EFFECT OF DE-IONIZED WATER IN LEACHING BISPHENOL A AND PHTHALATES FROM VIRGIN PLASTIC BOTTLES.

BY

ALADEJARE ADETOLA GIFT

PSC2105209

DEPARTMENT OF CHEMISTRY

FACULTY OF PHYSICAL SCIENCES

UNIVERSITY OF BENIN.

OCTOBER, 2025.

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SUPERVISOR: DR O. MOSES

A PROJECT SUBMITTED TO THE DEPARTMENT OF CHEMISTRY, UNIVERSITY OF BENIN, BENIN CITY, IN PARTIAL FULFILMENT OF THE REQUIREMENT FOR THE AWARD OF BACHELOR OF SCIENCE DEGREE (B.SC HONOURS) IN CHEMISTRY.

OCTOBER,2025.

CERTIFICATION

This is to certify that this project work was carried out and completed by ALADEJARE ADETOLA GIFT with matriculation number PSC2105209, Department of Chemistry, Faculty of Physical Science, University of Benin.

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PROF. E.E.I. IRABOR DATE

(HEAD OF DEPARTMENT)

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DR O. MOSES DATE

(PROJECT SUPRVISOR)

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ALADEJARE ADETOLA GIFT DATE

(PROJECT STUDENT)

DEDICATION

This project work is dedicated to God Almighty, who made this research work a reality. I also dedicate this project work to my parents, aunties, and friends for their immense support and every other person who contributed to the success of this work.

ACKNOWLEDGEMENT

Firstly, I give al glory to God for His strength, wisdom, provision, and protection all through the course of this project work. Without His Grace and Mercy this project work wouldn't have been a success.

My sincere appreciation goes to my supervisor PROF. O. MOSES, for his guidance, corrections, and constant encouragement until this project became a reality. His dedication to ensuring the accuracy of every stage of the project work was a source of inspiration to me throughout my journey, and for that I'm genuinely grateful.

I also want to appreciate the Head of Department, PROF.E.E.I. IRABOR, for his intentionality and endless efforts towards creating a safe, and conducive environment for the success of our lab work. This project wouldn't have been visible without his immense support.

My deepest appreciation goes to PROF. MRS. UKPEBOR for her endless support towards ensuring we finish well and strong, this project work wouldn't have been feasible without her help.

I would also like to extend my sincerest gratitude to the lecturers and staff of the Department of Chemistry for their significant contributions to my academic growth, as well as the knowledge and support they provided all through my academic journey.

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LIST OF ABBREVIATIONS

BPA- Bisphenol A

PAE- Phthalate acid esters

PVC- Polyvinylchloride

DBP- Dibutyl phthalate

DEP- Diethyl phthalate

BBP- Benzyl butyl phthalate

DEHP- Di(2-ethylhexyl) phthalate

DIOP- Diisooctyl phthalate

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ABSTRACT

This study explores how Bisphenol A (BPA) and different phthalates leach from unused plastic bottles when kept at a steady temperature of 40 °C in deionized water. The use of deionized water which is free from salts, ions, and organic matter, provided a clean, neutral environment that allowed a clear view of how these chemicals naturally migrate from plastics into water. Over a 96-hour period, BPA concentrations were measured using Gas Chromatography–Mass Spectrometry (GC–MS), with recorded values of 2.92, 2.40, 2.42, 2.74, and 2.96 µg/L at 0, 24, 48, 72, and 96 hours, respectively. The initially high BPA value was likely due to surface residues being quickly released into the water, while the slight drops at 24 and 48 hours suggest a brief stabilization or re-adsorption on the bottle surface. The subsequent rise at 72 and 96 hours indicates that BPA continued to diffuse from inside the plastic into the surrounding water which is a process encouraged by the constant heat.

Phthalates such as diethyl phthalate (DEP) and dibutyl phthalate (DBP) showed similar patterns, with their concentrations gradually increasing over time, confirming that additive migration is a slow but continuous process. Although the highest BPA concentration measured (2.96 µg/L) is far below the U.S. FDA's safety threshold of 5 mg/kg body weight per day, it is well above the extremely strict European Food Safety Authority (EFSA, 2023) limit of 0.2 ng/kg body weight per day. This finding suggests that even new, unused plastics can release trace amounts of potentially harmful chemicals when exposed to warm or storage conditions for extended periods. Overall, the study emphasizes the importance of monitoring plastic safety and highlights how everyday temperature exposure can influence the release of chemical additives into water, with potential implications for both health and the environment.

CHAPTER 1

1.0 Introduction

In recent years, the production of plastic waste in the environment has become a major issue in the world, and among the most dominant forms of plastic pollution are **microplastics**. **Microplastics** are tiny plastic particles less than 5 mm in diameter that are produced as a result of the breakdown of larger plastic materials or are manufactured intentionally for use in products such as cosmetics and cleaning agents.

Microplastics are widespread in marine, freshwater, and terrestrial ecosystems. Their small size leads to easy injestion by aquatic organisms, birds, and even humans, which often accumulates in food chains. (Thompson *et al.* 2004). However, the danger caused by microplastics is not limited to their physical presence alone, they also contain high amount of leachates which are chemical substances that can be released from the plastics into the environments when subjected to different weather conditions.

Leachates from microplastics may include additives such as flame retardants, plasticizers such as; Bisphenol A (BPA), Antimony, Phthalates, Polybrominated diphenyl ether (PBDE), etc. These chemicals when leached into the environment can interfere with hormonal systems, disrupt reproduction, affect human health through the food web, and be a major threat to aquatic life.

Despite growing awareness, there is limited information on the exact nature and quantity of

chemicals leached from microplastics under different environmental conditions. Factors such as pH, temperature, salinity, and exposure time can influence the rate and extent of leaching.

This study aims to determine the types of leachates and the concentrations of these leachates released from selected microplastic samples (PET), using appropriate analytical techniques under controlled laboratory conditions. Understanding these leachates is important to evaluate the full scope of microplastic pollution and support the development of effective regulatory and mitigation strategies.

1.1.1 Background Of Study

Plastics were first originated in the oil refineries during the course of production. They were formed on the body of the refinery machines by chemically bonded oil and gas molecules together to make monomers. In turn these monomers were bonded in long polymer chains to make plastics (**Polyethylene Terephthalate**), in a form of millions of phthalates which was melted at many factory plants and reformed into plastics bottles.

After several years of growth in the production of plastics, studies have shown that the use of plastics have led to a massive widespread of plastic pollution in our world today. As much as plastics have been of a great advantage to humanity at large, it has grown to become a threat to not just our livelihood but also to that of the aquatic life, and our ecosystem.

When plastics are dumped in the environment, they stay under different weather conditions which causes leaching of the chemical components from its makeup. Weather conditions such as **UV rays from sunlight** causes the leaching of toxic component that are on the surface of the plastic (polyethylene material), and **rainfall** which leads to the absorption of the water soluble leachates in rainwater. The wide spread of the rain water of absorbed leachates across the earth surface causes contamination of the ground water, soil, poisoning of the ecosystem and aquatic life.

Plastics are non-biodegradable (which means that they cannot be decomposed by microorganism), as a result they deteriorate into smaller particles called **microplastics.** These microplastics because of their size, spread wide and fast into the marine, freshwater, and terrestrial ecosystems, which further accumulates into the food chain. Their persistence due their non-biodegradability makes them deteriorate further into **nanoplastics** which are more dangerous as they are tiny enough to get into the blood stream of waterbodies, mammals, sand even humans, spreading through every organ in our body.

To reduce the growing problem of microplastics in our environment, scientists are now working on safer substitutes that can replace the harmful plasticizers used in making plastics. But before dealing with the plastics that already exist in nature, it's important to first understand how these plastics release their chemical additives through leaching. Studying this process helps researchers determine how much of these harmful substances have entered the environment and how to prevent more from leaching out before the plastics are properly recycled. Knowing the amount of leachates present over time will also make it easier to find ways to clean up polluted water bodies and reduce risks to human health.

In recent years, several studies have looked into how microplastics can absorb pollutants from their surroundings. However, there is still limited knowledge about how these plastics release their own chemical additives into water. According to a study by (Yan *et al.* 2021), polyvinyl chloride (PVC) plastics release dibutyl phthalate (DBP) into water, and the rate of leaching depends on factors like particle size, plasticizer content, and how old or weathered the plastic is. They also found that the acidity (pH) and salt concentration of the water have little impact on this release. Similarly, (Cao *et al.* 2022) estimated that between 57.8 and 16,100 kilograms of phthalate microplastics enter the oceans every year. Their research showed that different types of plastics release different kinds of phthalates, DBP was the main compound leached from PA, PP, and PET microplastics, while DEP was more common from PVC and rubber, and DBP also dominated in PE microplastics.

More recently, (Henkel *et al.* 2024) found that when PVC microplastics are exposed to

sunlight (photoaging), they release even higher amounts of di(2-ethylhexyl) phthalate (DEHP)—about 1.5 times more than before. They also discovered new harmful by-products like mono(2-ethylhexyl) phthalate (MEHP), phthalic acid, and phthalic anhydride. The researchers emphasized the need for more studies on how fast these chemicals leach out, as understanding their release rate is key to knowing the actual level of exposure in the environment.

1.1.2 Statement of problem

Prevalence of Endocrine disrupting compounds (Bisphenol A and Phthalates) in the environment

Many plastics because they are made up of non-renewable resources, are designed for single use. However, plastics take centuries to decompose and this as a result leads to a huge build up of waste on land, which eventually is drowned into the ocean.

In recent years, the negative impact of the use of plastics within the environment has become a major concern. Due to poor management practices, vast amounts of plastic waste are released into the oceans each year, largely originating from land-based sources such as mismanaged waste, urban runoff, and industrial activities.

In marine environments, plastic pollution threatens both ecosystems and human health by adsorbing pollutants and heavy metals, and by leaching additives like phthalates, Bisphenol A, and other flame retardants, which enhances chemical pollution. The leaching rate of such additives largely depends on particle size, molecular size, and physicochemical properties.

Among the various additives used in plastics, plasticizers constitute the largest group of auxiliaries, with phthalate esters (PAEs) being the most commonly used. Scientific research indicates that prolonged exposure to PAEs can result in hormonal disruptions, internal organ damage, reduced fertility, developmental disorders, and other adverse health effects in living organisms. (Abdi *et al.* 2021).

Research according to the United Nations Environment Program (UNEP) states that approximately 400 million tons of plastics are produced globally every year. Further

research shows that 330 billion single use plastic items are manufactured annually of which only 10% of these plastics undergoes recycling, 12% is subjected to incineration, and the remaining 79% finds its way to the ocean. (Rapa *et al.* 2024)

Global plastic production is predicted to grow rapidly worldwide, reaching 1.2 billion tons by 2060, as 442.5 million metric tons of plastic materials were generated in 2023 compared to 1.5 million metric tons produced in 1950 (Kushwaha *et al* 2024; Jaganmohan, 2024).

Plastic waste management systems will also be under additional strain because it is anticipated that by 2025, there will be over 250 million metric tons of plastic garbage in the environment (Kushwaha *et al* 2024; Miller *et al.*, 2023.). The Merely 9 % of the entire plastic waste generated is currently recycled or upcycled, while the remaining 22 % is disposed of as garbage and is considered improperly managed plastic waste (Babaremu *et al.*, 2022). The remaining 50 % is disposed of in landfills, 19 % is burned in incinerators, and the remaining 10 % is deposited in landfills. This as a result has led to the massive increase in the leaching of additives (Bisphenol A and Phthalates), and also its prevalence in the environment.

