Natural Resources for Human Health
eISSN: 2583-1194

Original Research

Received 02 May 2026
Revised 14 June 2026
Accepted 27 June 2026

Natural Resources for Human Health 2026, Vol. 6 (12s): 639–646

KEYWORDS:
Chemical migration; Plastic water bottles; Drinking water; FTIR spectroscopy; Chemical leaching; Storage temperature.

Chemical leaching Evaluation from Drinking Water bottles by using AT-FTIR Spectroscopic Method

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ABSTRACT: The study investigated the migration of chemical substances from plastic water bottles into stored drinking water under different storage conditions. Four commercially available plastic bottles were filled with distilled water and stored at room temperature and elevated room temperature. The sample were analysed using FTIR spectroscopy to detect chemical changes. FTIR spectra revealed additional absorption bands in bottled-water samples, particularly at 1630-1650 cm^{-1}, 1630–1650 cm^{-1}, 1460–1420 cm^{-1}, and 1295 cm^{-1}, indicating the presence of carbonyl, carbonate, amide, and aliphatic compounds. Increased peak intensity was observed in heat exposed sample, suggesting greater chemical migration at higher temperatures. The finding demonstrates the storage conditions, especially temperature, influence the release of plastic derived compounds into drinking water and may affect water quality. FTIR analysis proved effective in detecting these changes and assessing potential contamination.

1: INTRODUCTION

Plastic packing materials play an important role in the storage and distribution of drinking water due to their affordability, durability, and ease of handling. Among the various plastic used for beverages containers, polyethylene terephthalate (PET) is the most widely utilized because of its transparency, strength, and resistance to breakage. Despite these advantages, increasing attention has been directed towards the possibility of chemical migration from plastic containers into stored water.[1]

Chemicals migration occurs when substance present within plastic materials is transferred into the liquid it contains. This phenomenon can be influenced by environmental condition such as elevated temperature, prolonged storage, ultraviolet radiation, and repeated usage of the containers. During manufacturing, plastic is formulated with several auxiliary substances including catalysts, stabilizers, antioxidants, and processing additives. Under unfavourable condition, small quantities of these compounds may be released into the stored water.[2]

2: METHODOLOGY

The methodology of the study was designed to systematically investigate the leaching of chemicals substance from water bottles.[3]

2.1 Sample selection

Four different types of commercially available plastic water bottles were chosen for study to represent commonly used products.[4]

Table 1. Bottle Composition and Manufacturing Details of the Selected Sample

Samples	Name	Bottle composition	Manufacturer
Sample1	AQUA FINA	lightweight PET (polyethylene terephthalate) plastic	PepsiCo India Holdings Private Limited
Sample2	KINLEY	PET (Polyethylene terephthalate)	Hindustan Coca-Cola Beverages Private Limited (HCCB) and authorised Coca-Cola bottling partners.
Sample3	BISLERI	PET (Polyethylene terephthalate)	Bisleri International Pvt. Ltd. / plant-specific bottler india
Sample4	TUPPER WARE	Food-grade plastic	Tupperware India Pvt. Ltd.India.

2.2 Cleaning and preparation

All bottles were washed thoroughly and rinsed multiple times with distilled water to remove any contamination. Each bottle was filled with a fixed volume of distilled water (500 mL) and labelled properly.[5]

2.3 Experimental setup

The prepared sample were divided into two group:

Group1: stored in room temperature (≈25°C)

Group2: placed in a hot air oven and exposed to heat for 4 hours at 35-40 ^{0} C

Maintained different storage durations:

- 24 hours
- 72 hours
- 7 days

The setup was used to study the influence of temperature on chemical leaching.[6]

2.4 Sample collection

After the exposed period, water samples from both groups were collected carefully in clean containers to avoid contamination.[7]

2.5 Filtration process

The collected sample were filtered to remove any suspended particle before analysis.[8]

2.6 Analytical technique

The filtered sample were analysis using Fourier transform infrared (FTIR) spectroscopy. This technique helps in identically different functional groups present in the samples based on their characteristic absorption peaks. The spectra were recorded over the range of **4000–400 cm^{-1}**. Three replicates are used to ensure accuracy and reliability.[9]

2.7 Spectral preprocessing

The recorded FTIR spectra were inspected and compared with the corresponding distilled-water reference spectrum. The characteristic absorption bands observed in the test samples were identified based on their wavenumber positions.

2.8 Data recording and analysis

The obtained FTIR spectra were recorded and compared with standard distilled water. Differences in peaks position and intensities were used to identify the presence of leaching compounds.[10]

2.9 Statistical analysis

All experiments were conducted in triplicate. The experimental results were expressed as **mean ± standard deviation (SD)**. The results were compared among different bottle types and exposure conditions to observe variations in the measured parameters.

