ISSN 1996-3343

Asian Journal of Applied Sciences

http://knowledgiascientific.com

Knowledgia SCIENTIFIC
A Place to Publish Outstanding Research

OPEN ACCESS Asian Journal of Applied Sciences

ISSN 1996-3343
DOI: 10.3923/ajaps.2023.38.46

Research Article
Growth, Structural, Vibrational, Optical and Antibacterial Activity Studies on 4-Sulfamoylanilinium Chloride Semi-Organic Single Crystal

Chandran Muthuselvi, Meenakshi Sundaram Geetha and Nagarajan Mala

Department of Physics, Devanga Arts College, Aruppukottai, Tamil Nadu 626101, India

Abstract

Background and Objective: The organic-inorganic structure materials have been extensively analyzed due to their potential applications in material science. Sulfanilamide exhibits large pharmacological activities and is used to treat livestock diseases. This study explores the research findings and the work behaviour of sulfanilamide derivative crystal with hydrochloric acid. **Materials and Methods:** Using the slow evaporation technique, the semi-organic crystal of 4-sulfamoylanilinium chloride was grown at room temperature. The structural studies of the grown crystal were performed by using the single crystal XRD and powder XRD. The functional groups present in the crystal were confirmed from the IR and Raman vibrational spectroscopic study. In addition to these studies, optical, scanning electron microscopy with energy dispersive X-ray spectroscopy and antibacterial analysis was performed on the grown crystal. **Results:** Single crystal X-ray diffraction analysis revealed that the grown crystal was in an orthorhombic system. The appearance of sharp and strong peaks in powder XRD patterns confirmed the good crystallinity of the grown sample. The presence of -$[NH_3]^+$, -NH_2, -SO_2, C-N, C-S, C-H, C-C and C=C functional groups confirmed the formation of 4-sulfamoylanilinium chloride crystal in the salt form. From the analysis of the absorption spectrum, it was evident that the grown crystal had an optical band gap of 3.9 eV. The structural morphology consists of the rock-like morphology with distributed stones. The atomic and weight percentage of the grown crystal was confirmed from the EDX study. The 4-sulfamoylanilinium chloride crystal has high antibacterial activity against the *Escherichia coli*, *Klebsiella*, *Bacillus* and *Vibrio* bacterial strains at different concentrations. **Conclusion:** The semi-organic single crystals 4-sulfamoylanilinium chloride were successfully grown from the slow evaporation method and the orthorhombic crystal structure, pure crystallinity, vibrational modes of all functional groups, optical transparency, surface morphology with elemental composition and antibacterial effect against microorganisms were tested and confirmed in this present work.

Key words: 4-sulfamoylanilinium chloride salt, molecular structure, infrared spectroscopy, Raman spectroscopy, optical study, scanning electron microscopy with energy dispersive X-ray spectroscopy, antibacterial

Citation: Muthuselvi, C., M.S. Geetha and N. Mala, 2023. Growth, structural, vibrational, optical and antibacterial activity studies on 4-sulfamoylanilinium chloride semi-organic single crystal. Asian J. Appl. Sci., 16: 38-46.

Corresponding Author: Chandran Muthuselvi, Department of Physics, Devanga Arts College, Aruppukottai, Tamil Nadu 626101, India Tel: +919487672735

Competing Interest: The authors have declared that no competing interest exists.

Data Availability: All relevant data are within the paper and its supporting information files.

INTRODUCTION

The man-made synthetic medicinal compound of sulfanilamide also identified as sulphanilamide contains the sulfonamide and amino group in their structure[1]. The first developed sulfonamide was not used as an antimicrobial agent but it may be combined with other drugs to make them bactericidal[2]. Many classes of drugs which contain a sulfonamide structure are called sulfa drugs and they were used for the treatment of vaginal yeast infections mainly vulvovaginitis which was caused by *Candida albicans*[3]. The first sulfa drug, prontosil was used as an antibacterial agent to treat a variety of bacterial infections and sometimes it may be prescribed to treat urinary infections[4]. But this drug won't work for cold and flu viral infections[5]. Some developed important sulfanilamide-derived drugs include sulfamethazine, sulfadiazine, sulfamethoxazole, sulfasalazine, sulfisoxazole, sulfamerazine, sulfadimethoxine and sulfafurazole[6]. These derivatives were also used in combination with anti-malarial and antibacterial drugs to treat various diseases of human beings and animals[7]. Also, they have anticancer, antiviral, antidiabetic, antimicrobial and anti-inflammatory biological activities in a wide range. So, these drugs act as good bacteriostatic but they do not kill them which only inhibit the growth and multiplication of bacteria[8]. There was a large number of published works related to sulfanilamide derivative crystals in the organic and inorganic acids hybrid[9-12]. Taking into account all of the mentioned above, here we report the growth of 4-sulfamoylanilinium chloride single crystal using the slow evaporation method at room temperature. The experimental studies were also developed together with this crystal growth such as single crystal XRD, powder XRD, FT-IR, FT-Raman, UV-Visible-NIR spectroscopy, SEM with EDX and antibacterial activity studies.

