# CHEMISTRY FOR THE LIFE

# EDITOR DR. YASMEEN JUNEJO



# Chemistry for the Life

#### Editor

#### Yasmeen Junejo

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# PREFACE

Welcome to "Chemistry for the Life." This book embarks on a fascinating journey through the intricate and awe-inspiring world of chemistry, exploring the profound impact that chemicals have on our daily existence. As we navigate the realms of atoms and molecules, we uncover the hidden forces that shape the very fabric of life. Chemistry is often referred to as the central science, and for good reason. It provides the foundation for understanding the composition, structure, properties, and transformations of matter. In this exploration, we will delve into the heart of chemical principles, demonstrating their relevance and significance in shaping the world we live in.

This book is not just a compilation of formulas and reactions but a narrative that unfolds the narrative of chemistry in a way that is accessible and engaging. Whether you are a student delving into the subject for the first time or an experienced professional seeking a deeper understanding, "Chemistry for the Life" aims to demystify the complexities of this discipline.

Our journey begins by laying a solid foundation, introducing fundamental concepts and principles. From the basic building blocks of atoms to the intricacies of chemical bonds, we will navigate through the essential elements that form the basis of chemical understanding. As we progress, we will explore the diverse branches of chemistry and their applications in various facets of our lives. Moreover, we delve into the environmental impact of chemicals, exploring their role in climate change, pollution, and sustainable practices. The consequences of human activities on our planet are undeniable, and a deeper understanding of chemistry is essential for addressing these challenges and forging a sustainable future.

"Chemistry for the Life" is not merely an academic pursuit; it is a celebration of the wonders of the chemical world that surrounds us. Through vivid examples, real-world applications, and thought-provoking insights, this book aims to in still a profound appreciation for the beauty and importance of chemistry in our everyday lives.

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# INTRODUCTION TO CHEMISTRY: THE SCIENCE OF MATTER AND CHANGE

Yasmeen JUNEJO Mehmet ÖZASLAN

# **1. Introduction**

"Chemistry is a branch of science that studies the composition, structure, properties, and changes of matter". It is also a field of physical science that studies atoms and molecules, their interactions, and the transformations that they go through. Chemists explore the properties and behavior of substances, the changes they undergo in various conditions, and the energy changes that accompany these processes. We can also explain it as the science that helps us understand the nature of matter and how different substances interact with each other. It also plays a vital role in various scientific and industrial fields, such as medicine, materials science, environmental science, and energy production (Yao et al., 2022).

# 2. Importance of Chemistry in Everyday Life

#### a. Medicine and Healthcare:

- i. Drug Development: Chemistry is fundamental in the discovery and development of new medications, ensuring their effectiveness and safety.
- **ii.** Diagnostic Tools: Chemistry is behind various diagnostic tools like blood tests, X-rays, and MRIs, aiding in the detection and treatment of diseases.

# b. Food and Nutrition:

- i. Food Chemistry: Understanding food chemistry helps in food preservation, flavor enhancement, and nutritional improvement.
- ii. Nutritional Science: Chemistry is essential in studying the nutritional content of foods and creating balanced diets.

# c. Cleaning and Hygiene:

- i. Detergents and Cleaners: Chemistry is used to create effective cleaning products, making our surroundings hygienic.
- ii. Personal Care Products: Chemistry is involved in the formulation of cosmetics, soaps, shampoos, and other personal care items.

# d. Environmental Protection:

- i. Pollution Control: Chemistry helps in developing methods to monitor and control air and water pollution.
- ii. Green Technologies: Chemists work on developing eco-friendly solutions, such as renewable energy sources and biodegradable materials.

# e. Energy Production:

- i. Fossil Fuels: Chemistry is involved in the extraction and processing of fossil fuels, which are still major energy sources worldwide.
- ii. Renewable Energy: Chemistry plays a role in the development of solar cells, fuel cells, and other sustainable energy technologies.

# f. Materials and Technology:

- i. Materials Science: Chemistry contributes to the development of new materials with specific properties, leading to innovations in technology and industry (Figure 1).
- ii. Electronics: Chemistry is essential in the production of semiconductors and conductive materials used in electronic devices.

# g. Understanding Household Products:

i. Consumer Products: Chemistry helps consumers understand the composition and safe use of various household products, including paints, adhesives, and batteries.

# h. Agriculture:

- 1. Fertilizers and Pesticides: Chemistry is utilized in the development of fertilizers and pesticides, enhancing agricultural productivity.
- 2. Crop Science: Chemistry aids in studying plant metabolism and developing disease-resistant crop varieties.



Figure 1. Introduction of chemistry with their ores and purities.

# **3. Historical Development of Chemistry**

# a. Ancient Civilizations (Pre-1000 BCE):

- Alchemy in Egypt: The ancient Egyptians practiced early forms of chemistry, mainly in metallurgy, cosmetics, medicine, and embalming.
- Alchemy in Greece: Greek philosophers like Empedocles and Democritus proposed early theories about the composition of matter.

# b. Islamic Golden Age (8th - 13th Century):

- Islamic Scholars: Islamic scientists translated Greek and Roman texts into Arabic, preserving and expanding the knowledge of alchemy, medicine, and other sciences.
- Al-Razi (Rhazes): A Persian alchemist and physician, Al-Razi is often credited with the discovery of sulfuric acid and ethanol. He emphasized experimentation and systematic observation.

# c. Medieval Europe (12th - 16th Century):

- Alchemy in Europe: Alchemy spread to Europe and became a widespread practice among scholars seeking the Philosopher's Stone (a substance believed to grant immortality and transform base metals into gold).
- **Roger Bacon:** An English alchemist, philosopher, and Franciscan friar, Bacon advocated the scientific method and experimentation, laying the groundwork for modern chemistry.

# d. The Scientific Revolution (17th Century):

- **Robert Boyle:** Boyle's law, which describes the relationship between pressure and volume of a gas, is a fundamental principle in the study of gases. Boyle is often considered one of the pioneers of modern chemistry.
- Antoine Lavoisier: Known as the "Father of Modern Chemistry," Lavoisier established the law of conservation of mass, identified and named oxygen and hydrogen, and helped develop the modern system of chemical nomenclature.
- Joseph Priestley and Carl Wilhelm Scheele: Independently discovered oxygen and several other gases, contributing significantly to the understanding of gases and chemical reactions.

# e. The 18th and 19th Century:

- John Dalton: Dalton proposed the atomic theory, stating that matter is composed of indivisible particles called atoms. He also introduced the concept of chemical elements and their combinations.
- **Dmitri Mendeleev:** Mendeleev created the periodic table, organizing elements based on their atomic mass and predicting the properties of undiscovered elements.
- **Discovery of Elements:** Chemists isolated and identified numerous elements during this period, expanding the understanding of elemental properties.

# f. The 20th Century and Beyond:

- **Quantum Mechanics:** The development of quantum mechanics revolutionized the understanding of atomic and molecular behavior, explaining phenomena at the subatomic level.
- **Modern Chemistry:** Advancements in analytical techniques, computational chemistry, and materials science have expanded the scope of chemistry, leading to innovations in various fields, including medicine, electronics, and materials engineering.

# 4. Fundamental Concepts in Chemistry

# i. Matter and Its Properties:

- Matter is defined as everything that takes up space and has mass. It is made up of atoms and molecules.
- Physical properties (such as colour, density, and melting point) and chemical properties (such as reactivity and combustibility) are all characteristics of matter.

# ii. Atoms and Elements:

- Atoms: Atoms are the fundamental building components of matter. They are made up of a nucleus that contains protons and neutrons, as well as electrons that orbit the nucleus.
- Elements are substances that contain only one sort of atom. Each element has its own chemical symbol (for example, H for hydrogen, O for oxygen).

# iii. Chemical Bonds and Compounds:

- Chemical bonds are the forces that hold atoms together in molecules. Ionic bonds (made by the transfer of electrons) and covalent bonds (created by the sharing of electrons) are two types of bonding.
- Compounds are compounds made up of two or more separate elements that are chemically linked in specific ratios. Compounds include water (H2O) and carbon dioxide (CO2).

# iv. Chemical Reactions and Equations:

- Chemical reactions involve the breaking and building of chemical bonds, which results in the transformation of compounds into new substances with distinct properties.
- Chemical Equations: Chemical processes are depicted using chemical equations, which show the reactants on the left and the products on the right. Balanced equations guarantee mass conservation.

# v. The Mole Concept and Stoichiometry:

- The Mole: The mole is a unit of measurement for counting atoms, molecules, or ions. Avogadro's number of particles is included in one mole of any substance (approximately  $6.022 \times 10^{23}$ ).
- Stoichiometry: Stoichiometry involves the calculation of quantities in chemical reactions. It includes mass-to-mass calculations, limiting reactants, and percent yield.

# vi. Energy Changes in Chemical Reactions:

- Energy: Energy is involved in chemical reactions. Endothermic processes take in energy from their surroundings, whereas exothermic reactions expel it.
- Calorimetry: Calorimetry is the measurement of heat changes in chemical reactions, providing information about the reaction's energy changes.

#### vii. The Behavior of Gases:

- Gas Laws: Gas laws describe the behavior of gases under different conditions.
- Boyle's law (pressure and volume relationship)
- Charles' law (volume and temperature relationship).

# viii. Solutions and Their Properties:

- Solutions: Solutions are homogeneous mixtures composed of a solute (dissolved substance) and a solvent (dissolving medium). Solutions can be liquid, solid, or gas.
- Colligative Properties: Colligative properties, such as freezing point depression and osmotic pressure, depend on the number of solute particles in a solution (Akhter & Alam, 2023).





# 5. Chemical Reactions and Equations (Smith, 2020)

# **Chemical Reactions:**

- **a.** A chemical reaction is a process that transforms one or more chemicals into new ones with distinct chemical and physical properties.
- b. Combination Reactions: In these reactions, new compounds formed.  $A{+}B{\rightarrow}AB$
- c. Decomposition Reactions: In these reactions, compounds decomposed.  $AB{\rightarrow}A{+}B$
- **d.** Single Replacement Reactions: In these reactions, an element changes with another one.  $A+BC\rightarrow AC+B$
- e. Double Replacement Reactions: In these reactions, elements replace their places. AB+CD→AD+CB
- f. Combustion Reactions: In these reactions, substances release energies. Hydrocarbon+O\_2 \rightarrow CO\_2 + H\_2O

# 6. Chemical Equations:

- A chemical equation is a symbol that represents a chemical reaction.
   The reactants are on the left, and the products are on the right, divided by an arrow (→).
- Balancing Equations: The number of atoms of each element in a balanced chemical equation is the same on both sides of the equation.
   Balancing guarantees that the law of mass conservation is followed.
- Example: The imbalanced equation for hydrogen (H<sub>2</sub>) reacting with oxygen (O<sub>2</sub>) to generate water (H<sub>2</sub>O) as H<sub>2</sub>+O<sub>2</sub>→H<sub>2</sub>O.
- To balance it:  $2H_2+O_2 \rightarrow 2H_2O$ .

# 7. Chemical Reactions in Everyday Life:

- **a.** Metabolism: Chemical reactions occur in our bodies to break down food and convert it into energy. Digestion: Enzymes in our digestive system facilitate chemical reactions to break down complex molecules into simpler ones.
- **b.** Cellular respiration is the chemical interaction that occurs between glucose and oxygen to produce energy, carbon dioxide, and water.
- **c.** Photosynthesis is the process by which plants use sunshine to transform carbon dioxide and water into glucose and oxygen.
- **d.** Corrosion: Metals react with oxygen and moisture in the air, leading to rusting, which is a form of corrosion.

# 8. The Mole Concept and Stoichiometry (Ralph et al., 2022)

- a. The Mole Concept: In the field of chemistry, a mole is a unit of measurement that denotes a precise quantity of atoms, molecules, ions, or other particles. Avogadro's number of entities, about  $6.022 \times 10^{23}$ , is contained in one mole. This number is fundamental to chemistry because it allows scientists to count atoms and molecules on a macroscopic scale.
- **b.** Molar Mass: Molar mass, which is measured in grammes per mole (g/mol), is the mass of one mole of a substance. In atomic mass units (amu), it is mathematically equivalent to the mass of an atom or molecule. For instance, carbon (C) has a molar mass of about 12.01 g/mol.
- **c. Stoichiometry:** The computation of reactants and products in chemical reactions is known as stoichiometry. The mole ratios of reactants and products are provided by the balanced chemical equation, which serves as its foundation.
- 1. Steps in Stoichiometric Calculations (Khan, 2020):
- 2. Balancing the Equation: Ensure that the chemical equation is balanced, that is, that the number of atoms of each element on both sides is the same. Using the mole ratios from the balanced equation, convert moles of one substance to moles of another material in the reaction.
- **3.** Converting Moles to Mass: To convert moles to grammes, use the molar mass. This step is crucial for practical applications and real-world problems.

- 4. Converting Moles to Particles: Avogadro's number  $(6.022 \times 10^{23})$  can be used to convert moles to individual particles (atoms, molecules, ions, etc.).
- **5. Limiting Reactant Calculations**: Determine the limiting reactant in a reaction to find out how much product can be formed.
- **6. Percent Yield:** Calculate the percent yield, which represents the efficiency of a reaction concerning the amount of product obtained compared to the theoretical yield (the maximum amount predicted by stoichiometry).

# 9. Applications of Stoichiometry (Worrall et al., 2022)

- **a.** Chemical Synthesis: Stoichiometry is used in the laboratory to determine the appropriate amounts of reactants needed to synthesize a specific product.
- **b.** Reaction Efficiency: It helps in evaluating the efficiency of chemical reactions in industry, ensuring resources are not wasted.
- **c.** Environmental Chemistry: Stoichiometry is applied in environmental studies to calculate the quantities of pollutants produced in reactions, aiding in pollution control strategies.
- **d.** Medicine: Pharmaceutical industries use stoichiometry to design and manufacture drugs efficiently and economically.
- e. Food Industry: Stoichiometry is employed to determine the nutritional content of food products and to optimize food production processes.

#### **10. Summary**

In conclusion, "Introduction to Chemistry: The Science of Matter and Change" provides a comprehensive overview of the fundamental principles that underpin the fascinating world of chemistry. From the basic understanding of matter and its properties to the intricate concepts of chemical reactions and stoichiometry, this introductory exploration equips readers with a strong foundation in the science of chemistry. Throughout this chapter, we have delved into the historical development of chemistry, tracing its roots from ancient civilizations to the modern scientific era. We have explored the significance of chemistry in everyday life, elucidating its vital role in fields as diverse as medicine, agriculture, energy production, and environmental protection. The chapter has also elucidated key concepts such as atoms, elements, compounds, and chemical equations, providing readers with a clear understanding of the building blocks of matter and the language of chemical transformations. Moreover, the discussion on chemical reactions and stoichiometry has empowered readers to comprehend the quantitative aspects of chemistry. By mastering the mole concept and stoichiometric calculations, readers are prepared to tackle real-world problems, predict reaction outcomes, and analyze experimental results with precision. As we conclude, it is important to recognize that chemistry is not merely a scientific discipline; it is a dynamic force driving innovation, technological advancements, and sustainable solutions to global challenges. With a solid grasp of the concepts presented in this chapter, readers are well-equipped to embark on a journey of discovery, further exploring the intricate and awe-inspiring realm of chemistry. Whether pursuing careers in scientific research, medicine, engineering, or environmental conservation, the knowledge gained here serves as a strong foundation upon which future scientific endeavors can be built. In essence, "Introduction to Chemistry: The Science of Matter and Change" invites readers to marvel at the wonders of the microscopic world, encouraging curiosity, critical thinking, and a profound appreciation for the profound impact that chemistry has on our lives and the world around us. As we move forward, armed with this knowledge, the possibilities for exploration and innovation in the

realm of chemistry are boundless, promising a future filled with exciting discoveries and groundbreaking advancements.

# **Scientific Ethics Declaration**

The author say that she is responsible for the scientific, moral, and legal aspects of this chapter, which is published in In Junejo Y (Eds.), *Chemistry for the Life*. ISRES Publishing

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# CHEMICAL COMPONENTS OF POMEGRANTS OF DIFFERENT PHENOTYPES GROWN IN *TURKEY*

Sibel Bayıl OĞUZKAN Mehmet ÖZASLAN

#### **1. Introduction**

The pomegranate tree is a deciduous tree and has spread to regions similar to the Mediterranean climate, which is the most suitable climate for the cultivation of superior pomegranates. Pomegranate is a temperate climate plant and requires high temperature levels to reach proper maturity. The maturity index is the ratio of soluble dry matter to total acidity, and this index is used to classify pomegranates as sweet, tart and negative. Maturity indexes of 31-98 are grouped as sweet, 17-24 as bitter and 5-7 as minus species (Onur and et all., 1995; Oguz and et all., 2011). Pomegranate fruit consists of 75% moisture, 1.6% protein, ascorbic acid 16 mg/1000 g, ash 0.7%, 0.58% acidity and high amount of minerals (Özgüven and Yılmaz, 2000).

In our country, a significant increase has been observed in the production of pomegranate in recent years and in 1987, 44,000 tons of pomegranate was produced from 1,790,000 trees. While the number of fruit bearing trees was 3,610,788 in 2007, the number of fruitless trees was 3,367,316. According to 2007 data, 106,560 tons of pomegranate production was made. The average yield per tree was calculated as 30 kg. Production was 71,781 tons in the Mediterranean region, 18,841 tons in the Aegean and 11,247 tons in the Southeast Anatolia (Glozer and Ferguson, 2008). Pomegranate production in Gaziantep province Oğuzeli and Araban districts has an important place as a source of livelihood for farmers. There are 9 different phenotype pomegranate varieties produced in Oğuzel, and their local names are; It is named as camel tooth, red shell, muzzle sour, hicaz pomegranate, dirty lady, tail pomegranate, winter pomegranate, green skin, breast red. An average of 4,000 tons of pomegranate tooth, hicaz pomegranate and muzzle syrup are grown.

#### **1.1. Pomegranate Peel**

The peel of the pomegranate contains high amounts of polyphenols, punicalagin, a large polyphenol with a molecular weight greater than 1000, is the active ingredient in pomegranate and is part of an ellagitanin family that includes tannins, punicalin and gallagic acid. Although the peel rate of the pomegranate varies according to the species, it constitutes approximately 40% of the fruit.



Figure 1. Pomegrante Peel

Pomegranate peel, which is very rich in phenolic compounds, is a very valuable waste product of the fruit juice sector and has great potential in terms of functional components (Okumuş and et all., 2016). The edible part of the pomegranate fruit constitutes approximately 30% by weight of the whole fruit, and the active bioactive components are found at a very high rate in the peel and seed. It has been reported that the higher antioxidant activity of commercially sold pomegranate juices is due to the polyphenols transferred from the peel to the pomegranate juice as a result of pressing the fruit as a whole during production (Onurlubaş, 2007). It has been reported in different studies that pomegranate fruit peel contains a significant portion of tannins such as ellagic acid and gallic acid, which inhibit the proliferation of cancer cells. (Vardin,2008 ; Lansky and et all., 2005).

#### **1.2. Pomegrante Seed**

The seeds of pomegranate fruit vary between 40 and 100 grams per kilogram fruit weight, depending on the variety. Kernels contain 6.63-19.3% lipid on dry matter (Saravani and et al., 2014). In addition to lipids, there are lignin, cellulose and polysaccharides in the core (Jing and et all., 2012).



Figure 2. Pomegranate Seed

They determined that the fatty acid composition of the pomegranate seeds obtained from 7 regions of Spain is 4.16-26.5% saturated and 73.4-95.8% unsaturated fatty acids. The fatty acid composition of the seed oils of a total of 25 varieties of pomegranate, 8 of which are sweet, 3 of which is mayhos and 14 of which are minus species, grown in Iran were investigated. The fatty acid composition of sweet varieties of pomegranate seeds is 6.8-13.3% saturated and 86.7%-93.2% unsaturated, 6.4-12.1% unsaturated and 87.9-93.6% unsaturated, minus species consists of 4.8-26.8% saturated and 73.2-94.4% unsaturated fatty acids. determined (Anjaly and Mahedran, 2020).

# **1.3. Pomegranate Dice**

It is known that pomegranate fruit contains intense polyphenols in total and these components are present not only in its edible parts but also in its peel, seed and membranes.

It has been understood that the membranes covering the pomegranates are waste material in the consumption of the pomegranate fruit, and the analyzes of the components in its content have not been studied because no recorded data can be reached in the literature.



Figure 3. Pomegrante Dice

When we look at the literature, active substance determinations were made in the extracts of pomegranate seeds and peel obtained by using different extraction methods. There are studies explaining that pomegranate extracts have cytotoxic and apoptotic effects on some cancer cells (Fadavi and et all., 2004). The worldwide increase in interest in pomegranate and pomegranate-based products is not only related to the taste of the fruit, but also due to the fact that it has been proven in scientific studies that it prevents low-intensity and high-intensity cholesterol oxidation, reduces blood pressure and prevents the development of vascular occlusion. In the emergence of these beneficial effects of pomegranate-based products, reference is made to phenolic compounds with antioxidant properties (Anderson and et all., 2016).

Phenolic compounds show their beneficial effects by destroying free radicals. In recent years, the trend towards fruit juices such as grape juice and blueberry juice, which are high in phenolic antioxidants, has been increasing. Pomegranate juice is a popular fruit juice with the phenolic compounds it contains and the important biological activities it exhibits (Brays and et all., 2021 and Martinez and et all., 2006). It has been reported that consuming foods rich in polyphenolic compounds such as pomegranate has anti-proliferative, anti-angiogenic, anti-invasive and pro-apoptotic effects in some cancer cells in vitro and in vivo (Marı'a and et all., 2000, Kawaii and Lansky, 2004). In MCF7 and MB-MDA-231 cell lines, fermented pomegranate juice polyphenols were found to have 2 times more antiproliferative effect than fresh fruit pomegranate juice (Fadavi and et all., 2006).

It was stated that pomegranate juice extract inhibited cell viability/cell growth and increased apoptosis in PC3 cells in a dose-dependent manner, especially at a concentration of 10-100  $\mu$ g/ml and after 48 hours of incubation. In a study with human PC3 prostate cancer cells, pomegranate juice extract was reported to have antiproliferative and proapoptotic properties (Dalimov and et all., 2003). It has been reported that pomegranate fruit extract inhibits A549 cells in the G1 phase of the cell cycle in a concentration-dependent manner, by regulating the CKI cyclin-CDK system and inhibiting MAPK, NFkB and PI3K/Akt signal transduction. It has also been reported that pomegranate fruit extract has inhibitory effects on cell growth in A549 lung cancer cell line. It has been reported that especially pomegranate fruit extract has a concentration range of 50-150  $\mu$ gr/ml and as a result of 72 hours incubation, using MTT and trypan blue methods, cell viability is significantly reduced and cytotoxic effect (Melgarejo and Artes, 2000). The analyzes of the extracts obtained from the peel and seeds of nine different pomegranate species belonging to the province of İzmir were carried out using spectrophotometric and chromatographic techniques under optimum conditions. found has not been determined.

As a result, it has been understood that pomegranate peels are richer in phenolic compounds compared to other fruit skins and pomegranate seeds, and that pomegranate peel can be a very good source for the production of natural antioxidants with water and pressurized solvent extraction system (Sassano and et all.,2009). In another study, the total amount of phenolic substances was determined by making appropriate extractions of yellow-sweet pomegranate fruit peels obtained from the vicinity of Antalya. It has been determined that these fruit peel extracts have an inhibitory effect on cell proliferation by exerting cytotoxic and apoptotic effects on MCF-7 (human breast adenocarcinoma) cell line in a concentration and time-dependent manner (Deepa and et all., 2017). It has been shown in cell culture studies that it has antitumoral activity on cancer (El-Shaarawy and Nahapetian, 1983).

In many different studies, it has been reported that pomegranate juice, peel and seed have the potential to have antiprolerative, anti-apoptotic and cytotoxic effects on different types of cancer. There are studies in the literature on pomegranate fruits with genotypes belonging to two different regions cultivated in our country, and no determination, analysis or determination of the active substance has been made of the pomegranate variants of the Oğuzeli district, which has an annual production of 4,000 tons of pomegranate and is supported in rural development in terms of pomegranate production. In the literature, it has been reported that the juice, peel and seed of the pomegranate fruit have been examined in terms of bioactive components, especially the phenolic-based compounds in the peel have been investigated in terms of anticancer activity in different cell lines, and it has been reported that they have antitumoral activity.

#### **2.** Conclusion

The peel and seed, which make up approximately 40% of the pomegranate fruit consumed fresh and processed into fruit juice in our country, contain high amounts of phenolic compounds. The peel and seeds remaining during processing into pomegranate juice are industrially valuable waste products. Despite the active ingredient content, the peel, core and membrane parts are unfortunately in the category of waste material due to the limited conditions and knowledge of the farmers.

#### **Scientific Ethics Declaration**

The author say that she is responsible for the scientific, moral, and legal aspects of this chapter, which is published in In Junejo Y (Eds.), *Chemistry for the Life*. ISRES Publishing

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# CHEMICAL KINETICS: RATE OF REACTIONS IN CHEMISTRY

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#### Introduction

Chemical kinetics is considered a subfield of physical chemistry that is concerned with the rate at which chemical reactions proceed (Margaret, 2004). It has been found to have many applications in various fields such as engineering, biological and environmental sciences (Richard, 2001). Chemical kinetics provides valuable insight about the mechanisms of chemical processes; interestingly it can disprove a mechanism but cannot establish one with certainty (Keith, 1987).

This chapter covers the following areas of chemical kinetics:

- i. Factors affecting the rate of chemical reactions.
- ii. Rate laws
- iii. Order of chemical reactions
- iv. Half-life of reactions
- v. Theories and approximations of reaction kinetics.
- vi. Reactions and their mechanisms.
- vii. Chain reactions.

#### **Historical background**

The commencement of the first work on chemical kinetics was carried out by the German Chemist, Ludwig Wilhemy in 1850. He used the integrated rate law to determine the inversion of sucrose (Wilhemy, 1850). In 1864, Cato Guldberg and Peter Waage postulated the "law of mass action", which states that the rate of a chemical reaction is proportional to the concentration of reactants (Cato, Peter, 1864). Their work failed to investigate the kinetics of any one reaction.

# Factors affecting chemical reactions

There is a great variation in the rate at which reactants are consumed and products are formed. It is also worthy of note that chemical reactions are sensitive to temperature and will require constant temperature to proceed (Margaret, 2004).

The factors that affect the rate at which chemical reactions proceed include: nature of reactants, state of subdivision of the reactants, temperature, concentration, presence of catalyst.

#### **Nature of reactants**

The nature of the substrate determines the speed of a reaction. Reactions, under the same conditions, may proceed at different rates due to the nature of reactants. For example, sodium interacts entirely with air overnight when little particles of the metal iron are exposed to it, whereas iron is hardly impacted. Both the active metals calcium

and sodium produce hydrogen gas and a base when they interact with water. (Margaret, 2004).

# State of subdivision of the reactants

A finely divided solid has more surface area available for reaction than does one large piece of the same substance, so a liquid will react with it more quickly than with a large piece of the same solid. Reactions between two phases, with the exception of substances in the gaseous state or in solution, occur at the boundary, or interface, between them. As a result, the rate of a reaction between two phases depends to a great extent on the surface contact between them.

# Temperature

Fast chemical reactions are usually the result of high temperatures. The process of food spoilage is faster when it is left on the kitchen counter. However, the process is slowed down when the food is in a refrigerator due its low temperature. Hence the food remains fresh for a longer period of time. Hot plate is used in the lab to speed up chemical processes that proceed slowly at room temperature. In many instances, a homogeneous system's temperature increase of just 10 °C will roughly double a reaction's rate (Espenson, 2002).

# Concentration

Reactant's concentration influences the rate of a chemical reaction. An increase in the concentration of one or more of the reactants often increases the rate as well. For example, the decomposition of calcium carbonate (CaCO<sub>3</sub>) caused by its reaction with sulphur dioxide. The amount of sulphur dioxide in the air affects how quickly this reaction proceeds. In the following reaction, sulphur dioxide, an acidic oxide, reacts with airborne water vapour to yield sulphurous acid (Steinfeld, Francisco, and Hase 1999).

 $\begin{array}{c} SO_{2\,(g)} + H_2O_{(g)} \longrightarrow H_2SO_{3\,(aq)} \\ (1) \end{array}$ 

Calcium carbonate reacts with sulfurous acid as follows:

$$CaCO_{3 (s)} + H_2SO_{3 (aq)} \longrightarrow CaSO_{3 (aq)} + CO_{2 (g)} + H_2O (l)$$
(2)

Calcium carbonate degrades faster in highly polluted air than in unpolluted air due to the high concentration of sulphur dioxide in the former. Similar to how oxygen burns considerably more quickly in pure oxygen than in air that only contains 20% oxygen, phosphorus burns significantly more quickly in pure oxygen.

# **Presence of catalyst**

When hydrogen peroxide is poured on an open wound it causes foaming because tissues nearby function as catalysts, speeding up the breakdown of the peroxide. However, total degradation might take months in the absence of these catalysts. By reducing the activation energy without being consumed by the process, a material acts as a catalyst to speed up a chemical reaction. The bare minimum of energy needed for a chemical reaction to move ahead is known as activation energy. By offering a different road or mechanism for the reaction to follow, a catalyst speeds up the reaction process (Espenson, 2002).



Reaction coordinate

Figure 1. Plot showing the effect of the presence of a catalyst in a chemical reaction

The X-axis of a graph has is the "Reaction coordinate". The Y-axis is marked with the word "Energy". The blue horizontal line that covers the whole width of the graph is the "Reactants". Another brief blue line labelled "Products" marks the end of the curve. A higher level than the "Reactants" line is where the "Products" line may be seen. The horizontal line and the peak of the curve are connected by an arrow. "Uncatalyzed reaction activation energy" is the label on the arrow. There is a second, dark concave downward curve. This curve only reaches roughly two-thirds of the height of the initial curve, but it also intersects the blue line segments for reactants and products. Another arrow emerges from the horizontal line and points towards the second curve's peak. The name of this arrow is "Catalysed reaction activation energy"

#### **Half-life of reactions**

The time it takes for the concentration of a particular reactant to reach 50% of its initial concentration, or the time it takes for the reactant concentration to reach half of its initial value, is known as the half-life of a chemical reaction. It is commonly stated in seconds and is represented by the sign " $t_{1/2}$ ."

#### **Calculations involving half-life**

#### Problem 1:

A first order reaction takes 5 hours for 70% completion. Calculate the time required for 85% completion.

Solution:

 $k = \frac{2.303}{t} \log \left( \frac{[Ao]}{[A]} \right) \quad \dots \quad (i)$ let [Ao] = 100 M

When time =  $t_{70\%}$  then [A] = 30 M (given that  $t_{70\%}$  = 5 hours)

 $\Rightarrow$  at 85% completion,t<sub>85%</sub>, [A] = 15 M

$$k = \frac{2.303}{t_{85\%}} \log\left(\frac{100}{15}\right)$$
$$\implies t_{85\%} = \frac{2.303}{k} \log[6.7] ------ (ii)$$

To solve for k, we use:

$$k = \frac{2.303}{t_{70\%}} \log \left[\frac{100}{30}\right] \text{ (given } t_{70\%} = 5 \text{ hours)}$$
$$k = \frac{2.303}{5} \ge 0.5 = 0.24$$

Substitute the value of k into eqn (ii) to determine the t85%

$$\therefore t_{85\%} = \frac{2.303}{0.24} \times 0.8261 = 7.92 \text{ hours}$$

#### **Problem 2:**

Show that in the case of first order reaction the time required for 80% completion is nearly two times the time required for half completion. (Log 5 = 0.6989)

# Solution:

Using k = 
$$\frac{2.303}{t} log\left(\frac{[Ao]}{[A]}\right)$$
  
Let [A<sub>0</sub>] = 100  
 $\Rightarrow$  When t = t<sub>80%</sub> then [A] = (100 - 80) = 20  
t<sub>80%</sub> =  $\frac{2.303}{k} log\left(\frac{100}{20}\right)$   
t<sub>80%</sub> =  $\frac{1.6097}{k}$  ------ (i)  
But k =  $\frac{0.693}{t_{1/2}}$   
Substitute k into eqn (i): t<sub>80%</sub> =  $\frac{1.6097}{\frac{0.693}{t_{1/2}}}$ 

 $\therefore t_{80\%} \cong 2t_{1/2}$ 

#### **Order of Reaction**

An order of reaction is the sum or total of the exponents of reactant concentration in the rate. The order of a reaction cannot be in general predicted from the chemical equation.

:. Order of reaction is the sum powers of the reactant concentration.

Orders can be negative numbers (as in concentration  $l^{-1}$ ). A negative order implies that the concentration occurs in the denominator of the rate laws increasing the concentration of that species, usually a product, actually slows down the reaction because that species participates in a reverse reaction. An example is the decomposition of ozone, $O_3$  in the upper atmosphere

$$2O_{3(aq)} \rightarrow 3O_{2(g)}$$

The experimentally determined rate law for this reaction is

Rate = 
$$\frac{K[O_3]^2}{O_2} = K[O_3]^2[O_2]^1$$

#### Forms of Order of Reaction

Various forms of order of reaction include;

i. First-order Reaction: This is when the rate is directly proportioned to the concentration of reactant R as shown below

$$R \rightarrow \text{produc}; \text{Rate} = K[R]$$

- ii. Second- order Reaction: This is when the rate is proportional to the square of the reactant concentration  $e.g.2R \rightarrow product; rate = K[R]^2 or x + y \rightarrow product; rate = k[y][z]$
- iii. **Third-order Reactions:** This is when the rate is proportional to the cube of the reactant concentration e.g.

$$3R \rightarrow k[R]^3$$
; Rate =  $k[R]^3$ 

or

$$A + B + C \rightarrow product$$

Rate = K[a][B][C]

iv. **Zero-order Reaction:** This is when the rate remains regardless of the reactant concentrations e.g.

$$2NH_{3(g)} \rightarrow N_{2(g)} + 3H_{2(g)}$$

$$Rate = K[NH_3]^o$$

**N.B:** Concentration of the reactant in a zero-order reaction falls at a constant rate until it is exhausted or has been consumed or it falls abruptly to zero.

v. **Fractional-order Reaction:** This is when the exponent of the reactant concentration in a rate equation is a fraction. Example the oxidation of sulfur dioxide in the reaction

$$2SO_{2(g)} + O_{2(g)} \to 2SO_{3(g)}$$
$$Rate = K[O_2][SO_2]^{-1/2}$$

or

Generally, 
$$2R \rightarrow product$$
  
Rate =  $K[R]^{1/2}$ 

vi. **Pseudo-order Reaction;** This is when the order of a chemical reaction appears to be less than the true order due to experimental conditions e.g.

$$C_{12}H_{22}O_{11} + H_2O \to 2C_6H_{12}O6$$

Where  $[H_2 0]$  is constant

$$Rate = K'[C_{12}H_{22}O_{11}]$$
 Where  $K' = K[H_2O]$ 

In practice, the above reaction is second-order reaction but due to the condition of the experiment the reaction assumes a first order reaction as seen in the rate equation above. Hence, this reaction order is called pseudo-first order.

#### **Example 1**

1. Write the rate law for the consumption of për sulphate ions in the reaction and determine the order.

$$S_2 O_8^{2-} + 3I_{(aq)}^- \rightarrow 2S O_{4(aq)}^{2-} + I_{3(aq)}^-$$

With respect to each reactant

	initialconcmol/L		initial rate	
Exp.	$S_2 O_8^{2-}$	Ι-	$(mol \ of \ S_2 O_8^{2-}) L^{-1} s^{-1}$	

Chemistry for the Life				
1.	0.15	0.21	1.14	
2.	0.22	0.21	1.70	
3.	0.22	0.12	0.98	

#### Answer

Rate =  $K[S_2 O_8^{2-}][I^-]$ 

# Example 2

Write the rate law and determine the order of the reaction in a reaction of carbon monoxide and chlorine gas to produce highly toxic carbonyl chloride.
 CO<sub>(g)</sub> + Cl<sub>(g)</sub> → COCl<sub>2(g)</sub> Given the following data collected at a certain temperature

	initialconeme	ol/L	initial rate
Exp.	Со	Cl <sub>2</sub>	$(mol \ of \ 0)L^{-1}s^{-1}$
1.	0.12	0.20	0.121
2.	0.24	0.20	0.241
3.	0.24	0.40	0.682

# Solution for example 2

By comparing exp 1 and 2 Rate  $1 = K[Co]^{x}[Cl_{2}]^{y}$ Rate  $2 = K[Co][Cl_{2}]^{y}$ dividing both equations

$$\frac{Rate\ 2}{Rate\ 1} = \frac{K[Co]^x[Cl_2]^y}{K[Co]^x[Cl_2]^y}$$

Substituting the data obtained.

$$\frac{0.241}{0.121} = \frac{K[0.24]^{x}[0.20]^{y}}{K[0.12]^{x}[0.20]^{y}}$$

$$\frac{0.241}{0.121} = \left(\frac{0.24}{0.12}\right)^x$$
$$1.992 = 2^x$$

Taking the log of body sides

$$\log 1.992 = x \log 2$$

Divide both side by *log*2

$$\frac{\log 1.992}{\log 2} = \frac{\log 2}{\log 2}$$

$$x = \frac{\log 1.992}{\log 2}$$

$$x = \frac{0.2998}{0.3010}$$

$$x = 0.99$$

$$\approx x = 1$$

Reactant [Co] is first order

By comparing experiment 2 and 3

Rate 2 = 
$$K[Co]^{x}[Cl_{2}]^{y}$$
  
Rate 3 =  $K[Co]^{x}[Cl_{2}]^{y}$   
divide by Rate 2  
Rate 3 \_  $K[Co]^{x}[Cl_{2}]^{y}$ 

$$\frac{1}{Rate2} = \frac{1}{K[Co]^x [Cl_2]^y}$$

Substituting the data

$$\frac{0.684}{0.241} = \frac{K[0.24]^x[0.40]^y}{K[0.24]^x[0.20]^y}$$

$$\frac{0.684}{0.24} = \left(\frac{0.40}{0.20}\right)^{y}$$
$$2.84 = 2^{y}$$

Taking the log of body sides

 $\log 2.84 = y \log 2$ 

Divide both side by *log*2

$$y = \frac{\log 2.84}{\log 2}$$
$$y = \frac{0.4533}{0.3010}$$
$$y = 1.5$$

 $y \simeq = 2$ 

Reactant  $[Cl_2]$  is second order.

Rate =  $K[Co]^1[Cl_2]^2$  overall order

# **Solution for Example 1**

By comparing experiment 1 and 2.

Rate 1 = 
$$K[S_2 08^{2-}]^m [I^-]^n$$
  
Rate 2 =  $K[S_2 08^{2-}]^m [I^-]^n$ 

Divide by Rate 1

$$\frac{Rate\ 1}{Rate\ 2} = \frac{K[S_2O8^{2-}]^n[I^-]^n}{K[S_2O8^{2-}]^n[I^-]^n}$$

Substituting the data

$$\frac{1.70}{1.14} = \frac{K[0.22]^m [0.21]^n}{K[0.15]^m [0.21]^n}$$

$$1.491 = \left(\frac{0.22}{0.15}\right)^m$$

$$1.491 = 1.466^m$$

Taking the log of both side

$$\log 1.491 = m \log 1.466$$
$$m = \frac{\log 1.491}{\log 1.466}$$
$$\frac{0.173}{0.164}$$
$$m = 1.04$$
$$\approx m = 1$$

 $[S_2 O_8^{-2}]$  is a first order

By comparing experiment 2 and 3

Rate 2 = 
$$K[S_2O_8^{2-}]^m[I^-]^n$$
  
Rate 3 =  $K[S_2O_8^{2-}]^m[I^-]^n$ 

Divide by Rate 2

$$\frac{Rate \ 3}{Rate \ 2} = \frac{K[S_2O_8^{2-}]^m[I^-]^n}{K[S_2O_8^{2-}]^m[I^-]^n}$$

1

Substituting the data

$$\frac{0.98}{1.70} = \frac{K[0.2Z]^m [0.12]^n}{K[0.22]^m [0.21]^n}$$
$$0.576 = \left(\frac{0.12}{0.21}\right)^n$$
$$0.576 = 0.571^n$$

Taking the log of both side

$$\log 0.576 = n \log 0.571$$
$$n = \frac{+0.24}{+0.24}$$
$$n = 1$$

[I] is a first order.

**Exercise 2:** The following kinetic data were obtained for the reaction between hydrogen and chlorine gas at  $600^{\circ}$ C.

$$H_2 + Cl_{2(g)} \to 2HCl_{(g)}$$

	Initial $[H_2]$	Initial $[Cl_2]$	Initial rate
Exp.	mol/dm <sup>3</sup>	$mol/dm^3$	$mol/dm^2s^{-1}$
1.	0.15	0.075	$3.5 \times 10^{-3}$
2.	0.30	0.15	$1.4 \times 10^{-2}$
3.	0.15	0.15	$7.0 \times 10^{-3}$

- a. Deduce the order with respect to  $H_{2(g)}$  and  $Cl_{2(g)}$ . Give the overall order of the reaction.
- b. Write the rate law for the reaction.

#### **RATE LAW**

Chemists discover ways in reaction rate by determining the initial of a reaction, the instantaneous rate of change in concentration of a species at a very beginning of a reaction. Therefore, rate law is the way the rate of a chemical reaction varies with reactant concentration.

For example

$$xA + yB \rightarrow mY + nZ$$
  
 $xA + yB \rightarrow mY + nZ$ 

Rate law is

Rate  $\propto [A]^x [B]^y$ 

Rate =  $[A]^x [B]^y$ 

Where k is a constant, called the rate constant for the reaction. In chemical kinetics, the square brackets denote molar concentration, with units  $mol^{-1}L^{-1}$  retained.

#### Example 1: Write the rate law of the following reactions:-

(a)  $2N_2O \rightarrow 2N_2 + O_2$ (b)  $CH_3B_r + H_2O \rightarrow CH_3OH + B_r$ (c)  $C_{12}H_{22}O_{11} + H_2O \rightarrow 2C_6H_{12}O6$ 

#### Solution

(a) Rate =  $K [reactant]^n$ 

Rate =  $K\{N_2 0\}^2$ 

(b) Rate = 
$$K[CH_3B_r][OH^-]$$

(c) Rate =  $K[C_{12}H_{22}O_{11}[H^+]]$ 

**N.B:** Rate law is an experimentally determined characteristic of the reaction and cannot in general be written down from the stochiometry of the chemical equation for the reaction. Rate law is an empirical law.

#### **Exercise 1:**

Determine the rate law of the following equation:

(a) 
$$S_2 O_8^{2-} + 31_{(aq)}^- \rightarrow 250_{4(aq)}^{2-} + I_{3(aq)}^-$$
  
(b)  $B_r O_{3(aq)}^- + SB_{r(aq)}^- + 6H_{(aq)}^{\rightarrow +} \rightarrow 3Br_{2(aq)} + 3H_2 O_{(1)}$   
(c)  $Co_{(g)} + Cl_{2(g)} \rightarrow CoCl_{2(g)}$ 

#### **Theoretical Models in Reaction Kinetics**

#### **Collision Theory**

Based on this theory the first step in a chemical reaction involves collision between reactant molecules (Santosh, 2006). The reaction between molecules is based on the assumption that such reactants act as hard spheres during collision (Keith, 1987). It assumes that rate of a chemical reaction directly depends on the number of effective collisions of reactants in a unit of time. For effective collision to occur in any chemical reaction these assumptions must be satisfied (Eli, 2022).

- (i) There must be collision between molecules of the reactant species.
- (ii) There must be proper orientation of reactant molecules for effective collision to take place.
- (iii) A minimum amount of energy is required for breaking and formation of bonds, which is known as activation energy  $(E_a)$ .

The importance of molecular orientation for a reaction to take place is illustrated in the reaction scheme below.

$$CH_3^{8^+} - Cl^{8^-} + \stackrel{\leftrightarrow}{H^-} \rightarrow CH_3 - Cl + OH^-$$

Unfavourable reaction

considering the left hand side of the above reaction, the partially negative cholorine group will repel the negatively charged hydroxyl ion, causing ineffective collision. hence, the reaction does not proceed.

$$\underbrace{\overset{\text{Force}}{\xleftarrow}}_{H^{-} \overset{\text{Force}}{\leftrightarrow} \mathcal{C}^{8+}H_{3} - \mathcal{C}l^{8-}} \rightarrow \mathcal{C}H_{3} - \mathcal{O}H + \mathcal{C}l^{-}$$

Favourable reaction

From the above reaction scheme, the partially positive methyl group will attract the negatively charged hydroxyl ion near it. This attraction will lead o effective collision of reactant molecules and hence formation of the new product  $CH_3 - OH$  (methanol).

On the basis of the assumptions above rate can be expressed as the product of the three factors below.

Rate = collision frequency  $\times$  energy factor  $\times$  orientation factor

$$K = Zpf$$

Where collision frequency Z is expressed below for bimolecular reactions.

$$Z_{AA} = \pi \left(\frac{\sigma_A + \sigma_B}{2}\right)^2 \sqrt{\frac{8k_B T}{\pi\mu} n_A n_B}$$

(Bimolecular reactions)

When the reactant molecules are alike we have the expression below.

$$Z_{AA} = 2\sigma_{AA}n^2 \sqrt{\frac{\pi k_B T}{m}}$$

- $\sigma$  =diameter of reactant molecule
- n =number of molecules per unit volume (stochoimetry)
- m = mass of molecules
- $\mu$  =reduced mass of molecules
- T = temperature

 $K_{B=}$  Boltzman's constant =  $38 \times 10^{-23} J K^{-1}$ 

Energy factor f is expressed below as the ratio of affection collision to total collision.

$$f = \frac{z}{z_0} = e^{-E_a/RT}$$
$$f = e^{-E_a/RT}$$

Steric factor p is due to molecular arrangement in reactant molecules which could create hindrance during chemical reactions.

$$p = \frac{A}{z_{AB}} = \frac{\text{Pre} - \text{exponential factor}}{\text{collision frequency}}$$
; (0 < p < 1)

Hence in collision  $K = pZ e^{-E_a/RT}$  theory

#### **Transition State Theory**

This theory was established from the works of Erying and Polanyi in 1935which proposed that reactant molecules do not directly become products until an activated complex is formed (Eli, 2022, Santosh, 2006). The activated complex is specie that is not stable and splits to form products at a definite rate as follow.

Reactant  $\rightleftharpoons$  activated complex $\rightarrow$  product

e.g 
$$A + B \rightleftharpoons X^{\#} \to C + D$$

Therefore the equilibrium constant  $K^{\#} = \left[\frac{X^{\#}}{[A][B]}\right]$ 

According to the theory there is a minimum energy requirement to reach the activated complex ( $X^2$ ). This energy is referred to as the activation energy( $E_a$ ). This implies

that even when reactant molecules have the right orientation when colliding and do not have required energy to get to the transition state (activated complex), reaction will not proceed. The energy contribution that leads to formation of products from the activation complex depends on the vibrational frequency. Hence the rate expression at which the complex splits to form products is given below.

*Rate* =  $[X^{#}].v$ 

Since vibrational frequency  $v = \frac{K_B T}{h}$  and  $[X^{\#}] = K^{\#}[A][B]$ 

Then, Rate  $= \frac{K_B T}{h} K^{\#}[A][B]$ 

If k is the rate constant for the overall rection  $A + B \rightarrow$  product

Then, Rate = k[A][B]

By comparing the two rate expressions above

$$k = \frac{K_B T}{h} K^{\#}$$

h = plank's constant

 $k_B$  = Boltzman's constant

Based on thermodynamic considerations, the equilibrium constant of activated complex  $K^{\#}$  is related to the Gibb's function  $\Delta G^0 = \Delta H^0 - T \Delta S^0$ .

Therefore,  $K^{\#} = e^{(\Delta H^0 - T \Delta S^0)/RT}$ 

$$K^{\#} = e^{\frac{\Delta S^0}{R}} \cdot e^{-\frac{\Delta H^0}{RT}}$$

From  $E_a = RT + \Delta H - \Delta nRT$  when  $(\Delta n = 1)$ 

$$E_a = \Delta H^0$$

$$k^{\#} = e^{\Delta S^0/R}$$
 ,  $e^{-E_a/RT}$ 

When  $\Delta n \neq 1$ , then we have  $\Delta H^0 = E_a - RT(\Delta n - 1)$ 

Therefore  $k^{\#} = e^{\Delta S^0/R} e^{-E_a/RT} \cdot e^{-(\Delta n-)}$ 

For unimolecular reaction  $\Delta n = 0$ 

$$k^{\#} = e_{\cdot} e^{\Delta S^{0}/R} \cdot e^{-E_{a}/RT}$$

Since rate constant  $k = \frac{K_B T}{h} K^{\#}$ 

Then  $k = \frac{K_B T}{h} \cdot e \cdot e^{\Delta S^{\#}/R} \cdot e^{-E_a/RT}$ 

 $k = e \cdot \frac{K_B T}{h} \cdot e^{\Delta S^{\#}/R} \cdot e^{-E_a/RT}$ (Unimolecular reactions)

When  $\Delta n = -1$ ,

$$k^{\#} = e^{2} \cdot e^{\Delta S^{0}/R} \cdot e^{-E_{a}/RT}$$
  
 $k^{\#} = e^{2} \cdot \frac{K_{B}T}{h} \cdot e^{\Delta S^{\#}/R} \cdot e^{-E_{a}/RT}$ 

Generally, the rate constant in transition state theory is given by the expression below.

$$k = e^{-(\Delta n - 1)} \cdot \frac{K_B T}{h} \cdot e^{\Delta S^{\#}/R} \cdot e^{-E_a/RT}$$

#### **Arrhenius Equation**

The Arrhenius equation shows the temperature dependence of reaction rates and is mathematically derived from the collision rate expression  $k = Zp e^{-E_a/BT}$ 

Since 
$$p = \frac{A}{Z}$$
;  $Zp = A$ 

$$k = Ae^{-E_a/RT}$$
 Therefore,

Where A = pre-exponential factor,  $E_a =$  activation energy, R = gas constant 8.314 *Jmol*<sup>-1</sup> and T = temperature.

At variable temperature  $T_1$  and  $T_2$  the Arrhenius equation is expressed as follows;

$k_2 = c$	$-\frac{E_a}{P} \begin{bmatrix} 1 \end{bmatrix}$	1]	
$\frac{1}{k_1} = e$	$T_{1}$	$\overline{T_2}$	

#### **Solved Problems**

#### Problem 1

- (i) Calculate the decomposition rate constant of HI at 500k, given that activation energy is 150.0 kjmol<sup>-1</sup> and collision diameter of HI molecule is 3.5 Å.
- (ii) What is fraction of the molecules are activated at the given temperature?

#### <u>Solution</u>

$$2HI_{g \rightarrow}H_{2(g)} + I_{2(g)}$$

(i) Since at every collision we have two similar HI reactant molecules combining,

then  $k = p. Z_{AA} e^{-\frac{E_a}{RT}}$ 

$$k = 4\sigma^{2} \frac{N_{au}}{10^{3}} \left( \sqrt{\frac{\pi RT}{M_{A}}} \right) \cdot e^{-E_{\frac{a}{RT}}} (\text{in dm}^{3} \text{ mol}^{-1})$$

$$k = 4 \times (3.5 \times 10^{-3})^2 \times \frac{6.023 \times 10^{23}}{10^3} \times \left(\sqrt{\frac{22}{7} \times \frac{8.314 \times 500}{128}}\right) \cdot e^{-\frac{15000}{8.314 \times 500}}$$
$$k = 0.2553 \times 10^{10}$$

 $k = 2.553 \times 10^9 mol^{-1} dm^3 s^{-1}$ 

(ii) Fraction of molecules activated at 500k

$$f = e^{-\frac{150000}{4157}} e^{-36.0837}$$
$$f = 4.688 \times 10^{15} \text{molecules}$$

#### Problem 2

Given that  $\Delta s^{\#}$  for a reaction was calculated as  $-80.5 JK^{-1} mol^{-1}$  at a temperature 400*k*. Find the pre-exponential factor *A* of the reaction.

#### Solution

Generally from transition state theory

$$K = \frac{K_B T}{h} e^{\Delta S^{\#}/R} \cdot e^{-E_a/RT} \_ eq (i)$$

And from Arrhenius equation

$$K = Ae^{-E_{a/RT}} \_\_\_eq (ii)$$

By comparing both equations (i) & (ii)

$$A = \frac{K_B T}{h} e^{\Delta S^{\#}/R}$$

Given that

$$K_{B} = 1.38 \times 10^{-23} \ JK^{-1} \ mol^{-1}$$

$$T = 400k$$

$$h = 6.63 \times 10^{-34} \ Js$$

$$R = 8.314 \ Jk^{-1} \ mol^{-1} \ dm^{-3}$$

$$\Delta s^{\#} = -80.5 \ Jk^{-1} \ mol^{-1}$$

$$\Rightarrow A = \frac{1.38 \times 10^{-23}}{6.63 \times 10^{-34}} \ .e^{-80.5/8.314}$$

$$A = 8.3258 \times 10^{12} \ (e^{-9.6825})$$

$$A = 5.193 \times 10^{8} \ mol^{-1} \ dm^{3} \ s^{-1}$$
#### Problem 3

Food rots about 40 times more rapidly at 25<sup>°</sup>c than when it is stored at 4<sup>°</sup>c. Calculate the overall activation energy  $E_a$ , for the decomposition process.  $A[R = 8.3145 Jk^{-1} mol^{-1}]$ 

## **Solution**

Let the initial rate  $k_1 = k$ ,  $T_1 = 4^0 c = 277k$ 

Rate constant at  $25^{\circ}$ c be  $k_2 = 40k$ ,  $k_2 = 25^{\circ}c = 298k$ 

Given that  $R = 8.3145 \ Jk^{-1} \ mol^{-1}$ 

From Arrhenius theory at variable temperatures

$$\frac{k_2}{k_1} = e^{-\frac{E_a}{R}} \left[ \frac{1}{T_2} - \frac{1}{T_1} \right]$$
  

$$\Rightarrow E_a = \frac{-R in (k_2/k_1)}{\left[ \frac{1}{T_2} - \frac{1}{T_1} \right]} = \frac{-8.3145 in (40k/k)}{\left[ \frac{1}{298} - \frac{1}{277} \right]}$$
  

$$E_a = \frac{-8.8145 in 40}{0.00336 - 0.0036} = 122680 \text{ Jmol}^{-1}$$
  

$$E_a = 122.680 \times 10^3 \text{ Jmol}^{-1}$$
  

$$E_a = 122.68 \text{ KJmol}^{-1}$$

#### **Reaction mechanisms**

The microscopic process by which reactants are changed into products is known as a reaction mechanism. Every action is a simple reaction. Intermediaries are species that are created in one phase and consumed in another. The number of molecules that collide in each phase of an elementary reaction can be used to characterise it. The rate-determining step in a reaction system moves the most slowly (Atkins & Julio, 2006).

#### **Elementary reactions**

An elementary reaction is referred to as a one-step reaction with a single transition state and no intermediates. While complex reactions start with simple elementary reactions and build up to more complex ones; many elementary reaction steps can represent complex reactions. A reaction mechanism is made up of a series of simple reactions that shows the fundamental steps in a complex reaction. Elementary reactions can be described in terms of its molecularity (Petrucci, Harwood and Herring, 2002).

# Molecularity

The number of molecules involved in an elementary reaction is known as molecularity, and it is equal to the sum of the stoichiometric coefficients of the reactants in that reaction when there is an effective collision and the right orientation. A reaction may be unimolecular, bimolecular, or even tri-molecular depending on the number of molecules involved. Depending on the number of reacting species molecularity is classified into three: unimolecular, bimolecular and tri-molecular reactions

# **Unimolecular reactions**

This is a type of reaction in which a single reacting species changes form into several molecules.

A $\rightarrow$  P, where A is reactant and P is product. The rate of a unimolecular reaction can be described by the first order rate law:  $\frac{d[A]}{dt} = -k_r [A]$ 

# **Bimolecular reactions**

Two molecules collide in a bimolecular process, exchanging energy, atoms, or groups of atoms. Bimolecular reactions are second-order reactions because the rate of the reaction is dependent on the product of the concentrations of the two species involved.

 $A + B \rightarrow P$ 

rate =k[A][B] or rate= $k[A]^2$ 

Example:  $H_2 + Br_2 \rightarrow 2HBr_{(g)}$ 

rate=k[H<sub>2</sub>][Br<sub>2</sub>]

# **Termolecular reactions**

The simultaneous collision of three particles is necessary for a termolecular reaction. This kind of reaction is extremely rare since it requires synchronous collisions of all three reactants with enough energy and in the right orientation to generate a reaction. There are three possible third order reactions for termolecular processes.

 $A + A + A \rightarrow P \text{ or } A + A + B \rightarrow P \text{ or } A + B + C \rightarrow P$ 

rate =  $k[A]^3$  or rate=  $k[A]^2[C]$  or rate=k[A][B][C]

# **Chain Reactions**

**Definition of Chain reactions and rate law** 

Chain reactions are a collection of simple or elementary steps which are repeated severally

through the formation and consumption of intermediates in an overall reaction. Common chain

reactions include polymerization, combustion of hydrocarbon molecules and explosions

(Michel, 2011). Due to the complex nature of chain reactions, the mechanism involves initiation,

propagation, retardation and termination steps (Eli, 2022). The intermediate often known as

chain carriers are formed during the initiation step, which then attacks other molecules during

propagation. Each attack leads to formation of more chare carriers (intermediates). Then a chain carrier attacks a product molecule that was earlier formed to bring the chain reaction to an end in retardation and termination steps.

**Steady-State Approximation** 

This approximation proposes that concentrations of all intermediate species of a reaction are

constant and remain negligible throughout a reaction (Eli, 2022). The intermediate specie does

not appear in the overall reaction, which means it is produced and consumed during a chemical

reaction. In principle, the steady state approximation assumes that:

Rate of formation of intermediate = Rate of consumption of intermediate.

If the intermediate concentration is denoted by [I]

Then; 
$$\frac{d[I]}{dt} = -\frac{d[I]}{dt}$$

# Rate Law of reactions using steady state principle

The following are fundamental steps to follow in applying steady state principle for

law derivation in chain reactions (Eli, 2022).

(i) Check the proposed reaction steps (mechanisms) whether it balances the overall reaction.

(ii) Write rate expression using the slowest step in the reaction mechanism.

(iii) Express the concentration of all the reaction intermediates by using steady state principle below.

$$\frac{d[I]}{dt} \text{ produced} = -\frac{d[I]}{dt} \text{ consumed}$$

(iv) Replace the intermediate concentrations obtained in (iii) above into the rate expression in

(ii) above to eliminate all intermediates. It is worthy of note when the slowest step of the reaction mechanism does not involve an intermediate, then the rate law will not require the use of steady state approximation.

## Example 1:

Consider the reaction mechanism below in aqueous solution

$$NH_2NO_2 + OH^- \xleftarrow[k_1]{k_{-1}} H_2O + NHNO_2^- \text{ (fast)}$$
$$NH_2NO_2^- \xleftarrow[k_2]{k_2} N_2O + OH^- \text{ (slow)}$$

Assuming  $[H_2 0]$  is unitary (equals 1), derive the rate law for the reaction.

# **Solution**

From the reaction mechanisms with the slowest step

Rate =  $[NHNO_2^-]$ 

Since  $(NHNO_2^-)$  is an intermediate

Then, 
$$\frac{d[NHNO_2^-]}{dt} = k_1[NH_2 NO_2][OH^-] - k_{-1}[H_2O][NHNO_2^-] = 0$$
  
 $k_1[NH_2 NO_2][OH^-] = k_{-1}[H_2O][NHNO_2^-]$  (steady state pribiple)  
 $[NHNO_2^-] = \frac{K_1[NH_2 NO_2][OH^-]}{k_{-1}[H_2O]}$ 

Since  $[H_2 0] = 1$ 

$$[NHNO_{2}^{-}] = \frac{k_{1}}{k_{-1}} [NH_{2} NO_{2}] [OH^{-}]$$

Therefore, Rate =  $k_2 \left( \frac{k_1}{k_1} [NH_2 NO_2] [OH^-] \right)$ 

Rate 
$$k_2 \frac{k_1 k_2}{k_{-1}} [NH_2 NO_2][OH^-]$$

# Example 2:

The reaction  $H_{2(g)} + I_{2(g)} \rightarrow 2HI_g$  occurs through the following mechanism.

$$I_2 \xrightarrow[k_{-1}]{k_{-1}} 2I$$
 (fast)

$$I + I + H_2 \xrightarrow{k_2} 2HI$$
 (slow)

Derive the rate law for this reaction.

# **Solution**

The slow step above rate expression as follow

Rate =  $k_2 [I]^2 [H_2]$ 

Since (I) is the immediate specie

By steady state approximation  $\frac{d[I]}{dt} = 0$ 

$$K_{1}[I_{2}] - K_{-1}[I]^{2} = 0$$
$$\frac{K_{1}[I_{2}]}{K_{-1}} = 0$$
$$[I]^{2} = \frac{K_{1}}{K_{-1}} [I_{2}]$$

Substituting the expression for  $[I]^2$  into the rate law

$$Rate = k_2 \left(\frac{k_1}{k_{-1}} [I_2]\right) [H_2]$$

Rate = 
$$\frac{k_1k_2}{k_{-1}}[I_2][H_2]$$

#### **Conflict of interest**

The authors declare no conflict of interest.

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# STOICHIOMETRY CALCULATIONS WITH CHEMICAL FORMULAS AND EQUATIONS

Sajjad HUSSAIN Hammad KHAN Javaid Rabbani KHAN Ramesha TARIQ

#### Introduction

The way we express different states of matter and the variation take place in its chemical composition is not confined to use in chemistry class or chemical lab; it can be seen widely in scientific world. Think about chemical symbols, formulas, and equations as the universal language of science, showing up not only in chemistry but also in fields as varied as engineering, agriculture, pharmacy, geology, physics, biolog and medical sciences. Now, let's dive a bit deeper into the heart of this linguistic marvel called stoichiometry. In stoichiometry, we master the art of balancing chemical equations and uncovering the precise numerical relationships between the starting materials (*reactant*) and the resulting yields (*product*) (Vaz Jr, 2023)(Danzer, 2007). Imagine you're in a bakery, and you have a recipe that tells you how much flour, sugar, and eggs you need to make the perfect cake. Stoichiometry is like that recipe; it helps scientists and students predict, manage, and enhance chemical reactions just like a baker would whip up a delectable cake. So, whether you're formulating new materials in a lab or making delicious treats in the kitchen, stoichiometry is your trusty guide to ensure everything turns out as planned (Valcárcel Cases et al., 2018).

The term "stoichiometry" finds its roots in ancient Greek, where "stoicheion" (translated as element) and "metron" (interpreted as measure) come together to form its name. This linguistic history beautifully illustrates the core concept of stoichiometry, which is all about measuring and quantifying the elements and compounds that play a role in a chemical reaction. To put it simply, stoichiometry helps chemists figure out the exact amounts of starting materials needed, and the quantities of products generated. Stoichiometric calculations are the foundation upon which the entire building of chemical science stands, forming an essential scaffolding for comprehending and foretelling the consequences of chemical transformations. Imagine stoichiometry as the GPS of the chemical world, charting the precise course of atoms and molecules in their intricate choreography. It's not an overstatement to declare that stoichiometry holds a pivotal role in the realm of chemistry, not only by

unravelling the theoretical mysteries of reactions but also by providing a guiding star for practical applications across diverse industries (Mosher et al., 2023). Consider the example of pharmaceuticals: here, stoichiometry acts as a skilled pharmacist, ensuring that every ingredient in a medication plays its role in harmony, resulting in safe and effective drugs (Fahlman, 2023). Similarly, in the realm of energy production, stoichiometric insights optimize the combustion of fuels, like a master chef perfecting a recipe, ensuring maximum energy output with minimal waste. In essence, stoichiometry is the chemist's trusted companion, illuminating the path from the initial mixture of ingredients to the final product, whether it's a life-saving medicine or a sustainable energy source.

#### **Molecular mass /Weight and Molar Mass:**

Molar mass refers to the weight of one mole of a substance, usually stated in g/mol. It is same in numerical value to the molecular mass of a substance measured in amu. In chemical computations, molar mass is employed to establish the correlation with the mass of a compound and the quantity of moles it encompasses. As an illustration, the water (H<sub>2</sub>O) is approximately is 18 g/mol, indicating that a single mole of water molecules possesses a mass of 18 amu.

# The Mole:

The smallest amount of matter that can be consistently manipulated havinng an incredibly vast number of atoms. Consequently, in any practical scenario, we encounter substantial quantities of atoms, making it advantageous to have a unit for effectively expressing such large numbers.

The concept of quantifying specific quantities with units has a long history. Familiar units like a dozen (12 units) are well-known. In the International System of Units (SI), the mole (mol) is the standardized unit for measuring quantity of a substance. The amount containing the same entities as atoms present in 0.012 kg of pure carbon-12, even the smallest amount of matter has an astonishing number of atoms. In practical scenarios, dealing with these microscopic building blocks requires a convenient way to describe immense numbers of atoms, emphasizing the importance of the mole as a fundamental unit of measurement (Donald A. McQuarrie, Peter A. Rock, 2010).

It is accurately said as the quantity of compound containing an equivalent number of entities, be they atoms, molecules, as found in precisely 0.012 kilograms of pure carbon-12.

# 1mole = 6.02214179×10<sup>23</sup> particles

Avogadro's number, approximately  $6.0223 \times 10^{23}$ , is a tribute to the remarkable contributions of Amedeo Avogadro (1776–1856) to the field of chemistry. Avogadro's number defines what we call 'the mole'—a special unit that signifies a fixed quantity of stuff, with each piece of stuff having its own unique identity. Think of it this way: Just as we casually talk about a dozen eggs or a pair of aces in a deck of cards, we use the term 'a mole' to describe a certain number of atoms, molecules, ions, electrons, or any other tiny particles you can imagine. Imagine helium for a moment. It exists as individual helium atoms, so when we talk about 'one mole of helium,' we're actually talking about  $6.0223 \times 10^{23}$  helium atoms all hanging out together. Now, consider hydrogen, diatomic molecules. So, it means  $6.0223 \times 10^{23}$  H<sub>2</sub> molecules, which also amounts to twice that number,  $2(6.0223 \times 10^{23})$ , of individual H atoms.

Here's the magical part: Each type of atom, molecule, or ion has its own special weight, a unique characteristic mass. And because of this, 01 mole of any compound possesses a precise weight, no matter where you find it. This concept is vital in countless chemistry and science calculations. As mole is the quantity of particles present in 12 g of <sup>12</sup>C. The atomic mass unit, is established as 1/12th of a single <sup>12</sup>C atom's mass. This presents a straightforward yet potent principle: The mass of one mole of atoms from any pure element, measured in grams, precisely equals the element's atomic weight in amu. Therfore we termed the 'molar mass,' is denoted in units such as grams per mole (g/mol) or g mol<sup>-1</sup>.

**Example 1:** How many amu in 01 g of <sup>12</sup>C

$$\underline{2^{-1}} = 1.000 \text{ g} \ {}^{12}\text{C} \text{ atoms} \times \frac{1 \text{ mol} \ {}^{12}\text{C}}{12 \text{ g} \ {}^{12}\text{C} \text{ atoms}} \times \frac{6.022 \times 10^{23} \ {}^{12}\text{C} \text{ atoms}}{1 \text{ mol} \ {}^{12}\text{C} \text{ atoms}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ atom}} \times \frac{12 \text{ amu}}{{}^{12}\text{C} \text{ ato$$

 $= 6.022 \times 10^{23}$  amu

$$1 \text{ g} = 6.022 \times 10^{23} \text{ amu}$$
 or  $1 \text{ amu} = 1.660 \times 10^{-24} \text{ g}$ 

#### Molar Mass:

Molar mass, a vital concept in chemistry, represents the mass of a single mole of a substance and is typically represented in g/mol. This value is exactly equivalent to the

molecular mass, which is measured in amu for compounds. Molar mass plays a crucial role in chemical computations, helping us bridge the gap between mass and moles. Let's dive into this concept with a practical example. Imagine a glass of water,  $H_2O$ , a fundamental compound we encounter daily. Its molar mass is approximately 18 g/mol. This means that if we were to gather one mole of water molecules, we'd have a hefty 18 grams of water right there.

Chemists streamline calculations using a unit called a 'mole.' In essence, a mole is the amount of compound with a mass, measured in g, exactly same as to thier formula mass. Denoted by 'mol,' when benzene ( $C_6H_6$ ) has a formula mass of 78.11, its molar mass is readily identified as 78.11 g/mol. (Kenneth W. Whitten, Raymond E. Davis, Larry Peck, 2010).

Now, the magic happens when we need to switch between mass and moles in chemical calculations. Take benzene as an example again, with its formula mass of 78.11. This indicates that there are precisely 78.11 grams in one mole of  $C_6H_6$ . This insight provides us with two versatile unit conversion factors:

$$\frac{1mol C_6 H_6}{78.11g C_6 H_6} = 1, \qquad or \qquad \frac{78.11g C_6 H_6}{1mol C_6 H_6} = 1$$

We can use a special number to switch between grams and moles when dealing with substances like  $C_6H_6$ . It's like a magical bridge. If you have grams and want moles, you can use it one way, and if you have moles and want grams, you can use it the other way around. For example, let's say you have 100 g of benzene, and you want to figure out how many moles that is. You start with what you know, which is the 100 g, and then you use this special number to find the answer, which is the moles.

$$(100 g C_6 H_6) \times \frac{1 mol C_6 H_6}{78.11 g C_6 H_6} = 1.280 mol C_6 H_6$$

Note that the outcome is displayed with precision up to three significant digits. Furthermore, you have the option to determine the substance's mass when you have a specific quantity of moles at your disposal.

**Example 2:** Argon (Ar) gas is extracted from the air on an industrial scale. When we look at dry air, it contains a tiny 1.0 mole% of Argon, a whopping 78 mole% of Nitrogen (N<sub>2</sub>), and a significant 21 mole% of Oxygen (O<sub>2</sub>). Now, the question is,

how many kilograms of air do we need to extract just one kilogram of Argon? Ar has a mass of 40 amu, while Nitrogen weighs in at 14 amu.

## Solution:

$$N_{2} = 78 \times 28 = 2184 \ grams$$

$$O_{2} = 21 \times 32 = 672 \ grams$$

$$\frac{Ar = 1 \times 40 = 40 \ grams}{2896 \ grams}$$

$$g \text{ of } air = \left(\frac{2896 \, g \, air}{40 \, g \, Ar}\right) (1000 \, g \, Ar) = 72400 \, g = 72.4 \, kg$$

**Example 3:** You have a 30.0 gram sample of a unknown substance which consist of carbon (C), hydrogen (H), and oxygen (O). When you burn it (combustion), you get 25 g of  $CO_2$  and 30 g of  $H_2O$ . Calculate the oxygen molecules were used from the air during this process? Also, explain the way we capture  $CO_2$  and  $H_2O$  in this combustion experiment.

# Solution:

$$\begin{array}{rcl} Organic \ compound \ + \ O_2 & \rightarrow & CO_2 \ + \ H_2O \\ 30 \ g & + \ Xg \ \rightarrow & 25 \ g \ + \ 30 \ g \end{array}$$

Total Material Balance:

Thus X = 25 g

$$Molecule of X or O_2 from air = (25 g O_2) \left(\frac{1 mol of O_2}{32 g of O_2}\right) \left(\frac{6.02 \times 10^{23} Molecule of O_2}{1 mol of O_2}\right) = 4.8 \times 10^{23} molecules$$

OR

$$g \text{ of } C = (25 g CO_2) \left( \frac{12 g C}{44 g CO_2} \right) = 6.82 g \text{ of } C$$
$$g \text{ of } H = (30 g H_2 O) \left( \frac{2 g H}{18 g H_2 O} \right) = 3.3 g \text{ of } H$$

$$g \text{ of } O_2 = (30 g \text{ of compound}) - (6.82 g C) - (3.3 g H)$$

 $g of O_2 in sample = 19.88 g$ 

$$g of O_2 in \ product (H_2O \ and \ CO_2) = (25 \ g \ CO_2) \left(\frac{32 \ g \ O_2}{44 \ g \ CO_2}\right) + (30 \ g \ H_2O) \left(\frac{16 \ g \ O_2}{18 \ g \ H_2O}\right) = 44.85 \ g$$

$$g of O_2$$
 from  $air = g of O_2$  in product  $-g of O_2$  in Sample = 44.8  $g$  -19.88  $g$ 

$$O_2 \text{ molecules} = (25 \text{ g } O_2) \left(\frac{1 \text{ mol of } O_2}{32 \text{ g of } O_2}\right) \left(\frac{6.02 \times 10^{23} \text{ molecules of } O_2}{1 \text{ mol of } O_2}\right) = 4.8 \times 10^{23} \text{ molecules}$$

Upon burning a sample with ample oxygen, the resulting water and carbon dioxide traverse chambers containing various substances. Magnesium perchlorate absorbs the water, and the subsequent chamber sees sodium hydroxide interacting with carbon dioxide. Evaluating the mass increase of magnesium perchlorate and sodium hydroxide measures the quantities of water and CO<sub>2</sub> produced during combustion.

**Example 4:** Imagine you're in an exam hall with dimensions of 80 m in length, 75 m in width, and 50 m in height. Now, let's figure out the amount of carbon dioxide (CO<sub>2</sub>) present in kg. We know that the concentration of CO<sub>2</sub> in this room is 0.04% by volume, and the temperature (T) is 298 K, with the gas constant (R) being 8.314 J mol <sup>-1</sup> K<sup>-1</sup>. The pressure (P) is 101325 Pascals, where  $1Pa = 1N/m^2$ .

