ANALYSIS OF NAGONGERA WATER FOR PHTHALATES

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A RESEACH PROJECT REPORT SUBMITTED TO THE DEPARTMENT OF CHEMISTRY IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE AWARD OF BACHELOR OF SCIENCE EDUCATION DEGREE OF BUSITEMA UNIVERSITY

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DECLARATION

I, NAMBUBA ESTHER hereby declare that the research project titled "Analysis of Nagongera Water for Phthalates" is my own piece of work. The findings and conclusions presented in this report are based on rigorous scientific investigation and analysis.

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Nambuba Esther

Date: 22/08/2024

This research project work has been submitted to the department of chemistry with approval as research project supervisor:

…………………………………………………

Mr. Musagala Peter

Date: 22/08/2024

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In conclusion, this project would not have been possible without the collective efforts of everyone involved. Thank you for your dedication and commitment to advancing water quality research.

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ABSTRACT

This study was aimed at analyzing the presence of phthalates in different water sources using advanced analytical techniques. Specifically, I employed UV-VIS spectrometry and Fourier Transform Infrared (FTIR) analysis to investigate the following water types:

My findings revealed varying concentrations of phthalates across these water sources. The UV-VIS spectrometer allowed me to quantify specific phthalate compounds, while FTIR analysis provided insights into their chemical structures.

In conclusion, this study contributes valuable data to water quality management in Nagongera. The concentrations of were pond water 0.1015 mg/mL, stream water 0.0994 mg/mL, borehole water 0.0314 mg/mL, packed water 0.0352 mg/mL, and tap water 0.0410 mg/mL. Recommendations for minimizing phthalate contamination include regular monitoring, source-specific interventions, and public awareness campaigns. By understanding the phthalate profiles in different water types, we can safeguard community health and promote safe drinking water practices.

CHARPTER ONE

INTRODUCTION

1.1 Background to the Study

The first commercial plasticizers were synthesized in 1846, and in the late 1920s, di (2-ethylhexyl) phthalate (DEHP) was the first worldwide phthalic acid ester (PAE) introduced (Liu et al., 2021).

Other phthalates were gradually introduced in industrial processes due to the marked development of polyvinyl chloride plastics (PVC) (Y. Chen et al., 2013) and other polymers, such as polyethylene terephthalate (PET), polyvinyl acetates, cellulosic, and polyurethanes, which are softened by phthalates (Ruzickova et al., 2016). Polyvinyl chloride (PVC) was discovered in the late nineteenth century. Scientists at that time found the new plastic material unusual in that it appeared nearly inert to most chemicals (Manual, 2002).

The total worldwide production of phthalates increased from 1.8 tons in 1975 to more than 8 million tons in 2011 of which China and European countries have the highest phthalate utilization, accounting for approximately 1.5 and 1 million tons, respectively (Gao & Wen, 2016).

Historically DINP, DEHP, BBP, DBP, and DIHP have been the most important phthalates, however many of these are now facing regulatory pressure and gradual phase-outs. Almost all phthalates derived from alcohols with between 3 and 8 carbons are classed as toxic. This includes Bis (2-ethylhexyl) phthalate (DEHP or DOP), which has long been the most widely used phthalate, with commercial production dating back to the 1930s.

1.2 Statement of the problem

Phthalic acid esters (PAEs) are a class of lipophilic chemicals widely used as plasticizers and additives to improve various products' mechanical extensibility and flexibility. At present, synthesized PAEs, which are considered to cause potential hazards to ecosystem functioning and public health, have been easily detected in the atmosphere, water, soil, and sediments However, it has been pointed out that the use of phthalate ester may cause several risks such as its endocrine disruption, carcinogenic action or influence to the reproductive ability

This current approach will create awareness to people about the effects of taking water containing phthalates and emphasizing that they should drink water that has been properly filtered.

1.3 Objectives of the Study

The overall objective was to analyze Nagongera water for phthalates

The overall objective was achieved by the following specific objectives

i) To detect the presence of phthalates that leach into water.

ii) To quantify the amount of phthalates in different sources of water.

iii) To evaluate the preventive measures that can be undertaken to avoid water contamination by phthalates.

1.4 Justification of the Study

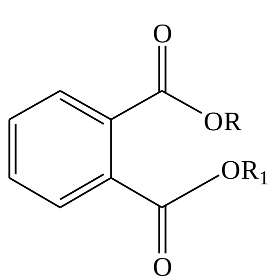
Exposure to phthalates compounds in water may have short-term and long-term health implications. Short-term exposure might include acute effects such as skin irritation, or respiratory issues. Long-term exposure to phthalates could potentially contribute to chronic health problems, including asthma, obesity, type11 diabetes, reproductive disorders, immune system dysfunction, and breast cancer. This study was to help ascertain the extent of these health implications and determine safe exposure limits.

To understand the specific vulnerabilities of groups such as women, children, and individuals with compromised immune systems, and determine whether additional protective measures are needed to safeguard their health.

