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.
      b. Atomic symbols are important representations and students need to know most of these symbols to function efficiently in the chemistry classroom.
   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.
      e. Ultimately, the atomic mass system is a relative one, based on the mass of a carbon-12 atom.

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 wave functions 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 wave functions 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. Definitions of ionization energy and electron affinity are important concepts for relating observable phenomena to periodic trends.
      c. 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 be 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.
      b. Atomic ratios within individual compounds, when related to periodic trends, can be used to identify what elements are present in a compound.
      c. The organization of the periodic table is identified with group numbers and names that are useful for categorization purposes beyond correlations with atomic structure.

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
depicts important concepts related to the volume of gas particles and
the interactions between them.

3. Many measurable properties of matter require bulk quantities, and
qualitative trends can be used to categorize these properties.
   a. Phases of matter are an important bulk quantity.
   b. Some properties of matter depend on individual atoms (or ions) of an
element, and others are meaningful only for bulk quantities of atoms.
   c. Trends in bulk properties, such as conductivity and reactivity, can be
used to identify elements present in an unknown substance.
   d. Some bulk properties are extensive and others are intensive.
   e. Important categorization schemes of matter, such as metal versus
nonmetal, are useful at both atomic and bulk scales.

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 $6.02 \times 10^{23}$.
   a. The translation between atomic-level understanding and macroscopic
understanding is facilitated by the concept of the 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 particulate level and the
macroscopic scale.
   a. Quantitative conversions with the concept of the moles are important.

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.

3. Measurements of radioactivity can be used to identify which unstable
isotopes are present in a sample and in what quantity.
   a. Radioactive half-lives are unique and may be used to identify what
isotopes are present.
   b. Radioactivity may occur via alpha, beta, gamma or other decay events
and the type of radioactivity observed is often an important component
of identifying the decaying isotope.
   c. In a mixture, the amount of a radioactive isotope can be determined via
quantitative measurement of radioactive events.
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.
      b. Symbolic representations of ions include the charge in addition to the atomic symbol, thereby imparting knowledge of both the number of protons and electrons present (and neutrons, if mass number is also given in the representation).
   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. Lattice structures of ionic substances display the alternation of opposite charges, which leads to a net attractive force.
      2. Covalent bonds can be distinguished from ionic ones and trends can be predicted based on the elements involved in the bonding.
         a. Bonds formed between two nonmetals tend to be covalent, while bonds formed between a metal and a nonmetal tend to be ionic in character.
      3. There is essentially a continuum of bonding behavior from ionic, through polar covalent, and ultimately nonpolar covalent bonding.
         a. Differences in electronegativity of elements involved in bonding can be used to predict the extent of charge separation when a bond forms.
         b. Electronegativity trends for elements have periodic tendencies, with electronegativity tending to increase towards the top and right of the periodic table, excluding the noble gas group.
   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 an 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.
b. Prior to bond formation, shared electrons may be either on one atom involved in the bond or both. The former distinguishes a coordinate covalent (or dative) bond.

C. *When chemical bonds form, the overall energy of the bonding atoms is lowered relative to free atoms, and therefore energy is released.*
   1. The net result of the formation of any stable chemical bond is a lowering of the energy of the system. If the energy is not lowered, the bond is not stable.
      a. Not all atoms combine to form stable chemical bonds, but when a bond forms it is always accompanied by a lowering of the energy.
   2. Graphical depiction of the potential energy for a chemical bond as a function of interatomic distance shows both the stabilization for intermediate distances and repulsion for very short distances.
      a. The energy of interaction between electrons and nuclei is captured graphically by plotting potential energy as a function of distance between atoms.
   3. Valence bond theory describes bonds in terms of overlap of electron wave functions.
      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, as 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.
      d. Molecular orbital theory helps account for unpaired electrons in molecules and can thereby explain the observation of paramagnetic behavior. $\text{O}_2$ is a common example.
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 amid 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 new compounds that have new properties based on structural and electronic features.
      1. Most compounds 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, some elements themselves may form chemical bonds so that their most 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.
      3. The formation of molecules may lead to pure substances, but often mixtures of molecules are observed.
         a. It is possible to depict the difference between a pure substance and a mixture, particularly at the atomic and molecular scale.

