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Synthesis, Characterization, Antimicrobial activity, and Applications of Trimethylphenylammonium Bromide

DEEPTHI B.V.[1]*, ISAC SOBANA RAJ. C[2] and SEEMA. A[3]

[1]*Research Scholar (21113112032008), Department of Chemistry & Research, Manonmaniam Sundaranar University Tirunelveli, Tamilnadu-627012, India.
[2]Associate Professor, Department of Chemistry & Research, Nesamony Memorial Christian College, Marthandam, Tamilnadu–629165, India.
[3]Assistant Professor, Department of Chemistry, Mar Ephraem College of Engineering and Technology, Elavuvilai, Tamilnadu-629172, India.
*Corresponding author E-mail: deepthibv1997@gmail.com

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ABSTRACT

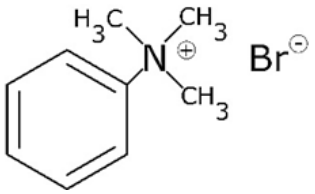
A quaternary ammonium compound destroys mold, bacteria, viruses, and fungi. Trimethylphenylammonium bromide, a novel quaternary ammonium compound, was synthesized in this study, and its absorbance wavelength and functional groups were determined through spectral characterization studies using FT-IR and UV-Visible spectroscopy. Additionally, the acidity and basicity of each synthesized concentration solution were determined by measuring pH fluctuations. Additionally, this article offers comprehensive action against two species of fungi, *Aspergillus flavus* and *Candida albicans*, as well as five distinct bacteria. Furthermore, a unique protein solubility test has been conducted. This article also discusses a few uses for Trimethylphenylammonium bromide solution. The effectiveness of Trimethylphenylammonium bromide in reacting against antimicrobial infections is highlighted in this article.

Keywords: Trimethylphenylammonium bromide, FT-IR, UV, Antibacterial, Antifungal.

INTRODUCTION

Organic compounds with four functional groups covalently bonded to a central nitrogen atom ($R4N^+$) are known as quaternary ammonium compounds (QACs). At least one long-chain alkyl group is present in these functional groups (R), with the remaining groups being either methyl or benzyl. Frequently shortened to quats, QACs are a class of organic molecules important in chemistry, biology, and industry, among other domains. These substances have a "quaternary" structure because a positively charged nitrogen atom (cation) is covalently bound to four alkyl or aryl groups. QACs are well known for their special qualities and wide range of uses. Among other things, they are frequently employed as catalysts, disinfectants, and surfactants. QACs' chemical makeup and characteristics make them indispensable in various sectors, including healthcare and agriculture, and they are still being actively researched and developed for several cutting-edge uses[1-9].

QAC is used in a variety of ways as a disinfectant. Trimethylphenylammonium bromide, an incipient QAC, was produced in this study using substances such as trimethyl amine and bromobenzene. Trimethylphenylammonium bromide has the chemical formula $C_9H_{14}BrN$, and the following is its molecular structure.



In this research, Trimethylphenylammonium bromide was synthesized in this study at varying concentrations, and spectral characterizations such as UV-Visible and FT-IR spectroscopy were used to determine the absorbance wavelength and functional groups contained in the synthesized quaternary ammonium compound. Additionally, this study also identified the pH fluctuations of Trimethylphenylammonium bromide. For antibacterial investigations, pathogenic microorganisms including *Pseudomonas aeruginosa, Klebsiella pneumoniae, Staphylococcus aureus, Escherichia coli*, and *Staphylococcus epidermidis* were assessed. The samples' antifungal activity was evaluated using *Aspergillus flavus* and *Candida albicans*.

Moreover, in some applications also done by this research, the prepared sanitizer was blended with copper nanoparticles and tested against five different bacterial and fungal pathogens. The bacterial and fungal activity is determined and soap is produced using a 0.4M Trimethylphenylammonium Bromide solution. All these results demonstrated the superior antibacterial and antifungal qualities of Trimethylphenylammonium bromide. Therefore, it can be applied to both bacterial and fungal dermatological conditions. The antibacterial and antifungal properties of synthesized QACs in molarity ranges are highlighted in this paper. The objective of this work is to create low molarity concentrations of QACs that can be used to make disinfectants that fight off diseases caused by bacteria and fungi.

