General Chemistry Anchoring Concepts Content Map

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The outline below delineates the anchoring concepts content map for general chemistry.

- I. Matter consists of atoms that have internal structures that dictate their chemical and physical behavior.
 - A. Atoms have unique chemical identities based on the number of protons in the nucleus.
 - 1. The number of protons specifies the atomic number, which is used as an identifier of the atom/element.
 - a. The atomic number is given in most periodic tables, so students should be able to provide the number of protons of any element.
 - 2. Atoms may have the same chemical identity but different masses and this explains the existence of isotopes.
 - a. Protons and neutrons sum to contribute the mass of an atom.
 - b. Atoms of one element have the same number of protons but can have differing numbers of neutrons. These are called isotopes.
 - c. Measures of mass are made at scales much larger than individual atoms, so elements have atomic masses that are the weighted average of all naturally occurring isotopes.
 - d. The isotopic abundance of any given element is not a constant of nature, and may vary depending on the origin of the sample being studied.
 - *B.* Electrons play the key role for atoms to bond with other atoms.
 - 1. For a neutral atom there are as many electrons as there are protons, but the electrons can be categorized as core (inner) and valence (outer) electrons.
 - a. Valence electrons, which determine the properties of elements, are correlated with the groups in the periodic table.
 - 2. The quantum model of the atom is capable of explaining many observations, and it organizes electrons into "orbitals", which are wavefunctions that are identified using quantum numbers.
 - a. The quantum mechanical model of the atom introduces the concept of orbitals, including atomic orbitals.
 - b. Quantum numbers specify the wavefunctions that are the orbitals.
 - 3. The occupation of atomic orbitals by electrons is summarized in the electron configuration, and this tool is helpful in understanding which atoms form chemical bonds, what type, and how many bonds they form.
 - a. Electron configuration is a shorthand notation that summarizes the orbital occupations of electrons in an atom or ion.

- b. Electron configuration notation for transition metal ions reflects that they can differ slightly from the patterns observed for main group ions.
- c. Electrons will occupy atomic orbitals following both the aufbau principle and Hund's rule.
- *C.* Atoms display a periodicity in their structures and observable phenomena that depend on that structure.
 - 1. Some properties of atoms, such as atomic radius, ionization energy, and electron affinity follow periodic trends.
 - a. Sizes of atoms and ions can be assigned and they demonstrate periodic trends.
 - b. In addition to atomic radii, other properties such as ionization energy, electron affinity, and effective nuclear charge are relatable to periodic trends.
 - 2. Effective nuclear charge is a useful model for explaining periodic trends in atomic properties.
 - a. Effective nuclear charge accounts for both the nuclear charge and the effect of shielding of that charge by core electrons.
 - b. Relative sizes of atoms and ionization energy can predicted based on effective nuclear charge.
 - 3. Reactivity trends of elements show periodic trends that are also relatable to the atomic structure of the atoms of the elements.
 - a. Elements in the same group have similar chemical and physical properties and valence electron configurations.
- D. Most information about atoms is inferred from studies on collections of atoms often involving an interaction with electromagnetic radiation.
 - 1. Electromagnetic radiation can be characterized by wavelength or frequency and different wavelengths of radiation are useful for different measurements of matter.
 - a. The interaction of photons with molecules and atoms provides information about energy levels.
 - b. Atomic spectra are unique for a given element.
 - 2. Kinetic molecular theory is an important bridge between particulate and macroscopic models of behavior.
 - a. Postulates of kinetic molecular theory can be listed for ideal gases, and their implications identified.
 - b. The manner in which these postulates for ideal gases fail for real gases depict important concepts related to the volume of gas particles and the interactions between them.
- *E.* Macroscopic samples of matter contain so many atoms that they are counted in moles.
 - 1. The mole is defined based on the relative mass scale for atoms, and this results in Avogadro's number being equal to 6.02×10^{23} .
 - a. The translation between atomic level understanding and macroscopic understanding is facilitated by the concept of a mole.
 - 2. Conversions involving the mole (molar mass, g/mol, mol/# of atoms, etc.) are critical to being able to describe matter at both the nanoscale and the macroscopic scale.