3. RESULT & DISSCUSION

The result was analysis to determine the effects of temperature and storage conditions on the leaching process. The presence of specific functional groups indicates contamination.

3.1 FTIR Report for Water Sample

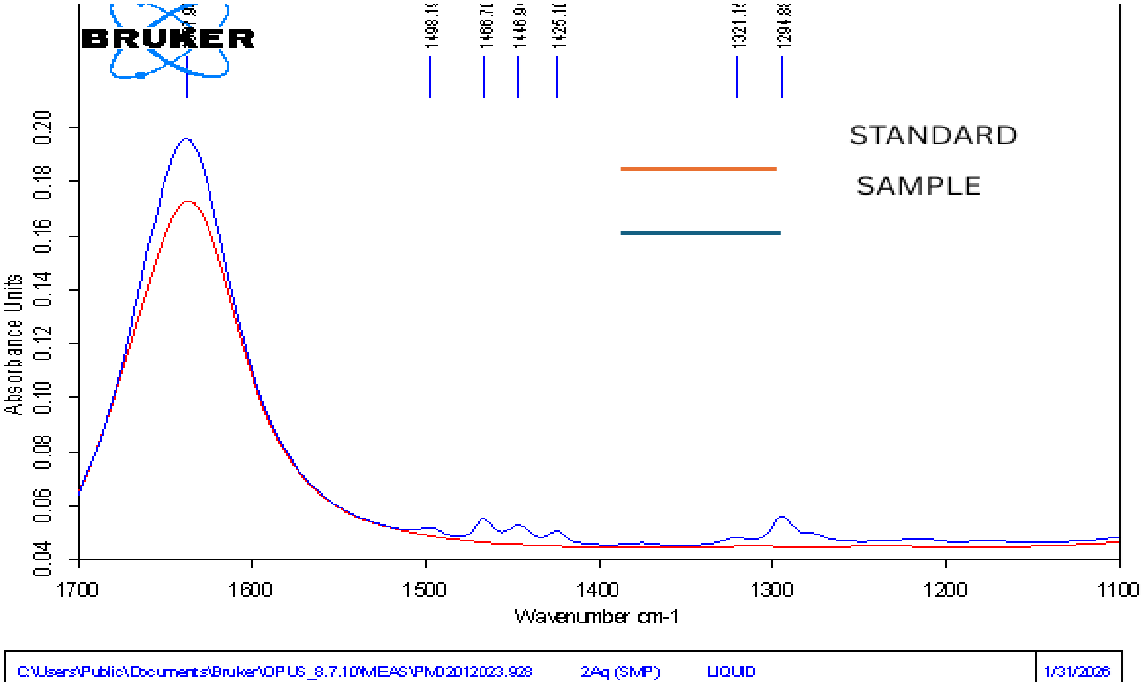

Figure 1. Sample 1

Table 2. FTIR Peak Assignments of Sample 1

Wave number	Bending / structing compound
1498.19	Carbonate (CO_3^{2-})
1466.7	Carbonate (CO_3^{2-})
1466.94	Carbonate (CO_3^{2-})
1321.15	Amide (R-CO-NR'$_2$)
1294.88	Amide (R-CO-NR'$_2$)

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eISSN: 2583-1194

The FTIR spectrum of the sample (blue line) shows a profile comparable to the standard (red line), indicating the presence of similar functional group. A broad absorption band is observed around 1638 cm-1, where the sample exhibits higher absorbance than the standard. Additional peaks are detected at approximately 1461 cm-1,1449 cm-1,1425 cm-1,1327 cm-1 and 1295 cm-1 in the sample spectrum. These peaks are more pronounced than those observed in the standard spectrum, suggesting the presence of additional chemical constituents. The overall similarity between the two spectra indicates that the basic composition remains unchanged, while the increase in absorbance and appearance of extra peaks confirm slight chemicals modification in the sample.

