u>: substance made of only one particle, fixed composition
 - <u>Mixture</u>: matter composed of different types of particles, varying composition
 - <u>Heterogeneous mixture</u>: when the composition varies from one section to another; components can be physically separated
 - <u>Homogeneous mixture</u>: when the composition is uniform throughout
 - <u>Solution</u>: a liquid homogeneous solution
 - Methods of separating mixtures
 - <u>Decanting</u>: method of separation of heterogeneous solution of an insoluble solid and a liquid (pouring the liquid off)
 - <u>Filtration</u>: method of separation of heterogeneous solutions of an insoluble solid and a liquid (sieving the liquid through)
 - <u>Distillation</u>: method of separation of homogeneous solutions by utilizing different boiling points
 - <u>Element</u>: a pure substance that cannot be broken down smaller
 - <u>Atoms</u>: the building blocks of matter, the smallest particle that has all the properties of that element
 - <u>Compound</u>: a substance composed of multiple atoms joined together chemically
 - <u>Molecules</u>: the combination of atoms by covalent bonds
 - <u>Formula units</u>: the unit that expresses the ratio of atoms in an ionic compound
- <u>States</u> of matter:
 - <u>Solid</u>: atoms vibrate but do not shift past one another; fixed volume and shape

- <u>Amorphous</u> (unstructured) or <u>crystalline</u> (structured in repeating pattern)
- <u>Liquid</u>: atoms move past one another freely but are packed together; fixed volume but not shape
- <u>Gas</u>: atoms move past one another freely and occupy all free space; free volume and shape
- Physical and chemical changes:
 - <u>Physical changes</u>: changes altering state or composition of a substance, but not composition
 - <u>Chemical changes</u>: changes that alter composition of a substance, usually through a chemical reaction
- Physical and chemical properties:
 - <u>Physical property</u>: a property that is displayed without changing a substance's molecular composition
 - Can be <u>intensive</u> (not based on amount of substance, e.g., density) or <u>extensive</u> (based on amount of substance, e.g., mass) properties
 - <u>Chemical property</u>: an intensive property that is displayed only when changing a substance's molecular composition (i.e., an observation relating to a chemical change)
- <u>Volatility</u>: property of a substance indicating its ability to boil (easy to boil = low boiling point = volatile)
- <u>Energy</u>: the capacity to do work
 - <u>Work</u>: the action of a force through a distance
 - Energy of a substance is sum of <u>kinetic energy</u> (energy of movement) and <u>potential</u> <u>energy</u> (stored energy associated with position or composition) associated with object
 - <u>Thermal energy</u> and movement are examples of kinetic energy
 - <u>Chemical potential energy</u> and position are examples of potential energy
 - <u>Law of conservation of energy</u> states that energy can change from one form into another, but cannot be lost— total amount in the universe is constant
 - Systems tend to move from high energy to low energy; high-energy systems are unstable
- <u>International Standard of Units</u> (SI) system based on <u>metric system</u> (as opposed to <u>English</u> <u>system</u>)

- Prefix Symbol Multiplier 10^{18} 1.000.000.000.000.000.000 Е exa 10¹⁵ \mathbf{P} 1,000,000,000,000,000 peta 10^{12} Т 1,000,000,000,000 tera 10⁹ G 1,000,000,000 giga 10⁶ 1,000,000 М mega 10³ 1,000 kilo k 10^{2} 100 hecto h 10^{1} deka da 10 10.1 d 0.1 deci 10^{-2} 0.01 centa С 10-3 0.001milli m 10-6 0.000,001 micro μ 10.9 0.000,000,001 nano n pico р 10^{-12} 0.000,000,000,001 micro micro μμ 10-15 0.000.000.000.000.001femto f 10^{-18} 0.000,000,000,000,000,001 atto а
- Unit multiplier prefixes:

- <u>Significant figures</u> are a system of preserving precision of data through measurements and calculations
 - They are measured so that every digit is estimated, except for the last (measurement plus guessed digit)
 - <u>Exact (counting) numbers</u> have infinite sigfigs, never lose precision
 - Multiply / divide → answer has # sigfigs of the multicand/multiplier/dividend/divisor with least sigfigs
 - Add / subtract → answer has precision to multicand/multiplier/dividend/divisor with least precision
- <u>Precision</u> "refers to how close a series of measurements are to one another or how reproducible they are"
 - <u>Systematic error</u> gives biased probability of too high or too low; higher precision but lower accuracy
- <u>Accuracy</u> "refers to how close the measured value is to the actual value"
 - <u>Random error</u> gives equal probability of too high or low; higher accuracy but lower precision
- <u>Dimensional analysis</u> is a method of converting between units by using <u>conversion factors</u>