The litter is typically discharged into aquatic or terrestrial habitats. Approximate estimates indicate that 22 % of the total produced plastic waste indicated above, or about 10 % of the trash that is illegally disposed off, ends up in the marine habitat where it will persist and collect over time. If the rapid increase in the amount of plastic garbage dumped into aquatic bodies continues at its current rate, scientists have already warned that by 2050, there will be more plastic than fish. Microplastics are fragments of any type of plastic <5 mm (0.20 in) in length, (Ghosh *et al.*, 2023) according to the U.S. National Oceanic and Atmospheric Administration (NOAA) **[10]** (Collignon *et al.*, 2014) and the European Chemicals Agency (Kushwaha *et al* 2024; ECHA, 2024).

Considering these challenges, our study on additive leaching under controlled conditions of temperature, contact time, and water, is aimed at understanding how plastics actually behave in real environmental settings. By simulating these conditions in the lab, we can observe how chemicals like Bisphenol A and phthalates migrate from plastics into water over time. This approach helps connect laboratory findings to what

truly happens in nature, providing insight that supports better risk evaluation and encourages the development of safer plastic materials and more effective waste management practices.

1.1.3 Justification Of Study

In recent years, cancer rates among humans have been increasing, and after several investigations into possible causes, scientists have linked microplastics as one of the major contributors. A study by (Marfella *et al.* 2024) reported that patients who underwent carotid endarterectomy which is a surgical procedure done to remove blockages in the arteries had about 58.4% of plastic particles present in the arterial plaques removed during surgery. This finding suggests a strong connection between microplastic exposure and human health issues.

It is estimated that around 51 trillion microplastic particles are floating on the ocean's surface, with about 70% eventually sinking to the sea floor, where their effects remain uncertain. Nanoplastics, which are extremely tiny particles smaller than 1 micrometer, are formed from the breakdown of larger plastics.

Their small size allows them to penetrate animal and human cells easily, raising serious concerns about their potential harm to both living organisms and the environment (Rapa *et al.*, 2024). Due to these discoveries, many studies have focused mainly on the physical effects of microplastics, while the chemical impact of leachates which include harmful plasticizers and additives has not been fully explored.

Recent findings by (Delaeter *et al.* 2022) and (Gardon *et al.* 2020) identified seven major chemical additives (leachates) commonly released from plastics. These include dimethyl phthalate (DMP), diethyl phthalate (DEP), dibutyl phthalate (DBP), diethyl hexyl

phthalate (DEHP), diisononyl phthalate (DINP), diisodecyl phthalate (DIDP), benzyl butyl phthalate (BBP), along with an antioxidant compound. Additionally, their research showed that both new and aged plastic materials used in pearl farming release about 20 types of polycyclic aromatic hydrocarbons (PAHs), which are known to be hazardous. Despite this, the dangers posed by these toxic chemicals are often neglected in plastic pollution discussions.

Understanding plastic leachates provides a clearer picture of the hidden risks associated with microplastic pollution. It also expands scientific knowledge on how plastics interact with the environment which is the main focus of this study. Moreover, this understanding helps in predicting potential risks to human health and the wider ecosystem. Since plastics continuously break down in marine environments, leachates are expected to be released throughout their lifetime. Therefore, identifying the source, behavior, and environmental effects of plastic leachates remains a top priority for future research on plastic pollution (Delaeter *et al.*, 2022).

1.1.4 Scope of work

The focus of this research was the effect of deionized water in leaching Bisphenol A and Phthalates in virgin plastic bottles. These virgin plastics were gotten with the help of ECO WASTE TO WEALTH COMPANY, Edo State.

Another major focus is the presence of the leached Bisphenol A, and Phthalates in the plastics and its effect on both the environment and the health of humans when subjected to storage.

This leaching agent (Deionized water) is a good representation of the environmental conditions that plastics are subjected to in our everyday life. In the leaching of virgin plastics, deionized water represents a neutral and controlled environmental condition that simulates natural freshwater or rainwater environments with minimal chemical interference. Since deionized water is free from dissolved salts, ions, and organic matter, it provides a chemically pure medium that allows for the assessment of the

tendency of plastics to release additives such as phthalates and Bisphenol A. This condition serves as a baseline reference for comparing the leaching behavior of plastics under other environmental scenarios, such as acidic, alkaline, or saline waters. Essentially, deionized water models an uncontaminated freshwater system, helping to understand how plastics may behave in natural, unpolluted aquatic environments.

This test summarizes the harmful effects of PET bottles to human health when used for the production and storage of consumable products.

1.1.5 Limitations

The time limitation of this research made it impossible to have a reference to work with when testing for the presence of leachates in the virgin plastics. It was intended to work with a longer period of time (2-6 months) and temperature however, the limited time frame to get the work done made it impossible.

Also, limited research has gone into the quantification of leachates from microplastics, this is as a result of the major focus that scientist have given to the environmental and health hazards of plastics without necessarily considering the root of the problem (the leaching process). This led to further restriction on our focus from the quantification of different leachates, to that of just Bisphenol A, and Phthalates.

1.1.6 Aim and Objectives

This study aims to determine the effect of deionized water in the leaching of Bisphenol A and Phthalates from Virgin (unused) plastics water bottles, as well as the

quantification and effect of these leachates to the environment.

It also aims to determine the effect of storage temperature and time on the leaching of Virgin (unused) plastics water bottles into drinking water, and the harmful effect of its consumption on human health.

The objectives of this project are to;

- Collect virgin plastic bottles and cut them into smaller bits
- Rinse the smaller bits of plastics to remove contaminants and avoid any form of contamination.
- Stimulate leaching in the virgin plastics using deionized water at constant temperature and time.
- Trap the leachates present in the solvent using Dichloromethane and drying of excess water using anhydrous sodium sulphate (Na2SO4)
- Determine the quantity of Bisphenol A and Phthalates present in the DCM sample using GC-MS.
- Determine the functional group present using FT-IR

1.2 LITERATURE REVIEW

1.2.1 History of Plastics

Plastics are synthetic polymers prepared by polymerization of monomers derived from oil or gas with the addition of different chemical additives. They are one of the most universally-used and multipurpose materials in the global economy due to their extraordinary properties such as versatility, lightweight, strength, durability, corrosion resistivity, high thermal and electrical insulation (Thompson *et al.* 2009).

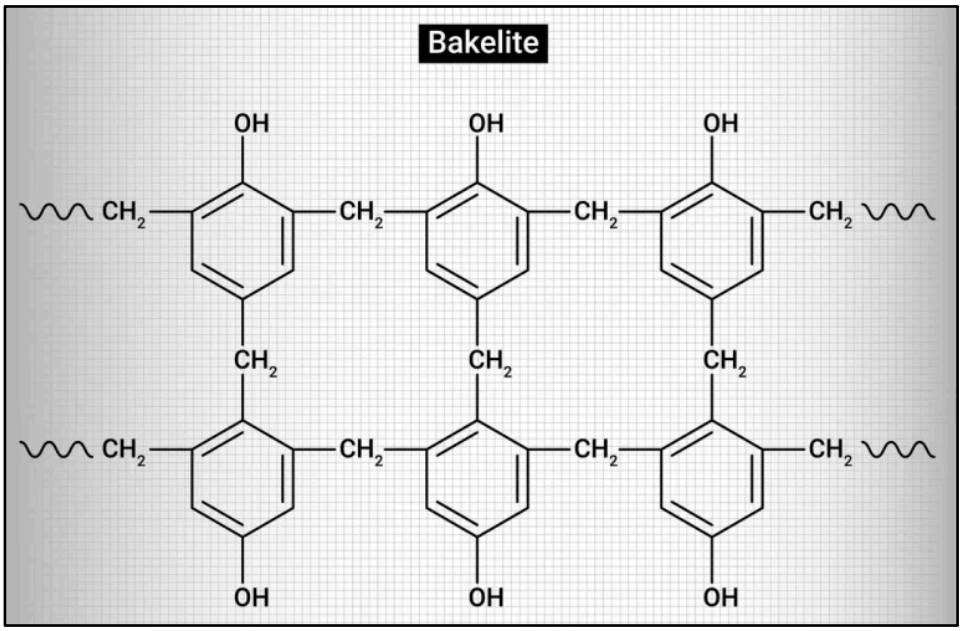
In 1862 Alexander Parkes an English chemist unveiled a new material called **parkesin.** It was made from cellulose, and had waterproof properties. It was also durable and could be made into various shapes. In 1868, an American named John Wesley Hyatt created a

material called **celluloid** made from cellulose which was used to make billiard balls (Bellis 2025). This material (**celluloid**) was also durable and was easily moldable to form different shapes, Hyatt's approach towards the creation of the celluloid was to mix nitrocellulose fibres from cotton with camphor, and a plant based wax. However, celluloid was highly flammable which made production risky, it also had the tendency to discolour and crack with age (Rodriguez 2025).

As a result of this risk, scientist began to research for a safer alternative which led to the production of a synthesized polymer called **Bakelite**. Leo Hendrik Baekeland a Belgian chemist invented the first synthesized plastics known as **Bakelite** in 1907, which was used in the production of telephones, radios and other household materials.

In 1909 Baekeland used the term **plastic materials** to describe products made from macromolecules (resins, elastomers and artificial fibers). (Chalmin. 2019). The ability of plastics to replace other materials effectively led to their use instead of expensive or luxury materials derived from endangered animals and plants. (Cambridge university press. 2024)

STRUCTURE OF BAKELITE

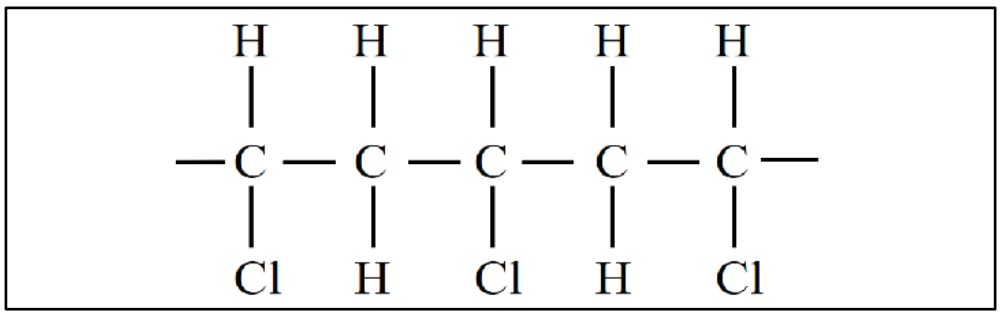


Years after bakelite was invented, other inventions of plastic occurred between two world wars. In 1913, cellophane was invented, followed by the production of polyvinylchloride (which was flexible) in 1927. In 1938, polystyrene and nylon took the center stage. Polystyrene was discovered by chance, and was used as a thermal insulation for buildings. Nylon was developed by a team of researchers led by the chemist Wallace Carothers, it was given the name Nylon by DuPont de Nemours.

