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Research Article

Synthesis, Characterization, and Antibacterial Evaluation of Novel Imidazolium Salts and Their Silver (I) N-Heterocyclic Carbene Complexes

Hasan M Marhoon *

Department of Chemistry, College of Science, University of Kufa, Najaf-54001, Iraq

Corresponding Author: *Hasan M Marhoon

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Abstract

Imidazolium salts are of great interest due to their unique structure and applications in the biological field, stemming from their nitrogen-derived heterocyclic carbene (NHC) mineral composition. This article presents a method for synthesising two imidazolium salts (L- and FT-IR spectroscopy, melting point analysis, and 1H/13C NMR spectroscopy were used to characterise the imidazolium salts and the two compounds). The formation of silver(I)-NHC compounds was confirmed by the disappearance of the characteristic C2-H acid proton signal in the 1H NMR spectra. Specific types of bacteria were used to study the antibacterial activity of compounds A and B. The results showed that the silver(I)-NHC compounds exhibited significantly enhanced antibacterial activity compared to the corresponding imidazolium salts. This improvement is attributed to the synergistic effect between the silver ion and the NHC ligand framework. These findings indicate that silver(I)–NHC complexes derived from imidazolium salts are promising candidates for further development as antibacterial agents.

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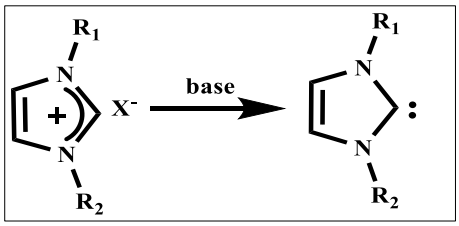
KEYWORDS: Antibacterial; E. coli; Heterocyclic Compound; Imidazolium; Silver.

INTRODUCTION

Imidazole (C3H4N2) is an aromatic heterocyclic compound with a five-membered ring containing two nitrogen atoms [1]. True stability is achieved when the associated proton is present in a renewable form. Imidazole is very soluble in water and air and plays an important role in biological systems, such as nuclear keychains, and maintenance is one such example [2]. Your imidazole source can serve as a baseplate and a plate. The nutrient corn produces DNA-only enhancement, which is important for non-nuclear carbinefic (NHC) DNA. Structural isolation can be catalyzed by monoammonium and can be easily protected by C2-activated carbinef (Scheme 1). It is made entirely of ions, catalysts, carbon dioxide absorbers, and biological activity agents [2].



Scheme 1: Deprotonation of imidazolium salts using a base.

Carbenes are neutral compounds containing a divalent carbon atom with two non-bonding electrons. Depending on their hybridization and spin state, carbenes exist as monomers or tertiary compounds with curved (sp2) or linear (sp) geometries [3]. Monomers are generally stable and exhibit a dimeric nature, while tertiary carbenes display dimeric properties. Electronic and spatial substitutions significantly influence the stability, orbital energies, and geometry of carbenes (Figures 2 and 3).

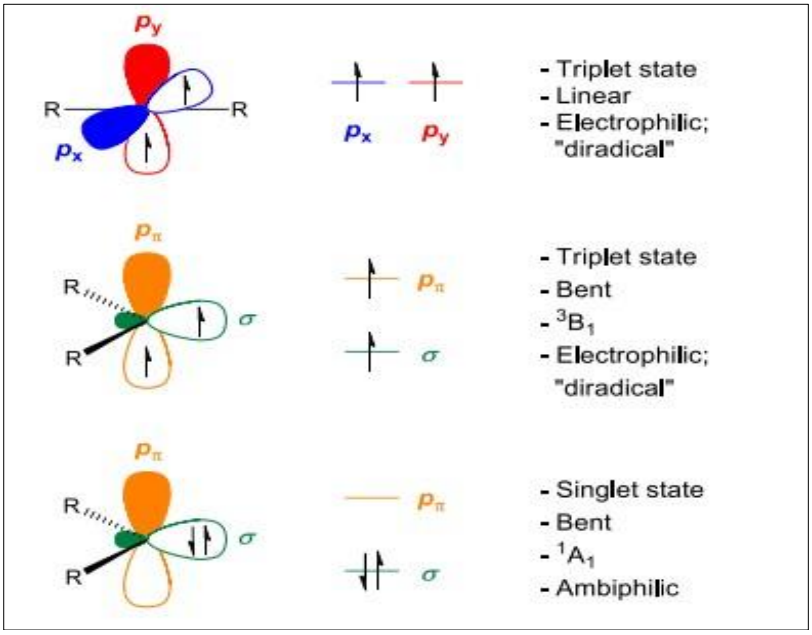


Fig 1: The effects of hybridisation and spin multiplicity of carbenes.

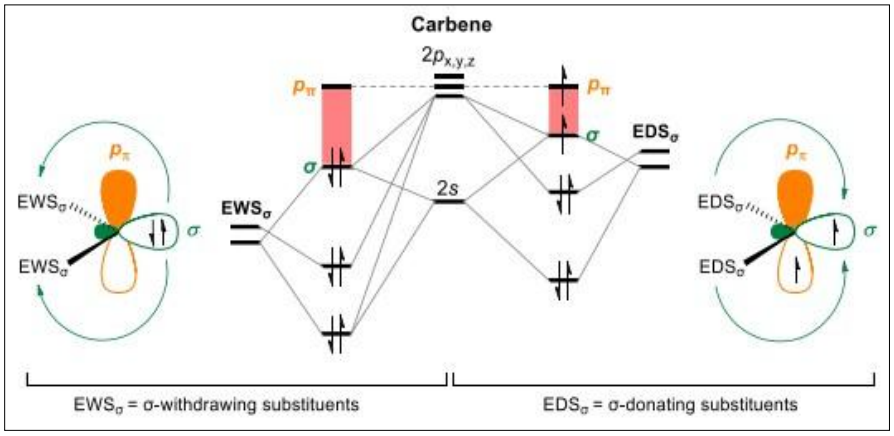


Fig 2: The influence of inductive effects on the size of the σ—pπ with σ-withdrawing.