MATERIALS AND METHODS

Study area: The 4-SAC crystals were harvested at the Research Department of Physics, Devanga Arts College, Aruppukottai, Tamil Nadu, India in December, 2022 and data were collected from January to February, 2023.

Chemicals used: Sulfanilamide > 99% (Sigma-Aldrich), Hydrochloric acid, ethanol and distilled water were purchased from Modern Scientific Company, a laboratory equipment supplier in Madurai, Tamil Nadu.

Computational details: The colorful 3D chemical structure of 4-SAC crystal was obtained using the Chem3D desktop modeling program (version 16.0).

Methods: Crystals of 4-sulfamoylanilinium chloride (4-SAC) were obtained by mixing the aqueous ethanol solution of sulfanilamide and hydrochloric acid (2 drops) at room temperature. The solution was stirred well for 2 hrs and filtered in the Petri dish. After 15 day's duration, the highly transparent colorless crystals were obtained by the slow evaporation process. The grown crystal and the chemical structure of the 4-SAC crystal were shown in Fig. 1 and 2, respectively.

Experimental details: The single crystal X-ray diffraction analysis was performed using Bruker SMART APEX CCD diffractometer with Mo Kα radiation (λ = 0.71073 Å). The FT-IR (Bruker-Alpha-Platinum) and FT-Raman (BRUKER: RFS 27) spectral data were recorded in the wavenumber range 4000–400 cm^{-1} at the Sophisticated Analytical Instruments Facility (SAIF), IIT Madras. The above three instrument's manufacture was Bruker India Scientific Pvt. Ltd., Bengaluru, Karnataka, India. The PXRD data were collected from the

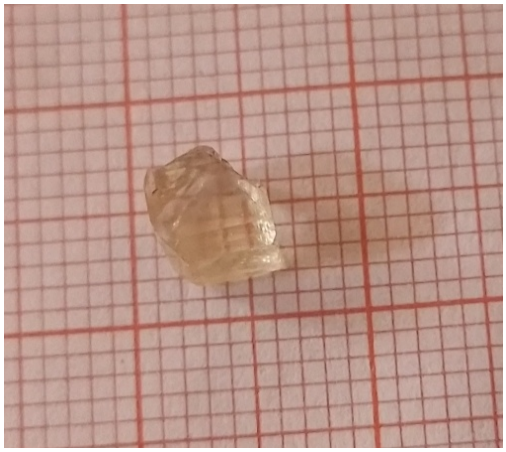


Fig. 1: Grown crystal of 4-SAC

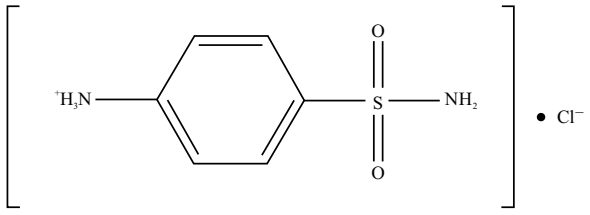


Fig. 2: Chemical structure for 4-SAC crystal

XPERT-PRO X-ray diffractometer (Malvern Panalytical Ltd., Malvern, United Kingdom) with Cu Kα radiation (1.54060 Å) at Alagappa University, Karaikudi. The SHIMADZU-UV 1601, manufactured by Shimadzu, Tokyo, Japan, a double beam spectrometer had been used to record UV-Vis-NIR spectrum in the wavelength range 190-1100 nm at Virudhunagar Hindu Nadars' Senthikumara Nadar College, Virudhunagar. The SEM with EDX data received from the CARLZEISS EVO18 (Carl Zeiss India Pvt. Ltd., Bangalore, Karnataka) scanning electron microscope at Kalasalingam University, International Research Centre, Krishnankoil, Tamil Nadu, India. The antibacterial activity study was performed by agar well diffusion method in Mueller Hinton Agar (MHA) plates with Dimethyl sulfoxide (DMSO) as a positive control at Sri Kaliswari College, Sivakasi, Tamil Nadu, India.

Statistical analysis: The Chem office suite 2016 version 16.0 software was used to produce scientific molecular 3D structures and properties of the compound. The graphical data was manipulated using the origin pro 8.6 software. The zone of inhibition was measured using a ruler by the naked eye without using any instrument. The diameter size was measured in millimeters.