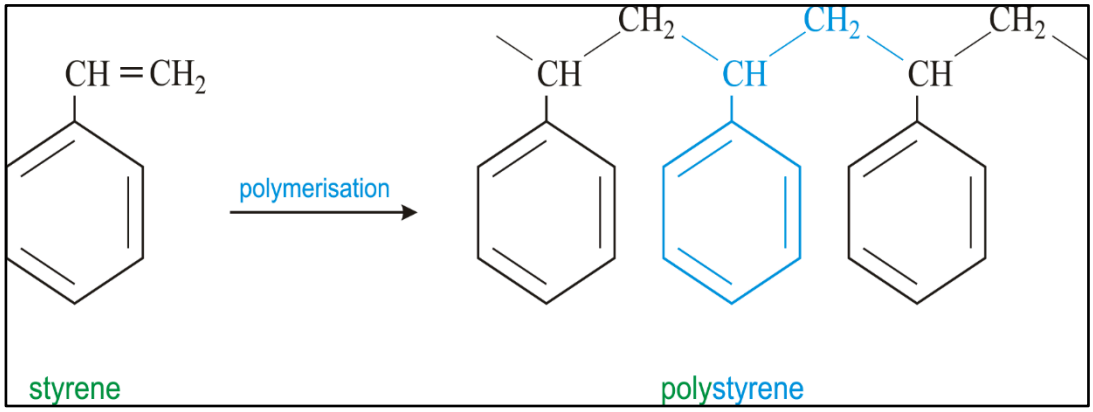
It is a super polyamide that forms very strong elastic threads which resist atmospheric agents and do not rot. it was a polymer designed to mimick silk. Nylon was used to produce GIs' parachutes during the World War II before it revolutionized the textile industry.

In 1933, Polyethylene was invented and became one of the most versatile plastics which was used and is still used today in the production of shampoo bottles, grocery bags, and also military applications. The discovery of low-density polyethylene was the result of research on resins by E.W. Fawcett and R.O. Gibson. (Chalmin. 2019).

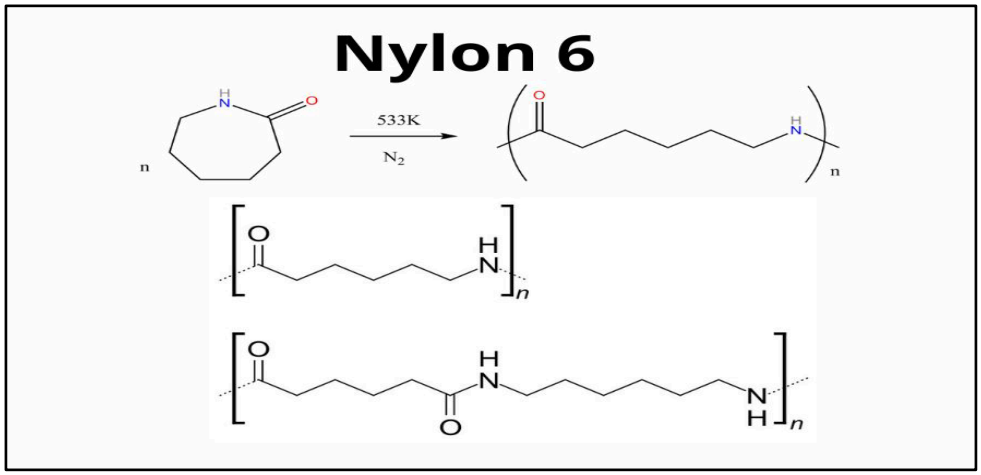
STRUCTURE OF POLYVINYLCHLORIDE



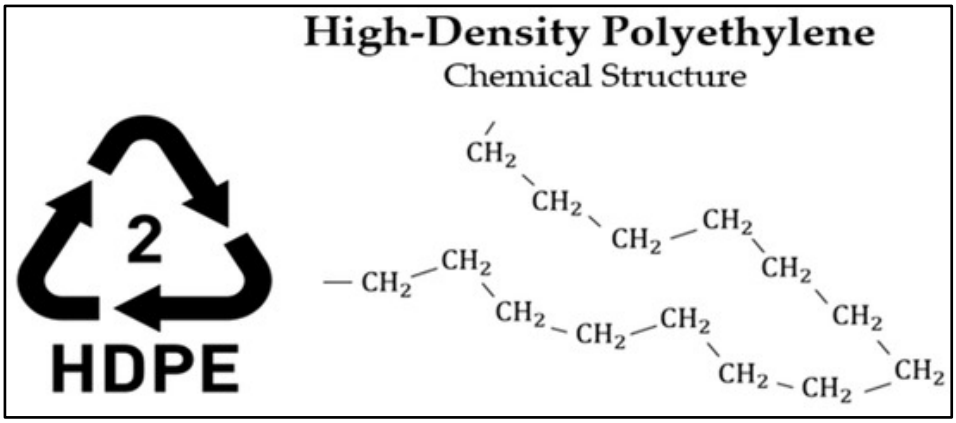
STRUCTURE OF POLYSTYRENE

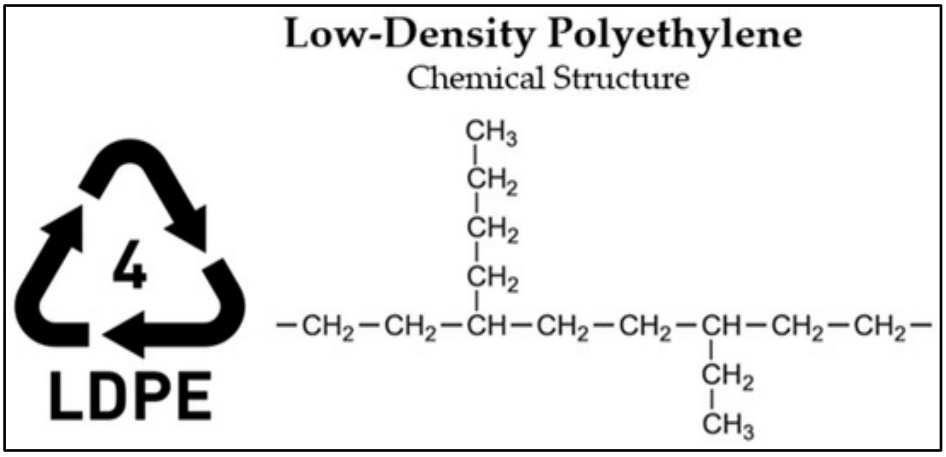


STRUCTURE OF NYLON



STRUCTURE OF POLYETHYLENE





1.2.2 Rapid growth in plastic production

After the World War II there was a massive outbreak in the production of plastics, according to the trade association PlasticsEurope, the worldwide plastic production grew from 1.5 million metric tons (about 1.7 million short tons) per year in 1950 to 275 million metric tons (about 303 million short tons) by 2010, and by 2018 production further grew to about 359 million metric tons (nearly 396 million short tons). The increase in production was as a result of the increase in the usage of these plastics, which led to about 4.8 million and 12.7 million metric tons (5.3 million and 14 million

short tons) to be discarded into the oceans annually by countries with ocean coastlines. (Moore. 2025).

Asides the use of plastics as a substitute for house hold appliances, grocery bags and so on, plastics were also used to produce plastic bottles for the storage of drinks, and water. The first plastic bottle was produced in 1968 (Vittel mineral water in France). (Philippe Chalmin. 2019). In developing countries, plastics are very cheap and affordable, and as a result of their durability they provide high-impact solutions, enhancing technology and the quality of life. Despite their advantages, the rapid expansion of the plastics industry and its production has raised environmental concerns. The characteristics that make plastics durable has posed to be one of the major threat to humans and their environment, especially in marine pollution and accumulation of non-biodegradable waste. (Stanley *et al.* 2025).

1.2.3 Increasing danger of Plastics and microplastics to the environment

Marine habitat

Plastic is a long chain of polymeric material whose molecules are very large, and is made up of endless series of interconnected links. They are materials that are derived mainly from petroleum and can be molded into different forms, cast, spun, or applied as a coating. However, because plastics are largely non-biodegradable, they persist in natural environment. (Moore. 2025].

Many plastics lurk around the environment as a result of their improper disposal, and when acted upon by different environmental conditions they form a heap of waste on terrestrial habitat (Illegal dumping of plastics on land) or float aimlessly on marine habitat (ocean).

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Since the earth is made up of 71% of water, the ocean has become the receiving body for much of the plastic waste generated on land. Several million tons of plastic wastes end up in the oceans every year, and most of it is as a result of improper disposal of plastic waste. An oceanographic study also gave an estimation that at least 5.25 trillion of individual plastic particles which weighed roughly 244,000 metric tons (269,000 short tons) were floating on the ocean surface. Another study also gave an estimation that 44 percent of plastic wastes in rivers and oceans, was made up of plastic bags, bottles, and food packages. (Moore. 2025).

The rapid increase of plastic pollution can kill animals in the marine habitat directly by entangling itself with them so much that they get stuck, and as a result die of starvation. It also kills them through ingestion; many animals often mistake some of these plastics for food and as a result consume them. Some of these plastics consumed can lead to suffocation if it get stuck In their throat or indigestion, which eventually leads to death.

Microplastics

As plastics are exposed to sunlight and seawater under high temperature and pressure, they become easy to breakdown. The larger plastics eventually break down into smaller particles called **microplastics**, and these microplastics because of their small sizes (which are less than 5 mm) become more available to zooplankton and other small marine animals.

These small pieces of plastic, make up a sizable fraction of plastic waste in the oceans. Studies have shown that microplastics are present in the organs of over 114 aquatic species, including the species that live only in the deepest parts of the ocean. (Moore. 2025)

Physicochemical processes such as wave action, photodegradation, and other weathering mechanisms gradually break down oceanic plastics into smaller fragments. These fragments are classified as macroplastics (>20 mm in diameter), mesoplastics (5–20 mm), microplastics (MPs, <5 mm), and nanoplastics (NPs, ranging from 1 μm to 1 nm) (Franzellitti *et al.,* 2019*;* GESAMP*,* 2016; Gunaalan *et al.* 2020). In addition to these, there are also primary micro, and nanoplastics materials that are intentionally produced and marketed as micro or nano sized particles for industrial applications (Ribeiro *et al.,* 2019; Gunaalan *et al.* 2020).

Research also estimated that at least 14 million metric tons (15.4 million short tons) of microplastics were present on the floor of the ocean in 2020, other research showed that the movement of deep-sea currents created dominant spots for microplastics in some parts of the oceans, for example; nearly two million microplastic pieces per square metre (about 186,000 pieces per square foot) is present in the Tyrrhenian sea that contained nearly two million microplastic pieces per square metre (about 186,000 pieces per square foot). (Gunaalan *et al.* 2020).

The leaching of additives from plastics released into the environment can expose wildlife to complex mixtures of chemicals, which include both substances already regulated under existing environmental laws and various contaminants of emerging concern (CECs) that may also pose potential risks (Gunaalan *et al.* 2020).

Recent studies estimate that marine plastics globally release approximately 23,600 metric tons of dissolved organic carbon (DOC) each year (Romera-Castillo *et al.,* 2018). DOC is an essential component of the marine trophic system, influencing the abundance, growth, and metabolic activity of both photosynthetic and heterotrophic microorganisms (Azam *et al.*, 1983a; Gunaalan *et al.* 2020). Consequently, the continuous increase in plastic pollution may significantly alter the composition, interactions, and functional diversity of marine microbial communities.

Approximately 60% of the dissolved organic carbon (DOC) released from plastics is readily bioavailable within five days. However, exposure to solar radiation reduces the lability of this plastic-derived DOC.

The leaching of plastics is believed to create localized zones of elevated DOC concentrations that can be quickly remineralized by marine microorganisms. Nonetheless, the fate of the remaining 40% of DOC that is not immediately utilized by bacteria remains uncertain. (Castillo *et al.,* 2018)

It has also been found that species such as; zooplankton, seabirds, and marine turtles, mistake plastic bits and trash items such as lighters, plastic bags, bottle caps, and cigarettes, for food and are quick to ingest them. (Moore. 2025).