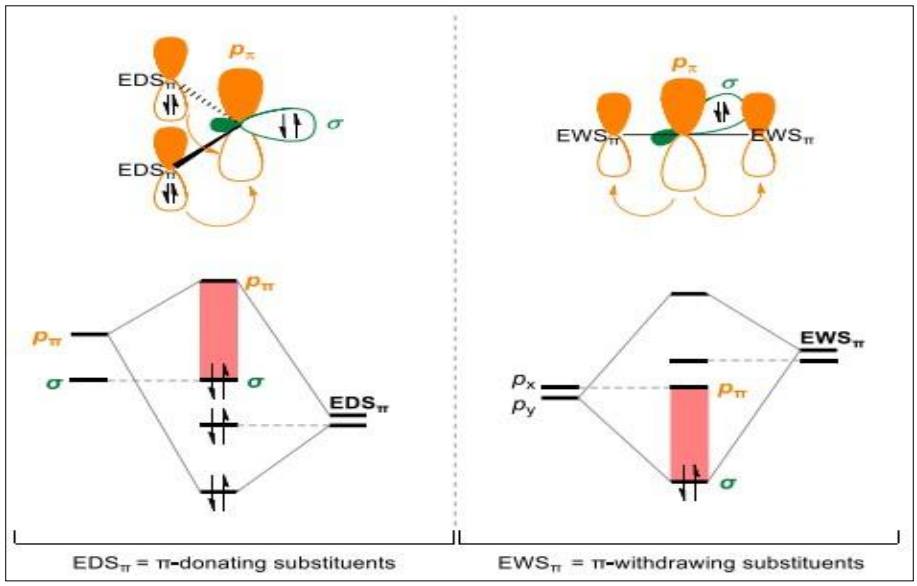
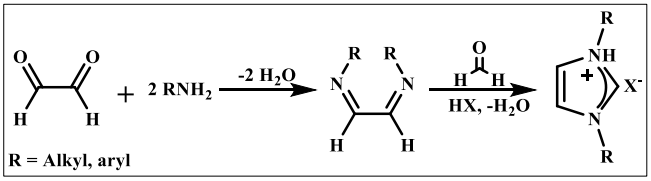


Fig 3: The influence of mesmeric effects on the size of the σ— pπ with π-donating.

Carbenes are classified into Fischer carbenes, Schrock carbenes, and stable carbenes. Fischer carbenes are stable π-acceptor electrophilic bonds, typically associated with late transition metals [4]. Schrock carbenes are nucleophilic bonds, associated with early transition metals in high oxidation states [5]. Stable carbenes, particularly nitrogen heterocyclic carbenes, are strong σ electron-donating cyclic bonds formed by the deprotonation of azole salts. Nitrogen heterocyclic carbenes (NHCs) are monophasic carbenes, stabilized by neighboring nitrogen atoms through inductive and mesomerizing effects [6]. Their stability was first demonstrated in 1991 by isolating free imidazole-2-ylidine [6]. The structural diversity of nitrogen heterocyclic carbenes arises from variations in the heterocyclic structure and nitrogen substitutions. Imidazolium salts, the basic precursors of NHC compounds, are manufactured either by stepwise N-alkylation or by multicomponent reactions involving amines, glyoxal, and formaldehyde (Diagram 2) [6].



Scheme 2: General representation of the synthesis of imidazolium salts by multi-component reaction.

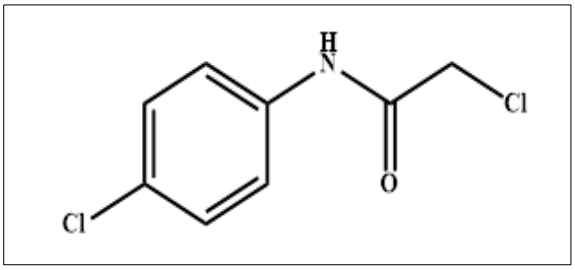
The stability of heterocyclic carbene compounds (NHCs) depends on both the electron-donating capacity of nitrogen atoms and the steric protection provided by the bulky substituents [7]. These properties allow NHCs to form strong complexes with transition metals and often outperform phosphine bonds in their stability under air and moisture. NHC-metal complexes can be synthesized by in situ deprotonation, free carbene coordination, or metal exchange via silver-NHC media. The good antibacterial activity of Silver(I)-NHC complexes are interested [8]. The biological activity of Silver and Ag(I)-NHC differs compared to simple silver salts [9]. Anticancer activity studies play an important role in recent studies, also highlighting their potential biological [10]. To conclude the study, the imidazolium salts and their derivatives represent a versatile class of compounds with crucial applications in coordination chemistry, catalysis, and medicinal chemistry, as evidenced by their well-defined structural properties and diverse synthetic methodologies [11]. Experimental Section (Abridged for Publication)

MATERIALS AND MEASUREMENTS

All reagents and solvents were purchased from commercial suppliers and used after purification.

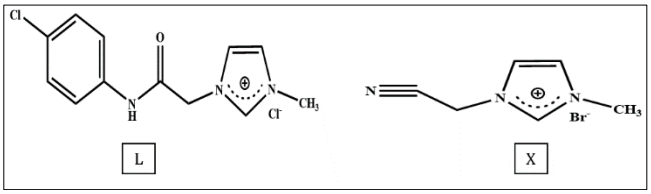
Synthesis of 2-Chloro-N-(4-Chlorophenyl) acetamide(R)

4-Chloroaniline (3.0 g, 0.021 mol) was dissolved in toluene (10 mL), followed by the addition of trimethylamine (1.5 mL). After stirring for 20 minutes, chloroacetyl chloride (1.6 mL, 0.014 mol) was added dropwise at room temperature. The reaction mixture was stirred for 30 minutes, then filtered and thoroughly washed with distilled water, and recrystallized from ethanol to obtain compound R as a white solid (yield 83%, melting point 130-133°C) [12].