RESULTS

Structural study: The 3D crystal structure of 4-SAC based on the crystallographic data obtained by single crystal XRD analysis was illustrated in Fig. 3. It has an orthorhombic structure with the space group of Pbnb and the lattice parameters were a = 7.4594 (5) (Å), b = 7.7269 (4) (Å), c = 31.6937(5) (Å), molecular weight = 208.66 g mol^{-1} and volume V = 1826.55 (10) $(Å)^3$. The obtained lattice parameters of 4-SAC were compared with the reported data of Zgolli *et al.*[9] (a = 7.4608 (2) (Å), b = 7.7278(2) (Å), c = 31.6940 (2) (Å) and V = 1827.35 (13) $(Å)^3$). The crystal structure of 4-SAC $[C_6H_9N_2O_2S^+Cl^-]$contains a sulfamoylanilinium cation with a protonated aniline group -$[NH_3]^+$ and a halide (chorine) anion. According to the study of Zgolli *et al.*[9] the 4-SAC crystal builds up a three-dimensional network through the N-H···Cl and N-H···O hydrogen bonds. Additionally, powder X-ray diffraction measurement was performed to verify the crystalline quality of 4-SAC crystal. The recorded powder X-ray diffraction patterns of pure sulfanilamide and 4-SAC crystals were shown in Fig. 4. Appearance of sharp and strong peaks confirms the good crystallinity of the grown sample. The 100% relative intensity peak appeared at 2θ = (25.9338°) which was compared with the pure sulfanilamide value of 2θ = 18.0608°. The shifted peak of the 4-SAC crystal confirms that the hydrogen atom from HCl was liberated and protonated with the aniline group of sulfanilamide -$[NH_3]^+$ which forms a sulfamoylanilinium cation. Also, the crystalline size of the 4-SAC crystal was calculated as 83 nm using the Debye-Scherrer formula which was compared with the pure sulfanilamide particle size of 54 nm. This powder X-ray diffraction study revealed that the addition of hydrochloric acid reacts with the sulfanilamide compound which increases the particle size of the 4-SAC crystal.

FT-IR and FT-Raman spectral study: The 4-SAC molecular structure has–$[NH_3]^+$, -NH_2, -SO_2, C-N, C-S, C-H, C-C, C=C and functional groups. The IR and Raman vibrational spectra of 4-SAC crystal were shown in Fig. 5a and b, respectively. The anti-symmetric vibrations of –$[NH_3]^+$ group were observed at 3258 and 3238 cm^{-1} in the FT-IR spectrum with a strong intensity band. Also, the symmetric vibration of the same mode was attributed at 3156 cm^{-1} and there is no counterpart in the FT-Raman spectrum for these modes. The deformation modes were assigned at 1524 cm^{-1} (scissoring), 1163 cm^{-1} (rocking), 934 cm^{-1} (wagging) and 544, 467 cm^{-1} (twisting) for -$[NH_3]^+$ group. The amide (-NH_2) symmetric stretching mode was observed at 3238 cm^{-1} in the IR spectrum and the mode corresponding to the antisymmetric stretching of the amide group was not identified in both spectra. The scissoring, rocking and wagging modes of the (-NH_2) group were assigned at 1630, 1423 and 660 cm^{-1} in the IR spectrum. The peaks in the region 1319 cm^{-1} (IR) and 1312 cm^{-1} (Raman) were caused by ν_{as} (-SO_2) vibration and also ν_s (-SO_2) vibration was identified at 1163 cm^{-1} (IR), 1156 cm^{-1} (Raman). The twisting and wagging vibrations of the -SO_2 group were observed in the lower wave number region. All the remaining functional group vibrations (C-N, C-S, C-H, C-C, C=C) were summarized in Table 1. All the above-mentioned characteristic vibrations were assigned according to the early reported related compound works[13,14-18].

