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1. LEC 1: FUNDAMENTALS 1 - AUG 25

SI = International System of Units

Different measurement devices provide different levels of precision or uncertainty. Use all known digit plus on estimated digit to properly record the uncertainty in measurement.

Precision - how close the measurements in a series are to **each other**

Accuracy - how close each measurement are to the **actual value**

Refer to significant figures rules when doing calculations.

2. LEC 2: FUNDAMENTALS 2 - AUG 27

Total mass of substance does not change during a chemical reaction.

Atom - electrically neutral , spherical entity composed of a positively charged nucleus surrounded by negatively charged electrons.

2.1. ELEMENTAL INFO FROM PERIODIC TABLE

Atomic number - # of protons = # of electrons Atomic mass - average mass of all nature occurring isotopes of an element

- Number of protons characterizes the element.
- Number of neutrons tells you if the element is an isotope.
- Number of electrons tells you if the element is an ion.



- A = mass number = # of protons + # of neutrons
- Z = atomic number = # of protons

- X = chemical symbol of the element

$$\text{atomic mass} = \sum \text{isotope mass} \times \text{fractional abundance}$$

2.2. IONIC AND COVALENT COMPOUNDS

Ionic compounds - usually metal + nonmetal, electrically neutral

- Metal atoms tends to lose electrons to form cations
- Nonmetal atoms tends to gain electrons to form anions

Covalent compounds - usually nonmetal + nonmetal, nonmetal bonding

Atoms lose electrons or gain electrons tends to form noble gas configuration (full outer shell of electrons).

Many transition metals form more than one cation.

Polyatomic ions - two or more atoms covalently bonded together with an overall charge.

3. LEC 3: FUNDAMENTALS 3 - SEP 1

$$1 \text{ mol} = 6.022 \times 10^{23} \text{ formula units} = \text{Avogadro's Number}$$

Atomic / Molecular Scale: we use the “atomic mass unit”, **amu**

Mass in amu cannot be determined easily using an analytical balance.

Macroscopic Scale: we use the “mole”, **mol** and grams, **g**

- **Atomic mass number** - the number of protons and neutrons in a atom.
 - unit: amu
- **Molecular mass** / formula mass - the average mass of a molecule
 - unit: amu
- **Molar mass** - the mass per 1 mole of substance in grams
 - unit: g/mol

4. LEC 4: FUNDAMENTALS 4 - SEP 3

A balanced chemical equation has the same number of atoms of each element on both sides of the equation.

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$

- The percent yield is always less than or equal to 100%.

5. LEC 5: FUNDAMENTALS 5 - SEP 10

Solution - homogeneous mixture of two or more substances

Solvent

- largest component of the solution
- can be solid, liquid, or gas

Solute

- smallest component of the solution
- can be solid, liquid, or gas

5.1. ELECTROLYTE AND NONELECTROLYTE SOLUTIONS

- Some compounds form aqueous solution can conduct electricity
 - compounds that break apart into ions when dissolved in water
 - e.g., NaCl, HCl, KOH
- Some compounds form aqueous solution DO NOT conduct electricity
 - compounds that do not break apart into ions when dissolved in water
 - e.g., sugar, alcohols
- **Strong electrolytes** dissolve and dissociate completely in water into ions (conduct electricity well)
 - HCl, HNO₃, HClO₄, H₂SO₄, NaOH, Ba(OH)₂, ionic compounds
- **Weak electrolytes** dissolve and dissociate partially in water into ions (conduct electricity poorly)
 - CH₃COOH, HF, HNO₃, NH₃, H₂O

- **Nonelectrolytes** dissolve in water but do not dissociate into ions (do not conduct electricity)
 - $(\text{NH}_2)_2\text{CO}$ (urea)
 - CH_3OH (methanol)
 - $\text{C}_2\text{H}_5\text{OH}$ (ethanol)
 - $\text{C}_6\text{H}_{12}\text{O}_6$ (glucose)
 - $\text{C}_{12}\text{H}_{22}\text{O}_{11}$ (sucrose)