1.5 Literature Review.

Phthalates are a family of compounds made from alcohols and phthalic anhydride. They are oily, colorless, odorless liquids that do not evaporate readily. Often called plasticizers, phthalates are used in the manufacture of plastics, including polyvinyl chloride plastics (PVC). Phthalates can prolong the lifespan or durability of plastics and increase the flexibility of some plastics. They can be found in hundreds of products such as toys, vinyl flooring, herbal pill coating, and plastic shower curtains. In addition, phthalates are also used as solvents. Phthalates are used in a variety of cosmetic products, such as nail polishes, perfumes, skin moisturizers and shampoos to enhance penetration and hold scent and/or color.

The general chemical structure of phthalates (R and $R_1 = C_nH_{2n+1}$) is

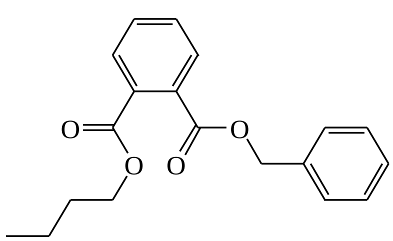
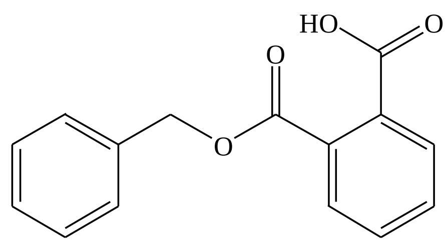
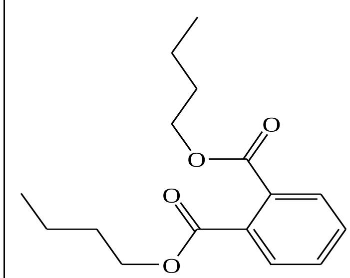
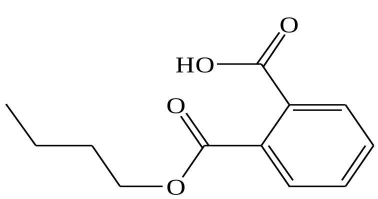
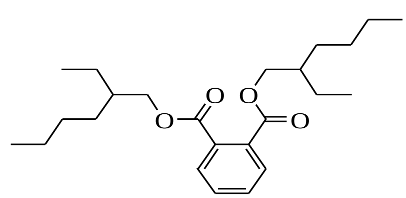
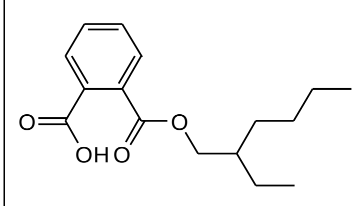
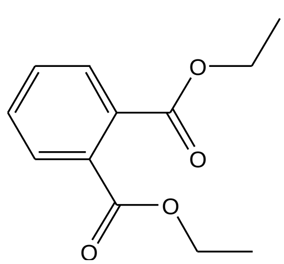
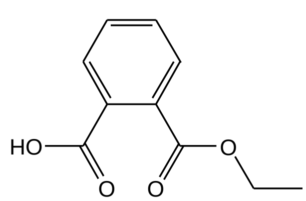
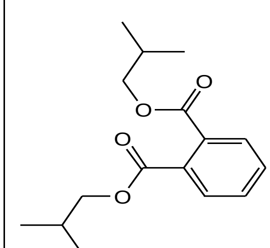


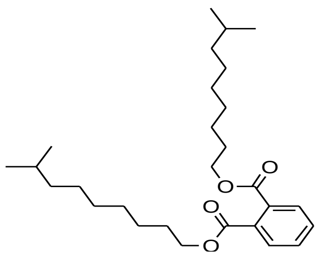
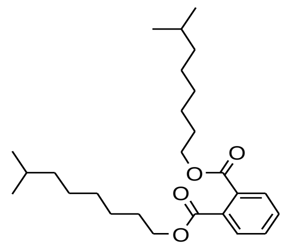
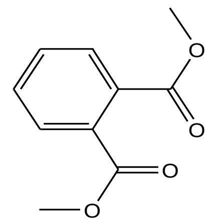
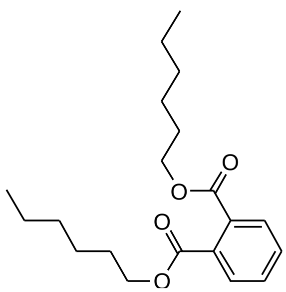
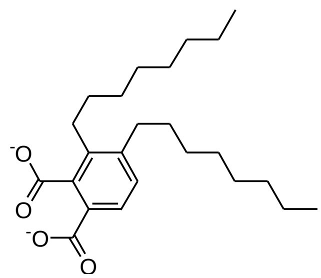
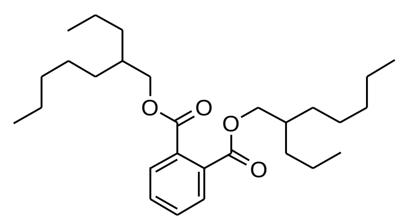
1.5.1 Examples of phthalates used.

The most frequently detected phthalates in different drinking water types that is to say mineral water, tap water, and fountain water) are DMP, DEP, DnBP, and DEHP (Net et al., 2015a).