Method 1:

$$P = 10^{5} Pa$$

$$V = 80m \times 75m \times 50m = 300000 m^{3}$$

$$R = 8.314 J mol^{-1}K^{-1}T = 298 K$$

$$n = moles of air in the room = ?$$

$$PV = nRT \Rightarrow n = \frac{PV}{RT} = \frac{101325 Pa \times 300000 m^{3}}{8.314 Pa m^{3} mol^{-1}K^{-1} \times 298 K} = 1.21 \times 10^{7} mol of air in the room$$

$$grams of CO_{2} = (1.21 \times 10^{7} mol of air) \times \left(\frac{0.04 mol CO_{2}}{100 mol air}\right) \times \left(\frac{44 g CO_{2}}{1000 g}\right) \times \frac{1kg}{1000 g} = 216 kg$$

#### Method 2:

$$grams of \ CO_2 = \left(300000 \ m^3\right) \times \left(\frac{100 \ L}{1m^3}\right) \times \left(\frac{0.04 \ L \ CO_2}{100 \ L \ air}\right) \times \left(\frac{1 \ mol \ CO_2}{2445 \ L \ CO_2 \ at \ 298 \ K}\right) \times \left(\frac{44 \ g}{1 \ mol \ CO_2}\right) \times \left(\frac{1 \ kg}{1000 \ g}\right) = 215 \ kg$$

#### Writing a Balance Chemical Equation:

Creating balanced chemical equations stands as a core skill within the realm of chemistry. These equations serve as precise portrayals of chemical reactions, effectively illustrating the amound and types of both the initial substances and the resulting compounds. The significance of balanced chemical equations in the field of chemistry cannot be overstated. They play a pivotal role for a variety of compelling reasons:

- Conservation of Mass: The conservation of mass, a cornerstone of chemistry, asserts that
  matter remains unaltered in quantity during chemical reactions. It firmly states that matter's
  inherent nature is persistence, as it can neither be conjured into existence nor obliterated.
  When we skilfully construct balanced chemical equations, we are meticulously orchestrating
  a symphony where the combined mass of the starting materials, referred to as reactants,
  harmoniously converges with the mass of the newly formed substances, aptly termed products.
  Thus, we're not creating matter; we're choreographing its elegant dance of transformation.
- 2. Stoichiometry: Balanced chemical equations are like treasure maps for chemists, revealing the hidden secrets of mole ratios in a chemical metamorphosis. These ratios, akin to magical incantations, unveil the precise quantities of substances needed or produced during the enchanting dance of atoms and molecules. For any experimental alchemist or aspiring soothsayer, this knowledge is indispensable, for it empowers them to wield their reactions with precision and foresee their mystical outcomes.
- Predicting Products: A well-orchestrated balanced chemical equation acts as a crystal ball, foretelling the future of a chemical reaction. It offers valuable insights into the substances that will emerge from the alchemical cauldron and the precise quantities in which they shall manifest under specific enchanting conditions.
- 4. *Quantitative Analysis:* Balanced equations are the alchemical keys to the realm of quantitative analysis. They empower practitioners to gauge the concentration of elixirs, divine the yield of reactions, and measure the efficiency of arcane chemical processes.
- 5. *Reaction Understanding:* Balanced equations provide a clear picture of chemical reactions. They help students to see how chemical reacts and transform into products.
- Communication: Balanced equations transcend linguistic barriers, serving as a universal tongue that unites chemists worldwide. They foster seamless communication, ensuring that scientists across the globe can comprehend and replicate experiments and rituals with unwavering accuracy.

There are different methos used for balancing a chemical equation, Some of the most commonly utilized methods include(Brown, Lawrence S., 2011):

- a) **Trial-and-Error Technique:** This approach is quite simple. You tweak the numbers in front of the chemicals in the equation until the count of atoms for every compound matches on either side of the chemical reaction.
- b) Redox Balancing: In redox reactions, which involve electron exchange, the half-reaction method is applicable. This technique involves dividing the overall reaction into oxidation and reduction reactions. Subsequently, the atoms on either side of reaction are balanced, and charges are individually balanced. Finally, the half-reactions are combined to yield the overall reaction.
- c) **Electron Transfer Balancing:** This method is used for redox reactions, and again we split the overall reaction into oxidation and reduction. During this kind of reaction, the oxidation state

of element changes and by putting suitable number of electrons to balance half reaction. Finally, both reactions are added to get the overall balance chemical equation.

d) Mathematical Approach: This is a more straightforward way to balance a very complex reaction in a short time. Here we make a set of equations to represent conversion of mass of each element in the reaction. Then using mathematical skill to solve these equations simultaneously to find the value of variables and coefficient for every element and compounds which ultimately gives us the balance chemical equation.

#### **Algebraic Method:**

The algebraic approach to balancing chemical equations is a valuable technique. It entails creating a set of linear equations to express the principle of mass conservation for every element within the reaction. This method proves especially handy when dealing with intricate chemical equations, as it offers a systematic solution instead of relying on trial-and-error or visual inspection. Now, let's break down the algebraic method into simple steps for a clearer understanding:

The algebraic method to balance a chemical equation is a useful method. Using this method, we can easily balance a very complex reaction within two minutes and in similar way we can also solve or balance a simple reaction in two minutes, and this is the only advantage and disadvantage of this mathematical approach. Here we supposed variables for each element in reactant and products and then we set linear equations to represent the main conversion of mass (reactant into product) in given reaction. Now we assume the value of one variable to find out the values of other variables. Then we solve this linear equation to find out the value of other variables (elements). The following is the schematic for easily understanding this method.



Figure 1. Breakdown of algebraic methods into simple steps

Example 5:

$$CaSO_{4} + CH_{4} + CO_{2} \rightarrow CaCO_{3} + S + H_{2}O$$
$$aCaSO_{4} + bCH_{4} + cCO_{2} \rightarrow dCaCO_{3} + eS + fH_{2}O$$

#### Solution:

Assume a = 1, then e = d = 1

Mass balance:  

$$Ca: a = d$$

$$S: a = e$$

$$O: 4a + 2c = 3d + f$$

$$C: b + c = d$$

$$H: 4b = 2f$$

$$Since,$$

$$b + c = 1 \rightarrow c = 1 - b$$

$$4 + 2(1 - b) = 3 + f$$
and,  

$$f = 3 + 2b$$

$$b = 3/4$$

$$c = 1 - 3/4 = 1/4$$

$$f = 6/4$$

[4+2c=3+f]

So,

$$CaSO_{4} + \frac{3}{4}CH_{4} + \frac{1}{4}CO_{2} \rightarrow CaCO_{3} + S + \frac{6}{4}H_{2}O$$
$$4CaSO_{4} + 3CH_{4} + CO_{2} \rightarrow 4CaCO_{3} + 4S + \frac{6}{4}H_{2}O$$

How do we balance charge in the algebraic method?

 $aMnO_{4}^{-} + bH^{+} + cFe^{2+} \rightarrow dMn^{2+} + eFe^{3+} + fH_{2}O$ Mass balance: For:  $Mn \rightarrow a = d$ For:  $Fe \rightarrow c = e$ For:  $O \rightarrow 4a = f$ For:  $H \rightarrow b = 2f$ Charge balance: -a + b + 2c = 2d + 3e

Assuming 
$$a = 1$$
, then  $\rightarrow -1 + b + 2c = 2 + 3e$   
 $-1 + 2f + 2e = 2 + 3e$   
 $-1 + 8 - 2 = e$   
 $e = 5, c = 5, a = 1, d = 1, f = 4, b = 8$ 

$$MnO_4^{-} + 8H^{+} + 5 Fe^{2+} \rightarrow Mn^{2+} + 5Fe^{3+} + 4H_2O$$

**Example 6:** Apply the algebraic way to balance the equation:

$$\operatorname{AsO}_{3}^{3-}(\operatorname{aq}) + \operatorname{Br}_{2}(\operatorname{aq}) + \operatorname{OH}_{(\operatorname{aq})}^{-} \to \operatorname{AsO}_{4}^{3-}(\operatorname{aq}) + \operatorname{Br}_{(\operatorname{aq})}^{-} + \operatorname{H}_{2}\operatorname{O}_{(\operatorname{aq})}^{-}$$

Solution:

$$aAsO_3^{3-} + bBr_2 + cOH^- \rightarrow dAsO_4^{3-} + eBr^- + fH_2O$$

Material Balance shows		Charge balance
As:	a = d	-3a-c = -3d-e
<b>O</b> :	3a + c = 4d + f	
Br:	2b = e	
H:	c = 2f	



Figure 2. Diagrammatic representation of limiting reactant pre and post reaction Limiting Reactant:

The limiting reactant has a prime importance in chemical reactions as well as in chemical industry as it decides the amount of product generated during any chemical process. The limiting reactant control the amount of yeild produced in a balance chemical equation. The other reactant which remains unreacted once the reaction complete is known as excess reactant. We can understand the concept by considering the following analogy:

Assume you are baking cookies. You have a limited supply of flour, sugar, and chocolate chips. These are the ingredients for your cookies. Flour and sugar are the limiting reactants here because they are the ones you run out of first. Once you've used up all your flour and sugar, you can't make any more cookies, even though you might still have plenty of chocolate chips left. The flour and sugar are like the limiting reactants, while the chocolate chips are the excess reactant. They remain unused because there's nothing left to react with once the flour and sugar are exhausted (Theodore Brown, H. LeMay, Bruce Bursten, Catherine Murphy, Patrick Woodward, 2012).

**Example 7:** Aluminum chloride, AlCl<sub>3</sub>, plays a crucial role in various industries such as rubber production, lubricant manufacturing, wood preservation, and paint formulation. It can be synthesized through a simple process: the direct combination of aluminum and chlorine:

$$2Al_{(s)} + 3Cl_{2(g)} \rightarrow 2AlCl_{3(s)}$$

To better understand this reaction, let's explore an example. Imagine you have 3.5 grams of aluminum (Al) and 5.2 grams of chlorine gas (Cl<sub>2</sub>) available for this reaction. Our goal is to determine the limiting reactant, find out:

- a) Which of the two reactants is the limiting one?
- b) How much of the excess reagent remains unused?
- c) What quantity of product will be produced?

## Solution:

In every stoichiometric calculation, the first crucial step involves finding the quantity of moles for each of the substances taking part in the reaction. This step is as fundamental as measuring ingredients for a recipe before cooking them, ensuring that you have the right amounts of each reactant, just like a chef measures out flour, sugar, and eggs before making a cake.

Moles of 
$$Al = (3.5g Al) \times \left(\frac{1mol Al}{26.98g Al}\right) = 0.1297 mol Al$$
  
Moles of  $Cl_2 = (5.2g Cl_2) \left(\frac{1 mol Cl_2}{71 g Cl_2}\right) = 0.0732 mol Cl_2$ 

Observing the balanced equation, we notice that when two moles of Aluminum react, they yield an equal amount of two moles of AlCl<sub>3</sub>. So, when we start with 0.1297 moles of Aluminum, it gives us precisely 0.1297 moles of AlCl<sub>3</sub>. In a similar fashion,

if we consider three moles of chlorine, they produce two moles of AlCl<sub>3</sub>. Thus, starting with 0.0732 moles of Cl<sub>2</sub>, we get  $2/3 \times 0.0732$  moles of AlCl<sub>3</sub>, which equals 0.049 moles of AlCl<sub>3</sub>. Now, what's interesting is that Cl<sub>2</sub>, with its 0.049 moles of AlCl<sub>3</sub> production, turns out to be the **limiting reagent** because it produces the least amount of AlCl<sub>3</sub>.

Now, Al is the excess reactant, so we can determine its quantity by:

#### 3 mol. of Cl<sub>2</sub> reacts with 2 mol. of Al

Hence, when you have 0.073 moles of Cl2, it will combine with 0.049 moles of aluminum (which is 2/3 of 0.073 mol)

Al = 0.13 mol.

Therefore, the remaining amount of Al or the amount of excess reactant = 0.13 - 0.049= 0.081 mol.

Remaining Amount of  $Al = mol Al \times molar mass of Al$ 

$$= (0.081 mol Al) \times \left(\frac{27 g Al}{1 mol Al}\right) = 2.2 g Al_{(s)}$$

Lastly, the g of product produced can be found as:

The mol of product calculated using the limiting reactant are 0.049 mol of AlCl<sub>3</sub>

To convert it into grams.

Amount of AlCl<sub>3</sub> produced in the reaction :

$$= (0.049 \, mol \, AlCl_3) \times \left(\frac{133.5 \, g \, AlCl_3}{1 \, mol \, AlCl_3}\right) = 6.54 \, g \, AlCl_{3(s)}$$

## A Fast Way to Identify Limiting Reactants:

A rapid approach to identify a limiting reactant involves determining its moles and dividing each reactant's moles by its reaction coefficient in the balanced chemical reaction. The reactant with the lowest result is the limiting reactant. This method streamlines limiting reactant identification by focusing on mole ratios.

**Example 8:** In the thermite reaction, either 20 g of  $Al_{(s)}$  or 52 g of  $Fe_2O_{3(s)}$  served as the limiting reactant. These masses equate to 0.325 moles of  $Fe_2O_3(s)$  and 0.740 moles

of Al<sub>(s)</sub>. Utilizing the coefficients in the balanced chemical reaction, let's analyze their reaction.

$$\operatorname{Fe}_{2}\operatorname{O}_{3}(s) + 2\operatorname{Al}(s) \rightarrow \operatorname{Al}_{2}\operatorname{O}_{3}(s) + 2\operatorname{Fe}(l)$$

**Solution:** To ascertain whether either of these substances is a limiting reactant, calculate the moles for each species and divide by its respective stoichiometric coefficient.

0.740 moles Al / 2 = 0.37 mol

and  $0.325 \text{ moles of Fe}_2O_3/1 = 0.325 \text{ mol}$ 

As the moles of  $Fe_2O_{3(s)}$  divided by its stoichiometric coefficient are fewer than the moles of Al(s) divided by its stoichiometric coefficient, we determine that  $Fe_2O_{3(s)}$  serves as the limiting reactant. This approach proves beneficial in solving problems with more than two reactants.

When the computed product quantity remains constant for distinct reactants, it implies you've determined the theoretical yield using both reactants, resulting in equivalent yields. In this scenario, neither reactant serves as the limiting reactant, as both can fully react to yield the same product quantity. The limiting reactant, which dictates the maximum product formation, is the one entirely consumed first, thereby restricting the reaction extent. When both reactants have the same theoretical yield of the product, it means that both reactants can react completely, and there is no limitation imposed by either of them. In summary, if the calculated amount of product is the same when considering both reactants, neither reactant is the limiting reactant, and both can be considered as "equally limiting" in the sense that they both contribute to the maximum possible yield of the product.

#### **Theoretical, Actual and Percentage Yield:**

When chemical reactions take place, we can anticipate the amounts of substances created by using the connection between the starting materials and the end products, which is explained through chemical equations. Nevertheless, in actual chemical reactions, things don't always go as planned because of a variety of factors.

#### **Theoretical Yield:**

Theoretical yield, in chemistry, describe the perfect quantity of yeilds expected from a reaction, considering the a balance chemical reaction. It's what we'd get if the reaction ran perfectly without any losses or issues. You can calculate it with this formula:

TY =(moles of limiting reactant) x (molar mass of product)

This represents the product yield obtained when the limiting reagent fully reacts, as shown in our earlier example.

#### **Actual Yield:**

The actual yield represents the real-world quantity of product obtained in a chemical reaction, considering practical limitations and inefficiencies. Factors such as incomplete reactions, side reactions, purification-related losses, impurities, and unexpected occurrences often result in the actual yield being less than the theoretical yield. Experimentally, the actual yield (AY) is determined through measurements.

#### **Percentage Yield:**

The performance of a chemical reaction and the corelation between actual and theoretical yields are gauged by the percent yield. Calculated with a specific formula, the percent yield quantifies the proportion of actual yield to theoretical yield.

Percentage yield = 
$$\left(\frac{Actual Yield}{Theoretical Yield}\right) \times 100$$

Calculating the percentage yield allows chemists to quantify the success of a reaction and identify areas for improvement in reaction efficiency. A percentage yield less than 100% indicates that the reaction did not proceed to completion or that some product was lost, or some undesired by-products were formed.

**Example 9:** A 30.5 g zinc (Zn) sample is reacted with higher quantity of nitric acid (HNO<sub>3</sub>) and produces 65.2 g of Zinc nitrate  $(Zn(NO_3)_2)$ .

$$Zn_{(s)} + 2 HNO_{3(aq)} \rightarrow Zn(NO_3)_{2(aq)} + H_{2(g)}$$

Find out the theoretical yield, the actual yield, and the percentage yield.

## Solution:

The theoretical yield of Zn(NO<sub>3</sub>)<sub>2</sub> is;

Theoretical yield = 
$$(30.5 \text{ g } Zn) \times \left(\frac{1 \mod Zn}{65.38 \text{ g } Zn}\right) \times \left(\frac{1 \mod Zn(NO_3)_2}{1 \mod Zn}\right) \times \left(\frac{189.36 \text{ g } Zn(NO_3)_2}{1 \mod Zn(NO_3)_2}\right)$$
  
=  $88.34 \text{ g } Zn(NO_3)_2$ 

The actual yield of  $Zn(NO_3)_2$  is the quantity produced, which, as mentioned, is 65.2 grams.

The percentage yield is given by:

% yield = 
$$\left(\frac{actual \ yield}{theoretical \ yield}\right) \times 100 = \left(\frac{65.2}{88.34}\right) \times 100 = 73.8$$
 %

Hence, we can conclude that the reaction has achieved approximately three-fourths of its maximum potential yield.

#### **Empirical and Molecular Formulas:**

Within the realm of chemical calculations, understanding the composition of compounds is a fundamental aspect of chemical analysis. Chemical formulas serve as concise representations of the elements present within a compound, as empirical and molecular formulas.

#### **Empirical Formulas:**

Empirical formulas represent the simplest whole-number ratio of atoms within a compound. These formulas give us a basic knowledge about comparable proportions of various elements in a compound and minimize the complexity of multiple atoms of the same element in a molecule. The empirical formula can be determined using experimentation and analysis. For example, molecular formula of Glucose is  $C_6H_{12}O_6$ . The Simplest or empirical formula would be  $CH_2O$  as it is showing the simple whole-number ratio of carbon (C), hydrogen (H), and oxygen (O) atoms.

#### **Molecular Formulas**

The molecular formulas give us a detailed representation of a compounds composition by representing the exact number and types of atom in compound. These describe an accurate detail of a compound which include number of atoms and their arrangement (Donald A. McQuarrie, Peter A. Rock, 2010). As we see in our previous example, that Glucose has  $C_6H_{12}O_6$  formula, there are 06 carbon, 12 hydrogen, and 06 oxygen atoms. Molecular formulas are important if we want to understand the exact configuration of a compound. The molecular formulas can easily be calculated from empirical formula by using following equation.

Molecular Formula =  $n \times Empirical$  Formula

Here in "n" is factor which can be determined as

n = molecular formula mass / empirical formula mass

For Example:

Let the Benzene, having empirical formula CH. Its molecular formula is  $C_6H_6$ .

Molecular formula mass of Benzene = 78 g/mol

Empirical formula mass of Benzene = 13

So n will be equal to 78/13 = 6

In this case, Molecular Formula for Benzene (CH)  $= 6 \times$  Empirical Formula (CH)

$$= C_6 H_6$$

**Example 10:** Upon complete combustion of 0.50 g of ascorbic acid commonly known as vit-C having C, H, and O atoms, resulting in 0.75 g of CO<sub>2</sub> and 0.205 g of H<sub>2</sub>O, deduce the empirical formula. With atomic masses: C (12 amu) and O (16 amu), if the molecular mass is 176 amu, establish the molecular formula.

#### Solution:

$$g \text{ of } C = (0.75 \text{ g } CO_2) \left(\frac{12 \text{ g } C}{44 \text{ g } CO_2}\right) = 0.204 \text{ g of } C$$
$$g \text{ of } H = (0.205 \text{ g } H_2 \text{O}) \left(\frac{2 \text{ g } \text{H}}{18 \text{ g } \text{H}_2 \text{O}}\right) = 0.022 \text{ g of } \text{H}$$
$$g \text{ of } O = (0.50 \text{ g of compound}) - (0.204 \text{ g } C) - (0.022 \text{ g } H)$$
$$g \text{ of } O = 0.274 \text{ g}$$
$$Mole \text{ of } C = (0.204 \text{ g } \text{C}) \left(\frac{1 \text{ mole } \text{C}}{12 \text{ g } \text{C}}\right) = 0.017 \text{ mol of } C$$

Mole of 
$$H = (0.022 \text{ g H}) \left(\frac{1 \text{ mole H}}{1 \text{ g H}}\right) = 0.022 \text{ mol of H}$$
  
Mole of  $O = (0.274 \text{ g O}) \left(\frac{1 \text{ mole O}}{16 \text{ g O}}\right) = 0.017 \text{ mol of O}$   
0.017 mole of  $C \cong 0.022$  mole of  $H \cong 0.017$  mole of  $O$   
dividing by lowest i.e0.017  
1 mole of  $C \cong 1.3$  mole of  $H \approx 1$  mole of  $O$   
multiply by lowest 3 to get whole number  
3 mole of  $C \cong 4$  mole of  $H \approx 1000 \text{ gc}$ 

So the empirical formula of the comound will be  $C_3H_4O_3$ 

The molecular mass is given i.e. 176 and the empirical formula mass is 88,

so the molecular formula must be  $\frac{176}{88} = 2$  times the empirical formula. Thus, the molecular formula is  $= 2(C_3H_4O_3) = C_6H_8O_6$ .

#### **Gas Stoichiometry:**

Chemical stoichiometry also the reactants and products chemical reactions in gaseous phase. While reactions involving gases share similarities with those involving solids and liquids, the incorporation of the Ideal Gas Law (PV=nRT) distinguishes them. Utilizing this law, we can compute the quantity of gas molecules present when armed with information on volume, pressure, and temperature(Andrew Burrows, John Holman, Simon Lancaster, Tina Overton, 2017).

Laboratory processes often encompass the formation or reaction of gases, necessitating chemists' competence in quantifying gaseous reactants and products, akin to their treatment of solids or solutions. Additionally, many crucial industrial reactions occur gaseous state. Gases readily combine, facilitate heating or cooling, and can be conveniently transported within manufacturing facilities through basic pumps and plumbing (Atkins, 2006).

Stoichiometric calculations for gas-involved reactions commonly involve the Ideal Gas Law Below is a comprehensive guide to executing stoichiometric computations.



#### *Here's is the illustrattion steps:*

**Example 11:** In the reaction  $2H_2 + O_2 \rightarrow 2H_2O$ , 5.0 moles of hydrogen gas (H<sub>2</sub>) react with high amount of O<sub>2</sub> gas Calculate the volume of water vapor (H<sub>2</sub>O) produced at 25°C and 1.00 atm.

#### Solution

Step 1: Balance the equation:  $2H_2 + O_2 \rightarrow 2H_2O$ .

Step 2: Convert temperature to Kelvin:  $25 \circ C + 273.15 = 298.15 \text{ K}$ .

*Step 3:* Compute the mol of H<sub>2</sub>:

$$n = \frac{(PV)}{(RT)} \rightarrow n = \frac{(1atm) \times (1L)}{(0.0821 L \cdot atm / (mol \cdot K) \times 298.15K)} \rightarrow n \approx 0.0406 \text{ moles of } H_2$$

*Step 4:* Apply stoichiometry:

Using the balanced equation, 2 moles of H<sub>2</sub> produce 2 moles of H<sub>2</sub>O.

*Step 5:* Calculate the volume of H<sub>2</sub>O:

Since 2 moles of  $H_2$  produce 2 moles of  $H_2O$ , and we have 0.0406 moles of  $H_2$ , we will also have 0.0406 moles of  $H_2O$ .

Now, applying PV=nRT to find Vol:

$$n = \frac{(PV)}{(RT)} \rightarrow 0.0406 \, moles = (1.00 \, atm) \times \frac{V}{(0.0821 \, L \cdot atm \, / \, (mol \cdot K) \times 298.15K)} \rightarrow V \approx 1.73 \, L.$$

So, approximately 1.73 L of water vapor are produced in the reaction.

## **Gas Stoichiometry Principles:**

Gas stoichiometry relies heavily on gas properties, especially molar volume, in elucidating the quantitative relationships between reactants and products during chemical reactions involving gases. Here's how these gas properties come into play (Ralph H. Petrucci, Carey Bissonnette, F. Geoffrey Herring, 2007):

- Molar Volume (V<sub>m</sub>): Molar volume signifies the space occupied by 01 mol of a gas under certain T and P, often denoted in L/mol. Particularly notable at STP, approximately 22.4 L/mol, it simplifies conversions between moles and volume in gas stoichiometry. For instance, having 2 moles of a gas at STP translates to a volume of 44.8 L (2 moles \* 22.4 L/mol).
- Ideal Gas Law: interrelates pressure (P), volume (V), moles of substance (n), and temperature (T) for a gas. It proves valuable for deducing unknown gas properties or calculating the quantity of gas involved in a chemical reaction. For example, it aids in determining the moles of gas generated in a reaction when furnished with volume, pressure, and temperature data.
- Stoichiometry Ratios: In the context of chemical reactions, balanced chemical equations offer stoichiometric coefficients that essentially delineate the mole ratios governing reactants and products. These ratios become particularly pivotal in gas stoichiometry, aiding in establishing the connection between the reactants and products.
- Combining Gas Laws: Gas stoichiometry frequently necessitates the integration of various gas laws like Boyle's law (P<sub>1</sub>V<sub>1</sub> = P<sub>2</sub>V<sub>2</sub>) or Charles's law (V<sub>1</sub>/T<sub>1</sub> = V<sub>2</sub>/T<sub>2</sub>) with stoichiometric ratios to solve for hitherto unknown variables. For instance, Boyle's law can be employed to deduce the final volume of a gas when initial volume and pressure values are provided, and pressure undergoes alterations during a reaction.

## **Complex Stoichiometric Problems:**

Below are the advanced stoichiometric problems involving multiple reactions and the combination of various stoichiometric principles, including mole ratios, reaction stoichiometry, and the Ideal Gas Law.

**1- Multiple Reactions:** 

**Example 12:** In a complex chemical process, ammonia  $(NH_3)$  is produced rom nitrogen  $(N_2)$  and hydrogen  $(H_2)$ . The reactions occur in two steps:

$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)} (Formation of ammonia)$$
$$2NH_{3(g)} \rightarrow N_{2(g)} + 3H_{2(g)} (Decomposition of ammonia)$$

Suppose you start with 5.0 moles of  $N_2$  and 15.0 moles of  $H_2$ . Calculate the final amount of ammonia and the remaining amounts of  $N_2$  and  $H_2$  after both reactions.

#### Solution:

Calculate the moles of NH<sub>3</sub> generated in the first reaction:

From the balanced equation, 1 mole of N<sub>2</sub> produces 2 moles of NH<sub>3</sub>.

Moles of NH<sub>3</sub> formed =  $(5.0 \text{ moles of } N_2) \times (2 \text{ moles of } NH_3 / 1 \text{ mole of } N_2) = 10.0$ 

## moles of NH<sub>3</sub>.

*Calculate the moles of NH*<sup>3</sup> *consumed in the second reaction:* 

From the balanced equation, 2 moles of NH<sub>3</sub> produce 1 mole of N<sub>2</sub>.

Moles of NH<sub>3</sub> consumed =  $(10.0 \text{ moles of NH}_3) \times (1 \text{ mole of } N_2 / 2 \text{ moles of NH}_3) =$ 

5.0 moles of N<sub>2</sub>.

Calculate the moles of  $H_2$  consumed in the second reaction:

From the balanced equation, 2 moles of NH<sub>3</sub> produce 3 moles of H<sub>2</sub>.

Moles of H<sub>2</sub> consumed =  $(10.0 \text{ moles of NH}_3) \times (3 \text{ moles of H}_2 / 2 \text{ moles of NH}_3) =$ 

15.0 moles of H<sub>2</sub>.

*Calculate the remaining moles of N*<sub>2</sub>*:* 

Initial moles of N<sub>2</sub> – Moles of N<sub>2</sub> consumed = 5.0 moles - 5.0 moles = 0 moles. *Calculate the remaining moles of H*<sub>2</sub>:

Initial moles of  $H_2$  – Moles of  $H_2$  consumed = 15.0 moles – 15.0 moles = 0 moles. So, after both reactions, you have 0 moles of  $N_2$  and 0 moles of  $H_2$  remaining, and you have 10.0 moles of NH<sub>3</sub>.

2- Combining Stoichiometric Principles:

**Example 13:** In the combustion of methane (CH<sub>4</sub>), 1.00 mole of CH<sub>4</sub> interact with 2.00 moles of  $O_2$  to generate CO<sub>2</sub> and H<sub>2</sub>O. Calculate the volume of CO<sub>2</sub> produced at STP when 4.00 moles of CH<sub>4</sub> are burned completely.

#### Solution:

Determine the moles of O<sub>2</sub>:

1 mole of CH<sub>4</sub> requires 2 moles of O<sub>2</sub>.

Moles of  $O_2$  needed = (4.00 moles of  $CH_4$ ) × (2 moles of  $O_2$  / 1 mole of  $CH_4$ ) = 8.00

moles of O<sub>2</sub>.

Use the Ideal Gas Law to find volume of CO<sub>2</sub> at STP:

Since 1 mole of any gas occupies 22.4 L

Vol of  $CO_2 = (8.00 \text{ moles}) \times (22.4 \text{ L/mol}) = 179.2 \text{ L}.$ 

So, 179.2 L of  $CO_2$  are produced when 4.00 moles of  $CH_4$  are burned completely at STP.

#### 3- Limiting Reactants and Percent Yield:

**Example 14:** In the synthesis of ammonia (NH<sub>3</sub>), 4.00 moles of nitrogen (N<sub>2</sub>) react with 12.0 moles of hydrogen (H<sub>2</sub>) as below:

$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$$

- a) Find the limiting reactant.
- b) Compute the moles of NH<sub>3</sub>.
- c) If the reaction goes to completion under the given conditions (no excess reactants), calculate the actual moles of NH<sub>3</sub> produced.
- d) The percent yield if 7.50 moles of NH<sub>3</sub> are obtained.

## Solution:

*a)* To find out the limiting reactant, we need to compare the moles of  $NH_3$  that can be produced from both  $N_2$  and  $H_2$ .

From N<sub>2</sub>: 4.00 moles of N<sub>2</sub> \* (2 moles of NH<sub>3</sub> / 1 mole of N<sub>2</sub>) = 8.00 moles of NH<sub>3</sub>.

From H<sub>2</sub>: 12.0 moles of H<sub>2</sub> \* (2 moles of NH<sub>3</sub> / 3 moles of H<sub>2</sub>) = 8.00 moles of NH<sub>3</sub>.

Both  $N_2$  and  $H_2$  produce 8.00 moles of  $NH_3$ , so there is no limiting reactant; both  $N_2$  and  $H_2$  are in excess.

*b) The maximum moles of NH*<sup>3</sup> *that can be produced are:* 

Moles of NH<sub>3</sub> produced =  $(4.00 \text{ moles of } N_2) * (2 \text{ moles of } NH_3 / 1 \text{ mole of } N_2) = 8.00 \text{ moles of } NH_3.$ 

c) If the reaction goes to completion under the given conditions with no excess reactants:

Moles of NH<sub>3</sub> produced =  $(4.00 \text{ moles of } N_2) * (2 \text{ moles of } NH_3 / 1 \text{ mole of } N_2) = 8.00 \text{ moles of } NH_3$ .

So, if the reaction goes to completion, 8.00 moles of NH<sub>3</sub> will be produced.

d) To calculate the percent yield, use the formula:

Percent Yield = (Actual Yield / Theoretical Yield) \* 100

Given that the actual yield is 7.50 moles of NH<sub>3</sub> and the theoretical yield is 8.00 moles (as calculated in part c):

$$Percent Yield = \left(\frac{7.50 \,moles}{8.00 \,moles}\right) \times 100 = 93.75\%$$

The percent yield is 93.75% when 7.50 moles of NH<sub>3</sub> are obtained.

#### 4- Gas Stoichiometry with Volume and Temperature Changes:

**Example 15:** A 5.00-liter container is initially filled with hydrogen gas (H<sub>2</sub>) at  $27^{\circ}$ C and 2.00 atm pressure. It reacts with excess oxygen gas (O<sub>2</sub>) to form water vapor (H<sub>2</sub>O):

$$2H_{2(g)} + O_{2(g)} \rightarrow 2H_2O_{(g)}$$

Calculate the final volume of the container after the reaction is complete if the temperature remains constant.

#### Solution:

To calculate the final volume of the container after the reaction is complete, we can use the ideal gas law, assuming that the temperature remains constant.

Initial volume  $(V_1) = 5.00 L$ 

Initial pressure 
$$(P_1) = 2.00$$
 atm

$$T(K) = 27^{\circ}C + 273.15 = 300.15 K$$

Initial moles of  $H_2(n_1) = ?$ 

The ideal gas law is given by: PV = nRT

We can find the initial moles of H<sub>2</sub> using the ideal gas law:

$$n_1 = (P_1 V_1) / (RT_1)$$
$$2H_{2(g)} + O_{2(g)} \rightarrow 2H_2 O_{(g)}$$

Since 2 moles of H<sub>2</sub> produce 2 moles of H<sub>2</sub>O, the mole ratio is 1:1. This means that if all the H<sub>2</sub> reacts, the number of moles of H<sub>2</sub>O produced will be the same as the initial moles of H<sub>2</sub>. So,  $n_1$  (initial moles of H<sub>2</sub>) will also be the initial moles of H<sub>2</sub>O formed. Now, we can use the equation below to find the final volume (V<sub>2</sub>) when the reaction is complete:

$$V_2 = (n_1 R T_1) / P_1 = \frac{(n_1 \times 0.0821 L \cdot atm / (mol \cdot K) \times 300.15 K)}{2.00 atm} \approx 7.82 L$$

Therefore, the final volume of the container after the reaction is complete, assuming constant temperature, is approximately 7.82 L.

## **Applications in Real-World Chemistry:**

Stoichiometry, a fundamental concept in chemistry, holds immense importance in various industries, including pharmaceuticals, agriculture, and environmental science. It serves as the quantitative foundation for optimizing processes, ensuring product quality, and addressing environmental concerns.

In the pharmaceutical industry, stoichiometry is indispensable for precise drug synthesis and formulation, guaranteeing the production of pharmaceutical compounds

with the desired purity and efficacy. In agriculture, stoichiometry aids in fertilizer production, determining the optimal nutrient ratios to promote plant growth while minimizing environmental impact. It also plays a crucial role in pesticide formulation, allowing for precise concentrations to control pests while safeguarding ecosystems.

Environmental science benefits from stoichiometry in pollutant monitoring and source identification, facilitating environmental impact assessments. It guides chemical dosing in wastewater treatment, ensuring efficient pollutant removal and reducing the generation of harmful byproducts. Stoichiometry is equally essential in the food industry, where it ensures accurate ingredient proportions and nutritional calculations to maintain product consistency. It also plays a vital role in brewing and fermentation processes, maintaining precise ratios for beverage and fermented food production.

Stoichiometric calculations inform various processes across different domains. In drug synthesis, they ensure precision and efficiency by minimizing waste and production costs. Stoichiometry aids in purity assessment by allowing chemists to compare actual yields to theoretical yields, guiding purification processes. In large-scale drug manufacturing, it ensures consistent product quality and reliability.

In the context of pollutant monitoring, stoichiometric calculations are indispensable for quantifying pollutant concentrations, facilitating regulatory compliance, and conducting environmental impact assessments. Furthermore, stoichiometry assists in source identification, as different pollutant sources release substances with distinct stoichiometric ratios, enabling accurate tracing of pollution origins. Stoichiometry significantly contributes to environmental impact assessments by revealing how pollutants disrupt natural systems, guiding conservation and remediation efforts. These diverse applications underscore the versatile and critical role of stoichiometry in various processes, from drug synthesis to environmental protection.

## Conclusion

This chapter has revealed a comprehensive exploration of fundamental concepts in quantitative chemistry. Beginning with mole, conversion of gram into mole and molecules and the chemical equations their balancing by algebraic method, we ventured into the world of mole concepts and Avogadro's number, enabling us to seamlessly convert between mass and moles. The concept of the limiting reactant revealed how one key component can determine the extent of a reaction, while actual and theoretical yield calculations shed light on real-world complexities in chemical processes. We also delved into empirical and molecular formulas, essential tools for

deciphering compound compositions, and applied these concepts to practical scenarios. Gas stoichiometry expanded our horizons to encompass gas-phase reactions, while complex stoichiometry problems showcased the versatility of these principles in solving real-world chemical puzzles. Stoichiometry's versatility enhances efficiency and sustainability in these fields, driving advancements in healthcare, agriculture, and environmental protection.

#### **Summary**

Stoichiometry is the common language of chemistry, chemical engineering and chemical technology explaining its principles, applications, and significance in understanding chemical reactions and their quantitative relationships. Preliminary it is establishing a solid foundation, elucidating crucial concepts like atoms, molecules, and moles. Stoichiometry operates at the atomic level, highlighting the mole concept's role in bridging macroscopic and microscopic areas. To calculate the quantity of reactants and its respective product we need a balance chemical equation which is showcasing how it reflects mass and mole conservation. Herein we elaborate an algebraic way to balance a very complex reaction in a very simple mathematical way. The Practical examples are discussed, and the provision of step-by-step solutions enhances understanding. Stoichiometric coefficients' vital role in chemical equations is detailed, enabling the calculation of reactant consumption and product formation. The chapter explores limiting reactants, explaining their influence on reaction extent. Discussions on identifying limiting reactants and calculating percent yield enhance efficiency assessment. Stoichiometry extends beyond theory; its practical applications span environmental science, pharmacy, and industry, including pollution control, pharmaceutical formulation, and chemical manufacturing. Real world problems encompass reaction stoichiometry and stoichiometry of gases catering to those seeking deeper insights. Exercises and problems engage readers in applying stoichiometric knowledge, with detailed solutions provided for reinforcement. This chapter underscores stoichiometry's pivotal role as chemistry's language. It facilitates comprehension and control of chemical transformations, applicable in laboratories and industrial processes. This concise yet comprehensive chapter equips readers with essential knowledge and problem-solving skills, making stoichiometry an indispensable resource for students as well as teachers and other readers.

#### **Scientific Ethics Declaration**

The authors say that they are responsible for the scientific, moral, and legal aspects of this chapter, which is published in *Chemistry for the Life*.

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**Conflict of Interest** 

The authors declare no conflict of interest.

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#### PH, ACID AND BASES IN CHEMISTRY

Oladoja A. AWOFISAYO

#### Introduction

pH is a fundamental concept in chemistry that measures the acidity or alkalinity of a solution. The term refers to the power of hydrogen? It quantifies the concentration of Hydrogen ions in solution. The pH and pH scale was introduced was introduced by Danish chemist Soren Peder Lauritz Sorensen in 1909. He developed the pH scale as a way to express the acidity or alkalinity of a solution, ranging from 0 to 14. They play a crucial role in understanding chemical reactions, biological processes, and various industrial applications. Compounds (organic and inorganic ) including drugs are classified as acids or bases based on the pH scale.

Sample	pН	рОН	[H]+(M)	рН
Solution				
	-1	15	10 <sup>1</sup>	
1M HCl	0	14	10 <sup>0</sup> or 1	
(Battery acid)				
Gastric Juice	1	13	10-1	
Lemon juice	2	12	10-2	
1M CH <sub>3</sub> COOH Vinegar	3	11	10-3	
Tomatoes	4	10	10 <sup>-4</sup>	
Black Coffee	5	9	10-5	
Milk	6	8	10-6	
Portable Water	7	7	10-7	
Ocean Water	8	6	10-8	
Baking Soda	9	5	10-9	
Milk of Magnesia	10	4	10 <sup>-10</sup>	
Milk of Magnesia	11	3	10-11	
Ammonia	12	2	10-12	

Bleach	13	1	10-13	
1M NaOH	14	0	10-14	
Caustic Soda				
	15	-1	10-15	

An illustration of the pH scale with common substance is as follows

pH 0-1 strong acids like HCl acid (Battery acid)

pH 2-3 lemon juice and Vinegar

pH 4-5 tomatoes and black coffee

pH 6 milk

pH 7 portable water

pH 8-9 Baking soda

pH 10-11 Ammonia solution

pH 12-14 Caustic soda and bleach

The pH of portable water is 7 which is neutral that is neither acidic nor basic. The presence of contaminants can thus lower the pH of water (acidic) or increase it (basic).

## Measurement

The pH of a solution can be determined by the pH paper (indicator strips), the Universal Indicator and the pH meter.

pH paper/Indicator strips are simple and cost effective tools used to determine the pH of a solution. They consist of a paper or plastic strip impregnated with a mixture of different chemical indicators. These indicators change their color in response to different pH values. The strips were developed in the 19<sup>th</sup> century when scientists began exploring natural dyes as pH papers. An example is the litmus paper which turns red in the acidic medium and blue in the basic medium. The pH indicator strips is available in various forms as the pH paper, the pH tape or the pH strips. They provide a rapid, qualitative and cost effective assessment of the pH of a solution. It is widely used in titrimetric methods. They have distinct colours for each pH and are provided with matching charts with the specific test strips provided. The strip is placed on the surface of the wet substance. Or a few drops

# **The Universal Indicator**

The measurement tool provides a more comprehensive analysis of pH values across the entire

These strips change colour depending on the pH of the solution. It is exhibits smooth color changes over a wide range of pH from 1 to 14. Examples examples include

Indicator	Low pH colour	Transition pH range	Description	High pH colour
m-Cresol Purple	Strong Acid	0.5-2.5	Red	Yellow
Thymol Blue	Strong Acid	1.2-2.8	Red	Yellow or Orange
2,4-Dinitrophenol	Strong Acid	2.6-4.0	Colourless	Yellow
Bromophenol blue	Strong Acid	3.0-4.6	Yellow	Blue
Methyl Orange	Weak Acid	3.1-4.4	Red	Yellow or Orange
Sodium Alizarin sulphonate	Weak Acid	3.7-5.2	Yellow	Violet
Bromocresol green	Weak Acid	3.8-5.4	Yellow	Blue
Methyl Red	Weak Acid	4.2-6.2	Red	Yellow
Bromocresol Purple	Weak Acid	6.0-7.6	Yellow	Blue
Alizarin	Weak Acid	5.5-6.8	Yellow	Red
p-Nitrophenol	Weak Acid	5.5-7.6	Colourless	Yellow
Bromothymol blue	Weak Acid	6.0-7.6	Yellow	Blue
Phenol red	Weak Acid	6.8-8.4	Yellow	Red
Cresol red	Weak Base	7.2-8.8	Yellow	Red
m-Cresol Purple	Base	7.4-9.0	Yellow	Purple
Thymol Blue	Base	8.0-9.6	Yellow	Blue
Phenopthalein	Strong Base	8.3-10.0	Colourless	Fuchsia
Thymophenopthalein	Strong Base	9.3-10.5	Colourless	Blue
Alizarin Yellow	Strong Base	10.2-12.0	Yellow	Red

# pH meters

These are electronic devices that provide a precise measurement of pH by measuring the voltage difference between a reference electrode and a glass electrode immersed in the solution. It is a highly precise and quantitative instrument used to measure the pH of a solution. It is developed from early 20<sup>th</sup> century with significant advancements occurring during the mid 20<sup>th</sup>.
## Application

## Water Quality Analysis

pH meters are extensively used in water quality analysis to determine the acidity or alkalinity of water samples. This is crucial in accessing the suitability of water for various purposes, such as drinking, irrigation and industrial processes. pH measurements help identify potential issue such as acid rain, pollution, or changes in natural water bodies. They also assist in monitoring the effectiveness of water treatment processes.

## Food and Beverage Industry

The pH of food and beverages plays a critical role in product quality, safety and preservation. pH meters are used to monitor and control acidity levels during food processing and manufacturing. They ensure that the desired pH is maintained in products such as fruit juices, dairy products, canned goods and fermented foods. pH meter measurements are included in quality control protocols and food safety regulations.

## Soil Analysis

pH meters ar e employed in soil analysis to determine the pH of soil samples. Soil pH affects nutrient availability, microbial activity and plant growth.pH measurements assist in soil fertility assessments, determination of lime or fertilizer requirements and identification of acidic or alkaline conditions. It is valuable for agricultural practices, horticulture and land management strategies.

### Pharmaceutical Research and Development

In pharmaceutical research and developments, pH meters are used to access the pH of drug formulations including solutions, suspensions and emulsions. pH pays a crucial role in drug stability, solubility, bioavailability and efficacy. The pH measurements helps to optimize drug formulations and ensure their quality and effectiveness.

## Medicine and Medical Diagnosis

pH is measured in the human body to diagnose certain medical conditions and monitor effectiveness of treatments for example, blood pH is titghtly regulated to maintain proper physiological functioning.

Test strips are used as diagnostic tools to test the urine

### **Chemical and Industrial Processes**

They are employed to monitor and control pH levels in chemical reactions, wastewater treatment plants, electroplating, paper and pulp manufacturing and many other industrial operations. Process efficiency, product quality and complying with environmental regulations

pH meters are used in various chemical and industrial processes.

## **Environmental monitoring**

Field studies and environmental monitoring programs to quickly access the pH of natural water bodies such as rivers, lakes and oceans.

### **Chemistry and Biochemistry**

pH is essential for understanding chemical reactions, enzyme activity and the behavior of acids and bases in solution.

## Food and Beverage Industry

pH is a critical parameter in food production, preservation and quality control. It affects taste, texture and microbial growth in various food products.

## Limitation

pH values do not give directly the concentration of the solution.

pH value of zero is obtained in a solution of strong acid.

pH value of an acid with low concentration is not above 8 but below the neutral pH 7.

## 1.Acid-Base Balance and Blood pH

A range of disorders can result from acid-base imbalance and these disorders are classified based on the cause and the direction of the pH change into respiratory or metabolic acidosis. Hydrogen ions with some other anions like serum sodium ion, potassium ions, sulphate, chloride ions and protein. The pH of the arterial blood is tightly regulated within a narrow range of 7.35 to 7.45. This balance is essential for proper oxygen delivery, enzyme function, and overall cellular metabolism. Acidosis (pH<7.35) or alkalosis (pH>7.45) can disrupt normal physiological processes and lead to serious complications as revealed below by the following examples.

## 2. Respiratory pH regulation

The respiratory system acts as a primary regulator of pH by controlling the elimination of carbon dioxide (CO2). Increased CO2 levels lead to acidosis, while decreased CO2 levels cause alkalosis. Conditions such as Chronic Obstructive Pulmonary Disease (COPD) can impair respiratory function, resulting in respiratory acidosis.

## **3.Gastric pH and Digestion**

The stomach maintains an acidic environment (pH 1.5-3.5) to aid in the digestion and breakdown of food. Alterations in gastric pH can impact the activity of digestive enzymes and the absorption of nutrients. Conditions like gastritis or the use of acid-suppressing medications can disrupt the normal gastric pH, leading to impaired digestion.

## 4.Urinary pH and Kidney Function

The Kidney help regulate the body's pH by selectively reabsorbing excreting hydrogen ions (H+) and bicarbonate ions (HCO3-). Changes in urinary pH can affect the formation of kidney stones and the elimination.

## 5.Vaginal pH

## 6.Tumorigenesis

### 7.Skin

### Application of the principle of pH

### **Acids and Bases**

Acids and Bases are important in various chemical processes which occur within our bodies and outside in our environment for instance the biochemical reactions that occur at the molecular level in our bodies, the synthesis and reactions carried out in the laboratory, industrial processes and others. The human body comprises of 70-75% water and drugs may be ingested which is first diluted, it's acid-base behavior can thus be described by the theory described by Bronsted and Lowry. Acid-base imbalance in the body can also result in various diseases A quatic life also depends on specific pH as pollutants from oil spillage or acid rain can alter the pH and destroy plants, microbes and fishes in the aquatic terrain. The quality of water obtained from boreholes and wells can be affected by dissolved mineral acids/bases and result in various neurological diseases, cognitive impairment in children. skin reactions/lesions, kidney damage, endocranial damage, reproductive disorders, cardiovascular problems and immunological issues upon ingestion provided the impurities are not dealt with to restore the pH. Soil contamination by acid rain can result in serious consequences on the vegetables and food produced. Corrosion in pipes made of lead has also result in grave consequences when the pip-borne water is consumed. The process in the Pharmaceutical industries must be carried out with utmost caution to the pH, acids and bases. Essentially, it can affect the totality of our lives.

Scientists from centuries past have discovered that the sour taste in certain fruits or substances have been attributed to acids for instance the sour taste of grape, lemon and some oranges is due to the presence of citric acid. The acid is capable of dissolving metals like lead, iron and zinc, can also dissolve organic dyes to generate definitive colors, turns blue litmus paper red and react with bases to form salts.

The relationship between the structure, composition and properties was studied extensively by chemists and Arrhenius (1859-1927) defined acids and bases. Bronsted-Lowry The Bronsted-Lowry theory defines an "acid" as any substance capable of yielding a proton (H+) and a "base " as a substance capable of accepting a proton. Arrhenius, a Swedish chemist however defined acids as substances that produce hydrogen (H+) ions in solution while bases produce hydroxide (OH-) ions in solution. An acidic solution therefore contains a higher proportion of Hydrogen (H+) ions than hydroxide (OH-) ions. Acids are corrosive and can cause damage to living tissues and materials, they react with metals to yield hydrogen gas and metal salts. They also react with bases to form salt and water. They are electrolytes and conduct electricity in aqueous solution. Bases on the other hand, are caustic

#### **Bases react with acids to form**

#### **Proton in water**

Water is a universal solvent. Commercially available HCl is 12M and contains 37-38% HCl. An acid like HCl dissociates in water to give a proton. It is highly soluble in water due to the dissociation into the constituent proton and Chloride ion. The resulting proton associates with water and is strongly bond between two molecules of water as discovered using the latest ultrafast spectroscopy. Ultrafast snapshots of protons using 2-D vibrational spectroscopy revealed many structural variations have been found and the structures persist not as the hydronium ion  $(H_3O^+)$ as generally believed but as "Zundel-like"  $(H_5O_2^+)$  and  $(H_9O_4^-)$ . These structures are important in computational models of transient water structure, oxidation-reduction reactions and generation of fuel from water. HCl has a low solubility in organic solvent like benzene.

### Illustration



The Bronsted-Lowry

Johannes Bronsted (1879-1947) - a Danish chemist and Thomas M.Lowry (1874-1936) described the reaction between acid- base reaction and proposed via independent study that it is related to their ability to transfer protons. They proposed independently in 1923 the definition of acids as substances capable of donating a proton and a base as a substance capable of accepting a proton. Hydrochloride in water thus acts as an acid by donating a proton to water which accepts the proton as a base. It can therefore be extrapolated to reactions occurring in non aqueous solvents (though with modification) as long as proton is donated by one and accepted by the other as exemplified by hydrochloric acid and ammonia, acetic acid in acetic acid, Ammonia in acetic acid

HCl + NH3 Cl - + NH4 +

CH3COOH + NH3 CH3COO-+NH4+

Ammonia acts as a base in the presence of acetic acid where the resulting species CH3COO- is the conjugate base of acetic acid and ammonium ion is the conjugate acid of the ammonia.

In non-aqueous solvents, the solvent molecules themselves can act as both a solvent and a base, A compound like Boron Trifluoride BF3 in ammonia

 $BF_3 + NH_3$  ( $BF_3.NH_3$ ) +  $NH4^+$ 

Here ammonia donates a proton to  $\rm NH_3$  and becomes  $\rm NH_4^+$  is the conjugate acid of ammonia.

It is important to know that the strength of an acid or base in non-aqueous solvent is often different from its strength in aqueous solutions. This is due to the effect of the solvent and its ability to protonate or deprotonate species. Identification of the acidbase pair in non-aqueous solvents .....

G.N. Lewis in 1923 described an acid as an electron pair acceptor while a base is an electron pair donor. Therefore non hydrogen compounds can be included in the definition of acids and bases for example

AlCl<sub>3</sub> + OR<sub>2</sub> Cl<sub>3</sub>Al:OR<sub>2</sub>

AlCl<sub>3</sub> is an acid by Lewis definition as it accepts electron pair from  $OR_2$  which functions as the base by donating the pair of electrons.

Acid, Base, Conjugate Acid and Conjugate Base

When an acid dissociates in an aqueous or non aqueous solvent by losing its proton, it is left with an extra pair of electrons that cannot be neutralized by the proton again. It is referred to as the "ionized" form of the acid and it is water soluble. Strong acids are completely ionized in solution while weak bases are partially ionized example is acetic acid. The acid dissociation constant can thus be calculated.

A large proportion of organic functional groups behave like acids. They contain functional groups like hydroxide (in phenol), Thiophenol, N-Aryl Sulphonamide, Aryl carboxylic acid, Sulphonic acid, Imide, Alkylcarboxylic acid, sulphonamide. Alkyl thiol, Sulphonic acid.

Compound	Acidic	Conjugate
	Functional Group	base
Ibuprofen	-COOH	Carboxylate
Naproxen	-COOH	Carboxylate
Acetylsalicylic acid	Acetyl (- COOCH3)	Carboxylate
Phenol	ОН	Phenolate
Indomethacin	-COOH	Carboxylate
Warfarin	-СООН	Carboxylate

Examples are tabulated below

Compounds with basic functional groups

Amphetamine	-NH2		
Cimetidine	-NH2		
Lignocaine	-CONH2		

Morphine	-NH2		
Diphenhydramine			
Guanidine			
Amidine			

Some organic functional groups that are considered neutral under physiologic conditions include alkyl alcohol R-CH<sub>2</sub>-OH, Amide R-CONH<sub>2</sub>, Amine oxide NRR'R"-O, Diarylamine Ar-NH-Ar, Ether R-O-R, Ester R-COOR', Ketone R-O-R', Aldehyde R-CHO, NitrileR-CN, Thioether R-S\_R', Sulphonic acid Ester R-SOOO-R', Quaternary ammonium RR'R"N, Sulphoxide RSOR', Sulphone RSO<sub>2</sub>R, Examples include Propanolol where the secondary alcohol group is located on the middle on the 3<sup>rd</sup> Carbon atom and the group plays a role in its interaction and Pharmacological properties.

## **Environmental Application**

Rainwater contains dissolved carbondioxide as carbonic acid hence pH  $\,$  is between 5 and 6  $\,$ 

H20 (l)+ CO2 (g)→ H2CO3 (aq)

H2CO3 (aq)  $\rightarrow$  H+(aq) +HCO3-(aq)

Acid rain is rainwater with a pH of less than 5 due to the presence of dissolved oxides sulphur dioxide SO2, Sulphur trioxide SO3 and Carbondioxide. CO2 is present in the atmosphere when released during respiration by living organism. It is also liberated during combustion of fuel and forest fires. However Sulphurdioxide and Sulphur trioxide are generated as industrial by products during the heating of ores (metal sulphides). The resultant effect varied as in the destruction of forests when the acid rain makes the plants susceptible to insect infestation and degradation. The soil is also damaged and lake water is acidified such that it cannot support life.

pH calculations involve

Kw = ionic product of water

Ka= Acid dissociation constant

Kb =Base dissociation constant

This is based on the exchange of proton.

Acid-Base Application in Pharmaceuticals

1 Analytical Procedures in Chemistry and Pharmacy

Analytical methods in Chemistry and Pharmacy depends on acid-base reaction such as acid-base titration which may involve dtrect titration for example standardization of 1M NaOH using sulphamic acid as a primary standard, or a back titration for example determination of Aspirin. The accurate determination of the strength of a standard solution is important for a successful analytical work . Sodium hydropxide is one of the most used standard solutions in acid-base titrations, and it must be standardized against a standard acid (for instance HCl) in the presence of a suitable indicator like methy orange or phenopthalein indicator. The acid HCl itself must have been standardized with exsiccated sodium bicarbonate which is the Analar.

A back titration consists of the addition of a definite excess of a standard volumetric solution to a weighed amount of the sample and the determination of the excess not consumed by the sample. Applied in the determination of the amount of Aspirin, Lactic acid and Ammonia solution.

## 2. Buffer systems

3. Acids and bases are used to dissolve insoluble medications for example Lidocaine hydrochloride injection U.S.P. is prepared by reacting Lignocaine with HCl. Niacin Injection U.S.P. is prepared by reacting Niacin with sodium hydroxide or sodium bicarbonate. Other solid acids that can be used are tartaric acid, citric acid and sodium dihydrogen phosphate. The sodium bicarbonate must be in the right particle size.

4. Preparation of effervescent mixtures where sodium bicarbonate is used as the source of carbondioxide.

## pH and aquatic life

It is one of the most important environmental factors limiting species distributions in aquatic habitats<sup>5</sup>. Different species flourish within different ranges of pH, with the optima for most aquatic organisms falling between pH 6.5-8. The pH of water determines the solubility and biological availability of chemical constituents such as nutrients and heavy metals. For example, in addition to affecting how much and what form of phosphorus is most abundant in the water, pH also determines whether aquatic life can use it. In the case of heavy metals, the degree to which they are soluble determines their toxicity.

Not only does the pH of a stream affect organisms living in the water, but a changing pH in a stream can also be an indicator of increasing pollution or some other environmental factor. Even small changes in pH can shift community composition in streams because pH alters the chemical state of many pollutants (e.g., copper, ammonia), changing their solubility, transport, and bioavailability. This can increase exposure to and toxicity of metals and nutrients to aquatic plants and animals.

### Summary

pH, Acids and Bases are fundamental concepts in chemistry. pH is used to measure the extent of acidity or alkalinity of a system , product, environment or the part of a human body. They play a crucial role in understanding chemical reactions, biological processes, reactions that occur in the body, living cell and microorganisms as well as various industrial processes. It determines the outcome of some reactions as certain reactions take place at specific pH while they do not at other pH while other conditions are constant for example neutralization reactions and hydrolysis.Lack of balance in pH in our body can result in diseases. Microorganisms also thrive at certain pH and enzymes within them may catalyze a reaction give rise to certain products at specific pH as in fermentation reaction. pH is important and its application spans across various industries like the chemical industry, industrial sector where it plays a role in water treatment, metal plating, paper and pulp industry, pharmaceutical industry (drug formulation, drug synthesis and drug delivery systems). Microorganisms thrive, grow and carry out basic processes like metabolism at specific pH while their growth are inhibited at other pH depending on the species. In conclusion, pH in general and acids and bases influences microbial growth, enzyme activity, metabolic pathways , pH stability during industrial processes and manufacturing of pharmaceutical drugs/drug products. It is essential to optimize the pH of any process or reaction via monitor and control to get the desired result.

### **Scientific Ethics Declaration**

The author say that she is responsible for the scientific, moral, and legal aspects of this chapter, which is published in In Junejo Y (Eds.), *Chemistry for the Life*. ISRES Publishing

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### **Conflict of Interest**

The authors declare no conflict of interest.

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# HETEROGENEOUS FENTON-LIKE PROCESS AND UTILIZED CATALYSTS

Memduha ERGUT

### Introduction

Nowadays, as a result of developing technology and increasing industrialization, permanent non-biodegradable pollutants are released into the receiving environment through the wastewater of various industries. Uncontrolled discharge of wastewater, which may contain organic dyes, halogenated aliphatic and aromatic compounds, agricultural chemicals, sulfur, and nitrogen-containing compounds, directly into the receiving environment causes widespread water pollution. Hence, water pollution has become one of the most striking environmental problems among the types of environmental pollution. Increasingly global chemical pollution of natural water is one of the main problems facing humanity due to its significant and unpredictable short and long-term effects on aquatic life and human health.

Depending on the intended use of wastewater, its compliance with water standards must be checked and its contaminant content must be reduced to the desired level. Therefore, it is necessary to develop effective, practical, and cost-effective removal methods that can meet wastewater discharge standards.

The majority of traditional treatment methods include various techniques such as adsorption (Senthil Kumar et al., 2019), coagulation (Sudoh et al., 2015), electrocoagulation (Senturk, 2013), ion exchange (Rengaraj et al., 2001), filtration (Muller et al., 1995), biological degradation (Joss et al., 2006), chlorination (Kim et al., 2003), and ozonation (Broséus et al., 2008). Although these methods are effective in the treatment of most anthropogenically contaminated water resources, they are not always effective on their own in bringing water containing toxic chemicals such as phenolic substances, textile dyestuffs, pesticides, organic solvents, pharmaceuticals, and household chemicals to legal and practically acceptable levels.

In recent years, the utilization of new methods called Advanced Oxidation Processes (AOPs) such as classical Fenton reaction (Fe(II)/H<sub>2</sub>O<sub>2</sub>), (Kallel et al., 2009); photo-Fenton reaction (Fe(II)/H<sub>2</sub>O<sub>2</sub>/UV) (Q. Liu et al., 2020); and ozonation (O<sub>3</sub>); (Amat et al., 2003); wet peroxide ozonation (O<sub>3</sub>/H<sub>2</sub>O<sub>2</sub>), (Ribeiro et al., 2017); (Lucas & Peres, 2009); heterogeneous/homogeneous Fenton-like processes (Xiao et al., 2016), and photocatalytic processes (TiO<sub>2</sub>/UV and ZnO/UV), (Tassalit et al., 2011) have aroused great attention in the removal of toxic and carcinogenic organic pollutants from natural water resources.

Advanced oxidation processes (AOP) are effective treatment methods that enable the complete transformation of toxic and biodegradable organic pollutants into non-toxic products such as carbon dioxide, water, and inorganic salts or less harmful compounds (Mazivila et al., 2019). Advanced oxidation processes (AOP) mainly produce and use hydroxyl radicals (OH•) to oxidize organic compounds. The OH• radical has an oxidation or standard reduction potential (2.8 V) higher than sulfate radicals, chlorine, permanganate, persulfate anion, and ozone (O<sub>3</sub>), but lower than only fluorine (3.03 V). The OH• radical is short-lived, can be produced simply, is a strong oxidant, shows electrophilic behavior, is easily available in nature, highly reactive, and is practically non-selective. It reacts with various classes of organic compounds, producing shorter chain length and simpler organic compounds (Guan et al., 2018).

Advanced oxidation processes offer many advantages over traditional methods. The biggest advantage of these methods is related to the conversion of organic substances into simpler compounds or  $CO_2$  and  $H_2O$ . Additionally, the lack of sludge production eliminates the need for an additional treatment stage. Advanced oxidation processes can treat wastewater containing dissolved organic compounds that are difficult to remove, with very low organic loads (in ppb) (Coha et al., 2021).

The Fenton process is one of the widely studied advanced oxidation processes in the treatment of various pollutants because of its simple operation, mild conditions, and fast formation rate of •OH, and it requires a short reaction time compared to other advanced oxidation processes. In the Fenton process, using iron as a catalyst offers advancement in terms of its being abundant and environmentally friendly nature, and lack of mass transfer limitation due to the homogeneous catalytic structure of the system. Nevertheless, the precipitation feature of iron and the difficulty of recovering the catalyst from the medium at the end of the reaction impose limitations on practical applications. For this reason, intensive studies have been conducted on the development of iron-containing material-based heterogeneous Fenton/Fenton-like catalysts (Asghar et al., 2015).

Heterogeneous Fenton/Fenton-like catalysts are emerging as excellent materials for applications related to water purification. Composite materials of magnetite and ferrites remain a winner in this area because of their easy separation and reuse, owing to their magnetic properties. Iron minerals supported on clay materials, carbon materials, zeolites, and mesoporous silica dramatically increase the catalytic degradation rate of contaminants by providing high surface area, good mechanical stability, and improved electron transfer (Thomas et al., 2021).

In this book chapter, the general aspects of the classical Fenton process and heterogeneous Fenton-like processes were introduced. Then, the utilized Fe-based catalysts such as natural mineral-based catalysts, nanocatalysts, bimetallic Fe-based catalysts, composite heterogeneous catalysts, and heterogeneous catalysts from industrial wastes in Fenton/Fenton-like processes were introduced briefly.

#### **Classical Fenton Reaction**

The conventional Fenton reaction, one of the advanced oxidation processes, is a catalytic process based on the formation of hydroxyl radicals (•OH) from hydrogen peroxide in the presence of a homogeneous catalyst (metal salt or oxide, usually iron). That is to say, Fenton's reagent (H<sub>2</sub>O<sub>2</sub> with Fe(II)/Fe(III) ions) in water produces •OH radicals (Matilainen & Sillanpää, 2010).

The Fenton process was first described in 1894 by H.J.H. Fenton. It was used by Fenton to study the redox reactions involved in the oxidation of tartaric acid (Sillanpää et al., 2018). However, its use as an oxidation process dates back to the 1960s (Dihingia & Tiwari, 2022).

The formation cycle of hydroxyl radicals via the Fenton reaction can be seen in Equations (1) - (7) (Cihanoğlu et al., 2015).

$$Fe^{2^+} + H_2O_2 \rightarrow \bullet OH + OH^- + Fe^{3^+}$$
(1)

$$Fe^{3+} + H_2O_2 \rightarrow Fe^{2+} + H^+ + HO_2 \bullet$$
 (2)

$$Fe^{3+} + HO_2 \bullet \longrightarrow Fe^{2+} + H^+ + O_2 \tag{3}$$

$$Fe^{2+} + \bullet OH \longrightarrow Fe^{3+} + OH^{-}$$
(4)

$$\bullet OH + \bullet OH \to H_2 O_2 \tag{5}$$

$$\bullet OH + H_2O_2 \rightarrow H_2O + HO_2 \bullet \tag{6}$$

•OH + organic molecules 
$$\rightarrow$$
 CO<sub>2</sub> + H<sub>2</sub>O (7)

As seen in Equations (1) – (7),  $Fe^{2+}$  ions initiate and catalyze the decomposition of H<sub>2</sub>O<sub>2</sub>, and hydroxyl radicals (•OH) are formed. Therefore, the degradation of contaminants is very fast in the first stage of the reaction. In the second stage, hydroperoxy radicals (HO<sub>2</sub>•) were also produced as intermediate radicals (Eq.2) and the rate of reaction began to decrease due to the consumption of Fe<sup>2+</sup> ions and the formation of Fe<sup>3+</sup> ions. This is because of generated HO<sub>2</sub>• (E°= 1.65 V) radicals which are weaker oxidants than that of •OH radicals (E°= 2.80 V), as a result of the interaction of Fe<sup>3+</sup> ions with H<sub>2</sub>O<sub>2</sub>. The formation of radicals continues as a complex reaction chain in the aqueous solutions. In the last step, produced •OH radicals attack the pollutant molecules breaking it down into CO<sub>2</sub> and H<sub>2</sub>O without showing selectivity by mineralization (Mirzaei et al., 2017).

The classical Fenton system, called the homogeneous Fenton process, is a widely used method due to its advantages such as being a simple method, requiring a short reaction time, availability of conventional equipment and ease of operation at ambient temperature and pressure. However, there are some limitations in terms of the Fenton system's utilization in industrial application areas. Since the concentration of the targeted contaminant in the actual wastewater is often quite high, the initial concentrations of iron and  $H_2O_2$  Fenton reagents must be increased in proportion to the concentration of contaminant to ensure complete mineralization of the component. Therefore, the operating cost of the system is increased. Also, Fenton oxidation cannot be applied to alkaline solutions and sludge with strong buffering capacity (Cihanoğlu et al., 2015). In addition, the removal of homogeneous catalyst (iron ions) from the medium at the end of the reaction causes more time and reagent consumption and therefore an increase in operating costs.

The physicochemical parameters such as initial pH, Fenton reagent concentration, and initial organic pollutant concentration are the driving forces affecting the Fenton process. The initial pH of the solution is one of the critical parameters. Because, although iron (II) species in aqueous solutions remain soluble even under neutral pH conditions, iron (III) species begin to form hydroxo species at  $pH \ge 4$ , thus causing the efficiency of the Fenton process to decrease. The optimum pH range that can provide optimum removal efficiency in the Fenton process is reported as pH (2 - 4) in many studies. (Dihingia & Tiwari, 2022). However, since actual wastewater samples are not available in this pH range, a large amount of acid must be added to adjust the pH of the wastewater samples before the Fenton process. This narrow operating range of pH could lead to the formation of different Fe<sup>3+</sup> complexes depending on the changes in the pH of the solution. Therefore, a neutralization step is required to remove the precipitate in the form of Fe(OH)<sub>3</sub> formed as sludge at the end of the reaction. This situation requires additional investments for the operation and appropriate design of the entire system. Another limitation is that iron ions may form complexes with substances such as EDTA found in real wastewater or possible by-products such as oxalic acid may be formed. Hence, catalyst deactivation can also occur with iron complexing agents such as phosphate anions in the homogeneous Fenton system. Therefore, reusability and regeneration of the homogeneous catalyst used in the reaction is not possible (Wang et al., 2016).

These disadvantages have led researchers to find alternative processes to minimize the limitations associated with the homogeneous Fenton process.

In this regard, the heterogeneous Fenton/Fenton-like process has become an attractive option due to the catalyst and target pollutants existing in different phases. The reactions mainly occur on the heterogeneous catalyst surface, where adsorption and diffusion processes occur. Moreover, the heterogeneous Fenton process enables operation over a wide pH range and prevents iron from leaching into the solution. Additionally, the efficiency of the process could be improved by several physical fields/phenomena that are successfully combined with photo, electro, microwave fields, cavitation, ultrasound, etc. (Dihingia & Tiwari, 2022).

#### **Heterogeneous Fenton-like Processes**

Heterogeneous Fenton-like processes are achieved by replacing the  $Fe^{2+}$  ion in the Fenton reagent with a solid catalyst, while homogeneous Fenton-like processes are based on the combination of  $H_2O_2$  with other metal ion/metal ion-organic ligand complexes (Babu et al., 2019). The development of heterogeneous Fenton/Fenton-like systems as an attractive method to homogeneous Fenton processes to prevent the limitations such as the high amount of iron released into the environment, the necessity of iron recovery to reduce the iron content to the desired level (about 2 ppm) to comply with water standards before the discharging, high  $H_2O_2$  consumption and high operating costs encountered in homogeneous Fenton processes (Wang et al., 2016).

The use of heterogeneous Fenton-like systems offers many advantages compared to homogeneous Fenton reactions. Heterogeneous Fenton reactions aim to enlarge the suitable operating pH range and reduce the problems associated with the separation of high concentrations of iron ions remaining after the treatment. In this context, magnetite (Fe<sub>3</sub>O<sub>4</sub>) can be given as an example a simple solid catalyst that can be easily separated from the solution at the end of the reaction owing to its magnetic properties. Therefore, in recent years, researchers have focused on the development of stable heterogeneous catalysts to increase the catalytic activity and long-term stability of the catalyst while preventing catalyst leaching (Mirzaei et al., 2017).

In the Fenton-like reactions, similar to the classical Fenton reaction in which Fe(II) takes part as a catalyst, Copper (Cu (II)), Cobalt (Co (II)), Manganese (Mn (II)), Cerium (Ce (III)), Aluminum (Al (III)) and Chromium (Cr (III)), etc., many other transition metal ions can also activate  $H_2O_2$  to form •OH radical in addition to Fe(III) (Fu et al., 2022).

The rate-limiting step of  $H_2O_2$  decomposition is also the reduction of transition metals (Eq.(8)). The reduced transition metals are then re-oxidized by  $H_2O_2$  to form highly active •OH (Eq. (9)).

$$M(X+1) + H_2O_2 \rightarrow M(X) + H^+ + \bullet OOH$$
(8)

$$M(X) + H_2O_2 \rightarrow M(X+1) + OH^- + \bullet OH$$
(9)

There are two kinds of •OH known as free •OH (without •OH) and surfacebound •OH (•OHads). Many transition metals can undergo a redox cycle in the presence of  $H_2O_2$  to form •OHads, which behave similarly to Fe in the Fenton-like reaction. However, dissolved transition metal ions tend to disperse in solution and break down  $H_2O_2$ , producing free •OH through a chain reaction. Thus, they significantly increase the efficiency of a heterogeneous Fenton-like reaction system (Liu et al., 2021).

In experimental studies, bimetallic oxides and their complexes are added to the heterogeneous catalytic system in solid form. Therefore, the Fenton-like process includes solution reactions and interfacial reactions. Different reactions in the Fentonlike system contribute to the degradation of organic pollutants by  $H_2O_2$  and bimetallic catalysts. It is known that Fe (II) reacts with  $H_2O_2$  to form •OH and at the same time Fe (III) is produced. Fe (II) produced by these reactions can participate in Fenton-like reactions to increase •OH formation (Fu et al., 2022). Bimetallic oxides and their complexes with binary reaction centers have been developed to increase the catalytic activity of Fenton-like reactions. In the bimetallic oxide/ $H_2O_2$  system, electron conversion between the two reaction centers easily forms active double reaction centers, that is, poor/rich electronic centers due to the different electronegativities of the doped metal ions, and inhomogeneous distribution of electron density. Organic matter and  $H_2O_2$  cluster around the electron-poor center and the electron-rich center, respectively (Dihingia & Tiwari, 2022; Wang & Tang, 2021a).

In the catalytic process, the electron-rich center reduces  $H_2O_2$  to form reactive oxidation species (e.g.,  ${}^1O_2$ ,  $O_2 \bullet^- /HO_2 \bullet^-$ , and  $\bullet OH$ ). The electron-poor center adsorbs pollutants and intermediates and then transfers the electrons provided by organic compounds to the electron-rich center. Therefore, adding metals with different electronegativity to form electron-rich centers and electron-poor centers can increase the catalytic activity and  $H_2O_2$  utilization efficiency (Dihingia & Tiwari, 2022; Fu et al., 2022; Wang & Tang, 2021a).

According to the literature, the decomposition of  $H_2O_2$  with bimetallic oxides and their complexes generally involves two states under different pH conditions. Under lower pH conditions (pH<4.5), the process is controlled by the redox cycle of transition metal ions (such as dissolved Fe (III)/Fe (II)) released from solid catalysts due to acidic pH conditions. Therefore, the solubility of the solid catalyst has a great impact on  $H_2O_2$  activation at low pH. On the contrary, at neutral and alkaline pH values, the contribution of dissolved metal ions to  $H_2O_2$  decomposition is negligible. Therefore, activation of  $H_2O_2$  at neutral and alkaline pH values may be a surface catalytic process (Kwan & Voelker, 2003).

In Fenton-like processes, iron-impregnated heterogeneous catalysts, natural and synthetic zeolites, mesoporous materials, columnar interlayer clays, Nafion films, and polymeric resins are frequently used as catalysts. Activated carbon, ashes, biochar, pumice particles, aluminates, etc. are widely used as supporting materials (Thomas et al., 2021).

Fenton-like processes can be supported by one or more different physical areas/phenomena to increment high efficiency in wastewater treatment. Photo@Fenton-like processes, electro@Fenton-like processes, cavitation@Fenton-like processes, and microwave@Fenton-like processes, etc., can be given examples of the mentioned Fenton-like processes (Dihingia & Tiwari, 2022; Miklos et al., 2018).

#### **Heterogeneous Fenton-like Catalysts**

A wide range of Fe-based materials have been developed and utilized as Fenton-like catalysts in the degradation of various organic pollutants in parallel with increasing knowledge on the synthesis and understanding of heterogeneous materials. Conventional Fe-based catalysts, such as iron oxides, zerovalent iron, iron sulfide, and oxychloride, are frequently used in heterogeneous Fenton reactions (Wang et al., 2016). All of these catalysts show different catalytic performances. This is expected because these catalysts exhibit different physicochemical properties. The physical properties of synthesized materials are affected from specific surface area, particle size, morphology, and synthesis strategies. The crystal structure of catalysts has a fundamental impact both on their catalytic performance and the content/value of Fe species (Scaria et al., 2021).