5.2. CONCENTRATION OF SOLUTIONS

Concentration

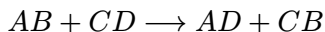
- Relative amount of solute and solvent in the solution
- quantitative amount of solute dissolved in solvent or solution

$$\text{Molarity (M)} = \frac{\text{moles of solute}}{\text{volume of solution (Liters)}}$$

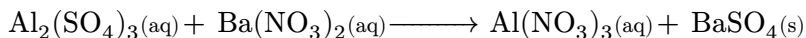
6. LEC 6: FUNDAMENTALS 6 - SEP 15

Double replacement reaction - two compounds react to form two new compounds by exchanging ions

General format:



Example:



The driving force of the displacement reaction is the formation of a stable product. This can be an insoluble solid precipitate.

- Full chemical equation - shows all reactants and products
- Ionic equation - write out all ions and states
- Net ionic equation - cancel out spectator ions

Neutralization reaction - acid + base $\rightarrow$ salt + water

6.1. DEFINITION OF ACID AND BASE

Acids - substance that produces H^+ when dissolved in water

- Strong acids ionize completely in water
 - HCl , HBr , HI , HNO_3 , HClO_4 , H_2SO_4
- Monoprotic acids - HCl , HNO_3
- Diprotic acids - H_2SO_4
- Triprotic acids - H_3PO_4

Bases - substance that produces OH^- when dissolved in water

7. LEC 7: THERMOCHEMISTRY 1 - SEP 17

$$\text{Universe} = \text{System} + \text{Surroundings}$$

$$\Delta E = E_{\text{final}} - E_{\text{initial}} = E_{\text{products}} - E_{\text{reactants}}$$

Law of Conservation of Energy: Energy can be converted from one form to another, but it can be neither created nor destroyed.

$$\Delta E_{\text{universe}} = \Delta E_{\text{system}} + \Delta E_{\text{surroundings}} = 0$$

- Endothermic: Transfer energy into the system
- Exothermic: Transfer energy out of the system

$$\Delta E = q + w$$

- heat (q) energy transferred because of difference in temperature
 - + means system **gains** heat
 - - means system **release** heat
- work (w) energy transferred when an object is moved by a force
 - + means work is done **on** the system
 - - means work is done **by** the system

7.1. STATE FUNCTIONS: E , H , P , V , T

state function - property of a system that determine only by the system's current state, regardless of how it arrived at that state

- symbols: $E, \Delta E, H, \Delta H, P, V, T$
- the change in a state function is independent of the path taken to reach that state

Enthalpy, H = the total energy or heat content of a system. Enthalpy represents the heat energy tied up in chemical bonds.

$$\Delta H = H_{\text{final}} - H_{\text{initial}} = H_{\text{products}} - H_{\text{reactants}}$$

- **Exothermic reaction:** $\Delta H < 0$, heat is released
- **Endothermic reaction:** $\Delta H > 0$, heat is absorbed

8. LEC 8: THERMOCHEMISTRY 2 - SEP 22

- Often the heat absorbed or released by a reaction is expressed in J or kJ.
- Usually the enthalpy change is expressed on a molar basis, in kJ/mol.

8.1. WAYS TO CALCULATE OR DETERMINE ΔH_{rxn}

1. Calorimetry

$$q = c \cdot m \cdot \Delta T \quad \text{and} \quad \Delta H_{\text{rxn}} = q_{\text{rxn}} / \text{mol}$$

2. Stoichiometry

Use ΔH_{rxn} provided for the reaction as written.

3. Hess's Law

Manipulate given reactions with ΔH_{rxn} values to find ΔH_{rxn} for reaction.

4. Use heats of formation (ΔH_f°)

$$\Delta H_{\text{rxn}}^\circ = \sum_n \Delta H_f^\circ(\text{products}) - \sum_m \Delta H_f^\circ(\text{reactants})$$

8.1.1. STANDARD ENTHALPY OF FORMATION

Standard enthalpy of formation: enthalpy change for the chemical reaction when 1 mol of a compound in its standard state 25°C is produced from its component elements in their **standard states**.