Some of the commonly used phthalates include

Table 1: Examples of phthalates

tBBzP: butyl benzyl phthalate 	MBzP: mono benzyl phthalate 	DnBP: di-n-butyl phthalate 
MnBP: mono-n-butyl phthalate 	DEHP: di-(2-ethylhexyl) phthalate 	MEHP: mono-(2-ethylhexyl) phthalate 
DEP: diethyl phthalate 	MEP: monoethyl phthalate 	DiBP: di-isobutyl phthalate 

DiDP: di-isodecyl phthalate 	DiNP: di-isononyl phthalate 	DMP: di-methyl phthalate 
DnHP: di-n- hexyl phthalate 	DnOP: di-n-octylphthalate 	DHPH: Di-(2-propylheptyl) phthalate 

1.5.2 Effects of phthalates

Despite their many uses and applications, phthalates have become major environmental concerns due to their genotoxicity, neurotoxicity, cytotoxicity, reproductive toxicity, and endocrine-disrupting effects which may affect human health from gestation to adulthood. Certain diseases such as breast, skin, liver and testicular cancer, diabetes, autism spectrum disorders, obesity, and thyroid function, are related to phthalate exposure (Benjamin et al., 2017).

1.5.2.1 Phthalates as endocrine disruptors

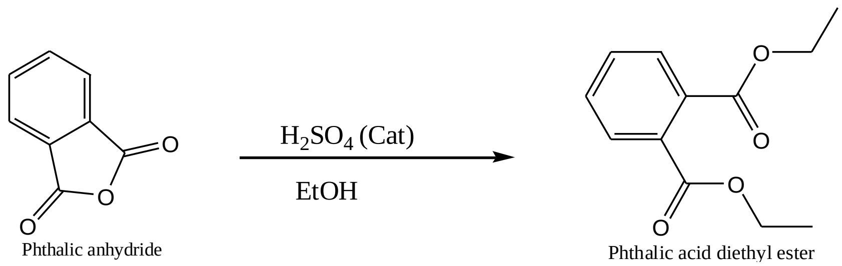
An endocrine disrupter is an exogenous agent that interferes with the synthesis, secretion, transport, binding, action, or elimination of natural hormones in the body that are responsible for the maintenance of homeostasis (biological stability), reproduction, development and/or behavior. Phthalates are capable of binding to the estrogen receptor. Human exposure to these endocrine disrupting compounds (EDCs) can occur through four major pathways (ingestion, inhalation, intravenous and dermal contact), where the first is the main route of exposure (Notardonato et al., 2018). In animal studies, several phthalates show antiandrogenic activity ((DHHS), 2005). Phthalates have been linked to adverse reproductive effects in male pubertal and adult rodents exposed in utero and during lactation, such as reduction in the weights of reproductive organs and a reduction in sperm count (Foster, 2006). There is also some evidence of reproductive toxicity in adult female rodents exposed to DEHP, such as prolonged estrous cycles and lowered circulating estradiol levels (Davis et al., 1994). In one human study, infant boys born to mothers with high phthalate urine levels were more likely to have smaller penises and scrotums and incomplete testicular descent (Swan, 2005). Boys born to mothers with the highest levels of phthalates were four to ten times more likely to have reduced genital development.

1.5.2.2 Phthalates as carcinogenic agents

In breast cancer cells, some phthalates have weak estrogenic effects and some have weak anti-estrogenic effects in the presence of 17beta-estradiol (Kim et al., 2004).

1.5.3 Production of phthalates

Phthalates are produced industrially by the acid catalyzed reaction of phthalic anhydride with excess alcohol. For example, the synthesis of diethyl phthalate is illustrative as below



1.5.3 Characteristics of phthalates

1.5.3.1 Durability

Extends a product's lifetime wear

1.5.3.2 Flexibility

Allows vinyl to bend and twist without cracking, an essential safety feature in products such as electrical and automotive cables

1.5.3.3 Low volatility

Using phthalates in applications where products are exposed to high temperatures enables products to be more resistant to degradation

1.5.3.4 Weather resistance

Makes products especially suitable for many outdoor applications

1.5.4 Properties of phthalates

phthalate esters, or phthalates, are a group of important derivatives of phthalic acids which are synthesized from phthalic anhydride and specific alcohols by Fischer esterification (Mathur, 1974).

PAEs based on hydrogen bond and van der Waals force interconnection are hydrophobic compounds with log K_{ow} ranging from 1.6 to 12 (Net et al., 2015b).

Most of the phthalate esters are colorless liquids with a low volatility, high boiling point, and poor solubility in water, but they are soluble in organic solvents and oils (Gani et al., 2017). These esters' general chemical structure consists of a rigid planar aromatic ring and two malleable nonlinear fatty side chains. The two side-chain groups can be the same or not, and there are approximately 30 types of different side chains, ranging from dimethyl phthalate to tridecyl ester (Autian, 1973).

Due to phthalate esters being widespread in the biosphere and potential hazards in relation to ecosystem functioning and public health, six PAEs have been listed as priority pollutants by the United States Environmental Protection Agency and the European Union (Das et al., 2020), including dimethyl phthalate, diethyl phthalate, di-n-butyl phthalate, butyl benzyl phthalate, di(2-ethylhexyl) phthalate, and di-n-octyl phthalate.