### Natural mineral-based catalysts

Natural mineral materials with special crystal structures and properties are used as alternative heterogeneous catalysts in Fenton-like processes due to their high catalytic activity and long-term stable structure. Fenton-like processes that use mineral materials as catalysts are called mineral-catalyzed Fenton-like processes, and goethite ( $\alpha$ -FeOOH), pyrite (FeS<sub>2</sub>), hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>), magnetite (Fe<sub>3</sub>O<sub>4</sub>), ferrihydrite, and lepidocrocite are the most commonly used natural iron-containing mineral materials as catalysts (Wang & Tang, 2021b; Wang et al., 2016b)

The advantages of using iron-containing minerals as catalysts are as follows:

- ✓ The catalyst can be easily separated from the medium at the end of the process by precipitation or filtration.
- ✓ Catalyst life can be extended by reusing the catalyst.
- ✓ The initial pH of the solution can be expanded to the neutral range (pH 5-9).
- ✓ The reaction system is not affected much by inorganic carbonate (Kamat & Meisel, 2002).

**Ferrihydrite** is a naturally occurring hydrous ferric oxyhydroxide. It is found in large quantities in the earth's crust. Ferrihydrite is used as a precursor during the preparation of geotite and hematite. The specific surface area of ferrihydrite is in the range of 250–275 m<sup>2</sup>/g. In Fenton reactions, higher surface area increases the contact between ferrihydrite and hydrogen peroxide, resulting in higher degradation efficiency (Thomas et al., 2021; Wang et al., 2016).

**Ferrites** are ceramic compounds formed by the combination of iron oxides with other transition metals. Ferrites are classified as garnet, hexagonal, and spinel ferrites according to their crystal structures. Among them, spinel ferrites have attracted much attention as heterogeneous Fenton catalysts for the removal of various organic pollutants. Spinel ferrites have a face-centered cubic lattice with the general formula  $M_xFe_{3-x}O_4$ , in which the oxide ions are arranged in a face-centered cubic manner and the metal ions are arranged in tetrahedral and octahedral regions (where one or more M, Zn, Mn, Co, etc. represents a divalent metal ion.) (Nidheesh, 2015).

**Geotite (\alpha-FeOOH)** is an iron oxyhydroxide found in soil and other low-temperature environments. Geotite is the main component of rust and bog iron ore. Among iron oxides, goethite is more widely used as a heterogeneous catalyst due to its properties such as (i) one of the most common forms of iron oxide, (ii) an environmentally friendly catalyst, (iii) one of the most chemically active compounds suspended in natural water, (iv) inexpensive, and (v) extremely high thermodynamic stability (vi) and low energy requirement (Nidheesh, 2015; Scaria et al., 2020).

**Shorl** (Black Tourmaline) is the most common form of tourmaline and is one of the most decorative black minerals known. Tourmaline is a crystalline borosilicate mineral combined with elements such as aluminum, iron, magnesium, sodium, lithium, or potassium. In addition to its natural iron transport feature, its pyroelectric and piezoelectric properties are also very good and positively affect the yield of Fenton-like processes (Nidheesh, 2015).

Hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) is a type of mineral that is common in many rock types. The iron content in hematite can be more than 70%, so it is an important type of iron ore.  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> is known as the most thermodynamically stable iron oxide at ambient conditions and is often the final stage of the transformation of other iron oxide phases. It crystallizes in the rhombohedral crystal system and exhibits a corundum structure isomorphic with  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. Hematite has attracted considerable attention as a heterogeneous Fenton catalyst due to its properties such as being a low-cost abundant mineral, its large surface area and high surface-to-volume ratio, its special morphology, well-defined topology, and its ability to be used as a feed material for iron production in a furnace without any environmental impact, even after losing its reactivity (Kwan & Voelker, 2003; Nidheesh, 2015; Wang & Tang, 2021b).

**Magnetite (Fe<sub>3</sub>O<sub>4</sub>)** is a mixed-valent oxide containing both divalent and trivalent Fe ions. It has an inverted spinel structure, where oxygen anions form a face-centered cubic (fcc) unit cell through regular cubic close-packing along the [111] direction, and iron cations occupy the interstitial regions (Wang and Tang., 2021b). Among all naturally occurring minerals on Earth, magnetite is the mineral with the most magnetic properties. Magnetite has attracted great attention in heterogeneous Fenton systems due to its structural iron ions, which play an important role in initiating the Fenton reaction according to the classical Haber-Weiss mechanism. Moreover; Fe<sub>3</sub>O<sub>4</sub> offers good conductivity due to rapid electron hopping between Fe<sup>2+</sup> and Fe<sup>3+</sup> centers in octahedral regions. This feature provides benefits for the Fe<sup>3+</sup>/Fe<sup>2+</sup> redox cycle. In addition, the ferrimagnetism of Fe<sub>3</sub>O<sub>4</sub> enables efficient separation of the catalyst from the reaction system (Munoz et al., 2015; Nidheesh, 2015).

**Maghemite (y-Fe<sub>2</sub>O<sub>3</sub>)** is another common ferrimagnetic oxide, usually formed by low-temperature oxidation of Fe<sub>3</sub>O<sub>4</sub> or dehydration of lepidocrosite. It has a similar spinel structure as Fe<sub>3</sub>O<sub>4</sub>, but with iron cation vacancy (V<sub>Fe</sub>) in the octahedral regions, which compensates for the oxidation of Fe<sup>2+</sup> ions. Like Fe<sub>3</sub>O<sub>4</sub>, y-Fe<sub>2</sub>O<sub>3</sub> offers strong magnetic separation and can be easily collected by an external magnetic field. However, y-Fe<sub>2</sub>O<sub>3</sub> without Fe<sup>2+</sup> ions presents a relatively lower catalytic performance compared to Fe<sub>3</sub>O<sub>4</sub>, as Fe<sup>2+</sup> catalytic sites are more active than their Fe<sup>3+</sup> counterparts in the heterogeneous Fenton process (Wang and Tang, 2021b).

**Pyrite (FeS<sub>2</sub>)** can often be found near coal and metal ore mines. Pyrite (FeS<sub>2</sub>), an iron sulfide mineral, has a high reactive capacity due to its high specific surface area and porosity. This makes pyrite susceptible to oxidation by an oxidizer (H<sub>2</sub>O<sub>2</sub>, Fe<sup>3+,</sup> and O<sub>2</sub>, etc.). FeS<sub>2</sub> can be easily oxidized by dissolved oxygen and/or H<sub>2</sub>O<sub>2</sub> in aqueous solution and simultaneously release Fe cations (Eq.10. and Eq.11.) This oxidative dissolution of FeS<sub>2</sub> allows the self-organization of Fe<sup>2+</sup>, which supports the partially homogeneous Fenton reaction along with its spontaneous reaction with Fe<sup>3+</sup> ions (Eq.

12.). However, unlike nZVI,  $FeS_2$  is less sensitive to pH and can induce the heterogeneous Fenton reaction in the alkaline state. More importantly, the release of  $H^+$  ions upon dissolution of  $FeS_2$  can lower the solution pH and reach the optimum pH condition for the Fenton reaction without adding extra acid.

$$2FeS_2 + 7O_2 + 2H_2O \rightarrow 2Fe^{2+} + 4SO_4^{2-} + 4H^+$$
(10)

$$FeS_2 + 7.5H_2O_2 \rightarrow Fe^{3+} + 2SO_4^{2-} + H^+ + 7H_2O$$
 (11)

$$FeS_2 + 14Fe^{3+} + 8H_2O \rightarrow 15Fe^{2+} + 2SO_4^{2-} + 16H^+$$
 (12)

The primary reaction mechanisms of the  $FeS_2/H_2O_2$  system are summarized as follows:

(i)  $Fe^{2+}$  ions bound to the FeS<sub>2</sub> surface initiate the heterogeneous Fenton reaction; (ii) Aqueous  $Fe^{2+}$  ions continuously released from the FeS<sub>2</sub> surface trigger homogeneous Fenton reactions; (iii) The autocatalytic reaction between FeS<sub>2</sub> and aqueous  $Fe^{3+}$  ions serves to provide aqueous  $Fe^{2+}$  ions (Song et al., 2022).

**Zero valent iron (ZVI),** has been shown a promising reactive medium in the removal of various pollutants in wastewater treatment due to its low cost, non-toxicity, efficiency, accessibility, and structural magnetic feature. ZVI is a reactive metal with a standard redox potential of 0.44 V, which can serve not only as a direct reducing agent but also as an electron donor in oxidative reactions. It is well known that ZVI is highly susceptible to corrosion in acidic solutions. Especially, when exposed to acidic oxygen aqueous solution, it can continuously activate dissolved oxygen (DO) to produce H<sub>2</sub>O<sub>2</sub> through the two-electron transfer reaction (Eq. (13)). The resulting H<sub>2</sub>O<sub>2</sub> can then be decomposed into H<sub>2</sub>O by another two-electron transfer from ZVI (Eq. (14)), or it can react with Fe<sup>2+</sup> ion and turn into •OH radical (Eq. (15)). Additionally, the Fe<sup>3+</sup> ion produced on or near the ZVI surface can be further reduced to Fe<sup>2+</sup> due to the electron-donating capacity of ZVI (Eq. (16)).

$$Fe^{\circ} + O_2 + 2H^+ \rightarrow Fe^{2+} + H_2O_2$$
 (13)

$$Fe^{\circ} + H_2O_2 + 2H^+ \rightarrow Fe^{2+} + 2H_2O$$
(14)

$$Fe^{2+} + H_2O_2 + H^+ \rightarrow Fe^{3+} + \bullet OH + 2H_2O$$
(15)

$$2Fe^{3+} + Fe^{\circ} \rightarrow 3Fe^{2+}$$
(16)

ZVI promotes the reduction of  $Fe^{3+}$  ions because it can act as a slow-release source of dissolved  $Fe^{2+}$  ions. Although ZVI in an oxygen-enriched solution (ZVI/O<sub>2</sub> system), it can spontaneously produce  $H_2O_2$  and form more radicals, the low yield of reactive oxidant as well as the loss in produced  $H_2O_2$  caused by two-electron reduction greatly limits ZVI applications in the field of water treatment (Fu et al.,2022). Therefore, various approaches have been investigated to improve oxidant production, such as the addition of a secondary metal or iron-chelating ligands. Furthermore, the addition of

 $H_2O_2$  is the most direct and effective method to promote the formation of reactive oxygen species (Wang and Tang, 2021b).

#### Nanomaterials-based heterogeneous catalysts

Today, thanks to the rapid developments in the field of nanotechnology, the number of studies on the use of reusable, low-cost nanoparticles with high catalytic activity due to their large specific surface area as heterogeneous Fenton-like catalysts is increasing day by day. Nanomaterials exhibit many advantages such as low diffusion resistance, easy accessibility to reactants, and having a large number of active centers owing to their large surface areas. The nanomaterials also exhibit distinct physical and chemical properties such as high recyclability, easy recovery, high stability, and dispersibility in Fenton-like degradation processes when they are used as catalysts (Wang et al., 2016).

Efficient degradations of various organic contaminants have been achieved by nanomaterial-catalyzed Fenton-like processes. For example, zero-valent iron nanoparticles, iron-containing bimetallic nanoparticles (Fe/Pd-NPs, Fe/Ni-NPs, Fe/Cu-NPs), nano  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>, CuO nanoparticles, ferrospinel nanonoparticles (ZnFe<sub>2</sub>O<sub>4</sub>, MgFe<sub>2</sub>O<sub>4</sub>, NiFe<sub>2</sub>O<sub>4</sub>, etc.,) have reported as catalysts in Fenton like degradation studies. Moreover, bimetallic catalysts prepared by adding other metal-based materials to Fe-based catalysts to increase the catalytic activity of Fe-based catalysts are widely used in heterogeneous Fenton/Fenton-like processes due to their more effective properties compared to mono-metallic catalysts (Mondal et al., 2020; Thomas et al., 2021; Wang & Tang, 2021b).

Bimetallic Fe-based catalysts can be divided into three main categories: Bimetallic Fe NPs, metal-doped iron oxides and mixed metal oxides, according to the way two different metal-based materials are mixed. Bimetallic Fe NPs based on Fe-M nanoalloys, where M represents another metal (e.g., Co, Ni, Cu, Pd, Ce), have been used for the activation of hydrogen peroxide. Metal-doped iron oxides are another important class of bimetallic Fe-based catalysts with excellent Fenton-like activity. In this category, the iron cation in the structure of iron oxides is isomorphically substituted by other metal cations of similar ionic radius, while retaining their original structure. Apart from the above-mentioned common properties of bimetallic catalysts, some foreign metal atoms (e.g. Ti, Nb, Sn, Mn, Co) can affect the electronic structure of neighboring iron atoms due to unequal charge substitutions. This may cause a valence change in the iron atom and the formation of oxygen vacancies for charge balancing. These oxygen vacancies can act as active sites for  $H_2O_2$  activation in the Fenton-like reaction, thus promoting the formation of •OH (Wang & Tang, 2021b).

Bimetallic Fe-based catalysts generally exhibit much better catalytic performance and pH tolerance than their monometallic form, as a result of the synergy that occurs when the two metallic components come together. Metal-based materials added to the catalyst structure generally cause significant changes in catalyst properties regarding particle size, surface area, pH tolerance, stability, adsorption ability, and catalytic activity (Wang & Tang, 2021). These improvements in catalyst properties can be attributed to the following reasons; (i) the addition of a second metal

can increase the surface area of the catalyst, (ii) the number of active sites on the catalyst surface can increase significantly by the addition of other transition metals, (iii) in most cases, the active metallic component with thermodynamically favorable redox pairs which not only spontaneously triggers Fenton-like processes but also aids in the regeneration of Fe(II) species and interfacial electron transfer through conjugation of redox couples (Thomas et al., 2021; Wang & Tang, 2021b).

In the bimetallic oxide/ $H_2O_2$  system, as a result of the inhomogeneous distribution of electron density due to the different electronegativities of the doped metal ions, electron conversion between the two reaction centers easily forms the active double reaction center, that is, poor/rich electronic centers. Organic matter and  $H_2O_2$  cluster around the electron-poor center and the electron-rich center, respectively. In the catalytic process, the electron-rich center reduces  $H_2O_2$  to form reactive oxygen species (ROS) (e.g.,  $O_2$ ,  $O_2$ •-/HO<sub>2</sub>•-, and •OH), while the electron-poor center adsorbs contaminants and intermediates and it then transfers the electrons provided by the organic substances to the electron-rich center. Therefore, combining different electronegative metals to form electron-rich and electron-poor centers can increase the catalytic activity and  $H_2O_2$  utilization efficiency (Fu et al., 2022; Wang & Tang, 2021b).

#### Composite heterogeneous catalysts

Conventional Fe-based catalysts have effectively demonstrated their potential in heterogeneous Fenton catalysis reactions but they have disadvantages such as relatively low catalytic activity at neutral pH conditions or low stability at acidic pH conditions. Therefore, several important strategies have been conducted to synthesize highly efficient Fe-based catalysts: i) having sufficient active sites for  $H_2O_2$  activation, ii) accelerating the reduction of Fe(III) to Fe(II), iii) showing high chemical stability over a long period and iv) applicability over a wide pH range. There are four main modification strategies reported in the literature to synthesize Fe-based catalysts that can meet these criteria, i) control of the microstructure, ii) use of support materials, iii) formation of the core-shell structure, and iv) incorporation of another metalcontaining component into the catalyst structure (Thomas et al., 2021; Wang et al., 2016).

### **Control of microstructure:**

The structure of the catalyst including morphology, size, and porosity has a significant impact on its physicochemical properties and surface reactivity. Since the heterogeneous Fenton reaction mainly involves the adsorption of  $H_2O_2$ , the conversion of  $H_2O_2$  into reactive oxidation species, and finally the desorption of reactive oxidation species on the catalyst surface, it can be assumed that these basic steps are closely related to the amounts of surface active atoms and their coordination environments. This dependence can be interpreted based on the particle size and anisotropic morphology of the catalysts. In general, smaller-sized catalysts have higher surface-to-volume ratios and more exposed active sites for contact with reactants. This results in higher adsorption capacity and catalytic activity. Different anisotropic morphologies of the same catalyst often have different exposed crystal

faces, which dominate the surface electronic and atomic structures and determine the reactivity, selectivity, and stability of the catalyst. Therefore, nanoscale catalyst particles with controlled crystallographic orientation can alter catalytic activity by selectively exposing desired reactive aspects. Controlled synthesis of catalysts with well-defined structures is a promising approach for the design of catalysts with desired performance (Wang & Tang, 2021b).

### **Core-shell structured nanocomposites:**

Another important strategy to develop more efficient and stable Fe-based catalysts is the synthesis of core-shell structured nanocomposites in which active nanoparticles (core) are encapsulated in other materials (shell). Fe-based catalysts with core-shell structures are materials of interest in heterogeneous Fenton/Fenton-like processes for the effective removal of various pollutants in water (Liu et al., 2020; Wang et al., 2015).

These catalysts are usually synthesized in a stepwise manner and can offer many advantages:

i) the presence of the shell not only prevents leaching and aggregation of the core during the catalytic reaction but also protects the core from the external conditions, ii) shell-core structure combines the advantageous properties of both core and shell to improve applicability, iii) possible synergy between core and shell enables higher performance from the heterogeneous Fenton reaction. Moreover, the physicochemical properties of the core-shell structure can be changed to suit the desired purpose by selecting appropriate core and shell components. This is especially important for the design and synthesis of Fenton-like catalysts with desired properties (Fu et al., 2022; Thomas et al., 2021). Shell materials are generally divided into two main classes inorganic and organic materials. While inorganic shell materials consist of silica and metal oxide, polymers are examples of organic shell materials. Among these, mesoporous silica shell is a very attractive material, as it allows the final core-shell materials to have a large surface area, and also improves the permeability of reagents to the inner active core. Shell can use the core as support to maximize the number of exposed active sites and thus achieve better catalytic performance by changing textural properties such as surface area, pore size, etc. (Fu et al., 2022).

### Using support materials:

The loss of Fe-based catalysts caused by iron leaching as well as their aggregation behavior may result from small interparticle distances, high surface energy, and strong anisotropic dipolar interactions, which inevitably reduces the beneficial properties of the catalyst in Fenton-like systems. The modification of traditional Fe-based catalysts using appropriate support materials is an effective approach to avoid these problems. In supported Fe-based catalysts, one of the important roles of support materials is to improve the dispersion and stability of catalyst particles and effectively prevent their aggregation during the reaction. Meanwhile, the support material with highly open pore structure and large surface area serves as an open channel for easy diffusion of reactants and products, which can

reduce the mass transfer resistance and increase the accessibility of reactants to the active sites of catalyst particles (Campanati et al., 2003; Thomas et al., 2021).

In some cases, interaction and/or synergistic effects may occur between support materials and catalyst particles, which may have a positive effect on the catalytic properties. The composite structure of the material increases the reusability of the active metal element in its structure, as it allows it to be easily separated from the reaction medium by the precipitation method after the reaction. For example, if we consider clay-based catalysts; clay is widely used as a catalyst support material because it is cost-effective compared to other catalyst support materials (Wang et al., 2016).

In recent years, various clay-based catalysts such as Fe/laponite, montmorillonite, Cu–Al/montmorillonite, and Fe/bentonite have been developed (Wang et al., 2016). In addition, the catalyst support material has also a significant effect on the catalyst activity. So far, various materials such as carbon materials, silica, and zeolites have been considered as the main support materials that can be used for the immobilization of Fe-based catalysts.

Carbon materials in the form of activated carbon (Rodrigues et al., 2017), carbon nanotubes (Liu et al., 2018), graphene-based materials (Xiao et al., 2016), activated carbon fibers (Liu et al., 2021), biochar (Li et al., 2017), and carbon aerogels or xerogels (Kharissova et al., 2015) are the most popular support materials for Febased catalysts due to their interesting properties such as large surface area, uniform pore distribution and physicochemical stability. More importantly, some of these materials have been reported to be efficient, metal-free catalysts for H<sub>2</sub>O<sub>2</sub> activation, although they have lower performance compared to Fe-based catalysts. Fe<sup>2+</sup>/AC (Mesquita et al., 2012),  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/S (Guo et al., 2010), CuO/Al (Atta et al., 2012), Fe<sup>2+</sup>/Magnetic NdFeB-AC (Wang et al., 2014), layered Fe-titanate (Chen et al., 2014), FeOOH–C (Zhang et al., 2011), Iron oxide/SiO<sub>2</sub> (Huang et al., 2013), Cu/MCM-41 (Lam et al., 2007), iron-loaded mangosteen (Laiju et al., 2014), and magnetite-based materials (Munoz et al., 2015) have been used as catalysts in heterogeneous Fenton-like processes in the literature.

#### Heterogeneous Catalysts Obtained from Industrial Wastes

Fly ash is a fine dust-like solid waste produced by modern power plants and steel mills. It is often disposed of as industrial waste, and annual production of coal fly ash is reported to be at least 200 million tonnes worldwide. Coal fly ash consists entirely of the non-combustible material in coal and a small amount of carbon remaining from the incomplete combustion of combustible material. According to the X-ray fluorescence spectroscopy analysis result, it was determined that coal fly ash contains SiO<sub>2</sub>, CaO, Al<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, MgO, K<sub>2</sub>O, P<sub>2</sub>O<sub>5</sub>, Na<sub>2</sub>O, SrO, ZrO<sub>2</sub> and ZnO components (Wang et al., 2016). In recent years, coal fly ash has been used exclusively in construction due to its complex composition. Although construction applications of coal fly ash have been successful, there is still a large amount of fly ash (70-75%) that remains unutilized and is simply disposed of in landfills and/or landfill lagoons, causing serious environmental problems. Therefore, to ensure effective removal of

coal fly ash, it is very important to develop new application areas where coal fly ash can be used (Wang et al., 2016).

The use of fly ash as a catalyst in heterogeneous Fenton-like processes has been investigated because it has a porous surface and active metal elements (such as iron elements) in its composition. Zhang et al. studied the heterogeneous Fenton-like degradation process of p-nitrophenol using coal fly ash containing 5.73% Fe<sub>2</sub>O<sub>3</sub> (%wt) as a catalyst. In the study, the highest p-NP removal (98%) was determined under optimum environmental conditions of pH=2.0, CH<sub>2</sub>O<sub>2</sub> = 166.5 mg/L, C p-NP = 100 mg/L, Ccatalyst = 10 g/L, and T= 25°C. Researchers indicated that the catalyst concentration should be increased to develop the stability and reusability of the catalyst (A. Zhang et al., 2012).

In addition to coal fly ash, the use of acid mine drainage sludge as a heterogeneous catalyst in electrochemical processes after combustion and milling has been reported (Alfaya et al., 2015).

### Conclusions

This chapter provides a general overview and fundamental mechanisms of conventional homogeneous Fenton's reaction, and heterogeneous Fenton-like reactions, and uses heterogeneous Fe-based catalysts in Fenton-like reactions. Conventional Fe-based catalysts such as zero-valent iron, iron oxides, oxyhydroxides, sulfides, and oxychloride have demonstrated their potential in heterogeneous Fenton catalysis. However, some problems have been reported such as relatively low catalytic activity under neutral pH conditions, high leaching of iron species from the catalyst under acidic pH conditions, and limited recyclability. So, the catalytic properties of conventional Fe-based catalysts can be improved by various modification strategies, such as microstructure controlling, the introduction of support materials, the formation of core–shell structure, and the addition of new metal-containing components. The catalytic mechanisms of various types of Fe-based catalysts as well as a brief description of synergistic effect were also discussed.

Considered from a future perspective, Fenton/Fenton-like processes with insitu production of  $H_2O_2$  have received increasing attention, in which  $H_2O_2$  was in-situ produced through  $O_2$  activation, then decomposed into hydroxyl radicals by Fenton catalysts. Therefore, in situ, synthesis of  $H_2O_2$  with iron-catalyzed heterogeneous Fenton-like reaction seems to be a cost-effective option since a single catalyst is used in the synthesis of  $H_2O_2$  and degradation process. In conclusion, the development of brand new materials with extraordinary catalytic efficiency which can in-situ produce the  $H_2O_2$  can provide significant opportunities in commercial-scale applications of the Fenton reaction thanks to improving the  $H_2O_2$  utilization and decreasing the operating cost of the reaction.

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#### **ESSANTIAL OMEGA FATS FOR LIFE**

### Ali ÇAPAN

#### Introduction

Oils are generally used in the production of necessities in the food, chemical, paint, cosmetics and pharmaceutical industries. Fats are one of the main nutrients that must be included in human nutrition. Fats provide more energy than other nutrients and they control body temperature by being stored under the skin in the form of fat when necessary. Fats are important for the synthesis of some hormones that regulate the body. Fats are responsible for the absorption of some vitamins, terpenes important for human health, some metals (iodine, manganese, iron, zinc, copper, phosphorus and calcium) and essential fatty acids that cannot be synthesised by the body. The importance of fatty acids in nutrition began in the 1920s and the first studies on Omega fatty acids began in the 1970s. In 1978, EPA obtained from seafood was mentioned. Omega-fatty acids were discovered both in diets and in blood. The fact that omega fatty acids have effective chemical and biological activities has increased the interest in omega fatty acids. In later studies, it has been stated that omega fatty acids and the metabolites formed by them reduce the risk of heart attack, regulate brain development and growth, especially in children, can be used to support disorders caused by brain functions such as Alzheimer's and forgetfulness, and contribute to the treatment of diseases such as cancer and tumours. However, these properties attributed to omega fatty acids should be supported by many more scientific studies ((Harris, et al., 2021; Cholewski, et al., 2018; Brasky, et et., 2013; Kohlmeier, 2015; Sanchez-Muniz., et al., 2003; Salar, et al., 2021; Lundsgaard, et al., 2020).

### 1. Chemical structure of fats

Fats are derived from plant and animal sources and can be found in solid and liquid form in nature. Since fats are apolar, hydrophobic and neutral compounds, they are soluble in organic solvents such as alcohol, dichloromethane, ether, benzene but not in water. Fats are obtained from the esterification reaction of glycerin and fatty acids. Glycerin (glycerol) is a trihydroxy alcohol and is called propane-1,2,3-triol. Glycerin is a polar compound in the form of a slightly sweet and non-toxic liquid. It is miscible with water and ethanol in all proportions; however, it is soluble in acetone. Glycerol is not found in mineral oils. Although glycerol is found in the same composition in all oil plants, fatty acids are different from each other. The fact that fatty acids are different from each other ensures that the chemical and biological properties of oils are different and gives diversity to oils (Salar, et al., 2021; Karaca et al., 2007; Tarhan, 2008; Akoh, 2002).



Figure 1. Esterification reaction

### 1.1 Chemistry of Fatty Acids

Fatty acids are carboxylic acids, usually consisting of a single carboxyl group (-COOH) and a straight hydrocarbon chain of alkyl (R-) groups. The alkyl (R) groups in the structure of fatty acids are variable, unique for each fatty acid. They differ from each other in terms of the number of carbons in the alkyl hydrocarbon straight chain, the number of double bonds, the location of the double bond, conjugation and isomerism. This difference expands the areas of use of both fatty acids and the oils they form in medicine, cosmetics, food and other industries. Fats are generally found in nature in the form of mixed glycerides. In nature, more than 450 fatty acids with 2-36 carbons, more than 40 of which are found in foods, have been identified and their chemical structure has been determined and many new fatty acids are waiting to be discovered. Fatty acids are usually analysed as methyl ester derivatives by gas chromatography-mass spectrometry (Nimal Ratnayake & Galli 2009; Brasky, et et., 2013; Kohlmeier, 2015; Karaca et al., 2007).



Figure 2. Representation of fatty acids

The first two-carbon organic acid is acetic acid. The last product formed as a result of the breakdown of fatty acids in the body is acetic acid. Acetic acid is finally broken down into water and carbon dioxide by burning as a result of the reaction. But acetic acid is not found in fats, the smallest four-carbon butyric acid in the structure of fats in nature, the longest chain 24-carbon member of the lignoceric (tetracosanoic) acid was found. Fatty acids with larger carbons are found in the fat of waxes (Luo, et at., 2023; Stachowicz, et al., 2023; Çelik, et al., 2004).



Figure 3. Representation of Acetic and Butyric Acids

There are many classifications of fatty acids, but they are commonly classified according to their carbon number, double bonds and bioactive properties. Fatty acids are classified according to the number of carbons as short chain fatty acids with carbon numbers between 3-7, medium chain fatty acids with carbon numbers between 8-13,

long chain fatty acids with carbon numbers between 14-24, and very long chain fatty acids with 21 or more carbon atoms. Long chain fatty acids are generally found in foods and are taken into the body through nutrition. Short chain fatty acids also contain fatty acids. Fatty acids with carbon number 9 and below are liquid under normal conditions. Fatty acids with carbon number more than 20 are usually found in the fats of vertebrates. Fatty acids with carbon number more than 6 form salts with metals by means of carboxyl groups and the salts formed with metals are called soap. Fatty acids are obtained from the reaction of these salts with acids (Nimal Ratnayake & Galli 2009; Cholewski, et al., 2018; Santin, et al., 2021; Luo, et at., 2023; Stachowicz, et al., 2023). Fatty acids are defined as monounsaturated if there is one (C=C) double bond between the straight chain aliphatic carbons of fatty acids, polyunsaturated if there is more than one (C=C) double bond and saturated fatty acids if there is no double bond. All bonds in the alkyl group of saturated fatty acids are sigma bonds (-C-C-), single bonds. Since each carbon atom is saturated with hydrogen, they cannot take other hydrogen into their structure. As the carbon number increases, melting points also increase. For this reason, oils containing more saturated fatty acids with long carbon chains are solid at room temperature. In addition, while their boiling points increase according to the increase in carbon number, their vapour pressures change in the opposite direction and decrease. Therefore, while the first members of the series can be distilled under normal pressure depending on their boiling point, the higher molecular members of the series, including lauric acid containing 12 carbon atoms, can only be obtained under vacuum and by water vapour distillation. Otherwise, high molecular members require very high temperature for boiling and break down before reaching boiling temperature. Since saturated fatty acids do not have double bonds, they are more stable against oxidation and have a longer shelf life. Saturated fatty acids found in nature usually consist of an even number of carbon atoms. Saturated fatty acids in the common diet have 4-24 carbon atoms. Palmitic acid (16 carbons) in vegetable oils and stearic acids (18 carbons) in animal fats are the most common saturated fatty acids. Margarine acid (17 carbons) and saturated fatty acids with 7, 9, 11 and 13 carbon atoms are also found in human hair (Nimal Ratnayake & Galli 2009; Nas, et al., 2001; Kohlmeier, 2015; Tarhan, Ö. 2008; Salar, et al., 2021; Kazaz, et al., 2022).



Figure 4. Palmitic and Streaic acid representation

Fatty acids are defined as monounsaturated if there is one (C=C) double bond between the straight chain aliphatic carbons and polyunsaturated if there is more than

one (C=C) double bond. Double bonds in polyunsaturated fatty acids usually repeat at three-carbon intervals. The shortest chain found in nature to date is 10-carbon unsaturated fatty acid and the longest chain is 30-carbon unsaturated fatty acid. Unsaturated fatty acid-containing triglycerides (fats) are liquid at room temperature and are very sensitive to oxidation light and heat treatments depending on the number of double bonds. Unsaturated fatty acids are a more active compound depending on the number of double bonds, which makes the shelf life shorter. Unsaturated fatty acids have mostly cis configuration. In general, since the atoms connected by double bonds cannot rotate around the axis of this bond, the chain of the fatty acid in the cis isomer state is bent at the double bond point and the freedom of movement of the carbon chain is reduced (Kohlmeier, 2015; Santin, et al., 2021; Luo, et at., 2023; Stachowicz, et al., 2023).

In the nomenclature of fatty acids, the name carboxylic acid may be used in addition to the main hydrocarbon chain, but this is more laborious and less common. There are many methods for the nomenclature of fatty acids. But most methods do not fully explain the chemical structure of fatty acids. In the systematic nomenclature of fatty acids, chemical properties are utilised to fully describe the structure. Firstly, the Latin name of the total carbon number of the fatty acid is written. Then anoic acid is added to alkane (saturated) fatty acids, enoic acid to alkene (unsaturated) fatty acids and inoic acid to alkyne (unsaturated) fatty acids. If there is more than one double bond in the straight chain of fatty acids, the number of carbon atoms is followed by the Latin number term (di-, tri-, tetra-, penta-, hexa-, etc.) followed by the suffix enoic. Double bond positions are indicated by numbers before the fatty acid name. In double bonds in fatty acids, the term cis (c or Z) is added before the double bond position number if the atoms are on the same side and trans (t or E) if they are on opposite sides. In addition, in systematic nomenclature, in case of unsaturated bond, branching, ring or substituted structure, carbon atoms are numbered starting from the carboxyl (-COOH) group in order to indicate these properties in the nomenclature ( Çelik, et al., 2004; Kazaz, et al., 2022; Kent, 2009; Çakmakçı, et al., 2012).

Fatty acids have specialised names that have developed over the years. The specialised names of fatty acids are more commonly used than the standard (IUPAC) terminology. The common names of fatty acids usually originate from botanical or zoological origins. However, it is easy to memorise these special names according to IUPAC nomenclature, but it is impossible to know the structure and properties of the fatty acid. Additional abbreviations are used to special names to understand the structure of the fatty acid. This abbreviation ( $\Delta$ ) is made according to the delta system. According to the delta system, double bonds are denoted by " $\Delta^{x}$ ", where x indicates the number of carbons from the carboxyl (-COOH) end of the double bond, and in the expression "a:b", "a" is the number of carbons and "b" is the number of double bonds. In abbreviated notation, unsaturated fatty acids are assumed to be in the cis form unless otherwise stated. The first carbon atom adjacent to the -COOH carbon is called the  $\alpha$ -carbon, the second the  $\beta$ -carbon, and the third the  $\gamma$ -carbon (Akoh, 2002; Nimal Ratnayake & Galli 2009; Brasky, et et., 2013; Kazaz, et al., 2022; Silva, et al., 2021; Garcia, et al., 2019; Yeşil, et al., 2017; Özdemir, et al., 2003; Kayahan, 2003; Nas, et al., 2001; Tarhan, Ö. 2008; Kümeli, 2006)



Figure 5. Genus trans isomer representation

Unsaturated fatty acids are classified by biochemists and nutritionists with omega ( $\omega$ ) and minus (n) markings to indicate the biological activity of fatty acids. Omega ( $\omega$ ) is the last letter of the Greek alphabet and has traditionally signalled the end. Therefore, starting from the methyl (CH<sub>3</sub>) group at the end of the aliphatic chain of the fatty acid, the carbon atom with the first double bond is indicated by the symbol ( $\omega$  or n). The discovery of omega compounds and the elucidation of their physical and chemical properties are important for a healthier life (Özdemir, et al., 2003; Kayahan, 2003; Çelik, et al., 2004; Kazaz, et al., 2022; Kent, 2009; Çakmakçı, et al., 2012; Göcen, 2018).

### 2. Omega Fatty Acids

Almost all naturally occurring unsaturated fatty acids have their double bonds in cis configuration and are positioned at 3,5,6,7 and 9 carbon atoms starting from the methyl group. The most widely known omega fatty acids are omega-9, omega-6 and omega-3. Less well known omega fatty acids are omega-5 and omega-7 fatty acids. Omega-7 and omega-5 fatty acids are remarkable in terms of their biological activity. Omega-5 and omega-7 fatty acids are especially important for youthful skin and healthy development of the body and are mostly of vegetable origin. The water solubility, melting point and susceptibility to oxidation of unsaturated fatty acids vary according to the degree of unsaturation and double bonds. Omega fatty acids are transformed into new metabolites in living metabolism by desaturase (oxygenase) enzyme that adds double bonds to the new acyl chain and elongase enzymes that elongate acyl chains. The cis-trans isomers of omega fatty acids determine their chemical and biological activities. Plants can synthesise  $\omega$ -3 and  $\omega$ -6 fatty acids and convert their metabolites to each other thanks to 12 and 15 desaturase enzymes. Animals have 5, 6 and 9 desaturase enzymes. Since animals do not have 12 and 15 desaturase enzymes, they cannot synthesise  $\omega$ -3 and 6 fatty acids. Since the human body cannot synthesise it, it is categorised as an essential fatty acid and must be taken from outside. However, humans can synthesise saturated and some monounsaturated

fatty acids from carbohydrates and proteins. Although all polyunsaturated fatty acids are known as essential fatty acids, linoleic acid (LA) and alpha-linolenic acid ( $\alpha$ -ALA) are the most important and are called "major essential fatty acids". Humans can only obtain LA and ALA from plant sources. Some animals can synthesise other essential fatty acids using LA and ALA as starting material. Today, thanks to scientific research, the existence of new omega fatty acids is revealed and their structures continue to be elucidated (Kazaz, et al., 2022; Erdoğan Orhan, İ. 2016; Okumuş, 2016; Ratnayake, et al., 2004; Patel, et al., 2020; Cholewski, et al., 2018; Silva, et al., 2021; Garcia, et al., 2019; Yeşil, et al., 2017; Salar, et al., 2021; Göcen, 2018).

### 2.1 Omega -9 Acids

Unsaturated fatty acids are called omega-9 fatty acids if there is a double bond between the ninth and tenth carbons when counted from the methyl group. Omega-9 fatty acids are generally characterised by a single double bond with a straight chain length ranging from 18 to 24 carbons. However, omega-9 fatty acids can also be polyunsaturated fatty acids such as mead acid 20:3  $\Delta^{5,8,11}$   $\omega$ -9 ((5Z,8Z,11Z)-eicosa-5,8,11-tricnoic acid). Omega-9 fatty acids usually have one double bond in their structure and therefore have a corner. Omega-9 fatty acids are widely used in food and chemical industries due to their unique chemical properties. Omega-9 fatty acids are found in almost all plants, including green algae, in certain proportions (Göcen, 2018; Sales-Campos, et al., 2013; Hernandez, et al., 2021; Spasibionek, et al.,2020).

### 2.1.1 Oleic Acid

The main source of monounsaturated Omega-9 fatty acid (OA) is oleic acid. When oleic acid is counted from the 18-carbon methyl group, there is a single double bond between the 9th and 10th carbons. Oleic acid C18:1  $\Delta^9 \omega$ -9 ((Z)-octadec-9-enoic acid), Elaidic acid C18:1  $\Delta^9 \omega$ -9 ((E)-octadec-9-enoic acid), Gondoic acid C20:1  $\Delta^{11} \omega$ -9 ((Z)-eicosa-11-enoic acid), Erucic acid C22:1  $\Delta^{13} \omega$ -9 ((Z)-docosa-13-enoic acid), Brassidic acid C22:1  $\Delta^{13} \omega$ -9 ((E)-docosa-13-enoic acid), Nervonic acid C24:1  $\Delta^{13} \omega$ -9 ((Z)-tetracosa-15-enoic acid) are converted into omega-9 fatty acids. Oleic acid is the main fatty acid in many vegetable oils such as olive oil (Çelik, et al., 2004; Spasibionek, et al., 2020; Hahn-Holbrook, et al., 2019). Oleic acid-rich oils are more shelf stable because they are more oxidatively stable and are more suitable as frying oils due to their high heat tolerance. It is also increasingly used in the field of biodiesel and biofuel. In the chemical industry, they are widely used in the production of azelaic acid monomer demanded for nylon production. Oleic acid provides glucose balance

in the body, regulates lipid levels and reduces the risk of cardiovascular disease (Göcen, 2018; Sales-Campos, et al., 2013; Hernandez, et al., 2021; Çelik, et al., 2004; Cholewski, et al., 2018; Salar, et al., 2021).



**Figure 6.** (Z)-octadec-9-enoic acid, oleic acid (OA) C18:1  $\Delta^9$ ,  $\omega$ -9 and n-5

#### 2.1.2 Elaidic acid

Elaidic acid C18:1  $\Delta^9 \omega$ -9 ((E)-octadec-9-enoic acid) is a trans oleic acid formed by the transformation of oleic acid. Elaidic acid, like oleic acid, has 18 carbons and a single double bond between carbons 9 and 10, but oleic acid is in the cis form while elaidic acid is in the trans form. Although the closed formulae of oleic acid and elaidic acid are the same, their chemical properties are different from each other because they are cis-trans. While oleic acid melts at 13 14°C, elaidic acid melts at 43°C. Erucic acid, another elongation product of oleic acid, is biodegradable to C22:1  $\Delta^{13} \omega$ -9 ((Z)docos-13-enoic acid) and forms environmentally safe products. Erucic acid has a single double bond at the 9th carbon after the 22-carbon methyl group and at the 13th carbon after the COOH group. One form of erucic acid, erusamide, is used as a lubricant in the production of plastic films such as polyethylene. They are also used as biodiesel, soap, emulsifier and surfactant. However, the rate of erucic acid in edible oils is determined as 2% of total fatty acids at most. Because the consumption of erucic acid has caused a decrease in the contractile ability of the heart muscle. Today, the main raw materials for erucic acid are rapeseeds and mustards containing 45-50% erucic acid. Scientific studies have also reported that Erucic and Elaidic acids cause cardiovascular diseases (Celik, et al., 2004; Lu, et al., 2020; Yan, et al., 2015; Saini, et al., 2016).



Figure 7. Conversion mechanism of oleic acid

#### 2.1.3 Nervonic acid
Nervonic acid C24:1  $\Delta^{15} \omega$ -9 ((Z)-tetracos-15-enoic acid) was first discovered in the brain of sharks and has been found in small concentrations in the nervous system of vertebrates, in the myelin sheath of the brain and in breast milk. In vegetable seed oils, it is less than 5% of total fatty acids. Nervonic acid is a very long-chain monounsaturated cis 15-tetracosenoic acid with 24 carbons. When counted from the COOH group, there is a single double bond between carbons 15-16. When counted from the methyl group, it is found in the form of omega-9 because there is a double between the 9th and 10th carbons. it is the monounsaturated analogue of lignoceric acid. Nervonic acid is synthesised in nature from oleic, palmitic and strearic acids by carbon chain elongation. it is an important component of lunaria oil. Nervonic acid has an important effect on brain development and protection and contributes to accelerating the development of infants. It can be used as an additional energiser in athletes. Nervonic acid C24:1  $\Delta^{15} \omega$ -9 has been reported to have positive results in patients with schizophrenia, Alzheimer's, Parkinson's and MS. Various studies have shown that NA supplementation supports the treatment of neurological diseases such as neurological disorders, which has further increased interest in nervonic acid (Lia, et al., 2019; Umemoto, et al., 2014; Tang, et al., 2013; Çelik, et al., 2004; Tvrzicka et al., 2011; Liu, et al., 2021; Kageyama, et al., 2021; Lewkowicz, et al., 2019; Hu, et al., 2021)



**Figure 8.** (E)-tetracos-15-enoic acid, Nervonic acid C24:1  $\Delta^{15}$ ,  $\omega$ -9 and n-9

## 2.2 Omega-7 Fatty Acids

The most common types of omega-7 fatty acids, which are less known than omega-3, 6 and 9 fatty acids, are Palmitoleic acid and trans Vaccenic acid fatty acids. Omega-7 fatty acids are monounsaturated fatty acids. When counted from the methyl group, it is found in the omega-7 form since the double bond is between the 7th and 8th carbons. Omega-7 fatty acids are suitable to be used as raw materials in the health field, polymer industry and energy field due to their chemical properties. The melting point of omega-7 fatty acids is lower than omega-9 fatty acids. Oils with high omega-7 content have been found to be superior in biodiesel use compared to oils containing other fatty acids. The usage areas of omega-7 acids have gradually increased. For

example, the use of  $\omega$ -7 fatty acids in the synthesis of 1-octene used in polyethylene production, biodiesel production, skin creams has become widespread. Vegetable oils showing high  $\omega$ 7 content are rare. The efforts of scientists to enrich vegetable oils with omega-7 fatty acids are promising (Herbst. 2015; Aruna et al., 2016; Garcia 2019; Grossmann, et al., 2010; Erdoğan Orhan, 2016; Çelik, et al., 2004; In-Bong, et al., 2018; Nguyen, et al., 2015).

### 2.2.1 Palmitoleic Acid

The source of omega-7 fatty acids is palmitoleic acid C16:1  $\Delta^9 \, \omega$ -7 (PAL (Z) hexadec-9-enoic acid). PAL C16:1  $\Delta^9$  is called an omega-7 fatty acid because it contains a double bond at the seventh carbon counting from the methyl group. PAL C16:1  $\Delta^9$  is cis 9-hexadec-9-enoic acid because it has a single double bond between carbons 9-10 when counted from the COOH group. Palmitoleic acid is also known as zoomeric acid. Palmitoleic acid is found in foods in two forms: cis palmitoleic acid and transpalmitoleic acid found in meats. PAL 16:1  $\Delta 9$  and its elongation products C18:1  $\Delta^{11}$ and C20:1  $\Delta^{13}$  are  $\omega$ 7 monounsaturated fatty acids. palmitoleic acid is a characteristic component of marine animal fats. Palmitoleic acid is obtained from cold-water fish, some yeasts, macadamia and sea buckthorn fruits (Herbst. 2015; Aruna et al., 2016; Garcia 2019; Grossmann, et al., 2010). In animals, fatty tissues use palmitoleic acid to communicate with distant organs. Palmitoleic acid has been increasingly used due to its antimicrobial, antioxidant and insulin resistance properties as well as its antiaging effects. However, research on palmitoleic acid is very limited (Erdoğan Orhan, İ. 2016; Çelik, et al., 2004; In-Bong, et al., 2018; Veronique, 2008; Demirok, et al., 2009).



Figure 9.(Z)-hexadec-9-enoic acid, Palmitoleic acid (PAL) C16:1  $\Delta^9 \omega$ -7 and n-7

#### 2.2.2 Trans-vaccenic acid

Trans-vaccenic acid C18:1  $\Delta^{11} \omega$ -7 ((E)-octadec-11-enoic acid) is another omega-7 fatty acid. TVA C18:1  $\Delta^{11} \omega$ -7 is an 18-carbon monounsaturated fatty acid with a double bond at the seventh carbon when counted from the methyl end and at the eleventh carbon when counted from the carboxyl end. TVA C18:1  $\Delta^{11} \omega$ -7 is a C18:1 $\Delta^{9} \omega$ -9 isomer of oleic acid and is a naturally occurring trans fatty acid. TVA has the same closed formula as oleic acid but different chemical and biological effects. It is

synthesised from palmitic acid (C16:0) via the production of C16:1 ( $\omega$ -7) by a desaturase and elongation by an elongase enzyme yielding C18:1 ( $\omega$ -7). In addition, linoleic acid is converted by biohydrogenation first to its cis-tyrance-isomer, then to vaccenic acid and finally to stearic acid (C18:0). It is the predominant trans fatty acid in human milk, ruminant fat and dairy products and various oilseeds. Trans-vaccenic acid (TVA, C18:1  $\Delta$ <sup>t11</sup>  $\omega$ -7) has been shown to protect against breast cancer in some studies. Biosynthetic evidence suggests that TVA is readily metabolised into conjugated linoleic acid (CLA) by the bacterial enzyme desaturase. Further scientific studies are needed to identify the health effects attributed to TVA (Duffy et al., 2006; Veronique, 2008; Herbst. 2015; Aruna et al., 2016; Garcia 2019; Grossmann, et al., 2010).



Figure 10. Trans-vaccenic acid metabolism

#### 2.3 Omega-6 Fatty Acids

omega-6 fatty acids are polyunsaturated fatty acids with the first double bond between the 6-7th carbon atoms from the methyl group of the hydrocarbon chain. Omega-6 fatty acids can have a straight hydrocarbon chain ranging from 18-22 carbons and at least two double bonds. The carbon number of omega-6 fatty acids and the location and position of the varying number of double bonds largely determine the degree of unsaturation and biological activity. Omega-6 fatty acids are used as supplements for healthy growth and development, for the regular functioning of heart and brain functions and in cancer treatment. Although omega-6 fatty acids play very important roles in many biological processes, humans and other mammals are essential fatty acids because they do not have enzymes to synthesise omega-6 fatty acids. omega-6 fatty acids should be taken into the body through diet (from vegetable oils and oil seeds). Due to excessive consumption of omega-6 in the diet, the  $\omega$ -6/ $\omega$ -3 balance in the body is disturbed and omega-3 intake is needed (John's, 2019; Santin, et al., 2021; Hahn-Holbrook, et al., 2019; Açıkgöz, 2006; Çelik, et al., 2004; Silva, et al., 2021;Stachowicz, et al., 2023).

# 2.3.1 linoleic acid

The main source of omega-6 ( $\omega$ -6) fatty acids is linoleic acid C18:2  $\Delta^{9,12} \omega$ -6 (LA; (9Z,12Z)-octadeca-9,12-dienoic acid), the shortest carbon chain. Linoleic acid (LA) has 18 carbons and two double bonds in the cis form. The daily energy from LA in the diet is around 7-8%. It is one of the essential polyunsaturated fatty acids needed by the human brain. linoleic acid (LA) regulates blood pressure, strengthens the immune system and is a precursor of lipoxin and speficic eicosanoids important for health. It is considered to be limiting in the elderly and in some disease states. It is also involved in the production of compounds with efflamaturising effects. Since omega-6 fatty acids are not synthesised by humans, they are obtained from plant sources and eggs and meat of poultry(Ceci, et al., 2021; Açıkgöz, 2006; Çelik, et al., 2004; Silva, et al., 2021; Stachowicz, et al., 2023).



Figure 11. (9Z,12Z)-octadeca-9,12-dienoic acid, Linolenic acid (LA) C18:2  $\Delta^{9,12}$  $\omega$ -6 and n-6

Omega-6. linoleic acid (LA) via desaturase and elongase enzymes, gamma-linolenic acid C18:3  $\Delta^{6,9,12}$   $\omega$ -6 (GLA; (6Z,9Z,12Z)-octadeca-6,9,12-trienoic acid), Dihomo gamma-linolenic C20:3  $\Delta^{8,11,14}$   $\omega$ -6 (DGLA: (8Z,11Z,14Z)-icosa-8,11,14-trienoic acid), Arachidonic acid C20: 4  $\Delta^{5,8,11,14}$   $\omega$ -6 (AA; (5Z,8Z,11Z,14Z)-icosa-5,8,11,14tetraenoic acid), Adrenic acid C22:4  $\Delta^{7,10,13,16}$   $\omega$ -6 (DTA; (7Z,10Z,13Z,16Z)- docosa-7,10,13,16-tetraenoic acid), Osbond acid C22: 5  $\Delta^{4,7,10,13,16}$   $\omega$ -6 (DPA; (4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoic acid) is converted into polyunsaturated omega-6 fatty acids Salar, et al., *202;* Stachowicz, et al., 2023; John's, 2019; Senning, 2019; Santin, et al., 2021).



Figure 12. LA metabolisation

# 2.3.2 GLA and DGLA Fatty Acids

Gamma-linolenic acid C18:3  $\Delta^{6,9,12}$   $\omega$ -6 (GLA; (6Z,9Z,12Z)-octadeca-6,9,12-trienoic acid) is a product of linoleic acid (LA; C18:2  $\Delta^{9,12}$   $\omega$ -6) formed by desaturase and rapidly converted to dihomo  $\gamma$ -linolenic acid C20:3  $\Delta^{8,11,14}$   $\omega$ -6 (DGLA: (8Z,11Z,14Z)-icosa-8,11,14-trienoic acid) by the enzyme elongase. GLA C18:3  $\Delta^{6,9,12}$ is an omega-6 fatty acid with three double bonds, including the first double bond of the 6th carbon from the 18-carbon methyl end. GLA is derived from vegetable oils such as donkey grass seed oil, blackcurrant, blackcurrant, evening primrose and borage oils. Evening primrose oil, which is in the form of gamma linoleic acid, is mostly marketed in the world. Since Gamma Linolenic Acid is an important precursor of prostaglandins and leukotrienes, it has effects such as delaying skin aging, moisturising, tightening and supporting hormonal balance. Creams containing GLA especially facilitate the treatment of skin problems due to stress and other factors. In addition, it has a positive effect on lowering LDL cholesterol and fat levels, increasing HDL cholesterol and preventing plaque formation. The physical addition of vegetable oils containing GLA to infant formula formulations has gained importance in recent years (Şahin Yeşilçubuk, et al., 2008; Çelik, et al., 2004; Santin, et al., 2021).



Figure 13. (6Z,9Z,12Z)-octadeca-6,9,12-trienoic acid, Gamma-linolenik asit GLA C18:3  $\Delta^{6,9,12}$ ,  $\omega$ -6 and n-6

Dihomo-gamma-linolenic acid C20:3  $\Delta^{8,11,14}$   $\omega$ -6 ((DGLA; (8Z,11Z,14Z)icosa-8,11,14-trienoic acid) is a natural product found in organisms. Dihomo gammalinolenic acid is converted to arachidonic acid C20:4  $\Delta^{5,8,11,14}$   $\omega$ -6 (AA; (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid) by the enzyme desaturase. DGLA C20:3  $\Delta^{8,11,14}$  The 20-carbon omega-3 fatty acid has three double bonds, all in cis form, and the first double bond is located at the 6th carbon from the methyl end. Dihomo gamma-linolenic acid is also called gamma-homolinolenic acid (DHLA). DGLA is a precursor molecule of prostaglandins and leukotrienes, and prostaglandins and leukotrienes help prevent various diseases through diet. In addition, according to recent studies, DGLA is a fatty acid that is a precursor of hormones that prevent cardiovascular, diabetes, skin diseases and immune inflammatory diseases (Şahin Yeşilçubuk, et al., 2008; Çelik, et al., 2004; Ceci, et al., 2021).



Figure 14. (8Z,11Z,14Z)-icosa-8,11,14-trienoic acid, Dihomo gama-linolenik DGLA C20:3  $\Delta^{8,11,14}$ ,  $\omega$ -6 and n-6

# 2.3.3 Arachidonic acid

Arachidonic acid ((5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid) can be directly ingested in the diet or synthesised in the body from linoleic acid (an essential fatty acid). Arachidonic acid (AA), which is obtained in the body from  $\alpha$  linolenic acid by metabolised elongation and desaturation enzymes, is C20:4  $\Delta^{5,8,11,14}$   $\omega$ -6, a 20-carbon eicosanoic acid in cis form with a  $\omega$ -6 sequence containing four double bonds. Arachidonic acid is the most widely used precursor in the synthesis of eicosanoids and initiates the biosynthesis of many eicosanoids. Arachidonic acid (AA) is found in animal fats such as liver, fish, egg lipids and peanut oils, and is rare in plant sources.

It is also stated that AA has an important role in the communication of the cells in the grey part of the brain and in the structure of the retina. Arachidonic acid is also a precursor of growth hormones and is necessary for the fluidity of fat in the vessels, and is responsible for 5-15% of phospholipid synthesis in the cell membrane. However, studies have shown that n-6 fatty acids, whose dietary intake is increasing today, increase the production of AA and its metabolites in our body. However, the development of many diseases has accelerated. Although it is not ignored that AA metabolites are important for body defence, it has been proven that excessive production of AA metabolites predisposes to diseases and adversely affects the course of diseases. This fatty acid, which has an important role in the development of diseases, should be taken into consideration and medical nutrition therapy should be organised taking into account these studies (Wainwright vd., 2001; Timmers, et al., 2011; Huang, et al., 2011; Göcen, 2018; Hendek, et al., 2012).



Figure 15. (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid, Araşidonikasit (AA) C20:4  $\Delta^{5,8,11,14}$   $\omega$ -6 and n-6

# 2.4 OMEGA-5 Fatty Acids Super (CLN)

Omega-5 fatty acids are Myristoleic acid, punisic acid and  $\alpha$ -Eleostearic acid. Punisic acid (PA) and  $\alpha$ -Eleostearic acid (ESA) are conjugated triene polyunsaturated fatty acids, while Myristoleic acid is monounsaturated fatty acids. Since the first double bond after the methyl group is between the 5th and 6th carbons, it is called omega-5 or n-5. Omega-5 fatty acids are taken from plant sources through diet. Omega-5 fatty acids are of interest due to their positive effects against tumours and especially prostate cancer (Kohlmeier., (2015; Erdoğan Orhan, 2016).

### 2.4.1 Myristoleic acid

Myristoleic acid C14:1  $\Delta 9 \oplus -5$  ((Z)-tetradec-9-enoic acid) is a monounsaturated fatty acid. Myristoleic acid has 14 carbons and is referred to as omega-5 fatty acid because its only double bond is located between carbons 5 and 6. It can be easily obtained from Myristicaceae plant seeds or biosynthesised from myristic acid by enzymes in organisms. Myristoleic acid C14:1  $\Delta^9 \oplus -5$  is rare in nature and has been reported to be effective against prostate cancer. Myristic acid (myristate) is a saturated tetradecanoic acid containing 14 carbons in a straight chain. Myristic acid 14:0 is found in nutmeg, palm seeds and butter. Myristate increases LDL cholesterol concentrations in plasma more than other saturated fatty acids Jun-Oh, et al., 2015; Salar, B., Kuruüzüm., 2021). (Jun-Oh, et al., 2015; Salar, B., Kuruüzüm., 2021).



Figure 16. Myristoleic acid metabolism

#### 2.4.2 Punicic acid

Punicic acid C18:3  $\Delta^{9c,11t,13t} \omega$ -5 ((9Z,11E,13Z)-octadeca-9,11,13-trienoic acid) is a super-conjugated linolenic acid (CLN) derivative and polyunsaturated fatty acid with three conjugated double bonds. Punicic acid C18:3  $\Delta^{9c,11t,13t}$  is an 18-carbon, triconjugated, omega-5 fatty acid with the first double bond at the 5th carbon from the methyl end. When counting from the carboxyl group, the double bond at carbon 9 is in cis form and the double bonds at carbons 11 and 13 are in trans form. This configuration of punicic acid is one of the features that determine its biological activity. Punicic acid is also called tricosanic acid. The most important source is the oil of pomegranate seed. It has been supported by various studies that punicic acid is antioxidant, anti-inflammatory, antidiabetic, lipid-lowering and effective against cancer. Especially those who have forgetfulness problems, those with fat accumulation problems and prostate cancer are positively effective against tumours. It is recommended to take Omega-3, -5 and -7 together (Karageorgou, et al., 2021; Kohlmeier., 2015; Erdoğan Orhan, 2016).



Figure 17. (9Z,11E,13Z)-octadeca-9,11,13-trienoic acid, Punisic acid (PA) C18:3  $\Delta^{9,11,13} \omega$ -5 and n-5

#### 2.4.3 *a-Eleostearic acid*

α-Eleostearic acid C18:3  $\Delta^{9c,11t,13t}$  ω-5 ((α-ESA; (9Z,11E,13E)-octadeca-9,11,13trienoic acid) is a long-chain olefin fatty acid containing a conjugated triene system.  $\alpha$ -ESA C18:3  $\Delta^{9c,11t,13t}$  is an 18-carbon, triple-linked, omega-5 fatty acid with the first double bond at the 5th carbon from the methyl end. When  $\alpha$ -ESA is counted from the carboxyl group, the double bond at carbon 9 is in cis form and the double bonds at carbons 11 and 13 are in trans form. This configuration of  $\alpha$ -ESA is one of the features that determine its biological activity. a-Eleostearic acid is the main constituent of bitter pumpkin seed oil, but catalpic acid gives the bitter taste of pumpkin. aeleostearic acid is obtained from the hydrolysis of Tung (Aleurites fordii) oil. α-ESA has a significant effect on tumour growth and may help to inhibit oxidative stress by lowering lipid peroxidation rates. ESA - effective against breast cancer. In fact, it has been reported that ESA has a strong effect against cancer in general CLA. ESA is recommended as a dietary supplement to prevent angiogenic diseases such as diabetes. Due to the high resistance of  $\alpha$ -ESA to heat and corrosion, its use in the coating industry has increased (Karageorgou, et al., 2021; Kohlmeier., 2015; Erdoğan Orhan, 2016; Simplício de Sousa, et al., 2013; Liu, et al., 2019).



Figure 18. α-Eleostearic acid metabolism

Plant-derived conjugated trienoic fatty acids are mainly  $\alpha$ -eleostearic ( $\Delta^{9c,11t,13t}$  18:3), catalpic acid ( $\Delta^{9t,11t-13c}$  18:3), punicic acid ( $\Delta^{9c,11t,13c}$ -18:3), calendic acid ( $\Delta^{8t,10t,12c}$  18:3) and jacaric acid ( $\Delta^{8c,10t,12c}$  18:3) with cis- and trans- geometric isomers. Conjugated fatty acids are classified as conjugated dienes, trienes and tetraenes according to the number of ordered double bonds in their structures. The bioactivity

of conjugated fatty acids is directly proportional to the number of ordered double bonds in their structure. Tetraenoic acids have stronger physiological activity than trienoic acids and trienoic acids have stronger physiological activity than dieonic acids. The strong biological activity of CLNA is thought to be due to its ability to convert into CLA isomers and undergo rapid oxidation. Conjugated trienoic fatty acids are found in small amounts in animal sources and are generally found in vegetable seed oils. Conjugated linolenic acids (CLN), especially in the form of C18-triene or C18-tetraene, constitute 40-80% of the total fatty acids in many seed oils. Conjugated eicosapentaenoic acid (CEPA) and conjugated arachidonic acid (CAA), which are tetraenoic acids containing four ordered conjugated double bonds, have been found in aquatic plants. The most common of the conjugated tetraene fatty acids is  $\alpha$ -parinaric acid and its geometric isomers are found in Makita tree seeds. There is a growing interest in CLN fatty acids. (Turpeinen, et al., 2002; Bohlin ve ark. 2003: Özgül-Yücel 2005; Tanaka, et al., 2011).



Figure 19. Conjugated trienoic fatty acids from plants

# 2.4.3 Conjugated Linoleic Acid (CLA)

Conjugated linoleic acid is an 18-carbon unsaturated fatty acid with two double bonds separated by a single bond. Conjugated linoleic acid (CLA) has 28 different isomers, especially linoleic acid. CLA is generally one of the isomer groups of octadecanoic fatty acid with two double bonds. The most abundant main isomer is (9Z,11E)-octadeca-9,11-dienoic acid. When CLA is counted from the 18-carbon carboxyl

group, it has two double bonds, one in cis form at the 9th carbon and one in trans form at the 11th carbon. CLA is known as rumenic acid. CLA C18:2  $\Delta^{9c,11t}$  is a fatty acid found in the fats and milk of ruminants and its content varies depending on the diet of the animals. For example, it has been determined that the CLA content in animals fed in pasture areas is higher than the CLA content in animals fed with ready-to-eat animal feed. Rumenic acid C18:2  $\Delta^{9c,11t}$  accounts for 90% of the total CLA in ruminant fat and most of the rest is made up of 7E, 9Z- and 10E, 12Z-octadecadienoic acid. (Demirok, et al., 2009; Turpeinen, et al., 2002; Kohlmeier., 2015). Erdoğan Orhan, 2016).



Figure 20. (9Z,11E)-octadeca-9,11-dienoic acid, Rumenic acid C18:2  $\Delta^{9,11}$ 

CLAs are metabolised from polyunsaturated fatty acids by biohydrogenation by rumen microorganisms during animal rumen metabolism. Two groups of bacteria are responsible for the metabolisation of biohydrogenation reactions. The first group of bacteria hydrogenates linoleic acid and linolenic acid and the main end product of this reaction is trans-11 C18:1 (vaccenic acid) fatty acid. The second group of bacteria uses trans-11 C18:1 fatty acid as the main substrate and produces stearic acid as the end product. The metabolism of trans11-octadecenoic acid (TVA) produces cis 9, trans11-linoleic acid. Some bacterial species are known to convert linoleic and linolenic acid into conjugated isomers (Duffy, et al., 2006; Erdoğan Orhan, 2016; Turpeinen, et al., 2002; Kohlmeier., 2015; Demirok, et al., 2009).



Figure 21. Role of rumen biohydrogenation in the production of Cis-9, trans-11 CLA in ruminant-derived fats

Rumenic acid is commonly found in natural sources in dairy products and vegetable oils such as corn oil, canola oil and sunflower oil. Unconjugated fatty acids can be converted into conjugated fatty acids by microorganisms. Since vegetable cooking oils are refined, the human body cannot produce CLA, so it can only meet its needs from beef and mutton and dairy products that it consumes daily. Since it has the ability to easily combine with phospholipids, it is considered to be the most biologically active isomer. CLA and omega fatty acids reduce triglyceride levels that play a role in heart attack and prevent vascular occlusion by providing blood fluidity. CLA is reported to have positive physiological effects against diseases such as obesity, antitumour, diabetes, hypertension and cholesterol. More detailed research on conjugated fatty acids is required. Apart from naturally occurring trans fatty acids, commercial trans fatty acids are produced. These are usually formed as a result of hydrogenation or refining of vegetable oils. While naturally occurring trans fats have positive effects on health, the negative effects of unnatural and dietary trans fats have also been reported(Arao ve ark. 2004; Erdoğan Orhan, 2016; Turpeinen, et al., 2002; Kohlmeier., 2015; Demirok, et al., 2009).

## 2.5 Omega-3 Fatty Acids

Omega-3 fatty acids are polyunsaturated fatty acids with the first double bond between the 3-4th carbon atoms from the methyl group of the hydrocarbon chain. Omega-3 fatty acids can have a straight hydrocarbon chain ranging from 18-24 carbons and at least double bonds. Omega-3 fatty acid has 8 isomers according to cis-trans isomer status. The number of carbons of omega-3 fatty acids and the location and position of the changing number of double bonds largely determine their chemical structure and biological activity. Omega-3 fatty acids are vulnerable to oxidation due to their double bonds and problems occur in storage conditions. Humans and animals do not have enzymes to synthesise Omega-3 fatty acids. Omega-3 fatty acids are essential fatty acids for humans, the body does not produce them and must be taken through diet for a healthy life. Aquatic organisms (such as algae, seaweed and fish) and plant seeds (such as flax, chia, and walnuts) are the main sources of omega-3 fatty acids. Omega-3 fatty acids are found in the cell membrane, brain, nervous system and regulate the immune system. Due to the cardiovascular, cancer and neurological effects of omega-3 fatty acids, new omega-3 sources and scientific studies are needed. Recently, studies have been carried out to synthesise omega-3 fatty acids through some microorganisms Cholewski, et al., 2018; Timmers, et al., 2011; Huang, et al., 2011; Göcen, 2018; Roke, 2017; Salar, et al., 2021).

### 2.5.1 Linolenic acid

Linolenic Acid C18:3  $\Delta^{9,12,15} \omega$ -3 (ALA; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid) is the main compound of omega-3 fatty acids. ALA is an unsaturated fatty acid containing three double bonds in its 18-carbon cis form and is an omega-3 fatty acid with the first double bond between carbons 3 and 4 from the methyl group of the straight chain.  $\alpha$ -linolenic acid C18:3  $\Delta^{9,12,15} \omega$ -3 is formed from oleic acid in plants by the action of enzymes. It is an essential fatty acid that is taken from the diet and cannot be synthesised in the body.  $\alpha$ -ALA, especially from plant sources such as canola, walnuts, flaxseed, etc., is transformed into metabolites important for health in the body Timmers, et al., 2011; Huang, et al., 2011; Göcen, 2018; Roke, 2017; Salar, et al., 2021).



Figure 22. (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid, Linoleic Acid (ALA) 18:2  $\Delta^{9,12,15} \omega$ -3 and n-3

Linolenic Acid C18:2  $\Delta^{9,12,15}$   $\omega$ -3 ((ALA; (9Z,12Z,15Z)-octadeca-9,12,15trienoic acid), stearidonic acid C20:4  $\Delta^{3,6,9,12}$   $\omega$ -3 ((SDA; (3Z,6Z,9Z,12Z)-icosa-C20:5  $\Delta^{5,8,11,14,17}$ 3,6,9,12-tetraene), eicosapentaenoic acid ω-3 ((EPA; (5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoic acid), docosapentaenoic acid C22:5  $\Delta^{7,10,10,13,16,19}$ ω-3 ((DPA; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19pentaenoic acid) and docosahexaenoic acid C22:6  $\Delta^{4,7,10,13,16,19}$   $\omega$ -3 ((DHA; (4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoic acid). (Stachowicz, et al, 2023; Göcen, 2018; Lopez, et al., 2023). The conversion of Linolenic acid (ALA), EPA and DHA in the human body is not fully efficient and must be taken from outside through diet or supplementation for a healthier life. While ALA is plant-derived omega-3, EPA and DHA are omega-3 fatty acids found in high amounts in marine organisms. Another omega-3 fatty acid, SDA, is found in borage and hemp oils. The EPA level of dietary supplementation of SDA, which is the product of desaturation of stearidonic acid,  $\alpha$ -linolenic acid, is higher than ALA supplementation, so it has recently attracted the attention of researchers. SDA was almost twice as effective as ALA in increasing cellular EPA concentration. But stearidonic acid, like α-linolenic acid, cannot replace pre-formed EPA and DHA (Göcen, 2018; . Roke, et al., 2017; Salar, et al., 2021 Dewhurst, et al., 2013; Cholewski, et al., 2018; Baker, et al., 2020; Roke, K. 2017; Ruxton, C. 2004: Dewhurst, et al., 2013).



**Figure 23.** Conversion of α-linolenic acid to longer-chain, polyunsaturated n-3 fatty acids

#### 2.5.2 Eicosapentaenoic Acid

Eicosapentaenoic acid C20:5  $\Delta^{5,8,11,14,17}$   $\omega$ -3 ((EPA; (5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoic acid) is a polyunsaturated omega-3 fatty acid. It is also called thymnodonic acid. The human body converts a hydrolytic portion of absorbed linolenic acid into EPA as a breakdown product. EPA is also the precursor of DHA. EPA, which is abundant in cold-water fish and breast milk, has been studied clinically for its ability to prevent heart attacks and strokes, making it one of the most popular PUFA supplements. The source of EPA in fish is the seaweed they feed on. EPA has also been reported to be found in trace amounts in purslane. Eicosapentaenoic acid is a US FDA approved drug for lowering triglyceride levels. It is used as an auxiliary substance to reduce blood clotting rate (Dewhurst, et al., 2013; Lopez, et al., 2023; Liua, et al., 2023; Cholewski, et al., 2018).



Figure 24. (5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoic acid, EPA 20:5  $\Delta^{5,8,11,14,17}$   $\omega$ -3 and n-3

### 2.5.3 Docosahexaenoic Acid

Docosahexaenoic acid C22:6  $\Delta^{4,7,10,13,16,19}$   $\omega$ -3 ((DHA; (4Z,7Z,10Z,13Z,16Z,19Z)docosa-4,7,10,13,13,16,19-hexaenoic acid) is a polyunsaturated omega-3 fatty acid. Since DHA has a large number of double bonds, it is sensitive to heat, light, oxygen, light and temperature and sensitive to storage conditions and has low permeability and bioavailability due to its low water solubility. Docosahexaenoic acid (DHA) is naturally produced in small amounts by our body from alpha-linolenic acid or obtained directly from dietary consumption such as breast milk, fish and algae oil. Docosahexaenoic acid is the most abundant polyunsaturated fatty acid in the brain, central nervous system and retina. DHA is also found in cell membranes in the body and helps to transmit messages between nerves. Studies have shown that exposure to human milk affects brain development and contributes to visual and motor development. In addition, DHA has been found to be an essential omega-3 fatty acid for healthy brain development, reducing the risk of cancer, better vision and heart health (Vu, et al., 2016; Liua, et al., 2023; Dewhurst, et al., 2013; Catalá, 2013; Su, et al., 2001; Weyland, et al., 2012; Serhan, 2014; Roke, 2017; Drouin, et al., 2018;).



Figure 25. (4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoic acid, DHA  $22:6 \Delta^{4,7,10,13,16,19} \omega$ -3 and n-3

#### **3.Essential Omega-6 And Omega-3 Balance**

Today, the use of vegetable oils rich in oleic (OA, omega-9) acid has increased due to nutrition. This has led to a decrease in the intake of omega-3 and an increase in heart diseases. In addition, the metabolisation of α-ALA, the main compound of omega-3 fatty acids and LA, the main compound of omega-6 fatty acids, which are essential fatty acids for humans, occurs with the same liver enzymes. The fact that omega fatty acids affect each other's reactions makes their consumption amounts different from each other and creates a competitive environment. This competition shows us that a balanced intake of essential fatty acids is vitally important. While anti-inflammatory agents such as (EPA) and (DHA) are formed as a result of ALA metabolism, bioactive compounds such as the precursor of eicosanoids (AA) are formed through GLA and DGLA via LA metabolism. However, the synthetic route for EPA and DHA production from  $\alpha$ -LA is not efficient. The conversion rate of ALA to EPA in the body is 8%, while the conversion rate to DHA is 1%. For adequate EPA and DHA, we need to obtain them from external dietary sources, especially from fish. The recommended daily intake of ALA is 1 g and the recommended daily intake of DHA and EPA is 250 mg each. While ALA is plant-derived omega-3, DHA and EPA type omega-3 fatty acids can be obtained from animal-derived foods. However, studies have shown that omega-6 fatty acids, whose dietary intake is increasing today, increase the production of AA and its metabolites in our body. In addition, the development of many diseases has accelerated (Sanchez-Muniz, J & C, Cuesta 2003; Roke, 2017; Mathieu-Resuge, et al., 2023). The recommended  $\omega$ -6 /  $\omega$ -3 ratio in the body is not less than 4: 1. Studies have shown that when the ratio between  $\omega$ -6 and  $\omega$ -3 essential fatty acids is at the

desired level, it has been determined that it has a healthier mind structure and brain functions work more regularly. It has been emphasised that  $\omega$ -3 supplementation can help in the treatment of depression and Alzheimer's. However, the subject is very broad and has not yet been sufficiently researched(Roke, 2017; Salar, et al., 2021; Veronique J. Barthet. 2008; Elbossaty, et al., 2018; Catalá, 2013; Mathieu-Resuge, et al., 2023; Stachowicz, 2023).



Figure 26. Metabolism of omega-3 and omega-6 PUFA synthesis from dietary LA

and A

### 4. Conclusion

In line with the increasingly important studies on omega fatty acids, we learn about the sources, chemical structure, function and use of omega fatty acids. Humans obtain omega fatty acids mostly from fish and to a lesser extent from cereals and plant products. It is very important to discover omega compounds and their derivatives, which have an important place in today's pharmaceutical industry. It is hoped that this study will encourage scientists to conduct further research that will eliminate this and many other doubts. In conclusion, fats and their main component fatty acids, which are one of the main food sources of human beings, are inadequately taken due to unhealthy and unbalanced nutrition. In addition, health problems such as heart disease, diabetes, alzheimer's, personality disorders, and stagnation in the development of intelligence arise due to the negative conditions brought about by technological developments. It is hoped that this compilation will contribute to further research by scientists.

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#### ATOMIC STRUCTURE AND THE PERIODIC TABLE

#### Tatheer FATIMA

#### Introduction

At the core of atomic structure and the periodic table importance lies the fundamental concept that all matter, regardless of its location or application, have atoms—the building blocks of the universe. These atoms, with their unique atomic structures and properties, collectively govern the behavior and interactions of matter on a global scale. Understanding the importance of atomic structure and the periodic table in comprehending the behavior of matter on a global scale is crucial for appreciating their significance in science, technology, and numerous aspects of our interconnected world (Stevens *et al.*, 2009). Atomic structure, as defined by the arrangement of protons, neutrons, and electrons within atoms, is the basis of chemistry. It provides insights into different ways of elements association to form compounds. These compounds, in turn, are essential in various industrial processes, from manufacturing to pharmaceuticals, influencing global economies and trade(Goodman et al., 2005).