- a. Quantitative conversions with the concept of the moles are important.
- b. The types of conversions that are important include the determination of empirical or molecular formulas.
- 3. The size scale of atoms is roughly the picometer scale, which helps explain why Avogadro's number is so large.
 - a. A sense of scale of sizes of atoms and the distance between the nucleus and electrons is integral to understanding fundamental concepts in chemistry.
- *F.* Atoms maintain their identity, except in nuclear reactions.
 - 1. Conservation of macroscopic mass in chemical reactions is due to the conservation of atoms.
 - a. Equations describing chemical reactions can be balanced based on conservation of atoms.
 - 2. Atoms change identity in nuclear reactions; it is possible to write nuclear equations that follow these changes.
 - a. Balancing nuclear reactions is based on the simultaneous conservation of both atomic and mass numbers.
- *G.* Ions arise when the number of electrons and protons are not equal, and can be formed from atoms.
 - 1. Anions form from atoms when additional electrons are added, while cations form from atoms when electrons are removed.
 - a. The charge on monoatomic anions and cations can often be predicted by their position in the periodic table.
 - 2. Ions have chemical properties that differ from the atoms from which they are derived.
 - a. The formation of ions often imparts stability to otherwise very reactive atoms.

II. Bonding: Atoms interact via electrostatic forces to form chemical bonds.

- A. Because protons and electrons are charged, physical models of bonding are based on electrostatic forces.
 - 1. Ionic bonding is described via the interaction of positive and negative charged ions via Coulomb forces.
 - a. The key attractive forces in ionic bonding give rise to the lattice energy which can be roughly predicted by the charges and sizes of the ions involved.
- B. Because chemical bonds arise from sharing of negatively charged valence electrons between positively charged nuclei, the overall electrostatic interaction is attractive.
 - 1. Electrons occupy "shells" so that the outer, valence electrons are the ones involved in chemical bonding.
 - a. Valence electrons are responsible for bonding.
 - b. The number of valence electrons shows periodic trends that result in predictable numbers of bonds being formed by atom.
 - 2. Covalent bonds arise when valence electrons are shared, in pairs, between nuclei.

- a. The build up of (negatively charged) electron pairs between (positively charged) nuclei leads to a bonding interaction.
- C. When chemical bonds form, the overall energy of the bonding atoms is lowered relative to free atoms, and therefore energy is released.
 - 1. Graphical depiction of the potential energy as a function of interatomic distance for a chemical bond shows both the stabilization for intermediate distances and repulsion for very short distances.
 - a. The energy of interaction between electrons and nuclei are captured graphically by plotting potential energy as a function of distance between atoms.
 - 2. Valence bond theory describes bonds in terms of overlap of electron waves.
 - a. The concept of atomic orbital overlap leading to chemical bonding as embodied in valence bond theory represents a useful tool for understanding the basic components of the quantum mechanics of bonding.
 - b. Sigma and pi bonds are a key way to distinguish chemical bonds obtained from valence bond theory.
- D. To break a chemical bond requires an input of energy.
 - 1. The energy required to break a chemical bond is the bond dissociation energy.
 - a. Bond dissociation energy is useful at the level of individual molecules; for calculations on macroscopic quantities, the value used is the bond dissociation enthalpy.
 - b. Bond dissociation enthalpies can be used to estimate the change in enthalpy for a reaction.
- *E.* A theoretical construct that describes chemical bonding utilizes the construction of molecular orbitals for the bond based on overlap of atomic orbitals on the constituent atoms.
 - 1. Molecular orbital theory describes chemical bonds via molecular orbitals derived from atomic orbitals.
 - a. In the quantum model of atoms and molecules, the combination of atomic orbitals leads to the formation of bonding and antibonding molecular orbitals.
 - b. Bond order can be defined in terms of the occupation of bonding and antibonding orbitals by electrons.
 - c. Hybrid atomic orbitals are useful in describing bonding, particularly for organic molecules.
- *F.* Covalent bonds can be categorized based on the number of electrons (pairs) shared. The most common categories are single, double, and triple bonds.
 - 1. Single bonds share one pair of electrons, double bonds share two pairs of electrons, triple bonds share three.
 - a. Bond energy increases as the number of shared pairs increases.
 - b. Bond length decreases as the number of shared pairs increases.
- G. Metallic bonding arises in many solids and fundamentally involves the sharing of valence electrons among many positively charged "cores" over extended distances.