Terrestrial habitat

Plastic pollution also affects terrestrial habitat as much as it does to that of marine. The presence of plastic bags, bottles food packs and other types of plastics causes a blockage in the drainage systems which brings about heavy flooding. Studies have also shown that Land birds have been found with plastics in their stomachs and also, terrestrial animals that feed on waste dump sites have been found to have intestinal blockages from plastic packaging. This is because the plastic wastes take up a large volume in their intestine which leads to the blockage.

The expansion of the waste dumpsites has led to its intrusion into residential areas thereby leaving the poor with no other choice than to live close to wastes or piles of residual plastics. This as a result has led to the detection of microplastics transported by wind to different parts of the world by researchers including the snow on high mountains, sea ice and in Antarctica. Microplastics also are a source of air pollution, which occurs in dust and airborne fibrous particles. The health effects of microplastics inhalation are unknown. (Moore. 2025).

Human health

The presence of microplastics have also been detected in beer, drinking water, and food products including; seafood and table salt. The presence of these microplastics in food

and water has raised concerns about their toxicity. In a research study concerned with the quantity of microplastics in human blood, the analysis of the blood sample of a subject group of 22 healthy people in the Netherlands was carried out. GC/MS was first used to identify the presence of several polymers such as; PP, PS, PE, and PET.

The blood analysis eventually concluded that 77% of the donors' blood contained quantifiable amounts of these plastics (PP, PS, PE, and PET) in their blood, and the authors stated the need to carry out further investigation so as to enlighten everyone on the health implications of microplastics (Jade *et al. 2025;* Leslie *et al.* 2022).

It was also recovered from stool samples of eight individuals from eight different countries who participated in a pilot study. Scientists have also detected microplastics in human tissues and organs however, the implication of its presence for human health was uncertain. (Moore. 2025).

1.3 Leachates

What are Leachates?

The pollution of plastics can also occur without being littered in the environment, and this can occur as a result of the release of the additives which were used during its manufacture into the content of the plastic, which will eventually be consumed by humans. (Moore. 2025). The release of these additives is also known as **leachates.**

Leachates are complex mixtures that contain various chemical additives, including some compounds now recognized as emerging contaminants. These substances are gaining attention because they pose serious risk to both the environment and human health, even though they haven't been fully addressed by current environmental laws. (Gunaalan *et al*. 2020).

During the manufacture of plastics, additives are incorporated into base polymers to enhance properties such as; flexibility, color, or heat stability which will be beneficial on production. Plastics may also contain residual substances such as catalysts,

monomers, NIAS, and solvents which emanate from the synthesis process. Non-intentionally added substances (NIAS) are chemicals in plastics which are present as a result of contamination, degradation, and accumulation of impurities during the process of manufacture or when it is in use. (James *et al. 2023*).

Chemicals such as; phthalates, bisphenol A (BPA), and polybrominated diphenyl ether (PBDE), are leachates used as additives in the manufacture of plastics, and have been studied closely and intensely for an expanded knowledge of its dangerous side effects to humans when consumed. With few exceptions, these leachates are physically mixed rather than chemically bonded to the polymer, allowing them to migrate through the material, reach the surface, and eventually leach into the environment. These leachates consist of mixtures of additives, some of which are classified as emerging contaminants or substances that have the potential to pose risks to human health and the environment but are not yet regulated. (Gunaalan *et al.* 2020).

The breakdown and degradation of plastics can promote the release of additive chemicals, many of which are not covalently bonded to the polymer matrix, making them more likely to leach into the environment (Kwan and Takada, 2016; Teuten *et al.*, 2009; Gunaalan *et al.* 2020).

A major category of these additives includes metals such as aluminium, chromium, cobalt, nickel, tin, and zinc, which are considered highly hazardous to human health (Capolupo *et al.,* 2020; Gunaalan *et al.* 2020). Among the organic additives, notable examples include Bisphenol A (BPA), phthalates, and brominated flame retardants (BFRs), which have been extensively documented to exert toxic effects on living organisms (Baršienė *et al.*, 2006; Bollmann *et al.,* 2012; Canesi and Fabbri, 2015; Balbi *et al.,* 2016; Wang *et al.*, 2020; Gunaalan *et al. 2020*).

1.3.1 Phthalates

Phthalates, also known as phthalic acid esters (PAEs), are chemical compounds used as additives in plastics to increase their flexibility and softness. They are formed when phthalic anhydride reacts with alcohol, resulting in a compound made up of a benzene ring with two carboxylic acid groups (Mankidy *et al.*, 2013; Arigo *et al.* 2023). Because of

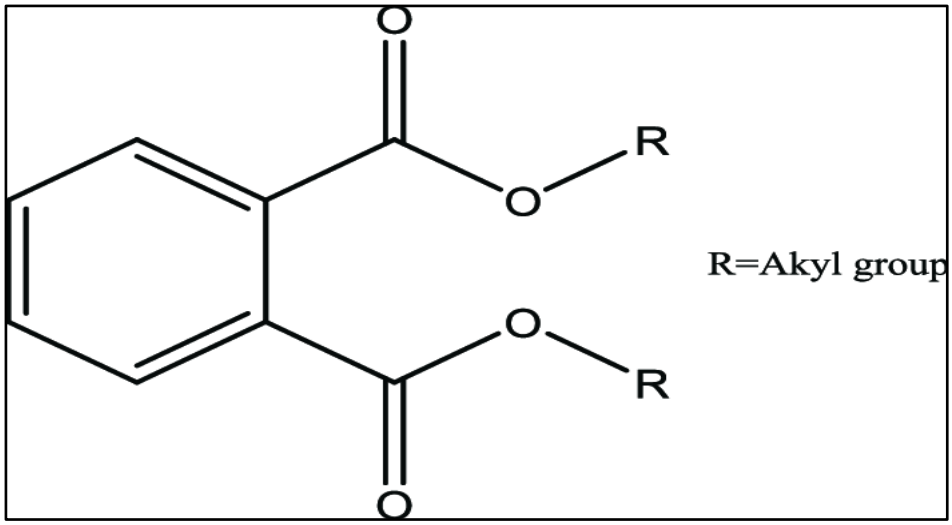
their covalent bonding nature, phthalates can easily be released into the environment through a process known as leaching, which occurs in soil, freshwater, marine environments, and sediments. These compounds are widely used in industries as plasticizers to improve the workability of polymers (Dutta *et al.,* 2020; Arigo *et al.* 2023). Studies have shown that about 7.5 million tonnes of plasticizers are used each year across various industries, including construction materials, leather production, medical equipment, perfumes, and cosmetics (Burgos-Aceves *et al.*, 2021; Arigo *et al.* 2023).

Phthalates are also used to improve texture, spreadability, and absorption in products. They are commonly found in polyvinyl chloride (PVC) plastics, which are used in packaging materials, hoses, and medical tubing (Przybylińska and Wyszkowski, 2016; Arigo *et al.* 2023).

Although phthalates do not persist for long periods because they break down through natural processes such as biodegradation, photodegradation, and anaerobic degradation, they are still easily released into the environment. Several studies have used human biomonitoring (HBM) to assess occupational exposure to different types of phthalates in work environments (Fréry *et al.,* 2020). Due to their durability and stability, these compounds are present in many consumer products and even in food items such as dairy, fish, and shellfish (Serrano *et al.,* 2014; Arigo *et al.* 2023). It is believed that food consumption is the main route of human exposure to phthalates, particularly through fatty foods like milk, butter, and meat.

There are various types of phthalates, including di(2-ethylhexyl) phthalate (DEHP), dibutyl phthalate (DBP), diethyl phthalate (DEP), di-isononyl phthalate (DiNP), di-isodecyl phthalate (DiDP), benzyl butyl phthalate (BBP), and dimethyl phthalate (DMP). Among them, dibutyl phthalate (DBP) has been identified as especially harmful to the environment and aquatic organisms (Zhang *et al.,* 2021). They are said to be found in flooring materials, cosmetics, pharmaceuticals, food packaging, medical devices, as well as perfumes.

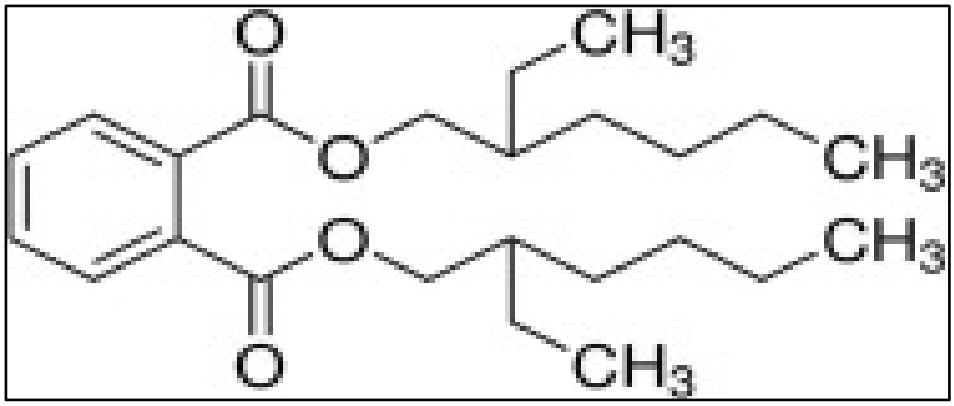
Structure of Phthalates



Types of phthalates and their uses

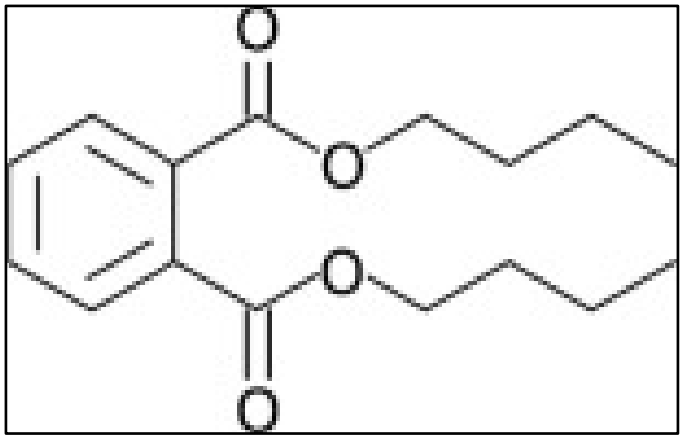
1. Di(2-ethylhexyl) phthalate (DEHP); It is a very flexible plasticizer for PVC and it is also used in the manufacture of medical devices, furniture materials, cosmetics, and personal care products. (Rowdhwal *et al.*2018)

Structure of Di(2-ethylhexyl) phthalate (DEHP)



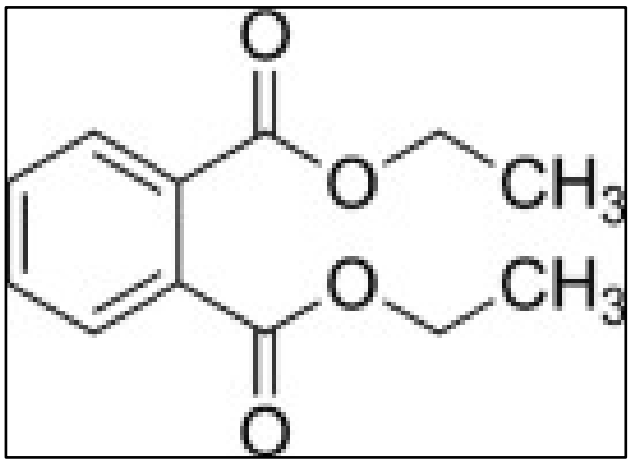
2. Dibutyl phthalate (DBP); Dibutyl phthalate (DBP) is a widely used plasticizer primarily applied in nitrocellulose lacquers and polyvinyl chloride (PVC) plastics to enhance their flexibility. It also functions as a solvent for dyes and pesticides, and serves as an industrial raw material in the production of anti-foaming agents, latex adhesives, and textile fiber lubricants. Due to its versatility, DBP is found in many everyday consumer products such as plastics, paints, adhesives, insect repellents, perfumes, hair sprays, and nail polishes. (Wei *et al.* 2011)