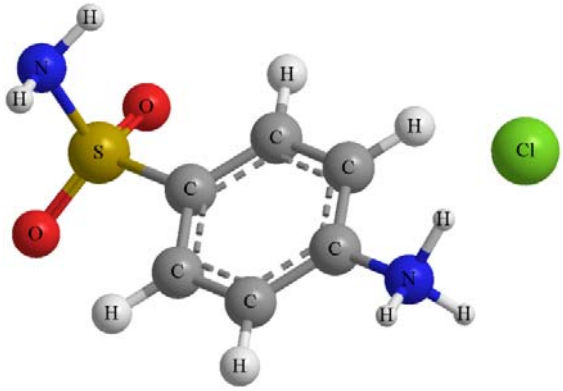


Fig. 3: Molecular structure of 4-SAC crystal

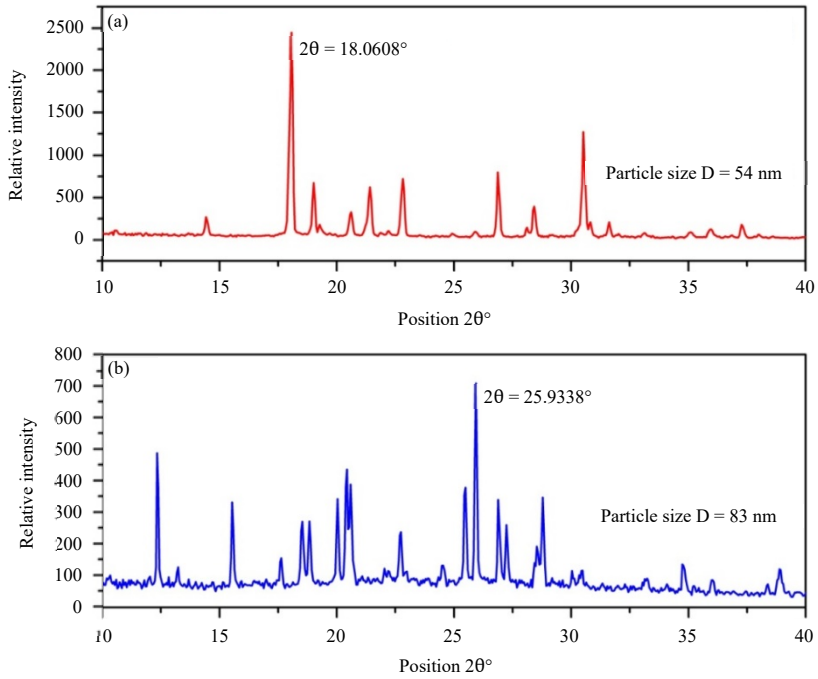


Fig. 4(a-b): Powder X-ray diffraction pattern for (a) 4-sulfanilamide and (b) 4-sulfamoylanilinium chloride crystals

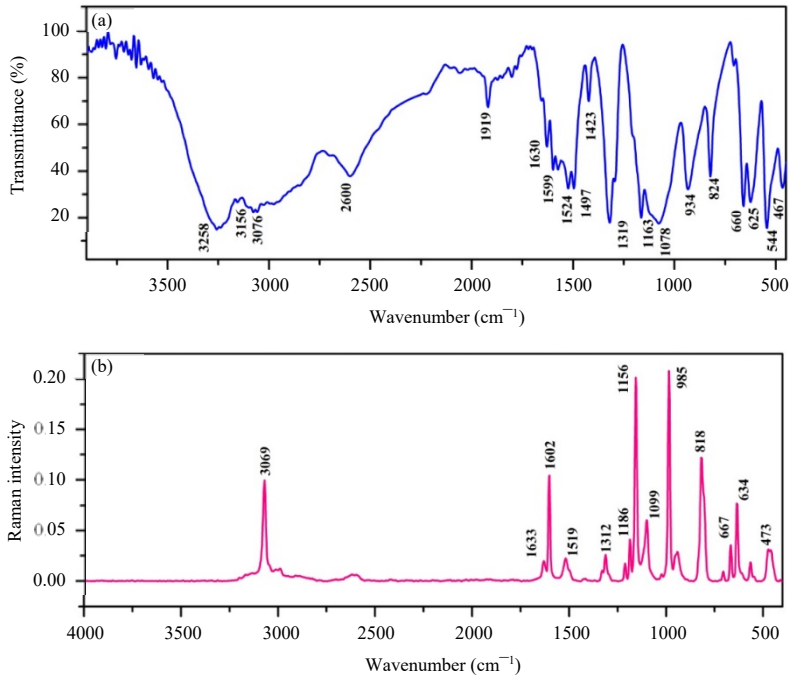


Fig. 5(a-b): (a) FT-IR spectrum and (b) FT-Raman spectrum of 4-SAC crystal

Optical study: The optical properties such as transmittance and optical bang gap were estimated using the UV-Visible spectroscopy in the wavelength range of 200-800 nm. The experimental UV-Visible absorbance spectrum (Fig. 6) showed an absorption maximum of 224 nm. Also, the crystal has a lower cut-off wavelength at 315 nm with high transparency in the entire visible region. The Tauc plot of $(\alpha h\nu)^2$ Vs photon energy ($h\nu$) was shown in Fig. 7. The optical band gap was