- 1. A simple model of metallic bonding invokes the concept of a "sea of electrons" that move relatively freely amidst the positively charged cores.
- 2. A more rigorous model of metallic bonding depicts electrons occupying bands.
 - a. The band gap between the valence band and conduction band can explain the difference between conductors, semiconductors, and insulators.
- III. Structure and Function: Chemical compounds have geometric structures that influence their chemical and physical behaviors.
 - A. Atoms combine to form compounds that have new properties based on structural and electronic features.
 - 1. Most molecules form using fixed ratios of atoms.
 - a. Mass percentages can be converted to atomic ratios.
 - b. The chemical formula reflects the atomic ratios.
 - 2. In addition to chemical compounds, elements may form chemical bonds so that the stable states are small molecules.
 - a. Some elements may have stable molecular forms (e.g., diatomics) that include multiple atoms.
 - b. Some elements have allotropes—multiple, stable forms.
 - *B.* Models exist that allow the prediction of the shape of chemicals about any bonding atom in a molecule.
 - 1. Using Lewis structures and VSPER theory, it is possible to roughly predict many chemical structures.
 - a. Lewis structures are an important model that allows one to keep track of bonding and nonbonding pairs of electrons in molecules.
 - b. The VSEPR model allows for the general prediction of shape about an atomic center in a covalent molecule.
 - c. Simple Lewis structure-level models of molecules are sometimes inadequate, and one key place where shortcomings occur can be explained by the concept of resonance.
 - C. Theoretical models are capable of providing detail structure for whole molecules based on energy minimization methods.
 - D. Symmetry, based on geometry, plays an important role in how atoms interact within molecules and how molecules are observed in many experiments.
 - *E.* Three-dimensional structures may give rise to chirality, which can play an important role in observed chemical and physical properties.
 - *F.* Reactions of molecules can often be understood in terms of subsets of atoms, called functional groups.
 - 1. Chemical formulas often designate the existence of functional groups in a molecule by listing those atoms as a group.
 - G. Many solid state, extended systems exist, and geometric structures play an important role in understanding the properties of these systems.
 - 1. Bonding types in solids include metallic bonding, ionic, and covalent network.
 - a. Many materials form crystalline solids that can be understood in terms of repeating (via translational symmetry) many units of a structure, called the unit cell.

b. Basic understanding of cubic unit cells provides a key example of this phenomenon, and should include some quantitative aspects.

IV. Intermolecular Interactions: Intermolecular forces—electrostatic forces between molecules—dictate the physical behavior of matter.

- A. Intermolecular forces are generally weaker, on an individual basis, than chemical bonds, but the presence of many such interactions may lead to overall strong interactions.
 - 1. Substances exist as a gas at room temperature when intermolecular forces are weak. Models for gas behavior can be quite general because these forces are small—the most common is the ideal gas model.
 - a. Gases have physical properties that are often independent of the identity of the gas; the conceptual understanding the relationships between these properties are important.
 - b. The quantitative relationships between properties of gases are summarized for most systems using the ideal gas law.
 - c. Gases in mixtures generally act as independent species that can be quantitatively described using partial pressure.
 - 2. Properties that depend on intermolecular forces include phase, vapor pressure, surface tension, etc.
 - a. Graphical summaries of the phase behavior of one-component systems, called phase diagrams, are useful tools for a compact understanding the phase behavior of these systems.
- *B.* For large molecules, intermolecular forces may occur between different regions of the molecule. In these cases, they are sometimes termed noncovalent forces.
- C. Intermolecular forces can be categorized based on the permanence and structural details of the dipoles involved.
 - 1. Key intermolecular forces include dispersion, dipole–dipole, and hydrogen bonding.
 - a. All common intermolecular forces can be understood in terms of models that invoke either permanent or instantaneous dipole moments.
 - b. Forces are present between molecules, and the categories of these forces (dispersion, dipole–dipole, and hydrogen bonding in particular) are important organizational ideas for conceptualizing physical properties of chemical systems.
 - c. Hydrogen bonding is a specialized form of intermolecular interaction that is important in the physical properties of water and in the intermolecular forces present in many living systems.
 - 2. VSEPR structure, coupled with concepts of bond dipoles, can be used to determine the presence of a permanent dipole.
 - a. In covalent bonding, electron pair sharing is not always equitable and the model of electronegativity differences allows one to explain when polar covalent bonds will form.
 - b. Permanent molecular dipoles may be inferred qualitatively by considering vector addition of bond dipoles and the geometries predicted via VSEPR theory.