Chapter 2: Atoms, Molecules, and Ions

- <u>Scanning tunneling microscopy</u> (STM) allows for the imaging of and moving of individual atoms and molecules
- <u>Law of conservation of mass</u> states that matter is neither created nor destroyed in a chemical reaction
- The atomic model developed through multiple scientists
 - Democritus (ancient Greece) thought that atoms were indestructible, tiny particles

- Dalton built upon the recent ideas of other scientists (such as Copernicus, Kepler, and Newton) to form a more modern atomic theory
- <u>Law of definite proportions</u> states that "all samples of a given compound, regardless of their source or how they were prepared, have the same proportions of their constituent elements"; ratio of elements in compound always the same
- <u>Law of multiple proportions</u> states that "when two elements (call them A and B) form two different compounds, the masses of element B that combine with 1g of element A can be expressed as a ratio of small whole numbers"
- J.J. Thomson discovered the <u>electron</u>, a negatively-charged subatomic particle
 - Cathode rays were shot from one side to another in a cathode ray tube and composed of electron particles
 - Electrons have electrical charge, which create an electric field
- <u>Robert Millikan</u> discovered the charge of an electron using the <u>oil drop experiment</u>, which suspended oil drops based on their charge and size
- <u>Rutherford</u> discovered the <u>nucleus</u> and the <u>proton</u>, which formed the dense, positively-charged center of an atom
 - <u>Chadwick</u> discovered that there were also <u>neutrons</u> in the nucleus
- The <u>atomic mass unit</u> (amu) is a common unit for measuring the mass of subatomic particles
 - 1/12 of the weight of a C-12 atom
- Elements are characterized by <u>atomic number</u> (Z) (number of protons in nucleus) and <u>chemical</u> <u>symbol</u> (1-3 letter representation, first letter capitalized)
 - Elements can vary in number of neutrons; <u>isotopes</u> have same # protons but varying neutrons
 - <u>Natural abundance</u> is the percentage of a certain isotope in a natural sample of an element
 - Sum of neutrons and protons = <u>mass number</u> (A) (approximately equal to atomic mass)
 - Isotopes can be represented like so: ${}_{6}^{12}C$ (for carbon with six neutrons) (mass number superscript, atomic number subscript, chemical symbol on right)
 - Isotopes can be represented like so: carbon-12 or C-12 (for carbon with six neutrons) (element name or formula and then mass number)
 - Isotopes only vary in nuclear stability; chemical and physical properties do not change (dependent on valence electrons and bonding)
 - Elements can vary in number of ions; <u>ions</u> have differing number of electrons and are charged accordingly
 - Positive ions (less electrons than protons) are called <u>cations</u>
 - Negative ions (more electrons than protons) are called <u>anions</u>
- Dmitri Mendeleev ordered the elements according to the <u>periodic law</u>, which states that elements arranged by increasing mass would have recurring (periodic) chemical patterns
 - Moseley later changed periodic law to order by increasing periodic number
- <u>Atomic mass</u> is the weighted average mass of the isotopes of an element based on their relative abundances

- <u>Mass spectrometry</u> involves the ionization of atoms and then shooting them in a trajectory altered by a magnet into a detector; the heavier particles are affected least and vice versa for the lighter particles
- A <u>mole</u> (mol) of a substance is <u>Avogadro's number</u> of it
 - An atom's <u>molar mass</u> is numerically equal in grams per mole as amu per atom (atomic mass)