MATERIALS AND METHODS

Materials

All the chemicals used were of analytical grade. The chemicals Trimethyl amine, Bromobenzene, Isopropyl alcohol, and glycerine were purchased from High Purity Laboratory Chemicals, Pvt. Ltd Maharashtra (India) and double distilled water is used throughout the experiment.

Synthesis of Trimethylphenylammonium bromide

Solutions of trimethyl amine and bromobenzene were used to prepare Trimethylphenylammonium bromide. These two solutions were combined in a 250 mL beaker and then heated to 78°C for 45 min at room temperature using a magnetic stirrer. After forty-five minutes, the solution was ready for further synthesis. Likewise, concentrations ranging from 0.1M to 0.8M were prepared using the same procedure[11].

Characterization studies

UV and FT-IR spectroscopy characterized the prepared quaternary ammonium compound using a Li-2900 UV-Visible spectrometer and an Invenio FT-IR spectrometer.

Biological Assay

The pathogenic bacteria and fungi such as *Staphylococcus aureus, Staphylococcus epidermidis, Klebsiella pneumonia, Escherichia coli*, *Pseudomonas aeruginosa, Aspergillus flavus, Candida albicans* were used for antibacterial and antifungal assay using disc diffusion method.

RESULTS AND DISCUSSIONS

UV–Visible spectroscopy

The UV-Visible spectrum of a prepared Trimethylphenylammonium bromide sample ranging from 0.1M to 0.8M concentration was tested at each concentration. UV-Visible absorption spectra were noticed to confirm the various absorbance wavelengths for synthesized quaternary ammonium compounds solution[22]. The spectra of synthesized quaternary ammonium compounds in different concentration ranges show absorption peaks between 300nm to 400nm. The different molarity concentrations and their absorbance wavelength of synthesized QACs results are shown in Table 1 and Figure 1.

Table 1: Absorbance wavelength of Synthesized quaternary ammonium compound

Concentration	Absorbance wavelength (nm)
0.1M	317
0.2M	340
0.3M	341
0.4M	342
0.5M	353
0.6M	365
0.7M	366
0.8M	366

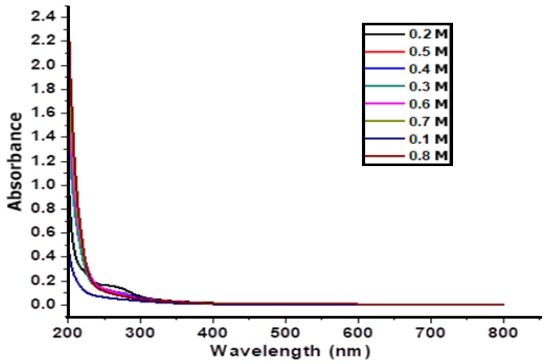


Fig. 1. UV-Visible spectrum of Trimethylphenylammonium bromide at 0.1M to 0.8M concentrations

FT-IR Spectra

The infrared studies identify the functional groups present in the prepared samples. Further, the formation of Trimethylphenylammonium bromide was confirmed by FT-IR analysis. The peaks are detected in the range from 3480 cm^{-1} to 517 cm^{-1}. The broad peak present in the range of 1042 cm^{-1} is due to the alkyl amine group[12-16]. The illustration of structural features using FT-IR is shown in Table 2. The explication of absorption peaks and their functional groups are given as a Figure 2.

Table 2: Absorption peaks and Functional groups are detected by TMPAB using FT-IR spectrometer

Absorption peak cm^{-1}	Functional groups
3480	O-H stretching
2311	C=C conjugated
2088	Adsorbed hydrogen atom
1643	C=O amide I band
1548	C-N amide II band
1510	C-N stretching of alkyl halides
1455	Stretching -C=O inorganic carbonate
1394	CH and CH_2 aliphatic bending group
1338	C-O
1316	C-O
1042	Alkyl amine
991	-CH=CH_2
649	Halogen compound (Cholorocompound C-Cl)
575	Halogen compound (Iodocompound C-I)
517	C-N stretching vibration of straight chain

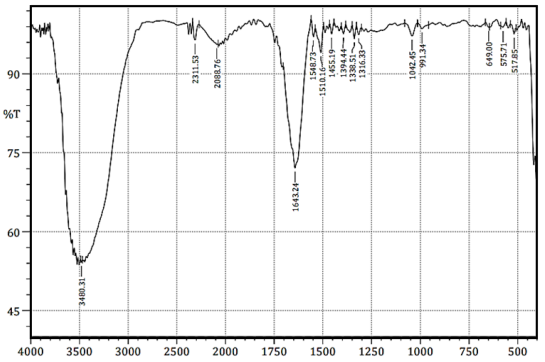


Fig. 2. FT-IR spectrum of prepared TMPAB at 0.8M concentration solution

pH Variation

Trimethylphenylammonium bromide solution is prepared from 0.1M to 0.8M concentrations. At each eight different concentrations were synthesized separately. Separate pH variations were taken for the synthesized quaternary ammonium compound. The pH value of the synthesized compound is below the range of 7. The pH variations of synthesized quaternary ammonium compound solutions are shown in Table 3.