- D. For condensed phases that are not structures of extended chemical bonds, the physical properties of the state are strongly influenced by the nature of the intermolecular forces.
 - 1. Solutions can be characterized as electrolytes or nonelectrolytes based on whether or not they conduct electricity.
 - a. The aqueous solutions of some solutes will conduct electricity.
 - 2. Solution behavior is largely dictated by intermolecular forces between solute and solvent molecules.
 - a. In a solution, there is a key distinction between solute and solvent molecules.
 - b. Intermolecular forces play a critical role in understanding the solubility of materials in each other. In the case of water as a solvent, the concepts of hydrophilic and hydrophobic summarize these ideas fairly succinctly.
 - c. Solutions have physical properties different from pure substances, and many of these properties are not dependent on the nature of the solute. Conceptual and quantitative understanding of such colligative properties is important.
 - 3. Quantitative understanding of solutions is usually predicated on calculations based on solute concentrations.
 - a. Calculations using molarity of solutions—including determination of molarity, making a solution of known molarity, and reaction stoichiometry of solutions—are key quantitative skills.
 - b. Depending on the nature of the quantitative property being determined, different concentration units may be needed when carrying out calculations related to solutions.
- *E.* The energy consequences of chemical reactions that take place in condensed phases (solution) usually must include intermolecular forces to be correctly/completely explained.
 - 1. Heats of solution and other thermodynamic factors (entropy of solution formation) are key factors in the formation of a solution.
 - a. Salts may dissolve either exothermically or endothermically.
- V. Chemical Reactions: Matter changes, forming products that have new chemical and physical properties.
 - A. In chemical changes, matter is conserved and this is the basis behind the ability to represent chemical change via a balanced chemical equation.
 - 1. A fundamental skill for chemistry is the ability to write a balanced chemical equation.
 - a. Chemical equations represent reactions symbolically so they must be balanced and accurately portray reactants and products.
 - b. Predicting the reactivity of chemicals is a key skill that ultimately involves the ability to write a balanced chemical equation.
 - 2. The chemical equation provides key information for quantitative problem solving in stoichiometry.
 - a. Stoichiometric calculations of chemical reactions are based on mole ratios determined from balanced chemical equations.

- b. Because chemical equations provide mole ratios, stoichiometry problems involving masses require the use of molar mass conversions.
- c. Because chemical equations provide mole ratios, stoichiometry problems involving solutions will require calculations using molarity and volume.
- d. Because chemical equations provide mole ratios, stoichiometry problems involving gases require using the ideal gas law for most systems.
- *B.* Chemical change involves the breaking or forming of chemical bonds, or typically both.
 - 1. Line structures of reactants and products can depict the changes in chemical bonds while conserving the number of atoms.
- C. Chemical change can be observed at both the particulate and macroscopic levels, and models exist that allow the translation between these two levels of observation.
 - 1. The visualization of chemical change at the particulate level enhances reasoning about stoichiometry and should include the concept of limiting reactants.
 - a. Schematic drawings at the particulate level are capable of depicting the inherent stoichiometry of a reaction, including whether or not limiting reactants must be accounted for.
- D. There are a large number of possible chemical reactions, and categories have been devised to organize understanding of these reaction types.
 - 1. Categories such as synthesis, decomposition, and double displacement are used to describe reactions.
 - 2. Oxidation–reduction reactions are important and include combustion.
 - a. Describing a reaction as oxidation–reduction is aided by establishing oxidation numbers of reactants and products.
 - b. Oxidation–reduction reactions are important to chemistry and are sometimes referred to as "redox" reactions.
 - c. Being able to identify an oxidation–reduction reaction often involves assigning oxidation numbers and includes concepts of oxidizing and reducing agents.
 - d. The oxidation–reduction of metals yields a measure of the activities of metals.
 - 3. Acid–base neutralization is an important category of reaction that includes several definitions.
 - a. Categorizing reactions in terms of acid–base chemistry, particularly in water, is important.
 - b. Categorizing acid–base reactions can be facilitated by a basic understanding of acid–base strength.
 - c. The definition of an acid as a proton donor and a base as a proton acceptor is a key concept of acid–base chemistry.
 - d. The definition of an acid as an electron pair acceptor (Lewis acid) and a base as an electron pair donor (Lewis base) is a key concept of acid–base chemistry.