B. Models exist that allow the prediction of the shape of chemicals about any bonding atom in a molecule.
   1. Many molecules exist with more than one isomer, species that have the same chemical formula but have atoms arranged differently in space.
      a. Structural isomers have distinctly different connectivity between atoms.
      b. Stereoisomers have the same connectivity between atoms but different spatial arrangements.
   2. Drawing Lewis structures is a common, simple model for describing atomic connectivity in molecules.
      a. Lewis structures are an important model that allows one to keep track of bonding and nonbonding pairs of electrons in molecules.
      b. 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. The octet rule is an important guide in the drawing of Lewis structures, but many molecules do not follow the octet rule.
3. Using the VSEPR (valence shell electron-pair repulsion) model in conjunction with Lewis structures makes it possible to roughly predict many chemical structures.
   a. The VSEPR model allows for the general prediction of shape about an atomic center in a covalent molecule.

C. Theoretical models are capable of providing detailed 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.
      a. The ability to identify functional groups in a molecule is an important skill for using representations.
      b. An important reason to define functional groups is that they allow the prediction of reactivity patterns.
   2. Functional groups are important in acid–base chemistry and strengths of acids and bases can often be understood in terms of functional groups.
      a. The strengths of oxoacids follow identifiable trends.

G. Periodic trends among elements can be used to organize the understanding of structure and function for related chemical compounds.
   1. Atoms and ionic sizes influence how solids, such as metals or ionic salts, pack into condensed structures.
      a. Lattice energy of ionic substances is influenced by the size of the ions involved; therefore, periodic trends in ionic sizes can predict trends in lattice energy.

H. 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.
      c. Metals, ionic solids, covalent network solids, and molecular solids have distinctive macroscopic properties that allow them to be categorized.
   2. Macromolecules exist and their properties are often understandable in terms of the units that comprise them.
      a. Polymers are macromolecules that are synthesized by repeated incorporation of a limited number of monomer units.
      b. Polymer properties are strongly influenced by their structures, including whether or not they are highly “branched.”
c. Natural polymers, such as polypeptides and polysaccharides, are important in biological chemistry.

3. The practical implications of solid and extended systems are diverse and often focus on the availability of a specific element within a compound.
   a. Refining of metal ores is an important practical chemical reaction that is normally designed to obtain a specific element.
   b. Chemical fertilizers may be small molecules, but are often ionic substances designed to deliver a specific element to crops.

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 of the relationships between these properties is important.
   b. Pressure is a key variable in describing gases; over time there have been many ways that the measurement of pressure has been carried out, leading to an array of units for measuring pressure.
   c. The quantitative relationships between properties of gases are summarized for most systems using the ideal gas law.
   d. 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 of the phase behavior of these systems.
   b. For pure substances, quantitative measurement of physical properties may allow the identification of the substance.
   c. Adhesion, cohesion, surface tension, and vapor pressure are observable bulk properties that rely on the same basic intermolecular forces present in the liquid.

3. When intermolecular forces only are overcome (broken), the chemical nature of the small molecules is not altered and the process is called a physical change.
   a. When a phase change occurs, the molecules involved do not change as they change phases.
   b. Physical and chemical changes are most easily distinguished at the atomic or molecular scale. If the molecules involved in the process do not change, it is a physical change. Otherwise it is a chemical change.
   c. For a given pure substance, the temperature at which a phase change occurs is a characteristic of that substance. Temperature does not change when a phase change is occurring, even though energy flow as heat is occurring.
B. For large molecules, intermolecular forces may occur between different regions of the molecule. In these cases, they are sometimes termed noncovalent forces.
   1. Macromolecules, including synthetics polymers and biochemical molecules, are examples of systems where nonbonding forces occur between atoms in the same large molecule.
      a. The specificity of base pairing in DNA and RNA is associated with hydrogen bonding interactions between nucleotide bases on opposite strands of the system.

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 the VSEPR model.

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.
      b. The origin of electrical conductivity in aqueous solutions is the solvation of ions because separate cations and anions can carry current in solution.
   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.

d. Gases are capable of dissolving in liquids and the extent of solubility is governed by the nature of the molecules involved and the pressure.
e. Mixtures can be characterized as homogeneous or heterogeneous.
f. Solutions are homogeneous mixtures that can be separated by physical means, such as distillation.
g. Solution behavior can have qualitative practical applications, such as water hardness.

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 and 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.
c. In some cases, a net ionic equation (in which spectator ions are removed) is an important tool in describing a chemical or physical process.

2. An important observation of reactions is that mass is conserved.
a. Conservation of mass in a chemical reaction can be observed in the laboratory or calculated based on the masses of the reactants and products.
b. When laboratory reactions include gaseous substances (including components of air), the conservation of mass must account for the mass of gases consumed or produced in the reaction.

3. 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.

   a. Precipitation reactions are common examples of double displacement reactions.

   b. Removal of waters of hydration of ionic solids is a category of reactions that finds common use in introductory chemistry laboratory classes.