1.5.5 Sources of phthalates in the environment.

The manufacture, use, and disposal of PVC and other phthalate-containing products have resulted in extensive environmental releases of phthalates.

Phthalates are not covalently bound to the polymer matrix, rather they usually remain present as a freely mobile and leachable phase; therefore, they can be lost from soft plastic over time and released to the environment during production and manufacture. Not surprisingly, phthalates can often be found in freshwater lakes and oceans (H. Chen et al., 2019), urban and suburban soil (H. Wang et al., 2017), the atmosphere and sediments.

The primary sources of phthalates in surface waters and sediments are industrial and municipal wastewater discharges, agricultural runoff and infiltrated leachate from landfills (Mukhopadhyay et al., 2021).

1.5.6 Exposure of humans to phthalates

People are exposed to these phthalates mainly through foods that are packaged in plastic (Clark, 2011). These phthalates can also enter food products when they are taken up by growing crops (Services, 2003). The ubiquitous use of phthalate esters in plastics, personal care products and food packaging materials results in widespread general population exposure. All populations of people, domestic animals, and wildlife regularly encounter opportunities for exposure to phthalates because of their widespread use.

1.5.6.1 Water

Phthalates are found in ground water and drinking water. From 1987 to 1993, according to EPA's Toxic Chemical Release Inventory, DEHP releases to land and water totaled over 500,000 lbs., of which about 5 percent was to water(Agency, n.d.).

1.5.6.2 Medications and nutritional supplements

Pharmaceutical preparations intended to treat diseases of the gastrointestinal tract, such as ulcerative colitis and colorectal cancer, are often coated with a polymer that allows the drug to be delivered directly to the colon or small intestine. This polymer may contain plasticizer phthalates such as DBP and DEP (Chourasia & JainSK, 2003). Other pharmaceutical products may also have phthalate plasticizers in their coatings, including some antibiotics, antihistamines and laxatives. Patented herbal preparations and nutritional supplements may also contain phthalates (Schettler, 2006).

1.5.6.3 Ingestion and inhalation

Intravenous injection tubing and solutions, and skin absorption are potential pathways of exposure. Human exposure to phthalates can occur as a result of direct contact or use of a product containing phthalates, through the leaching of phthalates from one product into another, as may occur with food packaging or intravenous fluids, or by general contamination of the ambient environment

1.5.7 Applications

Owing to their properties, approximately 80% of all phthalates are widely used as plasticizers in the polymer industry to increase flexibility and workability (J. Wang et al., 2013).

Diisononyl phthalate is commonly used in garden hoses, pool liners, flooring tiles, tarps, and toys. Additionally, butyl benzyl phthalate, as a component of materials, is extensively used in vinyl flooring, synthetic leather, inks, and adhesives (Gomez-Hens & Aguilar-Caballos, 2003).

1.5.7.1 Phthalates as polyvinyl chloride additives

Poly(vinyl chloride) is the second of the polyethylene among the highest sales plastic kinds materials, which are widely utilized in a wide range of industries containing, packaging, electronics, architecture, children's toys and transportation (Yousif et al., 2015). PVC contains ester compound type of plasticizer has been added and in particular the phthalate ester has been widely used as the superior plasticizer. Depending on the amount of plasticizer added, PVC can either rigid or extremely flexible. Phthalates are used as plasticizers for polyvinyl chloride resins, adhesives, and cellulose film coating.

1.5.7.2 Cosmetics and personal care products

Phthalates of lower molecular weight, such as dimethyl phthalate, diethyl phthalate, and di-n-butyl phthalate, are widely used in cosmetics and personal care products; dimethyl phthalate and diethyl phthalate allow perfume fragrances to evaporate more slowly, making the scent linger longer, and a small amount of di-n-butyl phthalate can make nail polish chip-resistant. Di-n-butyl phthalate is also used in cellulose esters, printing inks, latex adhesives, and insect repellents (Alnaimat et al., 2020).

1.5.7.3 Solvent and phlegmatizers

Phthalate esters are widely used as solvents for highly reactive organic peroxides. Thousands of tones are consumed annually for this purpose. The great advantage offered by these esters is that they are phlegmatizers, i.e. they minimize the explosive tendencies of a family of chemical compounds that otherwise are potentially dangerous to handle (Herbert et al., 1999). Phthalates have also been used for producing plastic explosives such as Semtex.

CHAPTER TWO

EXPERIMENTAL

2.1 Apparatus

FT-IR imaging was done using JASCO 6600 FTIR (Fourier transform infrared).

The UV-Vis spectrometer was used to detect and phthalates in water samples.

Whatman's filter paper (Grade-1-1001-110, 1001-125, 11 micron) was used to filter off big particles in the water sample matrix.

Beakers (Simax Czech Republic, 50-250 mL) was used to store the samples obtained from the sample area and during experimentation process.

Separating funnel (sadana brothers, 250 mL) was used for solvent extraction

Rotary evaporator was used to remove the organic solvent after solvent extraction

Analytical weighing balance (brand saffron 0.001 g accuracy) was used to weigh the chemicals

2.2 Materials

Chemicals that were used include dichloromethane that acted as the organic layer during solvent extraction of phthalates, anhydrous sodium sulphate that was used to remove any remaining water in the organic layer, sodium chloride that was used to saturate the sample so as to destabilize the formation of emulsions from the solvent.