Structure of Dibutyl phthalate (DBP)



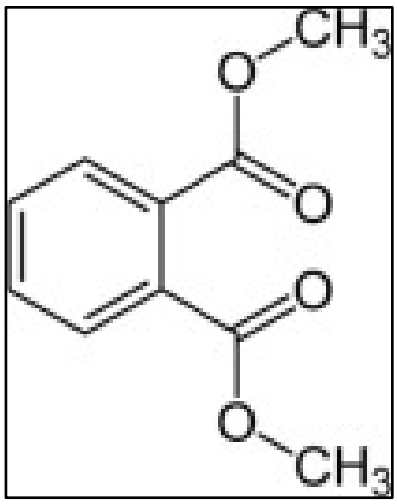
3. Diethyl phthalate (DEP); It adds flexibility and solvent properties in plastics and is also used in the production of personal care products, and cosmetics. (Leitz *et al.* 2009)

Structure of Diethyl phthalate (DEP)



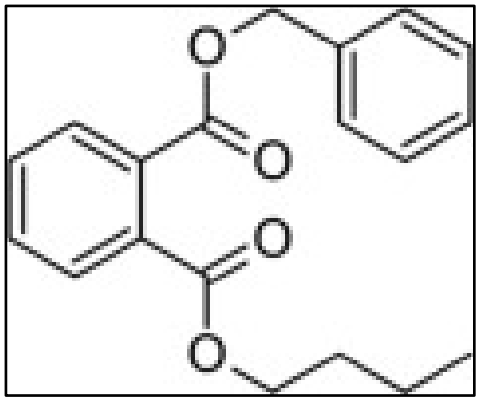
4. Dimethyl phthalate (DMP); It is used as a plasticizer and solvent in the manufacture of plastics and also in the production of Insect repellents, safety glass, and lacquer coatings.

Structure of Dimethyl phthalate (DMP)



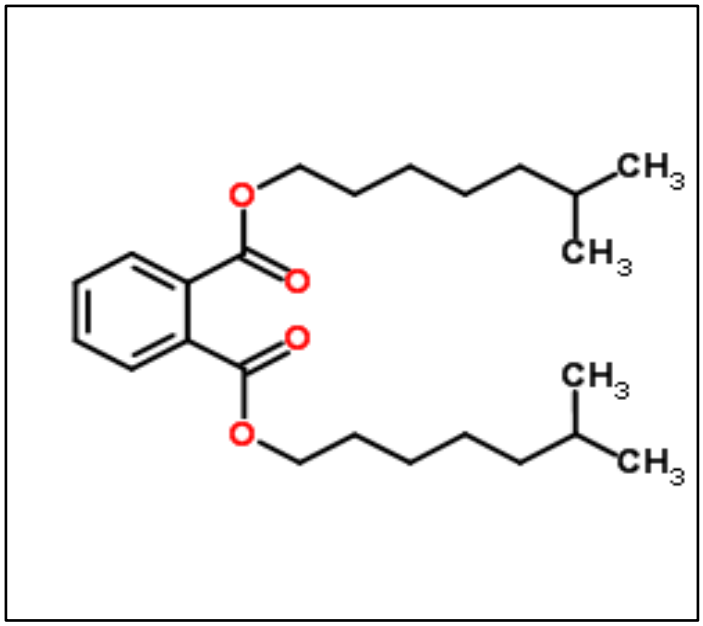
5. Benzyl butyl phthalate (BBP); It provides flexibility and adhesion and is also used in the manufacture of traffic cones, food conveyor belts, and artificial leather.

Structure of Benzyl butyl phthalate (BBP)



6. Diisooctyl phthalates; Diisooctyl phthalate (DIOP) is a high molecular weight phthalate ester that consists of a benzene ring with two carboxyl groups attached to two seven-carbon isooctyl ester chains positioned ortho to each other (HSDB, 2009). In Australia, DIOP is primarily imported for use in rubber formulations, particularly in the manufacture of automotive hoses and components (Luo *et al.* 2011). It is also distributed to research institutions and laboratories, where it serves as a reagent in biotechnology and pharmaceutical studies. Additionally, DIOP functions as a plasticizer in various materials, including vinyl, cellulose, and acrylic resins, as well as synthetic rubber, building insulation, children's toys (such as pacifiers and teething rings), and food-contact products (Saillenfait *et al.,* 2013).

Structure of Diisooctyl phthalates



Dangers of phthalates to the environment

Aquatic pollution caused by phthalic acid esters (PAEs) mainly comes from industrial and commercial wastewater, as well as plastic waste that contains these man-made compounds. Because most phthalates have a high n-octanol–water partition coefficient (Kow) and low vapor pressure, they do not evaporate easily but instead tend to spread and persist within different water bodies (Cao *et al.,* 2018; Zhang *et al.*, 2021). This makes it easy for them to move through aquatic systems and be absorbed by living organisms.

Once inside aquatic animals and other organisms, phthalates can trigger several

harmful effects, including immune system damage, metabolic disruption, hormonal (endocrine) imbalance, nerve damage, genetic toxicity, and developmental problems (Yu *et al., 2019;* Li *et al.,* 2020a; Xu *et al.,* 2020; Zhang *et al.,* 2021). Because of these serious health and environmental risks, both the United Nations Environment Programme (UNEP) and the International Maritime Organization (IMO) are currently studying the toxicity levels and public health impacts of these chemicals.

In response to the dangers associated with phthalates, the use of compounds such as benzyl butyl phthalate (BBP), di(2-ethylhexyl) phthalate (DEHP), dibutyl phthalate (DBP), and diisobutyl phthalate (DiBP) has been banned or restricted in children's toys and childcare products in several countries, including the United States and Canada. These regulations were established under the Consumer Product Safety Improvement Act (CPSIA, 2008) and the Dangerous Products Act (2010) (Zhang *et al* 2020; Zhang *et al.*, 2021)

1.3.2 Bisphenol A

Bisphenol A (BPA) is one of the most widely produced synthetic chemicals in the world, with an annual production of over 3.8 million tons. It is mainly used in making polycarbonates, epoxy resins, and thermal paper (Hoekstra and Simoneau, 2013). Because of its wide industrial use, BPA can be found in many everyday products such as water pipes, electronics, papers, and children's toys (Flint *et al.,* 2012; Huang *et al.*, 2012; Jaromir Michalowicz. 2014). It is also a common ingredient in food contact materials, including bottles, food packaging, and the protective coatings inside cans.

This means people are often exposed to BPA through food and drinking water (Yoshida *et al.,* 2001; Niu *et al.,* 2012; Markis *et al.*, 2013; Jaromir Michalowicz. 2014). Apart from ingestion, inhalation of household dust and direct contact during production can also expose workers and the general public to BPA (Geens *et al.,* 2009; He *et al.,* 2009; Jaromir Michalowicz. 2014).

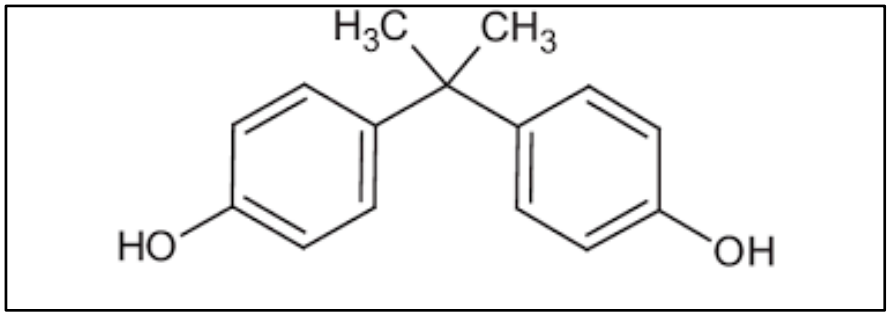
BPA has the ability to bind with several receptors in the body, such as estrogen,

androgen, aryl hydrocarbon, and peroxisome proliferator-activated receptors, all of which play roles in hormonal and metabolic regulation (Wetherill *et al.,* 2005; Iso *et al.,* 2006; Ziv-Gal *et al*., 2013). Because of its endocrine-disrupting properties, along with its potential to cause oxidative stress, DNA mutation, and epigenetic changes (Keri *et al.,* 2007; Richter *et al*., 2007; Tayama *et al.,* 2008; Moon *et al*., 2012), BPA can produce a wide range of toxic effects in both animals and possibly humans. It has been found to interfere with sex hormones, leptin, insulin, and thyroxin, leading to liver toxicity, immune system damage, genetic mutations, and even cancer (Meeker *et al*., 2010; Doherty *et al*., 2010; Clayton *et al.,* 2011; Zeinab *et al*., 2012).

BPA is also suspected to have neurotoxic and teratogenic effects, though research results in this area are not yet consistent (Yang *et al.,* 2009; Xing *et al.,* 2010; Ryan *et al*., 2010).

Bisphenol A is also used in the manufacture of clear, hard polycarbonate plastics, and strong epoxy coatings and adhesives. It is present in food can linings, medical devices, food packaging, bottles, and compact discs. Bisphenol A, and phthalates have been detected in humans and are known as endocrine disruptors which may lead to reproductive and developmental disorders. BPA interferes with different functions at the cardiovascular level thereby leading to cardiovascular disease, cancer, kidney disease, and birth defects. (Fonseca *et al.* 2022). It has also been found in the blood of pregnant women and placenta tissue, which indicates foetal exposure to BPA, and also found in feeding bottles which serves as the primary source of exposure for young children. (Jade *et al* 2025). BPA also replicates the natural female hormone estrogen.

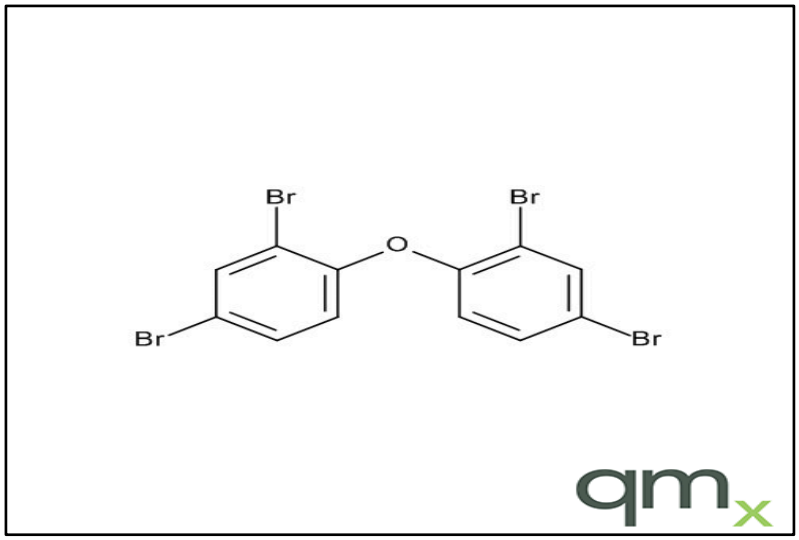
Structure of Bisphenol A



1.3.3 Polybrominated diphenyl ether (PBDE)

Polybrominated Diphenyl Ethers (PBDEs) are a group of brominated compounds widely applied as flame retardants in various materials such as electronic devices, textiles, transport components, and children's toys. Since PBDEs are not chemically bonded to the polymer matrix, they can easily be leached into the environment through leaching, volatilization, or physical abrasion, especially during use or disposal. At the end of a product's life cycle, this release becomes more pronounced as the materials degrade. Numerous studies have shown that the toxic impacts of PBDEs outweigh their functional advantages, as they exhibit neurotoxic properties and can interfere with endocrine and reproductive systems, with evidence also suggesting potential carcinogenic effects on both humans and wildlife. (Kostenko *et al.* 2024). The release of this chemical into the environment has become a major area of concern. (Moore. 2025).