Chapter 3: Mass Relations in Chemistry: Stoichiometry

- Compounds are very different than their component pieces
- <u>Empirical formula</u> is a chemical formula with the lowest ratios of elements
 Always the case for <u>formula units</u> (ions)
- <u>Molecular formula</u> is a chemical formula that actually occurs for molecules
 - May be the same as the empirical formula
- <u>Structural formula</u> shows bond angles (similar to Lewis structure)
- <u>Ball-and-stick model</u> shows bonding of particle and shows shape
- <u>Space-filling model</u> shows approximate proportions of atoms and how it would look in real life
- <u>Atomic elements</u> (e.g., Na) vs. <u>molecular elements</u> (e.g., BrINClHOF diatomics or S₆)
- <u>Common names</u> (e.g., water) vs. <u>systematic names</u> (e.g., dihydrogen monoxide (???))
- <u>Mass percent composition</u> is percentage of mass of element to mass of compound
- <u>Combustion analysis</u> is used to calculate empirical formulas of substances
 - \circ H \rightarrow H₂O
 - \circ C \rightarrow CO₂
 - $O \rightarrow H_2O$ and CO_2 (subtract sum of masses of Hs and Cs from original)
- Organic compounds mostly carbon and hydrogen (especially as hydrocarbons), sometimes N, O, S
 - \circ Carbon always forms four bonds (i.e., not substances like CO₂ w/ double bonds)
 - Hydrocarbons can have <u>functional groups</u> such as <u>hydroxyl</u> (-OH) groups
 - Hydrocarbons with same functional group form a <u>family</u>

Chapter 4: Chemical Quantities and Aqueous Solutions

- Reaction stoichiometry
- Limiting reactant, theoretical yield, and percent yield
- Solution concentration, molarity
 - <u>Stock solutions</u> are highly-concentrated solutions from which to make laboratory solutions of different concentrations
 - Use $M_1V_1 = M_2V_2$ to convert to lower molarity solution
- <u>Electrolytes</u> are substances that dissolve in water and conduct electricity as an aqueous solution
 - The better they dissolve, the stronger they are and the better the electricity they conduct
 - Often ionic compounds are good electrolytes
- <u>Precipitate reactions</u> happen when two solutes react to form a precipitate (an insoluble solid)
 - Molecular equations are the full equation

- Complete ionic equations have each aqueous compound as ions
- Net ionic equations have reacting elements only (i.e., without spectator ions)
- Acid-base and gas-evolution reactions
- Oxidation-reduction reactions
- Lab: Gravimetric Analysis of Calcium and Hard Water

Chapter 5: Gases

- Measurement of gases
- The ideal gas law
 - Boyle's Law (P-V), Charles' Law (V-T), Guy-Lussac's Law (P-T), Avogadro's Law (n-V)
- Gas law calculations
 - Dalton's Law (sum of partial pressures = total pressure)
- Mixtures of gases and partial pressures
- Stoichiometry of gaseous solution
- Kinetic Molecular Theory (KMT) of gases
 - Volume of gas particle is o
 - Average kinetic energy is proportional to temperature in kelvins
 - Kinetic energy = $\frac{1}{2}mv^2$
 - Collision of particles is elastic
- Mean free path, diffusion, and effusion of gases
 - Use root mean square velocity for velocity of gases
 - Mean free path decreases with pressure and particle size
 - Graham's law of effusion
- Real gases: the effects of size and intermolecular forces
 - At high pressures, volume is greater because of particle size and vice versa
 - At low temperatures, pressure is lower because of high intermolecular forces and vice versa
- *Lab*: Molar Volume of a Gas
- Interactive: PhET Virtual Lab-Gas Laws

Chapter 6: Thermochemistry

- First law of thermodynamics
- Heat, work, pressure-volume work
 - <u>Heat</u>: flow of energy through a distance
 - Transfer of energy between <u>system</u> and <u>surroundings</u> until it reaches thermal equilibrium
 - Internal energy (E) = KE + PE
 - E is a state function
 - <u>Pressure-volume work</u>: work is done when pressure or volume increases
 - There must be a change in temperature for this to happen
- Calorimetry and heat

- Enthalpies
 - $\circ \quad \underline{Enthalpy}(H) = E + PV$
 - $\Delta H = q$ (change in enthalpy = heat, pressure-volume work is cancelled out)
- Thermochemical equations
 - <u>Hess's Law</u>: adding and subtracting thermochemical equations and enthalpies of reactions
 - <u>Standard enthalpy of formation</u>: heat of forming one mole of compound at standard state (kJ/mol)
 - <u>Standard state</u>: 1atm and 25°C
- Relationship between heat and other forms of energy—measurement of first law of thermodynamics
- *Lab*: Designing a Hand Warmer
- *Lab*: Enthalpy of Reaction and Hess's Law