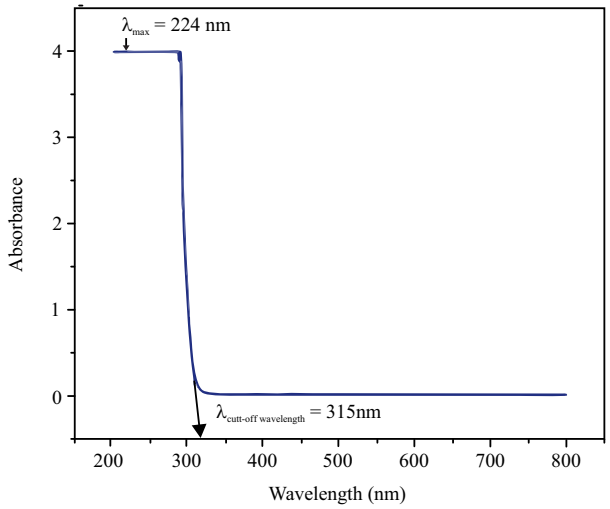


Fig. 6: Absorbance spectrum for 4-SAC crystal

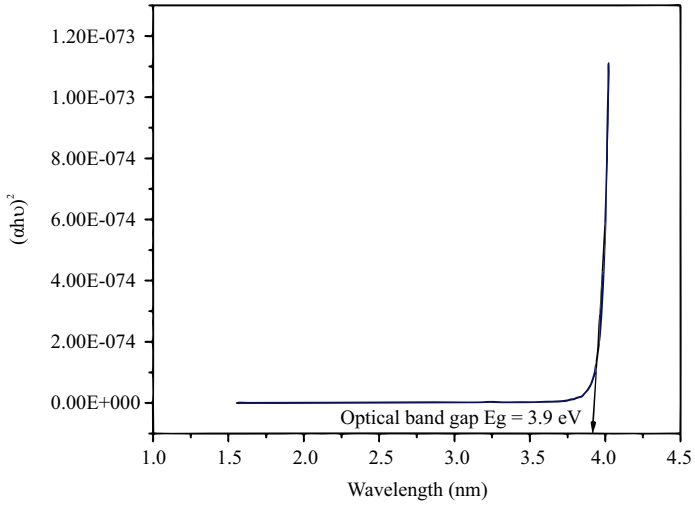


Fig. 7: Optical band gap for 4-SAC crystal

obtained from the intersection of extrapolation of the linear part of the curve with the photon energy axis. The optical band gap value was found to be 3.9 eV for 4-SAC crystal.

Morphology and elemental study: The SEM image of 4-SAC crystal has been shown with 5 kX and 20 kX magnifications at an acceleration voltage of 20 kV in Fig. 8a and b, respectively. The surface images of 4-SAC crystal show the rock-like morphology with distributed stones of approximately 2 µm (5 kX) and 1 µm (20 kX) in size. The EDX analysis of 4-SAC crystals was shown in Fig. 9 with their elemental composition. The composition was detected as for carbon = 43.7%, nitrogen = 15.6%, oxygen = 34.2% and sulfur = 6.6%. This study revealed that all the elements present in 4-SAC crystal without changing their atomic and weight percentage because only a hydrogen atom from the hydrochloric acid was added to the crystal structure of 4-SAC. In the EDX study, the hydrogen atom was not detected due to its low atomic number.

Antibacterial activity study: The antibacterial activity of 4-SAC crystal was determined by the agar well diffusion method against the *Escherichia coli*, *Klebsiella*, *Bacillus* and *Vibrio* bacterial strains. Figure 10 showed the results of the antibacterial activity with their zone of inhibition against the microorganisms tested for 15, 25 and 75 µL, concentrations. Also, the effective results have been presented in Table 2. The compound had shown high antibacterial activity against *Bacillus* (except 75 µL) and *Klebsiella* than *Vibrio* and *Escherichia coli* at all concentrations. This study showed that the 4-SAC crystal exhibits promising antibacterial potency.

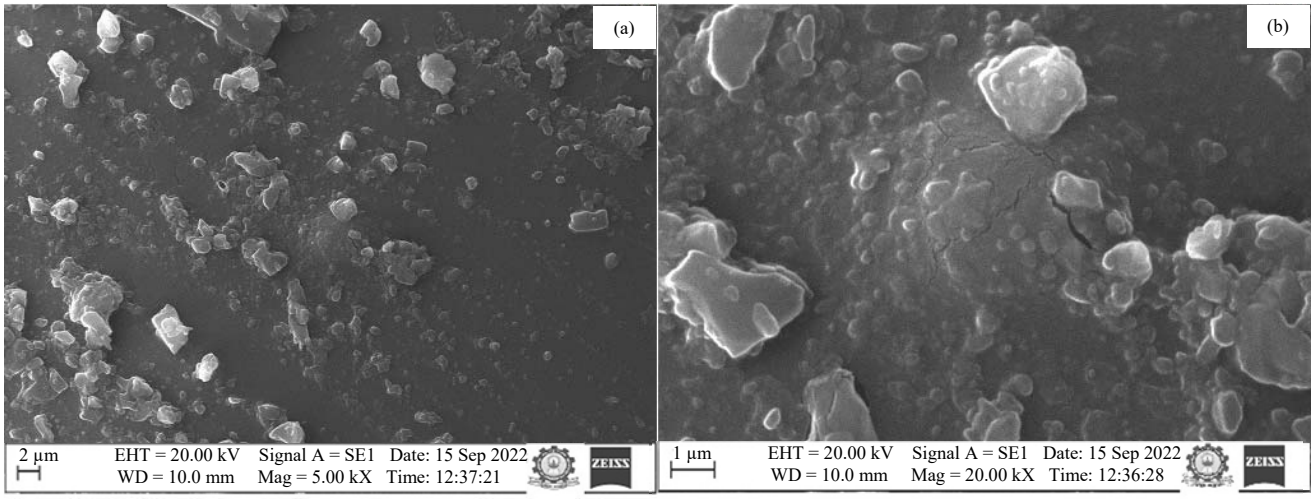


Fig. 8(a-b): SEM images of 4-SAC crystal with (a) 5 kX and (b) 20 kX magnifications