Acetone was also used to rinse the glassware so as to avoid contamination and the glassware were dried in an oven.

2.2.1 Anhydrous sodium sulphate

It was prepared by mixing 96% sulphuric acid (56 mL), sodium hydroxide (80 g) and distilled water.

80 g of sodium hydroxide is dissolved in a little distilled water, then 56 mL of 96% sulphuric acid was added

2.3 Procedures

2.3.1 Sample collection

Water samples were collected from National Water and Sewage Cooperation, Tororo that was tap water, underground water from the pond, borehole water from university borehole and packed water that was purchased from the shop and stream water.

Precautions were taken to avoid contamination during sample collection and processing. No plastic equipment was used and all glassware were precleaned.

2.3.2 Sample preparation

The samples were separately put in glass beakers, filtered off to remove the big particles and then put in the separating funnel.

An organic solvent (dichloromethane) was then added to the water sample in the separating funnel. (200mL of each water sample for phthalate esters analysis were extracted by liquid-liquid extraction in a separating funnel using 4x10mL dichloromethane)

Sodium chloride (4.0 g) was added to each sample and the mixtures were shaken vigorously to extract phthalates into the organic solvent phase.

The phases were allowed to separate for 7 hours, the organic phase containing phthalates was at the bottom.

The organic phase was drained into a clean container, leaving the water phase behind

The extraction process was 4 times repeated for better recovery.

Anhydrous sodium sulfate was added to the organic phase to remove any remaining water.

The dried organic phase was transferred to a rotary evaporator to remove the solvent at 45^{o}C and speed of 150 RMP.

The recovered samples were taken for UV-Vis spectrometric analysis.

Other samples were taken for FTIR Analysis

2.3.3 Instrument setup

The FTIR instrument was calibrated by passing infra-red radiations through the sample, adsorbed and the spectrum was obtained.

2.3.4 Spectrum acquisition

The infrared spectrum of the sample containing phthalates was obtained by placing it in the sample compartment of the FTIR instrument and running the analysis. This generated a spectrum showing the absorption of infrared light by the sample at different wavelengths.

Table 2: Functional groups and wave numbers

Origin(Functional group)	Group frequency, wavenumber (cm^{-1})
C-C	1350–1000
C-H in aromatics (out of the plane)	900-670
C-H	2820–2810
C-O-C	1140–1070
C=O	1680-1750
-OH	3400-3200

2.3.5 Compare with reference spectra

Compare the spectrum obtained from the sample with reference spectra of phthalates. This comparison can help in identifying the presence of phthalates in the sample based on characteristic absorption bands.

Peak identification: Look for specific absorption bands in the spectrum that are indicative of the presence of phthalates. Phthalates typically exhibit characteristic peaks in the FTIR spectrum due to the functional groups present in their chemical structure

CHAPTER THREE

RESULTS AND DISCUSSION

3.1 RESULTS

Table 3: sample results

Sample	Absorbance	Transmittance (%)	Concentration (mg/ml)
pond	0.297	50.4	0.1015
Stream	0.291	55.7	0.0994
Borehole	0.092	88.5	0.0314
Packed	0.103	70.3	0.0352
Tap	0.120	68.1	0.0410