The periodic table, with its systematic organization of elements, permits scientists to predict the chemical characteristics of elements, their reactivity, and their potential applications (Duffus, 2002). This predictive power is invaluable in designing new materials, developing sustainable technologies, and solving global challenges. The periodic table and atomic structure are universal concepts that transcend borders and languages. Scientists and researchers from around the world use this common framework to communicate their findings and collaborate on global issues (Ellemers, 2021). Whether it's addressing environmental concerns, advancing energy solutions, or researching new medical treatments, a shared considerate of atomic structure and the periodic table fosters international cooperation. Nuclear energy, both for electricity generation and medical applications, relies on a profound understanding of atomic structure and isotopes. In the quest for sustainable energy sources, atomic structure plays a pivotal role in the progress of nuclear fusion technologies to develop global energy production (Mathew, 2022).

Atomic structure informs our understanding of how pollutants interact with the environment, influencing climate change, water quality, and air pollution. This knowledge is vital for mitigating the global challenges posed by environmental degradation. Atomic structure is integral to the field of medical imaging, where techniques like MRI and PET scans rely on the behavior of atomic nuclei (Pellico et al., 2021). Additionally, the periodic table is indispensable to understand the chemical properties of drugs and their interactions within the human body, contributing to global healthcare advancements. The development of new materials with tailored properties, such as superconductors or lightweight alloys for transportation, is a global endeavor driven by a deep considerate of atomic structure and periodic trends (Kumar & Dixit, 2019). In essence, atomic structure and the periodic table serve as the universal language of science, fostering global collaboration and enabling innovations that touch every aspect of modern life. As our world becomes increasingly interconnected and reliant on scientific advancements, a grasp of these foundational concepts becomes ever more vital in addressing global challenges and driving progress on a global scale (Veers et al., 2019).

### **Historical Development**

The historical evolution of atomic models is a fascinating journey that spans centuries and encompasses contributions from scientists around the world (Swimme & Tucker, 2011). Here, we will explore this progression, highlighting key developments and emphasizing the global nature of scientific progress. Ancient Ideas (Pre-5th Century BCE): In ancient civilizations such as Greece and India, philosophers contemplated the nature of matter. Thinkers like Democritus anticipated that all matter have very tiny undividable units called "atomos," laying the groundwork for the concept of atoms. Ancient Chinese and Indian scholars also discussed the nature of the physical world and the existence of fundamental particles in their philosophical texts. Alchemical and Medieval Views (5th - 17th Century CE): During the Middle Ages, alchemists in various parts of the world required to transform base metals into noble ones and discover the new one (Campion, 2022). While their practices were often mystical, they contributed to early chemical knowledge and experimentation. Early Modern Insights (17th - 18th Century CE): In Europe, figures like Robert Boyle and John Dalton made significant contributions. Boyle's experiments with gases led to Boyle's law, which contributed to the understanding of gas behavior. Dalton's atomic

theory dipcted that matter composed of indivisible atoms, each have a unique mass (Chalmers, 2005).

Dalton's Atomic Theory (Early 19th Century): John Dalton's atomic theory, published in 1808, laid the foundation for modern atomic models. It postulated that elements consist of atoms, and compounds result from the combination of atoms in simple whole-number ratios (Constable, 2022). Thomson's Discovery of the Electron (Late 19th Century):British scientist J.J. Thomson's experiments with cathode rays in the late 19th century led to the discovery of the electron. This subatomic particle's existence challenged the idea of indivisible atoms. Rutherford's Nuclear Model (Early 20th Century): Ernest Rutherford, a New Zealand-born physicist working in the UK, conducted the famous gold foil experiment in 1909 (Bickerton et al.). His findings led to the proposal of the nuclear model of the atom, with a small, positively charged nucleus at its center. Bohr's Atomic Model (Early 20th Century):Danish physicist Niels Bohr expanded upon Rutherford's model, introducing the idea of quantized energy levels or electron shells. This model explained atomic spectra and was a crucial step in understanding atomic structure (Schwarz, 2013).

Quantum Mechanics (Early to Mid-20th Century): The development of quantum mechanics, involving scientists from various countries (including Werner Heisenberg, Erwin Schrödinger, and Max Planck), revolutionized our understanding of atomic and subatomic behavior (Nilesh et al., 2015). It introduced the concept of electron orbitals and probability-based descriptions of electron locations. Modern Quantum Mechanical Model (Mid-20th Century to Present): The modern quantum mechanical model of the atom, a culmination of global contributions, describes electrons as existing in three-dimensional probability distributions called orbitals. This model is the foundation of our current understanding of atomic structure (Mittemeijer, 2010). Throughout this historical journey, scientists from diverse backgrounds and locations played pivotal roles in advancing our understanding of atomic structure. The progression of ideas and experimental discoveries in atomic theory has been a truly global effort, demonstrating the collaborative nature of scientific progress and its profound impact on our world (Guo et al., 2016).

## **Modern Atomic Theory**

The current quantum mechanical atomic model, often referred to as the wavemechanical or the electron cloud model, represents a fundamental shift in our understanding of atomic structure. It unifies our understanding of atomic behavior and has had a profound impact on international research. The quantum mechanical atomic model is based on a branch of physics quantum mechanics which was developed in the early 20th century (Cresser, 2011). This model provides a comprehensive and accurate explanation of electrons within atoms. Here are its key features, In the quantum model, electrons do not revolve around the nucleus in specific pathways like solar system as suggested by the earlier Bohr model. Instead, electrons exist in quantized energy levels or electron shells around the nucleus. Within each energy level, electrons are described by probability distributions known as orbitals. Orbitals are defined as areas where electron are present with a high probability (Bliokh et al., 2017).

Quantum mechanics introduces Heisenberg's Uncertainty Principle, which states that it is not possible to instantaneously know the precise location and motion of an electron. This principle emphasizes the probabilistic nature of electron behavior. Electrons are described as both particles and waves. This wave-particle duality explains phenomena like electron diffraction and the quantization of energy levels. The development of the quantum mechanical model involved contributions from scientists around the world (Zaccaria et al., 2022). This model was not the work of a single individual or a single nation but the result of a collaborative international effort. Key contributors and their countries of origin include: Heisenberg formulated the matrix mechanics, a mathematical framework for quantum mechanics. Schrödinger developed wave mechanics, another mathematical approach to quantum mechanics. His Schrödinger equation describes the behavior of quantum systems (Khater et al., 2023). Planck's work on the quantization of energy, which he introduced in 1900, laid the foundation for quantum mechanics. De Broglie proposed the wave-particle duality of matter, suggesting that particles like electrons have both wave and particle characteristics. Although Bohr's atomic model was an intermediate step, it contributed to the understanding of quantized energy levels in atoms. Dirac's work on quantum field theory and the Dirac equation extended the scope of quantum mechanics. The collaborative efforts of these and many other scientists from various countries led to the formulation of a unified quantum mechanical model that could explain the behavior of atoms and subatomic particles with unprecedented precision (Shoup, 2018).

The quantum mechanical model revolutionized international research in several ways, Briefly the quantum mechanical model of the atom represents a monumental achievement in scientific collaboration. Its development involved scientists from diverse countries, and its impact extends to a wide range of international research fields, from fundamental physics to practical applications that shape our modern world. This model exemplifies the global nature of scientific progress and its potential to transform our understanding of the universe and improve our quality of life (Azarian, 2011).

### **Elements and Isotopes**

Significance of Atomic Number and Mass Number in Defining Elements and Isotopes: Elements are the fundamental building blocks of matter, and they are characterized by their unique chemical properties. Atomic number and mass number are two crucial concepts that play a significant role in defining elements and isotopes (Wray, 2018).

Atomic Number (Z): The atomic number of an element, symbolized as "Z," is an important property that discriminates one element from another. It represents the proton number in the nucleus of an atom. Since the protons in an atom is unique to each element, the atomic number is a key identifier. For example, hydrogen (H) has one proton thus its atomic no. is 1, while helium (He) has two protons in its nucleus thus possess 2 atomic number. The number of protons in nucleus specifies an element's chemical characteristics and its place on the periodic table (Greenwood & Earnshaw, 2012).

Mass Number (A): The mass number, denoted as "A," represents the total number of protons and electrons in an atomic nucleus. It is used to distinguish various isotopes of the same element. Isotopes are atoms having the same number of protons but a different number of neutrons. This variance in the number of neutrons results in isotopes with dissimilar mass numbers and, subsequently, different atomic masses. For instance, carbon has three isotopes: carbon-12, carbon-13, and carbon-14. These isotopes have the same number of protons but diverse mass numbers resulting in slightly different atomic masses (Baker, 2012).

**Significance:** The atomic number is the primary factor that identifies an element. For example, any atom with six protons is always carbon, regardless of its mass number.

This identification is crucial in chemistry and physics. The mass number distinguishes isotopes of the same element. Isotopes often have distinct physical properties, making them useful in various fields, such as radiocarbon dating using 14C isotopes (Atkins, 2010). Elements with the same atomic number exhibit similar chemical properties because the number of protons, which determines the element's chemical behavior, remains constant within an element. (Stacey, 2018).

### **Global Diversity of Elements and Isotopes in Various Industries**

Elements and isotopes have diverse applications across a wide range of industries worldwide due to their unique properties and versatility. Isotopes like uranium-235 (235U) and plutonium-239 (239Pu) are used as fuel in nuclear reactors to generate electricity. Elements like silicon are crucial in the production of solar panels, a key component of solar energy systems. Radioactive isotopes, such as technetium-99m (99mTc), are used in medical imaging techniques (Blake et al., 2003). Isotopes like cobalt-60 (60Co) and iodine-131 (131I) are used in radiation therapy to treat cancer. Stable isotopes like oxygen-18 (18O) and carbon-13 (13C) are used to trace the movement of pollutants in the environment, study climate change, and analyze groundwater flow. Elements like iron (Fe), aluminum (Al), and titanium (Ti) are essential in the manufacturing of alloys with specific properties. Elements like hydrogen (H) and oxygen (O) are used as propellants in rocket engines for space exploration (Pradhan et al., 2020).

Elements like nitrogen, phosphorus, and potassium are essential components of fertilizers used to enhance crop growth. Elements like silicon (Si) and gallium (Ga) are used in the production of semiconductors for electronic devices. Isotopes like deuterium (2H) are used in neutron-based detective systems. Isotopes like strontium-90 (90Sr) and cesium-137 (137Cs) can be used in radiological weapons (Holden et al., 2018). In conclusion, atomic number and mass number are fundamental in defining elements and isotopes, with each element having a unique atomic number and isotopes of the same element differing in mass number. The global diversity of elements and isotopes is harnessed across various industries, from energy production to healthcare, environmental monitoring, materials science, and beyond, highlighting their indispensable role in modern society (Kothari et al., 2021).

### **Understanding Electron Shells, Orbitals, and Electron Configurations**

Electron shells, are areas around the nucleus of an atom where electrons are found they also known as energy levels. These shells are labeled with numbers (n = 1, 2, 3, etc.) and are organized in order of increasing energy, with the innermost shell (n = 1) being the lowermost in energy. Each shell contain a specific number of electrons based on the  $2n^2$  formulation, in this formula 'n' represents the number of shells . For instance: First shell hold only 2 electrons(n=1), second shell has 8 electrons (n=2) and third shell possess 18 electrons(n=3) and so on (Kouwenhoven et al., 2001). Within each shell, electrons are further distributed into subshells, or orbitals. Orbitals are regions within a shell where electrons have the highest probability of being found. There are four types of orbitals: s, p, d, and f, each with an exceptional shape and orientation. The subshell contain 2, 6, 10 and 14 electrons respectively (Callister Jr & Rethwisch, 2020).

**Electron Configurations**: Electron configuration is a distribution of electrons in shells and orbitals of the atom. It is written using a notation such as the shell number (n), the subshell (s, p, d, f) and the electrons number in them (Kharub et al., 2010).

#### **Role of Electron Configuration in Chemical Reactions and Global Applications**

Electron configuration plays a fundamental role in chemical reactions. It determines the chemical properties of an element and how it will interact with other elements to form compounds. The outermost shell's electron configuration determines the number of valence electrons, which are involved in chemical bonding. Elements with similar valence electron configurations tend to exhibit similar chemical behavior (Clark, 2009). Elements with incomplete valence electron shells tend to form chemical bonds to achieve a stable electron configuration. For example, sodium (Na) has one valence electron (1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>6</sup> 3s<sup>1</sup>), and chlorine (Cl) has seven valence electrons (1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>6</sup> 3s<sup>2</sup> 3p<sup>5</sup>). Sodium donates its electron to chlorine, forming the ionic compound sodium chloride (NaCl). Electron configurations are used to construct Lewis structures, which help visualize how electrons are shared or transferred in molecules and predict molecular geometries (Gryn'ova et al., 2015).

Global Applications: Electron configurations are crucial in understanding and engineering materials with specific electronic properties. For example, the development of semiconductor materials relies on precise control of electron configurations for electronic devices (Pishtshev & Karazhanov, 2017). Catalysts in various industrial processes are designed based on the electronic configurations of the elements involved. Understanding electron configurations helps optimize catalysts for efficient chemical reactions. Electron configurations play a role in understanding chemical reactions in the environment, such as the transformation of pollutants or the behavior of elements in natural systems. Electron configurations are essential in drug discovery, as they influence how drugs interact with target molecules in the body. Electron configurations are crucial in the design of materials for energy storage (e.g., batteries) and energy conversion (e.g., photovoltaic cells) (Lv et al., 2022). Briefly, electron shells, orbitals, and electron configurations provide a framework for understanding how electrons are distributed in atoms and how this distribution influences chemical reactions. This knowledge is essential in various global applications, ranging from materials science and catalysis to environmental chemistry and pharmaceuticals, impacting industries and technologies that shape our modern world (Bratovcic, 2019).

# **Organization of the Periodic Table**

The periodic table is a fundamental tool in chemistry, providing a systematic and visual representation of the diversity of chemical elements. The key elements of its organization include periods, groups, and block notations (Malerba, 2005).

Periods(Horizontal Rows): Seven horizontal rows of the periodic table called periods (numbered 1 to 7). Each period shows different shells where electrons of the elements are arranged. All the elements in the period arranged on the basis of increasing atomic number and elements reside in the same energy level shows similar electronic confuguation. (Lee).

Groups(Vertical Columns): 18 vertical columns in the periodic table called groups or families (numbered 1 to 18). Elements in a roup have the same number of valence electrons, thus they possess similar chemical properties. These properties are responsible for reactivity and bonding behavior of the elemts. Some groups have specific names, such as the alkali metals (Group 1), alkaline earth metals (Group 2), halogens (Group 17), and noble gases (Group 18) (Fromm, 2020).

Block Notations: Groups 1 and 2, including helium (He), are part of the s-block. These elements have their outermost electrons in s-orbitals. Groups 13 to 18 are part of the

p-block. These elements have their outermost electrons in p-orbitals. Groups 3 to 12 are part of the d-block. These elements have their outermost electrons in d-orbitals and are often referred to as transition metals. The two rows at the bottom of the periodic table (lanthanides and actinides) are part of the f-block. These elements have their outermost electrons in f-orbitals and are often called inner transition metals (Das et al., 2023).

### The Periodic Table's Role in Classification and International Communication

The periodic table serves as a comprehensive reference for identifying and categorizing elements based on their atomic number and properties. This aids in the systematic study of elements and compounds. The periodic table reveals trends and patterns in element properties. For example, elements in the same group often exhibit similar reactivity, and elements in the same period display gradual changes in properties across the row. It allows scientists to predict the behavior of elements and compounds based on their positions in the table(Schwerdtfeger et al., 2020). For instance, knowing that oxygen is in Group 16 helps predict that sulfur, selenium, and tellurium (also in Group 16) will exhibit similar chemical behavior.

The periodic table provides a universal and standardized system for naming and organizing elements. This common language ensures that scientists, researchers, and industry professionals worldwide can communicate effectively without language barriers. It facilitates collaborative research and development across borders (Tomczewska-Popowycz & Taras, 2022). Scientists from different countries can work together seamlessly because they share a common framework for discussing elements and compounds. The periodic table is indispensable in the chemical industry for product development, quality control, and research. It enables the identification of raw materials, development of new compounds, and optimization of chemical processes on a global scale. The periodic table is a fundamental teaching tool in chemistry education (Sutrisno et al., 2020). It simplifies the learning process and enables students to grasp the relationships between elements and their properties. The periodic table is a globally recognized framework for organizing and classifying chemical elements based on their atomic properties. It plays a pivotal role in advancing science and industry by fostering international collaboration, aiding in element identification, and providing a standardized language for chemical communication. Its systematic structure has become a cornerstone of chemistry, enabling the understanding and manipulation of the diverse elements that make up our world (Jenkinson et al., 2022).

### Periodic Trends in Atomic Size, Ionization Energy, and Electronegativity

Atomic radius usually decreases in periods from left to right in periods and increases in group from top to bottom. Main reason of this trend is considered as, number of electronic shell increases in groups but in periods from left to right nuclear charge is increased. But in groups eclectron shells are also added thus size of atom increases(Mosher & Kelter, 2023). In general, ionization energy drops from top to bottom within a group and rises from left to right over time. Since this trend measures the energy needed to extract an electron from an atom, it is the opposite of atomic size. Higher ionization energy results from a decrease in atomic size and an increase in nuclear charge, which holds electrons more tightly and makes it harder to remove them. Ionization energy reduces as one moves down a group because atomic size grows and electrons are removed from the nucleus with less energy. (Schwarz et al., 2022). In general, electronegativity falls from top to bottom within a group and rises from left to right throughout a period. Energy require to remove an electron called electronegativity. Atoms become more electronegative as a result of an increased attraction for electrons brought on by an increase in nuclear charge during a time. Conversely, going down a group results in an increase in atomic size and energy levels, which lowers electronegativity since the outermost electrons are further away from the nucleus. (Viswanathan & Gulam Razul, 2023).

**Significance of the Atomic trends:** Smaller atoms in a period tend to form stronger and more compact bonds in chemical compounds. For example, the small size of carbon (C) allows it to form strong covalent bonds in organic molecules, making carbon-based compounds the basis of life and the chemical industry worldwide. Elements with high ionization energies, such as helium (He), are used in various applications, including cryogenics and cooling systems. Helium's low reactivity and high ionization energy make it ideal for supercooling applications, such as MRI machines and scientific research (Zhang et al., 2022). Electronegativity influences chemical reactions and bonding. For instance, the high electronegativity of oxygen (O) makes it an essential element in combustion reactions, as it attracts electrons and supports the burning of fuels in various industrial processes, including power generation and transportation. In biochemistry, electronegativity plays a role in the properties of biomolecules. The electronegativity of oxygen and nitrogen in amino acids influences the structure and function of proteins, enzymes, and DNA, affecting life processes globally (Yadav & Yadav, 2021). Catalysis in industrial processes often involves transition metals with varying electronegativities. For instance, platinum (Pt) and palladium (Pd) are used as catalysts in automotive catalytic converters, where their electronegativities influence the chemical reactions that reduce harmful emissions. Periodic trends in atomic size, ionization energy, and electronegativity have significant global implications in chemistry, industry, and daily life (Börner & Zeidler, 2023). These trends influence chemical behavior, reactivity, and the choice of materials in various industrial applications, from energy production to healthcare and environmental protection. Understanding these trends is crucial for optimizing processes, materials, and technologies on an international scale (Dixit et al., 2023).

### **Classification of Elements into Metals, Nonmetals, and Metalloids**

Elements are categorized into three primary groups based on their properties: metals, nonmetals, and metalloids. This classification is crucial in understanding the diverse behavior and applications of elements (Li et al., 2021). Metals are characterized by their luster, malleability, ductility, and excellent conductivity of heat and electricity. They are typically found on the left side and the middle of the periodic table, encompassing a majority of the elements. Some key properties of metals include: Metals often have a shiny appearance due to their ability to reflect light. They can be hammered into thin sheets without breaking. They can be drawn into wires without breaking. Metals allow to pass heat and electricity. They can easily lose electrons to form positively charged ions (cations) when they undergo chemical reactions (Chang et al., 2022). Common examples of metals include copper (Cu), iron (Fe), aluminum (Al), and gold (Au).

On the right side of the periodic table nonmetals are present, including elements like hydrogen, oxygen, nitrogen, and carbon. Nonmetals possess properties that are generally the opposite of metals: Nonmetals often lack luster and have a dull appearance. They are typically not malleable or ductile and tend to be brittle. Nonmetals are poor conductors of heat and electricity. Nonmetals tend to gain electrons to form negatively charged ions (anions) in chemical reactions (Maret & Blower, 2022).

Metalloids (Semimetals) are elements that exhibit properties intermediate between metals and nonmetals. They are typically found along the "staircase" line on the periodic table, including elements such as silicon (Si), germanium (Ge), and arsenic (As). Key characteristics of metalloids include: Metalloids can have properties of both good conductors and poor conductors of electricity, depending on their form and conditions. They may have a shiny or dull appearance. Metalloids can exhibit variable reactivity in chemical reactions (Medina-Cruz et al., 2020). Some metalloids, like silicon and germanium, are essential components in semiconductor devices used in electronics. the classification of elements into metals, nonmetals, and metalloids is a fundamental concept in chemistry with global significance. These categories influence the properties, behavior, and applications of elements in various fields, including industry, technology, energy production, and healthcare. Understanding these distinctions is essential for the development of materials and technologies that drive global progress and innovation (Halka & Nordstrom, 2019).

### **Unique Properties of Transition Metals**

Transition metals are elements found in groups 3 to 12 (or the d-block) of the periodic table. They exhibit several unique properties that distinguish them from other elements. Transition metals can exist in multiple oxidation states or charges, which makes them versatile in forming a wide range of compounds. For example, iron (Fe) can exist as Fe<sup>2+</sup> or Fe<sup>3+</sup> in various compounds. Transition metals have a strong tendency to form coordination compounds or complexes with ligands (molecules or ions) due to their ability to accept and share electrons. This is exploited in fields like catalysis and analytical chemistry (Liu et al., 2021). Many transition metal compounds are colorful due to the presence of unpaired electrons in their d-orbitals. These colors are exploited in pigments, dyes, and art. Transition metals are excellent catalysts, facilitating chemical reactions without undergoing permanent changes themselves. They play a vital role in industrial processes, such as the Haber-Bosch process for ammonia synthesis and catalytic converters in automobiles (Lah, 2021).

Inner transition metals consist of two series of elements, the lanthanides (from lanthanum to lutetium) and the actinides (from actinium to lawrencium). These elements have some unique characteristics. Inner transition metals fill their f-orbitals, leading to the distinctive electron configurations. For example, cerium (Ce) has the electron configuration [Xe]  $4f^2$   $5d^1$   $6s^2$ , which differs from the typical d-block

elements(Panda et al., 2023). Most actinides are radioactive, with unstable nuclei that undergo radioactive decay. This property has applications in nuclear power generation, medical imaging, and nuclear weapons. Uranium-235 (235U) and plutonium-239 (239Pu), both actinides, are essential in nuclear fission reactions, which are the basis for nuclear power plants and nuclear weapons (UZUN, 2022). The lanthanides are often referred to as rare earth elements because they are relatively abundant in the Earth's crust but were historically challenging to separate. They are essential in various technologies, including magnets, phosphors for screens, and catalysts. Transition metals and inner transition metals possess unique properties and have significant international contributions and applications across various industries, including catalysis, electronics, energy, medicine, and environmental remediation. These elements play a critical role in advancing science, technology, and global development (Gao et al., 2019).

The Inert Nature and Global Applications of Noble Gases Noble gases are a group of chemical elements located in Group 18 of the periodic table, also known as the noble gas group or the inert gases group. They include helium (He), neon (Ne), argon (Ar), krypton (Kr), xenon (Xe), and radon (Rn). These elements are characterized by their remarkable inertness, which arises from their stable electron configurations. This inert nature gives rise to a wide range of global applications in diverse fields (Schwarz et al., 2022). The inertness of noble gases can be attributed to their full outer electron shells. Specifically, they all have a stable configuration of valence electrons, making them chemically unreactive under normal conditions. This means they do not readily form compounds with other elements through chemical bonding, unlike most other elements (Winkler et al., 2016). Noble gases have various applications in (Zohuri & Zohuri, 2018)imaging, and more (Ballentine & Barry, 2017).

**Global Applications of Noble Gases:** Noble gases, particularly neon and argon, are widely used in lighting applications. When an electrical current is passed through a sealed tube containing these gases, they emit colorful and bright light. Neon lights, fluorescent lamps, and neon signs are common examples. The striking colors produced by noble gas discharges have made them essential in advertising and decorative lighting worldwide (Pareek et al., 2017). Helium and argon are critical in cryogenic applications, where extremely low temperatures are required. Helium is known for its use in cooling superconducting magnets in medical MRI machines and particle accelerators(Minervini et al., 2018). Argon is used in the cryogenic
preservation of biological samples and for cooling space telescopes. Argon is used as a shielding gas in welding processes to protect the weld area from atmospheric contamination, ensuring high-quality welds. It is also used in metal processing and manufacturing to create controlled atmospheres (Zohuri & Zohuri, 2018). Xenon-133, a radioactive isotope of xenon, is used in nuclear medicine for lung ventilation studies. It is inhaled by patients to allow imaging of lung ventilation and blood flow. Helium is utilized as a carrier gas in gas chromatography, a widely used analytical technique in chemistry and industry. Its low density and inert nature make it ideal for separating and analyzing chemical compounds. Helium is used to fill balloons, airships, and blimps because of its low density and non-flammable properties. It provides buoyancy for these aerial vehicles. A mixture of helium and oxygen, known as heliox, is used in deep-sea diving to reduce the risk of decompression sickness. Noble gases are used in radiation detectors due to their ability to produce flashes of light (scintillation) when ionized by radiation. Xenon is employed in xenon arc lamps used as intense light sources for photography and spectroscopy (Harris & Barnes, 2008). Argon is used as propellant in ion thrusters for spacecraft propulsion in deep space missions. Its inertness and high specific impulse make it advantageous for this purpose. The inert nature of noble gases, characterized by their stable electron configurations, has led to their widespread applications in various global industries and fields. From lighting to cryogenics, these elements play essential roles in advancing technology, scientific research, and everyday life. Their unique properties continue to drive innovation and improve the quality of life on a global scale (Germain et al., 2020).

#### Summary

The chapter has explored the fundamental concepts of atomic structure and the periodic table, highlighting their global significance in the field of chemistry. Key takeaways from this chapter include, atomic structure, including electron configuration, valence electrons, electronegativity, ionization energy, and atomic size, fundamentally influences the chemical behavior of elements. Periodic trends across the periodic table provide insights into how elements interact and form compounds. These principles of atomic structure and periodic trends have diverse global applications. From materials science and pharmaceuticals to environmental chemistry and clean energy technologies, the understanding of chemical behavior at the atomic level drives innovation, economic development, and improved quality of life

worldwide. The future of international scientific collaboration and innovation in the field of atomic structure and the periodic table holds great promise. As our understanding of atomic properties grows, we can expect the development of even more advanced materials with tailored properties. These materials will have applications in industries ranging from electronics and aerospace to healthcare and environmental technology. In conclusion, atomic structure and the periodic table are not merely abstract concepts; they are the foundation of modern chemistry and have a profound impact on our world. By fostering international collaboration and embracing emerging technologies, the global scientific community will continue to drive innovation, tackle global challenges, and shape the future of chemistry for the betterment of humanity. The future holds exciting opportunities for advancements that will benefit societies across the globe.

#### **Scientific Ethics Declaration**

The authors say that they are responsible for the scientific, moral, and legal aspects of this chapter, which is published in *Chemistry for the Life*.

#### **Conflict of Interest**

The authors declare no conflict of interest.

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#### SOLID, LIQUID AND GASES AND THEIR ROLE IN THE CHEMISTRY

#### Zobia ARIF

#### Introduction

Matter exists in four states that is solid, liquid and plasma, each of them have distinctive properties and behaviors. This chapter, aptly titled as "solid, liquid and gases", refers to the most fundamental and common states of matter that are present in our surrounding in our daily life. This chapter mainly refers to all the distinctive features properties of solids, liquid and gases along with their classification. It also explains the phase changes and heat changes involve in such inter conversions. We will discuss about the microscopic and macroscopic aspects of all the states of matter that ranges from motion, compressibility, density, kinetic energy, different phenomenon, laws that explains the relationship between different factors, response to change in temperature, pressure and other related factors. This chapter also explains the importance of these states of matter in our daily life as in cooking, washing, paints and dyes, DNA, RNA, proteins, lipids and other biological molecule's structures. In this chapter we will also discuss about the theories that explain the nature of bond and also their physical and chemical properties. This chapter also emphasizes about the graphical explanation of different laws that explains the relationship between common factors. Classification of each matter is also explained along with examples that are done on the different basis. Some other fundamental phenomenon are also discussed which have primary importance in daily life like boiling point, melting point, equilibrium, vapor pressure and evaporation etc.

#### 1. Solid:

Solid is a state of matter that has specific shape, particular volume, hard, strong attractive forces, negligible intermolecular distance, low compressibility and closely packed structure. Well order arrangement in case of solids is attained due to presence of cohesive force and adhesive forces.

#### **1.1 Classification of solid:**

Solids can be classified on the basis of different factors like:

- Arrangement of particles
- Nature of bond

#### **1.1.1 On the basis of arrangement of particles:**

Solids can be classified on the basis of arrangement or symmetry of particles i.e. atoms, ions or molecules.

### 1) Crystalline solid:

Those solids in which the atoms, ions or molecules are arranged in a definite manner and particles are arranged three dimensionally i.e. along x, y and z- axis. These solids have definite symmetry, regular arrangement and specific three dimensional regular geometric patterns. Crystalline solids have a sharp melting point and boiling point. These solids possess definite heat of fusion. For example, sugar, NaCl etc (Vippagunta et al., 2001).

## 2) Amorphous solid:

As the name indicates 'amorphous' meaning 'shapeless' indicates that these solids don't have any particular three dimensional arrangement of atoms, ions and molecules. These solids don't have any definite symmetry, no regular arrangement and no specific three dimensional regular geometric patterns. Amorphous solids don't have sharp melting point and boiling point. These solids don't possess definite heat of fusion. For example, rubber, glass etc (Baghel et al., 2016).

These solids have all the properties of solids except an ordered crystalline state. Many crystalline solids can be converted into amorphous solids by heating and then cooling the molten mass very rapidly and in this way molecules don't get time to arrange themselves, that's why, this conversion takes place.

Amorphous solids don't consist of long range of regularity but it contains small regions along the crystals where molecules, atoms or ions are well arranged and resembles to crystalline solids as of their regular arrangement and particular symmetry and such regions along the amorphous solids are called **crystallites**.

## **1.1.2 Properties of crystalline solids:**

## 1. Geometrical shape:

As the crystalline solids have definite order and arrangement of molecules, atoms or ions along three dimensional spaces that's why have definite and distinctive geometry. Crystalline solids have specific vertices (corners), axes (x, y, z), interfacial angles, faces (plane parallel surface) and edges (point where two faces match) that remain characteristic even when the solid is ground to fine powder (Vaida et al., 1988).

## 2. Melting point:

All the crystalline solids have characteristic sharp melting point because of order and symmetry and proper arrangement of components of solids and this is considered to be the identification sign for crystalline solids.

## 3. Symmetry:

When the crystalline solid is rotated along axes in 360 degree angle and faces, edges and angles undergo repetition then this is called symmetry. There are various types of symmetry like plane of symmetry, center of symmetry and axis of symmetry etc.

## 4. Habit of crystal:

The shape in which any crystal grows is called habit of crystal. When the liquid substance is condensed then thus saturated solution can be converted into solid. Solid

can be grown in different directions. If we want to grow crystal in same shape then condition in which the crystal is grown remain same and if we want to change the shape of crystal then conditions are varied. For example, if 10% urea as impurity is present in solution then needle shape crystals of sodium chloride are obtained instead of cubic crystals.

### 5. Anisotropy:

A process in which any physical property of any crystal shows variations along different directions is called anisotropy. Such properties like refractive index, thermal expansion, thermal and electrical conductivity etc that depend on direction are called 'anisotropic properties'. The orderly arrangement of molecule is different along different direction that's why some properties are anisotropic. For example, electrical conductivity of graphite is more in horizontal direction or in layers parallel to each other because arrangement of components in this direction allows electron to free easily but not perpendicular to layers due to restricted motion of electrons in this particular direction (Vaida et al., 1988).

## 6. Cleavage plane:

The crystalline solid can be broken from particular plane and such planes are called cleavage planes. As cleavage plane is an anisotropic property that varies along the direction. At a particular angle, cleavage planes are inclined to each other and this value of angle changes from one solid to other solid.

## 7. Transition temperature:

It is the temperature at which two crystalline forms of a substance or crystalline forms of any element co-exist with each other is called transition temperature. Transition temperature is always lesser than the melting point of substance or element.

For example, cubic grey tin can co-exists with tetragonal white tin at 13.2°C. Rhombic sulphur can be converted into monoclinic sulphur at 95.5°C. Orthorhomic potassium nitrate can be converted into rhombohedral potassium nitrate at 123°C.

### 8. Allotropy:

A process in which more than one crystalline form of an element co-exist is called allotropy. That element is called **'allotropic element'** and the crystalline forms of element are called **'allotropic forms'** or **'allotropes'**.

For example, carbon can exist in two allotropic forms that is diamond having cubic form and graphite having hexagonal form. Suphur also has two forms that is rhombic and monoclinic.

## 9. Isomorphism:

A process in which two different compounds exist in same or identical crystalline form is called isomorphism, the substances or compounds are called '**isomorphic compounds**' and the crystalline forms are called '**isomorph**' or '**isomorphic forms**'.

Crystalline form doesn't depend on nature or type of atom but it depends on number or ratio between atoms present in compound. These forms have different physical and chemical properties.

For example,  $NaNO_3$  and  $KNO_3$  have rhombohedral crystalline form and having atomic ratio that is 1:1:3.  $K_2SO_4$  and  $K_2CrO_4$  have same orthorhombic crystalline form

having ratio of 2:1:4. Similarly,  $CO_3^{-2}$  and  $NO_3^{-1}$  are triangular planar units having atomic ratio of 1:3 with similar charge that is -2.

#### 10. Polymorphism:

A process in which one compound can exist in more than one crystalline form is called polymorphism, the compound having different forms is called **'polymorphic compound'** and the forms are called **'polymorph'** or **'polymorphic forms'**.

Polymorphs have same chemical properties but different physical properties which is due to different physical arrangement of constituents along three dimensional space of solid.

For example, silver nitrate exists in rhombohedral and orthorhombic forms. Calcium carbonate has two crystalline forms that is trigonal and orthorhombic (Ford, 1945).

#### **1.2 Crystal lattice:**

A **crystal** is made up of components like atoms, ions or molecules. These atoms, ions or molecules are located at fixed or definite positions in three dimensional space in case of crystalline solid. Such fixed positions or sites are represented by points. Such definite points or positions in any crystal are called 'crystal lattice'. As 'array' means 'arrangement of components that may be atoms, ions or molecules along the fixed positions in three dimensional space for any crystal is called crystal lattice.'(Lifshitz & Kosevich, 1966)



#### 1.2.1 Unit cell:

"Unit cell is the smallest part of any crystal lattice that has all the features and characteristics of the complete crystal."

Unit cell is the smallest part of crystal lattice that forms the entire crystal structure on repetition along three dimensions. It is the smallest block and fundamental unit that contains all the structural properties of an entire crystal. If we want to get information about the complete crystal then we need to study unit cell as it has all the properties of complete system. Arrangement of any single unit cell actually gives us the information about the arrangement of whole crystal structure.

There are six parameters that give us the complete information about any unit cell and these parameters are called **crystallographic elements or crystallographic** 

**dimensions.** Size and shape of any crystal actually give us the information about these six quantitative aspects. These quantitative aspects or parameters are given below:

- 3 unit cell lengths
- 3 unit cell angles

Following are the three **unit cell lengths**:

- **a** is taken along x-axis.
- **b** is taken along y-axis.
- **c** is taken along z-axis.

As these unit cell lengths are also called 'unit cell axes' or 'unit cell edges'.

Following are the three **unit cell angles:** 

- $\alpha$  is present between length b and c.
- $\beta$  is present between length a and c.
- $\gamma$  is present between length a and b (Herbstein, 2000).



### 1.3 Crystal and their classification

All the types of crystals varied with respect to unit cell axes and unit cell angles along different edges. Here we are going to classify crystals on the basis of unit cell dimensions. There are seven different type of crystal system which is discussed below:

### 1.3.1 Cubic system:

In this crystal system all three unit cell axes are equal to each other as a=b=c and all these axes are perpendicular to each other that is  $\alpha = \beta = \gamma = 90^{\circ}$ .

For example, Diamond, Fe, Cu, Ag, Au, NaCl, NaBr etc.



#### **1.3.2 Orthorhombic system:**

In this crystal all three unit cell axes are not equal to each other as  $a\neq b\neq c$  and all these axes are at right angle to each other that is  $\alpha = \beta = \gamma = 90^{\circ}$ .

For example, iodine, rhombic, sulphur, barium sulphate etc.



#### **1.2.3 Tetragonal system:**

In this tetragonal system, two unit cell axes are equal to each other but third axes is either shorter or longer than other two axes as  $\mathbf{a=b\neq c}$  and three of the angles are perpendicular to each other and present at right angle to each other as  $\alpha = \beta = \gamma = 90^{\circ}$ .

For example, Sn, manganese dioxide, ammonium bromide etc.



**1.2.4 Monoclinic system:** 

In case of monoclinic system, all the unit cell lengths are not equal to each other as  $\mathbf{a}\neq\mathbf{b}\neq\mathbf{c}$  and two of the angles are of ninety degree while one of angle is either shorter or greater than ninety degree as  $\alpha = \gamma = 90^{\circ}$  and  $\beta \neq 90^{\circ}$ .

For example, borax, sulphur, sugar etc.



#### 1.4.5 Triclinic system:

In this crystal system, no unit cell length is equal and all are unequal to each other as  $a\neq b\neq c$  and all the unit cell angles are unequal to each other and no unit cell axes is at right angle to other axes as  $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$ .

For example, boric acid, potassium dichromate, copper sulphate etc.



#### 1.4.6 Hexagonal system:

In hexagonal crystal system, two of the unit cell axes are equal to each other but one of the unit cell axes is unequal as  $\mathbf{a=b\neq c}$  and two unit cell angles are equal to ninety degree but the third angle is equal to one hundred and twenty degree as  $\alpha = \beta = 90^{\circ}$  and  $\gamma = 120^{\circ}$ .

For example, graphite, zinc oxide, ice, zinc, cadmium etc.



#### 1.4.7 Rhombohedral system:

Rhombohedral system is also called trigonal system. In this crystal system, all the unit cell axes or lengths are equal to each other and all the three angles in this crystal system are equal but lie between ninety degree and one hundred and twenty degree as  $\alpha = \beta = \gamma > 90^{\circ}$  and  $< 120^{\circ}$  (Adamsky, 1958).



#### 1.5 Classification of solid on the basis of nature of bond

As in above topic, we have classified solids on the basis of shape of crystal or on the basis of unit cell dimensions but now we are going to classify solids on the basis of type of bonds present between atoms, ions or molecules present within the same compound or solid substance means 'cohesive forces'. There are four types of crystalline solid on the basis of nature or type of bond:

- covalent solid
- ➢ ionic solid
- metallic solid
- molecular solid

#### **1.5.1 Ionic solid:**

"Ionic solid is a type of crystalline solid that is made up of positive and negative ions which are connected to each other by ionic bond. These cations are connected to anions by strong electrostatic force of attraction which affects the properties of solid."

For example, sodium chloride, potassium chloride, sodium bromide, potassium bromide etc.

#### **Properties of ionic solid:**

#### 1) Physical state:

All the ionic solids exist naturally in **solid phase** instead of liquid or gas form. As these solids have well-arranged constituents i.e. ions in well-defined geometrical pattern along the whole crystal structure that's why these are crystalline solids which exist in solid form under ordinary conditions of temperature and pressure.

### 2) Hardness:

All the ionic solids have very hard structure because of symmetry and regularity along the crystal as well as the presence of strong bond i.e. ionic bond present between charged particles of ionic solid.

## 3) Melting point:

All the ionic solids have **high melting point and boiling point.** Both these factors are physical properties that depend on intermolecular forces rather than intramolecular forces. Ionic solids have ionic bond as intermolecular forces and also ionic bond as intramolecular forces so we can say that ionic solids have strong intermolecular forces i.e. ionic bond which is difficult to break so more energy is required that's why ionic solids have high melting point and boiling point.

### 4) Volatility:

Volatility is the ability of any specie to get vaporizes. Volatility is also a physical property that depends on intermolecular force which is ionic bond in ionic solids. As ionic bond is strong bond i.e. difficult to break so it's difficult to get vaporize so ionic solids have **low volatility**.

### 5) Nature:

Ionic solids don't exist in neutral independent form that's why ionic solids don't have molecular formula and don't exist in the form of molecules. So, ionic solids have formula unit mass and exists in the form of **formula unit**.

### 6) Density:

Ionic solids have **high density** because of strong intermolecular forces, greater attraction between opposite charges that result in close packing. Ionic solids occupy lesser or minimum space with negligible empty spaces due to the presence of non-directional intermolecular forces.

## 7) Radius ratio:

The structure of ionic solids depends on radius ratio of cations and anions. If two ionic solids have same radius ratio then there geometry would be same. For example, sodium chloride and cesium floride have same geometry because of same radius ratio.

### Radius ratio = radius of cation ÷ radius of anion

### 8) Electrical conductivity:

Ionic solids are poor conductor of electricity in solid state because in solid form positive and negative charges are unable to flow because of presence of stronger ionic bond between them but when these solids are converted into their respective solutions then these become good conductor of electricity due to presence of free positive and negative ions.

### 9) Brittleness:

Ionic solids are highly brittle as ionic solids have strong ionic bond but the layers can easily be separated from each other. The reason is, as opposite charges are present in alternative positions but when stress is applied to break layers, then layers slide on each other and similar charges come in front of each other due to which they repel each other. In order to minimize the repulsion between the layers, two layers get separated from each other very easily that's why we can say that ionic solids are highly brittle.



### **10) Solubility:**

Ionic solids are polar substance that's why soluble in polar solvents like water, chloroform etc according to 'like dissolves like'. But ionic solids are insoluble in benzene and other non-polar solvents because of opposite nature of ionic solids.

### 11) Rate of reaction:

Ionic solids show reactions called as 'ionic reaction' whose speed is fast. As these solids have polar, non- directional ionic bonds, which have greater attraction for any other reagent that's why rate of ionic reaction is fast.

### 12) Isomorphism and polymorphism:

Ionic solids have the ability to show the phenomenon of isomorphism and polymorphism (Salanne & Madden, 2011).

## 1.5.2 Structure of sodium chloride:

As we have already discussed that structure of any ionic crystal depends on the structure of ion and radius ratio. NaCl is a **face centered cubic** structure and consist of sodium and chloride ions. Na+ has 10 electrons while Cl<sup>-</sup> has 18 electrons. Thus Cl<sup>-</sup> is larger than sodium ion. In NaCl crystal, each Na+ ion is surrounded by six chloride ion which is present at the corners of a regular octahedron. So, the coordination number of sodium is six. Similarly, each chloride ion is surrounded by six sodium ions that are why coordination number of chloride is also six.

### Calculation of number of sodium and chloride ions per unit cell:

### Number of chloride ions:

The following figure shows that in NaCl crystal two types of chloride ions are present:

### • At the vertices:

8 chloride ions are present at the corners. Each of such chloride ion is shared by eight unit cells. So, in this way,

Share of one unit cell is = 8/8 = 1

### • At the faces:

6 chloride ions are present at the faces. Each of these is shared by 2 unit cells. So,

Share of one unit cell = 6/2 = 3



Hence, the one unit cell has 3 + 1 = 4 chloride ions.

#### Number of sodium ion:

The figure shows that in NaCl crystal two type of sodium ions are present.

• At the edges:

12 sodium ions are present along the edges, each of which is shared by four unit cells. So,

Share of one unit cell = 12/4 = 3

• At the centre:

1 sodium ion is present at the center, which is shared by only one unit cell. So, this complete sodium is the part of only one unit cell. Hence, one unit cell has 3 + 1 = 4 sodium ions.

### Total number of sodium and chloride ions:

One unit cell of NaCl has 4 sodium ions and 4 chloride ions. Thus, four sodium chloride formula units are present in one unit cell. Hence the ration of sodium and chloride is 1: 1.

#### Facts about NaCl:

- In NaCl, the distance between two similar ions is 5.63 Angstrom.
- Distance between two different ions is 5.63/2 = 2.815 Angstrom.
- In NaCl crystal, no independent NaCl molecule is present. However, NaCl molecule exists in vapor phase.
- The radius ratio of NaCl = 0.53 Angstrom (Vogt & Weiss, 2001).

#### 1.5.3 Lattice energy:

"It is the amount of energy that is released when one mole of the ionic crystal is formed from its gaseous ions is called lattice energy or enthalpy of lattice."

In this case reaction is exothermic that's why energy is assigned with a negative sign. This can also be defined as: "The amount of energy that is absorbed when one mole of gaseous ions are converted to form an ionic crystal." In this case, reaction is endothermic that's why value of energy is assigned a positive sign. Unit of lattice energy is KJ/mol (Kapustinskii, 1956).

For example:

Na<sup>+</sup>+Cl<sup>-</sup>NaCl $\Delta H$ = -787 KJ/molNaCl $\rightarrow$ Na<sup>+</sup>+Cl<sup>-</sup> $\Delta H$ = +787 KJ/mol

### **1.5.3 Covalent solids**

Covalent solids are the crystalline solids in which neutral atoms are held together by covalent bonds. These solids are also called 'atomic solids'. The atoms that form covalent solids are of different types and can also be of same type.

### Types of covalent solids:

- **Giant covalent solid:** solids in which atoms are combined together to form big molecules like macromolecules. For example, diamond, SiC etc
- Layered covalent solid: solids in which atoms are joined together to form separate layers. For example, graphite, iodine etc.

#### **Properties of covalent solids:**

Following are the properties of covalent solids:

- Covalent solids have a three dimensional network of atoms which are connected by covalent bond.
- Covalent bonds are comparatively weaker bond and also a dimensional bond that's why considerable free spaces are present in covalent solids because of their loose packing.
- Covalent solids are hard structures because of the presence of strong covalent bond.
- > They have high melting point and boiling point.
- > Covalent solids have strong covalent bond that's why these are less volatile.
- In case of covalent solids, no free ions or no free electrons are present that's why these are bad conductor of heat and electricity.

But graphite is a conductor when electrons move horizontally or parallel to layers as electrons can move parallel or linear to the plane but not vertically or perpendicularly to the plane because of restricted motion of electrons in this direction.

Covalent solids show covalent reactions and rate of covalent reaction is slow as compared to rate of ionic reactions.

- Covalent solids are soluble in non-polar solvents like benzene because of its non-polar nature but insoluble in water as its polar solvent,
- Covalent solid doesn't show the process of isomorphism and polymorphism (Ovshinsky & Adler, 1978).

### 1.5.4 Structure of diamond:

Diamond is an allotropic form of carbon in which carbon atom is tetravalent and having four strong covalent bonds. There are four valence electrons in carbon. The four un-hybrid orbital like 1s and 3p orbitals combine to give 4 sp3 hybrid orbitals.

As carbon is present in the form of tetrahedron so each carbon that has four hybrid orbitals which are directed towards each corner to give a **tetrahedron**. Many tetrahedron undergo **sp3-sp3 overlapping** with other tetrahedron to make a big or huge three dimensional structure of diamond.



As overlapping along the tetrahedron continuous and each carbon atom is connected via 4 covalent bonds and such characteristics allow diamond to exist in the form of a macromolecule as it is also known as **carbon polymer.** 

In diamond, all the bond angles are of **109.5 degree** and the bond lengths are **154pm**. Diamond has a face centered cubic structure (Robertson, 1992).

### **1.5.4 Molecular solid:**

"The solids in which atoms or molecules having polar or non-polar nature are connected through weak Vander-Waal's forces are called molecular solids."

There are two type of intermolecular forces are present in such solids i.e.

- Dipole-dipole forces
- Van der Waal's forces

For example, noble gases

### Types of molecular solid:

There are two types of molecular solids on the basis of type of intermolecular force i.e.

- **Polar molecular solid:** All solid that has positive and negative charges, polar and polar atoms are connected through dipole-dipole forces. For example, water, ice, sugar etc.
- Non-polar molecular solid: All the molecular solids that don't have polar nature or polar bond but neutral atoms or substance are connected by Van der Waal's forces. For example, iodine, suphur etc

#### **Properties of molecular solid:**

- X-ray analysis shows that molecular solids have regular arrangement of atom in a molecule.
- Weak intermolecular forces make molecular solids soft and more compressible.
- Molecular solids have low melting point and boiling point. Polar molecular solids have high melting point and boiling point as compare to non-polar molecular solids.
- These solids are more volatile because of the presence of weaker intermolecular forces.
- > These solids have low densities and have large empty spaces.
- Molecular solids are soluble in polar solvents and also in no-polar solvents as it depend on the nature of molecular solids.
- Sometimes, molecular solids are transparent to light. (Jones, 2019)

### **1.5.4 Metallic solids**

"The metallic solids are the solids in which metal atoms are connected by metallic bond." As metals consist of spherical shape atoms having larger spaces between them called '**interstices**, **crevices**, **and voids**'. These metals are arranged in either hexagonal close packing (ABAB or 1212) or cubic close packing (ABCABC or 123123).

### Theories of metallic bonding:

Following three theories explain the nature of metallic bond named as:

- Electron pool theory
- Valence bond theory
- Molecular orbital theory

Brief explanation of these above mentioned theories is given below:

#### • Electron pool theory:

This theory was presented by Loren and Drude. Electron pool theory is also called 'gas theory' as this theory suggests that all the metal atoms lose their electrons and these electrons then become free and mobile and become delocalized. These mobile electrons are not a part of any single atom rather belong to whole structure of metal. These mobile electrons form a pool or gas like structure in which electrons are dispersed in a sea of fixed positively charged nuclei which are present at definite positions. These positively charged nuclei generate a weak interaction with mobile and delocalized electrons which is called 'metallic bond'.



#### • Valence bond theory:

Valence bond theory is abbreviated as VBT which is presented by L.Pauling. According to this theory, metallic bonds are like covalent bonds but are more delocalized than covalent bonds.

### • Molecular orbital theory:

Molecular orbital theory is also abbreviated as MOT and called 'band theory'. Valence orbitals of metal atoms are combined or overlap to form delocalized orbitals that are called metallic bonds. This theory explains that, all the atomic orbitals of localized metals combine or overlap to generate equal molecular orbitals which are delocalized and spread over the whole structure of metal. Properties of metallic crystals are determined by the distance between bands of metal.

### **Properties of metallic solid:**

Following properties of metallic solid are explained on the basis of electron pool theory.

### 1) Electrical conductivity:

Metals are good conductors of electricity as these consist of free electrons which are delocalized and change position easily that's why can conduct electricity easily. As with increase in temperature, the metallic conductivity decreases because positive nuclei start oscillating and increase resistance in the flow of electron.

### 2) Thermal conductivity:

As the metallic solids are good conductors of heat because of the presence of delocalized, mobile and free electrons. As these electrons transfer heat from one part of the metal to other part, rapidly.

## 3) Metallic luster:

As the metals shine and produce a glow because of the mobile free electrons undergo excitation on gain of energy but when these electrons undergo deexcitation by the release of energy and this released energy produce luster or glow.



## 4) Malleable and ductile:

All these metals are soft in nature because of presence of delocalized metallic bond. This weak bond allows them to convert into sheets and wires (Singleton, 2001).

### 2. Liquid

Liquid is a state of matter which is least common because liquid can only exist within a specific range of temperature and pressure. Liquid has no specific shape but has specific volume, strong intermolecular forces than gases but weaker than solids, intermolecular distance of liquid is lesser than gases but more than solids and more compressible than solids but less compressible as compare to gases.

### 2.1 Type of bonds:

The nature and most of the properties of liquid depend on the **type of forces or bonds or attractive forces** which are of following two types:

- Intra molecular forces
- Inter molecular forces
  - 1) Intra molecular forces: As the word 'intra' indicates 'within the same molecule'. These are the type of forces which are present within the same molecules but among different or same kind of atoms. Such forces are stronger forces because of lesser distance between atoms and also these forces depend on electronic configuration of atom. Chemical properties and chemical composition of any liquid depend on intra molecular forces.

These forces are formed by losing electron, gaining electron or sharing electron in order to stabilize itself by following duplet rule or octet rule. Following are the main types of intra molecular forces:

- Covalent bond
- ➢ Ionic bond
- Coordinate covalent bond
- 2) Inter molecular forces: As the word 'inter' indicates 'between two molecules'. These are the type of forces which are present between two separate molecules which are either same type of molecules or different type of molecules. Such forces are weaker forces as compare to intra molecular forces because of relatively more distance among two separate molecules. These forces are simply electrostatic forces or attractive forces which are generated due to attraction between two opposite charged particles. Physical properties depend on inter molecular forces. Following are the types of inter molecular forces:
  - Dipole-dipole forces
  - Ion-dipole forces
  - Dipole-induced dipole forces
  - Instantaneous dipole-induced dipole forces
  - Hydrogen bond

As we are trying to explain the physical behavior of liquids which depends on inter molecular forces, so, we are going to explain all inter molecular forces in detail.

### **2.1.1 Dipole-dipole forces:**

'Dipole' represents any specie that has two poles or two kinds of charges i.e. positive end and negative end due to electronegativity difference. So these forces can be defined as the intermolecular forces which are present between two dipoles which may be of same type or different type.

These forces are developed when molecules of liquid on random motion came near to each other and then their opposite charges come in front of each other and this generates attraction between opposite charges of two separate molecules. These forces are strong inter molecular forces because of greater attraction between two opposite charges (Earles, 1995).

For example, intermolecular forces present between two HCl as it contains two poles, one is positive pole due to partial positive charge on hydrogen and negative charge on chloride ion.



As, intermolecular forces present in chloroform because chloroform is dipole and these forces are generated between negatively charged chloride of one chloroform and positively charged hydrogen of other chloroform.



#### **2.1.2 Ion-dipole forces:**

These are the type of electrostatic forces which are developed between ions having positive or negative charge with opposite charge of dipole. As these forces are also strong intermolecular forces due to the attraction between ion having complete charge and opposite charge present on any pole of dipole.

For example, ion-dipole forces are present between sodium ion and HCl as sodium in it is cation and partial negatively charged chloride present in HCl.



#### 2.1.3 Dipole-induced dipole forces:

These are the type of inter molecular forces in which opposite charges of two separate molecules i.e. dipole and other is induced dipole connect with each other. These forces

are relatively weaker inter molecular forces. These forces are also called 'Debye forces'.

In this case one molecule i.e 'dipole' already consist of two different charges which are partial positive and partial negative but the other molecule i.e. 'induced dipole' is any molecule which is neutral by nature but polarity is induced into it. **Induced dipole** is a neutral molecule in which nucleus is present in the center but electron density is present around the nucleus. When any dipole on random motion moves towards neutral molecule and either it's positive attract negatively charged electron density towards it that produce dipole into it or negative charge of dipole repels the electron density of neutral molecule which gets aside to minimize repulsion and as a result of it also polarity is induced into neutral molecule.



For example, water is a polar molecule having partial positive charge on hydrogen and partial negative charge on oxygen that's why it's a dipole, when put together with oxygen which is a non-polar molecule then oxygen is converted into dipole called 'induced dipole', then the forces generated between these two molecules called dipole-induced dipole forces.



#### 2.1.5 Instantaneous dipole-induced dipole forces:

These are the electrostatic forces which are generated between two separate species called 'induced dipole' and 'instantaneous dipole'. These forces are momentary forces and weakest intermolecular forces but common forces. These forces are also called 'London dispersion forces' as these are discovered by 'Fritz London'.

These forces are present in any specie which is entirely non-polar or a mixture of nonpolar species. As all the molecules are non-polar so all molecules move haphazardly and during this random motion, electron density of one molecule repel the electron density of nearby other non-polar molecules. In order to minimize this repulsion, electron density of one molecule moves aside and becomes polar at any instant is called **instantaneous dipole**. When this instantaneous dipole comes near other nonpolar and neutral molecule then also makes it polar because of repulsion of electron densities or attraction between opposite charges of instantaneous dipole and non-polar molecule is called **induced dipole (Earles, 1995)**.



#### 2.1.6 Factors affecting London forces:

Following are the major two factors that affect the London forces:

- Size of electronic cloud
- Number of atoms in a molecule

#### 1) Size of electronic cloud:

As the size of atom goes on increasing due to increase in number of electrons along with number of shells then we can say that electron density goes on increasing along with surface area or radius of atom. Number of intermolecular forces depends directly on surface area. For example, boiling point of noble gases and boiling point of halogens and other groups goes on increasing down the group even though number of intra bonds or valency remains same throughout a specific group remains same because as we move down the group in periodic table, elements arranged in such a way that size f atom goes on increasing, number of shells along with electrons increase, radius or surface area increase, polarzibility (ability of any atom to get distract its electronic cloud) increases that why number of inter molecular forces increases that's why boiling point increases and also physical state of elements changes from gas to liquid to solid along moving down the group.

#### 2) Number of atoms in a molecule:

As the number of atoms in a molecule increases this causes the increase of surface area and radius or size of molecule that's why number of inter molecular forces increases and causes to increase the melting and boiling point of any substance. For example, hexane has higher boiling point than ethane because of high carbon and hydrogen number (Buckingham & Utting, 1970).

#### 2.2 Hydrogen bonding:

"It is the type of electrostatic force which is present between electronegative elements like florine, oxygen and nitrogen of one molecule with hydrogen of another molecule. It is also a type of intermolecular force." Hydrogen bond is longer than normal covalent bond. Hydrogen bond is also stronger than dipole- dipole interaction but weaker than normal covalent bond. Its generally 20 times weaker than normal covalent bond. Hydrogen bond is a directional bond that results in the formation of long chains, rings and network of molecules.

### Hydrogen bonding in water:

As water molecule consist of electropositive element hydrogen and electronegative element like oxygen. As there are two hydrogen atoms in a molecule so it generates 2 hydrogen bonds per molecule.



Hydrogen Bonding in Water

### Hydrogen bonding in hydrogen floride:

As hydrofluoric acid consist of hydrogen and electronegative element that is florine. So, these atoms in separate molecules connect to give electrostatic hydrogen bond. As there is single hydrogen so it gives 1 hydrogen bond per molecule.



### Hydrogen bonding in ammonia:

Hydrogen bond is formed when electropositive element that is hydrogen of one molecule attracts the electronegative element that is nitrogen of other molecule. Ammonia molecule forms one hydrogen bond per molecule even though there are 3 hydrogen but due to relative lesser electronegativity of nitrogen that creates enough partial positive charge for hydrogen bonding on only a single hydrogen atom.



### **2.2.1 Applications of hydrogen bonding:**

Following are some of the main applications are given briefly:

- Due to presence of hydrogen bond, melting point and boiling point of molecules goes on increasing.
- HF is a weak acid as compared to HCl because of its stronger covalent bond.
- 3) Boiling point of hydrides of group IV-A to group-VII A is different than remaining members because of presence of hydrogen bond.
- 4) Water has highest boiling point than HF and ammonia because of formation of hydrogen bond.
- 5) Water and ethyl alcohol are highly miscible with each each other due to presence of hydrogen bond.
- 6) Hydrocarbons are insoluble in water due to different nature of solvent and substance.
- Soap and detergents show their cleansing action due to hydrogen bonding between their particles and material of stain on cloth.
- Ice floats on surface of eater because of its less dense structure and its 9% spaces increase due to creation of hydrogen bond.
- Living organisms like fishes etc grow and live inside the ice on surface due to hydrogen bond.
- 10) Structure of protein that is present in nails, hair, teeth etc due to the presence of hydrogen bond between amino acids.
- Structure of carbohydrates like glucose, sucrose, glycogen etc due to the hydrogen bond between hydrogen and electronegative elements.
- 12) Nuclotides like DNA, RNA have very stable molecular structure due to the presence of hydrogen bond.
- 13) Paints, dyes or other material attach to the other surface due to formation of hydrogen between them (Pimentel & McClellan, 1971).

### **2.3 Evaporation**

A process in which molecules of liquid get evaporated or converted to gas is called evaporation.

**Evaporation takes place at all temperatures.** Its reason, all molecules of liquid move randomly so possess different kind of kinetic energy. When molecules having high kinetic energy move towards the surface and break intermolecular forces of

liquid and escape the surface of liquid to get evaporated. This is the same reason for evaporation in general.

**Evaporation cause cooling.** Its reason, as mentioned earlier, that high kinetic energy molecules leave the surface of liquid and get evaporated. So, all the remaining molecules have low kinetic energy that's why produce cooling.

#### **Factors affecting evaporation:**

There are mainly these following factors that affect the rate of evaporation:

- surface area
- temperature
- strength of intermolecular forces
  - Surface area: As surface area increases, then there are more chances of more molecules of liquid to leave the surface and get evaporated that's why surface area has a direct relation with rate of evaporation and vice versa for lesser surface area.
  - 2) **Temperature:** as temperature decreases, then there's decrease in kinetic energy of molecules of liquid that's why less chances of less molecules to escape the surface to get evaporated that's why temperature also has the direct relation with rate of evaporation and vice versa for high temperature.
  - 3) Strength of intermolecular forces: As there are greater or stronger intermolecular forces then it refers to lesser rate of evaporation because it's difficult for more molecules to leave the surface of liquid to evaporate. So, strength of inter molecular forces has inverse relation with rate of evaporation (Borchman et al., 2009).

### 2.4 Vapor pressure:

"The pressure that is exerted by vapors on the surface of liquid when the container is closed during evaporation is called vapor pressure".

If the container is closed then the molecules of liquid having high kinetic energy leaves the surface to form vapors which is called "**evaporation**". As if vapors got stuck within the container then during random motion of vapors there are equal chances that these vapors got recaptured by liquid molecule and then this process is called "**condensation**". As these two processes are in opposite direction to each other and when the rate of evaporation becomes equal to rate of condensation then **equilibrium** is established in container.

### Factors affecting vapor pressure:

As surface area doesn't affects vapor pressure. So, following are the factors on which vapor pressure depends.

- Temperature
- Strength of intermolecular forces
  - 1) **Temperature:** As temperature of liquid increases then there are more chances for more liquid molecules to get out of the surface due to having greater energy to form vapors and greater number of vapors creates more vapor pressure.

For example, there is increase of vapor pressure of water from 4.579torr to 9.209torr for change of temperature from zero degrees Celsius to 10 degree Celsius.

2) Strength of intermolecular forces: If any substance has great intermolecular forces then it's difficult to break strong forces to get vaporize. So, evaporation decreases and vapor pressure too and vice versa for the weaker or lesser forces of attraction.

For example, isopentane has the highest vapor pressure and glycerol has the lowest.

We can measure vapor pressure of any liquid by using **manometer or manometric method** or by using **barometer (Borchman et al., 2009).** 

### **2.5 Boiling point:**

"Boiling point is the temperature at which vapor pressure of a liquid becomes equal to the atmospheric pressure".

"Boiling point also refers to the temperature that is required to convert liquid into vapors when internal pressure of a liquid becomes equal to the external pressure of the air"

A constant stream of bubbles comes out or moves toward the upper surface of the liquid because due to continuous heating increases the internal pressure of the liquid and this stream moves out of liquid to get vaporize according to pressure gradient that's why internal pressure becomes equal to external pressure.

Temperature of liquid becomes constant after reaching to boiling point, even on heating it doesn't change because after reaching boiling point of liquid, all the energy uses to break intermolecular forces so all the liquid could be converted into vapors which is why continuous heating doesn't affect temperature.

"The amount of the heat that is required to vaporize one mole of a liquid at its boiling point is called molar heat of vaporization". For example, molar heat of vaporization of water is 40.6 KJ/mol.

#### **Boiling point and external pressure:**

We can control or alter the boiling point of a liquid by changing the external atmospheric pressure as boiling point depends directly on the external atmospheric pressure. As the external pressure increases then more vapor pressure is required to balance or equalize with it that's why more energy, temperature or heat is required for greater evaporation that causes increase of boiling point of a liquid and vice versa.

For example, **boiling point of water** is different at different altitude because of different atmospheric pressure. Boiling point of water is 120 degree Celsius at 1489torr pressure and boils at 25 degree Celsius at 23.7torr. Similarly, boiling point of water at Mount Everest is 69 degree Celsius because of its low atmospheric pressure that is 323torr when compared to boiling point of water that is 98 degree Celsius at Murree hills having lower altitude and low atmospheric pressure that is 700torr.

It's one of the best application is **pressure cooker** as it's easy to cook food into it because it's a closed container having weight cause to increase the external pressure on the food which in result helps the food to absorb more heat and water which in return help in cooking food easily and quickly.

It's one other good example is **vacuum distillation** in which we actually decrease the external pressure on liquid so its boiling point also decreases which helps in easy distillation of any liquid without its decomposition. For example, the glycerin has boiling point 290 degree Celsius at 760torr pressure but undergo decomposition at this temperature. But under vacuum the boiling temperature of glycerin decreases to 210 degree Celsius at 50torr. So this method is useful because its economical and low temperature is required to purify without decomposition (Hilal et al., 2003).

### 2.6 Energetics of phase changes:

Whenever physical state of any matter changes, it causes the change in energy of system. This change is energy is mostly in the form of heat. "If physical or chemical change takes place at constant pressure then the heat changes during this process is also called enthalpy change that is represented by  $\Delta$ H. Its unit is KJ/mol. There are following types of enthalpy changes takes place during phase change:

### 1) Molar heat of fusion:

It is the amount of heat that is absorbed by one mole of a solid when it melts into

liquid form at its melting point at one atmospheric pressure. This is represented by  $\Delta H_f.$ 

### 2) Molar heat of vaporization:

It is the amount of heat that is absorbed by one mole of a liquid when it changes into vapors form at its boiling point at one atmospheric pressure. This is represented by  $\Delta H_{v}$ .

### 3) Molar heat of sublimation:

It is the amount of heat that is absorbed by one mole of a solid when it changes into vapors form at its particular temperature at one atmospheric pressure. This is represented by  $\Delta H_{s}$ .

### 2.6.1 Energy changes and intermolecular forces:

When atoms, molecules or solid substance melts then lesser distance change and lesser intermolecular forces got change to form liquid but during conversion of liquid to gases, drastic change in intermolecular forces and distance between molecules takes place which causes greater heat change in the system. But a much drastic change occurs during sublimation because in this molecules of solid having negligible spaces and strongest intermolecular forces has to convert to gases with least or weakest intermolecular forces and maximum distance. So, we can say that heat of sublimation is greater than heat of vaporization that is greater than heat of fusion.

Heat of vaporization of ammonia, water and HF is greater than other hydrides because of strong intermolecular forces and presence of hydrogen bonding. Also heat of vaporization of iodine is high than its remaining members because it's present on the bottom of the group with largest radius and surface area that represents presence of greater intermolecular forces.

Even two different states can co-exist at a particular temperature or particular range of temperature and the state at which two different phases co-exist is called **dynamic** equilibrium. For example, ice exists with liquid water at zero degrees Celsius (Hilal et al., 2003).

#### **3.Gases**

Gas is the simplest form of matter that doesn't have any specific shape or volume but can easily diffuse, effuse, compressible and also have low density with a lot of kinetic energy.

### 3.1 Gas laws

All the laws that tell us about the relationship between different factors like temperature, pressure, volume and number of moles are called gas laws. Following are the laws that we are going to discuss over here:

- Boyle's law
- Charles's law
- Avogadro's law
- Dalton's law of partial pressure
- Graham's law

### 3.1.1 Boyle's law

"This law states that volume of any gas is inversely proportional to the pressure when temperature and number of moles remain constant".

V α 1/P

V = k/P

PV = k .....(1)

So equation number represents another form of Boyle's law that is:

"The product of pressure and volume for any gas remains constant when temperature and no. of moles remain constant"

If initial conditions are applied on equation number (1) then:

 $P_1V_1 = k$  .....(2)

If final conditions are applied on equation number (1) ten:

 $P_2V_2 = k$  .....(3)

By comparing equation no 2 and 3 :

 $P_1V_1 = P_2V_2 = k$  .....(4)

This equation number (4) represents another form of Boyle's law and that is:

"The product of pressure and volume for initial conditions is equal to the product of pressure and volume for the final conditions and it remains constant when temperature and number of moles for any gas remains constant" (West, 1999).

#### **3.1.2 Graphical representation of Boyle's law:**

#### 1) Graph between pressure and volume:

Graph between pressure and volume is plotted by taking pressure as independent quantity on x-axis and volume on y-axis. This graph is also called "isotherm" as it is plotted at constant temperature to represent Boyle's law. A curve is formed in this graph that represents the inverse relation between pressure and volume. **By increasing temperature** to plot another isotherm, the curve I formed but at greater distance from volume axis. This can be explained by Charles's law that on increase in temperature the volume of gas also increase that's why curve of graph moves away from the volume axis.



#### 2) Graph between pressure and inverse of volume:

Graph is plotted by taking two variables that is inverse of volume (1/V) on x-axis and pressure (P) on y-axis. A straight line is formed that is passing through the origin that represents the direct relation between pressure and inverse of volume. So, with increase of pressure, inverse of volume also increases and vice versa.



#### 3. Graph between pressure and PV:

When a graph is plotted between P and PV then pressure is taken on x-axis and product of pressure and volume that is PV, which is constant at given temperature and number of moles, is taken on y-axis. By plotting graph, a straight that is parallel to x-axis or pressure axis is formed that represents that even by increasing pressure, the product remains constant due to decrease in volume (West, 1999).



# 3.1.3 Charles's law

This law states that:

"The volume of any gas is directly proportional to the temperature at constant pressure and number of moles."

Its mathematical form is

V α T .....(1)

$$V = kT$$

V / T = k .....(2)

Equation number 2 represents another form of Charles's law that is:

"The ratio between volume and temperature becomes constant when pressure and number of moles remain constant"

By applying initial conditions on equation (2):

 $V_1 / T_1 = k$  .....(3)

By applying final conditions on equation (2):

 $V_2 / T_2 = k$  .....(4)

By comparing equation (3) and (4):

 $V_1/T_1 = V_2/T_2 = k$  .....(5)

This equation number 5 represents that:

"Ratio between volume and temperature for initial conditions become equal to the ratio between volume an temperature for final conditions and it all becomes constant when pressure and number of moles".

#### Charles's law can be defined quantitatively as:

"At constant pressure, if temperature of any gas increases by 1 degree Celsius then volume is also increases by 1/273 from its original volume that is taken at zero degrees Celsius and vice versa for decreases in temperature by one degree Celsius."

#### 3.1.4 Graphical explanation of Charles's law:

When we plot a graph between variables then volume is taken on y-axis and temperature in absolute scale is plotted at x-axis. A straight line is formed that doesn't pass from origin which represents that both volume and temperature have direct relation with each other. If we extra plot this line and matches origin then it shows that origin represents **zero kelvin or absolute zero which is unattainable for real gases** because it's the coldest possible temperature for gases and all the gases get converted to liquid or solid before reaching this temperature and it's also against Charles's law (Limpanuparb et al., 2018).



### 3.1.5 Avogadro's law

Avogadro's law states that:

"Volume of any gas is directly proportional to the number of moles at constant temperature and pressure".

 $V \alpha n$  (P, T = constant)

This law can also be defined as:

"Equal number of moles of two or more different gases contains equal number of particles or molecules at standard temperature and pressure".

For example,

2g of hydrogen = 1mole =  $6.02 \times 10^{23}$  = 22.414dm<sup>3</sup> at STP

 $32g \text{ of oxygen} = 1 \text{ mole} = 6.02 \times 10^{23} = 22.414 \text{ dm}^3 \text{ at STP}$ 

All these different gases have different masses but same volume because the volume doesn't depend on mass of gas, size of gas, type or nature of gas but it only depends on number of moles of gas and number of molecules of gas which are same that's why volume remains same for different gases (Moya, 2019).

## 3.1.6 Dalton's law

Dalton's law of partial pressure of gases states that:

"The total pressure of mixture of gases is equal to the sum of partial pressure of each individual gas when volume and temperature remain constant".

 $P_t\!=p_a+p_b+p_c\ldots\ldots$ 

For example, if we consist of a mixture that contains hydrogen, oxygen and nitrogen gas then its pressure is called "total pressure of mixture of gases" and each gas individually in a separate cylinder exerts individual pressure that is called "partial pressure of gas". Suppose, if hydrogen gas exerts 200torr pressure, nitrogen exerts 300torr pressure and oxygen exerts 500torr pressure so the total pressure of a mixture is given by Dalton's law as:

 $P_t = p_{H2} + p_{O2} + p_{N2}$  $P_t = 200 + 500 + 300$  $P_t = 1000 torr$ 

This law suggests that:

"Partial pressure of any gas is directly proportional to the number of moles of that gas". The reason is because as having more number of moles has more number of molecules or particles which shows ore motion, having greater kinetic energy and exert more pressure.

As according to general gas equation:

PV = nRT

By keeping V, T constant for Dalton's law and R is already general gas constant then this equation shows:

P α n (Lord, 1986).

### **Applications of Dalton's law:**

### 1) Collection of gases over liquid:

Some gases are collected over water in the laboratory. These gases become moist after gathering water vapors from the surface. The vapor pressure that is
exerted by water vapors is called 'aqueous tension'. If Dalton's law is applied to this situation then we can say that total pressure exerted by the moist gas is equal to the sum of partial pressure exerted by the gas and partial pressure of water vapors.

 $P_{\text{moist}} = p_{\text{gas}} + p_{\text{water vapors}}$ 

 $P_{moist} = p_{gas} + aqueous tension$ 

 $P_{gas} = p_{moist}$  - aqueous tension

# 2) Respiration:

Dalton's law also explains the process of respiration as any as moves from area of high pressure to the area of low pressure, according to its natural pressure gradient. During inhalation, oxygen moves from area of high partial pressure of oxygen that is air having value 159torr to the area of low pressure that is lungs with partial pressure of oxygen that is 116torr. During exhalation, carbon dioxide moves from lungs to air in the same pressure gradient flow from 35torr in lungs to 0.3torr in air.

# 3) Respiration at higher altitude:

Breathing becomes difficult at higher altitude, due to low concentration of oxygen or air. Pilots also feel uncomfortable breathing because the partial pressure of oxygen is low in un-pressurized cabin as compare to 159torr.

# 4) **Respiration in deep sea level:**

Deep sea divers also take oxygen that is mixed in inert gas like helium or any other noble gas to adjust the partial pressure of oxygen according to requirement. 3atm pressure increases with every 100feet depth of sea that's why normal air can't be breathed in depth of sea. Moreover, the pressure of nitrogen increases in depth of sea which can also diffuse in the blood (Adair, 1928).