Table 3: pH variations for prepared quaternary ammonium compound

Concentrations	pH variations
0.1M	3.6
0.2M	3.4
0.3M	5.2
0.4M	4.7
0.5M	6.3
0.6M	6.5
0.7M	6.2
0.8M	6.4

Antibacterial Assay

While testing the antibacterial activity of the prepared quaternary ammonium compound named Trimethylphenylammonium bromide, it was found that five types of bacteria namely *Staphylococcus aureus, Staphylococcus epidermidis, Klebsiella pneumonia, Escherichia coli, Pseudomonas aeruginosa* at a concentration ranging from 0.1M to 0.8M. After studying the antibacterial assay, the prepared TMPAB solution acted more against bacteria namely Klebsiella pneumonia[17,18,19,20]. The antibacterial activity results are shown in Table 4 and Figure 3.

Antifungal assay

The QAC was found to be more efficacious against the fungus *Candida albicans* than against *Aspergillus flavus*. The fungi namely *Candida albicans* almost reach the standard value. The standard

value is decreasing the concentration level of fungal activity is increasing at the time the standard value is increasing the concentration level of fungal activity is decreasing. This solution is found to be one of the best anti-microbial agents[17,18,19,20]. The antifungal activity results are shown in Table 5 and Figure 4.

Table 4: The Antibacterial activity results for TMPAB

Bacteria	Zone of inhibition(mm) Concentration level								
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	Standard
Staphylococcus aureus	7	7	8	9	10	12	15	18	20
Staphylococcus epidermidis	7	7	9	11	12	13	14	14	20
Klebsiella pneumonia	9	10	10	11	15	16	20	22	25
Escherichia coli	8	9	9	10	11	13	15	17	25
Pseudomonas aeruginosa	6	7	8	9	10	11	11	12	25

Table 5: The Antifungal activity results for TMPAB

Fungal	Zone of inhibition(mm) Concentration level								
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	standard
Aspergillus flavus	8	8	9	11	12	12	13	15	25
Candida albicans	12	13	14	15	16	16	17	18	25