Structure of Polybrominated Diphenyl ether (PBDE)



Polybrominated diphenyl ether (PBDE) which is also an anti-androgen, disrupts thyroid hormones. The most vulnerable people to these hormone-disrupting chemicals are children and women of reproductive age. (Moore. 2025).

These compounds have also acted as an hormone disruption in terrestrial, aquatic, and marine animals in their distinguished habitat. They act against their reproduction and development, including the alterations in the number of their offsprings produced, larva development disruption, and delayed emergence in insects.

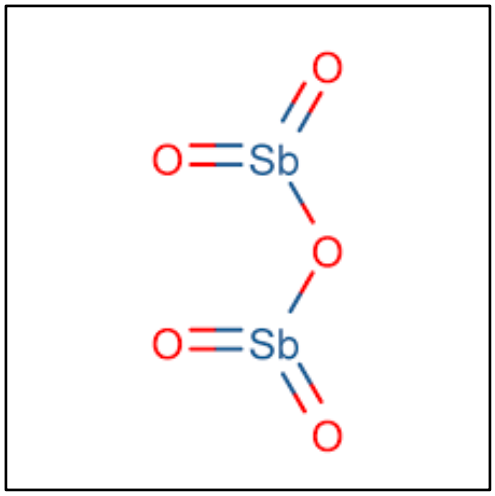
1.3.4 Antimony

Antimony (Sb) is a technologically important element commonly found in numerous manufactured products, especially in plastic materials. It serves multiple industrial purposes such as; functioning as a synergist with brominated flame retardants, a

catalyst in the production of polyethylene terephthalate (PET), and a coloring pigment in various polymers. Due to its widespread application, antimony has become ubiquitous in plastic-based products, contributing to its presence in the environment through leaching or degradation processes. (Filella *et al.*2020).

Antimony is a regulated contaminant that poses both acute and chronic health effects in drinking water. Antimony can leach out from PET plastics commonly used in making bottled drinking water. Although the leaching rate remains low at temperatures below 60 °C, exposure to higher temperatures can cause a significant and faster release of antimony into the water. Short-term exposure to antimony above the maximum contaminant level (MCL) may cause nausea, vomiting, and diarrhea, while long-term exposure has been linked to elevated blood cholesterol and reduced blood sugar levels. (Westerhoff *et al.* 2008).

Structure of Antimony Oxide (Sb_2O_5)



1.4 Analytical techniques used

Gas Chromatography - Mass Spectroscopy

GC-MS was used because it combines very good separation (GC) with specific molecular identification (MS). The GC column separates the many organic compounds that can leach from plastics (phthalates, bisphenol A and analogues, antioxidants, plasticizers, etc.), so they reach the mass spectrometer one at a time. The MS then produces fragmentation patterns (mass spectra) that helps identify compounds against spectral libraries and confirm identities by their characteristic ions. This combination makes GC–MS ideal for detecting and identifying low-level organic migrants from plastics. (Natalia P. Ivleva. 2021).

The function of the GC-MS involves:

- **Quantification for exposure assessment.** GC–MS gives quantitative results that feed into risk calculations (e.g., µg/L in leachate → estimated exposure). (Natalia P. Ivleva. 2021).
- **Detecting many migrants, including unexpected ones.** Studies that analyze plastic leachates often find dozens to hundreds of compounds; GC–MS (especially when combined with proper extraction and full-scan acquisition) helps reveal this chemical complexity so toxicity or hazard tests can be linked to real chemical exposure. (Natalia P. Ivleva. 2021).

FT-IR (Fourier-Transform Infrared)

FT-IR is used in this study because it helps to determine what kinds of chemical functional groups are present and also helps to quickly check the polymer type and surface chemistry changes caused by weathering or leaching. In FT-IR the functional group is determine by amount of infrared light absorbed by a sample at different wavelengths, each bond (C=O, O–H, C–H, C–O, etc.) absorbs in characteristic regions, so the resulting spectrum is like a fingerprint that can be compared with reference spectra to identify materials or major organic groups. (Campanale *et al.* 2023).

The function process of FT-IR includes;

- **Polymer identification** — I can confirm whether a piece is PE, PP, PET, PVC, PS, etc., by matching characteristic peaks (useful when determining the likely additive suite and source). (Campanale *et al.* 2023).
- **Functional-group detection in leachates or on plastic surfaces** — FT-IR shows carbonyl, hydroxyl, ester, and aromatic signals that help detect oxidation, hydrolysis or the presence of additives/contaminants at moderate concentrations. This is especially useful to detect signs of plastic ageing or

weathering that may increase leaching. (Campanale *et al.* 2023).

- **Screening / pre-screening of samples** — FT-IR is fast and low-cost for screening many samples to decide which ones need detailed GC-MS or LC-MS follow-up for specific additive quantification. (FT-IR is often used for total phthalate content screening, while GC-MS separates and quantifies individual phthalates.) (Andjelkovic *et al.* 2021).
- **Aging / degradation indices** — by measuring changes in the carbonyl and hydroxyl regions we can compute indices (Carbonyl Index, Hydroxyl Index, etc.) that quantify degradation and help explain increased leachability after weathering. (Campanale *et al.* 2023).

CHAPTER TWO

2.0 Materials and Methods

This chapter explains the materials and method employed in this study. The reagents, apparatus, plastic types, procedures adopted for the sample collection and preparation, as well as the experimental process for the leaching of Bisphenol A and Phthalates from virgin plastic bottles (PET) were highlighted.

Furthermore, the leaching conditions, leachate extraction, and analytical methods used were also described.

2.1 Materials

- Virgin plastic bottles
- Aluminium Foil
- Scissors
- Rubber Band
- Filter paper
- Hand gloves
- Paper tape

2.1.1 Reagents and Chemicals used

- De-ionized water
- Dichloromethane (DCM)

- Distilled water
- Anhydrous sodium sulphate (Na2So4)

2.1.2 Instrument and Apparatus used

- 250ml beakers
- 250ml conical flasks
- Separating funnel
- Plastic funnel
- Retort stand
- oven

2.2 Methodology

2.2.1 Collection of plastic samples

Virgin (unused) plastic samples were collected and cut into bits of reasonable size. It was further rinsed with de-ionized water for the removal of any form of surface contamination. After rinsing, it was dried in an oven within the temperature range of 30°C. The beakers were also rinsed with distilled water to avoid unforeseen contamination in the leachate sample that was to be prepared.

2.2.2 Preparation of Solvent Samples

5g of the bits of virgin plastics was measured and placed in 5 different beakers each labelled with representing different time frames (in hours) in increasing order (0hrs, 24hrs, 48hrs, 72hrs, 96hrs).

Each beaker which contained the bits of the virgin plastics were soaked with de-ionized water at the same time, and placed in the oven at a constant temperature of 40°C.

For 0 hours

The plastic bits were soaked in de-ionized water and allowed to stay in the oven for 60 seconds (1 minute) before it was filtered out from the solvent. The solvent was kept in the beaker and sealed with an Aluminium foil and rubber band to avoid any contamination.

For 24 hours

The plastic bits were soaked in de-ionized water and it was allowed to stay in the oven for 24 hours (1,440 minutes), after which it was filtered out from the solvent. The solvent was kept in the beaker and sealed with an Aluminium foil and rubber band to avoid any contamination.

For 48 hours

The plastic bits were soaked in de-ionized water and it was allowed to stay in the oven for 48 hours (2,880 minutes), after which it was filtered out from the solvent. The solvent was kept in the beaker and sealed with an Aluminium foil and rubber band to avoid any contamination.

For 72 hours

The plastic bits were soaked in de-ionized water and it was allowed to stay in the oven for 72 hours (4,320 minutes), after which it was filtered out from the solvent. The

solvent was kept in the beaker and sealed with an Aluminium foil and rubber band to avoid any contamination.

For 96 hours

The plastic bits were soaked in de-ionized water and it was allowed to stay in the oven for 96 hours (5,760 minutes), after which it was filtered out from the solvent. The solvent was kept in the beaker and sealed with an Aluminium foil and rubber band to avoid any contamination.

2.2.3 Leaching Condition

In the leaching of virgin plastics using deionized water, the deionized water represents a neutral and controlled environmental condition stimulated by pure freshwater or rainwater without chemical interference.

Since deionized water is free from dissolved salts, ions, and organic matter, it provides a chemically pure medium that makes it easy for researchers to have an indepth study or assessment on the tendency of plastics to release additives such as phthalates and Bisphenol A. This condition serves as a baseline reference for comparing the leaching behavior of plastics under other environmental scenarios, such as acidic, alkaline, or saline waters. However, DI water does not perfectly represent natural freshwater systems, which often contain ions, organic compounds, and slightly acidic conditions that can influence leaching behavior. As a result it serves primarily as a reference or control condition to compare how plastics might behave under more complex environmental scenarios such as acidic, alkaline, or saline waters. This controlled setup

provides valuable insight into the fundamental leaching characteristics of plastics before assessing them in real-world environments.

2.2.4 Extraction of Leachates from the Solvent samples

After the first procedure was carried out, the Aluminium foil was removed from each of the beakers and 50ml of the solvent samples was measured into a clean set of beakers. Dichloromethane (DCM) was measured and added to each of the measured samples in the ratio 1:1, after which it was stirred gently for 10-15 minutes. Dichloromethane is denser than water and as a result of this physical property it was used to trap the possible leachates present in the solvent sample. The was stirred gently and thoroughly to ensure every leachate present in the solvent sample was trapped by DCM.

After gentle and thorough stirring, it was made to settle for 5 minutes and two distinct layers was observed. The upper layer was the solvent sample made from the de-ionized water, and the second layer was the DCM sample with possibly trapped leachates.

The DCM in each of the five samples was separated from solvent samples made from de-ionized water into a clean conical flask, using a separating funnel. The separated DCM was then dried from excess water using anhydrous sodium sulphate (Na_2SO_4), it was then filtered and transferred into sample bottles which was taken for GC-MS and FT-IR analysis.

Fig 1.2. the two distinct layers observed in the conical flasks.

Fig 1.3. the separated DCM in beakers and separating funnel.

Fig 1.4 & 1.5 DCM samples transferred into sample bottles to be taken for analysis

2.3 Analytical Determination

Gas Chromatography- Mass Spectrometry (GC-MS)

Gas Chromatography–Mass Spectrometry (GC-MS) was used for the analytical determination of leachates because it is a very sensitive and reliable technique for identifying and quantifying organic compounds present in the sample. GC helps in separating the different chemical components in the leachate based on their volatility, while the MS detects and identifies each compound by its molecular structure and mass-to-charge ratio. This as a result makes it possible to accurately detect trace levels of additives such as phthalates and Bisphenol A that have leached out from plastics. Another advantage of using GC-MS is that it gives both qualitative and quantitative information of the leachates, thereby making it easy to know what compounds are present and how much of each is in the sample.