- *E.* Chemical change can be controlled by choices of reactants, reaction conditions, or use of catalysts.
 - 1. Utilizing solubility and/or precipitation reactions allows for the qualitative analysis of ions present in a solution.
 - a. Predicting the reactivity of chemicals is a key skill that can involve knowledge of solubility rules.
 - 2. Control of chemical reactions is often not fully accomplished, so details such as limiting reactants and percentage yields are important in characterizing what occurs.
 - a. Stoichiometric calculations must determine the limiting reactant when it is not clear that some reactant(s) are present in excess.
 - b. Stoichiometric calculations provide the theoretical yield, which can be used to determine percentage yield.
- *F.* Controlling chemical reactions is a key requirement in the synthesis of new materials.
 - 1. Modern materials represent an important example of the synthesis of new materials.
 - a. Some solid-state modern materials, including those that compose applications such as LEDs, do not require whole-number stoichiometry.

VI. Energy and Thermodynamics: Energy is the key currency of chemical reactions in molecular scale systems as well as macroscopic systems.

- *A.* Most chemical changes are accompanied by a net change of energy of the system.
 - 1. The role of kinetic versus potential energy is a key aspect of understanding how energy plays a role in chemical reactions.
 - 2. Energy changes can be considered in terms of heat and work.
 - a. Concepts related to energy in chemistry require careful definitions that are more precise than are used in everyday language.
 - b. In thermodynamic treatments of chemical systems, the definition of the system of interest versus the surroundings is important.
 - 3. There are a wide variety of energy units, so care must be taken to use consistent units when considering energy changes quantitatively.
 - 4. Within thermodynamics, it is important to distinguish between internal energy (the heat associated with a constant volume process) and enthalpy (the heat associated with a constant pressure process).
- B. Many chemical reactions require an energy input to be initiated.
 - 1. Reactive chemicals may remain stable for long times because the reactions they undergo must be initiated by some form of energy input, such as a spark or flame.
- C. The type of energy associated with chemical change may be heat, light, or electrical energy.
 - 1. Heat exchange is measured via temperature change.
 - a. Heat flow into the system is defined as endothermic and out of the system is defined as exothermic.
 - b. Heat flow is obtained from ΔT via molar heat capacity or specific heat.

- 2. The enthalpy of reaction is a measure of heat exchange for reactions carried out at constant pressure.
- 3. Electrochemistry is predicated on oxidation–reduction reactions, and involves physically separating the electron production of oxidation from the electron consumption of reduction.
 - a. Completion and balancing oxidation–reduction reactions requires both mass and charge balance, and often is facilitated by the concept of a half-reaction.
 - b. Oxidation–reduction reactions can be considered in two halves, and can be physically separated to form electrochemical systems.
- D. Breaking chemical bonds requires energy; formation of chemical bonds releases energy.
 - 1. While breaking a chemical bond is always endothermic, chemical energy can be released via reactions because bonds are both broken and formed in the course of the reaction.
- *E.* The forces that are associated with energy change in chemical processes are electrostatic forces.
 - 1. Moving charge in an external circuit (electrochemistry) provides one lever by which this concept is measured.
 - a. When an electrochemical system is built, it is possible to determine the cell potential.
 - b. Trends related to cell potential are summarized via tables of standard reduction potentials.
 - c. Calculations using standard reduction potentials can determine cell potential and the spontaneous direction of an electrochemical reaction.
 - $d. \ \ Nonstandard \ situations \ are \ addressed \ via \ the \ Nernst \ equation.$
 - e. External electrical energy can be used to drive an electrochemical system in the nonspontaneous direction. Quantitative information about stoichiometry of these systems can be derived from variables related to electricity flow.
- *F.* In accord with thermodynamics, energy is conserved in chemical changes, but the change of form in which the energy is present may be harnessed via natural or human-made devices.
 - 1. Pressure–volume (*PV*) work is a common means by which chemical changes, particularly combustion, are harnessed in human-made devices.
 - 2. Electrochemical cells provide one way that chemical change is harnessed in human-made devices (batteries).
 - a. Batteries and fuels cells are important applications of electrochemical systems.
- *G.* Thermodynamics provides a detailed capacity to understand energy change at the macroscopic level.
 - 1. Thermodynamic reasoning includes careful definitions of terms and variables.
 - a. Standard states of substances play a key role in thermodynamic calculations.
 - b. A key concept within thermodynamics is the state function, which can be defined as a quantity whose value is independent of its history.