2. Oxidation–reduction reactions are important and include combustion.

   a. Oxidation–reduction reactions are important to chemistry and are sometimes referred to as “redox” reactions.

   b. Being able to identify an oxidation–reduction reaction often involves assigning oxidation numbers.

   c. The use of oxidation–reduction reactions as a category includes the concepts of oxidizing and reducing agents.

   d. Completion and balancing of oxidation–reduction reactions requires both mass and charge balance and is often facilitated by the concept of a half-reaction.

   e. The oxidation–reduction of metals (with each other or with acids) yields a measure of the activities of metals.

   f. Materials that are combustible are undergoing oxidation–reduction reactions, often with oxygen in air.

3. Acid–base neutralization is an important category of reactions 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. Many chemical properties of elements follow periodic trends that can be used to strategically design reactions to achieve desired outcomes.

1. With some exceptions, elements in a single group or row on the periodic table have reactivity trends that vary in predictable ways when reacting with water or air.
   a. Reactivity trends vary in predictable ways as you move down and to the right on the periodic table, with a few exceptions.

F. 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.

G. 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; heat flow out of the system is defined as exothermic.
      b. Heat flow is quantitatively obtained from $\Delta T$ via molar heat capacity or specific heat and the mass of the substance involved.
      c. By convention, numerical estimates of exothermic processes carry a negative sign, while endothermic processes carry a positive sign.
      d. When observed in the laboratory, exothermic processes will show warming (heat evolved), while endothermic processes will show cooling (heat absorbed).
   2. The enthalpy of reaction is a measure of heat exchange for reactions carried out at constant pressure.
      a. Enthalpies of reaction, such as those incorporated in a thermochemical equation, can be used to calculate energy flow for a given amount of reactant or product.
   3. Electrochemistry is predicated on oxidation–reduction reactions, and involves physically separating the electron production of oxidation from the electron consumption of reduction.
      a. Oxidation–reduction reactions can be considered in two halves, and can be physically separated to form electrochemical systems.
      b. Electrical energy can be obtained from electrochemical systems operating as galvanic cells.

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.
      a. The extent of energy release or absorption is dictated by the bonds broken in the reactants and the bonds formed in the products.

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 fuel cells are important applications of electrochemical systems.

G. Thermodynamics provides a detailed capacity to understand energy change at the macroscopic level.

1. A key concept within thermodynamics is the state function, which can be defined as a quantity whose value is independent of its history.
   a. Standard states of substances play a key role in thermodynamic calculations.

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. Tabulated values for the calculation of thermodynamic variables often take advantage of the concept of the formation reaction.
   c. The concept of Hess’s law is useful in 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 of processes that lead to more random physical distributions of particles with an increase in entropy is valuable.
   c. An individual, nonspontaneous process can occur when linked to another process such that the combined events increase the entropy of the universe.

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 free 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. The Gibb’s free energy is defined in terms of enthalpy and entropy changes; students should be able to consider these components both quantitatively and qualitatively.
c. Calculations of Gibb’s free energy from tabulated values are important not only to obtain $\Delta G$, but often to estimate equilibrium constants or cell potentials as well.

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.

4. Thermodynamic spontaneity alone cannot predict whether a process will occur. Some spontaneous processes occur too slowly to be readily observed.
   a. Even spontaneous processes may not be observed if there is a large activation energy for the process to begin.

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.
         a. The reaction rate should incorporate reaction stoichiometry when it is defined.
      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.
      3. When solids are included in reactions, surface area is an important factor in the rate of reaction.
         a. A reactive solid with a large surface area will react more rapidly than the same solid with a smaller surface area.
   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. Under most circumstances, an increase in temperature leads to an increase in reaction rate.
   b. 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.
      c. Given a reaction mechanism and knowing the rate determining step allows the rate law to be inferred. This rate law must match the observed empirical rate law for a mechanism to be valid.
      d. A compatible rate law does not “prove” the correctness of a mechanism.
      e. Species that appear in a reaction mechanism but not in the overall reactions are called intermediates and their identification can provide important evidence about how well the mechanism describes the reaction.

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.
      a. In many cases, overcoming the activation energy is achieved by high-speed collisions between rapidly moving molecules in a sample.

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.
   b. Catalysts play an important role in applications, such as catalytic converters on cars, or environmental events, such as ozone depletion.

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.
   b. Because a catalyst lowers the activation energy, it affects both forward and reverse reactions.