For any physical or chemical process, if values for the standard heats of formation of all the reactants and products are known, the enthalpy change for the process can be calculated.

9. LEC 9: THERMOCHEMISTRY 3 - SEP 24

9.1. HESS'S LAW OF HEAT SUMMATION

Hess's Law states that the enthalpy change of an overall process is the sum of enthalpy changes of individual steps.

$$\Delta H_{\text{overall}} = \sum_n \Delta H_n$$

9.2. STOICHIOMETRY OF THERMOCHEMICAL EQUATIONS

A **thermochemical equation** is a balanced equation that includes the enthalpy change of the reaction ΔH_{rxn} .

- The **sign of ΔH** indicates whether the reaction is exothermic or endothermic. Reverse reaction reverses the sign of ΔH_{rxn} .
- The **magnitude of ΔH** is proportional to the amount of substance.

10. LEC 10: QUANTUM THEORY 1 - SEP 29

10.1. THE WAVE NATURE OF LIGHT

The energy of light is propagated by oscillating electric and magnetic fields as the light moves in space.

- frequency (ν): number of cycles the wave undergoes per sec (s^{-1} or Hz)
- wavelength (λ): distance between two "peaks" or "troughs"

Wavelength and frequency are inversely proportional.

$$c = \lambda\nu, \quad \nu = c/\lambda, \quad \lambda = c/\nu$$

Higher amplitude = brighter = more energy

Lower amplitude = dimmer = less energy

Planck's Radiation Law:

$$E = h\nu = \frac{hc}{\lambda}$$

- E - photon energy
- h - Planck's constant
- ν - frequency
- λ - wavelength

10.2. ELECTROMAGNETIC SPECTRUM

The waves of energy have oscillating electric and magnetic fields. Therefore, the radiation is called electromagnetic. There is no clean distinction between the types of light. The transitions are fluid.

Order of radiation

- Wave length from shortest to longest
- Frequency from highest to lowest
- Energy from highest to lowest

The order is:

- Gamma ray
- X-ray
- Ultraviolet
- Visible light
- Infrared
- Microwave
- Radio wave

10.3. DIFFRACTION FROM A GAS TUBE

- Electrically excited atoms emit a beam of light that is narrowed by a slit and refracted by a prism
- The line spectrum is a series of fine lines at specific wavelengths separated by black spaces.

- The atomic spectra of elements appear as colored lines. Each spectrum is characteristic for an element.

10.4. RYDBERG EQUATION

The Rydberg equation is a mathematical description that predicts the positions and wavelengths λ of the spectral lines in a series for an atom with a single electron.

$$\frac{1}{\lambda} = R \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

- R - Rydberg constant
- n_1 and n_2 are positive integers with $n_2 > n_1$

10.5. THE BOHR MODEL

Niels Bohr hypothesized that electrons orbit the nucleus in circular paths.

- “Bohr orbits” (flat circles) describe the physical motion and position of a one electron system.
- Each electron orbit is assigned a value of n .
- The lowest energy orbit is called the ground state ($n = 1$). The higher energy orbits are called excited states ($n = 2, 3, 4, \dots$).
- When the electron changes energy levels, it gains or loses energy as electromagnetic radiation (photons).

$$\Delta E = E_{\text{final}} - E_{\text{Initial}} = -2.18 \times 10^{-18} J \left(\frac{1}{n_{\text{final}}^2} - \frac{1}{n_{\text{initial}}^2} \right)$$

11. LEC 11: QUANTUM THEORY 2 - OCT 1

De Broglie wavelength:

$$\lambda = \frac{h}{mu}$$

- m - mass
- u - speed in m/s

When transitioning between energy levels, the energy change is proportional to the difference in the inverse squares of the orbit number (the principal quantum numbers).

$$\Delta E \propto \left| \frac{1}{n_{\text{final}}^2} - \frac{1}{n_{\text{initial}}^2} \right|$$

Meanwhile, recall that frequency is proportional to energy, and therefore inversely proportional to wavelength:

$$\Delta E \propto \nu \propto \frac{1}{\lambda}$$

11.1. THE QUANTUM MECHANICAL MODEL

Quantum Mechanical Orbital - a mathematical function Ψ from which we can determine different properties of electrons.