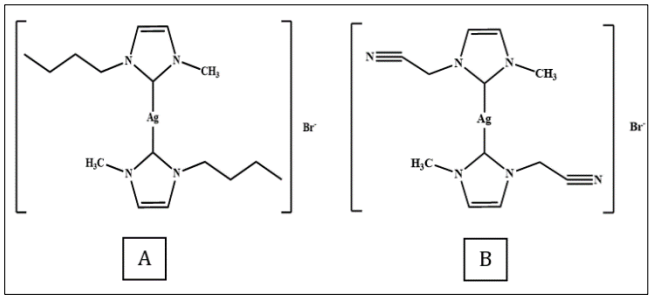
Synthesis of Imidazolium Salts (L, X)

The general alkylation method was used. Methylimidazole (1.0 g, ~0.012 mol) was dissolved in acetonitrile (5 mL), and then a suitable functional alkyl or halide was added to the acetonitrile (5 mL). The reaction mixture was heated under reflux at 90 °C for 24 hours. After evaporation of the solvent, the crude products were recrystallized from methanol to obtain the desired imidazolium salts: L (75%, melting point 125–127 °C, yellow ionic liquid), X (80%, melting point 120–125 °C, white solid).



Synthesis of Silver(I)–NHC Complexes (A, B)

Silver(I)–NHC complexes were prepared by in situ deprotonation using silver oxide. A methanolic solution (20 mL) of the corresponding imidazolium salt (L, X) was treated with Ag_2O (0.5–0.84 g). The reaction mixture was stirred for 10 hours at room temperature in the dark. After filtration through a slate, the solvent was removed under reduced pressure to obtain the corresponding Ag(I)–NHC complexes A and B in 71–76% concentrations as yellowish-white or pale solids (melting point 173–185 °C).



RESULTS AND DISCUSSION (SUMMARIZED)

1. Synthesis of Imidazolium Ligands (L, X)

Imidazolium salts were prepared using the SN_2 mechanism, in which the lone electron pair on the nitrogen atom of methylimidazole attacks alkyl halides (such as bromobutane, bromoacetonitrile, etc.). The high yield (70–83%) and sharp melting points confirm the purity and efficiency of this step. Fourier transform infrared spectroscopy confirmed the formation by the appearance of a characteristic valence coefficient (C=N) and the disappearance of the spectral bands of the starting materials.