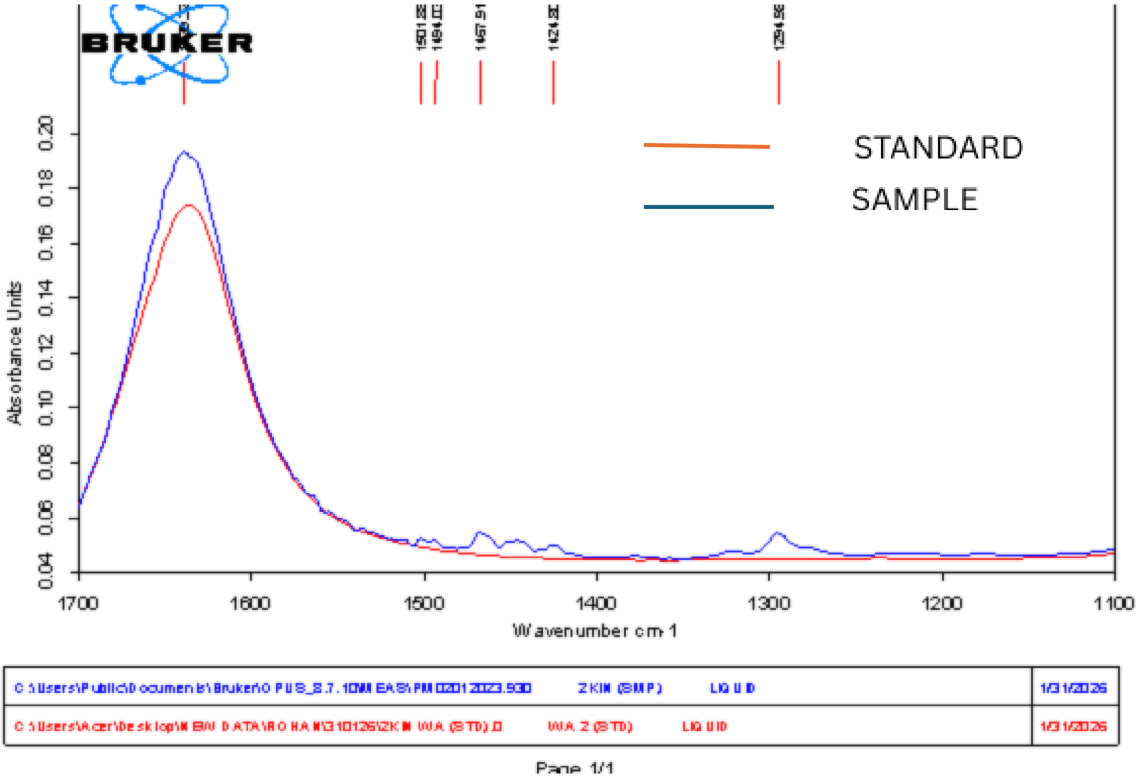

Figure 2. Sample 2

Table 3. FTIR Peak Assignments of Sample 2

Wave number	Bending / structing compound
1639.32	Amide carbonyl (C=O)
1501.88	Amide C–N
1494.03	Amide C–N
1467.91	Carbonate (CO_3^{2-})
1424.80	Aliphatic C–H (alkane)

The FTIR spectrum of the sample (blue line) shows a similar overall pattern to standard (red line) indicates the presence of related functional group. However, the sample exhibits slightly higher absorbance intensity, particularly around 1630-1650 cm-1, suggesting the presence of additional chemical constituents compared to the standard. minor absorption peaks are also observed in the regions of 1490-1420 cm-1 and around 1290 cm-1, which are less prominent in the standard spectrum. This variation indicates that the sample contains extra organic compounds or impurities that are not present in the standard. The

eISSN: 2583-1194

observation spectral differences confirm that chemicals substances have been introduced into the sample while the overall molecular structure remains comparable to the standard.