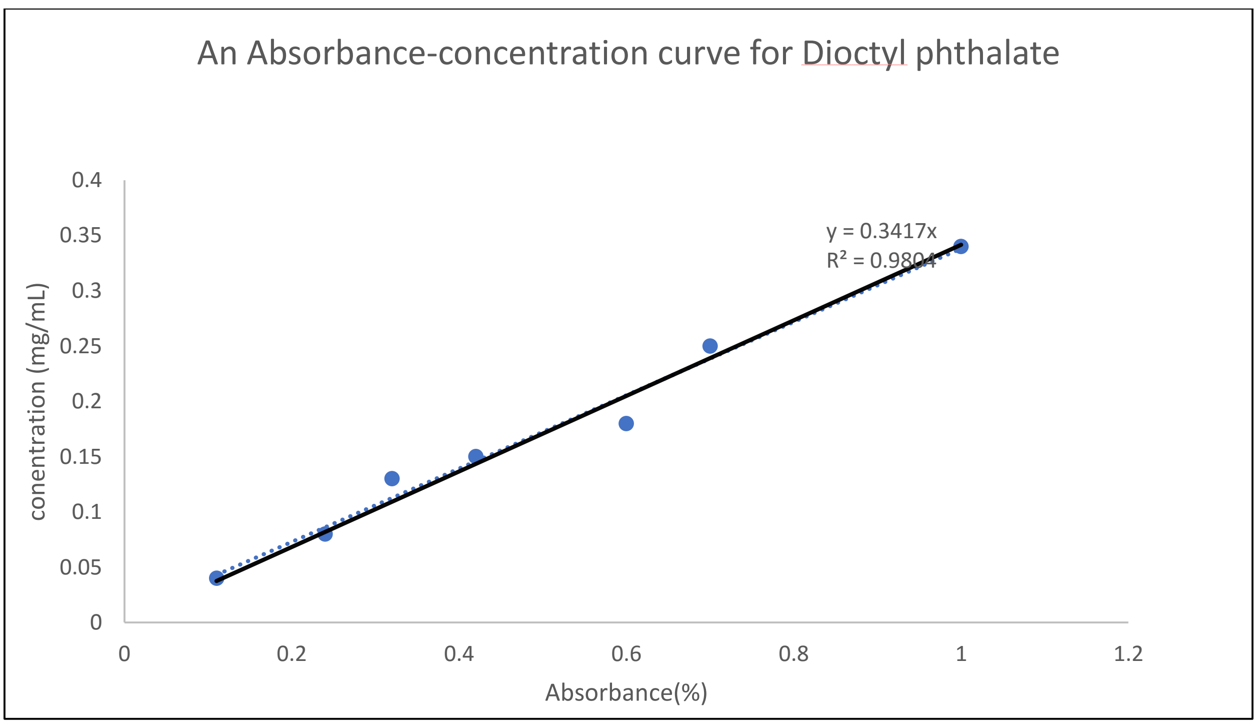


Figure 1: Stream water sample

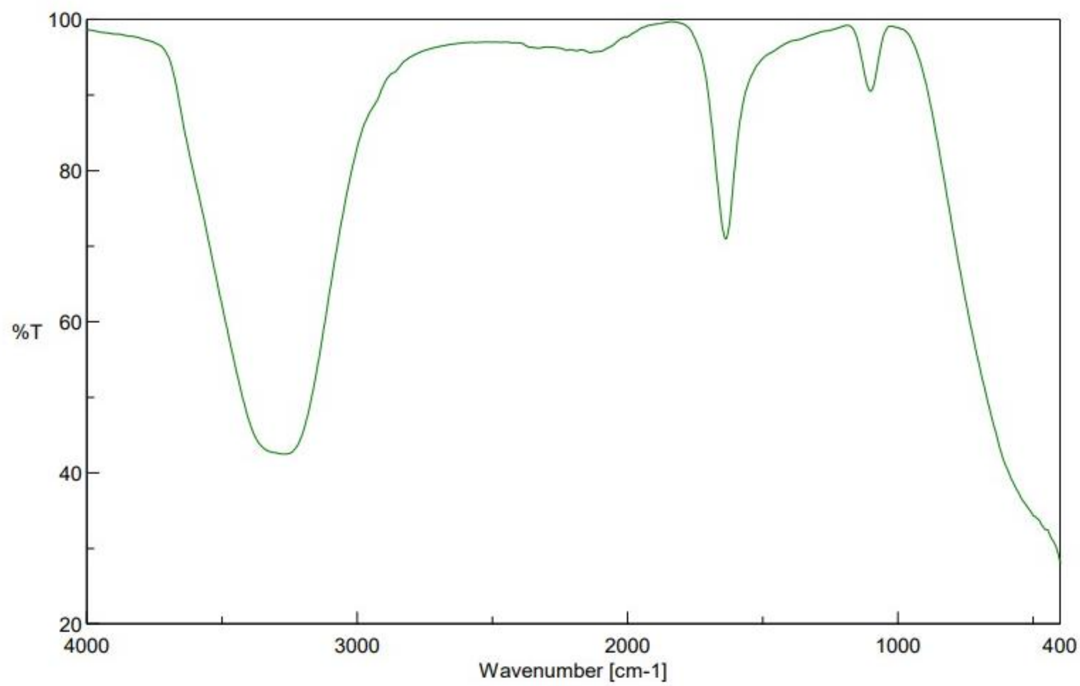


Figure 2: Packed water sample

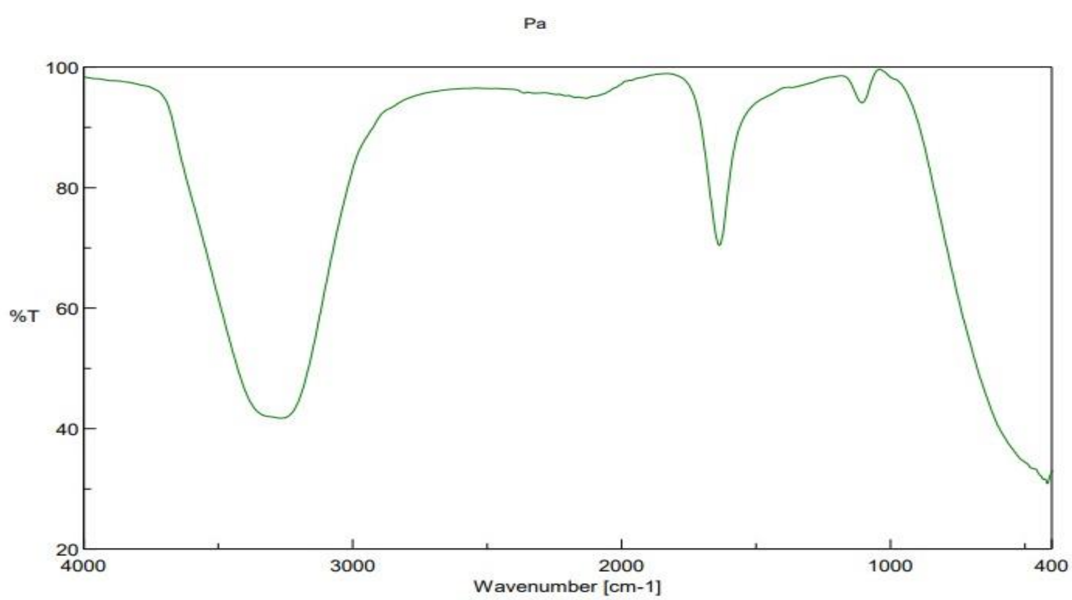


Figure 3: Pond water sample

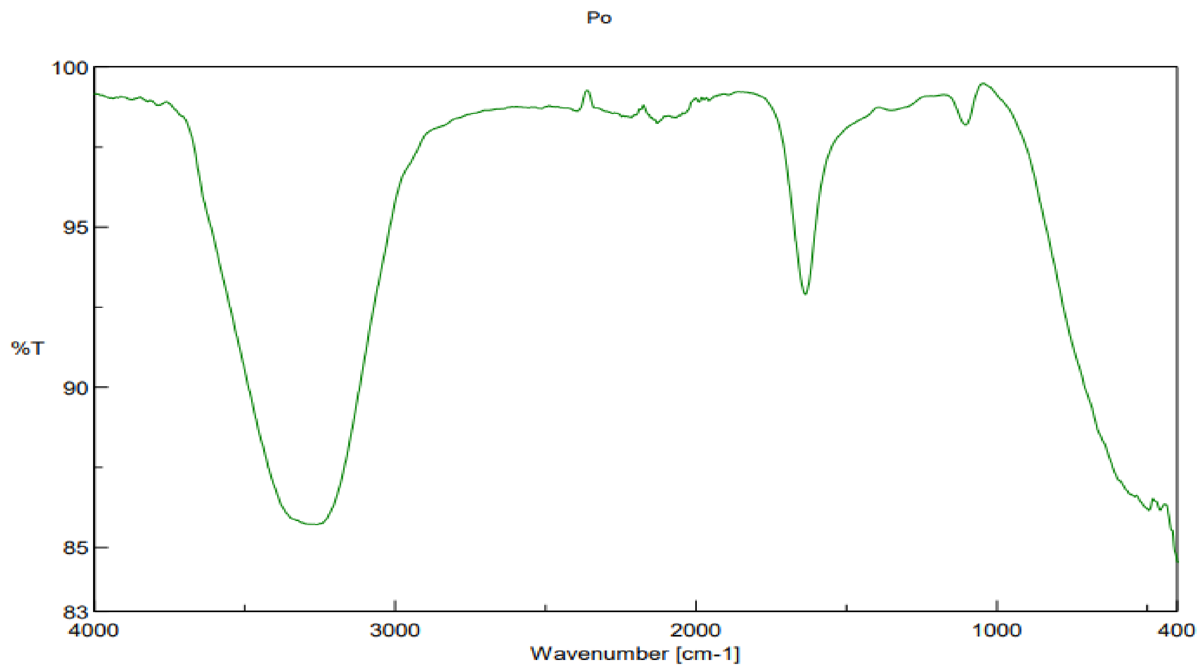


Figure 4: Borehole water sample

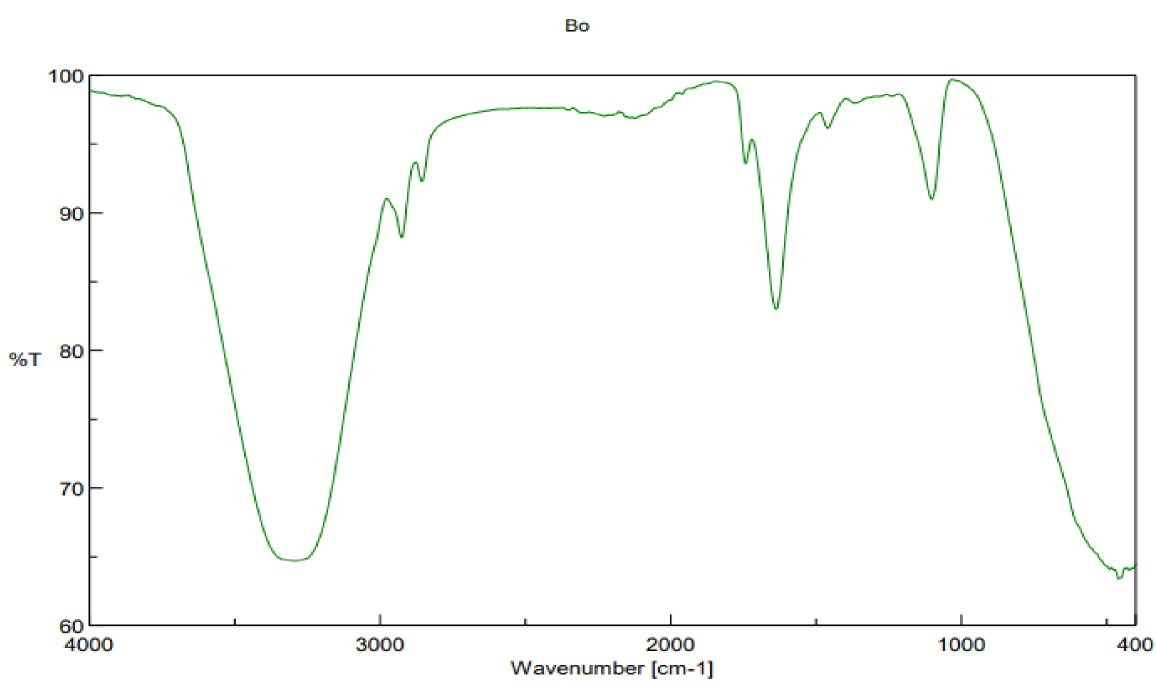
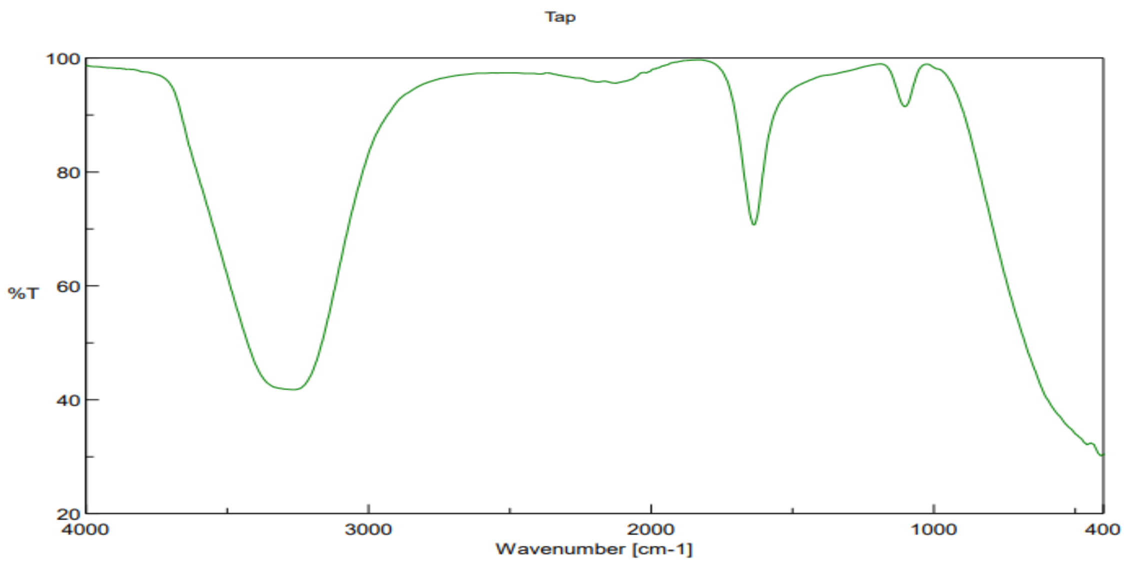


Figure 5: Tap water sample



3.2 DISCUSSION

According to the results obtained, the order of concentrations of phthalates in the water samples is; Pond water > stream water > tap water > packed water > borehole water.

This is because pond water is stagnant therefore phthalates concentration is high, followed by stream water due to flow from nearby trading centre water.

According to the results from FTIR water samples contained phthalates because the peaks obtained correlate with the ranges as follows;

Table 4: Water samples and wave numbers of the functional groups