- 2. Hess's law takes advantage of enthalpy being a state function to allow the determination of enthalpy change for a reaction based on combinations of more readily measured, or tabulated reaction enthalpies.
 - a. Enthalpy is a key thermodynamic state function for calculation of heat exchange for many processes; these calculations include Hess's law.
 - b. The concept of Hess's law is useful is calculating thermodynamic properties from both reactions and tabulated values.
- *H.* The tendency of nature to disperse, particularly in terms of energy distribution, is embodied in the state function called entropy.
 - 1. Spontaneous changes will always increase the entropy of the universe (practically speaking—the entropy of the system and surroundings).
 - a. The definition of entropy and the ability to calculate change in entropy for a reaction are important.
 - b. A qualitative, conceptual understanding that processes that lead to more random physical distributions of particles will increase entropy is valuable.
 - 2. Gibb's free energy is a state function that simultaneously calculates entropy for the system and surroundings, and is useful for determining whether or not a process occurs spontaneously.
 - a. Gibbs energy is defined in such a way that the calculation of it provides insight into whether a process is spontaneous with a single calculation.
 - b. There are several ways to calculate the change in Gibbs energy that should be known by students.
 - 3. The entropy of a perfect crystal at 0 K is 0.
 - a. Because the entropy has a specific value at 0 K, tabulated values for entropy need not be enumerated as changes relative to a standard reference state.
- *I.* Energy changes associated with nuclear chemistry are many orders of magnitude larger than those of classical chemical changes.
 - 1. Basic concepts related to energy in nuclear reactions derive from the conversion of mass to energy.
 - a. Nuclear chemistry arises when there are changes in the nuclei of atoms.
 - b. Mass deficits in nuclear reactions arise from the conversion of mass to energy and are calculated via the equation: $E = mc^2$.
 - c. Nuclear reactions give off radiation that may have biological effects.

VII. Kinetics: Chemical changes have a time scale over which they occur.

- A. Chemical change can be measured as a function of time and occurs over a wide range of time scales.
 - 1. The rate of the reaction must be defined in a manner that is not dependent on which reactant or product is used to measure it.
 - 2. Rate is generally defined as the change in concentration of a reactant or product as a function of time.
 - a. Chemical reactions may occur at a wide range of rates, and a key aspect of rate is related to the concentration of species involved in the reaction.