F. Reaction products can be influenced by controlling whether reaction rate or reaction energy plays the key role in the mechanism.
1. When reaction rate is the dominating factor for an observed process, it is said to be kinetically favored. When reaction energy is the dominating factor, it is said to be thermodynamically favored.
   a. Observing changes over time can sometimes distinguish between kinetically and thermodynamically favored processes.

VIII. Equilibrium: All physical and chemical changes are, in principle, reversible and 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 reactants).
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. Dynamic processes that achieve equilibrium may be phase changes or chemical reactions.
   a. Concentration versus time profiles can be used to demonstrate kinetic versus equilibrium realm.
   b. Equilibrium is dynamic because rates of opposing process are the same, but the rate is not commonly zero.

C. For chemical and physical processes, 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.
   c. The equilibrium constant, $K$, incorporates reaction stoichiometry as part of the ratio.
d. Calculations using equilibrium constants may determine $K$, or estimate equilibrium concentrations given initial concentrations of a system with a known value of $K$.

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. Very large or very small values of the equilibrium constant, $K$, indicate reactions strongly favoring products (in the former case) or reactants (in the latter).
   a. Reactions with very small values of $K$ will have little formation of products, while reactions with very large values of $K$ will proceed nearly completely to products.

2. 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 are considered fully ionized; weak acids have small $K$ values and are only partially ionized.
   b. For some reactions, particular acid–base chemistry, the concept of $pK_a$, $pK_b$, or $pK_w$ can both illustrate the relationship between the equilibrium constant of forward and reverse reactions, and provide qualitative reasoning for reaction extents.
   c. $K_{sp}$ values can be used to rank relative solubilities for sparingly soluble salts, or obtain numerical estimates of measureable solubility of these salts.

3. The equilibrium constant for a series of reactions is the product of the individual equilibrium constants.
   a. Qualitative analysis methods, such as the formation of complex ions, take advantage of differences in $K_{sp}$ or combined equilibrium constants to separate species dissolved in water.

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.
   b. Reasoning based on perturbations of equilibrium can be used to determine conditions that maximize product formation in a reaction.

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.
b. Systems achieve equilibrium when free energy is minimized.
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 acid–base chemistry; 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.
   d. Conjugate bases of weak acids are strong, and conjugate acids of weak bases are strong. Thus, salts of weak acids and bases affect pH.
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 is 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. Materials are frequently mixtures of chemical substances.
   1. Mixtures may be homogeneous or heterogeneous.
      a. Macroscopic samples of everyday objects and systems can serve as examples of homogeneous versus heterogeneous mixtures.
   2. Methods such as distillation and chromatography can be used to separate mixtures.
      a. A simple distillation apparatus can be used to separate mixtures in the laboratory.
B. Quantitative observation of matter can be made at a wide range of distance, energy, frequency, and/or time scales.
   1. Laboratory observations are made and then often understood in terms of particulate-level models.
      a. While molecular-scale observations are not generally made in the introductory chemistry laboratory, interpretation of results often invokes molecular-scale reasoning.
      b. Historically, the development of the atomic theory of matter was driven by experimental observations.
   2. Laboratory measurements are sometimes combined into ratios; for example, density is measured via a ratio of mass and volume.
a. Calculations that use density may include both the determination of the density from mass/volume data or the use of a known density with the measurement of either mass or volume.

b. Practical implications for density include the concept of buoyancy.

3. 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.

C. 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.

D. 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.

E. Chemical measurements are based on mass, charge, temperature, pressure, volume, or interaction with electrons or photons.
   1. Stoichiometry provides an example of mass measurements being used in the laboratory, particularly for percentage yield.
      a. Graphical analysis of reaction yields as a function of reagent amounts can reveal when a particular reactant is in excess and identify an unknown reaction stoichiometric ratio.
      b. Calculation of percentage yield is an important skill and may help determine the relative utility of a laboratory synthesis method.
   2. Practical implications of laboratory reactions include the ability to generate species of interest (such as oxygen) or release energy (by combustion of fuels).
      a. Common laboratory reactions to generate known species, such as oxygen, are an important component of descriptive chemistry.
      b. Many hydrocarbons can be used as fuels; the combustion of a hydrocarbon in air produces carbon dioxide and water.
   3. 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.
   4. Mass spectrometry can provide data that show the existence of isotopes of elements.
      a. Mass spectrum data can be used to illustrate the existence of isotopes of an element and the importance of isotopic abundances.

F. Observations are verifiable, so experimental conditions, including considerations of the representativeness of samples, must be considered for experiments.
1. Laboratory methods can be devised so that conditions limit the possibilities of measurement errors.
   a. Techniques in setting up and carrying out laboratory experiments are an important component of instruction in introductory college chemistry.
   b. Gaining familiarity with laboratory instruments and glassware is a key skill for the development of appropriate laboratory design methods.
   c. Errors in measurement can occur when techniques (such as meniscus reading or incomplete transfer of chemicals between vessels) arise in the laboratory.