# 3.1.7 Diffusion and effusion

"**Diffusion** is a natural process in which any gas moves from its area of higher concentration or pressure to the area of low concentration or pressure until concentration of gases on both sides becomes equal to form a homogenous mixture and uniform flow on both sides."

For example, spreading of rose fragrance or scent into the air.

"Effusion is a process in which gases escape out from a hole present in any container and in this case flow is also from area of higher concentration to the area of low concentration".

For example, puncture of tire.

# 3.1.8 Graham's law of diffusion

This is an empirical law that is presented by Thomas Graham which states that:

"The rate of diffusion or effusion of any gas is inversely proportional to the square root density of any gas by keeping the temperature and pressure constant" Rate of diffusion  $\alpha 1 / \sqrt{d}$ 

Rate of diffusion =  $k 1 / \sqrt{d}$ 

Rate of diffusion =  $k / \sqrt{d}$ 

Rate of diffusion  $\times \sqrt{d} = k$  .....(1)

This equation number '1' also gives another form of Graham's law:

"The product of rate of diffusion or effusion of gases and square root of density of gas remains constant when temperature and pressure become constant."

For gas 1, equation '1' becomes:

For gas 2, equation '1' becomes:

By comparing equation number '2' and '3':

This equation '4' can be written as:

 $R_1 / \sqrt{d_2} = R_2 / \sqrt{d_1} = k$  .....(5)

This equation number '5' can be written as :

 $d \mathrel{\alpha} M$ 

So,  $R_1 / \sqrt{M_2} = R_2 / \sqrt{M_1} = k$ 

(Mason & Kronstadt, 1967).

# 3.2 Ideal gas and non-ideal gas:

Ideal gas is defined as:

- Any gas that follows all the gas laws at all the given conditions of temperature and pressure.
- Any gas whose compressibility factor that is PV/ nRT becomes unity.
- Any gas that doesn't have any attractive forces or in which intermolecular attractive forces are negligible.
- Any gas whose actual volume of gas is negligible as compare to the total volume of container.
- No gas is actually ideal gas.
- In reality, ideal gases exist at low pressure and high temperature.

Non- ideal gas can be defined as:

- Any gas that follows all the gas laws at only particular conditions of temperature and pressure.
- Any gas whose compressibility factor that is PV/ nRT is not equal to unity.
- Any gas that doesn't have any attractive forces or in which intermolecular attractive forces are weak or lesser but not negligible.
- Any gas whose actual volume of gas is minimum but not negligible as compare to the total volume of container.
- All the gases are actually non-ideal gases or real gases.
- In reality, non- ideal gases exist at high pressure and low temperature.

#### **3.3 Ideal gas equation**

One of the equations for ideal gases is derived by using all the gas laws which are applicable to the ideal gases at all temperature and pressure which represents the relationship between all the factors like volume, temperature, pressure and number of moles of any gas.

According to Boyle's law:

 $V \alpha 1 / P$  (T, n = constant) .....(1)

According to Charles's law:

 $V \alpha T$  (P, n = constant) .....(2)

According to Avogadro's law:

 $V \alpha n$  (T, P = constant) .....(3)

By comparing equation 1, 2, 3:

V α 1/ P T n

 $\mathbf{V} = \mathbf{R} \ 1/\mathbf{P} \mathbf{T} \mathbf{n}$ 

V = R/PTn

PV = n RT .....(4)

This equation number 4 represents general gas equation or ideal gas equation in which R is general or ideal gas constant.

This equation '4' can be further derived for 1mole of gas, n =1mol and rearranging:

Equation '4' becomes:

PV / T = R .....(5)

For initial conditions, equation 5 becomes:

 $P_1V_1 / T_1 = R$  .....(6)

For final conditions, equation 5 becomes:

 $P_2V_2 / T_2 = R$  .....(7)

By comparing equation no. 6 and 7:

 $P_1V_1 / T_1 = P_2V_2 / T_2 = R$ 

The value and different units of 'R' can be calculated at different temperature pressure and volume as it is dependent on them (Laugier & Garai, 2007).

#### 3.4 Vander Waal's equation for non-ideal gases

Vander Waal's pointed out that non-ideal gases or real gases have intermolecular forces and also don't have negligible actual volume of gas as compared to the volume of container or volume of gas. So, he made two corrections into the ideal gas equation to modify it for non-ideal gases which are:

- Volume correction
- Pressure correction

#### 1) Volume correction:

Molecules of gas come closer to each other on applying high pressure or on high compression and then on coming closer to each other, repulsive forces also operates between molecules along with attractive forces. This represents that molecules have definite volume that can be small but no longer negligible. So, Vander Waal concluded that volume of gas can no longer be ignored in highly compressible form. If effective volume (occupied volume) of any gas is represented by 'b' then the volume which is free having no gas molecules that is represented by 'V<sub>free</sub>' is equal to the difference between 'b' and total volume of container or vessel that is represented by 'V<sub>vessel</sub>'.

 $V_{\text{free}} = V_{\text{vessel}} - b$  .....(1)

This 'b' also known as excluded volume which is constant and property of each gas. The value of 'b' is dependent on size of molecules of gas. This excluded volume is not equal to the actual volume of one mole of gas ' $V_m$ ' and it is four times the actual volume of molecules of gas.

 $b = 4 V_m$  .....(2)

#### 2) Pressure correction:

When the interior of gas molecules is attracted by all the other molecules from all the sides then these attractive forces got cancelled out. But the force of attraction is experienced by the other gas molecules on the molecule which is hitting or striking the wall of container. Consider a molecule A which is unable to create pressure on the wall of container due to the presence of attractive forces by type B molecules. Let the observed pressure on the wall of container is 'P'. This pressure is lessened than the actual total pressure 'P<sub>i</sub>' by an amount P'. So,

 $P = P_i - P'$ .....(3)

$$P_i = P + P'$$
 .....(4)

 $P_i$  is the 'ideal pressure' of any gas which is exerted when the attractive forces are absent. P' is the 'lessened pressure' due to the presence of attractive forces. It is also suggested that a part of pressure P is required to overcome the attractive forces.

The value of P' in terms of a constant 'a' which represents the attractive forces and the volume of vessel 'V' can be written as:

 $\mathbf{P'} = \mathbf{a} / \mathbf{V}^2$ 

This equation can be derived as:

P' can be determined by the attractive forces present between molecules A which is trying to strike the wall of container and molecules B that is pulling A behind by attractive forces. This net force od attraction is directly proportional to the concentration of A type molecules and concentration of B type molecules.

P'  $\alpha$  C<sub>A</sub>. C<sub>B</sub>

The concentration of any gas is dependent on number of moles of gas taken in unit volume. So concentration = n / V

P'αn/V.n/V

$$\mathbf{P'} = \mathbf{an^2} / \mathbf{V^2}$$

Here, 'a' is the proportionality constant that represents attractive forces. if above equation is written for one mole of gas then it shows that  $P' = a / V^2$ 

This equation shows that, greater the forces of attraction between molecules than smaller the volume of vessel and greater the value of lessened pressure P'.

So, equation '4' becomes:

 $Pi = P + a / V^2$  .....(5)

Equation derived for non-ideal gases by using above volume correction and pressure correction:

According to general gas equation for ideal gases: PV = nRT

For  $n = 1 \mod PV = RT$  PV = RT  $(P + a / V^2) (V - b) = RT$ This equation can be written for 'n' number of moles:  $(P + n^2a / V^2) (V - nb) = nRT$ 

(Sengers, 1974).

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# **BIOCHEMISTRY: ESSENTIAL MOLECULES FOR LIFE**

Muhammad SAFDAR Mehmet ÖZASLAN

# **1. Introduction to Biochemistry**

Biochemistry is the branch of science that explores the chemical processes and substances that occur within living organisms. It is a multidisciplinary science that combines principles from both biology and chemistry. The importance of biochemistry is necessary here to understand about biochemistry (Mougios, 2019).

# Importance of Biochemistry (Calderón-Ospina & Nava-Mesa, 2020):

- Understanding Life Processes: Actually, biochemistry helps in understanding the fundamental processes of life at the molecular level.
- **Disease and Medicine:** It provides deep understanding into the biochemical basis of diseases and is crucial for drug discovery and development.
- **Biotechnology:** Many techniques are essential in various biotechnological applications, including genetic engineering and protein production.
- **Nutrition:** It also explains the metabolic pathways and nutrient requirements necessary for life.

# **Basic Building Blocks:**

- Molecules of Life: It focuses on essential molecules such as proteins, carbohydrates, lipids, and nucleic acids.
- Proteins: They are made up of amino acids, that are involved in various biological functions. Carbohydrates: In biochemistry, sugars and starches provide energy and structural support.
- Lipids: In biochemistry, fats and membranes play roles in energy storage and cellular structure. Nucleic Acids: In biochemistry, nucleic acids carry genetic information and are vital for inheritance and protein synthesis (Minchin & Lodge, 2019).

#### **Enzymes and Catalysis:**

- Enzymes: Proteins operate as biological catalysts, accelerating chemical reactions in cells while remaining unconsumed.
- Importance: Enzymes are crucial for metabolism, allowing cells to perform necessary chemical transformations.
- Specificity and Regulation: Enzymes exhibit specificity for substrates and are regulated to maintain cellular balance.

# **Cellular Metabolism:**

• Metabolic Pathways: Biochemical reactions occur in organized pathways, such as glycolysis and the citric acid cycle, generating energy.

• Energy Currency: Adenosine triphosphate, or ATP, is the energy currency used by cells for both storing and exchanging energy.

# **Genetic Information and Protein Synthesis:**

- DNA Structure: DNA holds genetic instructions.
- RNA and Protein Synthesis: RNA molecules transcribe genetic information and guide protein synthesis through the process of translation.

#### **Biological Membranes:**

- Membrane Structure: Membranes are composed of lipids and proteins, providing structural integrity and regulating passage of molecules.
- Cell Signaling: Membranes are essential for cell signaling and communication.

# Modern Techniques:

- Biotechnological Advances: Techniques like gene cloning, PCR (polymerase chain reaction), and CRISPR-Cas9 revolutionize biochemistry research (Randazzo et al., 2021).
- Omics Technologies: Genomics, proteomics, and metabolomics analyze largescale biological data, enabling comprehensive understanding of organisms.

# **Interdisciplinary Nature:**

• Chemistry and Biology: Biochemistry bridges the gap between chemistry and biology, providing a molecular understanding of life processes.

**Medicine and Biotechnology:** Biochemical knowledge is applied in medicine for diagnostics and therapies, as well as in biotechnological industries.

# 2. Proteins

Amino acids, the building blocks of life, make up proteins, which are big, complicated molecules. As a result, they are essential to the composition, operation, and control of the body's tissues and organs (LaPelusa & Kaushik, 2020).

# **Structure of Proteins:**

- Amino Acids: Proteins are polymers of amino acids. There are 20 different amino acids, each with a unique side chain (R-group), which gives proteins their diverse functions.
- Peptide Bonds: Polypeptide chains are formed when amino acids are joined by peptide bonds.
- The primary structure of a polypeptide chain is its unique amino acid sequence. The genetic coding dictates this sequence.
- Secondary Structure: Hydrogen bonds between amino acids in the polypeptide backbone stabilise the formation of alpha helices or beta sheets in proteins.
- Tertiary Structure: Interactions between side chains of amino acids cause the polypeptide chain to fold in three dimensions. The protein's distinct form and function are derived from its structure. Quaternary Structure: A functional protein complex is formed when many polypeptide chains, or subunits, come together to form a protein.

#### **Functions of Proteins:**

- Enzymes: Proteins function as biological catalysts, accelerating chemical reactions without consuming any energy in the process.
- Structural proteins give cells and organisms structure and support. Collagen found in connective tissues and keratin found in hair and nails are two examples.
- Transport proteins: Help molecules pass through cell membranes (haemoglobin, for example, carries oxygen in blood).
- Hormones: Signalling proteins that control a range of physiological functions, including insulin's control over glucose metabolism.
- Antibodies are immune system proteins that identify and eliminate foreign entities, often known as antigens, such bacteria and viruses.
- Receptor Proteins: Located on cell membranes, they receive signals from the environment and facilitate cellular responses.
- Motor Proteins: Enable movement in cells, such as myosin in muscle contraction and kinesin in intracellular transport.

# **Protein Folding and Misfolding:**

- Protein Folding: Proteins must fold into specific three-dimensional shapes to be functional. Proper folding is essential for their biological activity.
- Protein Misfolding Diseases: Improper folding can lead to diseases like Alzheimer's, Parkinson's, and prion diseases, where misfolded proteins aggregate and disrupt cellular functions (Ribarič & Ribarič, 2019).

# **Protein Synthesis:**

- Transcription: The process in which genetic information from DNA is transcribed into RNA.
- Translation: RNA is translated into a specific sequence of amino acids, forming a polypeptide chain. This process occurs in ribosomes.

# **Protein Regulation:**

- Post-translational Modifications: Proteins can be modified after translation, altering their structure and function (e.g., phosphorylation, glycosylation).
- Protein Degradation: Proteins are degraded by proteases when they are no longer needed, regulating cellular processes.

# **Importance in Nutrition:**

- Dietary Proteins: Amino acids, which the body uses to create new proteins, are formed when diet-based proteins are broken down.
- Essential Amino Acids: Certain amino acids need to be taken from the food because the body is unable to synthesise them.

# **Biotechnological and Medical Applications:**

• Biotechnology: Proteins like enzymes are widely used in various industrial processes, including the production of food and pharmaceuticals.

• Medicine: Therapeutic proteins (e.g., insulin) are used to treat diseases, and protein-based drugs are vital in modern medicine

# 3. Carbohydrates

Carbohydrates are one of the major classes of biomolecules and are essential for life. They serve various critical functions in living organisms and play a central role in energy metabolism. Here are detailed notes on carbohydrates (Gerwig, 2021):

#### Structure:

Monosaccharides: They are the most basic type of carbohydrates that are incapable of being digested into smaller ones. Galactose, fructose, and glucose are a few examples.

Disaccharides are created when two monosaccharide molecules condense. Glucose + fructose, lactose + galactose, and maltose + glucose are examples of common disaccharides.

Large polymers made up of many monosaccharide units are called polysaccharides. Polysaccharides include cellulose, starch, and glycogen.

# **Functions:**

Energy Source: The body uses carbohydrates as its main energy source. Carbohydrates contain glucose, which is particularly crucial for the synthesis of energy in cells via glycolysis and cellular respiration.

Structural Support: Cells and organisms rely on carbohydrates to maintain their structural integrity. For example, the structural framework of plant cell walls is composed of cellulose.

Energy Storage: Excess glucose is stored in the form of glycogen in animals and as starch in plants. These stored carbohydrates can be broken down to provide energy when needed.

Cell Communication: Carbohydrates on the surface of cells play a role in cell recognition and communication. They are involved in processes such as immune response and cell adhesion. Nucleotide Sugars: Carbohydrates are essential components of nucleotides, which are building blocks of nucleic acids (DNA and RNA).

# **Types of Carbohydrates:**

Simple Carbohydrates: Also known as sugars, these include monosaccharides and disaccharides. They are quickly absorbed by the body and provide rapid energy.

Complex Carbohydrates: Polysaccharides are complex carbohydrates made up of many sugar units. They take longer to break down and provide sustained energy. Examples include starch and dietary fiber.

# **Dietary Importance:**

Sources: Grains, fruits, vegetables, legumes, and dairy products are among the foods that contain carbohydrates.

Dietary fibre is a kind of carbohydrates that the body does not break down. It is crucial for gastrointestinal health, helps with digestion, and gives the stool more volume.

Suggested Intake: Since they give the body energy for a variety of tasks, carbohydrates need to make up a sizeable portion of a diet that is balanced.

# Carbohydrate Metabolism:

Glycolysis: The breakdown of glucose into pyruvate, producing ATP and NADH. It occurs in the cytoplasm and is the first step in cellular respiration.

Gluconeogenesis: the production of glucose from precursors that are not carbohydrates. It supports the maintenance of blood glucose levels during fasting.

Glycogenesis and Glycogenolysis: Processes of glycogen synthesis and breakdown, regulating glucose storage and release in the body.

# **Carbohydrates in Health and Disease:**

Blood Sugar Regulation: Insulin, a hormone, helps regulate blood glucose levels. Imbalances can lead to diabetes.

Carbohydrate-Related Disorders: Conditions like lactose intolerance (inability to digest lactose) and celiac disease (gluten intolerance) involve problems with carbohydrate digestion.

# **Biotechnological Applications:**

Biofuels: Carbohydrates derived from plant materials are used in the production of biofuels such as ethanol.

Food Industry: Carbohydrates are used as sweeteners, thickeners, and stabilizers in various food products.

# 4. Lipids

Lipids are a varied collection of hydrophobic compounds that serve critical roles in cell and organism structure and function. Unlike carbohydrates and proteins, lipids are not defined by a specific chemical structure but by their solubility characteristics (Vázquez et al., 2019).

# **Types of Lipids:**

Fatty Acids: Long hydrocarbon chains having a carboxyl group at the end. In the hydrocarbon chain, saturated fatty acids contain no double bonds, whereas unsaturated fatty acids have one or more double bonds.

Triglycerides are made up of three fatty acids joined together by a glycerol molecule. In adipose tissue, they act as energy storage molecules.

Phospholipids are lipids that are similar to triglycerides but have a phosphate group connected to glycerol. Phospholipids are essential components of cell membranes.

Steroids: Lipids with a characteristic four-ring structure. Cholesterol is a vital steroid found in cell membranes and a precursor for hormones.

Waxes: Esterification of long-chain fatty acids to long-chain alcohols. Waxes are used to waterproof and protect plants and animals.

#### **Functions of Lipids:**

Energy Storage: Triglycerides store energy in adipose tissue. They provide a concentrated source of energy, important for organisms with high energy demands.

Structural Component: Phospholipids are the primary constituents of cell membranes, forming a lipid bilayer that separates the cell from its environment.

Insulation: Adipose tissue acts as an insulating layer, helping to maintain body temperature.

Protection: Lipids surround and protect vital organs in the body.

Signaling: Lipids function as signaling molecules (e.g., prostaglandins) that regulate various physiological processes.

Absorption of Fat-Soluble Nutrients: Lipids aid in the absorption of fat-soluble vitamins (A, D, E, and K) in the digestive system.

# Lipid Metabolism:

Fatty Acid Synthesis: Cells can synthesize fatty acids from acetyl-CoA. Excess energy is stored in the form of triglycerides.

Fatty Acid Oxidation: Fatty acids are broken down into acetyl-CoA through betaoxidation, generating energy in the form of ATP.

Cholesterol Metabolism: Cholesterol is synthesized in the liver and is vital for cell membrane integrity. Excess cholesterol can lead to atherosclerosis and cardiovascular diseases.

# **Health Implications:**

Dietary Fats: Different types of dietary fats (saturated, unsaturated, trans fats) have varying effects on health. Unsaturated fats, especially omega-3 and omega-6 fatty acids, are considered beneficial.

Cardiovascular Health: Imbalances in lipid levels, especially elevated LDL cholesterol ("bad" cholesterol), can increase the risk of heart disease and stroke.

Obesity: Excess calorie intake, especially from high-fat diets, can contribute to obesity, a condition associated with various health problems.

# Lipids in Biotechnology:

Biodiesel Production: Lipids from plant and microbial sources are used in the production of biodiesel, a renewable energy source.

Pharmaceuticals: Lipid-based drug delivery systems are utilized to enhance the solubility and effectiveness of certain drugs.

# 5. Nucleic Acids

Nucleic acids are complex macromolecules that carry and store genetic information. They are necessary for the continuation of life and serve as the foundation of heredity. Nucleic acids are classified into two types: deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) (Gautam, 2022).

# DNA (Deoxyribonucleic Acid):

Structure: DNA is a double-helix molecule made up of two nucleotide strands. A sugar (deoxyribose), a phosphate group, and a nitrogenous base (adenine, guanine, cytosine, or thymine) make up each nucleotide.

Base pairing is the process by which guanine (G) establishes hydrogen bonds with cytosine (C) and adenine (A) with thymine (T), resulting in complementary base pairs.

Function: All living things, including viruses, rely on DNA for their growth, development, and reproduction. It contains the genetic instructions necessary for these processes.

DNA replication is the mechanism via which DNA copies itself when a cell divides. It guarantees the transmission of genetic information from one generation to the next.

# RNA (Ribonucleic Acid):

Structure: Usually composed of ribose sugar and the bases adenine (A), guanine (G), cytosine (C), and uracil (U) rather than thymine (T), RNA is a single-stranded molecule.

# **Types of RNA:**

Transports genetic information from DNA to the ribosome, the location of protein synthesis, via messenger RNA (mRNA).

Transfer RNA (tRNA): During translation, it adds particular amino acids to the expanding polypeptide chain. One of the main parts of ribosomes, which are where protein synthesis takes place, is ribosomal RNA (rRNA).

Function: Gene control, protein synthesis, and other biological functions all depend on RNA. It serves as a messenger, transferring DNA instructions to regulate the production of proteins.

The process of creating an RNA molecule from a DNA template is called transcription. The genetic material from the DNA is transferred to the ribosome via this RNA, known as mRNA.

# Genetic Code and Protein Synthesis:

Genetic Code: The amino acid sequence in proteins is determined by the nucleotide sequences found in DNA and RNA. Certain codons, which are three-nucleotide sequences, carry this information in mRNA.

Translation is the process by which a particular sequence of amino acids is synthesised into a polypeptide chain using the information contained in mRNA. This process takes place in ribosomes.

#### **DNA Replication and Repair:**

DNA Replication: DNA replication is a significant process that is characterized as semi-conservative; each new DNA molecule is made up of one strand that was synthesized and one strand that was taken from the original molecule.

DNA Repair: The proof-reading systems are present in the cells. They have mechanisms to repair damaged DNA to maintain genetic stability. Therefore, errors in replication or damage due to multiple factors are being corrected (Kumari et al., 2021).

#### **Molecular Genetics and Biotechnology:**

Genetic Engineering: It is well known that the techniques such as gene cloning and genetic modification of organisms involve manipulating DNA for various functions, such as medical research, agriculture, and biotechnology.

Genomic Sequencing: It is also important that the determination of complete DNA sequence of an organism of genome is vital for understanding genetic traits and diseases in all species.

# **RNA World Hypothesis:**

It is a world hypothesis that RNA molecules were precursors to this life. It means that they are capable of self-replication and catalysing chemical reactions. It also suggests that RNA, not DNA, was the first genetic material for this life.

#### 6. Summary

In conclusion, the study of biomolecules in biochemistry reveals the intricate chemical processes that govern life. Proteins, carbohydrates, lipids, and nucleic acids are the fundamental building blocks of living organisms, each with unique structures and functions. Firstly, proteins composed of amino acids, are versatile molecules that serve as enzymes, structural supports, transporters, hormones, antibodies, and motor proteins. They play crucial roles in cellular processes and are essential for life. Secondly, carbohydrates including sugars and polysaccharides, are vital energy sources, providing quick energy through simple sugars and sustained energy through complex carbohydrates. They also contribute to structural support, cell recognition, and signalling within the body. Thirdly, lipids encompassing fatty acids, triglycerides, phospholipids, and steroids, fulfill roles in energy storage, cell membranes, insulation, protection, and signalling. They are essential components of cells and have significant implications for health and disease. Finally, nucleic acids such as DNA and RNA, store genetic information and govern the synthesis of proteins. DNA holds the instructions for an organism's development and functioning, while RNA acts as a messenger, transferring genetic information from DNA to proteins. Understanding nucleic acids is fundamental to genetics, evolution, and biotechnological

advancements. Collectively, these biomolecules showcase the complexity and elegance of life's molecular machinery. Biochemical knowledge not only deepens our understanding of biological processes but also underpins advancements in medicine, biotechnology, agriculture, and environmental science. Studying these biomolecules provides invaluable insights into the mechanisms of life, enabling us to unravel the mysteries of living organisms and develop innovative solutions to complex challenges in the world of science and beyond.

#### **Scientific Ethics Declaration**

The author say that she is responsible for the scientific, moral, and legal aspects of this chapter, which is published in In Junejo Y (Eds.), *Chemistry for the Life*. ISRES Publishing

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#### THERMOCHEMISTRY: ENERGY CHANGES IN CHEMICAL REACTIONS

#### Zobia ARIF

#### 1. Introduction

Thermochemistry is a branch of Chemistry that deals with the study of energy and energy changes as a result of absorption or emission of heat during conversion of reactant into product. Thermochemistry deals with qualitative and quantitative energy change that takes place during any reaction. Thermochemistry is also called **thermodynamics**.

#### **1.1 Types of reaction:**

Any process in which reactant is converted into product is called **chemical reaction**. In this case, we are classifying reaction on the basis of energy change.

- Endothermic reaction
- Exothermic reaction

#### 1.1.1 Endothermic reaction

'Endo' means 'inside' and 'therm' means 'heat'. As the name of reaction indicates that any process in which energy is required or absorbed into the system and direction of flow of heat is from surrounding to system. In this reaction, final energy of system is greater than initial energy of system. In endothermic reaction, energy of product is greater than energy of reactant as a result of absorption of energy from surrounding. This reaction is indicated by positive sign with value of energy in KJmol<sup>-1</sup>.In most of the cases, energy is required during bond breakage.

For example:

When one mole of nitrogen combines with one mole of oxygen to yield nitrogen oxide, 180.51 KJ of heat is absorbed by the system and the reaction is endothermic.

$$2NO + O_2 \rightarrow 2NO$$
  $\Delta E = 180.51 \text{ KJmol}^{-1}$ 

#### 1.1.2 Exothermic reaction:

'Exo' means 'outside' and 'therm' means 'heat'. As the name indicates that any process in which energy is released or evolved from the system and direction of flow of heat is from system to surrounding. In this reaction, final energy of the system is lesser than the initial energy of the system. In this exothermic reaction, energy of the product is lesser than the energy of the reactant as a result of release of energy from system. This reaction is indicated by negative sign along with value of energy that is taken in KJmol<sup>-1</sup>. In most of the cases, energy is released during bond formation. For example: The combustion of carbon in oxygen is an exothermic reaction as -393.7 KJmol<sup>-1</sup> energy is released during this process.

$$C(s) + O_2(g) \rightarrow CO_2(g)$$
  $\Delta E = -393.7 7 \text{ KJmol}^{-1}$ 

Now, we are classifying reaction on the basis of presence of energy or source of energy:

- Spontaneous process
- Non-spontaneous process

#### 1.1.3 Spontaneous process:

This process can be defined in two different ways. Any process which doesn't require energy to initiate or proceed reaction and second definition is as any reaction that requires energy to initiate any reaction but doesn't requires energy to proceed. It is unidirectional reaction. It is natural process, irreversible reaction and real process. In this case, reaction moves from a non-equilibrium state to equilibrium state. This is mostly represented by 'single headed arrow'.

For example:

- 1) Water flows from higher level to lower level.
- 2) Burning of candle

#### 1.1.4 Non-spontaneous process:

This process can be defined as any reaction that requires energy to get initiated and then also requires energy to proceed it. It is mostly bidirectional reaction. It is reverse of spontaneous reaction as it is an artificial reaction, reversible reaction and synthetic process. This reaction does not take place on its own. Some non-spontaneous processes can be made to take place by supplying energy to system from external sources. This reaction is mostly represented by 'double headed arrow'.

For example:

- 1) Water flows from lower level to higher level.
- 2) Transfer of heat from a colder body to hot body.

#### 1.2 System, surrounding and state function 1.2.1 System:

The term system is used for any specie or matter of universe that is under study or under test or under consideration. There are many classes of system on the basis of interaction:

- **Real system**: Matter under consideration during experimental work.
- Isolated system: Matter under consideration but having no ability to exchange

heat and matter with surrounding.

- Ideal system: Matter under consideration during pencil and paper work to
- Closed system: approach,
  solve problems related to thermodynamics.
  Matter under consideration and semi-permeable in

has the ability to exchange heat to surrounding but don't transfer mass across the boundary to surrounding (Lewis & Randall, 1963).

# 1.2.2 Surrounding:

The term surrounding is applied to any matter that is not under consideration or may be any portion of universe except system is called surrounding. Surrounding generally imply to more than one components like air, water bath in which system is immersed along with table, chair or other components on which system is placed.

# 1.2.3 Boundary or Wall:

Any imaginary or real surface that can separate the system from surrounding and present between them is called boundary. There are some types of walls or boundary like:

- Adiabatic wall: A boundary that is rigid enough and don't allow heat, energy or matter to pass from it provided, external force fields are absent.
- **Rigid wall**: A boundary whose positions and shapes are fixed.
- **Permeable wall**: A boundary that has the ability to pass energy as well as matter.
- Impermeable wall: A boundary that doesn't allow the passage of matter but can pass energy.
- **Diathermic wall**: A type of boundary which doesn't allow the passage of matter when held rigid but permits the transfer of energy or heat when external force fields are absent (Xu et al., 2022).

Consider a cup of tea that is under observation then this cup would be the system and air, table, chair etc except cup of tea would be under surrounding and the wall of cup or thin layer of air between cup and remaining air or surrounding is known as boundary.

Consider the reaction between zinc (Zn) and copper sulphate (CuSO<sub>4</sub>) solution. This can be called a system and the flask, air is known as surrounding.



#### 1.2.4 State and State Function:

As the **state of system** is actually the condition of the system. This state of system can be altered or changed due to different processes. As any system has a specific temperature, pressure or volume that is in the start of reaction which is known as initial state and when we change the condition then there's change in volume, temperature or pressure or other specific values of system so these values after experiment represent final state of any system. By comparing both states of system, we can describe change taking place in any system. As change in temperature can be determined by:

 $\Delta T$  = final temperature – initial temperature

$$\Delta T = T_2 - T_1$$

There are some properties of a system which depend on initial state and final state of a system but independent of path that brings about that change. Such properties of a system are macroscopic properties which are known as **state function**. These properties are represented by symbol ' $\Delta$ ' along with 'capital letter'. There are many properties which are stat function because change in them is caused by many different routes and methods, as temperature, pressure, volume, energy, enthalpy etc (Xu et al., 2022).

$$\Delta V = V_2 - V_1$$
$$\Delta P = P_2 - P_1$$
$$\Delta E = E_2 - E_1$$
$$\Delta H = H_2 - H_1$$

#### **1.3 Energy and forms of energy:**

Energy is the ability to do work. Total amount of energy that is present in any system is also called its **internal energy**. This energy can be in different forms like electrical energy, radiant energy, nuclear energy, chemical energy and thermal energy. Thermal energy is the result of motion of atoms and molecules of any system and the motion of atoms or molecules has a direct relation with thermal energy. We can measure thermal energy of any system by measuring the temperature of system.



Electrical energy is due to movement of electrically charged particles like cations, anions or free mobile electrons. A natural form of electrical energy is the production of lightning when the ground and cloud develops charge separation.



Radiant energy is the energy that is transferred to any system by light, microwaves, ultra waves and radio waves. This radiant energy can be converted into thermal energy as any system when exposed to bright sunlight or microwaves then it becomes warm.



Chemical energy is the energy that is due to specific array of atoms and is stored within the chemical compound.



Nuclear energy is the energy that is present in nucleus of an atom (Lewis & Randall, 1963).



# 1.3.1 Definition

Internal energy of any system can be defined in 3 different ways:

- Energy w.r.t state function
- Energy w.r.t types of energy
- Energy w.r.t forms of transferring energy
- Energy w.r.t state function: Energy is a state function because it's a macroscopic property and its value depends on initial state (E<sub>1</sub>) and final state (E<sub>2</sub>) but it doesn't depend on route or method that brought this change in energy. It is represented by symbol 'delta' along with capital letter that is 'E'. so change in energy is:

#### $\Delta E = E_2 - E_1$

2) Energy w.r.t types: Mainly two types of energy are present in the system that is 'kinetic energy' and 'potential energy'. Kinetic energy (K.E) is due to the movement or haphazard motion of molecules of reactant or system. As there is three types of motion of molecules so kinetic energy is of mainly three type's i.e.

Translational K.E	(due to translational motion)
Vibrational K.E	(due to vibrational motion)
Rotational K.E	(due to rotational motion)

Potential energy of a system is due to the rest of position of molecules of any system and in this case position of molecules is mainly due to the presence of bonds or attractive forces or Vander Wall's forces or London forces. So, energy is the sum of kinetic energy and potential energy.

$$\Delta E = K.E + P.E$$

- **3) Energy w.r.t forms of transfer:** Energy can be transferred between system and surrounding by crossing the boundary in two forms that is:
  - Heat (q)
  - ➤ Work (W)

Heat is not a state function and it can be defined as form of energy in which it is transferred from system to surrounding and surrounding to system across boundary. Heat is represented by 'q' and its unit is KJmol<sup>-1</sup>. Heat can be positive when the reaction is endothermic and it can be negative when the reaction is exothermic (Kulkarni & Tambade, 2017).

Work is also form of transferring energy and it is not a state function. Work is the product of force and distance i.e.  $W = F \times d$  but in thermodynamics, we take work in the form of pressure and volume so W = PV. Work is represented by 'W' and its SI unit is 'joule (J)'. Work can also be positive when work is done on the system and it can be negative when work is done by the system (**Parrondo et al., 2015**) So, energy is the sum of heat and work.

$$\Delta E = q + W$$

#### 1.4 First law of thermodynamics

First law of thermodynamics is also known as **'law of conservation of energy'** that states:

"Energy can neither be created nor be destroyed but it can only be converted from one form to another for but the amount or value of energy remains conserved".

In other words, energy can be transferred from system to surrounding and surrounding to system by crossing boundary in the form of heat and work but it cannot be destroyed or formed and its amount remains constant.

**Experiment:** Consider, a cylinder having a moveable but frictionless piston is taken as



in figure in which gas is enclosed having an initial volume  $(V_1)$  and on providing heat 'q' to the system, volume of system increased to  $(V_2)$  due to increase in temperature according to Charles's law, when system move the system upward by doing work. So change of energy of system can be written as:

Energy w.r.t state function:

Energy w.r.t types:

 $\Delta E = K.E + P.E \dots (2)$ 

Energy w.r.t forms of transfer:

 $\Delta E = q + W \dots (3)$ 

As, for this experiment, work is done in the form of pressure and volume:

 $W = F \times d$ 

When work is taken in pressure and volume form:

W = P V

As in this experiment, volume changes as  $\Delta V = V_2 - V_1$  due to heating and also work is done by the system so W is negative. So,  $W = -P \Delta V$ 

Put this value of 'W' in equation (3):

$$\Delta E = q + (-P \Delta V)$$

 $\Delta E = q - P \Delta V \dots (4)$ 

When the piston is fixed and kept in its original position then the volume becomes constant and no change in volume can be takes place. If, this condition applied then  $\Delta V = 0$ .

So, equation (4) becomes:

 $\Delta E=q - P(0)$ 

 $\Delta E = q \dots (5)$ 

In order to represent condition i.e. V=constant:

This equation shows that at constant volume, change in internal energy of a system becomes equal to the amount of heat absorbed by the system (Lewis et al., 2020).

#### **1.5 Enthalpy:**

Enthalpy is derived from a Greek word that is 'enthalpos' means 'heat content' of system. It can be defined as:

"Enthalpy is the sum of internal energy and work done of the system that itself is the product of pressure and volume. It shows the internal energy possessed by the gas and accompanying the work done by gas."

It is represented by 'H' and its unit is joule 'J'. As its mathematical formula is:

H = E + W .....(1)

As W = PV that's why equation (1) becomes:

 $H = E + PV \dots (2)$ 

As enthalpy is a state function that is represented by symbol ' $\Delta$ ' and change in enthalpy can be measured by using it. So by multiplying both sides of equation (2) with ' $\Delta$ ':

 $\Delta H = \Delta E + \Delta (PV)$ 

 $\Delta H = \Delta E + \Delta P V + P \Delta V \dots (3)$ 

As, the gas is kept at constant pressure,  $\Delta P = 0$ . So, equation (3) becomes:

 $\Delta H = \Delta E + (0) V + P \Delta V$ 

 $\Delta H = \Delta E + P \Delta V \dots (4)$ 

In case of liquids and solids, the change in state doesn't cause significant change in volume i.e.  $\Delta V= 0$ . So, for such processes  $\Delta H$  and  $\Delta E$  are same i.e.  $\Delta H=\Delta E$ .

According to first law of thermodynamics:

 $\Delta E = q + W \dots (5)$ 

Consider, a cylinder having a moveable but frictionless piston is taken as in fig (1.4) in which gas is enclosed having an initial volume ( $V_1$ ) and on providing heat 'q' to the system, volume of system increased to ( $V_2$ ) due to increase in temperature according to Charles's law, when system move the system upward by doing work. So change of energy of system can be written as:

As, for this experiment, work is done in the form of pressure and volume:

 $W = -P \Delta V$ 

 $W = F \times d$ 

When work is taken in pressure and volume form:

W = P V

As in this experiment, volume changes as  $\Delta V = V_2 - V_1$ 

due to heating and also work is done by the system so

W is negative. So,



Put value in equation (5):

 $\Delta E = q + (- P \Delta V)$ 

 $\Delta E = q - P \Delta V$ 

Put value of ' $\Delta E$ ' in equation (4):

 $\Delta H = q - P \Delta V + P \Delta V$ 

 $\Delta H=q$  .....(6)

In order to represent condition i.e. pressure is constant and  $\Delta P=0$ 

 $\Delta H = q_p$ 

This equation shows that at constant pressure, the enthalpy of a system is equal to the heat of reaction. As working with  $\Delta H$  is more suitable in most of the reactions than working with  $\Delta E$  because most of the reactions are carried out at constant pressure rather than constant volume (Ruscic & Bross, 2019).

#### 1.6 Classification of enthalpy

This classification of enthalpy is done on the basis of type and nature of reaction.

#### **1.6.1 Enthalpy of reaction:**

"The amount of heat that is released or absorbed when one mole of reactant is converted into product at standard temperature and pressure i.e. 25 °C and 1atm is called enthalpy of reaction. This is represented by  $\Delta H^0_r$ ."

In an exothermic reaction, the heat content or enthalpy of product is lesser than enthalpy of reactant due to release of heat so  $\Delta H$  is negative. In an endothermic reaction, the enthalpy or heat content of reactant is lesser than enthalpy of product because energy is absorbed in this case that's why value of  $\Delta H$  is positive.



All the reactants and products must be in their standard physical state. Its units are KJmol<sup>-1</sup>.

$$2 H_{2(g)} + O_{2(g)} \rightarrow 2 H_2O_{(l)}$$
  $\Delta H^0_r = -285.8 \text{ KJmol}^{-1}$ 

(Herman & Goodman, 1989).

#### **1.6.2 Enthalpy of atomization:**

"The amount of heat that is absorbed when one mole of element is converted into its own atoms at standard temperature and pressure that is  $25^{\circ}$  C and 1 atm. The enthalpy of atomization is taken in KJmol<sup>-1</sup> and it's always positive as it's and endothermic reaction. It is represented by  $\Delta H^{0}_{at}$ ."

For example, the standard enthalpy of atomization of hydrogen is given below (Lankhorst, 2002):

$$1/2 H_{2(g)} \rightarrow H_{(g)} \qquad \Delta H^0_{at.} = 218 \text{ KJmol}^{-1}$$

#### **1.6.3 Enthalpy of formation:**

"The amount of heat that is evolved or absorbed when one mole of a compound is formed from its respective elements at standard temperature and pressure i.e.  $25^{\circ}$  C and 1 atm when all the reactants are taken in standard physical states. Its unit is KJmol<sup>-1</sup> and is represented by  $\Delta H^{0}_{f}$ ." (Steele et al., 1992).

Enthalpy of formation can be positive and negative as reaction can endothermic as well as exothermic in this case. For example, enthalpy of formation of MgO is -692 KJmol<sup>-1</sup>.

$$Mg_{(s)} + 1/2 O_{2(g)} \rightarrow MgO_{(s)} \Delta H^0_f = -692 \text{ KJmol}^{-1}$$

#### **1.6.4 Enthalpy of neutralization:**

"The amount of heat that is evolved when one mole of reactant i.e. acid (any specie that donate proton) reacts with base (any specie that donate hydroxide ion) to form salt and water at standard conditions i.e.  $25^0$  C and 1 atm, when all the reactants and products are taken in standard physical states. Its unit is KJmol<sup>-1</sup> and it is represented by  $\Delta H_n^0$ ."

Enthalpy of neutralization is always negative as neutralization is always an exothermic reaction. Value of enthalpy of neutralization i.e. -57.4 KJmol<sup>-1</sup> is also constant for all the acid and bases because the property of donating proton remains same for all different acid and similarly all the bases donate hydroxide ion that results in the formation of water in all such reactions (Eatough et al., 1975).

For example:

$$NaOH_{(aq)} + HCl_{(aq)} \rightarrow NaCl_{(aq)} + H_2O \quad \Delta H^0_n = -57.4 \text{ KJmol}^{-1}$$

# **1.6.5 Enthalpy of solution:**

"The amount of heat that is released or absorbed when one mole of reactant i.e. solute and solvent to form solution at standard condition that is standard temperature=  $25^{\circ}$  C and standard pressure= 1atm, when all the reactants and products are present in their standard physical states. Its unit is KJmol<sup>-1</sup> and it is represented by  $\Delta H_{sol}^{0}$ ."

Enthalpy of solution can be positive and negative as formation of solution can be endothermic and exothermic process.

For example (Sanahuja & Cesari, 1984):

$$NH_4Cl_{(s)} + H_2O \rightarrow NH_4Cl_{(aq)} \quad \Delta H^0_{sol} = 16.2 \text{ KJmol}^{-1}$$

#### **1.6.3 Enthalpy of combustion:**

The amount of heat that is released when one mole of compound undergo burning in the presence of oxygen at standard conditions that is standard temperature=  $25^{0}$  C and standard pressure= 1atm, when all the reactants and products are present in their standard physical states. Its unit is KJmol<sup>-1</sup> and it is represented by  $\Delta H_{c}^{0}$ ."

Enthalpy of combustion is always an exothermic reaction and its value is always negative. For example (Kirklin et al., 1989):

$$C_{(\text{graphite})} + O_{2(g)} \rightarrow CO_{2(g)} \qquad \Delta H^0_c = -393.7 \text{KJmol}^{-1}$$

#### **1.7 Measurement of Enthalpy:**

As long as the heat exchange i.e. evolved or absorbed during any chemical reaction is considerable then we can determine it by using different kind of instruments which are called 'calorimeter'. These calorimeters are used to determine the accurate values of  $\Delta H$  for different reactions. We are going to discuss two calorimeters over here:

- Glass calorimeter
- Bomb calorimeter

#### **1.7.1 Glass calorimeter**

Glass calorimeter is an instrument that is use to determine enthalpy of reaction mainly enthalpy of neutralization and enthalpy of solution.

#### Instrumentation:

Glass calorimeter is made up of glass. It is an insulated container having two container i.e. outer container that contain water or cotton to act as barrier/ resistance or insulator between system and surrounding. It also contains stirrer for stirring and thermometer for measuring temperature.



#### Working:

Firstly, collect the sample whose enthalpy has to be measured. Weigh the sample and then place it into inner beaker and then set the whole assembly. Before starting the reaction, measure the initial temperature of sample i.e. initial temperature(T1) and after that keep on stirring the sample with the help of stirrer and keep on checking temperature of reaction media with the help of thermometer, as reaction proceeds allows the temperature to keep on changing but one the reaction stops, change in temperature also become equal to zero that indicates the completion of reaction.

the reaction stops, measure the final temperature (T2) with the help of thermometer. Change in temperature can be measured by:

$$\Delta T = T_2 - T_1$$

#### Calculation:

$$q = m \times s \times \Delta T$$

This above formula is use to determine hat or enthalpy of any system. As 'm' represents mass of sample, 's' represents specific heat of water whose value is 4.2 J K  $^{-1}$  g<sup>-1</sup> and ' $\Delta$ T' shows change in temperature (Aphecetche et al., 2003).

#### **1.7.2 Bomb calorimeter:**

Bomb calorimeter is an instrument that is use to determine the enthalpy and enthalpy change. Its wide application is to determine enthalpy of combustion.

#### **Instrumentation:**

Bomb calorimeter mainly consists of a cylindrical shape inner container that contains graphite coil that is connected with battery to help in combustion of sample. This cylindrical container is made up of steel and has an outer

protective layer that is called enamel for protection of

inner container from corrosion. A platinum crucible

contains weighed sample is place on graphite coil.

Upper side of container has a valve that helps the

inlet to open and close for the addition of 20 atm oxygen.

Then this inner container is placed into outer container

Having water or cotton and it also contains stirrer for



stirring and thermometer for the measurement of temperature.

#### Working:

First of all, collect sample and weigh it. After this, sample is placed in platinum crucible and put it on ignition/ graphite coil. Then oxygen is entered through inlet and temperature is measured initially by thermometer and noted as initial temperature (T1). Stirring is done by using stirrer and temperature is continuously measured by thermometer after regular intervals. After completion of process, final temperature (T2) is measured. Difference of temperatures gives change in temperature i.e

$$\Delta T = T_2 - T_1$$

#### Calculation:

$$q = m \times s \times \Delta T$$

'q' represents heat of any system, 'm' represents mass of sample, 's' represents specific heat of water and ' $\Delta$ T' represents change in temperature. As the product of mass and specific heat represent 'heat capacity' i.e. 'c'. **Heat capacity** is the ability

of any compound or specie to absorb temperature to raise its temperature by 1K. So, above formula can be written as (Miller & Payne, 1959):

 $q = c \times \Delta T$ 

#### 1.8 Hess's law of constant heat summation:

This law states that:

"If reaction takes place in more than one routes, then enthalpy of direct reaction becomes equal to sum of enthalpies of all the steps of indirect reaction."

We can also say that;

"Enthalpy change during any reaction remains same as it can take place in one step or in more than one step. So, enthalpy change becomes equal to zero as reaction can take place in any possible way, if initial and final conditions provided are same."

# *Example no.1:* Direct reaction:

$A \rightarrow D$	$\Delta H$

**Indirect reaction:** 

$A \rightarrow B$	$\Delta H_1$
$B \rightarrow C$	$\Delta H_2$
$C \rightarrow D$	$\Delta H_{3}$

According to Hess's law:

 $\Delta H = \Delta H_1 + \Delta H_2 + \Delta H_3$ 

Hess's cycle:



# *Example no.2:* Combustion of graphite:

**Direct reaction:** 

 $C + O_2 \longrightarrow CO_2$ 

 $\Delta H = -393.7 \text{ KJmol}^{-1}$ 

#### **Indirect reaction:**

$C + 1/2 O_2 \rightarrow$	CO	$\Delta H_1 = ?$
$\rm CO + 1/2O_2 \rightarrow$	CO <sub>2</sub>	$\Delta H_2 = -283 \text{ KJmol}^{-1}$

#### **Calculation:**

According to Hess's law:

 $\Delta H = \Delta H_1 + \Delta H_2$ 

 $-393.7 = \Delta H_1 + (-283)$ 

 $-393.7 + 283 = \Delta H_1$ 

 $-110.7 \text{ KJmol}^{-1} = \Delta H_1$ 

Hess's cycle:

 $C(s, graphite) + \frac{1}{2}O_2(g) \xrightarrow{(1)} CO(g) + \frac{1}{2}O_2(g) \xrightarrow{(2)} + \frac{1}{2}O_2(g) \xrightarrow{(3)} + \frac{1}{2}O_2(g)$ 

#### *Example no.3:* Formation of sodium carbonate:

#### **Direct reaction:**

**Calculation:** 

#### According to Hess's law:

 $\Delta H = \Delta H_1 + \Delta H_2$ 

-89.08 = -48.06 + (-41.02)

-89.08 = -89.08

Hess's cycle:



#### **Application of Hess's law:**

- Hess's law is used to calculate enthalpy of combustion for any reaction
- Hess's law is used to calculate enthalpy of formation of any reaction
- Hess's law is used to determine enthalpy of formation of any reaction.
- Hess's law can also be applied to determine enthalpy of reaction.
- Hess's law is used to calculate enthalpy of any individual step when reaction takes place in more than one route (Davik, 1980).

# **1.9 Future Horizons of Thermochemistry:**

As following are few future horizons of thermochemistry:

- Further work must be done on reservoirs, fuels and other fossils which are getting less, day by day, so these reservoirs could be reserved and restored too.
- Thermochemistry can help in production or generation of heat that can be used in further processes.
- Due to increase population, main goal of thermochemistry is to contribute in the efficient product of food, energy and heat so there requirements would be fulfilled.
- With the help of thermochemistry, different types of batteries, cells, solar cells and devices can be generated.

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# INDUSTRIAL CHEMISTRY: CHEMICALS AND TECHNOLOGY IN EVERYDAY LIFE

Ghashia AMEEN

# Introduction

The word "industry" is used to describe any economic activity that involves the production of a goods or service for human welfare. Chemicals are part of our lives since ages. We are surrounded by compounds and technology formulated from these chemicals. It will be not wrong to say that chemicals have made our world and life beautiful and easy, even our own body and all living organisms are beautiful creation of chemicals. If we discuss the development of first chemical industry, then we came to know that traces of first chemical industries were found in Middle Ages. They use basic knowledge and skills to synthesize some household items. First chemical industrial production started at late 1700 but still they were not able for large scale synthesis (Rowe, 1998). The evolution to modern chemical technology we are aware of came recently in the 19th and 20<sup>th</sup> century. Chemists play an important role in advancing industrial field by developing synthetic drugs, dyes, flavors, fiber, polymers, fertilizers, detergents, and cosmetics etc (Crini et al., 2020). So, synthetic chemistry plays an important role in developing technology. The chemical industry needed intensive research and development as it makes significant contributions to the economy. Despite all the benefits of these chemicals and technology in our daily life, it also has some of its drawbacks. Main drawback is environmental pollution. During any chemical reaction, many organic solvents, heavy metals, and harmful gases are released in the environment which affect plants and animals directly (Ukaogo et al., 2020). Hence, the chemical industry is regarded as one of the most extensively regulated sectors among all industries. Different strategies are used to reduce pollution by different industries and researchers which is not only helpful in reducing pollution but also increase yield and quality of product. Scientist are interested in using biological system for synthesizing different chemicals. It not only increases yield but also help to reduce pollution as there is no need to use toxic chemicals and solvents. So, it leads to a new branch of chemistry known as green chemistry. Another recent development in industrial chemistry is use of nanotechnology (Franco et al., 2021). Many heavy metals used in different reactions are not only expensive but also toxic to life. But when we study these metals at nanoscale their properties change. In this way scientist have replaced expensive and toxic metals with nanometals that are not only cheap but also increase yield.

# Chemicals used in our daily life

We daily come across a lot of chemicals that we use on daily basis. From the moment we wake up until we go to sleep, chemicals are at work, contributing to our comfort, health, and convenience. These chemicals come in various forms, serving purposes that range from cleaning to nourishment, construction to communication (Anastas & Zimmerman, 2019). Here, we explore the impact of these chemicals in our daily lives.

- Domestic cleaning products: We use surfactants, soaps, detergents, disinfectants for cleaning our homes. Synthetic chemicals are the basic ingredient for all these products. Soaps are a type of surfactant that consist of water-soluble salts derived from fatty acids, which can be either alkali or ammonium salts. Other additives used in soap manufacturing are Builders, Colorants, Fragrance, Antimicrobial agents, Citric acid, Oatmeal powder Calendula petals and many more to give them special properties and enhance their quality and activity (Achaw & Danso-Boateng, 2021b). On the other hand, detergents are used to clean oil and dirt from solid surfaces or cloths. These also contain synthetic chemicals like surfactants, cleansers (phosphates, zeolites), bleaches, enzymes, fabric brighteners, luminescent agents, and opacifying agents. Detergents are used for domestic, bathroom, toilet, glass, and bathroom cleaning. Four detergent types are amphoteric, cationic, anionic, and non-ionic (Kirsner & Froelich, 1998; Myers, 1992).
- **Personal care products:** Personal care products cover a wide range of items, such as skin and hair care products, UV protecting lotions, cleansers, bug repellents, perfumes, shampoos, conditioners, toothpaste, and so forth. Detergents, toothpaste, soaps, and deodorants all contain antimicrobial agents. sunscreens, soaps, conditioners, nail polishes, shampoos, shaving creams, detergents, and lotions contain cyclic volatile methyl siloxanes, Bisphenol A, and linear siloxanes (Allmyr et al., 2006; Dodson et al., 2012). Fragrances

contain a diverse range of organic compounds, including acetals, epoxides, alcohols, esters, amines, ethers, phenols, dioxanes, aldehydes, epoxides, amides, esters, carboxylic acids, heterocyclics, hydrocarbons, coumarins, lactones, nitriles, ketones, quinolines, pyrans, quinolines, and Schiff's bases (Bickers et al., 2003).

- Food Additives and Preservatives: Different chemicals are added in food for making them more healthier appealing, nutritious and for their preservation too. Saccharin is an artificial sweetener that is mostly used in food for diabetic patients as it is completely harmless and inert (Weihrauch & Diehl, 2004). When there is need to store food for long period, preservatives are added to control microbial growth. Most common food preservatives are table salt, sugar, Salts of sorbic acid, vegetable oils, propanoic acid and sodium benzoate (Bhargava, 2016).
- Medicines and Pharmaceuticals: This is one of the most important applications of chemical sciences as they help to keep us healthy and curing diseases. Every medicine that we use to treat a disease is a chemical compound that may be extracted from natural sources or artificially synthesized. Some plant derived drugs are Quinine (antimalarial), Cocaine (Local anaesthetic), and Digoxin (Cardiotoinc) (Fowler, 2006).
- **Polymers:** These are high molecular weight substances made of repeating units called monomers. They can be natural or artificial and straight chain or branched. Some examples of polymers are wool, cellulose, rubber, nylon, polythene etc. (Islam et al., 2020).
- Fertilizers and Pesticides: Agriculture is an important practice to fulfil human needs and fertilizers and pesticides help to overcome the emerging challenges in this field due to the increase in population and change in environmental conditions (Sharma & Singhvi, 2017). All these compounds are also chemical. So, we can see that our life is surrounded by chemical technology.

#### **Chemical Industries**

Industries are vital to modern life. The chemical industry is a significant sector that holds a significant role in our daily lives. Chemical industries play a crucial role in transforming raw materials into products that are in high demand and used in our daily lives. These goods, which are manufactured in chemical industries, are utilized in many other areas of life, including the food industry, agriculture, and the building and construction industry (Cui et al., 2019). The chemical industry can be categorized according to the primary raw materials, or the predominant products manufactured. Chemicals industries can be classified as organic and inorganic chemical industries (Sheoran et al., 2018). Heavy inorganics like sulfuric acid are examples of inorganic chemicals synthesized by inorganic chemical industry. Additionally, it also contains nitrogen, phosphorus, and potassium-based fertilizers (Monisha et al., 2022). The substances and materials utilized in advanced industries like electronics and pharmaceuticals, as well as the production of inorganic specialties like propellants, catalysts, and pigments, are examples of such components (Hout, 2023). Heavy organic chemical industries primarily manufacture petroleum fuels, petrochemicals, polymers, and other synthetic materials obtained from petroleum. Light organic industries primarily deal with the production of a range of chemicals, including but not limited to cosmetic products, dyes, pesticides, paints, pigments, soaps, detergents, pharmaceuticals, and other related goods (Okolie et al., 2021). Raw material for chemical industries is mostly obtained from nature. Air is a source of important industrial gases like O<sub>2</sub>, N<sub>2</sub>, Kr, Xe, Ne and Ar. From seawater we can obtain NaCl, Mg and Br. The great majority of elements are found in mineral ores, carbon, and hydrocarbons that come from the earth's crust (Bertau et al., 2023). In addition to being used as energy sources, coal, natural gas, and crude oil are transformed into countless compounds. Vegetation and animals contribute raw materials like sugar, fats, natural fibers, leather, oils, waxes and resins. Some important chemical industries are discussed below.

### **Fertilizer Industry**

Fertilizers have the potential to be incorporated into the soil to facilitate nutrient absorption via the roots. Additionally, they can be supplied by foliage feeding to enable absorption through the leaves. Fertilizers can occur naturally, such as in peat, saltpeter or mineral deposits, as well as synthesized through natural processes like composting (Assefa & Tadesse, 2019). Chemical processes, such as the Harber

Process, can also be used to manufacture them. Each nutrient or fertilizer has a distinct function in the growth of plants. Nitrogen is crucial for plants due to its role in protein metabolism and its ability to stimulate leaf and stem growth (Hu et al., 2021). Potassium is essential for the proper functioning of the metabolic system in plants. Potassium deficiency in plants leads to yellowing, wilting, leaf drop, and poor fruit development (de Bang et al., 2021). Phosphorus is essential for providing the energy needed for plant metabolism. A rich soil supply encourages root growth and fruit and flower production (Hossain et al., 2010; Karthika et al., 2018). Fertilizers are classified into three main groups according to the specific growth requirements of plants. Primary fertilizers typically include nitrogen, phosphorus, and potassium fertilizers. The nutrient requirements of plants for calcium, Sulphur, and magnesium are considerably lower compared to their requirements for primary fertilizers. Fertilizers containing these elements are commonly known as secondary fertilizers. Plants have lower requirements for elements such as copper, iron, manganese, zinc, boron, and molybdenum compared to secondary fertilizers. Fertilizers containing these elements are known as tertiary fertilizers (Delgado et al., 2016). Fertilizers can be categorized into two main types: organic and inorganic. Additionally, they can be further classified based on their origin, distinguishing between naturally occurring and manufactured fertilizers. In this section, we will focus on primary fertilizers.

- Nitrogen is a crucial plant nutrient. Although nitrogen constitutes 79% of the Earth's atmosphere, only a few plants, mainly legumes, possess the ability to directly utilize atmospheric nitrogen (Allito et al., 2015). In order to support the growth of these plants, we must supply them with artificial fixed nitrogen. Some important synthetic fertilizers include Ammonium sulfate, Urea, and Ammonium chloride. The list of nitrogen-based fertilizers includes ammonium nitrate, ammonium sulfate nitrate, calcium ammonium nitrate (CAN), sodium nitrate, calcium nitrate, potassium nitrate, calcium cyanamide, and ammonia (Nasr & Sewilam, 2018).
- 2. Phosphorus is considered to be the second most crucial element in fertilizers, ranking after nitrogen. It performs a pivotal function in the metabolic processes of all plants. Plant uptake of phosphorus occurs solely through root absorption from the soil. Phosphorus is absorbed by plants in the form of H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, HPO<sub>4</sub><sup>2-</sup>, or PO<sub>4</sub><sup>3-</sup>. The amount of phosphorus that is normally present

in native soils is rather low (Tian et al., 2021). Phosphate can be found in fertilizers in two different forms: those that are soluble in water and those that are soluble in citrate. The former is soluble in water, while the latter cannot be dissolved in water but can be dissolved in a solution that contains 2% neutral ammonium citrate (Chien, 1993). Some important phosphorus fertilizers include Superphosphate, Nitric Phosphate, Triple Superphosphate, Monoammonium Phosphate, Diammonium Phosphate, and Pulverized rock.

3. After nitrogen and phosphorus, potassium is the third most significant component in fertilizers. In plant physiology, potassium plays a variety of roles, including that as a regulator for a number of different chemical processes. It promotes root growth, strengthens stalks, aids in the formation of food substances such as sugars and starches, transports proteins, regulates respiration, helps plants retain water, and functions as a preventative measure against diseases (Kathpalia & Bhatla, 2018). The effectiveness of the process is diminished in the absence of co-nutrients such as nitrogen and phosphorus. Plants experiencing a potassium deficiency exhibit stunted growth, thinness, and display noticeable chlorosis and necrosis, particularly in the lower leaves. This may lead to a substantial decline in agricultural yields (Reed, 2019). Potassium is plentiful in the Earth's crust; however, its conversion into fertilizer-appropriate forms is challenging and costly. The primary potassium compounds utilized in the fertilizer industry are potassium chloride (muriate of potash), potassium-magnesium sulphates, potassium sulphate, and potassium nitrate with varying potassium to magnesium ratios (Achaw & Danso-Boateng, 2021a).

# **Pharmaceutical Industry**

The pharmaceutical industry is responsible for the production of medications. A substance is referred to as a "drug" if it is one that is meant to be used in the treatment or prevention of illnesses in both humans and animals (Ayukekbong et al., 2017). The pharmaceutical market is segmented into two categories. Ethical products are primarily distributed through prescription rather than being widely marketed to the general public. Over-the-counter (OTC) products are easily accessible. The latter usually refers to proven minor condition therapies (Perrot et al., 2019). In countries with modern healthcare systems, the distinction between these two categories is desirable and obvious. Explaining medicine names is necessary. Each active

ingredient has a chemical name. These names are long and only important to organic chemists. In the fields of pharmacology and medicine, it is advantageous to have a more concise nomenclature for general purposes. This type of name is commonly known as a generic name. Two groups of names, namely International Nonproprietary Names (INN) and United States Approved Names (USAN), are recommended by the World Health Organization (WHO) and the USAN Council, respectively (Heaton, 1993; Taylor, 2015).

In past, a significant proportion of pharmaceutical substances were obtained from natural origins, mostly botanical sources. It was later recognized that in order for these products to be effectively used as pharmaceuticals, they must be pure. Pharmaceuticals are manufactured using either synthetic methods or via the process of biosynthesis (Porta et al., 2016). Fermentation has historically served as a prominent technique for the production of crucial pharmaceutical categories, such as hormones, vitamins, and antibiotics. Microorganisms cultivated in regulated fermentation environments have the capacity to execute complex chemical conversions, hence leading to a more economically efficient manufacture of goods in contrast to solely chemical processes (Zhang et al., 2020). Genomic studies have revealed that certain groups of bacteria and fungi have multiple secondary metabolic process that are not active under standard laboratory growth conditions. Mixed fermentation is a method that can be used to maximize the metabolic capabilities of cultivatable microbes. This process involves the coexistence of neighboring microbes, which can enhance the production of secondary metabolites (Pettit, 2009). Here is an example of Antibiotics synthesized by mixed fermentation.

• A total of fifty-three marine bacteria species, which are known to inhabit surfaces, were cultivated in liquid medium alongside Streptomyces tenjimariensis, a marine bacterium renowned for its production of the antibiotics istamycin A and B. Among the 53 bacterial species that were subjected to testing, it was observed that twelve of them, accounting for 22.6% of the total, had the capability to stimulate the formation of istamycin. In addition to that, the expansion of competing colonies was prohibited by the use of this antibiotic (Slattery et al., 2001). The findings suggest that metabolites produced by marine bacteria play a role in suppressing the growth of competing species

Plants have long been used by humans as a source of therapeutic agents. Almost 80% of the worldwide population still depends on plants for primary healthcare. Even in Western medicine, where synthetic chemistry has made significant advancements, approximately 25% of prescription drugs are still derived from plants, whether by direct extraction or indirect synthesis (Jamshidi-Kia et al., 2018). Medicinal use of plants varies from crude preparations or extracts to refined extracts and isolated compounds.

- *Papaver somniferum* was used as an Analgesics. Codeine morphine isolated from this plant were the prime active constituents of *Papaver somniferum* (Singh et al., 2023).
- Digoxin from *Digitalis pupurea* is used as Cardiotoinc (Whayne, 2018).
- Quinine from Cinchona ledgerianais an Antimalarial drug (Fowler, 2006).

The demand for medicines increases as the population grows, and this demand is met through synthetic chemistry. With advancements in reactions and technology, it is now possible to synthesize naturally occurring compounds for disease treatment and meeting human needs. An antimalarial drug, like quinine, is now synthesized in laboratories.

# **Recent advances in chemical industries**

Technological advances, environmental concerns, and changing client demands make the chemical industry dynamic. The chemical business relies on scientific principles. The technologies used in the chemical industry have strong scientific foundations, and the industry's growth has been closely tied to scientific advancements. Following are some current developments and trends in the chemical industry:

# **Green Chemistry**

Green chemistry is one the most recent advancement in industrial field and it has taken up attention of the scientist as environmental pollution is increasing day by day. Organic solvents released from industries is one of the major causes of pollution. It is difficult or somehow impossible to run a chemical reaction in aqueous media. But these days scientist are able to tackle this problem to some extent. Cross coupling reactions play a significant role in the formation of carbon-carbon bonds and find widespread application in several industrial sectors (Hooshmand et al., 2020). One potential limitation associated with these reactions is waste produced due to use of organic solvents. Micellar catalysis uses surfactants in aqueous environments to create nanoreactors in organic media, enabling the conduction of traditional organic reactions in water, often at ambient temperature (Lipshutz et al., 2013). Supercritical fluids (SF) have also replaced many organic solvents in chemical reactions especially for extraction processes. SFs offer numerous advantages, such as the lack of hazardous waste, relatively low temperature needed for extraction, and the increased solvent power of SF. SF are non-flammable, non-carcinogenic, and non-toxic compared to organic solvents (Centi & Perathoner, 2003).

Green Chemistry Objectives	Industrial Chemistry objectives	Examples	References
Atom	Preventing waste	Selective	(Mäki-
economy (less	production by avoiding	hydrogenation of Citral	Arvela et
waste	side reaction	different alcohols over	al., 2002)
production)		Ni, Rh and Ru supported catalysts	
Avoid toxic	Replacing toxic solvents	Implementation of	(Constable
chemicals or	by green solvents	biocatalysts in	et al.,
solvents		oxidative processes avoiding use of toxic solvents	2007)
Use of renewable resources	Using natural resources to make reaction cheap and ecofriendly	Nanostructured cheap and sustainable carbonaceous materials	(Titirici & Antonietti, 2010)
		can be generated by hydrothermal	
		carbonization process	

 Table 1. Objectives of industrial chemistry in term of green chemistry

Simple and	The complexity of the	one-pot process on	(Climent et
safe process	process and the	single-site base	al., 2014)
	generation of	catalysts is the one-pot	
	intermediates may be	synthesis of 1,1-	
	minimized by using a	dicyano-2,4-	
	solid catalyst to facilitate	diphenylbutadiene	
	a single-step reaction, so	derivatives	
	avoiding the need for a		
	complicated multistep		
	reaction.		

# **Circular Economy**

As the global population is increasing, it is crucial to establish procedures for the management of natural resources. Circular economy (CE) aims to reduce waste production, improve the durability of products and materials, and restore natural systems. This gives the main principles of CE, which comprise reduce, reuse and recycle (Ghisellini et al., 2016). N<sub>2</sub>O is a greenhouse gas; however, it is also a valuable chemical that has been utilized for facilitating selective oxidation reactions. As a result, its potential reuse in adipic acid production has been recently explored, specifically through the Solutia-Borevskov process. N<sub>2</sub>O, a byproduct of the adipic acid process, is used in this method to synthesize phenol from benzene using ZSM-5 catalysts that include Fe. So, the cost of eliminating N<sub>2</sub>O is reduced by reusing it, which allows for higher plant productivity, cost reduction, and decreased hydrogen consumption (Centi, 2000).

#### **Bio-based Chemicals**

It is crucial to produce industrial chemicals from renewable biomass feedstock in order to tackle the fossil fuels depletion, climate change, and other environmental issues. A considerable amount of industrial chemicals derived from fossil resources can be replaced with bio-based chemicals. Platform chemicals are substances generated from biomass such levulinic acid, 5-hydroxymethylfurfural (5-HMF), sugar alcohols, furfurals, succinic acid, lactic acid, and phenols (Kohli et al., 2019). These chemicals can also be used to produce numerous significant compounds on a large scale.

#### **Biotechnology and Biocatalysis**

In terms of green chemistry, biocatalysis has a number of attractive qualities, such as the ability to operate under moderate conditions such as physiological pH and temperature. It utilizes environmentally friendly catalysts (enzymes) and solvents (often water), and also help in multifunctional molecules to achieve high activity and demonstrate stereo-, regio-, and chemo-selectivity (Markandan et al., 2023). Additionally, it does not include the additional steps of protection and deprotection needed in conventional organic synthesis. Synthesis of 6-aminopenicillanic acid is an illustrative example showing the advantages of substituting traditional chemistry with biocatalysis (Sheldon, 2005). This compound is used as a primary ingredient in the production of semi-synthetic antibiotics cephalosporin and penicillin. Its synthesis involves the hydrolysis of penicillin G (Benzylpenicillin) antibiotic (Wegman et al., 2001). The complicated composition of the molecules, which usually requires many reaction steps, is a key barrier encountered in the synthesis of medicines. Furthermore, this complexity tends to escalate as research progresses, posing additional challenges (Tao et al., 2009). The current objective is to prioritize environmental sustainability. Industrial biotechnology helps in 'greener' chemical syntheses. Biocatalysis is now widely used not just in the pharmaceutical business, but also in the food, cosmetic industries and feed (Naveed et al., 2021). Biotechnological synthesis of diverse compounds such as vitamins, anti-aging agents, scents, moisturizers, tastes, food additives, or de-pigmentation components is routinely carried out in the food and cosmetic industries employing single-enzyme systems, fermentation, or multi enzyme systems. Biotechnology is helpful since conventional chemical syntheses usually create undesirable racemic combinations and may fail to synthesize the intended product entirely (Vandamme & Soetaert, 2002).

# Nanotechnology

Nanotechnology holds the potential to deliver substantial advancements in advanced materials and manufacturing techniques and plays an significant role in ensuring the future competitiveness of national industries. Nanotechnology has enormous applications in the food industry and processing, including revolutionary instruments for pathogen detection, drug delivery systems for treatment, food packaging, and targeted delivery of bioactive substances to particular areas (Malik et al., 2023). Nanotechnology helps in food preservation and improve nutritional content

of food. Modern research has focused on investigating the application of nanoencapsulation in the delivery of various active compounds, including antioxidants, colorants, minerals, antimicrobials, drugs, vitamins, flavors, probiotic micronutrients and microorganisms (Ayala-Fuentes & Chavez-Santoscoy, 2021).

Encapsulation is a technique that is frequently used in food technology to effectively mask unfavorable tastes or odors, control interaction of active ingredients with the food matrix, manage the controlled release of these agents, guarantee their availability at a predetermined time and rate, and protect them from moisture and heat (Álvarez & Pando, 2021).

Nanotechnology can improve the performance of traditional building materials like steel and concrete. By carefully combining manufactured nanoparticles like carbon nanofibers and nanotubes with metal/metal oxide nanoparticles, concrete sustainability, strength and durability have seen notable increases (Abdalla et al., 2023). Additionally, nanoencapsulation techniques have been employed to create environment-responsive anticorrosion coatings. According to research conducted by Hanus and Harris (2013), nanotechnology can increase insulation, solar cell performance, and cooling systems. Traditional building materials like paint and cement are being improved with the help of nanomaterials by introducing new features like self-cleaning characteristics. Carbon nanotubes have much greater Young's modulus and tensile strength than steel, with carbon nanotubes weighing much less per volume compared to steel (See & Harris, 2007; Walters et al., 1999). Carbon nanotubes reinforce concrete at the nanoscale, unlike traditional steel reinforcement bars that operate at the macro scale. There are several uses for antimicrobial surfaces in building materials, including hospitals, childcare centers, and nursing homes. They assist in reducing the transmission of diseases and lowering chances of discomfort and illness. Antimicrobial nanoparticles come in a variety of forms, and some of them can operate as the main component of antimicrobial coatings(Biswas et al., 2023). Natural antimicrobial compounds like chitin, chitosan, and certain peptides, as well as metals and metal oxides including copper oxide (CuO), titanium dioxide (TiO<sub>2</sub>), magnesium oxide (MgO), copper (Cu), silver (Ag), and silver (Ag) are examples of nanoparticles. Additionally, engineered nanomaterials like carbon nanotubes (CNTs) and fullerenes are also included (Hanus & Harris, 2013).

### **Hydrogen Economy**

Hydrogen is gaining significant attention as a clean energy carrier with numerous benefits, making it a priority in future energy systems. A possible replacement for fossil fuels is hydrogen. Water is the only consequence of the reaction between hydrogen and oxygen, which releases energy either quietly in fuel cells or violently in heat engines (Genovese et al., 2023).

Hydrogen fuel  $(H_2)$  does not occur naturally. The majority of the hydrogen on Earth is present in chemical molecules. Water, hydrocarbons from deceased organisms, fossil fuels, and biomass all require chemical conversion to produce H<sub>2</sub>. Electrolysis from steam and hydrocarbons, ionic hydrides, water, metal acid reactions, and carbon are a few common processes for generating hydrogen (Muh et al., 2019). Hydrogen, similar to electricity, serves as an energy carrier and is required to be produced from a natural resource. Currently, the bulk of the hydrogen used in the world is created via a technique of steam reforming that use natural gas (Pareek et al., 2020). However, this process releases CO<sub>2</sub> in the environment. Even with the most economical manufacturing technique, steam reforming of methane, hydrogen is still four times more expensive than gasoline for the same amount of energy. The production from methane does not reduce the consumption of fossil fuels or the release of CO2 (Tashie-Lewis & Nnabuife, 2021). Hydrogen must be produced from non-fossil resources, including water, utilizing renewable energy sources in order to fully utilize the benefits of the hydrogen economy. Energy is needed to split the water molecule and release the hydrogen; however this energy is later recovered during the oxidation process to produce water. The energy needed to split water must originate from non-carbon sources in order to completely remove the usage of fossil fuels in this operation. These sources might be heat from a nuclear reactor or solar collector, electron-hole pairs formed in a semiconductor by solar radiation, an electric voltage generated by a renewable energy source like wind or hydropower, or nuclear or solar collector heat.(Crabtree et al., 2004) A remarkable advancement is the direct conversion of sunlight to H<sub>2</sub> using solar water splitting. Direct water electrolysis was made possible by a new and integrated photoelectrochemical-photovoltaic architecture. When lighted, this photoelectrochemical cell's integrated photovoltaic device, which is voltage biased, may immediately split water (Vilanova et al., 2020). The only source of energy for this photoelectrochemical cell is light, which it uses to split water. As a potential replacement for traditional fuels, hydrogen fuel has applications in standalone power generation, grid-connected hybrid renewable energy systems, and energy storage (Singla et al., 2021). It is a modern substitute for fossil fuels since it is clean, environmentally friendly, and has a greater energy density. Additionally, compared to the prices paid by electric utility companies across the world, the cost of producing power using hydrogen fuel cells is substantially cheaper. The control of the combustion rate of hydrogen gas is the only critical factor that needs to be addressed.