- Electron energy
 - proportional to Ψ
 - same energy for H atom as Bohr Model, different for multi-electron atoms
- spatial distribution
 - proportional to Ψ^2

11.2. THE QUANTUM NUMBERS AND ATOMIC ORBITALS AO

principal quantum number n

- a positive integer.
- indicates the **relative size and energy of the orbital** and therefore its relative distance from the nucleus
- describe the period number in the periodic table

angular momentum quantum number l

- integer from 0 to $n - 1$
- indicates the **shape of the orbital**
 - s - spherical, $l = 0$
 - p - dumbbell, $l = 1$

- three p orbitals: p_x, p_y, p_z
- d - cloverleaf, $l = 2$
 - five d orbitals: $d_{x^2-y^2}, d_{z^2}, d_{xy}, d_{xz}, d_{yz}$
- f - complex, $l = 3$

magnetic quantum number m_l

- integer from $-l$ to $+l$
- indicates the **spatial orientation of the orbital**

spin quantum number m_s

- either $+\frac{1}{2}$ or $-\frac{1}{2}$
- distinguishes between the two electrons that occupy the same orbit

12. LEC 12: QUANTUM THEORY 3 - OCT 6

12.1. RULES FOR FILLING ORBITALS

Hund's Rule: When degenerate (equal energy) orbitals are available, the lowest energy electron configuration has the maximum number of unpaired electrons with parallel spins.

Pauli Exclusion Principle: No two electrons in an atom can have the same set of quantum numbers. No more than two electrons may occupy the same atomic orbital, and they must have a different spin.

Aufbau Principle: Process of building up atoms by adding one proton at a time to nucleus, and one electron to lowest energy AO level.

12.2. ENERGY OF ORBITALS

- For a **1-electron** atom or ion
 - Example: H, He^+
 - Quantum energy agrees with the Bohr model
 - Energy depends only on n
- For a **multi-electron** atom or ion
 - Anything bigger than H
 - Bohr theory cannot predict these energies

Energy differences arise from:

1. nuclear attraction
2. electron repulsions
3. orbital shape

The interactions of these factors lead to shielding and penetration.

Shielding: electron repulsions counteract nuclear attraction somewhat

Penetration: how close the orbital is to the nucleus based on the radial probability distribution; closer to nucleus is lower energy

13. LEC 13: QUANTUM THEORY 4 - OCT 8

13.1. PARTIAL ORBITAL DIAGRAMS

Only show the highest energy.

Example: Al = $[1s^2 2s^2 2p^6] \underline{3s^2 3p^1}$

13.2. EFFECTS OF NUCLEAR CHARGE ON ENERGY LEVELS

Greater nuclear charge lowers the energy level.

lower energy level = stronger attraction

13.3. EFFECTS OF PENETRATION ON ENERGY LEVELS

$s < p < d < f$ for any given value of n
--

13.4. DETERMINING SHELLS AND ORBITALS

- Use periodic table
- Follow the diagonal rule
- Use

$$1s^2 \quad 2s^2 2p^6 \quad 3s^2 3p^6 \quad 4s^2 3d^{10} 4p^6 \quad 5s^2 4d^{10} 5p^6 \quad 6s^2 4f^{14} 5d^{10} 6p^2$$

Exceptions: Cr, Cu, Mo, Ag, Au

- Most are transition metals

13.5. TYPES OF ELECTRONS

Inner core electrons - Those electrons have in common with the previous noble gas

Outer electrons - Those in the highest energy level - highest n

Valence electrons - Those involved in forming bonds

Main group: valence = outer electrons

Transition metals: valence = outer electrons + d or f level electrons