Chapter 7: The Quantum-Mechanical Model of the Atom

- Schrödinger's cat
 - Presents the <u>quantum-mechanical model</u> of the atom, which presents light and particles as both particles and waves
- Light, photon energies, and atomic spectra
 - Light is <u>electromagnetic radiation</u>, with certain properties:
 - Amplitude (intensity)
 - Wavelength $(\lambda) = c/v$ (color)
 - Frequency (v) = c/λ (color)
 - Speed (c) = $v\lambda$
 - <u>Electromagnetic spectrum</u> contains all wavelengths/frequencies of electromagnetic radiation
 - Energy comparison (greater to lesser)
 - Gamma ray
 - X-ray
 - Ultraviolet ray
 - Visible light
 - Infrared waves
 - Microwaves
 - Radio waves
 - <u>Photoelectric effect</u> shows the particle nature of light
 - Light is made up of <u>photons</u>, bundles of light energy
 - Photons are <u>quantized</u>, with distinct amounts of energy
 - E = hv
- Atomic orbitals: shapes and sizes
- PES (photoelectron spectroscopy)
 - <u>Atomic spectroscopy</u>: study of electromagnetic radiation absorbed and emitted by atos
 - <u>Emission spectrum</u> is unique to every element

- Bohr created a model of the atom with quantized energy levels
 - Quantization of electrons shows wave nature

•
$$\Delta E = -2.18 \times 10^{-18} (\frac{1}{n^2} - \frac{1}{n^2})$$

- <u>de Broglie equation</u> for the wavelength of particles
 - $\circ \lambda = \frac{h}{mv}$
- <u>Uncertainty principle</u>: never observe both wave and particle natures of matter or light
 - This is the nature of the <u>particle-wave</u> duality
 - Particle nature and wave nature are <u>complementary properties</u>
- <u>Quantum numbers</u>: notation to indicate an electron's position in an atom
 - <u>Principle</u> (n): energy level (1 to 7)
 - <u>Angular momentum</u> (l): sublevel (0 to (n-1))
 - <u>Magnetic</u> (m₁): orbital position within sublevel (-n to n)
 - Spin (m_s): electron spin ($\pm \frac{1}{2}$)
- <u>Orbital</u>: probability map for up to two electrons, defined by Schrodinger's wave function
- <u>Probability density</u>: probability per unit volume of finding electron in space
- <u>Radial distribution function</u> (total radial probability): represents total probability of finding electron within spherical shell at distance r from nucleus



Graph of wavefunction and distribtuion function

- *Lab*: Discharge Lamps and Flame Tests
 - See atomic spectroscopy / photoelectron spectroscopy
- Lab: PES
 - See atomic spectroscopy / photoelectron spectroscopy

Chapter 8: Periodic Properties of the Elements

- Periodic table history
- Electron configurations and orbital notation
 - <u>Electron configuration</u> organized by <u>aufbau principle</u> (increasing energies)



- <u>Pauli exclusion principle</u>: no two electrons can have the same four quantum numbers; two electrons in same orbital must have opposite spins
- <u>Hund's rule</u>: orbitals in the same sublevel must fill themselves singly before filling doubly
- Energy levels in H are <u>degenerate</u> (have same energy); in other atoms, sublevels are degenerate
- Periodic trends: size and effective charge
 - <u>Coulomb's law</u>: $E = \frac{kq_1q_2}{d^2}$
 - Directly proportional to charge and inversely proportional to distance
 - Helps explain most of the periodic trends
 - Electron <u>shielding</u> leads to <u>effective nuclear charge</u>
 - ENC = total nuclear charge + charge of shielded electrons
 - <u>Penetration</u> decreases shielding
 - <u>Nonbinding atomic radius</u> (Van der Waals radius): half distance between two adjacent atoms
 - <u>Binding atomic radius</u> (covalent radius): half distance between two bonded atoms
- Ions: ionic radius and ionization energy
 - Electrons are lost based on distance from nucleus (energy level), not necessarily reverse aufbau
 - Atoms are either <u>paramagnetic</u> (odd # electrons) or <u>diamagnetic</u> (even # electrons); ions usually diamagnetic (with stable, even # of electrons)
 - Exceptions in ionization energy when moving from s to p sublevels (p is further away, easier to take away even though it has more protons and electrons)
 - <u>Electron affinity</u>: energy change associated with gain of electron
- Metallic character