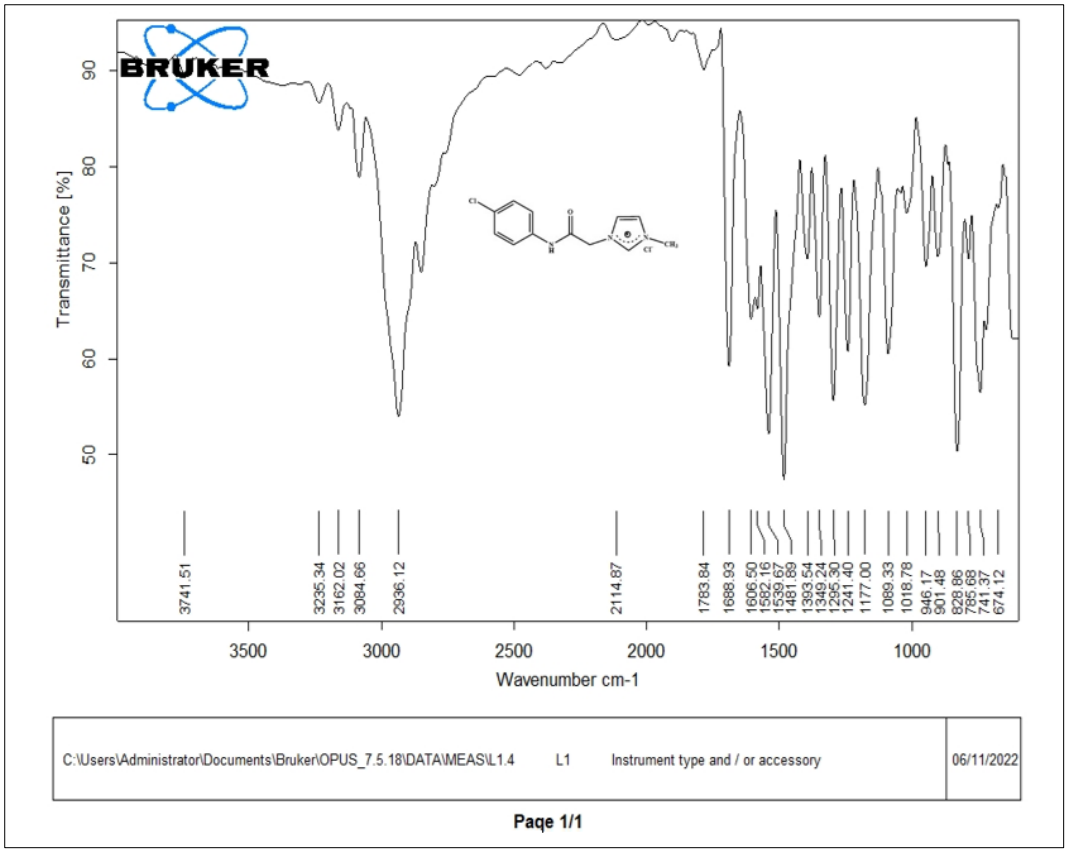


Fig 4: FTIR spectrum of the ligand L

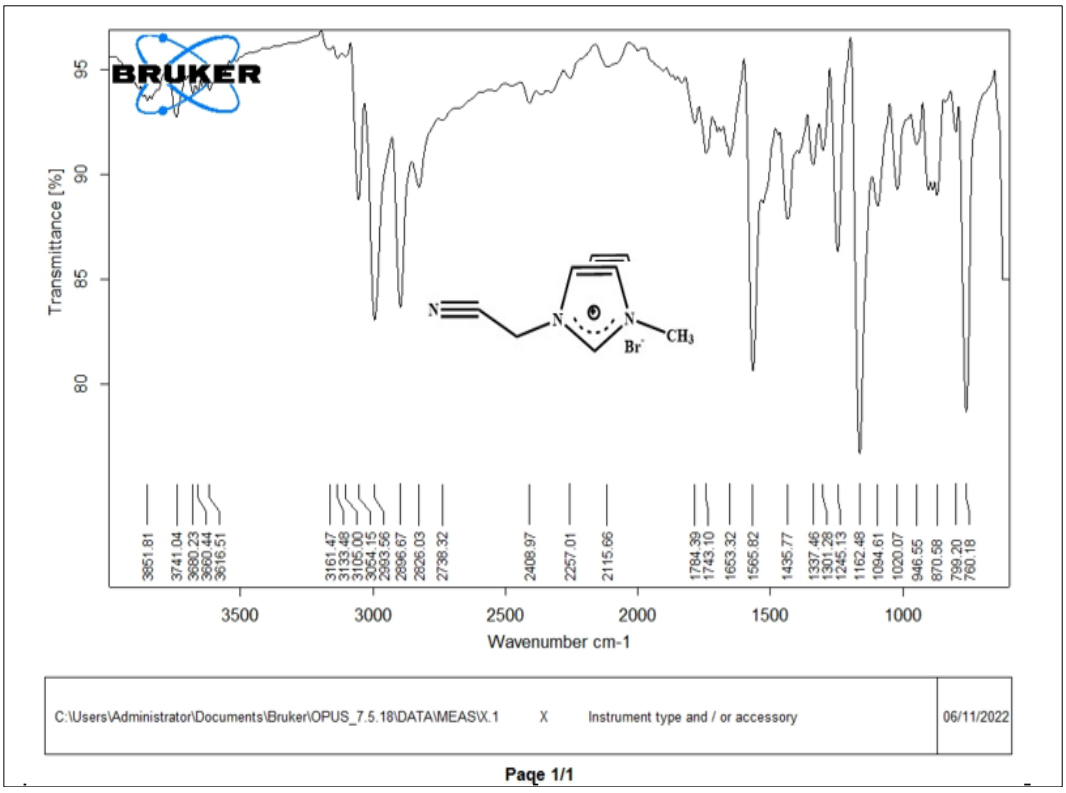


Fig 5: FTIR spectrum of ligand X.

Table 1: FTIR peaks of ligands

Com. No.	Molecular Formula	C-N	N-H	C-H ar.	C-H al.	C=O	C=N	C=C	CΞN
L	$C_{12}H_{13}Cl_2N_3O$	1295	3235	3085	2936	1689	1540	1482	------
X	$C_6H_8BrN_3$	1245	------	3161	2994 2896	-------	1566	1436	2409

Nuclear magnetic resonance analysis: The presence of a proton signal (C2-H) at approximately 9.25-9.46 ppm in proton nuclear magnetic resonance and NCHN carbon at 136-138 ppm in Carbon-13 nuclear magnetic resonance provided conclusive evidence of imidazolium nucleus formation.