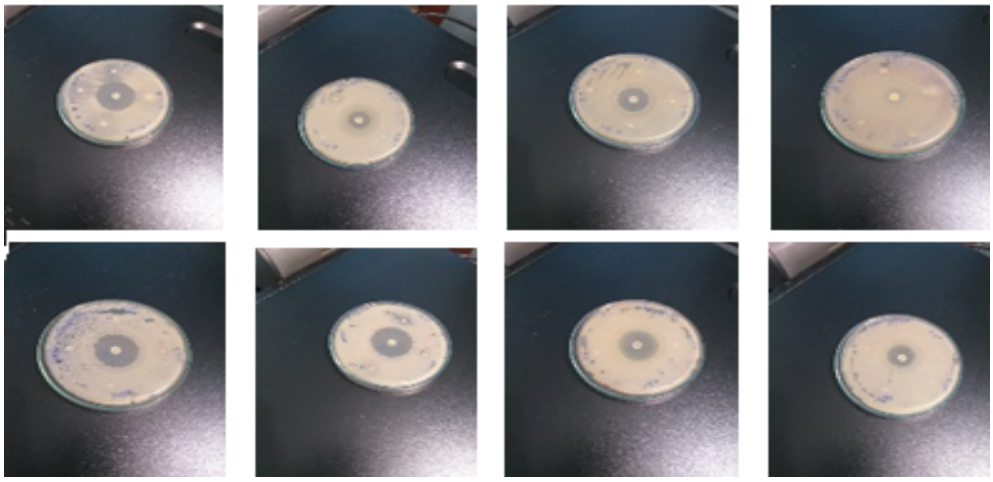


Fig. 3. Antibacterial activity results for TMPAB a

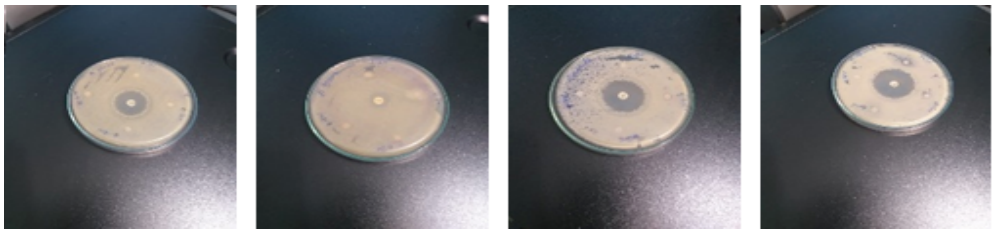


Fig. 4. Antifungal activity results for TMPAB

Protein Solubility Test

5 mL of Trimethylphenylammonium bromide solutions mixed with 3 g of membrane protein powder collected from soybean seeds. The eight concentrations were taken discretely in 8 beakers and kept in a magnetic stirrer for 45 minutes. After keeping it in a magnetic stirrer, the protein powder was dissolved in 20% in a 0.1M concentration, 30% to 95% in a 0.2M to 0.7M concentration, and 100% in a 0.8M concentration, making it a clear solution. Generally, a virus would be circumvented by proteins. In this research, a membrane protein was mixed with a Trimethylphenylammonium bromide solution. This membrane is one of the types of proteins that are circumvented by some viruses. In this, synthesized TMPAB at 0.8M concentration, 100% of the proteins

are dissolved. This shows an increase in quaternary ammonium compounds a particular concentration level that dissolves protein completely. Hence, it concludes that this Trimethylphenylammonium bromide solution may allow us to take measures against some viruses.

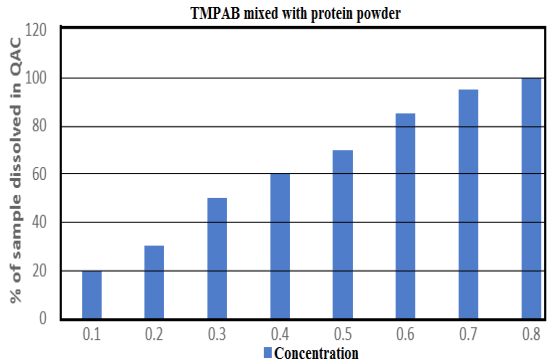


Fig. 5. Solubility of TMPAB mixed with protein powder

Utilization studies

In this study, the Trimethylphenylammonium bromide solutions are used to prepare hand sanitizer and soap. Then this sanitizer and soap are studied against five types of *Gram-positive* and *Gram-negative* bacteria, and two types of fungi.

Sanitizer

With a quaternary ammonium compound denominated Trimethylphenylammonium bromide, sanitizer was yielding a concentration of 0.1M to 0.8M concentration. This sanitizer was tested against bacteria like *Staphylococcus aureus, Staphylococcus epidermidis, Klebsiella pneumonia, Escherichia coli, Pseudomonas aeruginosa* and fungi like *Aspergillus flavus* and *Candida albicans*. As a result, the sanitizer was efficacious against five variants of bacteria and two variants of fungi. Keeping our hands clean is one of the best ways to prevent the spread of viruses[21]. Since this sanitizer acts against bacteria and fungi, we can surmise that it would additionally have virally acted. The antibacterial and antifungal results are shown in the Table. 6, 7 and Figure 5,6.

Table 6: The Antibacterial activity results for sanitizer prepared from TMPAB

Bacteria	Zone of inhibition(mm) Concentration level								
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	Standard
Staphylococcus aureus	8	9	10	10	12	13	16	19	20
Staphylococcus epidermidis	7	8	10	12	13	13	15	17	20
Klebsiella pneumonia	12	14	16	17	19	20	21	23	25
Escherichia coli	10	11	12	14	15	16	17	19	25
Pseudomonas aeruginosa	10	11	12	13	14	15	16	18	25

Table 7: The Antifungal activity results for sanitizer prepared from TMPAB

Fungal	Zone of inhibition(mm) Concentration level								
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	standard
Aspergillus flavus	9	9	10	12	13	14	15	17	25
Candida albicans	13	13	14	14	15	15	16	19	25