Chapter 9: Chemical Bonding I: The Lewis Model

- <u>Bonding theories</u> are different chemical models of atoms
 - <u>Lewis structures</u> are a bonding theory that represents molecules with dots, dashes, chemical symbols, and brackets (for ions)

- <u>Valence bond theory</u> is another bonding theory that treats an atom more in its quantum-mechanical state
- <u>Molecular orbital theory</u> is the third bonding theory that treats an atom and its electrons in the quantum-mechanical model
- Chemical bonds form because they lower the energy of a molecule and thus are more stable
 - A <u>chemical bond</u> is "the sharing or transfer of electrons to attain stable electron configurations for the bonding atoms" (according to the Lewis model)
- Ionic bonding and lattice energies
 - <u>Ionic bond</u> is when an atom is ionized by another and the two atoms attract one another according to Coulomb's law
 - Ions can be represented in the Lewis model by brackets with the charge indicated, like so: [№]⁺[:ä:]⁻
 - <u>Lattice energy</u> is the energy associated with the formation of the crystal lattice structure of an ionic compound
 - The creation of an ionic compound is always exothermic because it releases a lot of energy and becomes very stable as a crystal lattice structure because of the many nondirectional charges
 - The stronger the charges or the smaller the ionic radii, the stronger the lattice energy (according to Coulomb's Law)
 - High lattice energy of ionic compounds accounts for ionic compounds' high melting point, inability to conduct electricity as solids, and tendency to conduct electricity in solution
 - The <u>Born-Haber Cycle</u> can be used to calculate this
 - Heat of formation of the gaseous metal + the heat of formation of a single anion (if applicable, from diatomic molecule) + the ionization energy of the cation + the electron affinity of the anion + the lattice energy of the ionic compound = the heat of creation of the ionic compound



<u>^ The Born-Haber Cycle for CsF (used for calculating lattice energy)</u>

- Covalent bonding: Lewis structures
 - <u>Covalent bond</u> is when two atoms *share* electrons
 - A shared pair of electrons in a covalent compound is called a <u>bonding pair</u>
 - A bonding pair can be represented as two dots or a line
 - An unshared pair of electrons in a molecule is called a <u>lone pair</u>
 - A <u>double-bond</u> is when two atoms share four electrons; a <u>triple-bond</u> is when two atoms share six electrons; in both cases, the electrons count towards the octets of both atoms
 - The greater number of bonds, the stronger (more bonding pairs = more charge = higher Coulombic attraction) and shorter (also according to Coulomb's law) the bond
 - Bond attractions are directional (in contrast to nondirectional ionic bonds)
 - This means that there is less attraction and easier bonds to break between molecules, leading to low boiling points
 - The <u>Lewis model</u> consists of <u>Lewis (electron dot) structures</u>, which have atoms represented by their chemical symbol and with their valence electrons represented as dots
 - Examples: chlorine: [;]; oxygen: [;]
 - It has a high predictive power as to what is and is not likely to be a compound

- Eight valence electrons forms an <u>octet</u>, which is usually very stable, hence the <u>octet rule</u>
 - Octet rule has exceptions with odd numbers of electrons (<u>free radicals</u>), <u>incomplete octets</u> (such as BF₃ or H₂), and <u>expanded octets</u> (such as SO₃)
- Metallic bonding and the sea of electrons
 - <u>Metallic bond</u> forms between atoms of a metal and happen when the metals give up electrons to become cations and the electrons hold the metal together
- Electronegativity and bond polarity
 - <u>Electronegativity</u> is the "ability of an atom to attract electrons to itself in a chemical bond"
 - A higher electronegativity in one atom in a covalent bond than another can leads to a <u>polar covalent bond</u>
 - Polar covalent bonds lie between <u>pure covalent</u> and ionic bonds
 - H-Cl is a polar covalent bond: ⁺⁸ H^{---Cl⁻⁸}; the arrow points towards the more electronegative, and the delta-positive/delta-negative can also indicate the more electropositive or electronegative of the two, respectively
 - Electronegativity increases moving up and right in the periodic table
 - <u>Dipole moment</u> is when there is a difference in positive and negative charge
 - <u>Percent ionic character</u> is the "ratio of a bond's actual dipole moment to the dipole moment it would have if the electron were completely transferred from one atom to the other"
 - Over 50% percent ionic character (electronegativity difference > 1.7) means ionic
 - Less than 50% percent ionic character (electronegativity difference < 1.7) means covalent
- Resonance and formal charge
 - <u>Resonance</u> happens when more than one valid Lewis diagram can be drawn for a molecule
 - A <u>resonance hybrid</u> is an average, actual structure of a resonant molecule
 - <u>Formal charge</u> is "the charge [an atom] would have if all bonding electrons were shared equally between the bonded atoms"
 - $\blacksquare \quad FC = VE \frac{1}{2}BE LE$
 - Distinguishes between multiple valid Lewis structures or resonance structures to find the most likely one
 - The lower the formal charge, the better; on an ion, formal charges should sum to the overall charge of the ion; if charges are necessary, the most electronegative atom should hold the negative charge(s)
- Polarity of molecules
- *Lab*: What's in a Bottle?