# Challenges and environmental considerations of advancing technology

Technology has undeniably enhanced and streamlined our lives; however, it is not without its limitations. Addressing the challenges and environmental considerations associated with the advancement of technology is of utmost importance in the contemporary era. The following are essential headings to structure a comprehensive discussion on this particular topic:

### **Resource Depletion**

Resources depletion happens when natural resources are consumed at a faster rate than they can be replenished. The natural resources of a nation may be classed into two categories: non-renewable and renewable resources. Utilizing natural resources is essential for a country's economic growth. Current trends in energy and natural resource utilization, agricultural methods, and urban development indicate an urgent need for remedial action due to their unsustainable nature. The use of natural resources appeared unjustified, potentially leading to negative economic consequences for the country (Ogwu, 2019). The rapid population growth is speeding up the depletion of resources. Failure to address consumption patterns can result in irreversible climate change and hindered economic growth. This can be attributed to the rising social, economic, and environmental costs, along with a decline in productivity. Due to their desires for a greater quality of life, people in advanced countries have a larger demand for resources than is necessary for an adequate standard of living. As a result, they substantially harm the ecosystem by seriously overusing resources (Yu et al., 2023). However, because of their lower standard of living, people in emerging nations have a reduced need for resources. But because of their expanding population, lack of awareness about environment, and desire for a quick rise in living standards, they frequently participate in careless resource degradation. High consumption of these resources is also a big cause to environmental pollution, deforestation and soil erosion (Mittal & Gupta, 2015).

#### **Pollution and emission**

When used, household and personal care products emit chemicals into the indoor environment, exposing users to these substances through inhalation and skin contact. These substances are therefore important contributors to chemical emissions in the indoor environment. Volatile organic compounds, aldehydes, and semi-volatile organic compounds are some of these chemicals (Wei et al., 2022). To provide products distinct features and functions, chemicals are typically used as fragrances, solvents, preservatives, surfactants, and disinfectants. There are several linked health effects, including sensitization, endocrine disruption, reproductive toxicity, mutagenicity, carcinogenicity, and chronic toxicity.

Emissions of heavy metals into the environment can be caused by both manmade and natural factors. Mining operations are one of the main anthropogenic sources that contribute to emissions. Mercury is discharged into the environment through cosmetic products and other activities including the manufacturing of sodium hydroxide in addition to mining operations. The many industrial point sources, such as foundries and smelters, combustion byproducts, and transportation, are other sources of emission (Pacyna et al., 2010). Mercury is released during the degassing of the earth's crust, whereas lead is emitted during its mining and smelting operations, from automobile exhausts (by combustion of petroleum fuels treated with tetraethyl lead), and from old lead paints. When zinc is refined, a by-product called cadmium is released (Fu et al., 2019). Heavy metal contamination of surface and underground water sources causes significant soil pollution, and pollution levels increase when mined ore is spread out on the ground for hand dressing. Industrial items can also cause heavy metals contamination. Batteries, mirror coatings, outdated paints, and tiles may all expose you to lead. Artist paints and nickel/cadmium batteries are the main sources of cadmium exposure. organometallics, shampoos, antifungal substances, lotions, and disinfectants all contribute to mercury exposure (Pandey et al., 2016). These heavy metal depositions, such as cadmium, arsenic, lead, zinc, mercury, aluminum, and copper poisoning, can cause biotoxicity when volatile vapours and fumes are inhaled. This biotoxicity can lead to diarrhea, gastrointestinal (GI) disorders, hemoglobinuria, stomatitis, paralysis, tremor, ataxia, vomiting, depression, convulsions and pneumonia. (Duruibe et al., 2007)

Air pollutants are produced during burning of fossil fuels in different industries. Like textile industry contribute to environmental pollution by different ways. By directly discharging massive quantities of waste liquids and sludge that may include highly harmful components like metal-containing dyes or organic compounds, the textile industry pollutes soils and aquatic bodies (Islam et al., 2023). It contaminates indoor air because of air pollutants that are directly released, such as combustor fuel gases and chemical gases and vapors of some toxic or dangerous chemicals. These chemicals may include primary air pollutants, like volatile organic compounds and free gaseous chlorine, suspected photochemical precursors, like chlorine radicals, and other suspected secondary air pollutants that are formed in the gas phase by the action of the precursors mentioned above. Additionally, it generates a lot of solid waste (Müezzinoğlu, 1998).

Diabetics frequently use artificial sweeteners like sucralose. They are thought to contribute to the development of metabolic imbalances that result in obesity, lymphomas, cardiovascular disease, brain cancer and bladder, fatigue syndrome and leukemia because they alter glucose control (Grotz & Munro, 2009).

Humans living in heavily industrialized areas have higher mortality rates from lung cancer. High levels of benzo[a]pyrene and other polynuclear aromatic hydrocarbons, mostly of industrial origin, were present in the soil and air in these sites (Manzetti, 2013). Industries are a big cause of almost every type of pollution. So, care must be taken to control environmental pollution.

# Waste-water Management

Health of people and the environment are seriously threatened by the release of industrial waste that has not been completely treated and managed. The need for an adequate treatment strategy that can lead to cost- and environment-friendly waste management is becoming more and more crucial worldwide. Waste-water cleaning can be accomplished using a variety of conventional, cutting-edge, biological, and emerging treatment techniques.

- Adsorption is a physical treatment method with a long history that is effective in the recycling and treatment of organic, chlorinated and metallic contaminants (Velusamy et al., 2021).
- Electro-dialysis (ED) is a method of membrane separation that is used to separate anions and cations with the use of two charged membranes (cathode and anode). For the treatment of hazardous and inorganic pollutants, it is a highly acceptable and suitable approach (Chen et al., 2022).

- For the treatment of undesired cations and anions from industrial waste-water, ion exchange is a distinct, attractive approach (Swanckaert et al., 2022).
- Gravitational settling is a commonly used physical, operational treatment method called sedimentation that removes large, heavy particles suspended in wastewater (Saravanan et al., 2021).
- To purify industrial waste-water containing colloidal and suspended solids (SS), the coagulation method is used (Alekseev & Shambina, 2021).
- The separation of suspended and Dissolved Solids, carbonates, sulphates, metallic content and chloride impurities from industrial waste-water is mostly accomplished through precipitation and filtration (Saleh et al., 2022).
- Due to the efficient degradation of chlorinated, phenolic, and organic pollutants which are mostly present in industrial effluents, the oxidation approach associated with Fenton's reagent is becoming more and more significant (Ziembowicz & Kida, 2022).
- For the purpose of removing solid and organic impurities, the aerobic activated sludge process is frequently employed to treat large quantities of wastewater (Jagaba et al., 2021).
- Chemical treatment procedures known as advanced oxidation processes produce enough hydroxyl radicals to fully oxidize chemical substances. In order to considerably accelerate the deterioration, they employ catalysts like Mn, Fe<sup>+2</sup>/Fe<sup>+3</sup>, CCl, TiO<sub>2</sub>NiSO, and CuSO<sub>4</sub>, or powerful oxidizing agents (ozone/H<sub>2</sub>O<sub>2</sub>) as well as high-energy radiation (Rekhate & Srivastava, 2020).
- Photo-catalysis is a very innovative and successful treatment process for the elimination of the extremely harmful pollutants present in waste-water (Rathi et al., 2021). Metal and biological trash are regularly disposed of by using this process.
- Membrane filtration is a sophisticated physical separation process that is used to remove unwanted particles, microbials, sediments, and organic materials from waste-water (Sawunyama et al., 2023).

 Biotic reagents known as enzymes operate as catalysts for the conversion of substances into products by creating favorable circumstances that lower the reaction's activation energy. In compared to chemical and physical treatments, biological methods, including enzymatic digestion, are significantly superior, safer, and more successful for wastewater cleanup (Bharagava & Chowdhary, 2019).

### Solid Waste Management

Chemical industries generate toxic solid waste that must be disposed of properly to ensure public health and for the protection of the environment. This solid waste contains Paper and cardboard, packaging, Glass, car windshields, construction wastes, plastics, including splinters, wood, sawdust, fabric, municipal solid wastes from bars, heavy metals and leather from textile, food sector industries and restaurants, used tyres and hazardous wastes, printing ink, including car oil, disinfectants, paint, batteries, soluble cutting emulsion and varnish (Lambolez et al., 1994). This waste must be dumped in landfills in a controlled way to prevent soil and water pollution. These sites must have low coefficient of soil permeability, suitable hydrogeological characteristics of site, landfill cover etc.

# **Future Trends to control industrial pollution**

Cotton is grown globally as a major source of natural fiber. In cotton production systems, nitrogen management is difficult since it affects a cotton crop's yield, maturity, and its quality more than any other key nutrient (Khan et al., 2017). Excessive application of nitrogen can have negative environmental effects such as nitrate buildup in groundwater and the release of the highly potent greenhouse gas nitrous oxide, which is a major issue worldwide. So, slow-release fertilizers (such polymer-coated urea) may boost cotton yield while lowering environmental pollution.

One of the most widely used materials in the world economy is plastic. It is now an unavoidable component of the physical world. In general, synthetic organic polymers with a C-C bond-only backbone make up plastics, and coal, oil, and natural gas are their main raw materials (Brunner et al., 2018). Plastics have accumulated in lakes, land, and oceans for many years because they are difficult to organically degrade. There is more proof now than ever before that microplastics build not only in the environment but also in our diet. The management of plastic waste and the discharge of plastics into the environment, in addition to the mining and raw material transportation of plastic's, all contribute to greenhouse gas emissions. Currently, the majority of plastic trash is managed through recycling, burning, and landfilling. According to evidence, the incineration of plastic packaging trash resulted in net emissions that were expected to reach 16 million tons in 2015 (Shen et al., 2020). Bioplastic and biopolymers are considered as best solution to control plastic pollution (Muneer et al., 2021).

The Internet of Things (IoT) has given a possible opportunity to create robust industrial systems and applications by exploiting the spread of radio-frequency identification, mobile, wireless, and sensor devices (Gupta & Quamara, 2020). When IoT is used to create intelligent transportation systems, the transportation authority will be able to track each vehicle's present position, watch its movement, and predict its future location as well as any potential traffic. IoT projects have been implemented widely in a variety of industrial sectors, including food processing, agriculture, security surveillance, environmental monitoring, and others. The food industry is combining wireless sensor networks with radiofrequency identification to create automated systems for tracking, tracing, and monitoring food quality across the food supply chain (Da Xu et al., 2014).

Energy is one of the most important topics in the twenty-first century. Due to the accelerating depletion of fossil fuels and the rising environmental degradation brought on by vast fossil fuel usage, there is a critical need for efficient energy use and the search for renewable and clean energy sources that can replace fossil fuels. Energy storage, a step between the diverse, clean, and efficient use of energy, has generated concern and research interest globally. For fixed and mobile applications, hydrogen is a clean and re-usable energy source that only emits water. Today, a wide range of approaches, including nano-structuring, nano-/micro-combination, hybridization, configuration surface pore-structure management, design, modification, composition optimization, and inventive device design, may be used to produce advanced energy storage materials. Organic materials are increasingly being used for energy storage. The bulk of energy storage media under investigation today are made of inorganic materials, however from the viewpoints of sustainability and ecoefficiency, the development of renewable organic energy storage materials is vital. Secondly, the structure and compatibility of energy storage devices must be optimized.

# Summary

Industrial chemistry is a complicated mix of chemicals and technology that we use every day. It is where creation and production meet. Industrial chemistry supports everything from medications, plastics, and detergents to the technologies that power our homes, automobiles, and communication gadgets. Through this field, we've mastered the power of chemical reactions and turned simple materials into a wide range of goods and tools that make our lives better in countless ways. Industrial chemistry has also helped solve some of the biggest problems in society. It helps us to meet the needs of our world and its people, such as making products that are better for the earth, using cleaner energy sources, and making better materials. But it also has some of its side effects. Its biggest side effect is environmental pollution. There are responsibilities that come with the benefits of industrial chemistry. The right way to use chemicals in production, how they affect the environment, and safety are all very important. Researchers and experts in this field all are working for the betterment of this society. So, to make beneficial use of industrial products, everyone should pay their role to use products safely and then dispose off waste properly.

# **Scientific Ethics Declaration**

The authors say that they are responsible for the scientific, moral, and legal aspects of this chapter, which is published in *Chemistry for the Life*. ISRES Publishing.

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# **Conflict of Interest**

The authors declare no conflict of interest.

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# BASICS TO ADVANCED ANALYTICAL CHEMISTRY

Yasmeen JUNEJO Mehmet ÖZASLAN

# **Principles of Solvent Extraction**

Solvent extraction is a method of isolating and purifying compounds or elements from a mixture. It involves the transfer of a solute from one solvent phase to another solvent phase, typically from an aqueous phase to an organic phase or vice versa. Solvent extraction is based on the principles of distribution or partitioning, where the solute distributes itself between two immiscible solvents, depending on its solubility and the solvents' properties.

The solvent extraction process consists of several steps, including mixing the two phases, allowing them to separate, and finally collecting and recovering the desired component from the solvent phase. The partition coefficient, Kd, defined as the ratio of the solute concentration in the organic phase to that in the aqueous phase at equilibrium, describes the solute's distribution between the two phases.

Solvent extraction is commonly used to purify metals from their ores, such as the extraction of copper from copper ores using an organic solvent. The process involves leaching the ore with an aqueous solution containing the metal ion, followed by solvent extraction of the metal ion using an organic solvent such as an alkyl phosphine oxide.

The selection of the solvent system is crucial in the solvent extraction process. The solvent should be immiscible with the initial solvent phase and have a high affinity for the solute to ensure efficient extraction. The solvent should also be easy to separate from the solute and not react with the solute or other components of the mixture.

Solvent extraction is also used in the pharmaceutical industry to purify natural products and isolate drug compounds from impurities. It is a useful technique for useful basic, and neutral compounds from complex mixtures, such as plant extracts.

In conclusion, solvent extraction is a widely used separation technique based on the principles of distribution or partitioning. It is a useful technique for purifying metals from their ores, isolating drug compounds from impurities, and separating compounds from complex mixtures. The solvent system selection is a critical factor affecting the efficiency and selectivity of the solvent extraction process.

# **Analytical Separations**

Analytical separations are techniques used to separate and identify components of a mixture based on their physical and chemical properties. Analytical separations are used in various fields, including chemistry, biology, and environmental science, to determine the composition of complex mixtures.

There are several types of analytical separations, including chromatography, electrophoresis, and mass spectrometry. Each technique involves different principles and methods of separation and detection.

Chromatography is a separation technique based on the differential partitioning of a sample between two phases, one stationary and one mobile. The sample is introduced onto the stationary phase, which may be a solid or liquid and is then separated by the mobile phase, which is typically a liquid or a gas. The separated components of the sample are detected as they emerge from the column or other separation device. Chromatography can be further classified into different types, including gas chromatography (GC), liquid chromatography (LC), and ion chromatography (IC).

Electrophoresis is a technique that separates charged particles, such as proteins or DNA, in an electric field. The sample is placed on a gel matrix, and an electric field is applied, causing the charged particles to migrate through the gel at different rates. The separated components of the sample can be detected using various methods, including staining or labeling.

Mass spectrometry is a technique that separates and detects ions based on their massto-charge ratio. The sample is ionized, and the resulting ions are separated in a magnetic field based on their mass-to-charge ratio. The separated ions are then detected and quantified.
Analytical separations have many applications in industry, research, and medicine. For example, chromatography is used to produce pharmaceuticals to separate and purify drug compounds. Electrophoresis is used in genetics and genomics research to separate and analyze DNA fragments. Mass spectrometry is used in proteomics and metabolomics to identify and quantify proteins and small molecules in complex mixtures.

In conclusion, analytical separations are a vital set of techniques used to separate and identify components of complex mixtures based on their physical and chemical properties. These techniques are widely used in various fields, including chemistry, biology, and environmental science, to determine the composition of complex mixtures. The selection of the appropriate technique for a particular application depends on the nature of the sample and the information required.

### **Multiple Batch Extraction**

Batch extraction is the process of simultaneously extracting multiple pieces of data from a source. It is a common task in data analysis and is often used to extract data from databases, web pages, or other sources. Multiple batch extraction involves extracting data from multiple sources or multiple parts of a source in one go.

- **1. Identify the sources:** The first step in multiple batch extraction is identifying the sources from which you want to extract data. This could be multiple databases, web pages, or different sections of a single web page.
- 2. Define the extraction criteria: Once you have identified the sources, you must define the criteria for extracting data. This could include specifying the fields or columns you want to extract, setting filters or search criteria, or defining the range of data you want to extract.
- **3.** Choose a tool: Many tools are available for batch extraction, ranging from simple web scrapers to more complex data extraction software. Choose a tool that fits your needs and is compatible with the sources you are working with.
- 4. Set up the extraction process: Depending on the tool you are using; you may need to set up the extraction process by configuring the tool to connect to the source and specifying the extraction criteria.

- **5. Run the extraction:** Once the extraction process is set up, you can run the extraction and collect the data. Depending on the size of the data set, this may take some time.
- 6. Clean and analyze the data: After the data has been extracted, you may need to clean it up and organize it for analysis. This could involve removing duplicates, formatting the data, or merging it with other data sets. Once the data is clean, you can analyze it to gain insights or create reports.

Overall, multiple batch extraction can be a powerful tool for data analysis, allowing you to extract and analyze large amounts of data quickly and efficiently. However, it requires careful planning and attention to detail to ensure the data is extracted accurately and useful for analysis.

# **Counter Current Distribution**

Counter current distribution is a separation technique used in organic chemistry to separate components of a mixture. It involves the repeated extraction of a mixture with two immiscible solvents, each of which is placed in a separate phase. The process is based on mass transfer and partitioning principles, allowing for the isolation of individual components in a mixture.

- 1. Principles of mass transfer and partitioning: Counter-current distribution is based on the principles of mass transfer and partitioning. When a mixture is in contact with two immiscible solvents, its components partition the two phases based on their solubility in each solvent. This partitioning process is governed by the solvents' relative concentrations and the components' distribution coefficients in each solvent.
- 2. The process: The counter-current distribution process involves the repeated extraction of a mixture with two immiscible solvents, each of which is placed in a separate phase. The process is typically carried out in a series of separatory funnels containing the mixture and the two solvents. The two solvents are added to the funnel, which is shaken to mix the two phases. The mixture is then allowed to settle, separating the two phases.
- **3. Repeated extraction:** The separated phases are then transferred to the next funnel in the series and repeated. The solvents are added to the funnel

containing the separated phases from the previous funnel, and the funnel is shaken to mix the phases. The mixture is then allowed to settle, and the phases are separated again. This process is repeated until the desired separation is achieved.

- 4. Advantages of counter-current distribution: Counter-current distribution has several advantages over other separation techniques. It is a simple and inexpensive process that does not require specialized equipment. It is also a highly efficient technique, allowing for separating individual components in a mixture with a high degree of resolution.
- **5. Limitations of counter-current distribution:** While counter-current distribution is a highly effective technique, it does have some limitations. The process is time-consuming, as it requires repeated extractions. Its ability to separate components with similar partition coefficients is also limited.

Overall, counter-current distribution is a useful technique for separating components of a mixture based on their partitioning behaviour. While it does have some limitations, it is a powerful tool in the hands of an experienced organic chemist.

# Solvent Extraction by Flow Injection Method

Solvent extraction is a separation technique to isolate and purify compounds from complex mixtures. It involves using a solvent to selectively extract the target compound while leaving other components of the mixture behind. The flow injection method is a commonly used technique for performing solvent extraction, which involves using an automated system to deliver the sample to the solvent rapidly.

- 1. The principle of solvent extraction: Solvent extraction is based on the principle of partitioning, where the target compound selectively dissolves into the solvent while other components of the mixture are insoluble. This is achieved by mixing the sample with a suitable solvent and allowing the two phases to separate. The target compound selectively dissolves into the solvent, which can then be separated from the other components of the mixture.
- 2. **The flow injection method:** The flow injection method involves using an automated system to rapidly deliver the sample to the solvent. The sample is injected into a sample loop, which is then automatically switched to the solvent. The sample is then mixed with the solvent, allowing the target

compound to dissolve into the solvent selectively. The two phases are then separated, and the target compound can be further purified if necessary.

- 3. Advantages of solvent extraction by flow injection method: Solvent extraction by flow injection method has several advantages over other solvent extraction techniques. It is a rapid and efficient technique that can be automated, allowing for high-throughput analysis of samples. It also allows for the selective extraction of target compounds, resulting in higher purity and better recovery.
- 4. **Applications of solvent extraction by flow injection method:** Solvent extraction by flow injection method is commonly used in the analysis of environmental samples, such as water and soil, as well as in the analysis of pharmaceuticals and natural products. It is also used to analyse food and beverage samples to detect contaminants and additives.
- 5. Limitations of solvent extraction by flow injection method: Solvent extraction by flow injection method does have some limitations. The choice of solvent can greatly impact the efficiency and selectivity of the extraction. Additionally, the high flow rates used in the technique can lead to poor contact between the sample and the solvent, resulting in poor recovery and selectivity.

Overall, solvent extraction by flow injection method is a powerful technique for isolating and purifying target compounds from complex mixtures. Its ability to automate the process and deliver high-throughput results makes it a valuable tool in many areas of analytical chemistry.

# Solid-Phase Extraction by Flow Injection Method

Solid-phase extraction (SPE) is a technique to isolate and purify compounds from complex mixtures. It involves the uusinglid-phase material, such as a resin or silica gel, to selectively retain the target compound while other components of the mixture are washed away. The flow injection method is a commonly used technique for performing SPE, which involves using an automated system to rapidly deliver the sample to the solid-phase material.

1. The principle of SPE: Solid-phase extraction is based on the principle of partitioning, where the target compound selectively adsorbs onto the solid-

phase material. At the same time, other components of the mixture are washed away. This is achieved by passing the sample through a column containing the solid-phase material, allowing the target compound to interact with the stationary phase selectively.

- 2. The flow injection method: The flow injection method involves using an automated system to rapidly deliver the sample to the solid-phase material. The sample is injected into a sample loop, which is then automatically switched to the SPE column. The sample is then passed through the column, allowing the target compound to adsorb onto the solid-phase material selectively. The unbound components are washed away, and the target compound is eluted from the column using a suitable solvent.
- **3.** Advantages of SPE by flow injection method: SPE by flow injection method has several advantages over other SPE techniques. It is a rapid and efficient technique that can be automated, allowing for high-throughput analysis of samples. It also allows for the selective extraction of target compounds, resulting in higher purity and better recovery.
- **4. Applications of SPE by flow injection method:** SPE by flow injection method is commonly used in the analysis of environmental samples, such as water and soil, as well as in the analysis of pharmaceuticals and natural products. It also analyses food and beverage samples to detect contaminants and additives.
- 5. Limitations of SPE by flow injection method: SPE by flow injection method does have some limitations. The choice of solid-phase material and solvent can greatly impact the efficiency and selectivity of the extraction. Additionally, the high flow rates used in the technique can lead to channelling and poor contact between the sample and the solid-phase material, resulting in poor recovery and selectivity.

Overall, SPE by flow injection method is a powerful technique for isolating and purifying target compounds from complex mixtures. Its ability to automate the process and deliver high-throughput results makes it a valuable tool in many areas of analytical chemistry.

#### **Principles of Chromatography**

- 1. Chromatography is a separation process frequently employed in analytical chemistry to separate and purify complicated mixtures. Chromatography's fundamental premise is based on the differential distribution of components in a combination of mobile and stationary phases. The stationary phase is often a solid or liquid coated on a solid support, while the mobile phase is a fluid that travels through it. The mixture's components interact with the mobile and stationary phases.
- 2. Types of chromatography: Chromatography is classified into three types: gas chromatography (GC), liquid chromatography (LC), and ion chromatography (IC). The chromatography method used is determined by the nature of the sample being analysed as well as the qualities of the target substances.
- **3. Mobile phase:** The mobile phase is the fluid that flows through the stationary phase, carrying the mixture's components with it. The mobile phase used is determined by the nature of the sample being analysed as well as the qualities of the target molecules. The mobile phase in LC is often a solvent or a mixture of solvents, whereas the mobile phase in GC is typically an inert gas.
- **4. Stationary phase:** The stationary phase is the solid or liquid phase that is coated on a solid support and interacts with the mixture's components. The type of the material being analysed, as well as the properties of the target chemicals, influence the choice of stationary phase. The stationary phase in LC is often a solid or liquid coated on a solid support, whereas the stationary phase in GC is typically a high boiling liquid coated on a solid support.
- **5. Retention time:** The retention time is the time that a component of the mixture spends in the stationary phase before the mobile phase elutes it. The retention time is a function of the properties of the component, the properties of the stationary and mobile phases, and the flow rate of the mobile phase.
- 6. Separation factor: The separation factor is the degree of separation between two components in a mixture. It is a function of the retention times of the two components and is a measure of the selectivity of the chromatographic system.
- **7. Detection:** Chromatography is typically coupled with a detection method, such as mass spectrometry, UV-Vis spectroscopy, or fluorescence spectroscopy, to identify and quantify the components of the mixture.

Overall, chromatography is a powerful separation technique that is widely used in analytical chemistry. The chromatography principles involve the differential distribution of components between the mobile and stationary phases, which depends on the properties of the components and the stationary and mobile phases.

### Structure of Chromatography

Chromatography is a separation technique used in various scientific disciplines to separate and analyze complex mixtures of compounds. The technique relies on the differential interactions between a sample and a stationary phase (solid or liquid) and a mobile phase (gas or liquid), separating the sample into its individual components. Chromatography can be divided into several categories based on the nature of the stationary phase, the separation mechanism, and the mode of operation.

The basic structure of chromatography consists of the following components:

- 1. Stationary phase: The stationary phase is immobilised solid or liquid material on a support, such as a column or a thin layer on a solid substrate. The stationary phase can be selected based on its capacity to interact selectively with the sample components.
- 2. The mobile phase is the gas or liquid that transports the sample through the stationary phase. The mobile phase can be chosen based on its capacity to dissolve sample components as well as its interactions with the stationary phase.
- **3. Sample:** The sample is the mixture of compounds being analyzed by chromatography. The sample can be injected into the chromatography system using a syringe or an automatic sampler.
- **4. Detector:** The detector is the device that measures the concentration of the sample components as they exit the chromatography column. The detector can be chosen based on the properties of the sample components, such as their absorbance, fluorescence, or mass-to-charge ratio.
- **5. Data analysis:** The data generated by the detector can be analyzed using various methods, such as peak integration, spectral deconvolution, and statistical analysis. The data analysis can provide information about the sample components' identity, purity, and quantity.

The structure of chromatography varies greatly depending on the type of chromatography. The stationary phase in liquid chromatography, for example, can be a solid particle or a liquid deposited onto a solid support, whereas the stationary phase in gas chromatography is often a thin film sprayed onto a solid support. Additionally, the mode of operation can vary, such as in column chromatography, where the sample is separated by passing through a column packed with the stationary phase, or in thin-layer chromatography, where the sample is separated by migrating through a thin layer of stationary phase coated onto a solid substrate.

Overall, the structure of chromatography is diverse and can be adapted to suit a wide range of applications, making chromatography a powerful and versatile technique for the separation and analysis of complex mixtures of compounds.

# **Classification of Chromatographic Techniques**

Chromatography is a powerful separation process that is frequently utilised in a variety of scientific areas such as chemistry, biochemistry, and biotechnology. Chromatographic techniques rely on the differential interactions between a sample and a stationary phase (solid or liquid), separating the sample into its components.

Chromatographic techniques are grouped into numerous types based on the nature of the stationary phase, the mechanism of separation, and the mode of operation. In general, chromatography is divided into two types: liquid chromatography and gas chromatography.

# 1. Liquid chromatography (LC)

Liquid chromatography is a separation technique that uses a liquid stationary phase to separate a sample into its constituents. Liquid chromatography is divided into the following categories:

- Normal phase chromatography: The stationary phase is polar (e.g., silica gel) while the mobile phase is nonpolar (e.g., hexane) in normal phase chromatography. This chromatography method is effective for separating polar substances.
- **Reverse phase chromatography:** The stationary phase in reverse phase chromatography is nonpolar (e.g., C18) while the mobile phase is polar (e.g.,

water). This chromatography method is excellent for separating nonpolar substances.

- **Ion exchange chromatography:** In ion exchange chromatography, the stationary phase includes charged groups (for example, DEAE cellulose) while the mobile phase contains ions with opposing charges. This chromatography method is effective for separating charged compounds like proteins and nucleic acids.
- Size exclusion chromatography: In size exclusion chromatography, the stationary phase is porous, and the mobile phase is a buffer solution. This type of chromatography separates molecules based on their size.
- Affinity chromatography: In affinity chromatography, the stationary phase contains a ligand that specifically binds to the molecule of interest (e.g., an antibody). This type of chromatography is helpful for purifying proteins and other biomolecules.

# 2. Gas chromatography (GC)

Gas chromatography is a separation technique that involves using a gas as the mobile phase and a solid or liquid stationary phase to separate the sample into its individual components. Gas chromatography can be further classified into the following categories:

- Gas-solid chromatography: In gas-solid chromatography, the stationary phase is a solid (e.g., silica gel) and the mobile phase is a gas (e.g., helium). This type of chromatography is useful for separating volatile organic compounds.
- **Gas-liquid chromatography:** In gas-liquid chromatography, the stationary phase is a liquid (e.g., a silicone oil) coated onto a solid support (e.g., diatomaceous earth) and the mobile phase is a gas (e.g., helium). This type of chromatography is useful for separating nonpolar and moderately polar compounds.

Overall, chromatography is a versatile technique that can be used for a wide range of applications, including drug discovery, environmental analysis, and protein purification.

### Thin layer chromatography

Thin layer chromatography (TLC) is a chromatographic technique for separating and analysing compound mixtures. TLC is a rapid, easy, and low-cost technique that is widely used in chemistry, biochemistry, and environmental science.

TLC operates on the same basic concept as other chromatographic techniques in that a sample is separated based on its interactions with a stationary and mobile phase. A thin layer of a solid material, such as silica gel, alumina, or cellulose, is deposited onto a flat surface in TLC, such as a glass plate or a plastic sheet. The mobile phase is a solvent that moves up the thin layer due to capillary action.

The steps involved in performing TLC are as follows:

- 1. **Prepare the TLC plate:** A thin layer of the stationary phase is coated onto a flat surface, such as a glass plate or a plastic sheet. The thickness of the layer can vary depending on the type of TLC being performed, but it is typically between 0.1 and 0.5 mm.
- 2. Prepare the sample: The sample is dissolved in a solvent that is compatible with the mobile phase and spotted onto the TLC plate using a micropipette or a capillary tube.
- **3. Develop the TLC plate:** The TLC plate is placed in a container with a little amount of mobile phase that is allowed to travel up the plate via capillary action. The mobile phase interacts with the stationary phase as it advances up the plate, causing the components of the sample to segregate depending on their differential interactions with the stationary phase.
- 4. Visualize the separation: The TLC plate is taken from the container and dried once the mobile phase has reached the top. By exposing the plate to a visualisation reagent, such as iodine, ninhydrin, or UV light, the separated components can be seen. Each component will appear as a spot on the plate, with its position and intensity depending on its interactions with the stationary phase.

It is used as a preliminary separation step before more advanced techniques, such as HPLC or GC. TLC is relatively easy to perform and requires minimal equipment, making it an ideal technique for routine analysis and screening of large samples.

### **Column Chromatography**

Column chromatography is a common laboratory technique used to separate and purify chemical compounds from a complex mixture. The technique relies on the differential interactions between the sample components and the stationary phase, which is packed into a long, narrow column. The separated components are collected as they elute from the column and can be further analyzed or purified.

The basic steps involved in performing column chromatography are as follows:

- 1. Choose the stationary phase: The stationary phase is often a solid material packed into the column, such as silica gel, alumina, or a polymer. The stationary phase chosen is determined by the type of sample being separated and the desired separation method.
- 2. Pack the column: The stationary phase is packed into a long, narrow column using a slurry of the stationary phase in a suitable solvent. The column is typically packed from the bottom to the top, with a frit or other filter at the bottom to prevent the stationary phase from escaping.
- **3. Load the sample:** The sample is dissolved in a suitable solvent and loaded onto the top of the column. The sample is then allowed to enter the column and interact with the stationary phase.
- 4. Elute the column: The sample is eluted from the column by passing a solvent through the column. Depending on the desired separation mechanism, the solvent can be either a single solvent or a gradient of solvents. As the solvent passes through the column, the sample components interact with the stationary phase and are separated based on their differential interactions.
- 5. Collect the fractions: The separated components are collected as they elute from the column using a fraction collector or manually collecting the fractions. The fractions can be further analyzed or purified as needed.

Column chromatography can be performed using different modes of operation, such as gravity flow, flash chromatography, or preparative chromatography. Gravity flow chromatography is the simplest mode but is slow and requires careful flow rate control. Flash chromatography is a faster mode that uses compressed air to force the solvent through the column. Preparative chromatography is a larger-scale version of column chromatography used to purify larger quantities of material. Overall, column chromatography is a powerful and versatile technique widely used in various scientific disciplines for separating and purifying chemical compounds.

# Ion Exchange Chromatography

Ion exchange chromatography (IEC) is a method of separating ions depending on their charge. The approach is often used to purify and separate biomolecules with a net charge at a certain pH, such as proteins and nucleic acids. The principle of IEC is based on the reversible binding of ions to charged stationary phases, which can be either cationic or anionic.

The basic steps involved in performing IEC are as follows:

- Choose the stationary phase: The stationary phase is typically a resin that is charged either positively (cation exchange) or negatively (anion exchange). The choice of stationary phase depends on the type of ions being separated and the desired separation mechanism.
- 2. Pack the column: The stationary phase is packed into a column, similar to the process of column chromatography. The sample is then loaded onto the top of the column.
- **3. Wash the column:** The column is washed with a buffer solution that matches the pH and ionic strength of the sample. This step ensures the stationary phase is fully equilibrated and ready to bind the sample ions.
- **4. Elute the column:** The sample is eluted from the column by passing a salt or pH gradient. As the salt or pH changes, the ions in the sample are displaced from the stationary phase and eluted from the column. The eluted fractions can be collected and further analyzed or purified.

IEC can be performed in different modes of operation, such as analytical, preparative, and continuous ion exchange chromatography. Analytical IEC is used to separate and analyse small quantities of ions or biomolecules. In contrast, preparative IEC is used to purify and isolate larger quantities of biomolecules. Continuous ion exchange chromatography is used for the production of large-scale biopharmaceuticals.

IEC has several advantages, including high resolution and specificity, compatibility with a wide range of biomolecules, and the ability to handle complex mixtures.

However, the technique has limitations, such as low sample loading capacity and the potential for non-specific binding. IEC is a powerful and widely used technique for separating and purifying charged biomolecules.

### **Electrophoresis**

Electrophoresis is a technique used to separate charged molecules based on their size and charge. It is commonly used in molecular biology and biochemistry to separate and analyze nucleic acids, proteins, and other charged molecules. The principle of electrophoresis is based on the migration of charged particles in an electric field, where the charge, size, and shape of the molecules determines the direction and rate of migration.

The basic steps involved in performing electrophoresis are as follows:

- Choose the electrophoresis medium: The electrophoresis medium is a gel or a solution that contains a matrix of charged particles, such as agarose or polyacrylamide. The choice of medium depends on the type of molecules being separated and the desired resolution.
- 2. **Prepare the sample:** The sample is prepared by mixing the charged molecules with a buffer solution and a loading buffer that contains a tracking dye. The loading buffer helps to visualize the sample during electrophoresis.
- **3. Load the sample:** The sample is loaded onto the electrophoresis medium using a pipette or a gel loading apparatus. The sample is loaded into a well or a slot in the medium.
- **4. Apply the electric field:** The electrophoresis medium is placed in a chamber filled with buffer solution and connected to a power supply. When the electric field is applied, the charged molecules in the sample migrate through the medium towards the oppositely charged electrode.
- **5. Visualize the separated molecules:** After electrophoresis, the separated molecules can be visualized using a staining solution, such as ethidium bromide for nucleic acids or Coomassie blue for proteins. The separated molecules can also be transferred to a membrane for further analysis.

Electrophoresis can be performed using different modes of operation, such as **agarose gel electrophoresis, polyacrylamide gel electrophoresis (PAGE), and capillary electrophoresis**. Agarose gel electrophoresis is used to separate large nucleic acids, such as genomic DNA, while PAGE is used to separate proteins and smaller nucleic acids. Capillary electrophoresis is a high-resolution technique used to separate small molecules, such as amino acids and carbohydrates.

Electrophoresis has several advantages, including high resolution, sensitivity, and versatility. However, the technique also has limitations, such as the potential for band distortion, variable band intensity, and the need for specialized equipment. Overall, electrophoresis is a powerful and widely used technique for the separation and analysis of charged molecules.

# **Multiple Batch Extraction**

Batch extraction is the process of simultaneously extracting multiple pieces of data from a source. It is a common task in data analysis and is often used to extract data from databases, web pages, or other sources. Multiple batch extraction involves extracting data from multiple sources or multiple parts of a source in one go.

- **7. Identify the sources:** The first step in multiple batch extraction is identifying the sources from which you want to extract data. This could be multiple databases, web pages, or different sections of a single web page.
- 8. Define the extraction criteria: Once you have identified the sources, you must define the criteria for extracting data. This could include specifying the fields or columns you want to extract, setting filters or search criteria, or defining the range of data you want to extract.
- **9.** Choose a tool: Many tools are available for batch extraction, ranging from simple web scrapers to more complex data extraction software. Choose a tool that fits your needs and is compatible with the sources you are working with.
- **10. Set up the extraction process:** Depending on the tool you are using, you may need to set up the extraction process by configuring the tool to connect to the source and specifying the extraction criteria.

- **11. Run the extraction:** Once the extraction process is set up, you can run the extraction and collect the data. Depending on the size of the data set, this may take some time.
- **12. Clean and analyze the data:** After the data has been extracted, you may need to clean it up and organize it for analysis. This could involve removing duplicates, formatting the data, or merging it with other data sets. Once the data is clean, you can analyze it to gain insights or create reports.

Overall, multiple batch extraction can be a powerful tool for data analysis, allowing you to extract and analyze large amounts of data quickly and efficiently. However, it requires careful planning and attention to detail to ensure that the data is extracted accurately and is useful for analysis.

# **Analytical Separations**

Analytical separations are techniques used to separate and identify components of a mixture based on their physical and chemical properties. Analytical separations are used in a variety of fields, including chemistry, biology, and environmental science, to determine the composition of complex mixtures.

There are several types of analytical separations, including chromatography, electrophoresis, and mass spectrometry. Each technique involves different principles and methods of separation and detection.

Chromatography is a separation technique based on the differential partitioning of a sample between two phases, one stationary and one mobile. The sample is introduced onto the stationary phase, which may be a solid or a liquid, and is then separated by the mobile phase, which is typically a liquid or a gas. The separated components of the sample are detected as they emerge from the column or other separation device. Chromatography can be further classified into different types, including gas chromatography (GC), liquid chromatography (LC), and ion chromatography (IC).

Electrophoresis is a technique that separates charged particles, such as proteins or DNA, in an electric field. The sample is placed on a gel matrix, and an electric field is applied, causing the charged particles to migrate through the gel at different rates.

The separated components of the sample can be detected using a variety of methods, including staining or labeling.

Mass spectrometry is a technique that separates and detects ions based on their massto-charge ratio. The sample is ionized, and the resulting ions are separated in a magnetic field based on their mass-to-charge ratio. The separated ions are then detected and quantified.

Analytical separations have many applications in industry, research, and medicine. For example, chromatography is used in the production of pharmaceuticals to separate and purify drug compounds. Electrophoresis is used in genetics and genomics research to separate and analyze DNA fragments. Mass spectrometry is used in proteomics and metabolomics to identify and quantify proteins and small molecules in complex mixtures.

In conclusion, analytical separations are a vital set of techniques used to separate and identify components of complex mixtures based on their physical and chemical properties. These techniques are widely used in various fields, including chemistry, biology, and environmental science, to determine the composition of complex mixtures. The selection of the appropriate technique for a particular application depends on the nature of the sample and the information required.

# **Principles of solvent extraction**

Solvent extraction is a method of isolating and purifying compounds or elements from a mixture. It involves the transfer of a solute from one solvent phase to another solvent phase, typically from an aqueous phase to an organic phase or vice versa. Solvent extraction is based on the principles of distribution or partitioning, where the solute distributes itself between two immiscible solvents, depending on its solubility and the solvents' properties.

The solvent extraction process consists of several steps, including mixing the two phases, allowing them to separate, and finally collecting and recovering the desired component from the solvent phase. The partition coefficient, Kd, which is defined as the ratio of the concentration of the solute in the organic phase to that in the aqueous phase at equilibrium, describes the solute's distribution between the two phases. Solvent extraction is commonly used in the purification of metals from their ores, such as the extraction of copper from copper ores using an organic solvent. The process involves leaching the ore with an aqueous solution containing the metal ion, followed by solvent extraction of the metal ion using an organic solvent such as an alkyl phosphine oxide.

The selection of the solvent system is crucial in the solvent extraction process. The solvent should be immiscible with the initial solvent phase and have a high affinity for the solute to ensure efficient extraction. The solvent should also be easy to separate from the solute and not react with the solute or other components of the mixture.

Solvent extraction is also used in the pharmaceutical industry for the purification of natural products and isolation of drug compounds from impurities. It is a useful technique for the separation of acidic, basic, and neutral compounds from complex mixtures, such as plant extracts.

In conclusion, solvent extraction is a widely used separation technique based on the principles of distribution or partitioning. It is a useful technique for the purification of metals from their ores, the isolation of drug compounds from impurities, and the separation of compounds from complex mixtures. The selection of the solvent system is a critical factor that affects the efficiency and selectivity of the solvent extraction process.

**Analytical spectrophotometry** is a technique used in analytical chemistry to determine the concentration and properties of a substance in a sample by measuring the absorption or transmission of electromagnetic radiation. This technique involves using a spectrophotometer, which measures light intensity as a function of wavelength or frequency.

There are several types of analytical spectrophotometry, each of which is suited to measuring specific properties of a sample. Some of the most common types of spectrophotometry include:

- **1. Ultraviolet-visible (UV-Vis) spectroscopy:** measures the absorption of ultraviolet and visible light by a sample, and is used to determine the concentration of chromophores, such as proteins and nucleic acids.
- 2. Infrared (IR) spectroscopy: measures the absorption of infrared radiation by a sample, and is used to identify functional groups in organic molecules and to determine the structure of complex molecules, such as proteins and polymers.
- **3.** Fluorescence spectroscopy: measures the emission of light by a sample after it has been excited by a light source, and is used to study the properties of fluorescent molecules, such as fluorescent dyes used in biological imaging.
- **4.** Atomic absorption spectroscopy (AAS): measures the absorption of light by free atoms in a sample, and is used to determine the concentration of metals in a sample.

Analytical spectrophotometry is a widely used and powerful technique in analytical chemistry, allowing for the determination of the concentration and properties of a wide range of analytes in various types of samples. It has numerous applications in fields such as environmental analysis, clinical chemistry, and biochemistry.

### **Examples of Analytical Spectrophotometry**

Here are some examples of analytical spectrophotometry:

- 1. Protein quantification using UV-Vis spectroscopy: UV-Vis spectroscopy is commonly used to quantify the concentration of proteins in a sample. This technique is based on the fact that proteins contain aromatic amino acids (such as tyrosine and tryptophan) that absorb light in the UV-Vis range. By measuring the absorbance of light at a specific wavelength (e.g., 280 nm), the concentration of protein in a sample can be determined.
- 2. Identification of unknown organic compounds using IR spectroscopy: IR spectroscopy is a powerful tool for identifying unknown organic compounds. Each functional group in an organic compound absorbs infrared radiation at a specific frequency, which produces a unique fingerprint that can be used for identification. The compound can be identified by comparing the IR spectrum of an unknown compound to a database of known spectra.

- **3.** Quantification of DNA using UV-Vis spectroscopy: UV-Vis spectroscopy can also be used to quantify the concentration of DNA in a sample. DNA absorbs light at 260 nm, so the concentration of DNA in a sample can be determined by measuring the absorbance of light at this wavelength. This technique is commonly used in molecular biology research.
- 4. Determination of trace metal concentrations in environmental samples using AAS: AAS is a highly sensitive technique that can be used to measure trace concentrations of metals in environmental samples. The sample is atomized and the free atoms absorb light at a specific wavelength, which allows the concentration of the metal to be determined. This technique is commonly used in environmental monitoring and quality control.

Overall, analytical spectrophotometry is a powerful and versatile technique that can be used to quantify and identify a wide range of compounds in various types of samples. It has numerous applications in research, industry, and environmental monitoring.

- **1.** Ultraviolet-visible (UV-Vis) spectroscopy: Properties of light and its interaction with matter
- Ultraviolet-visible (UV-Vis) spectroscopy is a technique used to measure the absorption of ultraviolet and visible light by a sample. To understand how UV-Vis spectroscopy works, it is important to first understand the properties of light and how it interacts with matter.
- Light is a form of electromagnetic radiation, which travels in waves and is characterized by its wavelength and frequency. The wavelength of light determines its color, with shorter wavelengths appearing blue and violet, and longer wavelengths appearing red and orange. The frequency of light is inversely proportional to its wavelength, meaning that shorter wavelengths have higher frequencies.
- When light passes through a sample, it can be absorbed, transmitted, or reflected. The amount of light that is absorbed or transmitted depends on the properties of the sample, including its chemical composition and structure.
- In UV-Vis spectroscopy, a sample is exposed to light in the UV-Vis range, typically between 200-800 nm. The sample absorbs some of the light, which

reduces the intensity of the light that is transmitted through the sample. The amount of light absorbed by the sample at a specific wavelength can be quantified by measuring the absorbance of the light using a spectrophotometer.

- The amount of light absorbed by a sample at a specific wavelength is proportional to the concentration of the absorbing species in the sample, as well as the path length of the sample and the molar absorptivity of the species. This relationship is described by the Beer-Lambert law:
- $A = \varepsilon lc$
- where A is the absorbance of the light,  $\varepsilon$  is the molar absorptivity of the absorbing species, l is the path length of the sample, and c is the concentration of the species.
- UV-Vis spectroscopy is commonly used to measure the concentration of chromophores, which are molecules that absorb light in the UV-Vis range. Chromophores include molecules such as proteins, nucleic acids, and pigments. By measuring the absorbance of light at a specific wavelength that corresponds to the chromophore, the concentration of the chromophore in a sample can be determined.

# 2. Infrared (IR) spectroscopy: Properties of light and its interaction with matter

- Infrared (IR) spectroscopy is a technique used to measure the absorption, transmission, and reflection of infrared radiation by a sample. To understand how IR spectroscopy works, it is important to first understand the properties of light and how it interacts with matter.
- Infrared radiation is a type of electromagnetic radiation with longer wavelengths than visible light. It is characterized by its frequency, which is inversely proportional to its wavelength. IR radiation can be divided into three regions: near-IR (NIR), mid-IR (MIR), and far-IR (FIR).
- When IR radiation passes through a sample, it can be absorbed, transmitted, or reflected. The amount of IR radiation that is absorbed or transmitted depends on the properties of the sample, including its chemical composition and structure.

- In IR spectroscopy, a sample is exposed to IR radiation, typically in the mid-IR range (4000-400 cm-1). The sample absorbs some of the IR radiation, which reduces the intensity of the radiation that is transmitted through the sample. The amount of IR radiation absorbed by the sample at a specific wavelength can be quantified by measuring the transmittance or absorbance of the radiation using a spectrophotometer.
- The amount of IR radiation absorbed by a sample at a specific wavelength is proportional to the concentration of the absorbing species in the sample, as well as the path length of the sample and the molar absorptivity of the species. This relationship is described by the Beer-Lambert law:
- $A = \log(Io/I) = \varepsilon lc$
- where A is the absorbance of the IR radiation, Io is the intensity of the incident radiation, I is the intensity of the transmitted radiation, ε is the molar absorptivity of the absorbing species, I is the path length of the sample, and c is the concentration of the species.
- IR spectroscopy is commonly used to identify and characterize the chemical composition of a sample, including functional groups and chemical bonds. Different functional groups and chemical bonds absorb IR radiation at specific frequencies, which produces a unique fingerprint that can be used for identification. By comparing the IR spectrum of an unknown sample to a database of known spectra, the sample can be identified.

# 3. Fluorescence spectroscopy: Properties of light and its interaction with matter

- Fluorescence spectroscopy is a technique used to measure the absorption and emission of light by a sample. To understand how fluorescence spectroscopy works, it is important to first understand the properties of light and how it interacts with matter.
- Light is a form of electromagnetic radiation, which travels in waves and is characterized by its wavelength and frequency. The wavelength of light determines its color, with shorter wavelengths appearing blue and violet, and longer wavelengths appearing red and orange. The frequency of light is

inversely proportional to its wavelength, meaning that shorter wavelengths have higher frequencies.

- When light passes through a sample, it can be absorbed, transmitted, or reflected. The amount of light that is absorbed or transmitted depends on the properties of the sample, including its chemical composition and structure.
- In fluorescence spectroscopy, a sample is exposed to the light of a specific wavelength, which causes the sample to absorb some of the light. This absorbed energy promotes an electron to a higher energy state. The electron then relaxes back to its ground state, emitting light of a longer wavelength than the excitation light. This emitted light is called fluorescence.
- The amount of fluorescence emitted by the sample depends on the concentration and properties of the fluorescent molecules in the sample, as well as the intensity of the excitation light and the detection sensitivity of the instrument. The fluorescence emission spectrum can be measured using a spectrofluorometer.
- Fluorescence spectroscopy is commonly used in biochemistry and biophysics to study the properties and behavior of fluorescent molecules, such as proteins and nucleic acids. Fluorescent molecules can be used as probes to study the interaction of biological molecules with each other and with their environment. By measuring the fluorescence emission of a sample, information about the sample's structure, conformation, and binding interactions can be obtained. Fluorescence spectroscopy can also be used to quantitatively analyse fluorescent molecules, such as in immunoassays or DNA sequencing.

# 4. Atomic absorption spectroscopy (AAS): Properties of light and its interaction with matter

- Atomic absorption spectroscopy (AAS) is a technique used to measure the concentration of atoms in a sample by measuring the absorption of light by the atoms. To understand how AAS works, it is important to first understand the properties of light and how it interacts with matter.
- Light is a form of electromagnetic radiation, which travels in waves and is characterized by its wavelength and frequency. The wavelength of light

determines its color, with shorter wavelengths appearing blue and violet, and longer wavelengths appearing red and orange. The frequency of light is inversely proportional to its wavelength, meaning that shorter wavelengths have higher frequencies.

- When light passes through a sample, it can be absorbed, transmitted, or reflected. The amount of light that is absorbed or transmitted depends on the properties of the sample, including its chemical composition and structure.
- In AAS, a sample is vaporized and atomized using a flame or plasma. The atoms in the sample are then excited by exposing them to light of a specific wavelength, which causes the atoms to absorb some of the light. The amount of light absorbed by the atoms is proportional to their concentration in the sample. The amount of light absorbed by the sample can be quantified by measuring the decrease in the intensity of the incident light using a spectrophotometer.
- The wavelength of the light used in AAS is specific to the element being measured, as different elements absorb light at different wavelengths. By measuring the absorption of light at the characteristic wavelength for a particular element, the concentration of that element in the sample can be determined.
- AAS is commonly used in analytical chemistry to measure the concentration of metal ions in a sample. It is particularly useful for analyzing trace amounts of metals in environmental and biological samples. AAS can also be used to determine the purity of chemicals and to monitor industrial processes.

# **Analytical Spectrophotometry: Relation Between Frequency**

- Analytical spectrophotometry involves the measurement of the interaction between light and matter, with the goal of determining the chemical composition, structure, or concentration of the sample being analyzed. The frequency of light plays a crucial role in this process, as it determines the energy of the light and how it interacts with the sample.
- The frequency of light is related to its wavelength by the formula  $c = \lambda v$ , where c is the speed of light,  $\lambda$  is the wavelength, and v is the frequency. This means that light with a shorter wavelength will have a higher frequency and vice versa.

- When light passes through a sample, it can be absorbed, transmitted, or reflected. The amount of light that is absorbed or transmitted by the sample depends on its chemical composition and structure, as well as the frequency of the incident light.
- In fluorescence spectroscopy, a sample is excited by light of a specific frequency, causing it to emit light of a different frequency. The frequency of the emitted light is lower than that of the incident light, due to the energy lost during relaxation of the excited state. The relationship between the frequency of the incident light and the emission of the sample is described by the Stokes shift, which is the difference between the excitation and emission wavelengths.
- In atomic absorption spectroscopy, a sample is vaporized and atomized, and the atoms in the sample are excited by light of a specific frequency. The frequency of the incident light is specific to the element being measured, as different elements absorb light at different frequencies. The amount of light absorbed by the atoms is proportional to their concentration in the sample.
- In summary, the frequency of light plays a critical role in analytical spectrophotometry, as it determines the energy of the incident light and how it interacts with the sample. The relationship between the frequency of the incident light and the absorption, emission, or excitation of the sample depends on the specific spectroscopic technique being used.

# **Analytical Spectrophotometry: Relation Between Frequency**

- In analytical spectrophotometry, the frequency of light plays a crucial role in determining the chemical composition of a sample. The frequency of light is related to the energy of the light wave, which in turn affects how the light interacts with matter.
- The relationship between frequency and energy is described by the equation E
  = hv, where E is the energy of the light, h is Planck's constant (6.626 × 10^-34 joule-seconds), and v is the frequency of the light. This equation shows that the energy of the light is directly proportional to its frequency. In other words, the higher the frequency of the light, the greater the energy of the light wave.

- This relationship between frequency and energy is important in many analytical techniques. For example, in UV-Vis spectroscopy, a sample is exposed to light in the UV and visible regions of the electromagnetic spectrum. The light interacts with the sample, and the amount of light absorbed or transmitted is measured. The amount of light absorbed or transmitted depends on the energy of the light, which is determined by its frequency.
- Infrared (IR) spectroscopy is another analytical technique that relies on the frequency of light. In this technique, a sample is exposed to infrared radiation, which causes molecular vibrations within the sample. The frequency of the infrared radiation is chosen to match the natural frequency of the molecular vibrations in the sample. The amount of light absorbed or transmitted by the sample depends on the strength of these vibrations, which in turn depends on the chemical composition of the sample.
- The relationship between frequency and wavelength is also important in analytical spectrophotometry. The wavelength of light is related to its frequency by the equation λ = c/v, where λ is the wavelength, c is the velocity of light, and v is the frequency. This means that light with a higher frequency (and shorter wavelength) has a shorter wavelength than light with a lower frequency (and longer wavelength). The relationship between frequency and wavelength is used to determine the range of frequencies or wavelengths that will interact with a given sample in a particular analytical technique.

# Analytical Spectrophotometry: Relation Between Wave Number

- In analytical spectrophotometry, wave number (v) is a unit of measurement used to describe the frequency of light. The wave number is defined as the reciprocal of the wavelength of the light, multiplied by a factor of 10<sup>7</sup> to convert from meters to centimeters. The relationship between wave number, frequency, and wavelength is given by the equation:
- $\tilde{v} = 1/\lambda \ge 10^7 = v/c \ge 10^7$
- where v
   is the wave number, λ is the wavelength, v is the frequency, and c is
   the velocity of light.

- The wave number is particularly useful in infrared (IR) spectroscopy, where it is commonly used to describe the frequency of molecular vibrations. In IR spectroscopy, a sample is exposed to infrared radiation, which causes molecular vibrations within the sample. The frequency of the infrared radiation is matched to the natural frequency of the molecular vibrations in the sample. The amount of light absorbed or transmitted by the sample depends on the strength of these vibrations, which in turn depends on the chemical composition of the sample.
- The wave number is a convenient way to describe the frequency of these molecular vibrations because it is directly proportional to the energy of the vibration. Stronger molecular vibrations have higher wave numbers, while weaker vibrations have lower wave numbers. The wave number is also used to identify specific functional groups within a molecule based on their characteristic vibrations.
- In summary, wave number is a unit of measurement used to describe the frequency of light in analytical spectrophotometry. It is particularly useful in IR spectroscopy for describing the frequency of molecular vibrations. The wave number is directly proportional to the energy of the vibration and is used to identify specific functional groups within a molecule based on their characteristic vibrations.

# Lambert-Beer's law

- Lambert-Beer's law (also known as Beer-Lambert law or Beer's law) describes the relationship between the concentration of a solute in a solution and the amount of light absorbed or transmitted by the solution. The absorbance (A) of a solution is directly proportional to the solute concentration (c) and the path length (l) of the solution, and inversely proportional to the amount of light (I) transmitted through the solution, according to the law. The law is stated mathematically as:
- $A = \epsilon c l$

- where A is the solution's absorbance, is the molar absorptivity or extinction coefficient (a constant that depends on the chemical identity of the solute and the wavelength of light), c is the solute concentration in moles per litre (M), and l is the solution's path length in centimeters.
- The law covers all electromagnetic radiation, including visible, ultraviolet, and infrared light. It is often used in analytical chemistry to calculate the concentration of a solute in a solution based on the solution's absorbance of light at a specific wavelength.
- For example, let's consider a solution of a colored compound that absorbs light at a wavelength of 500 nm. A spectrophotometer is used to measure the absorbance of the solution, which is found to be 0.5. The path length of the solution is 1 cm. The molar absorptivity of the compound at 500 nm is known to be 1000 M^-1 cm^-1. Using Beer's law, we can calculate the concentration of the compound in the solution:
- $A = \epsilon c l$
- $0.5 = (1000 \text{ M}^{-1} \text{ cm}^{-1}) \text{ x} (\text{c}) \text{ x} (1 \text{ cm})$
- c = 0.0005 M
- Therefore, the concentration of the colored compound in the solution is 0.0005 M.

### Limitations of Lambert-Beer's law

While Lambert-Beer's law is a useful principle for quantitative analysis, it has some limitations that should be considered. Here are some of the limitations:

1. Valid only within a certain concentration range: Lambert-Beer's law is valid only within a certain concentration range, typically up to about 1 absorbance unit (AU). The law may not hold properly at higher concentrations due to interactions between the solute molecules, leading to deviations from the linear relationship between absorbance and concentration.

- 2. Valid only for monochromatic light: The law assumes that the light source is monochromatic (i.e., of a single wavelength). In practice, most light sources are polychromatic (i.e., consisting of multiple wavelengths), so the law may not be accurate for all wavelengths.
- 3. Valid only for dilute solutions: The law assumes that the solution is dilute (i.e., the solute molecules are well separated from each other), so that the absorption of each molecule is independent of the others. The law may not hold true for concentrated solutions or with strong intermolecular interactions.
- 4. **Assumes homogeneity of the sample**: The law assumes that the sample is homogeneous, with no spatial variations in concentration or other physical properties. For samples with spatial variations, the absorbance may vary with position and the law may not be applicable.
- 5. Sensitivity to experimental conditions: Lambert-Beer's law is sensitive to experimental conditions, such as temperature, pH, and solvent composition. Any changes in these conditions can affect the molar absorptivity and the accuracy of the law.

Overall, while Lambert-Beer's law is a useful principle for spectrophotometric analysis, it is important to be aware of its limitations and to ensure that the experimental conditions are appropriate for the application.

### Single beam spectrophotometer

A single-beam spectrophotometer is a type of spectrophotometer that is widely used in analytical chemistry to measure the absorbance of a sample. It measures the absorbance of light at a particular wavelength, which can be used to determine the concentration of a solute in a solution. Here's an explanation of how a single-beam spectrophotometer works:

- 1. Light Source: The spectrophotometer uses a light source that emits a beam of light, typically a tungsten filament lamp, a deuterium lamp, or a light-emitting diode (LED).
- 2. Monochromator: The beam of light is then passed through a monochromator, which is a device that separates the light into its component wavelengths. This is typically done using a diffraction grating or a prism.

- **3. Sample Holder:** The monochromatic beam of light is then directed through a sample holder containing the sample. The sample holder is typically a cuvette made of quartz or glass with a path length of 1 cm.
- **4. Detector:** After passing through the sample, the light is detected by a photosensitive detector, such as a photodiode or a photomultiplier tube. The detector measures the intensity of the light, which is typically converted to an electrical signal that can be displayed on a computer or a chart recorder.
- **5.** Calibration: Before analyzing a sample, the spectrophotometer is calibrated using a blank solution, which is a solvent that does not contain the solute of interest. The blank solution is used to set the instrument to zero absorbance at the selected wavelength.
- 6. Absorbance Measurement: Once the instrument is calibrated, the sample is placed in the sample holder and the absorbance is measured. The absorbance is calculated as the negative logarithm of the ratio of the intensity of the light before and after passing through the sample, according to the Lambert-Beer's law equation A = log(Io/I), where A is the absorbance, Io is the intensity of the incident light, and I is the intensity of the transmitted light.
- 7. Calculation of Concentration: The absorbance of the sample is then used to calculate the concentration of the solute using the Lambert-Beer's law equation C = A/εl, where C is the concentration, ε is the molar absorptivity, and l is the path length of the sample holder.

In summary, a single-beam spectrophotometer is a relatively simple device that uses a light source, a monochromator, a sample holder, and a detector to measure the absorbance of a sample. It is widely used in analytical chemistry for quantitative analysis of various solutes in solution.

# **Double Beam Spectrophotometer**

A double-beam spectrophotometer is a type of spectrophotometer that is commonly used in analytical chemistry for quantitative analysis of various solutes in solution. It is similar to a single-beam spectrophotometer but has two separate beams of light used to simultaneously measure the sample and the reference. Here's a detailed explanation of how a double beam spectrophotometer works:

- 1. Light Source: The spectrophotometer uses a light source that emits a beam of light, typically a tungsten filament lamp, a deuterium lamp, or a light-emitting diode (LED).
- 2. Monochromator: The beam of light is then passed through a monochromator, which is a device that separates the light into its component wavelengths. This is typically done using a diffraction grating or a prism.
- **3. Beam Splitter:** The monochromatic beam of light is then directed through a beam splitter, which divides the light into two separate beams: the sample beam and the reference beam.
- **4. Sample Holder:** The sample beam is directed through a sample holder containing the sample. The sample holder is typically a cuvette made of quartz or glass with a path length of 1 cm.
- **5. Detector:** After passing through the sample, the sample beam is detected by a photosensitive detector, such as a photodiode or a photomultiplier tube. The detector measures the intensity of the light, which is typically converted to an electrical signal that can be displayed on a computer or a chart recorder.
- 6. **Reference Holder:** The reference beam is directed through a reference holder containing a blank solution, which is a solvent that does not contain the solute of interest. The reference holder is also typically a cuvette made of quartz or glass that has a path length of 1 cm.
- **7. Reference Detector:** After passing through the reference holder, the reference beam is detected by another photosensitive detector, which measures the intensity of the light.
- **8.** Calibration: The spectrophotometer is calibrated using the blank solution in the reference holder before analysing a sample. The blank solution is used to set the instrument to zero absorbance at the selected wavelength.
- **9.** Absorbance Measurement: Once the instrument is calibrated, the sample is placed in the sample holder and the absorbance of the sample beam and the reference beam are simultaneously measured. The absorbance is calculated as the negative logarithm of the ratio of the intensity of the sample beam and the intensity of the reference beam, according to the Lambert-Beer's law equation  $A = \log(Io/I)$ , where A is the absorbance, Io is the intensity of the incident light, and I is the intensity of the transmitted light.

10. Calculation of Concentration: The absorbance of the sample is then used to calculate the concentration of the solute using the Lambert-Beer's law equation C = A/εl, where C is the concentration, ε is the molar absorptivity, and l is the path length of the sample holder.

In summary, a double-beam spectrophotometer is a more advanced type of spectrophotometer that uses two separate beams of light to simultaneously measure the sample and the reference, improving the measurement's accuracy and precision. It is widely used in analytical chemistry for quantitative analysis of various solutes in solution.

### **Difference Between Single and Double Beam Spectrophotometers**

Single-beam and double-beam spectrophotometers are both commonly used in analytical chemistry for quantitative analysis of various solutes in solution. Still, they differ in how they measure a sample's absorbance. Here are some key differences between the two:

- 1. Optical Design: In a single-beam spectrophotometer, there is only one path for light, which passes through the sample and then to the detector. In contrast, a double-beam spectrophotometer splits the beam of light into two separate paths: one for the sample and the other for a blank/reference solution. This allows for simultaneous measurement of the sample and the reference, which can improve accuracy and precision.
- 2. Stability: A single-beam spectrophotometer is typically less stable than a double-beam spectrophotometer. This is because changes in the intensity of the light source or the detector can affect the measurement's accuracy since no reference measurement is being taken. In contrast, a double-beam spectrophotometer takes a reference measurement, which can help to correct for changes in the intensity of the light source or detector.
- **3.** Calibration: A single-beam spectrophotometer requires frequent calibration since the light source and detector can drift over time, leading to inaccurate measurements. In contrast, a double-beam spectrophotometer is typically calibrated once daily since the reference measurement can help correct any drift in the light source or detector.

- 4. Sample Throughput: A single beam spectrophotometer can measure only one sample at a time, which can limit the speed of analysis. In contrast, a double-beam spectrophotometer can measure two samples simultaneously, increasing the analysis speed.
- **5.** Cost: Double-beam spectrophotometers are typically more expensive than single beam spectrophotometers due to their more complex optical design and additional components.

In summary, while both single-beam and double-beam spectrophotometers are helpful for the quantitative analysis of solutes in solution, double-beam spectrophotometers offer some advantages over single-beam spectrophotometers in terms of stability, speed of analysis, and accuracy but come at a higher cost.

# Lasers and Lamps as Sources of Light in Spectrophotometry

- Lasers and lamps are two common sources of light used in spectrophotometry, each with its own advantages and limitations.
- Laser sources provide intense, monochromatic light with a narrow wavelength range, making them useful for various analytical applications, such as fluorescence and Raman spectroscopy. They can also provide high power density, which can benefit certain applications requiring high sensitivity or precision.
- However, laser sources can be expensive and may require specialized knowledge to operate and maintain. Additionally, they typically provide a limited range of wavelengths, which can make them less versatile than broadspectrum light sources like lamps.
- Lamps, on the other hand, provide a broad spectrum of light with a range of wavelengths, which makes them useful for a wide range of applications in spectrophotometry, such as UV-Vis and IR spectroscopy. They are also relatively inexpensive and easy to operate.
- However, lamps may not provide the same level of intensity as laser sources, which can limit their sensitivity and precision in some applications. They may also require frequent replacement, particularly if they are used frequently or at high intensity, which can increase their cost over time.

• In summary, both lasers and lamps have their own advantages and limitations as light sources in spectrophotometry, and the choice of the source depends on the specific application and the analysis requirements.

### **Monochromators in Spectrophotometry**

- Monochromators are an important component of many spectrophotometers, particularly those used for UV-Vis and fluorescence spectroscopy. A monochromator is a device that selectively filters and isolates a narrow range of wavelengths from a broader light spectrum. It then excites a sample or measures its absorption or emission properties.
- A typical monochromator is made up of three major parts: an entry slit, a diffraction grating or prism, and an exit slit. Only a narrow beam of light enters the monochromator through the entrance slit, which is then dispersed into its constituent wavelengths by the diffraction grating or prism. After that, the exit slit selects only a restricted range of wavelengths to get through to the sample or detector.
- Monochromators can be manually or electronically adjusted to select a specific wavelength range for measurement, which allows for greater flexibility and precision in spectrophotometric analysis. Some advanced spectrophotometers also have multiple or tunable monochromators, which can provide even greater flexibility in selecting specific wavelength ranges.
- Overall, monochromators play a critical role in spectrophotometric analysis by allowing for precise control and selection of the wavelengths used for measurement, which is essential for the accurate and reliable analysis of samples.

# **Detectors in Spectrophotometry**

In spectrophotometry, detectors are used to measure the intensity of light transmitted or absorbed by a sample at different wavelengths. The choice of the detector depends on the wavelength range of interest and the sensitivity required for the application.

Some commonly used detectors in spectrophotometry include:

- **1. Photomultiplier tube (PMT):** This is a high-sensitivity detector that can detect very low levels of light. PMTs are often used in fluorescence spectroscopy because of their high sensitivity to low-level light emissions.
- 2. Charge-coupled device (CCD): This detector is commonly used in UV-Vis spectrophotometers. It consists of an array of photodiodes that can be read out electronically. CCDs have good sensitivity, and their signal-to-noise ratio is also high.
- **3. Photodiode array (PDA):** This detector is similar to the CCD but contains multiple photodiodes arranged in a linear array. PDAs are often used in high-resolution UV-Vis spectrophotometers.
- **4. Integrating sphere:** This detector measures diffuse reflectance and transmittance. It comprises a hollow sphere with a diffuse reflective inner surface and a small aperture for sample entry.
- 5. Infrared detectors: Infrared detectors are used in infrared spectrophotometers. Several types of infrared detectors include thermocouples, Golay cells, and pyroelectric detectors. These detectors are sensitive to the infrared range of the electromagnetic spectrum.

Overall, the choice of the detector in spectrophotometry depends on the specific application and the range of wavelengths of interest.

# **Photomultiplier Tubes in Spectrophotometry**

- Photomultiplier tubes (PMTs) are widely used in spectrophotometry due to their high sensitivity and low noise characteristics. PMTs work by converting light photons into electrical signals, which are then amplified by a series of dynodes.
- In spectrophotometry, PMTs are often used in applications where the sample emits low light levels, such as in fluorescence or Raman spectroscopy. PMTs are also used in detectors for liquid chromatography and capillary electrophoresis.
- PMTs have several advantages over other detectors in spectrophotometry. They have high sensitivity to low levels of light, a wide dynamic range, and a fast response time. They are also less affected by ambient light and have low dark currents.

 However, PMTs also have some limitations. They are more expensive than other detectors, can be affected by magnetic fields, and require a high-voltage power supply. They are also sensitive to temperature changes, which can affect their stability and performance.

### **Photodiode Array**

- A photodiode array (PDA) is a type of detector used in spectrophotometry that contains an array of photodiodes arranged in a linear pattern. PDAs are commonly used in high-resolution UV-Vis spectrophotometers.
- When light enters a PDA, it is dispersed by a diffraction grating or prism, and each wavelength of light falls on a different photodiode. The electrical current generated by each photodiode is proportional to the amount of light that falls on it. The resulting signal from each photodiode is then combined to produce a spectrum of the sample.
- PDAs offer several advantages over other detectors in spectrophotometry. They have a high spectral resolution, which makes them useful for analyzing narrow spectral features. They also have a fast acquisition time and a large dynamic range, which allows them to detect a wide range of light intensities.
- One limitation of PDAs is that they are more expensive than some other detectors, such as photomultiplier tubes or charge-coupled devices. They are also more complex to operate and require specialized electronics for signal processing. However, their high spectral resolution and fast acquisition time make them ideal for applications that require high precision and speed, such as in pharmaceutical or environmental analysis.

# **Charged Couple Device**

• A charged-coupled device (CCD) is a type of detector used in spectrophotometry that consists of an array of photodiodes that can be read out electronically. Each photodiode in the array is sensitive to a specific wavelength range of light. When light strikes the photodiodes, it creates an electrical charge that is then transferred from one photodiode to the next in a process known as "charge-coupling."

- CCDs are widely used in UV-Vis spectrophotometers because they offer several advantages over other types of detectors. They have high sensitivity, fast response times, and low noise. They also have a high signal-to-noise ratio, making them ideal for low-level light detection.
- CCDs are particularly useful in applications that require detecting weak signals, such as in fluorescence spectroscopy or analysing samples with low concentrations. They can also measure multiple wavelengths simultaneously, making them ideal for spectral scanning.
- One limitation of CCDs is that they are sensitive to temperature fluctuations, which can affect their performance. They also have a smaller dynamic range than other types of detectors, such as photomultiplier tubes (PMTs). However, the high sensitivity and low noise of CCDs make them an excellent choice for many types of spectrophotometry applications.

### **FT-IR Spectroscopy**

- Fourier Transform Infrared (FT-IR) Spectroscopy is a technique used in analytical chemistry to obtain information about the vibrational modes of molecules. It is based on the interaction of infrared radiation with matter, and the resulting absorption or transmission spectra can be used to identify and quantify the presence of various functional groups and chemical bonds in a sample.
- In FT-IR spectroscopy, a beam of infrared light is directed through the sample and the resulting transmitted or absorbed light is measured. The signal is then analyzed using a Fourier Transform algorithm to generate a spectrum that shows the intensity of the absorbed or transmitted light as a function of the frequency or wavelength of the radiation. The resulting spectra are highly specific to the sample's chemical composition and can be used for qualitative and quantitative analysis.
- FT-IR spectroscopy is widely used in a range of applications, including pharmaceuticals, polymers, food, and environmental analysis. It can be used to analyze solids, liquids, and gases, and is particularly useful for analysing complex mixtures.
- One major advantage of FT-IR spectroscopy is its high sensitivity and selectivity. It can detect very small amounts of analytes and provide detailed information about their chemical structure. It is also a non-destructive technique, meaning samples can be analyzed without alteration or destruction.
- However, FT-IR spectroscopy does have some limitations. It is often limited in its ability to provide information about the spatial distribution of analytes, and it may not be suitable for analysing highly absorbing or scattering samples. Additionally, the interpretation of spectra can be complex and requires expertise in the field of vibrational spectroscopy.

#### **Fourier Analysis in FT-IR**

- In FT-IR spectroscopy, Fourier analysis is used to transform the raw data from a time-domain signal (the interferogram) into a frequency-domain spectrum. This is done using a mathematical technique called a Fourier transform, which converts the interferogram data from the time domain into the frequency domain.
- The interferogram is obtained by measuring the interference pattern of a beam of infrared light that has passed through a sample and a reference. This interference pattern contains information about the absorption of the sample at different frequencies. By performing a Fourier transform on the interferogram, this information can be extracted and presented in the form of a frequency-domain spectrum.
- The resulting FT-IR spectrum shows the intensity of the absorbed or transmitted light as a function of the frequency or wavelength of the radiation. The peaks in the spectrum correspond to the different vibrational modes of the molecular bonds in the sample, and can be used to identify and quantify the presence of various functional groups and chemical bonds in the sample.
- In FT-IR spectroscopy, Fourier analysis is an essential part of data processing and interpretation, allowing for the extraction of valuable information from the raw interferogram data.

#### **Interferometry in FT-IR**

- Interferometry is a technique used in FT-IR spectroscopy to obtain a highly precise and accurate measurement of the transmitted or reflected light intensity from a sample. In FT-IR spectroscopy, interferometry is used to measure the interference pattern between a sample beam and a reference beam of infrared light.
- The interferometer is the key component of an FT-IR spectrometer, and it consists of several mirrors that split the incoming infrared light into two beams. One beam is directed to the sample, while the other is directed to a reference mirror. After reflecting off the sample and the reference mirror, the beams are recombined at a detector, which measures the resulting interference pattern.
- The interference pattern is known as an interferogram, containing information about the sample's absorbance or transmittance at different frequencies. The interferogram is then processed using a Fourier transform to generate a spectrum that shows the intensity of the absorbed or transmitted light as a function of the frequency or wavelength of the radiation.
- Interferometry in FT-IR spectroscopy has several advantages. It provides highly accurate and precise measurements of the intensity of the transmitted or reflected light, and it is capable of measuring the entire spectrum of the sample in a single measurement. This allows for rapid and efficient analysis of complex samples.
- However, interferometry also has some limitations. It requires a highly stable and accurate interferometer, which can be expensive and difficult to maintain. Additionally, interferometry is sensitive to environmental factors such as temperature and vibration, which can affect the accuracy and precision of the measurements.