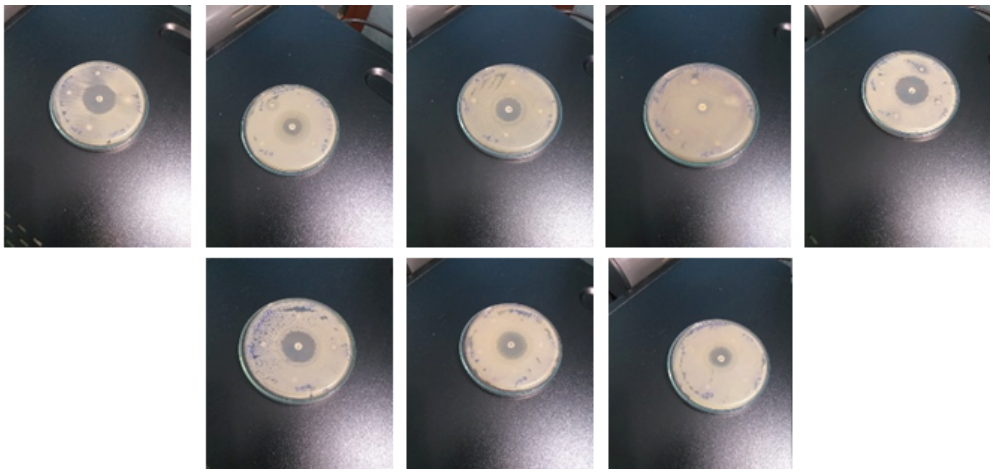


Fig. 6. Antibacterial activity results for sanitizer prepared from TMPAB

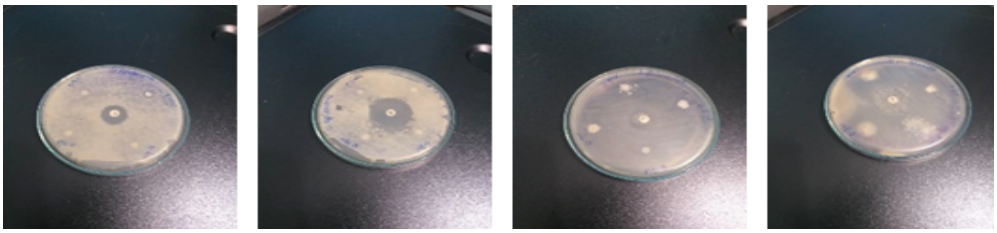


Fig. 7. Antifungal activity results for sanitizer prepared from TMPAB

Soap

In a 0.4M concentration with TMPAB solution, Soap was generated. That was tested against five types of bacteria and two types of fungi. In this research, successfully acted against *Pseudomonas aeruginosa* bacteria and *Candida albicans* fungi more than other bacteria and fungi[21]. Hence, this soap can be used against the dermal infection of some bacteria and fungi.

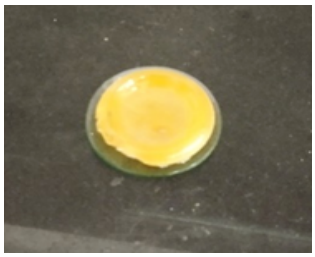


Fig. 8. Image of soap prepared by using TMPAB solution

Table 8: The Antibacterial activity results for soap prepared from TMPAB

Bacteria	Trimethylphenylammonium bromide for 0.4M	Standard
Staphylococcus aureus	14	35
Staphylococcus epidermidis	15	23
Klebsiella pneumonia	14	15
Escherichia coli	21	30
Pseudomonas aeruginosa	15	20

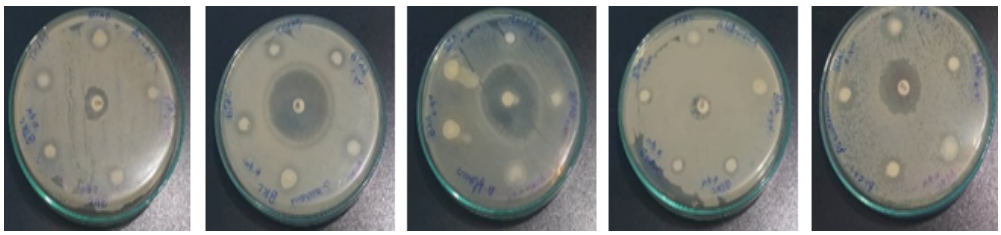


Fig. 9. Antibacterial activity results for soap prepared from TMPAB

Table 9: The Antifungal activity results for soap prepared from TMPAB

Fungi	Trimethylphenylammonium bromide for 0.4M	Standard
Aspergillus flavus	12	35
Candida albicans	20	35