Chapter 10: Chemical Bonding II: Molecular Shapes, VSEPR, and Molecular Orbital Theory

• VSEPR theory: the five basic shapes

- <u>Valence Shell Electron Pair Repulsion</u> (VSEPR) theory is based off the idea that electron groups repel themselves through coulombic forces
 - Lone pairs occupy more space (more repulsion) than bonding pair
- <u>Electron geometry</u> based on all electron groups; <u>molecular geometry</u> based on bonded groups
 - They are the same when all electrons of atom involved in bonds (0 lone pairs)

	VSEPR Geometries				
Steric No.	Basic Geometry 0 Ione pair	1 Ione pair	2 lone pairs	3 lone pairs	4 lone pairs
2	XEX Linear				
3	X E X Trigonal Planar	E X < 120° Bent or Angular			
4	X Imm, E 109° X X Tetrahedral	X/IIII.E X < 109° Trigonal Pyramid	X E X << 109° Bent or Angular		
5	X 120° X E X X X X X X X X X X X X X	< 90° X Xiii < 120° E X Sawhorse or Seesaw	X 90° X X T-shape	X 180° E X Linear	
6	$X = \frac{X = 90^{\circ}}{X_{H_{H_{ens}}} + \frac{1}{2} \times \frac{1}{2} $	<90° Xhun, and X Square Pyramid	90°X/101. EastHX 90°XXXX Square Planar	X Minus Emult EXX X < 90° T-thape	Linear X 180°

- Lone pairs
- Molecular geometries
- Shape and polarity
 - If polar bonds and unsymmetrical, probably polar
- Hybridization
- <u>Valence bond theory</u>: theory based on the idea of electrons in quantum-mechanical orbitals

• Lowest interaction energy (potential energy is at certain distance with substantial overlap but without too much nuclear repulsion



- Two half-filled orbitals overlap to form bond
- <u>Hybridization</u>: degenerate "hybrid" orbitals
 - Minimizes energy by maximizing overlap
 - Depends on number of electron groups (not bonding pairs):
 - Two electron groups: sp
 - 3: sp²
 - $4: sp^3$
 - 5: sp³d
 - $6: sp^3 d^2$
 - Rotation of double or triple bonds will break molecular geometry, not allowed
- Molecular orbital theory: electron delocalization
- Lab: Molecular Modeling

Chapter 11: Liquids, Solids, and Intermolecular Forces

- Solids (crystalline)
- Liquids
- Gases
 - This state can be induced by pressure changes (lower pressure) to solids or liquids, and vice versa
- KMT
 - See <u>Chapter 5</u>
- Phase changes

- Vaporization and melting (fusion) are endothermic
- Vaporization continues until <u>dynamic equilibrium</u> is reached
 - <u>Vapor pressure</u> is pressure exerted by vapor of liquid at dynamic equilibrium
 - Vapor pressure correlates exponentially with temperature

• Clausius-Clapeyron equation:
$$ln(P_{vap}) = -\frac{\Delta H_{vap}}{R}(\frac{1}{T}) + ln(\beta)$$

- System attempts to keep equilibrium
- <u>Critical point</u> is when <u>supercritical fluid</u> exists
 - Over critical temperature and critical pressure
- <u>Sublimation</u> is direct phase change from solid to gas (and vice versa with <u>deposition</u>)
 - Happen even below boiling point, but often slowly
- <u>Phase diagram</u> represents phase changes at different pressures and temperatures
 - Example:



- Water's phase diagram is unique because of the positive slope of the liquid/solid line because the liquid is more dense
- Surface tension, capillary action, viscosity
 - <u>Surface tension</u>: the "energy required to increase surface area by a unit amount"
 - <u>Viscosity</u>: ability of liquid to flow
 - Measured in poise (P)
 - Increased by higher intermolecular forces, longer or less regular molecular shape, lower temperatures
 - <u>Capillary action</u>: movement of a liquid up a narrow tube
 - Requires higher adhesive forces than cohesive forces
 - Rises until cohesive and adhesive forces are balanced by gravity
 - Rises higher in a narrower tube
- Intermolecular attractions

- Because of Coulomb's law, greater distance between molecules than between atoms of molecule make intermolecular attractions much weaker than intramolecular attractions
- <u>X-ray diffraction</u> uses trigonometry and an interference pattern from atoms to determine space between planes
 - <u>Bragg's Law</u> calculates distance between layers using specific wavelength of light and angle
- Regular arrangement of atoms in crystalline solid = <u>crystalline lattice</u>
 - Crystalline lattices can be represented by a <u>unit cell</u>, a repeating structure of a few atoms



- <u>Packing efficiency</u> is percentage of total space that the atoms occupy
 - <u>Hexagonal closest packing</u> (in hcp and ccp) is the highest packing efficiency
 - Used in hexagonal cubic cell and face-centered (which is like a diagonal hexagonal closest packing) (face-centered is <u>cubic closest packing</u>)
- There are different types of crystalline solids
 - <u>Molecular solids</u> (e.g., ice)
 - <u>Ionic solids</u>: maximize coordinate # and accommodate charge neutrality
 - Usually the more disproportionate the sizes of the ions, the lower the coordination number
 - <u>Atomic solids</u>:
 - Non-binding atomic solids (only noble gases in the solid phase)
 - Metallic solids

- <u>Network covalent atomic solids</u> (e.g., diamond or graphite)
- <u>Band theory</u>: a solid bonding model
 - Electrons are delocalized over the entire crystal (not just atom or orbital)
 - Electrons form a band known as the <u>valence band</u>
 - There is also the <u>conduction band</u> formed of the unfilled, higher-energy orbitals that electrons can use to freely move around the crystal
 - The <u>band gap</u> is small in metals, medium in semimetals, and large in nonmetals
 - In semimetals, the band gap can be controlled using <u>doping</u>
 - Elements with more valence electrons can be doped as impurities to create <u>n-type semiconductors</u> (negative charge because more electrons in conductive band), and vice versa for <u>p-type semiconductors</u>
 - Different semiconductors can be combined to form <u>p-n</u> junctions, which are common computer components
 - P-n junctions can act as diodes or amplifiers in electronics
- Lab: Clausius-Clapeyron Equation

Formulas

- Heat of Reaction Shortcuts:
 - Using Hess's Law: $\Delta H_{rxn}^{o} = \sum n_p \Delta H_f^{o}(products) \sum n_r \Delta H_f^{o}(reactants)$
 - Using bond energies:

 $\Delta H_{rxn}^{o} = \sum (bond \ energies \ of \ reactants) - \sum (bond \ energies \ of \ products)$

- Formal charge: $FC = VE \frac{1}{2}BE LE$
 - \circ FC = formal charge
 - \circ VE = valence electrons
 - BE = bonding electrons
 - \circ LE = lone electrons
- Enthalpy: H = E + PV
 - \circ H = enthalpy
 - \circ P = pressure
 - \circ V = volume
- Pressure-Volume Work: $w = -P\Delta T$
 - \circ w = work
 - \circ P = pressure
 - \circ T = temperature
- Ideal Gas Law: $PV = n \times RT$
 - \circ P = pressure (atm)
 - \circ V = volume (L)
 - \circ n = moles