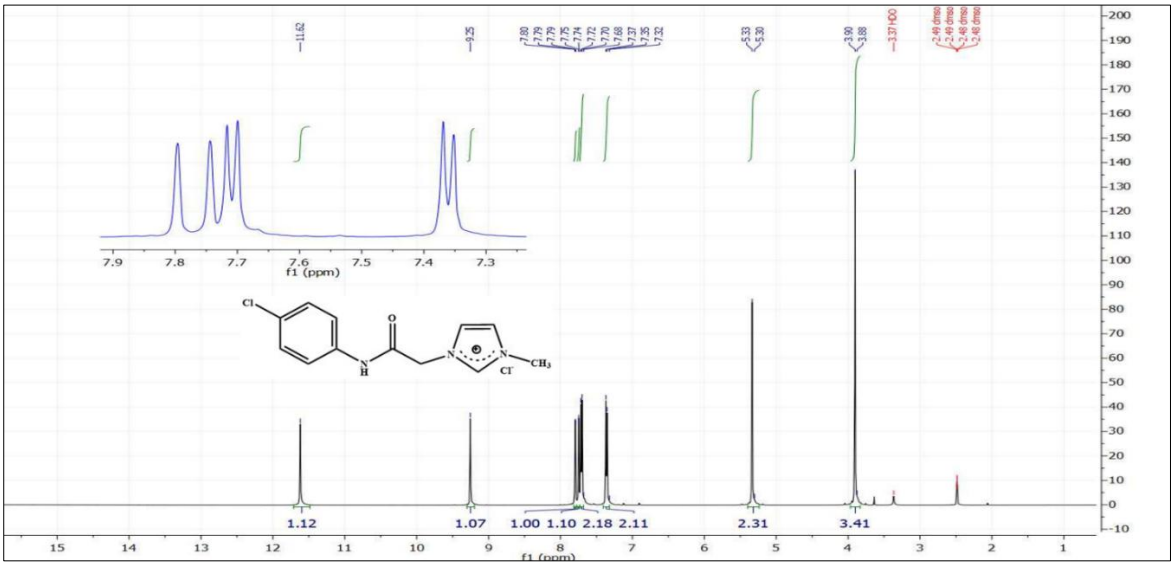


Fig 3.9: [1]HNMR full spectrum of ligand L

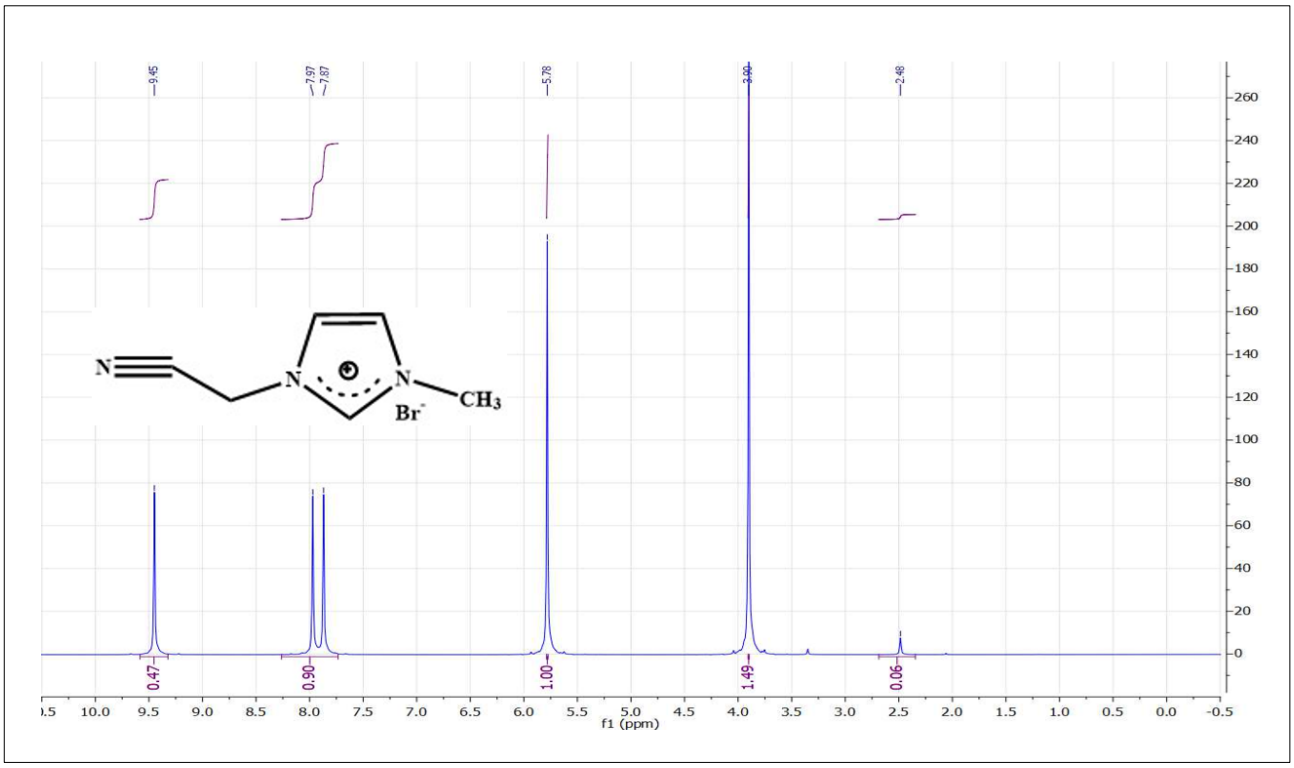


Fig 6: 1H NMR spectrum of ligand X.

Table 2. ^{1}HNMR (500 MHz) data of ligands.

Functional group	^{1}HNMR Chemical shift range (ppm)	
	Ligand L	ligand X
NH-amide	11.62	----------
N**CH**N	9.25	9.45
Ar-H	7.3 - 7.4	----------
CH=CH-imidazole ring	7.75 – 7.80	7.97, 7.87
CO-**CH_2**-N	5.33	----------
CH_3 –terminal	3.67	3.90
N-**CH_2**-CN	----------	5.78
CH_2-imidazole	----------	----------
CH_3-CH_2-CH_2-	----------	----------
Carbonyl-CH_3	----------	----------

2. Silver(I)–NHC Complexes (A, B)

Fourier transform infrared spectroscopy confirmed the successful bonding of the nitrogen-containing heterocyclic carbene to the silver(I) center. In the spectra of the Ag(I)–NHC complexes, the disappearance of the characteristic imidazolium C2–H stretching band (bonded to the N–H) observed in the free bonds indicates proton loss and the formation of an Ag–C bond for the carbene. Furthermore, the C=N stretching vibrations showed marked shifts compared to the corresponding bonds, reflecting changes in electron density in the imidazole ring upon bonding to silver(I).

The remaining functional group bands, including C–H and carbonyl vibrations, were largely conserved with only minor shifts, indicating that the bonding occurs selectively at the carbene carbon atom without significant changes to the bond structure. These spectral characteristics are consistent with previously described silver(I)–NHC complexes and confirm the formation of stable Ag–C bonds.