- B. Empirically derived rate laws summarize the dependence of reaction rates on concentrations of reactants and temperature.
 - 1. The "order" of a reaction is derived from the exponent on the concentration term of a given reactant in the rate law.
 - a. Rate laws are always determined experimentally, and the methods of initial rates or graphical depiction of rates provide the key method for determining rate laws.
 - b. Once known, a rate law can be used to quantitatively predict concentrations of species involved in a reaction as a function of time.
 - c. The kinetics of nuclear processes is first order and can be quantitatively treated, often by indicating the half-life of a nuclear reaction.
 - 2. The temperature dependence of the reaction rate is contained in the rate constant. This temperature dependence is often well modeled by the Arrhenius model.
 - a. Empirical fits of temperature data in kinetics can be used to estimate the activation energy.
- *C.* Most chemical reactions take place by a series of more elementary reactions, called the reaction mechanism.
 - 1. The reaction stoichiometry does not imply the species actually involved in a reaction.
 - 2. It is possible to devise a series of reactions that, when summed, yield the overall reaction and provide a mechanism for how the reaction occurs.
 - a. Chemical reactions often occur via multiple steps, called the reaction mechanism.
 - b. One step in a mechanism, the rate determining step, is often much slower than others and this slow step tends to determine the overall reaction rate.
- D. An elementary reaction requires that the reactants collide (interact) and have both enough energy and appropriate orientation of colliding particles for the reaction to occur.
 - 1. The collision theory of reactions indicates that collisions result in products only if there is enough energy and if the orientation of the reactants is appropriate.
 - a. The number of particles involved in a collision defines the reaction as unimolecular, bimolecular, or termolecular.
 - b. At the molecular scale, reactions are required to overcome an energy barrier, called the activation energy, in order to take place.
 - 2. The energy required to initiate a reaction is called the activation energy.
 - 3. A representative geometric structure at this point in the reaction progress is called the transition state.
- *E.* Catalysis increases the rate of reaction and has important applications in a number of subdisciplines of chemistry.
 - 1. A catalyst is defined as an agent that increases the rate of the reaction while not being consumed by the reaction.
 - a. Catalysts can be either homogeneous or heterogeneous.

- 2. A catalyst increases the rate of the reaction by providing a new reaction pathway with a lower activation energy.
 - a. Catalysts provide an alternative reaction pathway that lowers this activation energy.
- *F.* Reaction products can be influenced by controlling whether reaction rate or reaction energy plays the key role in the mechanism.
- VIII. Equilibrium: All chemical changes are, in principle, reversible; chemical processes often reach a state of dynamic equilibrium.
 - A. Both physical and chemical changes may occur in either direction (e.g., from reactants to products or products to reactant).
 - 1. Phase changes are reversible and provide a good example of dynamic equilibrium.
 - a. Interpretation of phase diagrams can be tied to the understanding of equilibrium concepts.
 - B. When opposing processes both occur at the same rate the net change is zero.
 - 1. Opposing process may be phase changes or chemical reactions.
 - a. Concentration versus time profiles can be used to demonstrate kinetic versus equilibrium realm.
 - *C.* For chemical reactions, the equilibrium state can be characterized via the equilibrium constant.
 - 1. The equilibrium constant can be used in calculations that determine the amount of reactants or products present at equilibrium for a given initial state.
 - a. The equilibrium state is characterized by a constant, designated *K*, which provides quantitative information of the extent of a reaction and is related to the ratio of the concentrations of reactants and products.
 - b. The equilibrium constant, *K*, is a function of temperature.
 - 2. Solubility of solids, particularly ionic solids, provides an example of chemical equilibrium.
 - a. Dissolving of solids in water provides an example of equilibrium systems, for which quantitative understanding via K_{sp} can be derived.
 - b. There are limitations related to using molarity as the unit of concentration in this type of equilibrium problem, so answers obtained are subject to error.
 - D. When the equilibrium constant is very large or small, products or reactants, respectively, are primarily present at equilibrium. Systems with K near 1 have significant amounts of both reactants and products present.
 - 1. Because the equilibrium constant is determined for the reaction as written, the reverse reaction has the inverse equilibrium constant.
 - a. Strong acids have very large *K* values and insoluble substances have very small *K* values.
 - 2. The equilibrium constant for a series of reactions is the product of the individual equilibrium constants.
 - *E.* If perturbed, a system at equilibrium will respond in the direction that tends to offset the perturbation.