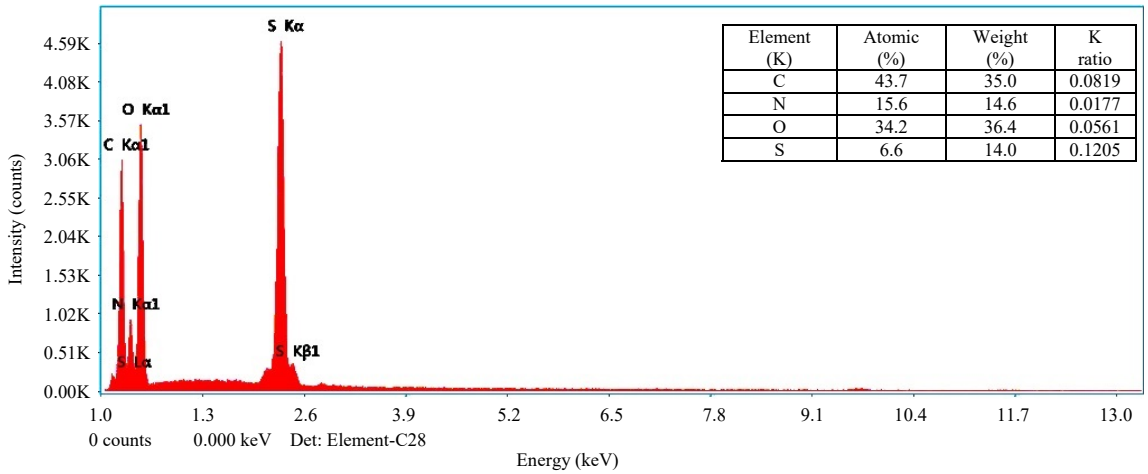
Table 1: Wavenumber assignments for 4-SAC crystal in FT-IR and FT-Raman spectra

FT-IR ($\bar{\upsilon}$/cm^{-1})	FT-Raman ($\bar{\upsilon}$/cm^{-1})	Assignment
3258 (s)	-	υ_{as}–$[NH_3]^+_{Aniline}$
3238 (s)	-	υ_s (–NH_2)$_{Amide}$
3156 (m)	-	υ_s–$[NH_3]^+_{Aniline}$
3098 (m)	-	υ (C-H)
3076 (m)	3069 (s)	υ (C-H)
3057(m)	-	υ (C-H)
3026 (w)	-	υ (C-H)
2899 (w)		
2851 (w)	-	υ (N–H···O)
1630 (m)	1633 (m)	ρ (-NH_2)$_{Amide}$
1599 (m)	1602 (s)	υ (C-C)
1574 (m)	-	υ (C-C)
1524 (m)	1519 (m)	ρ-$[NH_3]^+_{Aniline}$
1497 (m)	-	υ (C=C)
1423 (w)	-	υ (C=C), τ (–NH_2)$_{Amide}$
1319 (s)	1312 (m)	υ_{as} (-SO_2), υ (C–N), β(C-H)
-	1186 (m)	β(C–H)
1163 (s)	1156 (m)	τ-$[NH_3]^+_{Aniline}$, υ_s (-SO_2)
1078 (s)	1099 (m)	γ(C-H)
934 (m)	985 (s)	ω-$[NH_3]^+_{Aniline}$
824 (m)	818 (m)	Ring breathing mode
660 (m)	667 (m)	ω(-NH_2)$_{Amide}$
625 (m)	634 (m)	υ (C-S)
544 (s)	-	t-$[NH_3]^+_{Aniline}$
467 (m)	473 (m)	t-$[NH_3]^+_{Aniline}$

s: Strong, m: Medium, w: Weak, υ: Stretching, υ_s: Symmetric stretching, υ_{as}: Anti symmetric stretching, β: In-plane bending, γ: out-of-plane bending, ρ: Scissoring, τ: Rocking, ω: Wagging and t: Twisting

Table 2: Effect of the 4-SAC on the growth inhibition of different microorganisms tested

	Diameter inhibition (mm) with different concentrations (µg/mL)		
Microorganisms	15 (mm)	25 (mm)	75 (mm)
Escherichia coli	16	20	25
Klebsiella	30	27	34
Bacillus	16	36	-
Vibrio	30	18	25



Element (K)	Atomic (%)	Weight (%)	K ratio
C	43.7	35.0	0.0819
N	15.6	14.6	0.0177
O	34.2	36.4	0.0561
S	6.6	14.0	0.1205