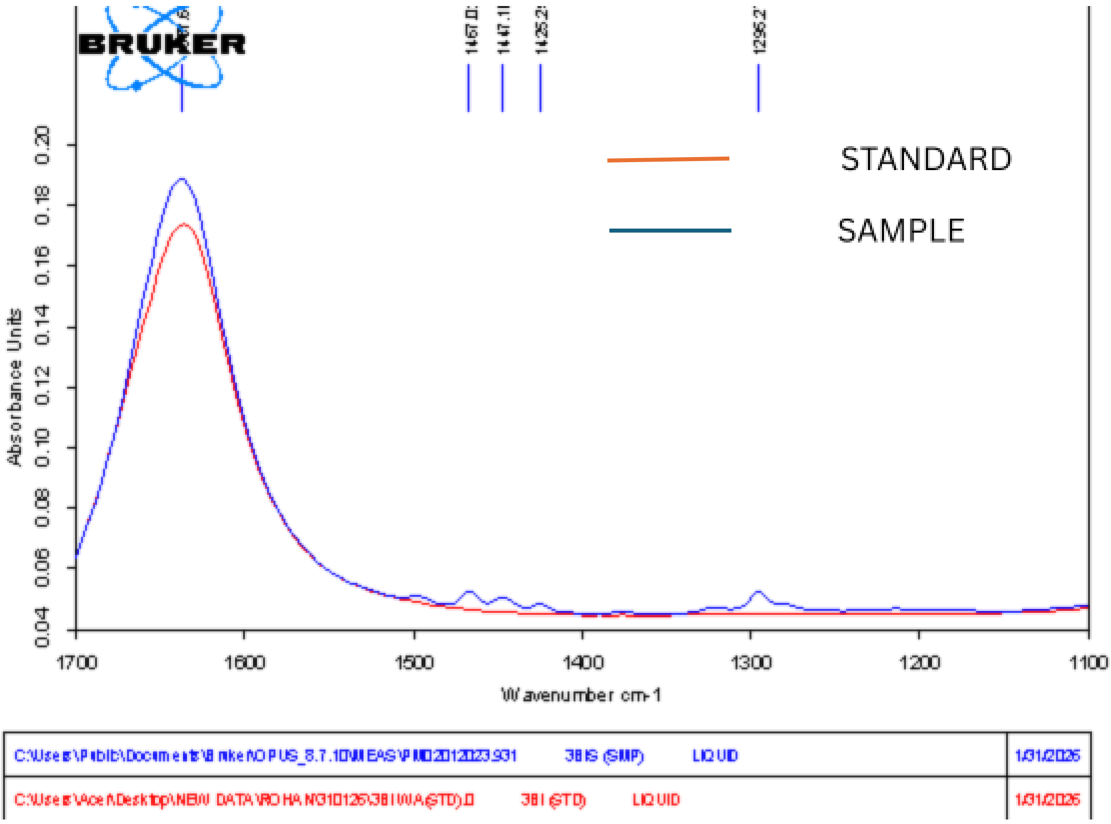

Figure 3. Sample 3

Table 4. FTIR Peak Assignments of Sample 3

Wave number	Bending / structing compound
1687.60	Quinone carbonyl (C=O)
1467.02	Carbonate group (CO_3^{2-})
14447.10	Aliphatic C–H
1425.25	Aliphatic C–H
1295.27	Amide (C–N / N–H) group

The FTIR spectrum of the sample (blue line) shows a profile like that of the standard (red line), indicating the presence of comparable functional group. A broad and intense absorption band is observed near 1630-1650 cm-1 in both spectra; however, the sample exhibits slightly higher absorbance intensity. Additional weak peaks are visible in the sample around 1467 cm-1,1425 cm-1 and 1295 cm-1, suggesting the presence of minor chemical constituents not evident in the standard. The slight increase in peak intensity and the appearance of these extra bands indicates that the sample contains additional compounds while maintaining a similar overall chemical structure to the standard.