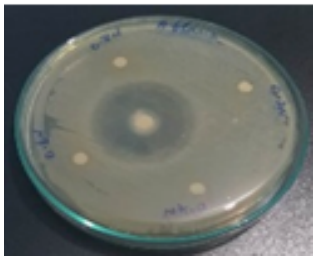


Fig. 10. Antifungal activity results for soap prepared from TMPAB

Copper Nanoparticles Blended with Sanitizer

The incipiently composed sanitizer was mixed with four different sizes of copper nanoparticles and its bacterial and fungal activities were assessed. On sizes[33,30,] 27, and 26, the sanitizer was taken in 0.8M, 0.6M, 0.4M and 0.2M respectively. These solutions are kept in a magnetic stirrer for 1 hour. Then it was proven that the copper nanoparticles and sanitizer have the faculty to act as disinfectant.

Table 10: The Antibacterial activity results for sanitizer mixed with copper nanoparticles

Bacteria	Concentrations 0.2M	0.4M	0.6M	0.8M	standard
Staphylococcus aureus	7	7	9	10	25
Staphylococcus epidermidis	7	7	9	10	14
Klebsiella pneumonia	9	9	9	9	25
Escherichia coli	7	7	7	14	20
Pseudomonas aeruginosa	7	9	11	13	30

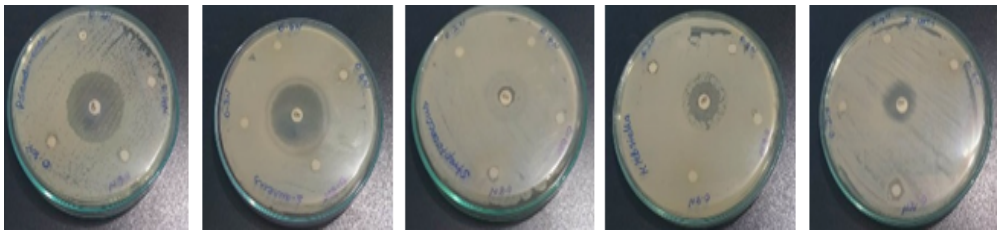


Fig. 11. The antibacterial activity results for sanitizer mixed with copper nanoparticles

Table 11: The Antifungal activity results for sanitizer mixed with copper nanoparticles

Fungi	Concentrations				
	0.2	0.4	0.6	0.8	std
Aspergillus flavus	7	7	9	9	35
Candida albicans	7	9	9	13	30

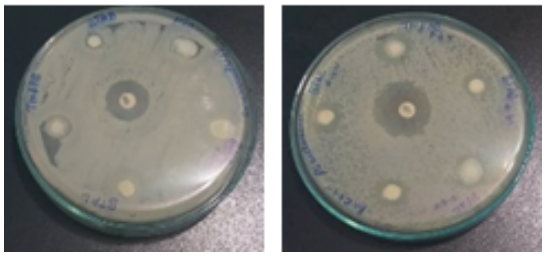


Fig. 12. The antifungal activity results for sanitizer mixed with copper nanoparticles

CONCLUSION

There are several uses for quaternary ammonium compounds as a disinfectant. because it prevents congenital illnesses during the COVID-19 virus. Quaternary ammonium compounds were used in soap, sanitizer, and other cleaning supplies. The absorbance wavelength found in the eight distinct molarity concentrations in this study is explained by UV-Visible spectroscopy, and the functional groups in these quaternary ammonium compounds were verified by FT-IR spectroscopy. Additionally, a QAC called Trimethylphenylammonium bromide was used to make soap and hand sanitizer, and additional research was conducted on the bacterial and fungal activities of the substance. Trimethylphenylammonium bromide thus effectively inhibited two kinds of fungus and five types of bacteria. Trimethylphenylammonium bromide combined with four different sizes of copper nanoparticles was used to make a hand sanitizer. Its antibacterial activity was evaluated to see what kinds of bacteria and fungi it could combat. Therefore, at very low concentrations, trimethylphenylammonium bromide functions as a disinfectant against a variety of infectious disorders.

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Conflict of Interest

The authors declare that they have no conflicts of interest.

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