#### **Noise and Control in FT-IR**

 Noise is a common issue in FT-IR spectroscopy, and it can significantly affect the accuracy and precision of the measurements. In FT-IR spectroscopy, there are several sources of noise, including electronic noise, detector noise, and background noise.

- Electronic noise can be reduced by using high-quality electronic components, such as low-noise amplifiers and analog-to-digital converters. Detector noise can be reduced using high-quality detectors with low noise levels, such as liquid-nitrogen-cooled mercury cadmium telluride (MCT) detectors. Background noise can be reduced by using appropriate background subtraction techniques, such as the use of a reference sample or a blank sample.
- In addition to these hardware-based noise reduction techniques, there are also several software-based noise reduction techniques that can be used in FT-IR spectroscopy. These include averaging multiple scans, smoothing the spectrum using digital filters, and using advanced signal processing techniques like wavelet transforms.
- To control noise in FT-IR spectroscopy, it is important to design and optimize the experimental setup carefully, and to use appropriate noise reduction techniques during data processing. This may include optimizing the sample preparation and handling, selecting appropriate instrumental settings, and using appropriate data processing techniques.
- Overall, controlling noise in FT-IR spectroscopy is essential for obtaining accurate and precise measurements, and it requires careful attention to the experimental design and data processing techniques.

### **Classical Analytical methods: Acid-Base**

- The acid-base titration method is a traditional analytical method for determining the concentration of an unknown acid or base solution by reacting it with a known concentration of acid or base solution. The acid-base process is a neutralization reaction that creates salt and water. When the acid and base are totally neutralized and the solution is neither acidic nor basic, the reaction has achieved its equivalence point.
- The acid-base titration method requires several steps. First, a known volume of the unknown solution is placed in a flask or beaker. A suitable indicator is added to the solution to help determine when the equivalence point is reached. Then, a known concentration of the titrant (either an acid or a base) is slowly added to the solution while stirring until the endpoint is reached, as indicated by the change in color of the indicator.

- The endpoint of the reaction is the point at which the acid and base are completely neutralized, and the solution is neither acidic nor basic. At this point, the amount of titrant added equals the amount of the unknown solution present. The concentration of the unknown solution can then be calculated using the stoichiometry of the neutralization reaction and the volume and concentration of the titrant solution.
- An acid-base titration is a widely used analytical method due to its simplicity, speed, and accuracy. It can be used to determine the concentration of a wide range of acids and bases and is particularly useful for determining the concentration of weak acids or bases, which are difficult to measure using other analytical methods.

#### **Complexometric and Redox Titrations**

- Complexometric titration is a classical analytical method used to determine the concentration of metal ions in a solution by reacting them with a known amount of a chelating agent (complexing agent) that forms a complex with the metal ions. The chelating agent typically has multiple donor atoms that form coordination bonds with the metal ion. The formation of the metal-chelate complex is indicated by a color change or other observable property.
- The endpoint of the complexometric titration is reached when all of the metal ions have reacted with the chelating agent and are present in the form of the metal-chelate complex. The concentration of the metal ion can then be calculated based on the stoichiometry of the reaction and the amount of chelating agent added.
- Redox titration is another classical analytical method used to determine the concentration of a substance in a solution by reacting it with a known amount of an oxidizing or reducing agent. Redox titrations are typically used to determine the concentration of substances that are capable of undergoing oxidation or reduction reactions. The endpoint of the redox titration is reached when all of the substance being analyzed has reacted with the oxidizing or reducing agent and the stoichiometric equivalence point has been reached.
- Redox titrations can be carried out using a variety of oxidizing or reducing agents, depending on the substance being analyzed. Common oxidizing agents

used in redox titrations include potassium permanganate, potassium dichromate, and iodine. Common reducing agents used in redox titrations include sodium thiosulfate, ascorbic acid, and ferrous ammonium sulphate.

• Overall, complexometric and redox titrations are widely used classical analytical methods due to their simplicity, speed, and accuracy. They can be used to determine the concentration of a wide range of substances and are particularly useful for analyzing metal ions and substances capable of undergoing oxidation or reduction reactions.

#### **Gravimetric Analysis**

- Gravimetric analysis is a classical analytical method used to determine the amount of a substance present in a sample by measuring its mass. This method involves isolating the substance of interest in a pure form, typically by precipitation or volatilization, and then weighing the resulting solid or gas.
- In gravimetric analysis, a known sample volume is taken, and the substance of interest is separated from the other components of the sample. The separated substance is then collected and weighed, and the mass of the substance is used to calculate its concentration in the original sample.
- Gravimetric analysis requires careful attention to experimental details to ensure accurate and precise results. The sample must be carefully prepared and weighed, and the conditions of the separation process must be controlled to ensure complete isolation of the substance of interest. In addition, the purity of the separated substance must be confirmed through additional tests, such as melting point determination or chemical analysis.
- Gravimetric analysis is commonly used in the analysis of metals, particularly in the determination of the composition of alloys. It is also used in the analysis of inorganic compounds, such as salts and minerals. While gravimetric analysis is a time-consuming and labor-intensive method, it is a highly accurate and precise method for the determination of the amount of a substance present in a sample.

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## BASICS TO ADVANCED ENVIRONMENTAL CHEMISTRY

Yasmeen JUNEJO Mehmet ÖZASLAN

#### **Atmospheric Pollution**

The presence of hazardous substances in the air we breathe is referred to as atmospheric pollution, commonly known as air pollution. These compounds can be gases, particles, or biological molecules that are harmful to human, animal, and environmental health.

Examples of atmospheric pollutants include:

- Particulate matter is defined as small particles of solid or liquid substances suspended in air. These can be emitted by construction sites, wildfires, or vehicle exhaust. Particulate particles can enter the lungs and cause respiratory issues.
- Carbon monoxide (CO): A colorless and odorless gas created by incomplete combustion of fossil fuels. It is extremely poisonous and can result in severe headaches, dizziness, and even death in high quantities.
- When fossil fuels are used, Sulphur dioxide (SO2) is created, mainly in power plants and industry. It can irritate the lungs and contribute to acid rain.
- Nitrogen oxides (NOx) are gases created by the combustion of fossil fuels, particularly in transportation. They can contribute to smog and acid rain generation, as well as respiratory difficulties.
- When nitrogen oxides and volatile organic compounds (VOCs) combine with sunlight, ozone (O3) is generated. It can cause respiratory issues and contribute to smog development.
- VOCs are chemicals that are emitted by items such as paints, solvents, and cleaning agents. They can contribute to smog formation and be hazardous to human health.
- As a result, air pollution can have major consequences for human health and the ecosystem. It is critical that we take actions to reduce our pollution emissions and enhance the quality of the air we breathe.

### The atmosphere and Atmospheric Pollution

• The atmosphere is the layer of gases that surrounds and holds the Earth together. It is mostly made up of nitrogen (78%), oxygen (21%), and trace amounts of other gases such carbon dioxide, water vapors, and neon.

- The atmosphere is separated into layers, each with its own set of properties and functions. The troposphere, the lowest layer, is where weather occurs and the majority of the Earth's air pollution is found. The stratosphere is located above the troposphere and contains the ozone layer, which is critical in protecting the Earth from damaging ultraviolet radiation.
- The atmosphere is critical to the survival of life on Earth. It maintains the planet's temperature, provides oxygen for breathing, and shields it from dangerous radiation.
- Human activities such as fossil fuel combustion and deforestation have released large amounts of pollutants into the atmosphere, contributing to atmospheric pollution and climate change. To preserve a healthy and sustainable ecosystem for future generations, we must limit our pollution emissions and conserve the environment.

## **Composition of Atmospheric Pollution**

The components of atmospheric pollution, also known as air pollution, can be categorized into two main types: primary pollutants and secondary pollutants.

- **1. Primary pollutants**: These are pollutants that are released into the atmosphere directly from a source. Primary pollutants include the following:
- Particulate matter is defined as tiny particles of solid or liquid materials suspended in the air.
- Carbon monoxide (CO): A colourless and odourless gas created by incomplete combustion of fossil fuels.
- Sulphur dioxide (SO2) is a gas created by the combustion of fossil fuels, mainly in power plants and industry.
- Nitrogen oxides (NOx): Gases created by the combustion of fossil fuels, particularly in transportation.
- VOCs (volatile organic compounds): Chemicals emitted by items such as paints, solvents, and cleaning agents.
- **2.** Secondary pollutants are those that develop in the atmosphere as a result of chemical interactions between main pollutants and other substances. Secondary pollutants include the following:
- Ozone (O3): A gas generated by the reaction of nitrogen oxides with volatile organic compounds (VOCs) in the presence of sunshine.
- Sulfuric acid (H2SO4): An acid generated when sulphur dioxide in the atmosphere combines with water.
- Nitric acid (HNO3): An acid generated in the atmosphere when nitrogen dioxide combines with water.

- Photochemical smog: A pollutant combination created by the reaction of nitrogen oxides and volatile organic compounds (VOCs) in the presence of sunshine.
- Because these pollutants can impair human health, animal health, and the ecosystem, it is critical that we minimize our emissions of these pollutants and enhance the quality of the air we breathe.

## **Role of Temperature in Atmospheric Pollution**

Temperature plays an important role in atmospheric pollution as it can affect the chemical reactions and physical processes that occur in the atmosphere. Some of the ways that temperature can influence atmospheric pollution are:

- **Temperature inversions:** When a layer of warm air builds above a layer of cool air, contaminants in the bottom layer become trapped. This can happen on calm, clear nights when the ground cools quickly, resulting in significant concentrations of pollutants in urban areas.
- Chemical reactions: Temperature can affect the rate of chemical reactions that occur in the atmosphere. For example, some chemical reactions that produce ozone (a secondary pollutant) are faster at higher temperatures, while others are slower. The temperature can also affect the stability of some pollutants, such as nitrogen oxides, which can break down at higher temperatures.
- Volatile organic compounds (VOCs): Temperature can affect the rate at which volatile organic compounds (VOCs) evaporate from sources such as paints, solvents, and cleaning agents. Higher temperatures can increase the evaporation rate, leading to higher VOC concentrations in the air.
- Climate change: Temperature is also a key factor in climate change, which can significantly impact atmospheric pollution. As temperatures warm, it can change weather patterns, such as more frequent and severe heatwaves, droughts, and wildfires. These events can release more pollutants into the atmosphere and lead to higher concentrations of pollution.
- As a result, the temperature can play a complex role in atmospheric pollution, and it is important to understand how it can influence the sources, concentrations, and chemical reactions of pollutants in the air. By reducing our emissions of pollutants and mitigating climate change, we can help to improve the quality of the air we breathe and protect the health of the environment.

### **Role of Pressure in Atmospheric Pollution**

Pressure is an important factor in atmospheric pollution as it can affect the movement and behavior of air pollutants in the atmosphere. Some of the ways that pressure can influence atmospheric pollution are:

- Atmospheric mixing: Pressure differences between different regions of the atmosphere can cause air to move, which can lead to the mixing of pollutants. For example, high pressure systems can create sinking air that traps pollutants near the surface, while low pressure systems can create rising air that disperses pollutants.
- **Emissions:** Pressure can affect the emissions of pollutants from sources such as vehicles and industrial processes. For example, higher pressure can increase the combustion efficiency of engines, leading to lower emissions of pollutants such as carbon monoxide (CO) and nitrogen oxides (NOx).
- **Particle formation:** Pressure can also affect the formation of particles in the atmosphere. Some types of particles, such as ammonium sulfate and ammonium nitrate, are more likely to form at higher pressures, while others, such as sea salt particles, are more likely to form at lower pressures.
- **Transport:** Pressure can influence the transport of pollutants in the atmosphere. For example, high-pressure systems can create stable atmospheric conditions that prevent the vertical mixing of pollutants, leading to higher concentrations near the surface. Low-pressure systems, on the other hand, can transport pollutants over long distances.

Finally, pressure can play a complex role in atmospheric pollution, and it is important to understand how it can influence the behavior and concentrations of pollutants in the air. By reducing our emissions of pollutants and promoting sustainable practices, we can help improve the quality of the air we breathe and protect the environment's health.

### **Role of Free Radicals in the Atmosphere**

Free radicals play an important role in atmospheric chemistry, particularly in forming and degrading air pollutants. Free radicals are highly reactive species that have unpaired electrons, and they can interact with other molecules in the atmosphere to form new compounds or break down existing ones. Some of the ways that free radicals can influence atmospheric pollution are:

- Ozone formation: Free radicals such as hydroxyl radicals (OH) and nitric oxide (NO) are important intermediates in the formation of ozone (O3), a secondary pollutant that can cause respiratory problems and other health issues. In the presence of sunlight, reactions involving these free radicals can form ozone from primary pollutants such as nitrogen oxides (NOx) and volatile organic compounds (VOCs).
- **Oxidation:** Free radicals can also contribute to the oxidation of pollutants in the atmosphere, breaking down their molecular structure and making them less harmful. For example, hydroxyl radicals can react with a wide range of pollutants, including VOCs and carbon monoxide (CO), to produce less harmful compounds such as water and carbon dioxide.
- **Pollution degradation:** Free radicals can also contribute to the degradation of pollutants in the atmosphere. For example, the reaction of hydroxyl radicals

with polycyclic aromatic hydrocarbons (PAHs), which are a class of pollutants commonly found in vehicle exhaust and industrial emissions, can break down these compounds into less harmful substances.

• Atmospheric lifetime: The presence of free radicals can also affect the atmospheric lifetime of pollutants. Free radicals can react with pollutants to either break them down or transform them into other compounds that may be more or less harmful. This can affect how long pollutants persist in the atmosphere and how far they can travel before they are degraded.

Therefore, free radicals play a complex role in atmospheric chemistry and can influence air pollutants' formation, degradation, and behavior. By understanding these processes, we can develop strategies to reduce emissions of pollutants and mitigate their impacts on human health and the environment.

### **Temperature Inversion**

Temperature inversion is a weather phenomenon in which the temperature of the atmosphere rises with height rather than falling. This results in the formation of a layer of warm air that traps pollutants and can contribute to poor air quality. Some examples of temperature inversion are:

- Winter Inversion: During winter months, temperature inversion can occur frequently in areas with high pressure systems and clear skies. In this scenario, the ground cools off rapidly at night due to radiative cooling, while the air above it remains warmer. This creates a stable layer of warm air that traps pollutants close to the ground, leading to increased levels of particulate matter, sulfur dioxide, and other pollutants.
- **Mountain Valley Inversion:** Mountain valleys can also experience temperature inversion, where cold air gets trapped in the valley, and the warmer air stays above it. This can create a situation where pollution generated in the valley accumulates, leading to poor air quality.
- Urban Inversion: Cities with tall buildings can also experience temperature inversion, where the heat generated by human activities, such as cars and factories, is trapped by the buildings. This creates a layer of warm air that can trap pollutants near the surface, leading to increased levels of ozone and other pollutants.
- **Coastal Inversion:** Coastal regions can also experience temperature inversion, where warm air from the ocean is trapped under a layer of cooler air. This can lead to increased levels of pollutants near the coast, as the warm air traps pollutants close to the ground.

As a result, temperature inversion can significantly impact air quality and human health, and it is important to monitor and mitigate its effects by reducing emissions of pollutants and promoting sustainable practices.

## **Photochemical Smog**

When sunlight interacts with specific air pollutants, especially nitrogen oxides (NOx) and volatile organic compounds (VOCs), it can produce photochemical smog. A complex mixture of dangerous compounds, such as aldehydes, ozone, and other secondary pollutants, are produced by the reactions. Some examples of photochemical smog are:

- Los Angeles: The city of Los Angeles is well known for its high levels of photochemical smog, particularly during the summer months. The city has a large number of vehicles, which produce significant amounts of NOx and VOCs, and its location in a valley surrounded by mountains can trap the pollution, leading to elevated levels of ozone and other pollutants.
- **Mexico City:** Mexico City is another urban area with high levels of photochemical smog. The city has a high population density and a large number of vehicles, which contribute to high levels of NOx and VOCs. The city's high altitude also contributes to the formation of photochemical smog, as the intense sunlight at high altitudes can lead to more chemical reactions in the atmosphere.
- **Beijing:** Beijing is a rapidly growing city in China that has experienced significant air pollution problems in recent years, including high levels of photochemical smog. The city has a large number of vehicles and industries, which produce significant amounts of NOx and VOCs. In addition, the city's geography, surrounded by mountains and with limited wind circulation, can trap the pollution and lead to increased levels of ozone and other pollutants.
- **London:** While London has significantly reduced air pollution in recent years, it still experiences episodes of photochemical smog during hot summer days. The city's transportation sector, particularly diesel vehicles, is a significant source of NOx and VOCs. The city's location, with prevailing winds coming from continental Europe, can also bring in pollutants from other regions.

Finally, photochemical smog is a complex and harmful type of air pollution that can significantly impact human health and the environment. Reducing NOx and VOCs emissions and promoting sustainable practices to mitigate the effects of photochemical smog is important.

### Particulate Matter in the Atmosphere

Tiny particles hanging in the air are known as particulate matter, or PM, and they are one kind of air pollution. These particles can consist of a multitude of substances, such as chemicals, dust, pollen, and soot. Because particulate matter can enter the lungs deeply and create respiratory issues, it can be dangerous to human health. Some examples of particulate matter in the atmosphere are:

- **Dust Storms:** Dust storms are a natural source of particulate matter in the atmosphere. They occur when strong winds pick up dust and other particles from the ground and suspend them in the air. Dust storms can happen in arid and semi-arid regions around the world, such as the Sahel region in Africa or the southwestern United States.
- **Industrial Pollution:** Industries that burn fossil fuels or use certain manufacturing processes can produce significant amounts of particulate matter. For example, coal-fired power plants and smelters can release large quantities of soot and other particulate matter into the air.
- Vehicle Emissions: Cars, trucks, and other vehicles are a significant source of particulate matter in the atmosphere. Diesel vehicles, in particular, produce high levels of particulate matter. The particles can come from the tailpipe emissions or from the wear and tear of tires and brakes.
- Wildfires: Wildfires can produce significant amounts of particulate matter, as burning vegetation releases particles into the air. In addition, the smoke from wildfires can carry particulate matter over long distances, impacting air quality in regions far from the fire.

Overall, particulate matter is a complex and harmful type of air pollution that can have significant impacts on human health and the environment. It is important to reduce emissions of particulate matter and promote sustainable practices to mitigate the effects of this type of pollution.

# **Industrial pollutants**

- Industrial pollutants are harmful substances released into the environment due to industrial processes. These pollutants can include a wide range of chemicals, gases, and particles that can have serious negative impacts on human health, ecosystems, and the planet as a whole.
- Several sources of industrial pollutants include factories, power plants, chemical plants, and waste disposal sites. These industries can release a variety of pollutants into the air, water, and soil, depending on the processes they use and the types of chemicals and materials they handle.
- Sulphur dioxide, nitrogen oxides, carbon monoxide, and particulate matter are examples of industrial air pollutants. These pollutants can cause respiratory troubles, heart disease, and other health concerns, as well as contribute to climate change and acid rain.
- Water pollutants from industrial sources can include heavy metals, organic compounds, and toxic chemicals, harming aquatic life and contaminating drinking water supplies. Soil pollutants can include hazardous waste materials, such as heavy metals and chemicals, which can leach into the soil and groundwater and affect both human health and the environment.
- There are a variety of regulations and policies in place to try to limit industrial pollution and reduce its impacts. These can include emissions standards, waste

disposal regulations, and pollution prevention programs. Additionally, many technologies and practices are available to help industries reduce their pollution levels, such as cleaner production processes, recycling, and waste minimization.

• Overall, industrial pollutants are a significant problem that can seriously impact human health and the environment. It is important for industries to take steps to reduce their pollution levels and for governments to enforce regulations and policies to protect the public and the planet.

#### **Atmospheric Aerosols**

- Atmospheric aerosols are tiny particles that are suspended in the air. These particles can come from natural sources, such as dust, volcanic activity, and forest fires, as well as from human activities, such as fossil fuel combustion, industrial processes, and transportation.
- Atmospheric aerosols can positively and negatively affect the environment and human health. Depending on their composition and location, they can act as both cooling and warming agents in the atmosphere. For example, sulfate aerosols from fossil fuel combustion can reflect sunlight back into space and have a cooling effect, while black carbon aerosols from burning wood or diesel fuel can absorb sunlight and have a warming effect.
- In addition to their role in climate change, atmospheric aerosols can also affect air quality and human health. Fine particulate matter (PM2.5), which is a type of atmospheric aerosol, can penetrate deep into the lungs and cause respiratory and cardiovascular problems. Other health effects of atmospheric aerosols include increased risk of asthma, lung cancer, and premature death.
- Atmospheric aerosols can also impact visibility, reducing the clarity and color of the sky, and contribute to acid rain and eutrophication, which can harm aquatic ecosystems.
- The composition and behavior of atmospheric aerosols are complex and can vary depending on their source, size, and chemical makeup. Scientists use sophisticated instruments and models to study atmospheric aerosols and their impacts on the environment and human health.
- Overall, atmospheric aerosols are an important and complex component of the Earth's atmosphere that can positively and negatively impact the environment and human health. Understanding their behavior and impacts is crucial for developing effective policies and strategies to address air quality and climate change issues.

### Acid Rain and its Major Sources

Any precipitation with a pH of less than 5.6, which is regarded as acidic, is referred to as acid rain. This is usually brought on by the atmosphere's concentration of nitrogen oxides (NOx) and sulphur dioxide (SO2), which combine with water, oxygen, and other substances to generate nitric acid and sulfuric acid.

The following are the main sources of nitrogen oxides and sulphur dioxide that cause acid rain:

- Fossil fuel combustion: Sulphur dioxide and nitrogen oxides are released into the environment in significant quantities when coal, oil, and gas are burned in factories, power plants, and automobiles.
- Transportation: Sulphur dioxide and nitrogen oxides are released into the atmosphere in large quantities by cars, trucks, and other fossil fuel-burning machinery.
- Industrial processes: Sulphur dioxide and nitrogen oxides can also be released in significant quantities during manufacturing and other industrial processes that consume fossil fuels, such as the production of steel and cement.
- Natural sources: Acid rain is caused by the atmospheric release of sulphur dioxide and nitrogen oxides from volcanic eruptions and wildfires. These natural sources, however, typically have a far lesser effect than human activity.

Significant negative impacts are included.

- Damage to forests: Acid rain causes plants, including trees, to become more susceptible to disease, pests, and other stresses by thinning their leaves and needles.
- Lake and river acidification: Acid rain can increase the acidity of lakes and rivers, which can be harmful to fish and other aquatic life.
- Corrosion of infrastructure and buildings: Acid rain can harm infrastructure like roads and bridges as well as erode building materials like marble and limestone.
- Numerous nations have enacted laws and policies aimed at lowering sulphur dioxide and nitrogen oxide emissions in order to combat the problem of acid rain. These include incentives for switching to greener energy sources, such wind and solar power, and emissions regulations for cars and power plants.

### **Mechanisms of Acid rain**

A complicated chain of chemical reactions in the atmosphere produces acid rain. The main mechanism is the emission of nitrogen oxides (NOx) and sulphur dioxide (SO2) as a result of human activities such industrial processes, transportation, and the burning of fossil fuels. Acid rain is created when these gases combine with water

vapour, oxygen, and other substances in the atmosphere to produce sulfuric and nitric acids (H2SO4 and HNO3, respectively).

The following are the steps involved in the formation of acid rain:

- **Emissions:** Burning fossil fuels, driving, and conducting industrial operations are some of the human activities that cause SO2 and NOx to be released into the atmosphere.
- **Transformation:** Nitric acid and sulfuric acid are produced in the atmosphere when SO2 and NOx combine with water, oxygen, and other substances. Sunlight and other atmospheric variables promote these processes.

 $SO2 + H2O + O2 \rightarrow H2SO4$ 

 $NOx + H2O + O2 \rightarrow HNO3$ 

- **Deposition:** Once formed, sulfuric acid and nitric acid can be deposited back to the earth's surface in the form of acid rain, snow, fog, or gas-phase particles.
- The impacts of acid rain can be seen in various ways, including the acidification of lakes, rivers, and soil; damage to forests and vegetation; corrosion of buildings and infrastructure; and health impacts on humans and wildlife. To address the problem of acid rain, regulations and policies have been implemented in many countries to reduce emissions of SO2 and NOx, including the use of cleaner technologies and energy sources, as well as emissions standards for power plants and vehicles.

### **Control measures for Acid rain**

- Reducing the emissions of nitrogen oxides (NOx) and sulphur dioxide (SO2) from human activities, such as the burning of fossil fuels, transportation, and industrial processes, is the first step in controlling acid rain. The following are some preventative steps that can be taken to lessen acid rain:
- Use of cleaner energy sources: Using nuclear, solar, wind, hydropower, and other cleaner energy sources can help cut down on SO2 and NOx emissions from power plants and other industrial operations.
- Fuel switching: Using natural gas, low-sulfur coal, or other alternative fuels can help power plants emit fewer SO2 emissions.
- Retrofitting existing facilities: To lower SO2 and NOx emissions, technologies like scrubbers and selective catalytic reduction (SCR) systems can be installed in power plants and other industrial facilities.
- Energy efficiency: Reducing energy consumption and, consequently, SO2 and NOx emissions can be achieved by making houses, buildings, and industrial operations more energy-efficient.
- Emissions requirements: Transportation, industrial facilities, and power plants can all have their emissions limits set by laws and policies. The maximum

quantity of SO2 and NOx that can be released into the environment is limited by these regulations.

- International cooperation: Addressing acid rain is a worldwide issue that requires international cooperation. Cooperation among nations can be used to set and meet goals for reducing emissions and encourage the use of cleaner energy sources.
- Education and awareness: Spreading knowledge about acid rain's causes and consequences can help people become more aware of the issue and be inspired to take steps to lower their own SO2 and NOx emissions.
- By implementing these control measures, it is possible to reduce the emissions of SO2 and NOx and mitigate the impacts of acid rain on the environment and human health.

## Effects of acid rain on Buildings and Vegetation

Acid rain can have damaging effects on buildings and vegetation. Here are some of the impacts of acid rain on buildings and vegetation:

- **Buildings:** Acid rain can cause corrosion and degradation of building materials such as limestone and marble, which are commonly used in historical buildings and monuments. The sulfuric acid in acid rain reacts with the calcium carbonate in limestone and marble, causing it to dissolve and deteriorate over time. This can result in the loss of architectural detail and weakening structural components.
- Vegetation: Acid rain can damage or kill vegetation by leaching important nutrients such as calcium and magnesium from the soil. The acidic soil can also release aluminum, which is toxic to plants. The leaves and needles of trees and plants can become discolored and weakened, making them more susceptible to disease and pests. Acid rain can also cause forest decline, which is the gradual deterioration of forest ecosystems over time.
- Aquatic life: Acid rain can cause lakes, rivers, and streams to lose pH, increasing the acidity of the water. Fish, amphibians, and aquatic plants are among the aquatic creatures that may suffer from this. Aluminium from the soil can be released by acid rain, and fish and other aquatic life may find it poisonous.
- **Human health:** The effects of acid rain can also be detrimental to human health. Acid rain's sulphur dioxide and nitrogen oxides can exacerbate respiratory conditions like asthma and bronchitis by causing smog to accumulate.
- To mitigate the impacts of acid rain on buildings and vegetation, it is important to reduce emissions of sulfur dioxide and nitrogen oxides. This can be done through the implementation of emissions standards, the use of cleaner energy sources, and the adoption of energy-efficient practices. Additionally, measures such as liming, which involves the addition of calcium carbonate to soil, can be used to neutralize the acidity of the soil and improve plant health.

### **Global Warming**

The average surface temperature of the Earth has been rising throughout time, mostly as a result of human activity-induced increases in greenhouse gases (GHGs) in the atmosphere. This phenomenon is known as global warming. Methane (CH4), nitrous oxide (N2O), fluorinated gases, and carbon dioxide (CO2) are the primary greenhouse gases that cause global warming. Earth's temperature rises as a result of these gases' ability to trap heat in the atmosphere and keep it from escaping into space.

Burning fossil fuels like coal, oil, and gas produces a lot of CO2 into the atmosphere, which is the primary driver of global warming. By releasing greenhouse gases into the atmosphere, other human activities including deforestation, agriculture, and industrial processes also contribute to global warming.

The impacts of global warming are numerous and far-reaching. Some of the key impacts include:

- Rising temperatures: As a result of global warming, heat waves occur more frequently and with greater intensity, and extreme weather events like floods, droughts, and wildfires occur more frequently.
- Sea levels increase as a result of glaciers and ice caps melting due to rising temperatures. This poses a threat to the survival of certain island nations and can result in floods in low-lying coastal areas.
- Modifications in precipitation patterns: In certain areas, changes in precipitation patterns brought on by global warming may result in more frequent and severe droughts and floods.
- Effects on ecosystems: Certain plant and animal species may go extinct as a result of ecological disruption brought on by global warming. Food security and agricultural output can also be impacted by variations in temperature and precipitation patterns.
- Effects on human health: The proliferation of disease-carrying insects like mosquitoes, respiratory issues brought on by air pollution, and heat-related ailments are just a few of the ways that global warming may harm people's health.
- Lowering GHG emissions is essential to combating global warming. This can be achieved by switching to greener energy sources, like hydropower, solar power, and wind power, as well as by increasing energy efficiency and implementing sustainable land-use techniques. Enacting laws and policies that support the deployment of low-carbon technologies and encourage emissions reductions is also crucial. To lessen their carbon footprint, people should also consume less energy, drive less, and consume a diet higher in plant-based foods.

## **Major Greenhouse Gases**

The gases that trap heat in the Earth's atmosphere and cause global warming are known as greenhouse gases, or GHGs. The principal greenhouse gases consist of:

- Carbon dioxide (CO2): CO2 is the most significant greenhouse gas, accounting for more than 60% of the warming effect generated by all GHGs. CO2 is produced by the combustion of fossil fuels, deforestation, and other human activities.
- Methane (CH4): Methane is the second most major GHG, accounting for approximately 20% of the warming effect induced by all GHGs. CH4 is created by natural processes such as organic matter decomposition, as well as human activities such as livestock husbandry and natural gas production and transportation.
- Nitrous oxide (N2O): Nitrous oxide accounts for approximately 6% of the warming effect generated by all GHGs. Natural processes such as the nitrogen cycle and human activity produce N2O.
- Fluorinated gases are synthetic gases that include hydrofluorocarbons (HFCs), perfluorocarbons (PFCs), and sulphur hexafluoride (SF6). They are employed in a variety of industrial and commercial applications. Despite accounting for a minor part of GHG emissions, they are extraordinarily strong and have a far larger warming effect than CO2.
- Water vapor: Water vapor is the most abundant GHG in the atmosphere, but its concentrations are largely determined by temperature and other factors. While human activities do not directly control it, its concentrations can be influenced by changes in other GHGs.
- To address the issue of global warming, it is necessary to reduce the emissions of these greenhouse gases. This can be done by reducing our reliance on fossil fuels, promoting energy efficiency, adopting sustainable land-use practices, and using low-carbon technologies. It is also important to promote policies and regulations that encourage emissions reductions and to increase public awareness about the impacts of climate change.

### **Mechanism of Greenhouse**

The Earth's atmosphere contains molecules known as greenhouse gases (GHGs), which trap solar heat and prevent it from escaping into space. This process is known as the greenhouse effect. The average surface temperature of the Earth would be around  $-18^{\circ}C$  (0°F) without the greenhouse effect, which is too chilly for the majority of life forms.

The mechanism of the greenhouse effect can be explained as follows:

• Short-wave radiation is emitted by the sun, travels through the atmosphere, and eventually reaches the Earth's surface. Some of this radiation is absorbed by the surface, which then radiates long-wave radiation again.

- Some of this long-wave radiation is absorbed by greenhouse gases in the atmosphere, which include carbon dioxide (CO2), methane (CH4), and water vapour (H2O), and they trap this energy there.
- The Earth's surface and lower atmosphere warm as a result of the trapped heat, and some of that heat is then radiated back into space.
- Nonetheless, a portion of the heat is retained in the atmosphere due to greenhouse gas trapping, resulting in a net rise in temperature.
- The amounts of greenhouse gases in the atmosphere dictate how strong the greenhouse effect is. The concentrations of greenhouse gases (GHGs) in the atmosphere have increased due to human activities including the burning of fossil fuels and deforestation, which has strengthened the greenhouse effect and raised Earth's temperature.
- Although the greenhouse effect occurs naturally, human activity has intensified it, which is causing climate change and a number of negative effects, such as rising sea levels, more frequent and severe weather events, and a decline in biodiversity. As a result, addressing the causes of climate change and reducing greenhouse gas emissions are crucial.

### **Global impact of Major greenhouse gasess**

- The primary greenhouse gases that have a big worldwide impact on climate change and the environment are carbon dioxide (CO2), methane (CH4), nitrous oxide (N2O), and fluorinated gases.
- CO2 (carbon dioxide): More than 60% of the warming effect induced by all greenhouse gases is attributed to CO2, the most significant greenhouse gas. Land-use changes, deforestation, and the burning of fossil fuels are some of the main human-caused factors contributing to the increase in CO2 concentrations in the atmosphere. Because CO2 causes rising global temperatures, an increase in sea level, and modifications to weather patterns, it has a considerable impact on climate change.
- Methane, or CH4, is the second most significant greenhouse gas and accounts for 20% of the total warming effect that greenhouse gases produce. Natural processes like the breakdown of organic matter and human activities like raising cattle and producing and moving natural gas both result in the generation of CH4. Because CH4 has a warming potential 28 times greater than CO2 over a 100-year time horizon, it has a substantial impact on climate change.
- About 6% of the warming effect resulting from all greenhouse gases is attributed to nitrous oxide (N2O). Both natural processes like the nitrogen cycle and human activity like farming and burning fossil fuels produce N2O. Because N2O has a warming potential 265 times larger than CO2 over a 100-year time horizon, it has a considerable impact on climate change.

- Gases with fluorine: Fluorinated gases are synthetic gases utilized in a variety of industrial and commercial applications. These gases include sulphur hexafluoride (SF6), hydrofluorocarbons (HFCs), and perfluorocarbons (PFCs). Despite contributing very little to greenhouse gas emissions, they are incredibly powerful and warm the planet far more than CO2. Because fluorinated gases have warming potential hundreds to thousands of times larger than that of carbon dioxide, they have a considerable impact on climate change.
- These main greenhouse gases have a substantial worldwide influence and are the cause of climate change, which has a number of detrimental effects on the environment, the economy, and society. In order to lessen these effects and encourage a more sustainable future, it is critical to cut greenhouse gas emissions and address the root causes of climate change.

#### Ozone

Ozone is a colorless gas made up of three oxygen atoms (O3). It is a highly reactive molecule that is naturally occurring in the Earth's atmosphere. It is formed from the action of sunlight on oxygen in the presence of pollutants emitted by human activities, such as cars and power plants.

### **Effects of Ozone**

The effects of ozone can be both beneficial and harmful, depending on where it is located and at what concentration. Here are some of the effects of ozone:

- 1. Beneficial effects: Ozone in the stratosphere (the layer of the atmosphere between 10 and 50 km above the Earth's surface) plays a vital role in protecting life on Earth by absorbing most of the harmful ultraviolet radiation from the sun. This prevents skin cancer, cataracts, and other health problems.
- 2. Harmful effects: Ozone in the troposphere (the layer of the atmosphere closest to the Earth's surface) can cause respiratory problems, such as coughing, wheezing, and shortness of breath. It can also aggravate existing lung conditions, such as asthma and bronchitis. Ozone pollution is a major problem in many cities around the world, and exposure to high levels of ozone can lead to health problems, including chest pain, nausea, and reduced lung function.
- **3.** Environmental effects: Ozone pollution can harm crops, trees, and other plants. It can also reduce the yield of agricultural crops and decrease the quality of timber. Ozone depletion in the stratosphere allows more harmful ultraviolet radiation to reach the Earth's surface, which can damage the DNA of plants and animals, reduce crop yields, and disrupt ecosystems.
- **4. Industrial effects:** Ozone is a powerful oxidizing agent and can be used in a variety of industrial processes, such as water treatment, chemical synthesis, and disinfection. However, high concentrations of ozone can be dangerous to workers and can damage equipment.

**5. Medical effects**: Ozone therapy is a controversial alternative medical treatment that involves injecting or inhaling ozone gas to treat a variety of medical conditions. There is little scientific evidence to support the effectiveness of this treatment, and it can be dangerous if not administered properly.

#### **Stratospheric Ozone-Ozone Hole**

Stratospheric ozone is a layer of ozone gas that is found in the stratosphere, which is the layer of the Earth's atmosphere that is located between 10 and 50 kilometers above the surface of the Earth. This layer of ozone plays an important role in protecting the Earth from the harmful effects of ultraviolet (UV) radiation from the sun.

The "ozone hole" refers to a thinning of the stratospheric ozone layer over Antarctica that was first discovered in the 1980s. The ozone hole is caused by the release of manmade chemicals, such as chlorofluorocarbons (CFCs), into the atmosphere. These chemicals break down in the atmosphere and release chlorine and other chemicals that destroy ozone molecules.

The ozone hole occurs primarily over Antarctica because of the extremely cold temperatures in that region. During the Antarctic winter, a polar vortex forms over the continent and isolates the air inside from the rest of the atmosphere. This polar vortex prevents the mixing of air with the surrounding atmosphere, which leads to the formation of an area of extremely low ozone concentrations.

The ozone hole has had a significant impact on the Earth's climate and has led to an increase in UV radiation reaching the surface of the Earth, which can cause skin cancer, cataracts, and other health problems. However, since the discovery of the ozone hole, the international community has taken steps to reduce the production and use of ozone-depleting chemicals, which has led to a gradual recovery of the ozone layer.

### Stratospheric Ozone-CFCs

Chlorofluorocarbons (CFCs) are a group of man-made chemicals that were widely used in the past in refrigeration, air conditioning, and aerosol products. CFCs are chemically stable and have a long atmospheric lifetime, which means they can remain in the atmosphere for several decades to centuries.

CFCs are one of the main contributors to the depletion of stratospheric ozone. When CFCs are released into the atmosphere, they can be transported to the stratosphere, where they are broken down by the intense UV radiation. This breakdown releases chlorine atoms, which then react with ozone molecules to form chlorine monoxide and oxygen molecules. Chlorine monoxide can then react with other ozone molecules to form more oxygen, leading to a net reduction in the amount of ozone in the stratosphere.

The depletion of stratospheric ozone has significant consequences for the Earth's climate and human health. The loss of ozone allows more harmful UV radiation to reach the Earth's surface, which can increase the incidence of skin cancer, cataracts, and other health problems. The reduction of ozone in the stratosphere also leads to cooling of the stratosphere and warming of the troposphere, which can affect weather patterns and the Earth's climate.

The production and consumption of CFCs have been regulated internationally under the Montreal Protocol, which was signed in 1987. The Montreal Protocol sets out a timetable for the phasing out of the production and use of CFCs and other ozonedepleting substances. As a result of the Montreal Protocol, the production and consumption of CFCs have been significantly reduced, and the ozone layer is expected to recover over the coming decades.

### **Stratospheric Ozone "Ozone Protection"**

Protecting the stratospheric ozone layer is important to ensure the Earth's protection from harmful UV radiation. Here are some of the ways that stratospheric ozone can be protected:

- Minimize the use of ozone-depleting substances: It is recommended to minimize or completely stop using ozone-depleting substances including halons, hydrochlorofluorocarbons (HCFCs), and chlorofluorocarbons (CFCs). Reducing the manufacturing and consumption of these drugs has been successful due to the 1987 signing of the Montreal Protocol, an international accord.
- **Promote the use of alternatives:** The use of substitutes for ozone-depleting substances, such as hydrofluorocarbons (HFCs) and other fluorinated gases, can help to reduce the demand for ozone-depleting substances.
- **Properly dispose of ozone-depleting substances:** Ozone-depleting substances should be disposed of properly to prevent their release into the atmosphere. This includes the proper handling and disposal of refrigeration and air conditioning equipment that contains these substances.
- Educate the public: Education and awareness campaigns can help to inform the public about the importance of protecting the ozone layer and the actions they can take to reduce their own contribution to ozone depletion.
- Monitor the ozone layer: Regular monitoring of the ozone layer can help to identify changes in its thickness and concentration, as well as any potential threats to its protection.

By taking these actions, we can protect the stratospheric ozone layer and ensure that it continues to provide essential protection for life on Earth.

## **Biological Consequences of Ozone Depletion**

Ozone depletion can have a number of biological consequences, primarily due to the increased levels of ultraviolet (UV) radiation reaching the Earth's surface. Here are some of the potential biological consequences of ozone depletion:

- Skin cancer: One of the main risk factors for skin cancer is UV radiation exposure. With less ozone in the atmosphere to absorb UV radiation, there is an increased risk of skin cancer, especially in regions closer to the equator.
- **Eye damage:** Exposure to UV radiation can also damage the eyes, leading to cataracts and other eye conditions.
- Weakened immune system: Studies have shown that exposure to UV radiation can weaken the immune system, making individuals more susceptible to infections and diseases.
- **Crop damage:** Increased UV radiation can damage crops, leading to reduced yields and lower quality produce.
- **Marine ecosystem disruption:** UV radiation can also have harmful effects on marine ecosystems, such as reducing the growth and productivity of phytoplankton, which are a key food source for many marine organisms.
- **Disruption of terrestrial ecosystems:** Increased UV radiation can also disrupt terrestrial ecosystems, such as altering plant communities' composition and reducing certain species' reproductive success.
- Overall, the biological consequences of ozone depletion can seriously impact human health, food security, and the functioning of ecosystems. It is, therefore, important to continue to take action to protect the ozone layer and prevent further depletion.

# Water Pollution and Wastewater Treatment

When hazardous substances are added to water, they contaminate lakes, rivers, seas, and groundwater, rendering it unfit for human use and upsetting aquatic ecosystems. Human waste, industrial and agricultural processes, and urbanization are the main causes of water contamination.

One of the primary methods for reducing water pollution is wastewater treatment. Wastewater is the water that has been used in households, industries, and agriculture, which contains a variety of pollutants such as organic matter, pathogens, nutrients, and toxic chemicals. Wastewater treatment involves several processes that remove these pollutants and make the water safe for reuse or release into the environment.

The basic steps involved in wastewater treatment are as follows:

• **Initial Treatment:** In this stage, physical procedures including grit removal and screening are used to remove big particles and debris from the wastewater.

- **Primary Treatment:** During this phase, suspended solids in the wastewater are allowed to sink to the bottom of enormous tanks and be removed as sludge. The residual liquid, referred to as effluent, is directed towards further processing.
- Secondary Treatment: In this step, the effluent is treated with biological processes that break down organic matter using microorganisms such as bacteria and protozoa. This process is usually done in aerated tanks where oxygen is provided to support the growth of microorganisms. The effluent is then sent for tertiary treatment.
- **Tertiary Treatment:** In this step, the effluent is further treated to remove any remaining pollutants using advanced physical, chemical, and biological processes such as sand filtration, chemical precipitation, and disinfection. This makes the water suitable for reuse or release into the environment.

There are several types of wastewater treatment systems, including conventional treatment, extended aeration systems, sequencing batch reactors, and membrane bioreactors. The choice of treatment system depends on the type and amount of pollutants in the wastewater, as well as the level of treatment required.

Wastewater treatment is a crucial process for ensuring clean water supplies, protecting public health, and preserving the environment. However, it is also important to reduce the amount of pollutants entering wastewater systems through the implementation of pollution prevention measures and sustainable practices.

# Municipal, Industrial and Agricultural Sources of Water Pollution

Water pollution can come from various sources, including municipal, industrial, and agricultural activities. Here are some examples of each:

- **Municipal sources:** Municipal sources of water pollution include the discharge of untreated or inadequately treated wastewater from households, commercial establishments, and municipal sewage treatment plants. Other sources may include stormwater runoff from urban areas, which can carry pollutants such as oil, grease, and debris into water bodies.
- **Industrial sources:** Industries such as chemical plants, petroleum refineries, and manufacturing facilities can generate large volumes of wastewater that contain pollutants such as heavy metals, organic compounds, and toxic chemicals. If these wastes are not properly treated before discharge, they can contaminate nearby water bodies and harm aquatic life.
- Agricultural sources: Agricultural activities can also contribute to water pollution through the use of fertilizers, pesticides, and other chemicals that can leach into groundwater or runoff into nearby water bodies. Livestock farming can also generate large volumes of animal waste that can pollute water bodies if not properly managed.

In addition to these sources, other factors can contribute to water pollution, such as erosion and sedimentation from construction sites, mining activities, and natural disasters such as floods and landslides.

Reducing water pollution requires a comprehensive approach that involves regulatory measures, pollution prevention, and sustainable practices. This can include implementing stricter regulations on discharges from industrial and municipal sources, promoting the use of environmentally friendly products and practices in agriculture, and improving wastewater treatment and stormwater management systems. Education and awareness-raising campaigns can also help encourage individuals and communities to adopt more sustainable behaviors and reduce their environmental impact.

### **Heavy Metals and Water Pollution**

- Heavy metals are metallic elements that have a density greater than 5 g/cm3 and are toxic to humans, animals, and plants at certain levels. Some common heavy metals that can cause water pollution include lead, cadmium, mercury, arsenic, chromium, and copper. These metals can enter water bodies through various sources, such as industrial discharges, municipal wastewater, agricultural runoff, and atmospheric deposition.
- Heavy metals in water can have harmful effects on human health and the environment. They can accumulate in aquatic organisms and enter the food chain, causing biomagnification and bioaccumulation. Exposure to heavy metals through contaminated water can cause a range of health problems such as neurological disorders, kidney damage, and cancer. In addition, heavy metals can have negative impacts on aquatic ecosystems, causing reduced biodiversity and impaired ecological functions.
- Several methods can be used to remove heavy metals from water, including physical, chemical, and biological processes. These include sedimentation, filtration, adsorption, precipitation, and ion exchange. Some of these methods may be more effective for certain types of metals and at certain concentrations. For example, reverse osmosis and ultrafiltration are commonly used to remove metals such as lead, while ion exchange is more effective at removing metals such as arsenic and chromium.
- Preventing heavy metal pollution in water requires a range of measures, including reducing industrial discharges, properly treating wastewater, and implementing agricultural best practices to reduce runoff. In addition, improving public awareness of the risks associated with heavy metal contamination and promoting sustainable practices can help to reduce the use and release of heavy metals into the environment.

## **Eutrophication**

- When excessive amounts of nutrients, such as nitrogen and phosphorus, get into a body of water, it can cause eutrophication, which is the development of algae and aquatic plants. This overabundance of plant growth may cause the water's oxygen content to drop, harming aquatic life and perhaps killing fish and other creatures.
- Eutrophication can occur naturally, but it is often accelerated by human activities such as agriculture, urbanization, and wastewater discharges. Excessive use of fertilizers in agriculture can result in runoff that carries excess nutrients into nearby water bodies, while urbanization can increase the number of impervious surfaces and reduce the ability of water to naturally filter nutrients. Wastewater discharges can also be a significant source of nutrients, particularly in areas where sewage treatment facilities are inadequate or non-existent.
- The effects of eutrophication can vary depending on the severity and duration of the nutrient loading. In some cases, excess nutrients can lead to harmful algal blooms that can produce toxins that are harmful to humans and animals. These blooms can also lead to the death of fish and other aquatic organisms due to oxygen depletion. In addition, excessive plant growth can reduce water clarity, making it difficult for aquatic plants to photosynthesize and for fish to find prey.
- To address eutrophication, a range of management strategies can be employed. These can include reducing nutrient inputs from agriculture and urban sources, improving wastewater treatment facilities to remove nutrients, and implementing best practices for land use and development. In some cases, physical interventions such as dredging and oxygenation may be necessary to improve water quality. Public education and awareness-raising campaigns can also help to encourage individuals and communities to adopt more sustainable practices and reduce their impact on water quality.

### **Detergents and Phosphates in Water**

- Detergents are household and industrial cleaning products used to remove dirt and stains from various surfaces. Many detergents contain phosphates, which are a type of nutrient that can contribute to water pollution.
- When detergents containing phosphates are used and then washed down the drain, they can end up in nearby water bodies. In water, phosphates can promote the growth of algae and aquatic plants, leading to a process known as eutrophication. This process can cause a number of environmental problems, including oxygen depletion, reduced water quality, and harm to aquatic organisms.

- Many countries have banned or restricted the use of phosphates in laundry and dishwasher detergents to address the problem of phosphates in water. In some cases, this has been done through government regulations, while in other cases, the detergent industry has voluntarily reduced or eliminated the use of phosphates.
- Many detergent manufacturers have also developed alternative formulations that do not contain phosphates. These alternative products can be just as effective at cleaning, but have a reduced impact on water quality. In addition, consumers can reduce their use of detergents and ensure that any products they use are phosphate-free. This can include using lower amounts of detergent, washing full loads of laundry or dishes, and using environmentally friendly cleaning products.

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Water Quality Criteria (WQC)
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Water quality criteria (WQC) are guidelines that provide a basis for assessing and managing water quality. These guidelines are established by regulatory agencies and other organizations and are based on scientific knowledge and available data.

The primary purpose of water quality criteria is to protect human health and aquatic life. The criteria provide numerical values for various water quality parameters, such as temperature, pH, dissolved oxygen, nutrients, and toxic substances. These values are designed to ensure that water quality is sufficient to support healthy aquatic ecosystems and protect human health.

The development of water quality criteria involves a rigorous scientific process that includes:

- Identifying the water quality parameters that are of concern and assessing their potential impacts on aquatic life and human health.
- Conducting laboratory and field studies to determine the effects of different levels of exposure to these parameters on aquatic life and human health.
- Using this information to establish numerical values for each parameter that are protective of aquatic life and human health.
- Periodically reviewing and updating the criteria based on new scientific information and changing environmental conditions.

Water quality criteria are used by regulatory agencies to develop water quality standards and permit limits. Water quality standards are legal requirements that specify the maximum allowable levels of various water quality parameters in a water body. Permit limits are specific to individual sources of pollution, such as industrial or municipal wastewater dischargers, and are designed to ensure that these sources do not exceed the applicable water quality standards.

In addition to regulatory use, water quality criteria can also be used by water resource managers, scientists, and other stakeholders to evaluate the condition of water bodies

and identify areas of concern. They can also be used to develop management strategies, such as best management practices and restoration plans, to improve water quality.

Overall, water quality criteria are an important tool for protecting and managing water resources. By providing clear guidelines for acceptable water quality parameters, they help ensure that water bodies are healthy and support a range of beneficial uses.

#### Water Purification

Water purification is removing unwanted substances, such as contaminants, impurities, and pollutants, from water to make it safe for human consumption or other specific purposes. Water purification aims to produce high-quality water that meets specific standards for health, aesthetics, and other properties.

There are several different methods of water purification, each of which may be used alone or in combination with other methods, depending on the quality of the source water and the desired final product. Some common methods of water purification include:

- **Filtration:** In order to get rid of particles, silt, and other contaminants, water is passed through a filter. A variety of materials, such as sand, gravel, activated carbon, and ceramics, can be used to make filters.
- **Reverse osmosis:** This method eliminates dissolved particles, minerals, and other impurities from water by forcing it through a semi-permeable membrane under pressure.
- **Distillation:** This process turns water into steam by boiling it, which is subsequently condensed back into water. Impurities with a boiling point greater than water are eliminated by this method.
- **Chlorination:** To eliminate bacteria and other pathogenic microorganisms, a little amount of chlorine is added to water.
- **UV treatment:** In order to eradicate any potential bacteria, viruses, and other germs from the water, ultraviolet radiation is used.
- **Chemical treatment:** In order to rid water of impurities, such as flocculants, which cause particles to cluster together and settle out of the water, chemicals are added.
- Water purification is a critical process for ensuring access to safe, clean drinking water. It is used by municipalities, private companies, and individuals to treat water from a variety of sources, including rivers, lakes, groundwater, and municipal water supplies. The specific methods used for water purification depend on the quality of the source water and the intended use of the purified water.

## Primary, Secondary and Advanced Water Treatments

The process of making water suitable for human eating or other particular uses involves filtering out pollutants, impurities, and other undesirable materials. A vital part in guaranteeing the safety and purity of water is played by various water treatment methods, such as basic, secondary, and advanced treatment.

- **Primary Treatment:** The primary treatment is the first stage of the water treatment process. It involves the physical removal of large solids and organic matter from the water. This is typically done through a process called sedimentation, in which the water is allowed to settle, and the solids sink to the bottom. This process can be enhanced by adding chemicals called coagulants, which cause the solids to clump together and settle more quickly. After primary treatment, the water still contains dissolved and suspended particles, as well as microorganisms.
- Secondary Treatment: Secondary treatment is the second stage of the water treatment process, which is designed to remove dissolved and suspended organic matter, as well as microorganisms, that remain after primary treatment. This is typically done through biological treatment, which uses microorganisms to break down organic matter in the water. The most common type of biological treatment is called activated sludge, in which water is mixed with bacteria-rich sludge and air in a tank, allowing the bacteria to consume organic matter and produce clean water. After secondary treatment, the water is much cleaner but may still contain some dissolved solids and microorganisms.
- Advanced Treatment: Advanced treatment is the final stage of the water treatment process, which is used to remove any remaining contaminants and improve the quality of the water to meet specific standards for health, aesthetics, and other properties. Advanced treatment methods can include a variety of processes, such as filtration, chemical treatment, UV treatment, and reverse osmosis. Some common advanced treatment processes include:
- **Filtration:** This involves passing water through a filter that removes particles, sediment, and other impurities.
- **Chemical Treatment:** This involves adding chemicals to water to remove contaminants, such as flocculants that cause particles to clump together and settle out of the water.
- **Reverse Osmosis:** This is a process that uses pressure to force water through a semi-permeable membrane that removes dissolved solids, minerals, and other contaminants.
- Ultraviolet Treatment: This involves using ultraviolet light to kill bacteria, viruses, and other microorganisms that may be present in the water.

Advanced treatment is critical for ensuring that water meets specific standards for human consumption or for other specific purposes, such as industrial use or irrigation. In summary, primary, secondary, and advanced treatments are essential components of the water treatment process. By combining these treatment methods, water can be purified to meet specific standards and provide safe, clean water for a variety of uses.

## **Removal of Nitrogen and Phosphorous Compounds from Polluted Water**

Although phosphorus and nitrogen are necessary elements for plant growth, excessive concentrations of these minerals in water bodies can lead to eutrophication, or the overgrowth of algae and other aquatic plants. Reduced oxygen levels in the water can result from this, endangering aquatic life and rendering the water unfit for human consumption. Thus, it is crucial to remove phosphorus and nitrogen molecules from contaminated water in order to preserve water quality.

There are several methods for removing nitrogen and phosphorus compounds from polluted water, including:

- 1. Biological Nutrient Removal (BNR): BNR is a process that uses bacteria to remove nitrogen and phosphorus compounds from wastewater. This process involves two stages: the first stage is called anoxic, in which bacteria consume organic matter in the wastewater while using nitrate as an electron acceptor; the second stage is called aerobic, in which bacteria consume remaining organic matter and convert nitrogen to gas.
- 2. Chemical Precipitation: Chemical precipitation is a process that uses chemicals to remove nitrogen and phosphorus compounds from water. This process involves adding chemicals, such as alum or ferric chloride, to water to form insoluble compounds that settle to the bottom of the water.
- **3. Membrane Filtration:** Membrane filtration is a process that uses membranes to remove nitrogen and phosphorus compounds from water. This process involves passing water through a membrane that filters out nitrogen and phosphorus compounds, as well as other contaminants.
- 4. Constructed Wetlands: Constructed wetlands are engineered systems that use plants, soil, and microorganisms to remove nitrogen and phosphorus compounds from water. This process involves allowing water to flow through a wetland, where plants and microorganisms remove nitrogen and phosphorus compounds.
- **5. Ion Exchange:** Ion exchange is a process that uses a resin to remove nitrogen and phosphorus compounds from water. This process involves passing water through a resin, which exchanges ions with the nitrogen and phosphorus compounds, removing them from the water.

In conclusion, removing nitrogen and phosphorus compounds from polluted water is essential for maintaining water quality and preventing eutrophication. The methods for removing nitrogen and phosphorus compounds from water include biological nutrient removal, chemical precipitation, membrane filtration, constructed wetlands, and ion exchange.

#### **Organic Matter in Water and Its Decomposition**

Organic matter in water refers to any material of natural or synthetic origin that contains carbon-based compounds. Organic matter can enter water bodies from various sources such as sewage, industrial effluent, agricultural runoff, and natural processes such as decaying plants and animals. Organic matter in water can be beneficial as it provides a food source for aquatic organisms, but it can also be problematic as it can cause water quality issues.

The decomposition of organic matter in water occurs through a process known as microbial decomposition. Microbial decomposition involves the breakdown of organic matter by microorganisms such as bacteria and fungi. During decomposition, microorganisms break down organic matter into simpler compounds such as carbon dioxide, water, and inorganic nutrients such as nitrogen and phosphorus. This process releases energy that microorganisms can use for growth and reproduction.

The decomposition of organic matter in water can positively and negatively affect water quality. On the one hand, microbial decomposition can help to break down organic matter, reducing the amount of pollutants in the water. It can also help to cycle nutrients, such as nitrogen and phosphorus, which can be beneficial for aquatic life.

On the other hand, the decomposition of organic matter can lead to a depletion of dissolved oxygen in the water. As microorganisms consume organic matter, they use up dissolved oxygen in the water. This can lead to hypoxia, or low oxygen levels, which can be harmful to aquatic organisms. Hypoxia can also lead to the release of toxic substances from sediments into the water.

In conclusion, the presence of organic matter in water can have both positive and negative effects on water quality. While microbial decomposition can help break down organic matter and cycle nutrients, it can also lead to a depletion of dissolved oxygen in the water, which can harm aquatic life. It is therefore important to manage sources of organic matter in water to maintain healthy water quality.

### Land Pollution with Examples

Land pollution is the degradation of land resources, usually caused by human activities such as industrialization, urbanization, and agricultural practices. Land pollution can have a significant impact on soil quality, water quality, and the health of humans and wildlife. Here are some examples of land pollution:

- Industrial waste: Industries such as manufacturing, mining, and chemical production generate a large amount of waste materials that can be harmful to the environment. These waste materials may contain toxic substances, heavy metals, and other hazardous materials that can contaminate the soil and groundwater.
- Agricultural practices: Agricultural practices such as excessive use of fertilizers, pesticides, and herbicides can lead to soil pollution. The use of these chemicals can also contaminate the groundwater and other water sources, leading to water pollution.
- Landfills: Landfills are sites where waste materials are buried in the ground. Improperly managed landfills can pollute the soil, groundwater, and air with hazardous chemicals and toxic gases.
- **Deforestation:** The removal of trees for industrial or agricultural uses is known as deforestation. This approach may result in diminished soil fertility, soil erosion, and a decline in biodiversity.
- **Mining activities:** Mining activities can lead to soil erosion, soil compaction, and the release of toxic substances into the soil and groundwater.
- Urbanization: Urbanization is the expansion of urban areas into rural areas. This can lead to land degradation, soil erosion, loss of biodiversity, and increased pollution.
- **Construction activities:** Construction activities such as excavation, grading, and demolition can lead to soil erosion, soil compaction, and the release of hazardous materials into the soil.

These are just a few examples of land pollution. It is important to address the causes of land pollution and take measures to prevent and mitigate its impact on the environment and human health.

### **Soil and Mineral Resources**

Soil and mineral resources refer to the naturally occurring materials found in the earth that are used for various purposes. Soil resources primarily refer to the layer of topsoil that covers the earth's surface and supports plant life, while mineral resources include a wide range of valuable materials such as ores, gemstones, metals, and fossil fuels.

Soil resources are important for agriculture, as they provide the nutrients and moisture needed for crops to grow. They also help regulate the earth's climate by absorbing and storing carbon dioxide from the atmosphere. However, soil resources can be depleted or degraded through overuse, erosion, or contamination, which can have negative impacts on the environment and human health.

Mineral resources, on the other hand, are valuable for their economic and industrial uses. For example, metals like iron and copper are used in construction and manufacturing, while fossil fuels like oil and coal are used for energy production. However, mining and extraction of mineral resources can also have negative environmental impacts, such as habitat destruction and pollution.

In conclusion, soil and mineral resources play important roles in supporting human civilization, but it is important to manage them sustainably to minimize negative impacts on the environment and ensure their availability for future generations.

## **General Principles of Metal Extraction**

General principles of metal extraction refer to the basic principles that underlie the process of obtaining metals from their ores. Several different methods are used to extract metals, depending on the metal's properties and the ore's nature. However, some general principles apply to all metal extraction processes. In this response, we will discuss these general principles in detail.

- The concentration of the Ore: Most ores contain a small percentage of the metal in them, and therefore, before the extraction process can begin, the ore must be concentrated. This is typically done through a process called 'beneficiation,' which involves crushing the ore into small pieces and then using a technique like flotation or magnetic separation to remove impurities.
- **Reduction of the Metal Oxide:** The next step in the extraction process is to reduce the metal oxide to its elemental form. This is usually done using a reducing agent, which is a substance that can donate electrons to the metal oxide and thereby reduce it. The reducing agent used depends on the metal being extracted. For example, carbon is commonly used to reduce iron oxide to metallic iron.
- **Purification of the Metal:** After the metal has been reduced, it is often impure and needs to be purified. Purification can be done through a variety of techniques, depending on the metal and the impurities. For example, electrolysis can be used to purify copper, while fractional distillation can be used to purify mercury.
- **Refining:** Refining is the final step in the metal extraction process. It involves further purification of the metal, often through electrolysis or chemical methods. This step is crucial for obtaining high-purity metals that can be used in various applications.

In addition to these general principles, there are several other factors that can influence the metal extraction process, such as the cost of the raw materials, the availability of the required chemicals, and the environmental impact of the process.

Overall, the general principles of metal extraction involve concentrating the ore, reducing the metal oxide to its elemental form, purifying the metal, and refining it to obtain a high-purity product. The specific techniques used in each step depend on the metal being extracted and the nature of the ore.

### Heavy metals contamination of soil

Heavy metals are naturally occurring elements that can be found in the soil. They include elements such as lead, arsenic, cadmium, mercury, and chromium. These

metals can be harmful to human health and the environment if they are present in excessive amounts. Heavy metals can enter the soil through various sources such as industrial activities, agricultural practices, mining activities, and waste disposal sites.

Contamination of soil with heavy metals can have several negative impacts. Here are some of the most important:

- 1. Toxicity to Plants: Heavy metals can be toxic to plants, affecting their growth and reducing crop yields. This can have significant economic implications for agriculture.
- 2. Soil Pollution: Heavy metals can cause soil pollution, which can have longterm impacts on soil fertility, plant growth, and microbial activity. The metals can also affect the physical and chemical properties of soil, making it less suitable for plant growth.
- **3. Water Pollution:** Heavy metals can leach from contaminated soil into nearby water sources, causing pollution and affecting aquatic life. This can be a significant environmental problem, especially in areas where water is used for drinking or irrigation.
- 4. Human Health Impacts: Heavy metals can be harmful to human health, especially if they enter the food chain through contaminated plants or animals. Some heavy metals, such as lead and mercury, are known to cause serious health problems, including neurological disorders, cancer, and developmental delays in children.

Preventing heavy metal contamination in soil requires a multifaceted approach that involves both reducing the sources of contamination and managing contaminated sites. Some of the measures that can be taken include:

- **1. Reducing Industrial Emissions:** Governments can regulate industrial activities to reduce emissions of heavy metals into the environment.
- 2. **Proper Waste Disposal:** Proper disposal of hazardous waste is crucial in preventing soil contamination. Waste disposal sites should be managed properly to prevent leaching of heavy metals into the soil.
- **3.** Soil Testing: Soil testing can help identify contaminated areas and provide information on the type and extent of contamination.
- **4. Remediation Techniques:** Remediation techniques such as soil washing, phytoremediation, and soil stabilization can be used to reduce the levels of heavy metals in contaminated soil.

Therefore, heavy metal contamination of soil is a significant environmental problem that requires a comprehensive approach to address. Prevention and management strategies must be implemented to minimize the risk of contamination and protect human health and the environment.

## **Toxicity of Heavy Metals**

Heavy metals are naturally occurring elements that can be toxic to living organisms in high concentrations. Here are some of the most common heavy metals and their associated toxicities:

- 1. Lead: Lead is a highly toxic metal that can cause damage to the nervous system, kidneys, and reproductive system. Children are particularly vulnerable to lead exposure, which can cause developmental delays, learning disabilities, and behavioral problems.
- 2. Arsenic: Arsenic is a toxic metalloid that can cause skin lesions, cancers of the skin, bladder, lung, and liver, and damage to the cardiovascular system, nervous system, and kidneys.
- **3. Cadmium:** Cadmium is a toxic metal that can cause damage to the kidneys, liver, and bones. It can also cause cancer and has been linked to cardiovascular disease.
- 4. Mercury: Mercury is a toxic metal that can cause damage to the nervous system, including tremors, memory loss, and developmental delays in children. It can also cause damage to the kidneys, lungs, and immune system.
- **5.** Chromium: Chromium is a toxic metal that can cause lung cancer, respiratory problems, and skin irritation. Hexavalent chromium is particularly toxic and has been linked to an increased risk of lung cancer.

The toxicity of heavy metals depends on several factors, including the route of exposure, the duration of exposure, the dose, and the individual's susceptibility. Heavy metals can enter the body through ingestion, inhalation, or skin contact. Once inside the body, they can accumulate in various organs and tissues, causing damage over time.

To prevent the toxic effects of heavy metals, it is important to minimize exposure. This can be achieved through several measures, such as using protective equipment in industrial settings, avoiding contaminated food and water sources, and properly disposing of hazardous waste. In addition, monitoring and testing for heavy metals in the environment and in food and water sources can help identify potential exposure risks and prevent toxicity.

# **Bio-Accumulation of Heavy Metals**

Bioaccumulation of heavy metals refers to the process by which these metals accumulate in the tissues of living organisms over time, leading to potentially harmful levels of exposure. Heavy metals can enter the food chain through various pathways, such as contaminated soil or water, and can be taken up by plants or ingested by animals.

Once ingested, heavy metals can accumulate in the tissues of organisms, including muscle, liver, and kidney. This can result in a gradual increase in the concentration of
the metal in the organism's body over time. The accumulation of heavy metals in the body can have several negative effects, including toxicity and reproductive problems.

Bioaccumulation of heavy metals is particularly problematic in aquatic environments, where metals can accumulate in the tissues of fish and other aquatic organisms. This can have significant health implications for humans who consume contaminated seafood. For example, high levels of mercury in certain fish species, such as tuna and swordfish, can lead to neurological problems and developmental delays in children.

Bioaccumulation can also occur in terrestrial environments, where animals can ingest contaminated soil or plants. This can lead to high levels of heavy metals in the animal's tissues, which can be transferred to humans who consume the animal's meat or milk.

To prevent bioaccumulation of heavy metals, it is important to minimize exposure in the environment. This can be achieved through several measures, such as reducing industrial emissions of heavy metals, properly disposing of hazardous waste, and monitoring and testing for heavy metals in food and water sources. In addition, reducing the consumption of contaminated seafood or meat from animals that have been exposed to heavy metals can help minimize the risk of exposure.

### **Organic Matter in Soil**

Organic matter in soil refers to the decomposed remains of plants and animals that provide a source of nutrients and support for soil organisms. Organic matter is a vital component of healthy soil and plays an important role in soil fertility, water holding capacity, and nutrient cycling.

Organic matter in soil can be divided into two categories: living and dead. Living organic matter includes plant roots and soil organisms, such as bacteria, fungi, and insects. Dead organic matter includes plant residues, such as leaves and stems, and animal remains, such as bones and feathers.

Microorganisms like fungi and bacteria are involved in the intricate process of decomposing organic waste in soil. The organic stuff is broken down by these microbes into simpler substances like water, carbon dioxide, and nutrients like phosphorus and nitrogen. Organic matter breaks down to produce nutrients that are vital to the growth and development of plants.

The presence of organic matter in soil is important for several reasons. First, organic matter can improve soil structure and water holding capacity. This can increase soil fertility by improving nutrient availability and promoting plant growth. Second, organic matter can help to reduce soil erosion by improving soil aggregation and stability. Finally, organic matter can help to reduce greenhouse gas emissions by storing carbon in the soil.

Organic matter levels in soil can be increased through several practices, such as adding compost, using cover crops, and reducing tillage. These practices can help to promote the growth of soil organisms and increase the amount of organic matter in the soil. Maintaining adequate levels of organic matter in soil is important for sustainable agriculture and maintaining soil health over the long term.

maintaining soil health over the long term.

#### Macro and Micro-Nutrients in Soil

Both macro and micronutrients are vital elements of soil that are necessary for the growth and development of plants. Micronutrients are needed in smaller proportions than macronutrients, which are needed in relatively larger amounts.

### **Macro-nutrients:**

- 1. Nitrogen (N): Nitrogen is required for the formation of chlorophyll, which is essential for photosynthesis. It is also a component of amino acids, which are the building blocks of proteins.
- 2. Phosphorus (P): Phosphorus is required for cell division and growth, and is a component of nucleic acids, which are essential for genetic information.
- **3. Potassium (K):** Potassium is required for osmoregulation and helps to regulate water uptake and loss in plants. It also plays a role in the formation of carbohydrates and proteins.
- **4. Calcium (Ca):** Calcium is required for cell wall formation and helps to regulate cell division and growth.
- 5. Magnesium (Mg): Magnesium is required for the formation of chlorophyll and plays a role in the regulation of enzyme activity.

#### **Micro-nutrients:**

- 1. Iron (Fe): Iron is required for the formation of chlorophyll and plays a role in the regulation of enzyme activity.
- **2.** Zinc (Zn): Zinc is required for the regulation of enzyme activity and plays a role in the formation of proteins.
- **3.** Manganese (Mn): Manganese is required for the formation of chlorophyll and plays a role in the regulation of enzyme activity.
- **4.** Copper (Cu): Copper is required for the formation of chlorophyll and plays a role in the regulation of enzyme activity.
- 5. Boron (B): Boron is required for the formation of cell walls and plays a role in the regulation of carbohydrate metabolism.
- 6. Molybdenum (Mo): Molybdenum is required for the conversion of nitrogen into a usable form for plants.

# **Ion-Exchange in Soil**

Ion exchange is a process that occurs in soil where positively charged ions (cations) are exchanged for other cations of similar charge that are present in the soil solution. This exchange process is a critical mechanism for nutrient uptake by plants and for maintaining soil fertility.

Soil particles, such as clay and humus, have negatively charged surfaces. These negatively charged surfaces attract positively charged ions, such as calcium (Ca2+), magnesium (Mg2+), potassium (K+), and ammonium (NH4+), from the soil solution. As plants take up these cations, they are replaced by hydrogen ions (H+), which are released by the roots into the soil solution. This exchange process is known as cation exchange.

Cation exchange is an important mechanism for nutrient uptake by plants because it allows them to acquire essential nutrients, such as calcium, magnesium, and potassium, from the soil. Additionally, cation exchange can help to maintain soil pH by regulating the release of hydrogen ions into the soil solution. The amount of cation exchange that occurs in soil is influenced by several factors, such as soil texture, pH, and organic matter content.

In addition to cation exchange, anion exchange also occurs in soil, which involves the exchange of negatively charged ions (anions), such as nitrate (NO3-) and phosphate (PO43-), for other anions that are present in the soil solution. However, anion exchange is generally less important than cation exchange for plant nutrition because anions are usually more readily available in the soil solution.

Overall, ion exchange is an important mechanism for maintaining soil fertility and ensuring that plants have access to the essential nutrients they need for growth and development.

# Soil pH and Nutrients Availability

The acidity or alkalinity of the soil is measured by its pH, which can have a big impact on the availability of nutrients for plant growth. Because soil pH influences various elements' solubility and ability to be absorbed by plant roots, it has a significant impact on the availability of nutrients in soil.

In general, most plants prefer a slightly acidic soil pH between 6.0 and 7.0. When the soil pH is too high (alkaline), certain nutrients such as iron (Fe), manganese (Mn), and zinc (Zn) become less available to plants, while other nutrients such as calcium (Ca), magnesium (Mg), and potassium (K) become more available. Conversely, when the soil pH is too low (acidic), certain nutrients such as phosphorus (P) become less available, while other nutrients such as aluminum (Al) and manganese (Mn) become more available.

Nutrient availability in soil is also affected by the interactions between different elements. For example, the availability of calcium (Ca) and magnesium (Mg) can be influenced by the amount of available potassium (K) in soil, as these nutrients compete for uptake by plant roots. Similarly, the availability of phosphorus (P) can be influenced by the presence of other elements such as iron (Fe), aluminum (Al), and calcium (Ca).

Therefore, it is important to maintain the proper pH level in soil to optimize nutrient availability for plant growth. Soil testing can help to identify nutrient deficiencies and pH imbalances, and guide fertilization practices to maintain the appropriate pH level for the specific crops being grown. In addition, amendments such as lime can be added to increase the pH of acidic soil, while sulfur can be added to decrease the pH of alkaline soil. Maintaining a balanced pH level in soil is crucial for healthy plant growth and maximum yield.

# **Green Chemistry**

Green chemistry, sometimes referred to as sustainable chemistry, is a method of creating and designing chemicals with the goal of minimizing or completely doing away with the usage of dangerous materials. It entails creating chemical systems and goods that are safe for human health, effective, and the environment.

# The principles of green chemistry include:

- 1. Designing chemical processes to be safe and efficient
- 2. Using renewable feedstocks and minimizing waste
- 3. Reducing or eliminating the use of hazardous substances
- 4. Using safer solvents and reaction conditions
- 5. Designing products for reusability or biodegradability
- 6. Minimizing energy use and greenhouse gas emissions

Green chemistry can benefit both the environment and the economy by reducing the amount of waste generated and decreasing the use of non-renewable resources. It can also lead to the development of new technologies and industries.

**Examples of green chemistry** include the development of biodegradable plastics, the use of enzymes in industrial processes, and the creation of safer and more efficient pharmaceuticals.

#### **Atom Economy in Green Chemistry**

• In green chemistry, the term "atom economy" describes how well a chemical reaction uses all of the constituent atoms to generate the intended output or products while producing the least amount of waste. It is computed by

multiplying by 100 after dividing the molecular weight of the intended product by the molecular weight of all reactants utilized in the reaction.

- A high atom economy indicates that the reaction has a high efficiency in converting the starting materials into the desired product(s), while generating minimal waste. This is important because it reduces the number of resources required for a reaction, as well as the amount of waste generated, which can lead to environmental pollution.
- The principles of green chemistry place a strong emphasis on the value of optimizing atom economy in chemical reactions because doing so can result in more efficient and sustainable manufacturing processes. Chemists can minimize the use of hazardous ingredients and reduce energy consumption by developing reactions with high atom economy. This can result in cost savings and environmental benefits.
- In addition, a high atom economy can also be achieved by using renewable resources, such as biomass or carbon dioxide, as starting materials, which can further increase the sustainability of the reaction. Overall, atom economy is a critical consideration in green chemistry, as it can help to minimize waste and reduce the environmental impact of chemical processes.