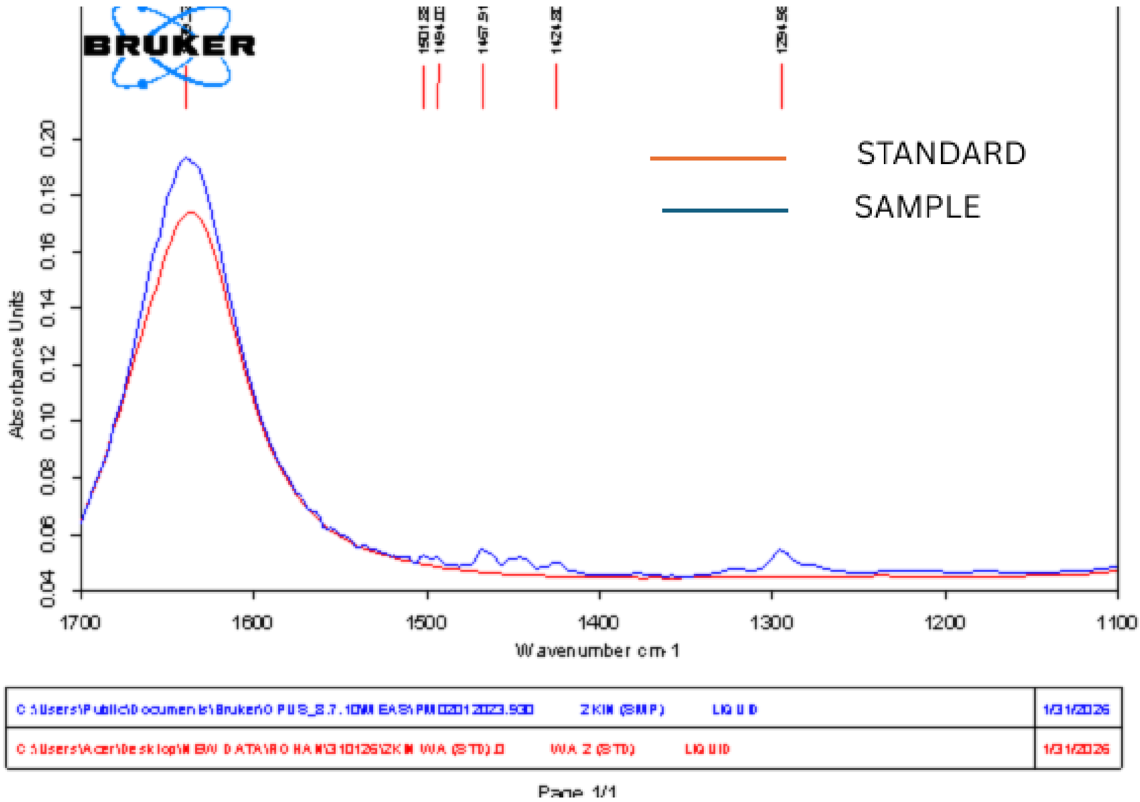

Figure 4. Sample 4

Table 5. FTIR Peak Assignments of Sample 4

Wave number	Bending / structing compound
1687.64	Quinone carbonyl (C=O)
1466.92	Carbonate (CO_3^{2-})
1446.76	Carbonate (CO_3^{2-})
1425.16	Carbonate (CO_3^{2-})
1294.80	Amide (C–N / N–H) group

The FTIR spectrum of the sample (blue line) exhibits a pattern closely related to that of the standard (red line), indicating the presence of similar chemical functionalities. A prominent absorption band is observed near 1634 cm-1 in both spectra, with the sample showing a slightly greater absorbance intensity. Additional weak absorption peaks are present in the sample at approximately 1467 cm-1, 1452 cm-1, 1426 cm-1, and 1295 cm-1 which are either absent or less intense in the standard spectrum. These spectral variations suggest the presence of supplementary chemical components in the sample. The overall similarity of the spectra indicates that the primarily composition remains comparable to the standard, while the additional peaks reflect minor compositional changes.

3.2: DISCUSSION

Fourier Transform Infrared spectroscopy was employed to evaluate the chemical composition of water samples stored in different plastic bottles. The spectral profile of distilled water was used as a reference and compared with spectra obtained from the experimental samples. Variations between the control and test spectra indicated the presence of additional chemical species in the bottled-water samples. The FTIR spectra of the experimental samples displayed several absorption bands that were not observed in the control sample. These bands corresponded to functional groups related to carbonyl, carbonate, amide, and aliphatic compounds. The occurrence of these groups suggests that molecular fragments originating from the plastic packaging material were transferred into the stored water.

Carbonyl-associated absorptions observed in certain samples may be linked to oxidative degradation products generated during storage. Carbonate-related peaks indicate the presence of inorganic constituents, while amide-associated bands suggest nitrogen-containing compounds. The identification of aliphatic functional groups further supports the presence of organic residues derived from polymeric materials or additives.

Differences in spectral intensity among the samples indicate that the composition of the bottle material may influence the extent of chemical migration. Some bottles exhibited a greater number of characteristic absorption bands, suggesting variability in polymer formulation and manufacturing processes.

4: CONCLUSION

The present investigation examined the migration of chemical substances from plastic water bottles into stored drinking water. Four commercially available bottle samples were evaluated under controlled storage conditions, including ambient temperature and heat exposure. FTIR spectroscopy was utilized to identify functional groups associated with compounds released from plastic materials.

Comparison of the FTIR spectra revealed the presence of additional absorption bands in the bottled-water samples when compared with distilled water. These bands corresponded to carbonyl, carbonate, amide, and aliphatic functional groups, indicating the introduction of both organic and inorganic compounds into the water.

The experimental observations demonstrated that storage temperature influences the extent of chemical migration. Samples exposed to elevated temperature exhibited stronger spectral responses, suggesting enhanced release of chemical constituents from the plastic matrix.

ACKNOWLEDGEMENTS

The authors sincerely acknowledgement Vinayaka Missions College of Pharmacy, Salem, Tamil Nadu, India, for providing the necessary facilities, technical support and guidance to conduct this study.

AUTHOR CONTRIBUTIONS

M.KUMAR: project administration, validation

K. AATHISH, A. AJEETH KUMAR: Conceptualization, sample collection

E. ABINAYA, A. ANITHA: Methodology, Data collection

R. AKILAN, T. ARUN: FT IR analysis, Data interpretation

K. ARAVINDH: Visualization, manuscript review and editing

DATA AVAILABILITY STATEMENT:

Data supporting the findings of this study are available from the corresponding author upon reasonable request.

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