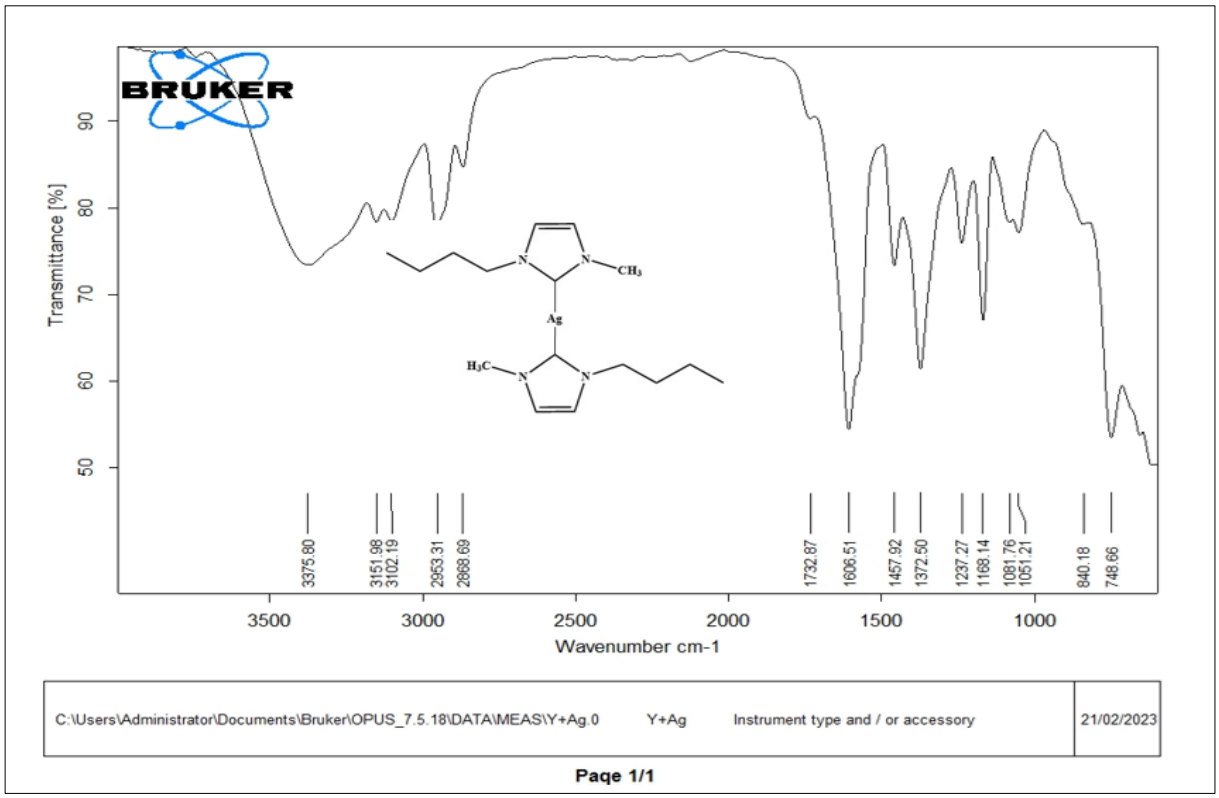


Fig 7: FTIR spectrum of complex A.

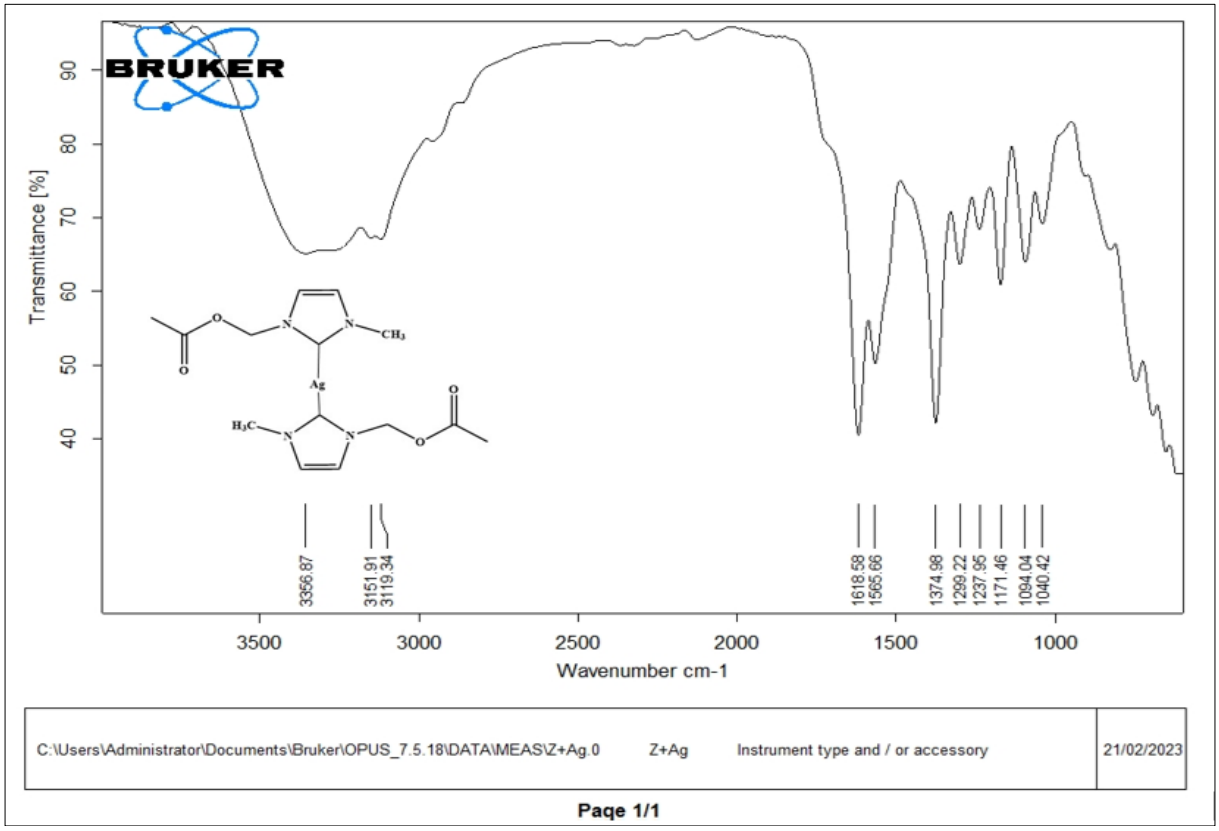


Fig 8: FTIR spectrum of complex B.