Fourier Transform Infrared Spectroscopy (FT-IR)

Fourier Transform Infrared Spectroscopy (FT-IR) was also used to analyze leachates because it helps identify the functional groups and chemical bonds present in the compounds that have leached out from plastics. FT-IR works by measuring how the sample absorbs infrared light at different wavelengths, thereby producing a spectrum that serves as a kind of chemical fingerprint. This helps to determine the types of organic compounds released, such as phthalates and Bisphenol A, based on their characteristic absorption peaks. Another reason FT-IR was used is because it is fast, simple to use, and requires little or no sample preparation, making it very useful for confirming the presence of specific chemical groups in the leachate samples.

CHAPTER THREE

3.0 RESULTS AND DISCUSSION

3.1 RESULTS

This study assessed the concentration of Bisphenol A and Phthalates in virgin (unused) plastic bottles using de-ionized water as a neutral medium to stimulate its leaching. The results obtained from the Gas Chromatography- Mass spectroscopy (GC-MS) analysis is presented the Table 3.1

Sample ID	Concentration in µg/L

	BPA	DBP	DEP	BBP	DEHP	DIOP	TOTAL PHTHALATES
UNUSED DI 0HRS	2.92	2.34	0.32	2.89	4.12	4.12	13.79
UNUSED DI 24HRS	2.4	2.67	1.48	1.23	6.5	6.5	18.38
UNUSED DI 48HRS	2.42	2.94	1.02	1.22	6.54	6.54	18.26
UNUSED DI 72HRS	2.74	2.89	0.82	2.78	5.54	5.54	17.57
UNUSED DI 96HRS	2.96	2.96	0.85	2.14	5.54	5.54	17.03

Table 3.1 Concentration of Bisphenol A and Phthalates in µg/L for the leached solvent samples from virgin (unused) plastic bottles using De-ionized water.

3.2 DISCUSSION

3.2.1 Bisphenol A

At a regulated temperature of 40 °C with cooling at intervals, the observed variations in Bisphenol A concentrations from unused plastic bottles (2.92 → 2.40 → 2.42 → 2.74 → 2.96 µg/L) can be attributed to reflect the interplay of diffusion, analytical factors, and temperature changes. The relatively high initial value results from the quick desorption of residual surface BPA, while the gradual increase after 24 h and 48h reflects the slower diffusion of BPA from the polymer interior into the surrounding water phase, a process typical of polycarbonate-based materials at moderate temperature. Continuous temperature monitoring is recommended to confirm thermal stability, as even small deviations could influence diffusion rates.

Overall, the pattern indicates a diffusion-driven leaching process approaching dynamic

equilibrium under near-isothermal conditions.

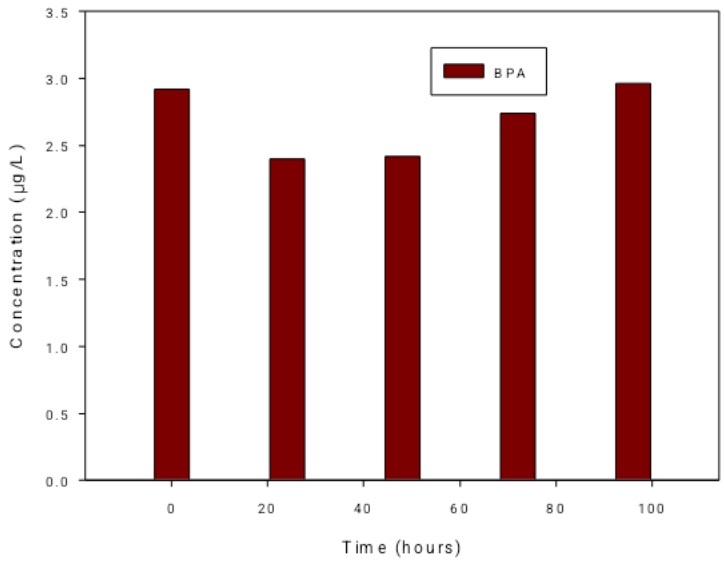


Fig 3.2. Concentration of Bisphenol A obtained from the sample

The slight dip observed at 24h and 48h may result from short-term adsorption to container walls or transient equilibrium effects, possibly within the expected analytical uncertainty range (±10 %). These fluctuations are characteristic of a diffusion-controlled leaching process approaching equilibrium under isothermal conditions.

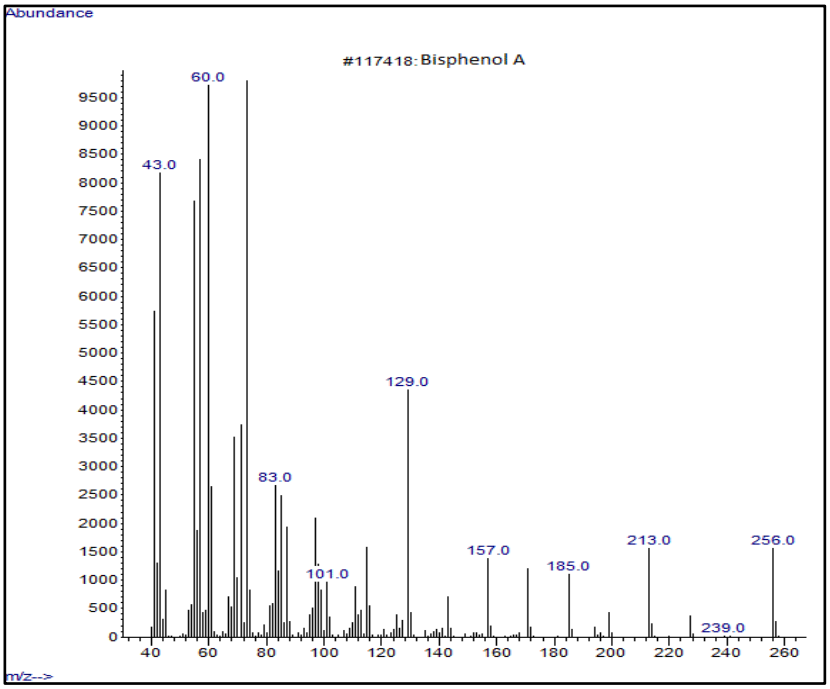


Fig 3.3 Spectrogram diagram of Bisphenol A detected by the GC-MS

Studies have shown that multiple heating and cooling can increase BPA release by several folds under severe conditions, while moderate cycling tends to produce reversible fluctuations. (Le *et al.*2008). Studies have also shown that constant regulated heating for a longer period of time (i.e 6days at 70deg/celsius) can lead to a massive increase in the release of BPA. Consequently, stepwise sampling, replicate testing, and surface characterization are essential to distinguish temporary diffusion effects from lasting polymer degradation. (Cao and Corriveau. 2008).

The observed variations in Bisphenol A (BPA) concentrations from unused plastic bottles under regulated temperature can be closely related to our day-to-day use of plastics, where plastics are frequently exposed to various thermal conditions.

In everyday life, plastics such as water bottles, food containers, and packaging materials often undergo series of heating, such as being left in a hot car, or refilled with warm liquids. These scenarios mimic the thermal stress conditions described in the experiment and can similarly influence the rate of BPA migration into consumables.

For instance, during warm conditions (around 40 °C or higher), polymer chains become more flexible, which increases the diffusion of residual BPA toward the surface.

Over time, long storage patterns of unused plastic bottles within storage temperature may cause microstructural changes or mild degradation of the plastic, leading to a gradual increase in BPA release with continued use. This pattern explains why older bottles or containers, even if originally safe, may begin to leach more BPA after prolonged or improper use.

According to a 2014 report from the U.S. Food and Drug Administration (FDA), exposure of less than 2.25 *milligrams* per pound (5 mg per kg) of bodyweight per day are safe (CFSAN, HFS-275. 2014), and with the concentration of the BPA released in 1 day (24 hours) (2.40µg/L/0.00240mg/pounds), it might be considered safe. Most people are only exposed to 0.1-2.2 *micrograms* per pound (0.2-0.5 micrograms per kg) of bodyweight per day (CFSAN, HFS-275. 2014).

However, some emerging research suggests that even at “safe” levels, the consistent exposure to BPA may cause or contribute to a variety of health problems.

These findings emphasize the importance of proper plastic use and handling. Consumers are advised to avoid heating plastic bottles or storing them under high-temperature conditions, as these actions can accelerate chemical migration. Furthermore, the results underscore the need for manufacturers to design more thermally stable, BPA-free materials to minimize human exposure to endocrine-disrupting chemicals during daily plastic use.

3.2.2 Phthalates

The results show the concentrations of five phthalates; **Dibutyl phthalate (DBP), Diethyl phthalate (DEP), Benzyl butyl phthalate (BBP), Di(2-ethylhexyl) phthalate (DEHP), and Diisooctyl phthalate (DIOP)** which were leached from unused plastic bottles into deionized water over a 96-hour period.

At the initial time (0 h), all phthalates were already present in small amounts, indicating that even unused bottles contain trace residues capable of migrating into water immediately. As time progressed, changes were observed in the concentrations of these compounds. **DBP** showed a gradual increase from 2.34 µg/L to 2.96 µg/L by 96 h, suggesting continuous but moderate leaching. **DEP** exhibited a sharp rise from 0.32 µg/L at 0 h to a peak of 1.48 µg/L after 24 h, followed by a decline to 0.85 µg/L, indicating rapid initial migration and subsequent equilibrium or re-adsorption. **BBP** fluctuated with a noticeable drop at 24–48 h but later increased again, implying irregular diffusion or variable solubility behavior.

The higher concentrations of **DEHP** and **DIOP** (both reaching around 6.5 µg/L at 48 h) show that these high-molecular-weight phthalates are more abundant in the polymer matrix and continue to migrate steadily over time.

However, their levels slightly decreased after 72 h, possibly due to saturation of the leaching medium or stabilization of the polymer–water interface.

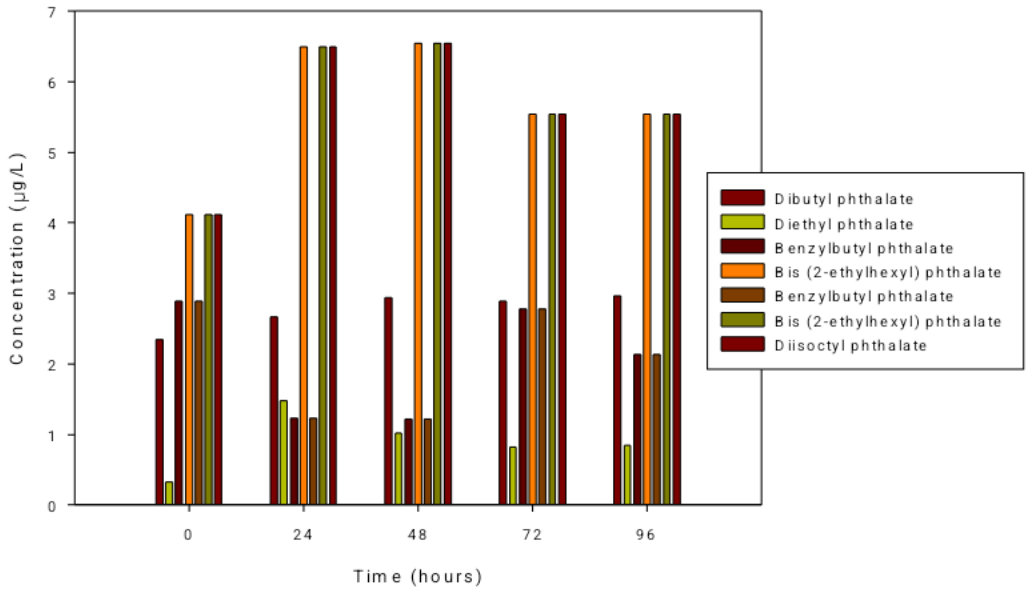


Fig 3.4 Graphical representation of the concentration of DBP, DEP, BBP, DEHP, DIOP

Overall, the data indicate that phthalate leaching occurs even in unused plastic bottles and is time-dependent. The patterns suggest that leaching is influenced by the physicochemical properties of each phthalate particularly molecular weight, solubility, and interaction with the polymer matrix.