# **Integrated Pests Management Control**

**Integrated Pest Management (IPM)** is a pest control strategy that aims to manage pests using a combination of techniques that minimize the use of chemical pesticides and reduce the impact of pest management on the environment. The goal of IPM is to prevent pests from becoming a problem and to minimize the damage caused by pests when they do occur.

The key principles of IPM include:

- **1. Monitoring and identification of pests:** Regular monitoring of pests is essential to identify their presence and the extent of the infestation.
- **2. Prevention:** Implementing measures to prevent pests from entering and establishing in the area, such as sealing cracks and crevices and removing potential sources of food and water.
- **3.** Cultural control: Modifying the environment to make it less hospitable to pests, such as removing breeding sites or planting pest-resistant crops.
- **4. Biological control:** Introducing natural enemies of the pests, such as predators, parasites, or pathogens, to reduce their population.
- **5.** Chemical control: Using chemical pesticides only when necessary, and selecting pesticides that are selective, low-toxicity, and have a short residual effect.
- 6. Integration of control methods: Combining different pest control techniques in a coordinated and complementary manner to achieve the best results.

IPM emphasizes the use of non-chemical methods whenever possible, and the judicious use of chemical pesticides as a last resort. This approach minimizes the risk

of developing pesticide resistance in pests, reduces the impact of pesticides on nontarget organisms, and promotes the use of environmentally sustainable pest management practices.

**Examples of Integrated Pests Management Control** 

There are various examples of Integrated Pest Management (IPM) control strategies that can be implemented in different contexts. Some examples are:

- 1. Agricultural IPM: Crop rotation, intercropping, planting pest-resistant crop types, and employing natural enemies of pests like parasitic wasps and ladybirds to manage pest populations are all examples of integrated pest management (IPM) in agricultural contexts.
- 2. Urban IPM: In urban settings, IPM can involve measures such as sealing cracks and gaps in buildings to prevent pest entry, removing food sources and breeding sites, and using non-toxic baits and traps to control pests.
- **3.** Forest IPM: In forest settings, IPM can involve the use of pheromone traps to monitor pest populations, selective pruning to remove infested branches, and the use of biological controls such as fungal pathogens or parasitic wasps to reduce pest populations.
- 4. IPM in stored products: In storage settings, IPM can involve the use of proper storage techniques, such as cleaning and drying grains, using airtight containers, and maintaining appropriate temperatures and humidity levels to prevent pest infestation.
- **5. IPM in livestock production:** In livestock settings, IPM can involve practices such as sanitation measures, vaccination of animals, and the use of biological controls such as nematodes or fungi to control pest populations.

In each of these examples, IPM involves a combination of techniques that aim to reduce pest populations and minimize the use of chemical pesticides, while taking into account the specific context and needs of the system.

# **Ionic Liquids and Green Chemistry**

Ionic liquids are a type of fluids with melting points lower than 100°C that are made completely of ions. A growing number of people are now considering them as a viable substitute for conventional organic solvents because of their special qualities, which include high temperature stability, low volatility, and adjustable qualities.

Ionic liquids have several potential applications in green chemistry due to their properties. They can be used as a solvent for green chemistry reactions, replacing hazardous organic solvents. Ionic liquids can also be used as a separation medium in green chemistry processes, such as extraction and chromatography.

Furthermore, ionic liquids can be designed to be more environmentally friendly by selecting the appropriate combination of cation and anion, and by minimizing their toxicity and potential for bioaccumulation. For example, some ionic liquids are

derived from naturally occurring substances, such as amino acids or sugars, and can be biodegradable.

Ionic liquids also have the potential to be recycled and reused, which can lead to cost savings and reduce waste. Moreover, their unique properties can allow for the development of new and more sustainable chemical processes, such as the use of ionic liquids as a reaction medium for biomass conversion.

Overall, ionic liquids have significant potential in green chemistry due to their unique properties and ability to replace traditional hazardous solvents, leading to more sustainable and environmentally friendly chemical processes.

**Super Critical Extraction Technology** 

Supercritical fluid extraction (SFE) is a green chemistry technique that uses supercritical fluids, usually carbon dioxide, to extract target compounds from a variety of matrices. The steps involved in supercritical fluid extraction are as follows:

- **1. Loading:** The sample matrix containing the target compound is loaded into the extraction vessel.
- 2. Pressurization: Carbon dioxide is then pumped into the extraction vessel to increase the pressure and temperature above the critical point of carbon dioxide (31°C and 73 atm).
- **3.** Extraction: The supercritical carbon dioxide acts as a solvent and extracts the target compounds from the sample matrix. The extracted compounds dissolve in the supercritical carbon dioxide and are carried to the collection vessel.
- **4. Separation:** After extraction, the supercritical carbon dioxide containing the extracted compounds is depressurized and passes through a separator, where the extracted compounds are separated from the carbon dioxide.
- **5.** Collection: The extracted compounds are collected in a collection vessel or fraction collector.
- **6. Purification:** The extracted compounds may require further purification using techniques such as liquid chromatography or distillation.

Supercritical fluid extraction has several advantages over traditional extraction techniques. It is a green chemistry technique that is non-toxic, non-flammable, and produces minimal waste. It is also highly selective and can be used to extract specific compounds from complex matrices, while leaving other compounds behind. Additionally, supercritical fluid extraction can be used to extract both non-polar and polar compounds, making it a versatile extraction technique.

# **Applications of Super Critical Extraction Technology**

Supercritical extraction technology is a process that uses supercritical fluids as a solvent to extract compounds from a variety of materials, including plants, herbs, and spices. The supercritical fluid used in this process is typically carbon dioxide (CO2),

which is heated and pressurized to its supercritical state, where it has properties of both a liquid and a gas.

Here are some of the applications and benefits of supercritical extraction technology:

- 1. Extraction of natural products: Supercritical extraction technology is widely used to extract natural products from a variety of materials, such as plants, herbs, and spices. The process is gentle and efficient, and it can extract compounds without damaging them, unlike traditional extraction methods such as steam distillation.
- 2. Food and beverage industry: Supercritical extraction technology is used in the food and beverage industry to extract natural flavors and fragrances from plant materials. It can also be used to extract caffeine from coffee beans and tea leaves, as well as other compounds such as vitamins, antioxidants, and fatty acids.
- **3. Pharmaceutical industry:** Supercritical extraction technology is used in the pharmaceutical industry to extract active compounds from medicinal plants. It is also used to extract essential oils, fatty acids, and other compounds from plant materials for use in pharmaceutical formulations.
- **4. Environmental applications**: Supercritical extraction technology is used in environmental applications to extract pollutants from soil and water. It can also be used to extract oil and gas from shale formations.
- **5. Benefits:** Supercritical extraction technology has several benefits over traditional extraction methods, including higher yields, shorter extraction times, and lower solvent consumption. It is also a green technology, as it uses a non-toxic and non-flammable solvent (CO2) that can be easily recycled.

In conclusion, supercritical extraction technology is a versatile and efficient process that has a wide range of applications in various industries. Its benefits include high yields, short extraction times, and a green approach to extraction.

# **Green Synthesis**

**Green synthesis** refers to the development of chemical processes for the synthesis of various compounds and materials that are environmentally friendly and sustainable. Green synthesis aims to minimize the use of hazardous chemicals, reduce energy consumption, and generate less waste.

It can be applied to a variety of fields, including pharmaceuticals, materials science, and nanotechnology. Examples of green synthesis include using renewable resources as raw materials, using non-toxic solvents, and using catalysts that are benign to the environment.

It has several advantages over traditional chemical synthesis methods. It is a more sustainable and environmentally friendly approach that can reduce the negative impact of chemical synthesis on human health and the environment. It also has the potential to reduce costs and increase efficiency, making it an attractive alternative to traditional synthesis methods.

It means synthesizing chemical compounds using sustainable and environmentally friendly methods. The following are some examples of green synthesis:

- **Plant extracts:** The use of plant extracts in green synthesis is a popular approach. Plants are a rich source of natural compounds such as flavonoids, alkaloids, and terpenoids, which have various biological activities. These compounds can be extracted using sustainable methods such as water or ethanol extraction. They can then be used to synthesize nanoparticles, drugs, and other compounds.
- **Microorganisms**: Microorganisms such as bacteria and fungi can be used in green synthesis. They produce enzymes and other bioactive compounds that can be used in the synthesis of various compounds. For example, some bacteria produce enzymes that can be used to convert biomass into biofuels.
- **Green solvents:** Solvents play a critical role in chemical synthesis. However, many solvents used in conventional synthesis are toxic and harmful to the environment. Green solvents such as water, ethanol, and supercritical carbon dioxide are gaining popularity as they are non-toxic and have a low environmental impact.
- **Nanoparticles:** Nanoparticles can be synthesized using green methods. For example, green synthesis of silver nanoparticles can be achieved using plant extracts or microorganisms. These nanoparticles have various applications in areas such as drug delivery and wastewater treatment.
- **Catalysis**: Green catalysis is a process of catalysis that involves the use of non-toxic and renewable catalysts. These catalysts can be synthesized using sustainable methods such as plant extracts or biomass. Green catalysis has various applications in organic synthesis and chemical manufacturing.

In conclusion, green synthesis is a rapidly growing field that offers sustainable and environmentally friendly methods for chemical synthesis. The above examples are just a few of the many approaches that are being developed to achieve this goal.

# **Recycling and Green Chemistry**

Recycling and green chemistry are two complementary approaches that aim to reduce the environmental impact of chemical processes and products.

The process of turning waste resources into new products is known as recycling. It is a crucial strategy for lowering the quantity of garbage that pollutes the environment and landfills. Recycling can be done at various stages of the product lifecycle, including manufacturing, use, and disposal.

On the other hand, the development of chemical products and processes that minimize or completely do away with the use and production of dangerous materials is known as "green chemistry." It involves the use of sustainable and non-toxic chemicals and materials, and the development of efficient and environmentally friendly processes.

The relationship between recycling and green chemistry can be seen in the concept of "closed-loop recycling." This approach involves the recycling of materials in a way that minimizes the use of virgin resources and the generation of waste. For example, the recycling of plastic bottles can be done using a process that uses non-toxic solvents and energy-efficient methods, such as supercritical CO2. The recycled plastic can then be used to make new bottles or other products.

Another example of the relationship between recycling and green chemistry is in the use of renewable resources for the production of chemicals. For instance, biomass such as agricultural waste or forestry residues can be used to produce bio-based chemicals through sustainable and non-toxic processes.

In conclusion, recycling and green chemistry are two complementary approaches that can help reduce the environmental impact of chemical processes and products. By using sustainable and non-toxic chemicals and materials, and by designing efficient and environmentally friendly processes, we can create a more sustainable future for our planet.

### **Examples of recycling**

The practice of turning waste resources into new goods or materials is known as recycling. Recycling preserves natural resources, lowers greenhouse gas emissions, and lessens the quantity of garbage that ends up in landfills. Here are some examples of recycling:

- **Paper recycling:** Paper is one of the most commonly recycled materials. It can be recycled into new paper products, such as newspapers, cardboard, and tissue paper. Recycling one ton of paper can save 17 trees, 380 gallons of oil, 3 cubic yards of landfill space, and 4,000 kilowatts of energy.
- **Plastic recycling:** Plastic recycling is the process of recovering waste plastic and reprocessing it into useful products. Some of the most commonly recycled plastics include PET bottles, HDPE containers, and PVC pipes. Recycling plastic can help to reduce the amount of plastic waste that ends up in landfills and oceans.
- **Glass recycling:** Glass can be recycled into new bottles and jars, as well as insulation, road aggregate, and other products. Recycling glass conserves natural resources and reduces energy consumption, as it takes less energy to recycle glass than to make new glass from raw materials.
- Metal recycling: Metal recycling involves recovering and processing scrap metal to create new products. Metals such as aluminum, copper, and steel can be recycled into new products, such as cans, car parts, and building materials. Recycling metal helps to conserve natural resources and reduce greenhouse gas emissions.

• Electronic waste recycling: Electronic waste (e-waste) includes discarded electronic devices such as computers, cell phones, and televisions. E-waste recycling involves recovering valuable materials from these devices, such as gold, silver, and copper. Recycling e-waste can help to reduce the amount of electronic waste that ends up in landfills and prevent the release of toxic materials into the environment.

In conclusion, recycling is an important way to reduce waste, conserve natural resources, and protect the environment. By recycling materials, we can create a more sustainable future for our planet.

# **Carbon dioxide sequestering**

Carbon dioxide (CO2) sequestering refers to the capture and long-term storage of CO2 from the atmosphere or industrial processes to mitigate climate change. Here are some methods of CO2 sequestration:

- 1. Geological sequestration: Using this technique, CO2 is injected underground into geological formations such deep saline aquifers and depleted oil and gas reservoirs. Dissolution and mineralization are two examples of the physical and chemical processes that combine to store CO2 in these formations.
- 2. Ocean sequestration: This method involves the injection of CO2 into the deep ocean, where it is dissolved and stored in the form of bicarbonate ions. This process is limited by concerns over the potential impact on marine ecosystems.
- **3. Mineral carbonation:** This method involves the reaction of CO2 with naturally occurring minerals, such as magnesium and calcium silicates, to form stable carbonates. This process is slow and requires high temperatures and pressures, but has the potential to permanently store CO2.
- 4. **Bio-sequestration:** This method involves the use of plants and trees to capture and store CO2 through photosynthesis. The carbon is stored in the biomass and in the soil. This process is limited by the amount of land available for planting and the potential for carbon to be released back into the atmosphere through deforestation or other land-use changes.
- **5.** Carbon capture and utilization: This method involves the capture of CO2 from industrial processes and its use in the production of fuels, chemicals, and other products. This process can reduce emissions and create economic benefits, but it does not permanently store CO2.

In conclusion, CO2 sequestration is an important strategy for mitigating climate change by reducing greenhouse gas emissions. While several methods are being developed and tested, there is still a need for further research and investment to fully develop and scale up these technologies.

# Applications and benefits of Carbon dioxide sequestering

Carbon dioxide (CO2) sequestration has several potential applications and benefits for mitigating climate change and reducing greenhouse gas emissions. Here are some examples:

- 1. Reducing greenhouse gas emissions: Through the collection and storage of CO2 from the environment and industrial processes, CO2 sequestration can aid in the reduction of greenhouse gas emissions. This can lessen the chance of global warming and assist to alleviate the effects of climate change.
- **2. Enhanced oil recovery:** CO2 sequestration can be used to enhance oil recovery by injecting CO2 into oil reservoirs. The CO2 dissolves in the oil, making it less viscous and easier to extract.
- **3.** Agricultural applications: CO2 sequestration can be used to enhance plant growth and increase crop yields. The CO2 can be injected into greenhouses or used to fertilize crops, which can increase photosynthesis and plant growth.
- **4. Industrial applications:** CO2 sequestration can be used in industrial applications to reduce emissions from power plants, cement production, and other manufacturing processes. This can help to reduce the environmental impact of these industries and improve their sustainability.
- **5.** Carbon credits: CO2 sequestration can generate carbon credits, which can be sold on carbon markets to companies and organizations looking to offset their emissions. This can provide financial incentives for companies to invest in CO2 sequestration technologies and reduce their carbon footprint.

In conclusion, CO2 sequestration has the potential to provide several benefits for mitigating climate change and reducing greenhouse gas emissions. While there are still challenges to be addressed, such as the scalability and cost-effectiveness of these technologies, continued research and development can help to unlock the full potential of CO2 sequestration.

# Water-Based Paints and Green Chemistry

Water-based paints are an example of green chemistry in the paint industry. Waterbased paints, also known as latex paints, are a type of paint that use water as the solvent instead of traditional solvents like oil or mineral spirits. These paints are environmentally friendly and non-toxic, as they do not contain harmful chemicals like volatile organic compounds (VOCs) that are present in oil-based paints.

Water-based paints are available in a variety of finishes such as matte, eggshell, satin, and gloss, and are suitable for both interior and exterior applications. They dry quickly, have a low odor, and are easy to clean up with soap and water. They are also resistant to fading and cracking, making them a durable option for painting projects.

Water-based paints are versatile and can be used on a variety of surfaces such as drywall, wood, metal, and concrete. They are often used for painting walls, ceilings,

trim, and furniture, and can be tinted to a wide range of colors. In addition, they are often more affordable than oil-based paints and require less preparation and cleanup.

Here are some of the benefits of using water-based paints:

- 1. Reduced VOC emissions: Water-based paints emit significantly less VOCs than solvent-based paints, which reduces their impact on indoor and outdoor air quality.
- 2. Improved health and safety: Water-based paints are less harmful to human health than solvent-based paints, as they do not contain the harmful chemicals found in VOCs.
- **3. Lower environmental impact:** Water-based paints have a lower environmental impact than solvent-based paints, as they release fewer pollutants into the air and water.
- **4. Increased durability and quality:** Water-based paints are highly durable and provide a high-quality finish, making them a viable alternative to traditional solvent-based paints.
- 5. Cost-effective: Water-based paints are often more cost-effective than solventbased paints, as they require fewer coats and dry faster, reducing the amount of time and resources needed for painting.

Overall, water-based paints are a prime example of how green chemistry can help to develop environmentally friendly products that are safer for human health and the environment. As more companies and industries adopt green chemistry principles, we can reduce our impact on the environment and improve the sustainability of our products and processes.

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# ENVIRONMENTAL CHEMISTRY, CHEMICALS IN THE ENVIRONMENT

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## Introduction

During the early 1970s, a groundbreaking perspective emerged to shed light on the environmental implications of chemicals. Spearheaded by Hamelink and colleagues (1971), this perspective challenged the prevailing notion that the accumulation of organic compounds in living organisms was solely driven by ecological factors. Instead, they put forth the idea that the chemical's inherent properties played a pivotal role. Over time, this concept underwent significant expansion, revealing that the distribution of chemicals in the environment is influenced by both their intrinsic characteristics and the surrounding environmental conditions(Escher et al., 2020). This realization underscores the intricate interplay between chemical properties and the environment in shaping the behavior and fate of chemicals within ecosystems. Environmental chemistry has gained recognition among scientists in recent years as a comprehensive field of study encompassing the behavior and potential negative impacts of chemicals released into the environment. While the concept itself is not novel, its widespread adoption highlights the significant value placed on understanding the behavior and potential harm caused by chemical substances when they are introduced into natural ecosystems. Extensive research has been conducted to investigate natural chemical processes occurring in various environmental sectors, including soil, water, and the atmosphere. Additionally, considerable attention has been given to understanding the environmental behavior of contaminating chemicals. These studies aim to reveal the interactions between chemical compounds and their surrounding environment, shedding light on their fate, transport, transformation, and potential impacts on ecosystems (Manzetti et al., 2014). By exploring these aspects, scientists strive to gain a deeper understanding of the complex dynamics within the natural environment and the implications of contaminant release.

Environmental chemistry, characterized by its interdisciplinary nature, emerges as one of the most diverse branch within the field of chemistry. It seamlessly incorporates

elements from related disciplines such as organic chemistry, analytical chemistry, physical chemistry, and inorganic chemistry. Furthermore, it extends its reach into diverse domains including biology, toxicology, biochemistry, public health, and epidemiology. This multidisciplinary approach is essential for comprehending and addressing the interactions between chemicals and the environment. By combining knowledge and methodologies from various scientific fields, environmental chemists have gained a comprehensive understanding of the behavior, impacts, and potential risks of chemical substances in both natural and human-dominated ecosystems (Des W. Connell, 2005).

Environmental Chemistry is defined as the field of study that focuses on investigating the sources, reactions, transport, effects, and fates of chemical species in water, soil, air, and living environments. It also examines the influence of technology on these processes. Its objective is to understand the complex interactions between chemicals and the environment, and to assess the impacts on ecosystems and human health (Stanley E. Manahan, 2006). Environmental Chemistry also devise suitable methodologies that can be implied to solve the problems associated with the environment.

#### **Green Chemistry**

In recent years, there has been a notable shift within the environmental movement, moving beyond a sole focus on pollution, its effects, and mitigation strategies, to embrace a broader perspective of sustainability. This contemporary approach is commonly referred to as "green" and emphasizes environmentally friendly practices. When applied to the field of chemistry, this shift is manifested in the practice of green chemistry, which promotes the use of inherently safer and more environmentally sustainable chemical science. So, Green chemistry refers to the implementation of chemical science and manufacturing practices that prioritize sustainability, safety, and minimal pollution(Lancaster, 2002). It emphasizes the efficient use of materials and energy while striving to generate little to no waste.

#### **Principles of green chemistry**

By embracing green chemistry principles, the goal is to develop environmentally friendly processes that minimize the environmental impact associated with chemical production and usage(Stanley E. Manahan, 2006).By prioritizing green chemistry

principles (presented below in figure 1), we can strive towards a more sustainable and environmentally conscious future(Anastas & Warner, 1998).



Figure 1. Principles of green chemistry

### **Importance of Green Chemistry**

As the global population continues to grow and strain the finite resources of our planet, the adoption of green science and technology has become critically important. Meeting the needs of a large population with limited resources requires a shift towards sustainable practices and solutions. The practice of green science and technology offers innovative approaches to minimize environmental impact, conserve resources, and promote long-term sustainability. By prioritizing and implementing green practices, we can address the challenges of providing for a growing population while minimizing our ecological footprint and ensuring a healthier future for both humanity and the planet(Manahan, 2010).

#### Why Green Chemistry?

In traditional environmental science, the focus had been on the hydrosphere, atmosphere, geosphere, and biosphere—the realms of water, air, earth, and life. Human activities were often regarded as undesirable disruptions to these spheres, leading to pollution and negative consequences. However, this perspective is limited, and we must now recognize the inclusion of a fifth sphere, known as the anthrosphere. The anthrosphere encompasses the creations and actions of humans—the things we make and do. By acknowledging the significance of the anthrosphere, we broaden our understanding of the interactions between human activities and the environment,

enabling us to address the complex environmental challenges we face today(Stanley E. Manahan, 2006).

#### **Applications of Green Chemistry**

Green chemistry is referred as the approach in which the chemical science and manufacturing techniques are modified in a way that is environmentally friendly, utilize least amount of materials and energy while producing little or no waste. In order to achieve the goals of green chemistry, the manufacturing processes and techniques are modified or redesigned completely in order to gain sustainability. Green chemistry is all about innovation for the protection of human health and environment. Green chemistry finds application across diverse industries such as chemicals, pharmaceuticals, paper, polymers, textiles, and pigments. It holds significance in energy research, contributing to the creation of innovative methods for manufacturing solar cells, fuel cells, and energy storage batteries. Moreover, green chemistry plays a pivotal role in nanoscience and technology. The central aim of green chemistry is waste minimization in the chemical sector, driving the innovation of various environmentally friendly catalysts.

#### **Environmental Pollution**

The Industrial Revolution (1760-1840) marked a turning point as rapid industrialization led to widespread pollution from factories and coal burning, causing environmental degradation(Rifkin, 2011). In 1952, London's Great Smog claimed thousands of lives, underscoring the severe consequences of air pollution and prompting the implementation of clean air regulations (Bell et al., 2004). The devastating Minamata Disease outbreak in Japan (1956-1960s) demonstrated the dire effects of industrial wastewater contamination, emphasizing the need for stricter environmental safeguards (Harada, 1995). Rachel Carson's groundbreaking book "Silent Spring" (1962) exposed the harmful effects of pesticides on ecosystems, fueling the environmental movement (Carson, 2002). The infamous Cuyahoga River fire (1969) in Cleveland, Ohio, became a symbol of the perils of industrial pollution and galvanized efforts to restore environmental health (2001). The Bhopal Gas Tragedy in India (1984) highlighted the catastrophic consequences of industrial accidents, leading to increased awareness of industrial pollution's human toll (Dhara & Dhara, 2002). Major oil spills such as the Exxon Valdez (1989) and Deepwater Horizon (2010) disasters brought attention to the devastating impact of oil pollution on marine ecosystems (Koper & Terpstra, 1991; Rauh et al., 2011). Lastly, the Fridays for Future movement (2018-present), initiated by Greta Thunberg, has mobilized global youth activism, demanding urgent action against climate change and pollution (Hanna-Attisha et al., 2016).

#### What is Environmental pollution?

Environmental pollution is the introduction of harmful substances or energy into the environment, resulting in adverse effects on ecosystems and human health (USEPA, 2019). Pollution arises from various sources, both natural and anthropogenic. Natural sources include volcanic eruptions, wildfires, and biogenic emissions (Andreae, M. O., 2019; Field, R. D., 2016). Anthropogenic sources, however, play a major role in pollution. These sources encompass industrial activities, transportation emissions, energy production, and improper waste management(Hijazi et al., 2019; Lelieveld et al., 2015).

Environmental pollution manifests in various forms, including air pollution, water pollution, and soil pollution. Air pollution refers to the contamination of the air with harmful substances, such as particulate matter, nitrogen oxides, sulfur dioxide, volatile organic compounds, and ozone, which have detrimental effects on human health and the environment (Dockery & Pope, 1994; Murray et al., 2020). Water pollution occurs when pollutants, including industrial effluents, agricultural runoff, sewage, and chemical contaminants, contaminate freshwater bodies, coastal areas, and groundwater, leading to ecological imbalances and health risks(Braat, 2016). Soil pollution involves the accumulation of hazardous substances, such as heavy metals, pesticides, and industrial waste, in the soil, resulting in soil degradation and contamination that can adversely affect agricultural productivity and ecosystem health. Understanding the different types of environmental pollution is crucial for developing effective strategies to mitigate their impacts and protect human and ecological well-being. As shown below in Fig. 5 below, environmental contamination exists and can be transfer between different ecosystems(Puri et al., 2023).



Figure 2. Transfer of contaminants in different ecosystems

As shown in Fig. 3 below, the COVID-19 pandemic and subsequent lockdown measures imposed worldwide have had profound effects on the environment (Venter et al., 2020). With reduced human activities and restrictions on travel and industrial operations, there have been noticeable improvements in air quality, reduced pollution levels, and changes in ecological dynamics. Studies have shown significant decreases in air pollutants such as nitrogen dioxide (NO<sub>2</sub>) and particulate matter (PM<sub>2.5</sub>) during the lockdown period (Collivignarelli et al., 2020; Liu et al., 2021). The impact of these observations has motivated researchers to explore the potential of sustainable practices and innovative solutions to mitigate pollution even beyond the pandemic. It has triggered investigations into cleaner energy alternatives, sustainable transportation systems, and more efficient waste management strategies. The pandemic has served as a catalyst for innovative research and policy discussions aimed at building a more resilient and sustainable future (Rupani et al., 2020).

When we talk about environment, we are concerned about all the factors that are included in the environment. It involves all the ecosystems and every type of pollution. Here is a complete description of the types of pollutions:

#### **Atmospheric Pollution**

Atmospheric pollution, also known as air pollution, refers to the presence of substances in the atmosphere resulting from human activities or natural processes (pollutants), that can cause harmful effects on human health, the environment, and the climate. Pollutants can be in the form of gases, tiny particles or they can be of different

chemical nature that becomes a part of the air in order to cause pollution. These pollutants are produced by various sources, including industrial processes, transportation, energy production, agricultural activities, as well as natural events such as wildfires or volcanic eruptions. Air pollution can contaminate both indoor and outdoor environments and encompasses any chemical, physical, or biological agent that alters thenatural characteristics of the atmosphere. Its detrimental impacts extend to air quality, ecosystem integrity, climate patterns, and human well-being (USEPA, 2019; WHO, n.d.).

# **Tropospheric Pollution**

Tropospheric pollution is also referred to as air pollution. It is the contamination of the lowest layer of the Earth's atmosphere, known as the troposphere. From the earth's surface this layer extends to an altitude of about 10-15 kilometers. Tropospheric pollution involves both gaseous and particulate matter that are released into the air because of human activities and natural processes. Following are the main types of tropospheric pollutants:



Figure 3. The mapping displays global distribution of ground-level air pollution anomalies in 2020. Ground station measurements of (A) NO2, (B)O3, and (C) PM2.5 anomalies are utilized. Anomalies are defined as deviations from 3-year baseline levels for the same dates in the January-May 2020 period, without accounting for weather variability. Insets depict the density distributions of baseline and 2020 data periods, with vertical lines indicating median values.

#### Gaseous air pollutants

Air pollutants are typically classified into several categories based on their chemical composition and sources (War et al., 1998; WHO, n.d.):

- 1. **Nitrogen oxides (NOx),** including nitrogen dioxide (NO<sub>2</sub>) and nitric oxide (NO), are highly reactive gases formed from the combustion of fossil fuels and contribute to the formation of photochemical smog and acid rain(Almetwally et al., 2020).
- 2. Sulfur oxides (SOx), primarily sulfur dioxide (SO<sub>2</sub>), are emitted during the combustion of sulfur-containing fossil fuels, such as coal and oil, and are associated with respiratory and cardiovascular health issues(Nieder & Benbi, 2022).
- 3. **Carbon monoxide (CO)** is a colorless, odorless gas produced by incomplete combustion of carbon-based fuels, and its high levels can be harmful to human health(Manahan, 2010).
- 4. Volatile organic compounds (VOCs) encompass a wide range of organic chemicals that easily vaporize, including hydrocarbons and other volatile substances emitted by industrial processes, vehicle exhaust, and solvents.
- 5. **Ozone (O<sub>3</sub>)** is a secondary pollutant, as presented below in Fig. 3(Sicard et al., 2023), it is formed through complex photochemical reactions involving nitrogen oxides and volatile organic compounds(Erickson et al., 2020). While ozone in the upper atmosphere plays a beneficial role in blocking harmful UV radiation, ground-level ozone is a harmful component of smog and can cause respiratory problems and lung damage(Markozannes et al., 2022).

#### **Particulate Pollution**

Particulate matter (PM) refers to fine solid or liquid particles suspended in the air, such as dust, soot, and aerosols. These particles are classified by their size, with  $PM_{10}$  representing particles with a diameter of 10 micrometers or less, and  $PM_{2.5}$  indicating particles with a diameter of 2.5 micrometers or less (Wark et al., 1998). Particulate matter are released into the air as a result of combustion processes, vehicle emission, industrial activities, and natural sources such as dust, forest fire, volcanic eruptions and pollen.

#### Health effects of particulate pollution

- **Respiratory problems:** PM<sub>2.5</sub> can penetrate deep into the lungs and can cause respiratory problems such as, asthma, bronchitis, and chronic obstructive pulmonary disease (COPD).
- Heart Issues: Particulate matter have to potential to enter the bloodstream and cause inflammation. This poses the risk of heart attacks, strokes, and other cardiovascular diseases.
- **Premature death:** Particulate matter have impact on respiratory and cardiovascular health, and its long-term exposure can eventually increase the risk of premature death.

#### **Environmental and Climate impact**

- **Reduce Visibility:** Especially in the urban areas, particulate pollution contributes to hazy conditions and thus reduce the visibility.
- Climate Effects: Particulate matter can affect the local and regional climate patterns, because some particulates such as black carbon, absorbs sunlight and contributes to the global warming.

#### **Stratospheric Pollution**

Stratospheric pollution refers to the presence of harmful substances in the stratosphere, the atmospheric layer located approximately 10 to 50 kilometers above the Earth's surface. One notable aspect of stratospheric pollution is the depletion of the ozone layer, which plays a crucial role in protecting life on Earth from harmful ultraviolet (UV) radiation(Erickson et al., 2020). The primary cause of the ozone hole is the release of ozone-depleting substances (ODS), particularly chlorofluorocarbons (CFCs), into the atmosphere(Manisalidis et al., 2020). CFCs were widely used in various industrial and consumer applications, such as refrigeration, aerosol propellants, and foam-blowing agents. These substances are stable enough to reach the stratosphere, where they undergo photodissociation due to UV radiation, releasing chlorine and bromine atoms. These atoms then catalytically destroy ozone molecules, resulting in the thinning of the ozone layer(Karadan et al., 2023).Ozone (O<sub>3</sub>) formation and breakdown in the stratosphere involve complex photochemical reactions. Ozone is formed through the Chapman cycle, which begins with the dissociation of molecular oxygen (O<sub>2</sub>) by high-energy UV-C radiation (wavelengths

shorter than 240 nanometers). The dissociated oxygen atomscan then react with other O<sub>2</sub> molecules, forming ozone. The process of ozone formation is balanced by its destruction. Ozone can be broken down by reactions with naturally occurring compounds like nitrogen oxides (NOx) and hydrogen atoms. However, the introduction of ODS into the stratosphere upsets this equilibrium(Adcock, 2020). The chlorine and bromine atoms released from ODS act as catalysts in ozone destruction cycles, leading to the formation of the ozone hole, particularly over Antarctica(Adcock, 2020).



Figure 4. O3 and other air pollutants from atmospheric chemical reactions and other natural and anthropogenic sources.

#### How to control air pollution?

Air pollution is a serious global issue, that need serious efforts to get controlled, otherwise it can cause serious health issues for the living beings. In order to control air pollution, we need a combination of policy measures, advancement in technology and individual efforts. Here are some strategies that can control or reduce air pollution effectively:

# 1. Policies and Regulations

- Strict emission standards for the industries, vehicles, power plants, and other sources of pollution should be enforced and implemented.
- To restrict activities contributing to air pollution, such as burning of waste and open field burning, it is the need of the time to establish and strengthen laws for it. Proper law and order can be a contributing factor for pollution control.
- Instead of coal, cleaner fuels such as natural gas should be encouraged to use, and the use of renewable energy sources (solar and wind power) should be promoted.

# 2. Vehicle Emission Control

- The use of electric vehicles (EVs) should be promoted.
- Inspection of the vehicles should be done regularly to ensure that the vehicles are not producing any hazardous chemicals that can add to the air pollution.
- Try to reduce the private vehicles on the road by investing in the public transport. This can be a very promising factor towards environmental sustainability.

# 3. Industrial Pollution Control

Industries are the most contributing factor towards air pollution, and it is required to adapt serious strategies to minimize the pollutants coming out of industries. Following are some measures that needs to be implemented:

- Pollution control technologies such as scrubbers and filters should be used to avoid or reduce emissions.
- The industries should be far away from cities where there is minimum human population to avoid the threats that can be posed to human health through the chemicals coming out of the industries.
- Adsorption techniques should be used at industrial level to ensure that the waste coming out of industries is free from hazardous effluents
- 4. Promote Clean Energy
- Solar, wind, hydroelectric, and nuclear power should be used to generate energy instead of the use of fossil fuels.
- For renewable energy projects and energy efficient technologies, incentives and subsidies should be offered.
- 5. Urban Planning and Design
- Cities should be planned in such as way that minimizes the traffic congestion and encourage walking, cycling, and the use of public transport.
- It is the absolute necessity to develop green spaces and urban forests that will act as natural air filters.
- 6. Waste Management
- In order to reduce the need of open burning and landfilling, proper waste management practices, such as recycling should be promoted.
- Such technologies should be implied that can convert the waste into useful energy without releasing pollutants in the environment.

- 7. Public Awareness and Education
- Through the use of educational campaigns, awareness should be raised about the causes and consequences of the air pollution.
- Personal practices that can adds to the control of air pollution, such as using public transport, recycling, reducing energy consumption, and avoiding burning of waste should be encouraged.
- 8. Research and Innovation
- Investments should be made in research and development of advanced pollution control technologies.
- We should support the innovation in areas like air quality monitoring, pollution reducing devices, and clean energy production.
- 9. International Collaboration
- It is a good idea to collaborate with the neighboring countries to address the pollution issues.
- Collaborate with researchers globally that are working for the development to technologies that can be helpful to reduce pollution.
- **10. Air Quality Monitoring**
- Air quality monitoring systems should be established to track pollution levels and identify the causes of the pollution.

It is important to note that controlling air pollution requires multiple efforts on governmental and at individual level, and by adopting the above-mentioned strategies a significant contribution can be made to reduce the air pollution, and improving the air quality.

# Water Pollution

Access to clean and safe drinking water is of utmost significance for human health and overall well-being of the living(WHO, 2019). Contaminated water sources can pose severe health risks, leading to waterborne diseases, such as cholera, typhoid, and diarrhea, which contribute to millions of deaths each year(Prüss-Ustün et al., 2019).Furthermore, inadequate access to safe drinking water impacts vulnerable populations, exacerbating socio-economic disparities and hindering sustainable development(UN, 2015). To address this global challenge, international standards and guidelines for drinking water have been established to ensure the provision of safe and high-quality water to communities worldwide(WHO, 2017). These standards, developed by organizations like the World Health Organization (WHO) and regulatory bodies such as the United States Environmental Protection Agency (EPA), aim to safeguard human health by setting limits for various contaminants and parameters in drinking water(USEPA, 2020; WHO, 2017). Adhering to these international standards is crucial for preventing waterborne illnesses and promoting public health on a global scale.

Water pollution is referred as the addition of pollutants in the water bodies such as, river, lakes, etc., that imposes serious threats to the health of human beings, plants and animals. These pollutants came from different sources and are different in nature some can be toxic to highly acidic in nature that can even lead to the death of the water bodies and have the capability to disturb or completely destroy the food chain.

#### **Toxic Chemicals in Water**

Contamination of water sources with toxic chemicals presents a significant risk to human health and the environment. Industrial activities, agricultural practices, and improper waste management contribute to the presence of these harmful substances in water. This article provides an in-depth exploration of the most concerning toxic chemicals found in water and their potential health effects.

Water resources contamination with chemicals is a pressing issue that has been extensively studied and documented by various reliable sources. The EPA plays a significant role in monitoring and addressing contamination concerns, providing valuable information on specific contaminants, such as lead and copper in water distribution systems (EPA, 2021). The WHO offers comprehensive guidelines on drinking water quality, including information on various chemical contaminants like arsenic and disinfection byproducts (WHO, 2018). The International Agency for Research on Cancer (IARC) provides insights into the potential health risks associated with drinking water disinfectants and contaminants, offering guidance on mitigating those risks (IARC, 2014). The United States Geological Survey (USGS) conducts extensive research and monitoring of water resources, examining pesticide contamination and its impact on groundwater (USGS, 2020). These sources, among others, provide valuable insights into the identification, prevention, and remediation of chemical contamination in water resources, helping to inform policies and protect human health and the environment.

**Lead Contamination:** Lead is a highly toxic heavy metal that can enter water through old lead pipes, plumbing fixtures, and solder. Even at low levels, lead exposure can have severe health consequences. Children are particularly vulnerable to lead poisoning, as it can impair their development, lead to learning disabilities, and cause behavioral problems. In adults, lead exposure is associated with increased blood pressure, kidney damage, and reproductive issues (EPA, 2021).

**Arsenic Contamination:** Arsenic is a naturally occurring element found in rocks and soil. It can contaminate groundwater and surface water sources, particularly in regions with geological arsenic deposits. Chronic exposure to arsenic through drinking water has been linked to a range of health problems. Skin lesions, cardiovascular diseases, neurodevelopmental disorders in children, and various types of cancer, including skin, lung, bladder, and kidney cancer, are among the health effects associated with arsenic exposure (WHO, 2018).

**Disinfection Byproducts:** Water treatment plants often use chlorine as a disinfectant to eliminate harmful bacteria and viruses. However, when chlorine reacts with organic matter present in water, it can lead to the formation of disinfection byproducts (DBPs). Trihalomethanes (THMs) are a group of DBPs that have raised concerns due to their potential health risks. Long-term exposure to high levels of THMs through drinking water has been associated with an increased risk of bladder cancer. Studies have also suggested links between THMs and adverse reproductive outcomes, such as preterm birth and low birth weight (IARC, 2014).

**Pesticide Pollution:** Pesticides are chemicals used in agricultural practices to control pests and increase crop yields. However, these substances can contaminate water sources through runoff and leaching into the soil. Prolonged exposure to pesticides in drinking water has been associated with a range of health issues. Organophosphates and organochlorines, two common classes of pesticides, have been linked to neurological disorders, hormone disruption, reproductive problems, and an increased risk of certain cancers. Monitoring by the United States Geological Survey (USGS) has revealed the widespread presence of pesticides in groundwater across various regions in the United States (USGS, 2020).

**Conclusion:** Toxic chemicals in water pose a significant threat to human health and the environment. Lead, arsenic, disinfection byproducts, and pesticides are among the most concerning contaminants found in water sources. Protecting water quality

requires comprehensive efforts from governments, regulatory bodies, industries, and individuals. This includes implementing and enforcing strict regulations on industrial and agricultural practices, upgrading infrastructure to prevent lead contamination, promoting alternative disinfection methods to minimize DBP formation, and adopting sustainable agricultural practices that reduce pesticide use and runoff. Regular monitoring and public awareness are essential to identify and address emerging contaminants, safeguarding water resources and ensuring the well-being of communities.

### **Causes of water pollution**

Water pollution arises from various sources(some of them are shown below in Fig. 3) (Mitiku, 2020) some of them are described here. Industrial discharges are a major source of water pollution, releasing contaminants such as heavy metals, organic chemicals, and pollutants from manufacturing processes(EPA, 2021). Sewage treatment plants also contribute to water pollution through the discharge of inadequately containing treated wastewater pathogens, nutrients, and pharmaceuticals(Huang et al., 2020). Additionally, agricultural runoff is also a significant contributor, carrying pesticides, fertilizers, and sediment into water bodies, resulting in nutrient enrichment, harmful algal blooms, and degraded water quality (Carpenter et al., 1998). Waste disposal practices, including improper disposal of solid waste and dumping of hazardous substances, further contribute to water pollution by leaching harmful chemicals into groundwater and surface water(Jambeck et al., 2015; UNEP, 2020).



Figure 5. Major causes of water pollution

# **International Standards of Drinking Water**

In order to provide guidance on safe and healthy drinking water, the World Health Organization (WHO) has played its role by setting international standards for the quality of drinking water. The standards are written in the WHO's "Guidelines for Drinking water Quality". The guidelines are kept up to date to ensure the quality imrovement according to the latest research and development. The standards are then modified at the country level, and each country change them according to their own national standards. Following are some main points that shows the important standards set by the WHO:

### 1. Microbial Parameters

Total Coliforms: Not detected in a 100mL sample of drinking water.

Escherichia coli (E.coli): Absence in a 100 mL sample of drinking water.

Heterotrophic Plate Count (HPC): The recommended limit is no more than 100 colony-forming units (CFU) per mL.

### 2. Chemical Parameters

Arsenic: The advised concentration should not exceed 10 micrograms per liter ( $\mu$ g/L).

Lead: The recommended concentration is less than or equal to 10  $\mu$ g/L.

Nitrate: The recommended concentration is 50 mg/L or less.

Fluoride: The suggested limit is no more than 1.5 mg/L.

Mercury: The advised concentration should not exceed 6  $\mu$ g/L.

#### 3. Physical Parameters

Turbidity: The recommended level is 5 nephelometric turbidity units (NTU) or less.

**Color:** While no specific guidance value is provided, the color should not indicate contamination or pose a health risk.

# 4. Radiology Prameters

Radon: The acceptable level is 100 Bq/L (becquerels per liter) or less.

# 5. Disinfection By-products

**Trihalomethanes (THMs):** The suggsted limit is no more than 100  $\mu$ g/L, measured as the sum of four THMs.

### 6. Emerging Contaminants

The guidelines also consider emerging contaminants such as pharmaceuticals and substances known for their potential to disrupt the endocrine system. Specific guideline value may not be available due to ongoing research in these areas.

These are some main key parameters according to the WHO and these guidelines are used by the authorities in each country for customizing the drinking water quality standards at national level.

### How to control water pollution?

Addressing water pollution challenges requires a collective effort and strong adherence to established standards.Collaborative action involving governments, international organizations, communities, and stakeholders to effectively tackle water pollution issues. Cooperation among countries in sharing best practices, knowledge exchange, and joint research initiatives can contribute to effective pollution control and prevention strategies(UNESCO, 2020). Here are some strategies that are effective for controlling or reducing water pollution:

- 1. International Standards and Guidelines
- Adherence to international standards and guidelines for water quality, such as those developed by the WHO and regulatory bodies like the USEPA, is crucial (USEPA, 2020; WHO, 2017). It is essential to ensure proper implementation and enforcement of these standards, which set limits for various contaminants and parameters in drinking water, safeguarding human health (Li & Wu, 2019). The basis of these standards are extensive research and scientific evidence.
- It is the basic right of the public to have access to clean and safe drinking water. International standards play an important role to ensure the safety of water. They works as a barrier for various pollutants, such as microbial contaminants (bacteria, viruses), chemical substances (heavy metals, pesticides), and physical parameters (turbidity, pH), that are the causes of water pollution. If these standards are strictly followed, they play the key role to prevent water borne diseases.
- 2. Wastewater Treatment

- The industrial and domestic waste water should be treated properly before discharging. In order to do this the waste water treatment plants should be maintained and upgraded regularly.
- In order to remove some specific pollutants such as nutrients, heavy metals, and pharmaceuticals, advanced treatment technologies should be implemented.
- In today's world wastewater that is coming out of industries is filling with a lot of carcinogenic substances such as organic azo dyes, that are non-biodegradable. In order to remove these substances from water advanced methods are being used such as nanotechnology is proven to be the most effective. Advancement is being made in this field to get the most effective results.
- 3. Industrial Best Practices
- In order to reduce pollution at the source, industries should be encouraged to adopt cleaner production methods, recycling, and waste reduction.
- Pollution prevention plans should be introduced at industrial level, that have to potential to identify and the address the potential pollution risks.
- 4. Agricultural Practices
- Sustainable agricultural practices should be promoted that can reduce the use of harmful fertilizers and pesticides. The use of natural fertilizers should be promoted because they don't pose any environmental issue.
- In order to prevent sediment and nutrient runoff from fields, erosion control measures such as contour plowing and cover crops should be implemented.
- 5. Hazardous Waste Management
- The hazardous materials should be prevented from entering water bodies, because they can pose serious health issues for not only humans but for plants and animals as well. They can even cause the complete depletion of marine life. So, to prevent this from happening the hazardous materials should be properly disposed of.
- Safe disposal practices at domestic and industrial level can be established with the development of hazardous waste collection centers.
- 6. Community Education
- Awareness among the communities about the importance of preventing water pollution can also help to prevent water pollution.
- Proper education should be given to common people about the safe waste disposal practices at domestic level.

# 7. Monitoring and Enforcement

- Establishment of water quality monitoring system in order to track the pollution levels and identify pollution sources is also a very promising factor.
- The rules and regulations should be strictly implemented through regular inspections, fines, and penalties for the non-compliance.
- 8. Research and Innovation
- Government should invest in research and development of novel technologies that can help to reduce or control water pollution.
- New and effective solutions should be explored such as nanotechnology and bioremediation. These methods are very effective for targeting specific pollutants.
- 9. International Collaboration
- Collaborations should be made with the neighboring countries to address the water pollution issues, and collective efforts should be made to look for effective strategies to eradicate the pollutants from the water to overcome water pollution.
- International collaborations should be made at the global level to address the problems a country is facing individually, and experts from all around the world should work together to look for effective solutions,

#### **10. Better Infrastructure**

• Government should invest for the upgradation and expansion of sewage infrastructure, in accordance with the growing population and to reduce the overflows.

By following these strategies and modifying them according the situation in each region of the world, it is possible to control water pollution effectively at domestic and industrial level.

# **Soil Pollution**

"Soil is referred to as the complex and dynamic natural resource that makes the top layer of the surface of Earth". It is the outermost layer of the earth's crust and is mainly consists of organic, inorganic minerals as the major components, other than this its composition also includes: water, air and some microorganisms. Soil plays a pivotal role for the sustainability of life on earth by providing the foundation for the growth of plants, which ultimately is responsible for the sustainability of the ecosystems and agriculture. Following are the main components and characteristics of soil:

- **Inorganic materials:** They constitute the bulk of the soil. They are materials that result from the disintegration of the various rocks that make up the earth's crust, such as igneous, sedimentary and metamorphic rocks by chemical and mechanical factors. Nitrogen, phosphorous, potassium, manganese, lead, copper, zinc, iron, aluminum, sodium and potassium salts are the necessary elements for plants that determine the quality of the soil whether it is calcareous, saline, iron, or neutral (S. H. H. Al-Taai, 2021).
- Organic materials: These materials consist of plant and animal wastes such as animal excrement (such as feces, blood, skins, roots and remains of plants, leaves, stems, carcasses of dead animals, etc.) They are broken down and transformed over time into humus. Humus is one of the main fertilizers of soil. Soil is a mobile world that contains large and microscopic organisms. They are part of the biosphere. They contribute to the aeration of the soil and change its chemical composition. Bacteria absorb nitrogen and fix it in the soil to absorb it by the plant because plants are unable to absorb it from the air directly. Therefore, the soil must be preserved and not polluted (S. H. H. Al-Taai, 2021).
- Water: Soil has the ability to retain varying amount of water in it. This ability is associated with the texture of the soil and the composition of organic and inorganic minerals in it. Water is also a very important component of soil, because it is essential for the growth of plants, ad is also vital for the hydrological cycle of earth.
- Air:Soil contain pores, and these pores have air entrapped in it. This air is very important for the gaseous exchange between plant roots and the microorganisms. This air allows the roots to take up oxygen and release carbon dioxide.
- Living Organisms: Soil contains multiple type of living organisms including, bacteria, fungi, insects, earthworms, and other microorganisms. These organisms play their role for maintaining the nutrient value and overall health of the soil. They are also responsible for doing decomposition.

#### **Causes of Soil Pollution**

Soil pollution, stemming from various causes and sources, poses significant environmental and human health challenges.

Agricultural practices play a major role in soil pollution. The excessive use of chemical fertilizers and pesticides in farming can result in the accumulation of these

substances in the soil. When not managed properly, these chemicals can leach into the soil, contaminating it and affecting its quality. In addition, agricultural runoff, which includes sediment, nutrients, and pesticides, can find its way into nearby water bodies, further contributing to soil pollution.

**Industrial activities** are another prominent source of soil pollution. Improper disposal of industrial waste, including chemicals, heavy metals, and toxic byproducts, can lead to contamination of nearby soil. Accidental spills, leaks, and improper storage and handling of hazardous materials can also introduce these pollutants into the soil environment. Industries such as mining, manufacturing, and energy production are particularly prone to generating soil pollution due to their waste disposal practices.

**Contaminated landfills** represent yet another significant source of soil pollution. As landfills accumulate various forms of waste over time, the chemicals and pollutants present in the waste can seep into the surrounding soil. This can result in long-term contamination that affects the soil quality and the underlying groundwater, leading to broader environmental concerns.

# Impact of Soil Pollution on the Quality of Soil

The impact of soil pollution on soil quality is detrimental and far-reaching. Pollutants alter the soil's natural composition and balance of nutrients, degrading its fertility. Soil structure can be affected, leading to increased compaction or erosion. The presence of toxic substances in the soil hinders the growth and development of plants. Contaminants can interfere with root development, nutrient uptake, and overall plant health. Consequently, crop productivity can be significantly reduced, posing risks to food security and agricultural sustainability.

Moreover, soil pollution has implications for the broader ecosystem and the food chain. Toxic chemicals found in contaminated soil, such as heavy metals, pesticides, and industrial pollutants, can persist for extended periods. They can be taken up by plants and subsequently transferred to herbivores and then to higher-level consumers through the food chain. This bioaccumulation of pollutants can lead to adverse health effects in humans and wildlife that consume contaminated plants or animals.

Addressing soil pollution requires a multifaceted approach. Implementing sustainable agricultural practices, such as organic farming and integrated pest management, can reduce reliance on chemical inputs and minimize soil pollution. Proper waste

management strategies and regulations for industrial activities are essential to prevent the release of hazardous substances into the soil. Additionally, remediation techniques, such as soil monitoring, soil remediation technologies (e.g., soil washing, bioremediation), and land reclamation efforts, are crucial in mitigating the effects of soil pollution and restoring contaminated lands.

In conclusion, soil pollution is a pressing environmental issue caused by various factors, including agricultural practices, industrial waste disposal, and contaminated landfills. Its impact on soil quality, plant growth, and the food chain is significant. Recognizing the presence of toxic chemicals in soil and understanding their potential risks is crucial for effective management and remediation efforts to ensure the long-term health and sustainability of soil ecosystems and human well-being. Soil pollution is a topic of great importance for researchers and environmental enthusiasts due to its significant impact on human and animal life. The chemical and physical alterations in soil composition are a result of the introduction of foreign substances. Factors such as the excessive use of pesticides and chemical fertilizers, acid rain deposition, and the improper disposal of solid and liquid waste from factories contribute to the degradation of soil fertility and organic matter content (S. Al-Taai, 2021).

The research examines several crucial aspects related to soil pollution, including the definition of environmental pollution with a specific focus on soil pollution. It also highlights key soil pollutants, such as radioactive contamination, which has global significance due to its detrimental effects on soil, plants, animals, and humans. Industrial and domestic waste pollution is addressed, considering the proximity of factories to residential areas and water bodies. Additionally, natural phenomena like volcanic activity, fires, and mining play significant roles in soil pollution, leading to the loss of organic matter and soil fertility. The impact of pesticides, fungicides, and chemical fertilizers on soil health and agricultural crops is explored, as well as the use of untreated wastewater for irrigation, which contributes to soil pollution through the proliferation of harmful insects and plants(Abubakar et al., 2022).

Environmental pollution encompasses all undesired alterations that occur in the environment, whether partial or complete, due to human activities. It is a broad term that encompasses various ecological changes caused by human actions. Soil pollution is specifically characterized by the entry of foreign substances into the soil, resulting in chemical and physical changes. These changes can arise from the use of pesticides,
fertilizers, and the impact of acid rain, which alters the soil's pH and can release radioactive particles. Soil pollution leads to the disruption of soil layers and the alteration of its natural characteristics, hindering analysis and increasing the level of radioactivity. Agricultural land pollution refers to the degradation of agricultural land, including changes in its chemical, biological, and physical properties. This pollution negatively affects living organisms on the land surface, including humans, animals, and plants (Soil Contamination and Human Health : A Major Challenge for Global Soil Security, n.d.).

#### **Industrial Waste**

In the context of industrial waste, environmental chemistry plays a crucial role in understanding the effects of chemical pollutants, analyzing them, and treating them.

Industrial waste is a complex environmental problem, as it varies in types and chemical components. It includes organic compounds, heavy metals, and toxic substances, which can have a negative impact on the environment and living organisms. The characteristics of industrial waste depend on the originating industry, production processes, and materials used (Alshammari et al., 2008).

Effective management of industrial waste requires a deep understanding of chemistry to ensure safe and efficient handling. Key steps in industrial waste management include identifying the waste's chemical components, classifying, storing it securely, and transporting it safely. It also involves using chemical analysis techniques to assess the impact of the waste on the environment and selecting the best methods for its treatment and disposal (Srivastava, 2021).

Environmental chemistry in the context of industrial waste aims to develop techniques and processes that address the environmental challenges associated with such waste. Scientists aim to reduce industrial waste generation by improving production processes and efficiently utilizing resources. Additionally, they strive to develop safe and sustainable techniques for the disposal of industrial waste, including bioremediation, chemical degradation, and recycling.

In summary, environmental chemistry plays a crucial role in understanding and treating industrial waste and its impact on the environment. A comprehensive approach to managing industrial waste relies on a deep understanding of chemical reactions and the application of chemical techniques to address these environmental challenges safely and effectively. Green chemistry is now being considered the only solution of the industrial waste. Industrial development is necessary for the survival of any country so we can not just shut down the industry for the sake of environmental sustainability. Extensive research is being done in this area to develop or design such industrial processes and reactions that promises little or no waste at all. These methods are being implemented already in a lot of industries; with the development of this field, it can be considered that in the near future the global issue of pollution will be controlled.

# **Impact of Chemical on Enzymes**

Chemicals can interact with enzymes in environmental systems, leading to various effects on enzyme activity and ecological processes. Enzymes are biological catalysts that play a crucial role in facilitating biochemical reactions in living organisms and maintaining ecological balance. The interaction between chemicals and enzymes can occur through several mechanisms, including enzyme inhibition, activation, or alteration of enzyme structure(Paraschiv et al., 2022).

Chemicals can potentially affect enzyme activity by interfering with the active site of the enzyme or its cofactors. This interference can lead to inhibition, where the chemical molecule binds to the enzyme and prevents its normal functioning. Inhibition can be reversible or irreversible, depending on the strength of the interaction between the chemical and the enzyme. Some chemicals may also act as activators, enhancing the enzyme's activity and promoting specific biochemical reactions (Åqvist et al., 2017).

The effects of chemicals on enzyme activity can have significant ecological implications. Enzymes are involved in key metabolic processes in organisms, such as nutrient cycling, energy production, and detoxification. Any disruption in enzyme activity caused by chemicals can impact these essential ecological processes. For example, inhibition of enzymes involved in nutrient cycling can affect the availability and distribution of nutrients in ecosystems, leading to imbalances and ecological disturbances (Filipiak & Filipiak, 2022).

Chemicals can also impact enzyme activity in non-target organisms, including microorganisms, plants, and wildlife. Pesticides, heavy metals, and industrial pollutants are examples of chemicals that can have detrimental effects on enzyme activity in various organisms. These effects can lead to physiological and ecological consequences, such as reduced growth, reproductive abnormalities, and population declines.

Understanding the interaction between chemicals and enzymes in environmental systems is crucial for assessing the potential risks and impacts of chemical pollution. It involves studying the mechanisms of enzyme-chemical interactions, evaluating the toxicity and bioaccumulation potential of chemicals, and assessing their long-term effects on ecological processes and biodiversity (Patra et al., 2022).

The interaction between chemicals and enzymes in environmental systems can have significant implications for enzyme activity and ecological processes. Understanding these interactions is essential for evaluating the effects of chemical pollution on ecosystems and developing strategies for sustainable environmental management.

#### **Chemical Toxicology**

Chemical toxicology is the branch of science that studies the adverse effects of chemicals on living organisms. It plays a critical role in assessing the risks associated with exposure to environmental chemicals and determining their potential impact on human health and the environment. By studying the toxicological properties of chemicals, scientists can evaluate their potential hazards, establish safe exposure limits, and develop strategies for risk management and environmental protection (Vandenberg et al., 2023).

One of the key aspects of chemical toxicology is understanding the various routes of exposure to toxic chemicals. These routes include inhalation, ingestion, dermal contact, and injection. Inhalation occurs when chemicals are inhaled as gases, vapors, or particulate matter in the air. Ingestion refers to the intake of chemicals through the mouth via food, water, or contaminated objects. Dermal contact involves the absorption of chemicals through the skin. Injection occurs when chemicals are directly introduced into the body through needles or other means (Hubbard et al., 2022).

Toxic chemicals can have a range of health effects depending on the dose, duration of exposure, and individual susceptibility. They can target specific organs or systems in the body, leading to acute or chronic toxicity. Acute toxicity refers to immediate adverse effects that occur shortly after a high-dose exposure. These effects can include nausea, respiratory distress, organ damage, or even death. Chronic toxicity, on the

other hand, refers to long-term effects resulting from repeated or prolonged exposure to lower doses of toxic chemicals. Chronic exposure can lead to various health problems, such as cancer, reproductive disorders, neurological impairments, or endocrine disruptions(Arpornchayanon et al., 2022).

Furthermore, toxic chemicals can have ecological impacts by affecting wildlife, ecosystems, and the overall balance of the environment. They can bioaccumulate in the food chain, where they become more concentrated as they move up through different organisms. This bioaccumulation can lead to adverse effects on wildlife populations and disrupt ecological processes.

Understanding chemical toxicology is essential for assessing the risks associated with environmental chemicals. It involves conducting toxicity studies using animal models, cell cultures, and computational models to determine the toxicological properties of chemicals. These studies help establish dose-response relationships, identify potential hazards, and provide data for risk assessment and regulatory decision-making(Spurgeon et al., 2020).

Chemical toxicology plays a crucial role in assessing the risks of environmental chemicals on human health and the environment. It involves studying the routes of exposure, understanding the potential health effects of toxic chemicals, and evaluating their ecological impacts. By comprehensively examining the toxicological properties of chemicals, scientists can make informed decisions to mitigate risks and protect public health and the environment(Woodruff et al., 2023).

## **Strategies to Control Environmental Pollution**

Strategies to control environmental pollution encompass a range of approaches aimed at reducing and mitigating pollution across various sectors. One key strategy is pollution prevention, which focuses on minimizing or eliminating the generation of pollutants at their source. This involves adopting cleaner production processes, promoting sustainable practices, and implementing efficient waste management systems to prevent pollution from being released into the environment (EPA, 2021).

## 1. Regulations and Legislation

Regulatory measures play a crucial role in controlling pollution by establishing and enforcing environmental regulations and standards. These regulations set limits on pollutant emissions, prescribe treatment requirements for wastewater and air emissions, and impose penalties for non-compliance. By enforcing these measures, governments and regulatory bodies ensure that industries and individuals adhere to environmentally responsible practices (OECD, 2019).

# 2. Environmental impact assessments (EIA)

Environmental impact assessments (EIA) are essential in assessing and managing potential pollution risks associated with new projects, developments, or policies. EIAs help identify potential adverse environmental impacts, allowing decision-makers to implement preventive or mitigative measures before pollution occurs. This includes evaluating the environmental consequences of proposed actions, considering alternative approaches, and engaging stakeholders in the decision-making process (UNEP, 2017).

# 3. Technological solutions

Technological advancements and innovation play a critical role in pollution control. Developing and adopting cleaner technologies can significantly reduce pollutant emissions and minimize environmental impacts. This includes investing in renewable energy sources, implementing more efficient industrial processes, and employing advanced waste treatment methods. Additionally, research and development efforts focus on finding innovative solutions to address pollution challenges (IEA, 2020).

## 4. Community awareness

Public awareness and education initiatives play a vital role in pollution control. Increasing environmental literacy and promoting awareness of pollution's consequences can lead to behavior changes, sustainable practices, and support for pollution control initiatives. Educational programs, public campaigns, and community engagement efforts help empower individuals and communities to make informed choices that contribute to pollution reduction. Public participation and involvement create a sense of environmental responsibility and promote collective action for a cleaner environment (UNESCO, 2017).

# 5. Waste Management

Waste management is one of the most important strategy that can be adopted when it comes to pollution control. If the waste is properly disposed off it can save the disaster it can create. Recycling should be encouraged to the maximum level because it is the only way that can reduce the waste and thus can reduce the pollution cause by the waste disposal. Moreover, composting and organic waste management should be promoted in this way we can reduce landfilling.

# 6. Habitat Conservation

Serious efforts should be made at governmental level to conserve the natural habitat, including forests, coral reefs, and the wetlands. These habitats plays vital role for absorbing pollutants so by conserving these habitats pollution can be controlled or reduced. Moreover, instead of make cities by cutting forests, the government should make tall buildings in which there are apartment housing this can help to accommodate more people with minimum space used. Strict laws should also be established and implemented for the conservation of natural habitats.

# 7. Green Technologies

All the hose appliances should be replaced by the energy efficient appliances, and the use of environmentally friendly technologies should be promoted, such as green building materials. In order to clean the contaminated sites, innovative methods should be used such as bioremediation or phytoremediation.

## **Summary**

Overall, a combination of pollution prevention, regulatory measures, environmental impact assessments, technological advancements, and public awareness and education efforts are crucial for effective control of environmental pollution. Implementing these strategies in a comprehensive and integrated manner helps mitigate pollution's adverse effects on human health and the environment.

The study of environmental chemistry stands as a crucial discipline, shedding light on the intricate connections between chemicals and our surroundings. This chapter has illuminated how these connections often lead to diverse types of pollution, which, in turn, present significant challenges to ecosystems, human well-being, and the overall health of our planet.

Pollution, whether it takes the form of air, water, or soil pollution, is a pressing global issue that demands immediate attention and concerted action. The repercussions of uncontrolled pollution are far-reaching, encompassing the depletion of natural

resources, the proliferation of health ailments, and even the disruption of global climate patterns.

Nevertheless, there is reason for optimism. As we have explored, there exists a multitude of strategies and remedies available to effectively combat pollution. These strategies encompasses a blend of rigorous environmental laws, innovative technological breakthroughs, and individual accountability. By instating and upholding strict environmental regulations, we ca hold both industries and individuals responsible for their environmental footprint. Moreover, progress in pollution prevention, waste management, and sustainable practices has the potential to significantly curtail pollution at its source.

In conclusion, even though dealing with environmental pollution is challenging, it is not impossible. By working collaboratively, coming up with innovative solutions, and most importantly staying committed to eco friendly actions, we can reduce the harmful effects of pollution and create a cleaner, healthier, and more robust planet. The path to a pollution-free world starts with each of us, and together, we can make a significant difference in our environment.

# **Scientific Ethics Declaration**

The authors say that they are responsible for the scientific, moral, and legal aspects of this chapter, which is published in Current Studies in Health and Life Sciences 2023.

## **Conflict of Interest**

The authors declare no conflict of interest.

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## Green Chemistry in Daily Life and Its Effects on Health

Ali SERT Mumin POLAT

#### Introduction

The opportunities that come our way, especially with urbanization, industrialization and the latest advances in technology, cause people to face some health problems. Pollutions in oxygen and water and food can sometimes turn into weapons and leave us with diseases . We need to know that chemicals are not only found in laboratory environments, but also in almost all materials we use. In order for a person to be basically healthy, the safety of the food he eats and especially clean water are very important. The safe foods mentioned here are those that do not pose any danger to individuals in terms of physical, chemical and biological risks if kept for a certain period of time. The century we live in has replaced our most needed nutrition with industrial and processed foods. Well, in addition to these nutritions, we also need to look at the damage caused by chemistry or chemistry laboratories in our field of work. In this work area, the production and use of some chemicals increases the risk of occupational accidents and occupational diseases. In order to prevent and prevent occupational accidents and occupational diseases in Turkey, Occupational Health and Safety Law No. 6331 came into force and was put into practice in 2012. With the law, A, B and C certified OHS experts emerged, and businesses were categorized as less dangerous, dangerous and very dangerous according to the type of danger (Yavuz, 2020).



Figure 1. Harmful chemicals

Green chemistry; It is a package of 12 principles aimed at chemical products and processes that use materials with very high efficiency and low dose toxicity, especially those that cause less environmental pollution. Design, production, use and final disposal of chemical products and processes It is a branch of chemical science that aims to reduce or completely eliminate the use or formation of hazardous substances throughout their life cycle, including The main purpose of this new generation of chemistry, which emerged in the 1990s, is to stop the effects of industrial waste at the beginning rather than later, that is, to reduce or even eliminate pollution at the source. For this reason, green chemistry **is also called sustainable chemistry or environmental chemistry.** (Chen et al.,2020; Ivankovic et al., 2017; Ribeiro et al.,2015;Sheldon, 2014).



Figure 2. 12 effects of Green Chemistry

If we look at the last 150 years of chemistry, unfortunately green chemistry is a fairly new concept. This concept started in 1990 with the prevention movement, which aims to reduce or eliminate pollution at its source, instead of eliminating the benefits of developing technology while also eliminating its harms later. US Environmental Protection Universal pollution prevention efforts taken by the Agency (EPA) are identified as inventory controls, process control, in-process recycling, household modifications and green chemistry. In the 2000s, this concept began to be used by the academic community and was taught in classes (Çakmak et al.,2012; Sheldon, 2012).

# **1-Prevention of Waste**

Waste Management; minimization of domestic, medical, hazardous and nonhazardous wastes, separate collection at the source, intermediate storage, creation of transfer centers for wastes when necessary, transportation, recovery, disposal of wastes, operation of recovery and disposal facilities and closure, post-closure maintenance, monitoring and control processes. It is a management style that includes Regardless of the field in which the waste hierarchy is applied, it is based on the 'prevention' step. Prevention, as we can understand from its name, aims to intervene in waste before it occurs. In order to do this, it is necessary to determine the steps in the production processes where waste may occur. New rules and solutions are sought for processes that have the capacity to create waste in production. Every stage is inspected to prevent waste generation (Sheldon, 2017; Tank et al.,2005).



Figure 3. Waste Management

#### **2-Atomic Economy**

Atomic economics, Prof. It is a concept related to the efficiency of reactions, introduced by Trost in 1995. It is the economic yield of the event that will occur in a chemical reaction process. For example, if all of a substance turns into the product we expect, the efficiency of this process is 100%. However, if extra by-products are formed during the reaction, the yield will inevitably decrease. For this reason, the concept of atomic economy is an important method to ensure the transformation of the raw material to be used into the desired product with almost 100% efficiency. According to this concept; Production processes should be designed to maximize the amount and energy of all materials entering the production process in the final product. This is only possible with processes that have minimum by-products and waste. Atomic optimization ensures fully efficient use of raw materials. Every atom that is not wasted is beneficial for both the environment and the producer. In this context; There are danger elements in many places where chemicals are used. Minimizing or eliminating them is one of the main goals of green chemistry. It is very important to develop synthesis routes for the use and production of substances that pose little or no harm to humans and the environment (Anastas & Eghbali, 2010;Armenta et al.,2008).

## **3-Designing Less Harmful Chemical Syntheses**

The main function here is that during any synthesis, substances that are at least toxic or not at all toxic to the environment and humans should be used. In chemical reactions, reagents that are often dangerous and toxic to human health and the environment are used. If the chemicals used are carcinogenic, national and international legislation must be taken into consideration and necessary measures must be taken to eliminate the risk in the workplace environment or to eliminate the exposure of the employee. (Gilbertson et al.,2015; Topraksever, 2023).

## **4- Designing Safer Chemicals**

Almost everyone comes into contact with chemicals that can be harmful if not used properly. Many deaths, and perhaps a hundred times as many accidents, occur as a result of careless use of chemicals. Industrial toxicology examines the chemicals in the air and water and their harmful effects based on factories. Economic toxicology plays a role in the examination of chemicals found in substances such as drugs, food, cosmetics and fertilizers. In addition, forensic toxicology generally examines the results in cases involving death or serious injuries Reducing toxicity is one of the fundamental rules in chemistry. The real challenge here is knowing what makes a molecule toxic. Toxicity can be an even greater concern when considering chemicals that have never been produced before. The science of toxicology allows us to predict or test the toxicity level of a molecule. According to Eurostat, more than 300 million tons of chemicals were consumed in the EU in 2018, and more than half of this amount was classified as harmful to health. There is recorded data on more than 20,000 individual chemicals in the EU under the registration, evaluation, authorization and restriction of chemicals regulation (Khetan et al., 2007; Topraksever, 2023).

# 5- Safer Solvents and Excipients

Auxiliary substances such as solvents and separating agents should be used as little and harmless as possible. One of the most important sources of risk, especially in chemistry laboratories, is the chemicals present. Almost all of these substances, especially solvents, are volatile, flammable and/or toxic , posing a risk to human and environmental health. Solvents are chemicals that attract much attention within the scope of green chemistry (Clarke et al., 2018; Topraksever, 2023; Ahluwalia et al., 2004).

Recommended Solvents	Problem Solvers	Hazardous Solvents
✓ This	✓ benzyl alcohol	✓ diisopropyl ether
✓ methanol	✓ tetrahydrofuran	✓ methyltertbutyl
✓ ethanol	✓ methyltetrahydrofuran	ether
✓ i -propanol	✓ methylcyclohexane	✓ dimethoxymethane
✓ n - utanol	✓ xylene	<ul> <li>✓ dichloromethane</li> </ul>
✓ t -butanol	✓ dimethylpropylene	<ul> <li>✓ dimethylformamide</li> </ul>
✓ ethylene glycol	urea	✓ dimethylacetamide
✓ nail polish remover	✓ DMSO	✓ n -methyl-2-
$\checkmark$ methyl ethyl ketone	✓ formic acid	pyrrolidone
✓ methyl isobutyl	✓ acetic acid	✓ sulfolane
ketone	<ul> <li>✓ acetic anhydride</li> </ul>	✓ methoxyethanol
		✓ pyridine
		✓ triethylamine

Table 1. Recommended, Problem, Hazardous Solvents

# 6- Design for Energy Efficiency

A perspective with a supply and demand side index should be adopted to understand the benefits of energy efficiency and how the full potential of energy efficiency can be realized. Energy requirements for chemical processes should be minimized by using ambient pressure and temperature whenever possible. Design for energy reduction is in many ways inherently tied to design for material efficiency (Real, 2012).

## 7- Use of Renewable Raw Materials

Raw materials should be sourced from renewable raw materials wherever technically and economically possible. Renewable raw materials are obtained from resources that can renew themselves in an average of 10 years or less. These raw materials are in contrast to materials such as fossil fuel derivatives, which will take millions of years to regenerate(Jessop, 2011).

# 8-Reducing derivatives

One of the main principles of green chemistry is to avoid the use of chemical derivatives in the synthesis of target molecules. Unnecessary derivatization in the chemical process (e.g. chemicals used for blocking or protection purposes in chemical production ) should be minimized and avoided as much as possible. Because derivatization will bring about additional chemical use and therefore additional waste (Karagölge et al., 2019).

# 9-Catalysis:

This is because most chemical processes; Catalysts may be needed to either accelerate reactions, increase selectivity or reduce energy requirements. Currently available catalysts are often expensive, toxic, or based on metals. Green catalysts must have the following properties. It should have some common features such as:

- $\checkmark$  high activity,
- ✓ selectivity
- $\checkmark$  determination,
- ✓ separation
- ✓ ease of reuse(Gilbertson et al.,2015).

# **10- Design for Degradation**

The degradation of chemical products must be designed to be harmless. Unfortunately, many chemical products actively used in today's world can remain in nature without degrading for tens or even hundreds of years . Our goal here is to ensure that this period is shorter in green products and that they degrade in a way that is harmless to the environment or human health.

## **11-Full Time Analysis for Pollution Prevention**

In particular, analytical methods should be developed to ensure continuous monitoring and control of the production process in order to minimize or completely eliminate the formation of by-products as much as possible. To date, the application of environmental analysis has been directed towards measuring and characterizing environmental problems after they have been created.

## 12- Safer Chemistry for Accident Prevention

An international study has been created on this issue and they are actively working on it. Among these, the Major Accident Hazards Bureau (MAHB), working under the Joint Research Center of the European Commission, carries out studies on major industrial accidents within the European Union and keeps the accident inventory. The Organization for Economic Co-operation and Development (OECD) chemical accidents working group, established within the UN , worked together with many other organizations (ILO, IMO, UNECE, UNEP, UNOCHA and WHO) to develop the "OECD Guidelines for Prevention, Preparedness and Response for Chemical Accidents (OECD). Guiding principles for chemical Accident Prevention , Preparedness oath Response ) has prepared. This guide has been written in a flexible way that can be applied in all facilities that use, produce, store or dispose of hazardous chemicals, and it provides advice to the competent authorities on industrial and chemical accidents and to all sectors that may be affected by an industrial accident (Sheldon, 2017).

## What to Do

In particular, it is necessary to support private and public studies that work on the protection of the environment, to recover materials through recycling projects, to increase the production of energy-saving products, to produce and use environmentally friendly products, to have waste units for all kinds of chemical waste, and to provide relevant support.

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