Fig. 9: Elemental analysis for 4-SAC crystal

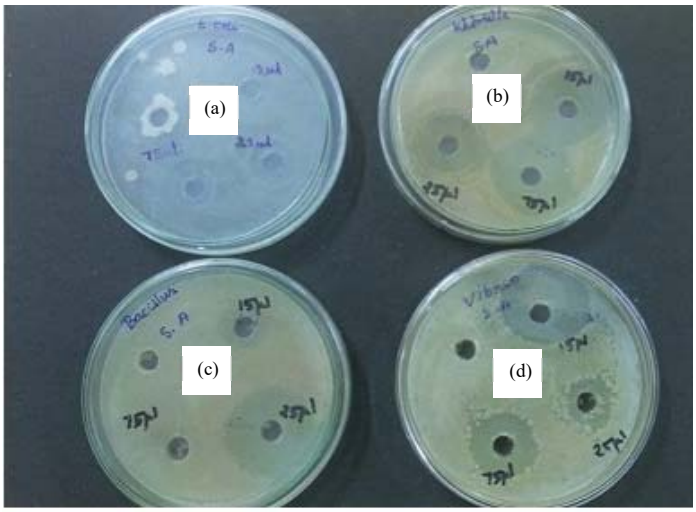


Fig. 10(a-d): Photographic view showing inhibition region of 4-SAC crystal against, (a) *Escherichia coli*, (b) *Klebsiella*, (c) *Bacillus* and (d) *Vibrio* microorganisms at 15, 25 and 75 µg/mL concentrations

DISCUSSION

This work demonstrates that the investigation of structural, vibrational frequency, optical band gap, morphology with elemental composition and antimicrobial activities of 4-SAC crystal. All these results were summarized and discussed.

In the present study, the 4-SAC crystal was grown using the slow evaporation method without changing the crystal system reported by Zgolli *et al.*[9] in the year 2010. But there was no report for the additional studies such as vibrational, optical, surface morphology with elemental composition and antibacterial activity studies. Ravikumar *et al.*[10] and Pandiarajan *et al.*[11] reported the crystal structure of sulfa drugs with inorganic acid hybrid (i.e., sulfate and nitrate). The crystal structure and spectroscopy study of 4-sulfamoylanilinium dihydrogen phosphate was reported by Muthuselvi *et al.*[12,13]. The functional groups wavenumber assignment of 4-sulfamoylanilinium cation was exactly matched with the already reported values by researchers[13-18]. Also, the optical and scanning electron microscopy studies showed that the 4-SAC crystal had high transparency in the entire visible region with the rock stone like shape. For the first time, the antibacterial study was done for the title compound which revealed that the compound had effective antibacterial activity against some tested bacteria than the parent sulfanilamide compound except *Escherichia coli*.

The antibiotic resistance compound of sulfa drug is commonly used to treat various bacterial infections. The synthetic antibacterial sulfa drug combination is used to treat infections including urinary tract infections, shigellosis, bronchitis and middle ear infections. But they produce blood problems if take a long time period. The crystal structure of sulfanilamide derivatives with inorganic acid was only reported in the salt form, but there is no report for these compounds in the organic acid hybrid. In the future, this study will discover new sulfanilamide compounds with the organic acid combination and enhance their antibacterial activity.

CONCLUSION

Using the slow evaporation technique, the semi-organic crystal of 4-sulfamoylanilinium chloride was grown at room temperature. The crystal system of orthorhombic with space group Pbnb was confirmed from the single crystal X-ray diffraction study. The crystal structure has a sulfamoylanilinium cation and a chloride anion which were interlinked through hydrogen bonding. Also, the powder XRD study confirmed the good crystalline nature of the crystal. The various functional groups present were confirmed by FT-IR and FT-Raman spectroscopy studies. In UV-visible study, the optical transparency was examined which shows that in the visible region, the crystal has 100% transparency. The optical band gap was found at 3.9 eV. The surface morphology and the presence of elemental composition were confirmed by SEM with the EDX study. The 4-SAC crystal shows good antibacterial activity against various standard bacterial strains (*Escherichia coli*, *Klebsiella*, *Bacillus* and *Vibrio*). This study will help the researcher to discover new sulfa drug compounds which could be of great importance in the pharmaceutical and medicinal fields.

SIGNIFICANCE STATEMENT

This study realizes the synthesis of an organic-inorganic hybrid that can play a widespread role in medicinal chemistry. This study will help the researcher to synthesize the novel sulfanilamide derivative drug compounds with different organic and inorganic acid combinations. These combination sulfa drugs may use to treat and prevent bacterial infections in humans and animals.

ACKNOWLEDGMENT

The authors sincerely acknowledge their gratitude to the Management and Principal of Devanga Arts College, Aruppukottai, Tamil Nadu, India for their consent and support during their research work.