2. The preparation of solutions and accurate determination of their concentrations are important components of defining experimental conditions.
   a. Correct uses of volumetric glassware and/or dilution methods are important techniques in the preparation of solutions for chemical experimentation.
   b. Determination of solution concentration is often carried out via titration with a standard.

G. Fidelity of inferences made from data requires appropriate experimental design and data analysis.

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.

3. Proper laboratory procedures record all observations and correct recording errors with cross-outs rather than erasures.
   a. Appropriate methods for keeping a laboratory notebook are important in the instruction of introductory college chemistry.

4. Calibration with samples of known quantities is a common method for determining unknowns in a laboratory setting.
   a. Construction and use of calibrations curves is an important laboratory skill.
   b. Standardization of laboratory solutions is a form of calibration that is an important laboratory skill.

H. Chemistry experiments have risks associated with them, so chemical safety is a key consideration in the design of any experiment.

1. Knowledge of appropriate safety apparatus is important knowledge for any work being done in the laboratory.
   a. Students should be able to identify and use safety equipment in the laboratory.

2. Knowledge of chemical hazards and safety procedures associated with chemicals is important in the chemistry laboratory.
a. Assessing the hazards associated with chemical procedures, such as the dilution of strong acids or heating of chemicals, is an important skill for introductory chemistry courses.

b. Appropriate storage and labeling of chemicals is a constant component of good chemical safety practices. This includes understanding safety terminology and the language, signs, and symbols commonly found in Safety Data Sheets and on labels.

c. Basic knowledge about handling of exposure to chemicals due to spills or other accidents is an important component of chemical safety.

d. Basic knowledge of and appropriate use of personal protective equipment, such as safety goggles, gloves, and lab coats, are important features of chemical safety.

e. Basic knowledge of the possible hazards of chemicals, such as flammability, toxicity, and corrosiveness, is an important component of chemical safety.

f. Basic knowledge of the routes of exposure for chemicals, such as inhalation, ingestion, and dermal routes, is an important component of chemical safety.

3. Appropriate disposal of chemical waste is a key component of chemical safety and hygiene.

   a. Appropriate disposal of chemical waste is needed in any laboratory and students should know general guidelines related to chemical waste handling.

4. Students should develop an “awareness” of chemical safety when conducting experiments that involves continual consideration of hazards and risks due to chemicals, chemical procedures, and physical hazards that may be present.

   a. The concept of a “culture of safety” is an increasingly important component of chemical education.

5. Radioactive chemicals require additional knowledge related to risks and use of radioactive materials must include appropriate protective measures.

   a. Exposure to different forms of radiation pose different levels of risk, and students should have a general knowledge of these differences.

X. Visualization: Chemistry constructs meaning interchangeably at the particulate and macroscopic levels.

   A. Many theoretical models 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.
a. Schematic drawings can depict key concepts at the particulate level, such as mixtures versus pure substances, compounds versus elements, or dissociative processes.

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 $^{12}$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 entry point into the importance of statistical reasoning at the general chemistry level.
   2. Many macroscopic observables are the result of gradients in a key, molecular-scale quantity.
      a. Gradients in temperature result in the flow of energy as heat.
      b. Concentration gradients lead to diffusion or osmosis.

D. Quantitative reasoning within chemistry is often visualized and interpreted graphically.
   1. Energy profiles for reaction progress include both kinetic and thermodynamic information.
      a. Students should be able to distinguish exothermic and endothermic reaction depictions from an energy profile representation.
      b. Students should be able to identify the concept of activation energy within an energy profile representation.
   2. Manipulation of data (e.g., taking the natural log or the inverse of the data) as part of graphical depictions can be helpful in making appropriate inferences of the phenomena the data represent.
      a. Direct plots of experimentally measured quantities are sometimes able to provide key inferences, but in other cases data manipulation tends to make the interpretation easier.
      b. Some experimentally observed phenomena, such as absorbance or transmission of light, may be recorded either directly or as an inverse of the observation.
      c. When data of interest can range over several orders of magnitude, logarithms are often useful in helping graphical interpretations.

E. Mathematical equations provide a tool to visualize chemical and physical processes.
   1. Rearrangement of common mathematical expressions can either isolate variables or identify relationships that enhance understanding of the system being described.
      a. The ideal gas law can be manipulated to show the relationship between the molar mass and density of a gas.
BIBLIOGRAPHY