- R = gas constant ((0.08206 L*atm/mol*K)) depends on which units you use, affects other units in equation for other variables
- T = temperature (K)
- Van der Waals Equation: $(P + a(\frac{n}{a})^2)(V nb) = nRT$
 - a, b = constants dependent on substance
 - (rest of constants same as ideal gas law)
 - Know the concept about how real gases compare to ideal (write how here, and why)
- Combined Gas Law: $\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$
 - P = pressure (any unit)
 - V = volume (any unit)
 - T = temperature (K)
- Root Mean Square Velocity: $\mu = \sqrt{\frac{3RT}{M}}$
 - \circ μ = root mean square velocity, used to find velocity
 - \circ R = ideal gas constant
 - T = temperature (K)
 - \circ M = molar mass
- Dipole Moment: $\mu = qd$
 - $\circ \mu = dipole moment$
 - \circ q = charge
 - \circ d = distance
- Probability density: $\psi^2 = \frac{probability}{unit volume}$
 - $\circ \Psi = \text{probability density}$
- Radial distribution function: *radial probability at radius* $r = \psi^2 \times (volume \ of \ shell \ at \ r)$
- Coulomb's Law: $F = k \times \frac{q_1 q_2}{d^2}$
 - F = electromagnetic attraction between particles
 - \circ k = Coulomb's constant
 - \circ q₁ and q₂ = (signed) charges of particles
 - d = distance between particles
- Change of Molarity Function: $M_1V_1 = M_2V_2$
 - \circ M = molarity
 - \circ V = volume

Constants

• Ideal gas constant (R)

$$R = \frac{0.08206atm \times I}{mol \times K}$$

$$R = \frac{8.314J}{K \times mol}$$

• Joule (J)

$$\circ \quad J = k \times \frac{m^2}{s^2}$$

• Avogadro's constant (N_A) \circ $N_A = 6.022 \times 10^{23}$

- Planck's constant
 - 6.626 x10⁻³⁴ Js
- Speed of light
 - 3.00 x10⁸ m/s

Other things to know

- How to calculate specific heat, or use it
 - \circ ~ Also know other aspects of calorimetry such as c_{cal} (how to calculate?), q_{cal}, etc.
- Basic elements and symbols
- Polyatomic ions

TABLE 2.5 Common Polyatomic Ions					
lon	Name	lon	Name		
Hg_{2}^{2+}	Mercury(I)	NCS ⁻	Thiocyanate		
NH_4^+	Ammonium	CO_{3}^{2-}	Carbonate		
NO_2^-	Nitrite	HCO ₃ ⁻	Hydrogen carbonate		
NO_3^-	Nitrate		(bicarbonate is a widely		
SO_{3}^{2-}	Sulfite		used common name)		
SO_4^{2-}	Sulfate	ClO ⁻	Hypochlorite		
HSO_4^-	Hydrogen sulfate	ClO_2^-	Chlorite		
	(bisulfate is a widely	ClO ₃ ⁻	Chlorate		
	used common name)	ClO_4^-	Perchlorate		
OH^-	Hydroxide	$C_{2}H_{3}O_{2}^{-}$	Acetate		
CN^{-}	Cyanide	MnO_4^-	Permanganate		
PO_{4}^{3-}	Phosphate	$Cr_2O_7^{2-}$	Dichromate		
HPO_4^{2-}	Hydrogen phosphate	CrO_4^{2-}	Chromate		
$H_2PO_4^-$	Dihydrogen phosphate	O_2^{2-}	Peroxide		
		$C_2 O_4^{2-}$	Oxalate		

• Solubility rules

Soluble Ionic Compoun	ds	Important Exceptions None	
Compounds containing	NO ₃ ⁻		
	$C_{2}H_{3}O_{2}^{-}$	None	
	CI-	Compounds of Ag ⁺ , Hg ₂ ²⁺ and Pb ²⁺	
	Br ⁻	Compounds of Ag ⁺ , Hg ₂ ²⁺ and Pb ²⁺	
	I-	Compounds of Ag ⁺ , Hg ₂ ²⁺ and Pb ²⁺	
	SO4 ²⁻	Compounds of Sr ²⁺ , Ba ²⁺ , Hg ₂ ²⁺ and Pb ²⁺	
Insoluble Ionic Compounds		Important Exceptions	
Compounds containing	S ²⁻	Compounds of NH4 ⁺ , the alkali metal cations and Ca ²⁺ , Sr ²⁺ and Ba ²⁺	
	CO3 ²⁻	Compounds of NH4 ⁺ and the alkali metal cations	
	PO4 ³⁻	Compounds of NH4 ⁺ and the alkali metal cations	
	OH-	Compounds of the alkali metal cations, and NH ₄ ⁺ , Ca ²⁺ , Sr ²⁺ and Ba ²⁺	

- How to calculate empirical formulas
- How to balance a chemical reaction

Jonathan Lam Dr. Nuzzo AP Chemistry p. 3

• Systematic and hydrocarbon nomenclature