REFERENCES

1. Ovung, A. and J. Bhattacharyya, 2021. Sulfonamide drugs: Structure, antibacterial property, toxicity, and biophysical interactions. Biophys. Rev., 13: 259-272.
2. Supuran, C.T., A. Casini and A. Scozzafava, 2003. Protease inhibitors of the sulfonamide type: Anticancer, antiinflammatory, and antiviral agents. Med. Res. Rev., 23: 535-558.
3. Fernández-Villa, D., M.R. Aguilar and L. Rojo, 2019. Folic acid antagonists: Antimicrobial and immunomodulating mechanisms and applications. Int. J. Mol. Sci., Vol. 20. 10.3390/ijms20204996.
4. Rama, A., L. Lucatello, C. Benetti, G. Galina and D. Bajraktari, 2017. Assessment of antibacterial drug residues in milk for consumption in Kosovo. J. Food Drug Anal., 25: 525-532.
5. Banerjee, J., S. Seetharaman, N.L. Wrice, R.J. Christy and S. Natesan, 2019. Delivery of silver sulfadiazine and adipose derived stem cells using fibrin hydrogel improves infected burn wound regeneration. PLoS ONE, Vol. 14. 10.1371/journal.pone.0217965.
6. Arshad, M.N., H.M. Faidallah, A.M. Asiri, N. Kosar and T. Mahmood, 2020. Structural, spectroscopic and nonlinear optical properties of sulfonamide derivatives; experimental and theoretical study. J. Mol. Struct., Vol. 1202. 10.1016/j.molstruc.2019.127393.
7. Hosseini, S.V., N. Tanideh, J. Kohanteb, Z. Ghodrati, D. Mehrabani and H. Yarmohammadi, 2007. Comparison between alpha and silver sulfadiazine ointments in treatment of *Pseudomonas* infections in 3rd degree burns. Int. J. Surg., 5: 23-26.
8. Dibbern Jr, D.A. and A. Montanaro, 2008. Allergies to sulfonamide antibiotics and sulfur-containing drugs. Ann. Allergy Asthma Immunol., 100: 91-101.
9. Zgolli, D.Z., H. Boughzala and A. Driss, 2010. 4-sulfamoylanilinium chloride. Acta Crystallogr. Sec. E: Crystallogr. Commun., Vol. E66. 10.1107/s1600536810019471.
10. Ravikumar, B., S. Pandiarajan and S. Athimoolam, 2013. Bis(4-sulfamoylanilinium) sulfate. Acta Crystallogr. Sec. E: Crystallogr. Commun., Vol. E69. 10.1107/s1600536813007216.
11. Pandiarajan, S., S. Balasubramanian, B. Ravikumar and S. Athimoolam, 2011. 4-sulfamoylanilinium nitrate. Acta Crystallogr. Sec. E: Crystallogr. Commun., Vol. E67. 10.1107/s1600536811038827.

12. Muthuselvi, C., N. Mala, N. Srinivasan, S. Pandiarajan and R.V. Krishnakumar, 2014. Crystal structure of 4-sulfamoylanilinium dihydrogen phosphate. Acta Crystallogr. Sec. E: Crystallogr. Commun., E70: o997-o998.
13. Muthuselvi, C., S. Pandiarajan, S. Athimoolam, R.V. Krishnakumar and A. Manikandan, 2017. Structural and optical properties of NLO material: 4-sulfamoylanilinium dihydrogen phosphate. Adv. Sci. Eng. Med., 9: 931-942.
14. El-Mansy, M.A.M., M.S. El-Bana and S.S. Fouad, 2017. On the spectroscopic analyses of 3-hydroxy-1-phenyl-pyridazin-6(2H)one (HPHP): A comparative experimental and computational study. Spectrochim. Acta Part A: Mol. Biomol. Spectrosc., 176: 99-105.
15. Dede, B., D. Avcı and S. Bahçeli, 2018. Study on the 4-ethoxy-2-methyl-5-(4-morpholinyl)-3(2H)-pyridazinone using FT-IR, ^{1}H and ^{13}C NMR, UV-vis spectroscopy, and DFT/HSEH1PBE method. Can. J. Phys., 96: 1042-1052.
16. Anitha, R., S. Athimoolam, M. Gunasekaran and K. Anitha, 2014. X-ray, vibrational spectra and quantum chemical studies on a new semiorganic crystal: 4-chloroanilinium perchlorate. J. Mol. Struct., 1076: 115-125.
17. Raut, S.D., M. Ubaidullah, S.F. Shaikh, M.M. Abdulhameed, B. Pandit, A. Tyagi and D. Kumar, 2022. Synthesis, crystal structure, quantum calculation and Hirshfeld surface analysis of 4-bromoanilinium oxalate hemihydrate single crystal. J. Mol. Struct., Vol. 1252. 10.1016/j.molstruc.2021.132087.
18. Thakral, S., R. Narang, M. Kumar and V. Singh, 2020. Synthesis, molecular docking and molecular dynamic simulation studies of 2-chloro-5-[(4-chlorophenyl)sulfamoyl]-*N*-(alkyl/aryl)-4-nitrobenzamide derivatives as antidiabetic agents. BMC Chem., Vol. 14. 10.1186/s13065-020-00703-4.