Table 3: FTIR peaks of Ag(I) complexes

Com. No.	Molecular Formula	N-H	C-H ar.	C-H al.	C=O	C=N	CΞN	C=C
A	$C_{16}H_{28}AgBrN_4$	-----	3152	2869	-----	1607	-----	1607
B	$C_{14}H_{20}AgBrN_4O_4$	-----	3152	3119	1748	1566	-----	1619

Silver complexes were prepared by in situ proton removal of imidazolium salts using Ag_2O. important results: we indicate that the successful production of Ag-C (carbene) leads to the disappearance of acidic C2-H proton signal in the proton NMR spectra.

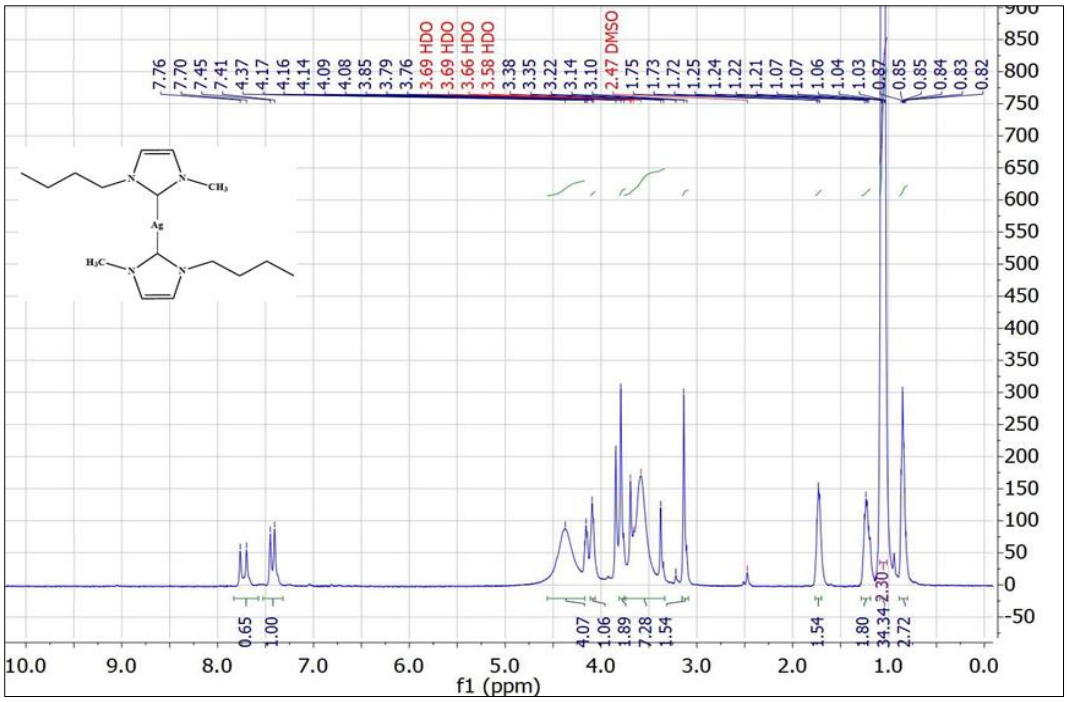


Fig 9: [1]HNMR spectrum of complex A

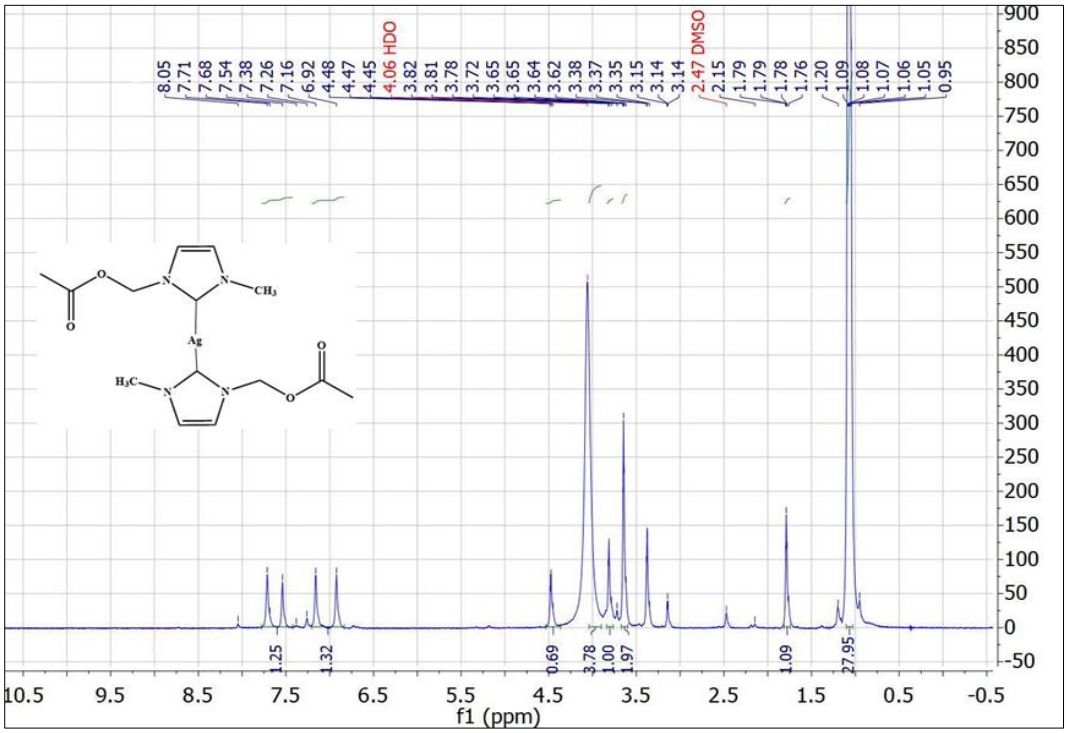


Fig 10: [1]HNMR spectrum of complex B.

Table 4: ^{1}HNMR (500 MHz) data of Ag(I) complexes.