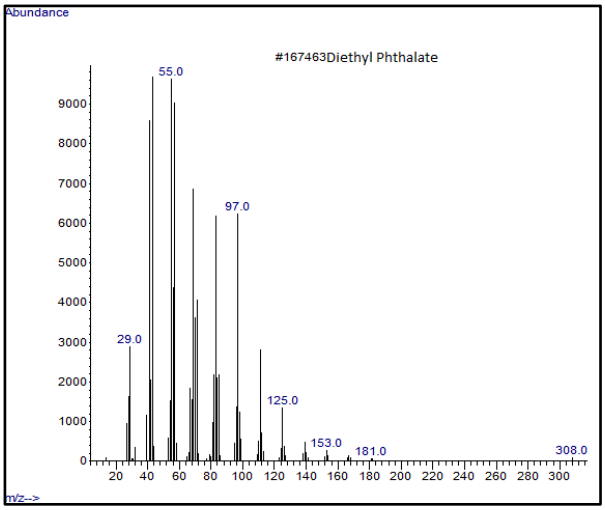


Fig. 3.5 diethyl phthalate

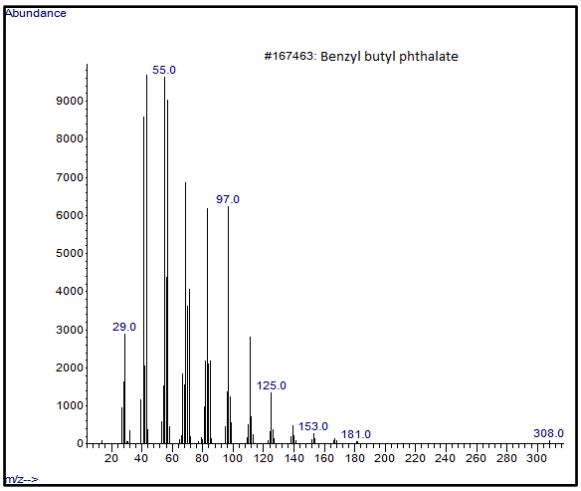
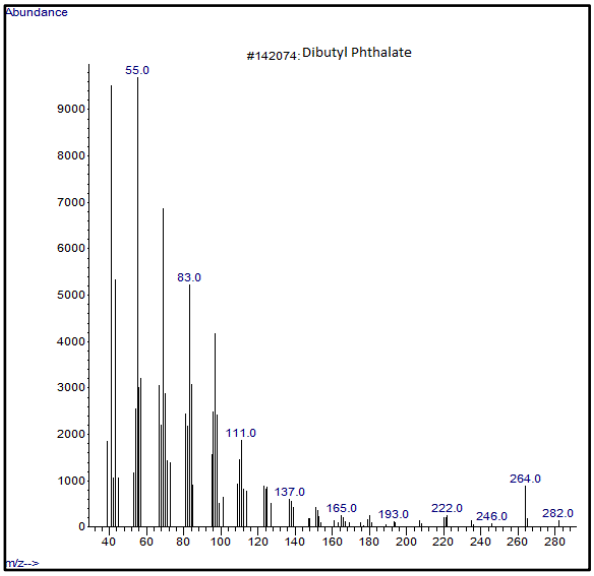


Fig. 3.6 benzyl butyl phthalate



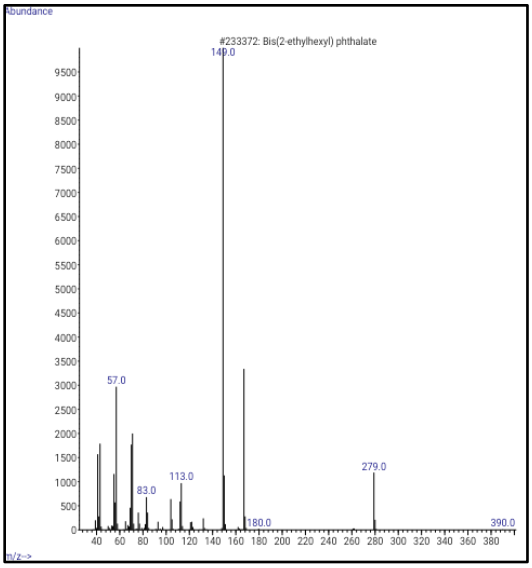


Fig. 3.7 dibutyl phthalate

Fig. 3.8 bis (2- ethylhexyl) phthalate

The figures above are the spectrogram of DEP, BBP, DBP, and DEHP in GC-MS.

The observed leaching of phthalates such as DBP, DEHP, and DIOP from unused bottles into deionized water suggests that similar migration could occur when these plastics come into contact with real drinking water, especially under warmer or prolonged storage conditions. This means that chemicals designed to make plastics flexible and durable can slowly move into the liquid we consume.

An example that explains this is when a water bottle left in a hot car for several hours develops a slightly different taste or smell, this can be a sign of additive migration, similar to what the experiment detected in controlled conditions, as increase in temperature enhances its release. (Liu *et al*. 2020).

The same concept applies to food stored in plastic containers, microwaving food in plastic bowls, or using soft plastic wraps. Over time, especially under heat or sunlight, phthalates can leach out and enter the food or drink. Although the levels detected may be small, continuous exposure from various sources in daily life can add up.

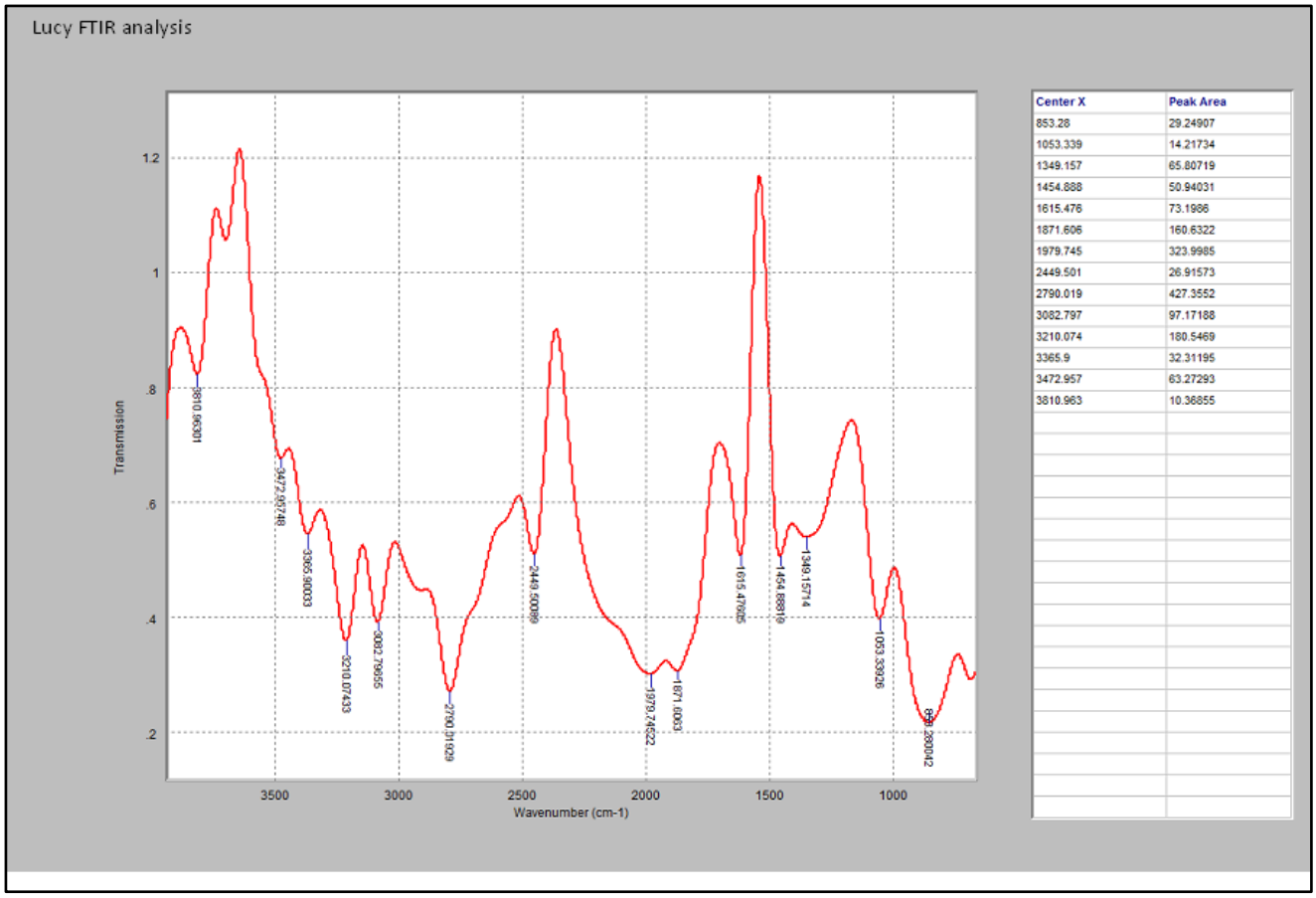


Fig 3.8 FTIR spectrogragh of Bisphenol A and Phthalates

Although there is no universal "standard concentration" for phthalates, as regulations by each country is different. Instead, legal limits often restrict concentrations to 0.1% by weight or less for certain products, such as toys and food containers. (Perestrelo *et al.* 2021).

Therefore, the laboratory observation that unused plastic bottles release measurable

quantities of phthalates reflects a real-world issue of chemical migration from plastics into consumables. It emphasizes the importance of proper plastic use, avoiding prolonged storage of food or water in plastic containers, and preferring phthalate-free or glass alternatives for safer, long-term storage.

3.3 CONCLUSION AND RECOMMENDATION

In conclusion, this study shows that virgin plastics already contain measurable amounts of Bisphenol A (BPA) and phthalates such as DBP, DEP, BBP, DEHP, and DIOP, even before they are used or exposed to the environment. The presence of these chemicals in leachates from unused plastic bottles proves that additives can migrate into water under simple and neutral conditions like contact with drinking water during the process of its storage with respect to time and temperature.

This means the release of such substances is a natural property of the plastic itself, not just a result of weathering or repeated use. The changes in concentration of DEHP, DBP, BBP, DOIP, and DEP over time and temperature suggest that the leaching of these chemicals can persist over long storage time. Heavier phthalates like DEHP and DIOP remained in higher amounts for longer periods, while lighter ones like DEP moved out more quickly and then stabilized. (Mastanjević *et al*. 2025).

The detection of BPA also shows that some of the building blocks of plastics can still move into water with influence of time and temperature. (Marsolea *et al*. 2023). However, the total amount of phthalates leached was higher than Bisphenol A and this indicates that when these bottles are eventually used by customers, a high amount of phthalates will be consumed.

Finally, this study has pointed out the need to pay more attention to the safety of plastic

materials used for storing food and drinks. Even though the amounts released may seem small, their

continuous presence and buildup in the environment and human body can pose health risks. (Marsolea *et al*. 2023).

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