Origin (Functional group)	Stream water sample	Packed water sample	Pond water sample	Borehole water sample	Tap water sample
-OH	3300	3300	3300	3300	3300
C=O	1700	1600	1600	1600	1600
C-O-C	1100	1100	1100	1100	1100
C-H	-	-	-	2800	-

The predominant peaks of phthalates were obtained using FTIR spectroscopy indicating that phthalates were present because the peaks shown in table 4 above shows the wave numbers corresponding to the functional groups that are present in phthalates.

The recommended levels of phthalates in drinking water are <0.006ppm

CHAPTER FOUR

CONCLUSIONS AND RECOMMENDATION

4.1 Conclusions

In conclusion, the concentrations of phthalates were as follows: pond water 0.1015 mg/mL, stream water 0.0994 mg/mL, borehole water 0.0314 mg/mL, packed water 0.0352 mg/mL, and tap water 0.0410 mg/mL. Borehole water sample had the lowest concentration of phthalates because it comes from underground and since phthalates are got from plastics, borehole water rarely gets in contact with phthalates.

4.2 Recommendations

Since borehole water had the lowest concentration of phthalates of 0.0314 mg/mL, I therefore recommend that borehole water should be used for domestic use. Implement regular monitoring of water sources to detect any phthalate contamination. Educate the community on safe water practices and the importance of using clean water. Encourage proper waste disposal to prevent phthalate contamination.

Advocate for strict regulations on industrial and agricultural practices that contribute to phthalate pollution.

Collaborate with local authorities to enforce water quality standards.

I also recommend that one should use HPLC (High performance liquid chromatography) so as to quantify the levels of phthalates in the water samples since FTIR spectroscopy and UV-Vis spectroscopy could not quantify the levels of phthalates.

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