Functional group	^{1}HNMR Chemical shift range (ppm)	
	Complex A	Complex B
NH-amide	-------	-------
Ar-H	-------	-------
CH=CH-imidazole ring	7.45 – 7.76	7.26, 7.71
CO-**CH$_2$**-N	-------	4.5
CH$_3$ –terminal	3.14	3.15
N-**CH$_2$**-CN	-------	-------
CH$_2$-imidazole	4.37	-------
CH$_3$-CH$_2$-CH$_2$-	0.85-1.25-1.72	-------
Carbonyl-CH$_3$	-------	1.08

4. Antibacterial Activity

The results reveal that synthesized imidazolium salts (L, B) show good improvement in the antibacterial properties. The silver ions in the structure of silver (I)-NHC compounds play an important role in high activity, which is known for its relatively broad antibacterial activity. The bacterial cell membranes are affected by Silver ions (interaction), inhibiting important enzymatic processes and disrupting DNA replication. The metallic center is stabilized by the reaction between the NHC and silver and produced anew bond, enhancing antibacterial activity and interaction with bacterial cells. In another hand, with an ionic nature and limited interaction with microbial membranes, the imidazolium salts show moderate antibacterial activity. The improvement in biological activity by stable Ag-C (carbene) bonds in compounds A and B suggests a synergistic effect between the silver ion and the NHC bond. These observations are consistent with previous findings. Published studies on silver(I)-NHC systems confirm their potential use as effective antimicrobial agents.

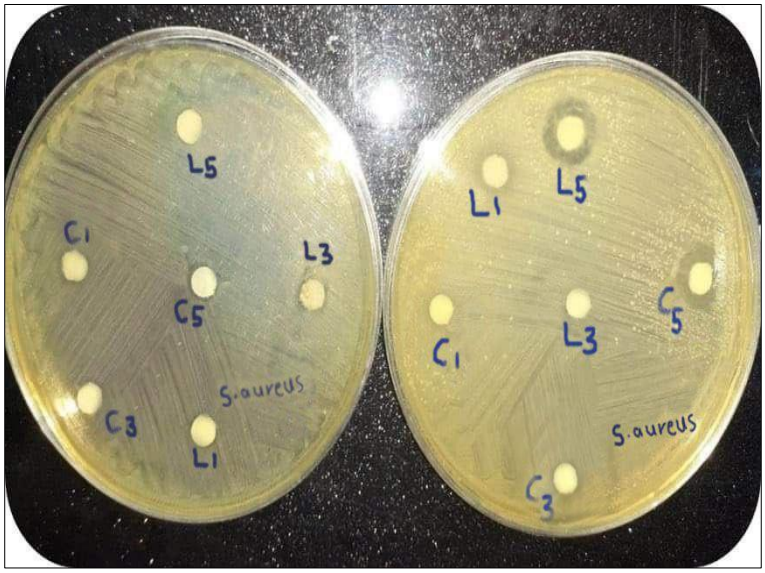


Fig 11: Antibacterial activities of compounds (C1, C3, C5, L1, L3, and L5) against Staphylococcus aureus.

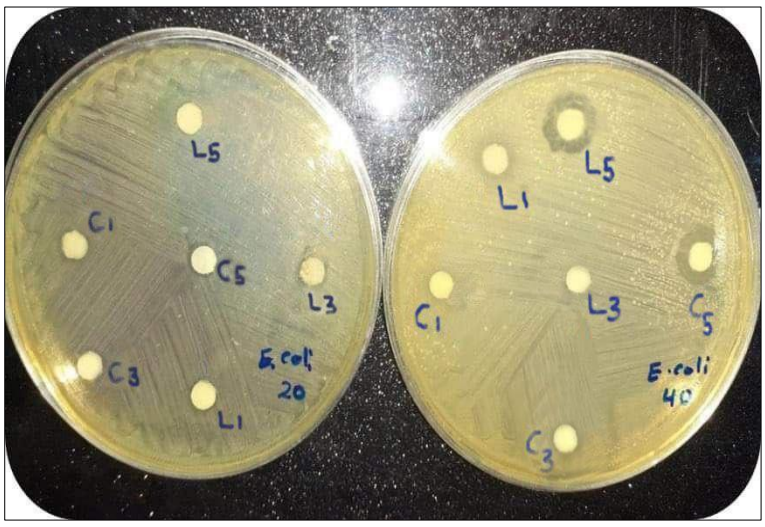


Fig 12: Antibacterial activities of compounds (C1, C3, C5, L1, L3, and L5) against Escherichia coli.

CONCLUSION

The starting materials of novel imidazolium salts used for the preparation of silver (I) complexes with nitrogen-containing heterocyclic carbene were successfully prepared in this study. Different Spectroscopic analyses techniques using nuclear magnetic resonance (NMR) and infrared Fourier transform techniques (FTIR) confirmed the successful bond formation and efficient coordination of silver across the carbon atom in the carbene, as evidenced by the disappearance of the characteristic C2-H proton signal. THE Antibacterial evaluation showed that the imidazolium salts have lower activity than silver(I) complexes with nitrogen-containing heterocyclic carbene. This improvement highlights the important role of silver coordination and the stabilizing effect of nitrogen-containing heterocyclic carbene bonds in enhancing antimicrobial efficacy. Overall, the results of this work indicate that silver (I) complexes with nitrogen-containing heterocyclic carbene derived from imidazolium salts are promising systems for further investigation in coordination chemistry and antimicrobial applications. Future studies focusing on the relationship between structure, activity, and biological mechanisms may contribute to the development of new and effective antibacterial agents.

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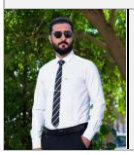
About the corresponding author



Hasan M. Marhoon is a faculty member in the Department of Chemistry, College of Science, University of Kufa, Najaf, Iraq. His academic interests include chemical sciences, experimental analysis, and interdisciplinary research. He is actively engaged in teaching, research, and academic development within higher education.