- 1. The direction of change in a system that is perturbed from equilibrium is predictable—it will change so as to minimize the perturbation.
 - a. The ability to predict the direction a reaction will progress for a given perturbation is a key concept.
- *F.* Thermodynamics provides mathematical tools to understand equilibrium systems quantitatively.
 - 1. The equilibrium constant is related mathematically to the change in free energy.
 - a. Calculations of the equilibrium constant of a system from the free energy of that system are important.
 - 2. For electrochemical systems, the cell potential is also related to the change in free energy.
- *G.* Equilibrium concepts have important applications in several subdisciplines of chemistry.
 - 1. Many reactions categorized as acid-base are described via equilibrium.
 - a. Acid–base chemistry, particularly in water, forms an important example of equilibrium systems. Conceptual and quantitative understanding of this form of equilibrium system is important.
 - b. The laboratory technique of titration serves as a key example for acidbase chemistry and interpretation of titration curves, both conceptually and quantitatively, is an important tool for chemists.
 - c. $\,\,$ pH is used in quantitative descriptions of acid–base chemistry.
 - 2. Buffers resist changes in pH because both the acid and base of a conjugate pair are present.
 - a. Weak acid–base systems are capable of forming buffer systems that tend to resist changes in the pH of the system.
 - b. Conceptual and quantitative understanding of buffers are important.
 - 3. Protein–substrate binding can serve as another example of the application of equilibrium concepts.

IX. Experiments, Measurement, and Data: Chemistry is generally advanced via experimental observations.

- A. Quantitative observation of matter can be made at a wide range of distance scales and/or time scales.
 - 1. Laboratory observations are made and then often understood in terms of particulate-level models.
 - 2. Laboratory observation of reaction rates helps to establish the concept of reaction time scales empirically.
 - a. Rate laws and reaction order are determined using empirical rate data.
- *B.* Because there are a large number of compounds, a system of naming these compounds is used.
 - 1. A system of nomenclature is applied based on the classification of the substance.
 - a. Anyone who works with chemicals needs to be able to name compounds, including binary inorganic compounds, acids, and some organic chemicals.

- C. Experimental control of reactions plays a key role in the synthesis of new materials and analysis of composition.
 - 1. One key way to control reactions is to control the amount of reactants by varying concentrations.
 - a. Le Châtelier's principle is demonstrated by varying the concentration of one species and observing the outcome on the overall reaction.
- D. Chemical measurements are based on mass, charge, or interaction with electrons or photons.
 - 1. Stoichiometry provides an example of mass measurements being used in the laboratory, particularly for percentage yield.
 - 2. Atomic line spectra provide important evidence that led to the quantum model of the atom.
 - a. Spectral data can be used to demonstrate quantized energy levels in atoms in the gas phase.
 - 3. Mass spectroscopy can provide data that shows the existence of isotopes of elements.
 - a. Mass spectrum data can also be used to illustrate the importance of isotopic abundances.
- *E.* Observations are verifiable, so experimental conditions, including considerations of the representativeness of samples, must be considered for experiments.
- F. Fidelity of inferences made from data requires appropriate experimental design.
 - 1. Data can be characterized by both accuracy and precision.
 - a. While the words "accuracy" and "precision" can be used nearly interchangeably in everyday life, in the laboratory they have specific meanings that must be understood.
 - 2. Error in data can be either random or systematic.
 - a. Significant figures are used to reflect the level of error.
 - b. Standard deviation is relatable to the level of error.
- X. Visualization: Chemistry constructs meaning interchangeably at the particulate and macroscopic levels.
 - A. Many theoretical constructs are constructed at the particulate level, while many empirical observations are made at the macroscopic level.
 - 1. Kinetic molecular theory provides an important bridge for the particulate and macroscopic levels.
 - a. Gases provide an important example of bridging particulate and macroscopic description at the general chemistry level through kinetic molecular theory.
 - b. The diffusion and effusion of gases may be understood in terms of kinetic molecular theory and described quantitatively through Graham's laws.
 - 2. Understanding the relationship between symbolic, macroscopic, and particulate representations of matter and reactions is important.
 - B. The mole represents the key factor for translating between the macroscopic and particulate levels.

- 1. The mole is a measurable quantity that is set by the choice that $^{12}\mathrm{C}$ has a mass of exactly 12 amu.
- *C.* Macroscopic properties result from large numbers of particles, so statistical methods provide a useful model for understanding the connections between these levels.
 - 1. The idea that the Boltzmann distribution is a distribution function can provide an entrée into the importance of statistical reasoning at the general chemistry level.
- D. Quantitative reasoning within chemistry is often visualized and interpreted graphically.
 - 1. Energy profiles for reaction progress include both kinetic and thermodynamic information.
 - 2. Manipulation of data (e.g., taking natural log or inverse) as part of graphical depictions can be helpful in making appropriate inferences of the phenomena the data represent.

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