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Research Article

Novel Vinyl Substituted N-Heterocyclic Carbene Silver(I) Complex: Synthesis and Structural Characterization

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Abstract – Transition metal complexes of N-heterocyclic carbenes (NHCs) containing benzimidazole have been at the center of intensive research in organometallic chemistry and homogeneous catalysis over the years [1]. The electronic and steric properties of NHC complexes can be easily modified. This makes carbene complexes indispensable in homogeneous catalysis. These complexes also have greater stability against air, moisture and heat compared to their phosphine analogues [2]. In addition to catalysis, M-NHC complexes are also widely used in the medical field. In addition to their antimicrobial effects, these compounds have also been shown to be active against cancer. Research on the antimicrobial and anticancer properties of silver has continued to increase in recent years and there are now many different silver complexes that exhibit a wide spectrum of antimicrobial and anticancer activity [3]. The current research work aims to provide alternatives to some products. In this study, a new 1-(4-vinylbenzyl)-3-(alkyl)-5,6-dimethylbenzimidazol-2-ylidene]silver(I) complexes were synthesized. The structures of all compounds were characterized by ^{1}H NMR, ^{13}C NMR and IR spectroscopy techniques.properties.

Keywords – Silver, Benzimidazolium, Ag-NHC, Synthesis, Characterization.

I. INTRODUCTION

Among the various metal ions, a large group of metal and their complexes were used as a individual aid in treating different conditions. preliminarily copper, arsenic trioxide, gold and mercury sulphide were employed for treating leukaemia, psoriasis, rheumatoid conditions and syphilis. In organometallics, it's well known that the ligands can have significant goods on the complexes. Metal complexes with unique characteristics, including reactivity, different collaboration routes and redox capability, showed tremendous eventuality in cancer remedy. These complexes showed a better cytotoxic action than the ligands through reactive oxygen species (ROS) product, cell membrane revision, inhibiting DNA replication, affecting electron transport and anxiety of enzyme action and altering redox eventuality of the cell [1-6].

Because of the neutral nature of electron benefactors, NHCs can bind with metal ions through the σ-donation. It also plays a significant part in the exploration field, particularly in catalysis, because of its better stability and easy derivability. Ulmost studies have displayed the imidazole- grounded nexus, but some benzimidazole derivations were infrequently studied. Ag- NHC complexes parade a slow- release rate of tableware. Arduengo and associates have designed the first Ag- NHC complex with the operation of free carbenes, but its conflation was limited due to some complications in getting free carbenes. It has

been reported that the capability of the Ag- NHCs in the transmetallation response as a carbene transfer agent facilitates the conflation of various metal- NHC complexes [4,7-9].

In this work, we synthesized of a new series of 1-(4-Vinylbenzyl)-3-(2,2-dimethoxyethyl)-5,6-dimethylbenzimidazo-2-ylidene]silver(I) complexes and investigated their in vitro antibacterial, antifungal and anticancer properties.

II. MATERIALS AND METHOD

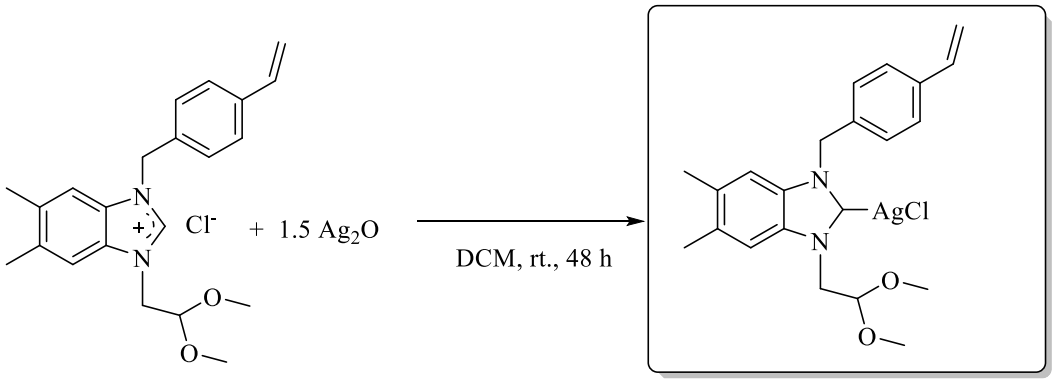
All reactions for the prepared compounds were carried out under argon in flame-dried glassware using standard Schlenk techniques. Chemicals and solvents were purchased from Sigma-Aldrich and Merck. The solvents used were purified by distillation over the drying agents indicated and were transferred under Ar: Et_2O (Na/K alloy), CH_2Cl_2 (P_4O_{10}), hexane, toluene (Na). Elemental analyses were performed by ElementarVario EL III Carlo Erba 1108. The melting points of the complexes and NHC precursors were determined using Stuart automatic melting point apparatus (SMP-40). IR spectra were recorded with a PerkinElmer Spectrum 100 GladiATR FT/IR spectrophotometer. ^1H, ^{13}C NMR spectra were recorded in $CDCl_3$ or DMSO-d6 solutions operating on a Bruker Avance III HD 400 MHz NMR spectrometer. Coupling constants (J values) are given in hertz. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, m = multiplet signal.

General synthesis of Ag-NHC complexes

Ag_2O (1.5 mmol) and the precursor salt (1 mmol) were diluted in 20 mL of CH_2Cl_2 and stirred at 25 ºC for 48 h. The solution was then run through a pad of Celite for filtering. In vacuo, half of the dichloromethane was evaporated, and the mixture of CH_2Cl_2 and Et_2O crystallized the crude complex (1:5).

1-(4-Vinylbenzyl)-3-(2,2-dimethoxyethyl)-5,6-dimethylbenzimidazolium chloride (1mmol) and Ag_2O (1.5 mmol) were diluted in 20 mL of CH_2Cl_2 and stirred at 25 ºC for 48 h. The solution was then run through a pad of Celite for filtering. In vacuo, half of the dichloromethane was evaporated, and the mixture of CH_2Cl_2 and Et_2O crystallized the crude complex (1:5).

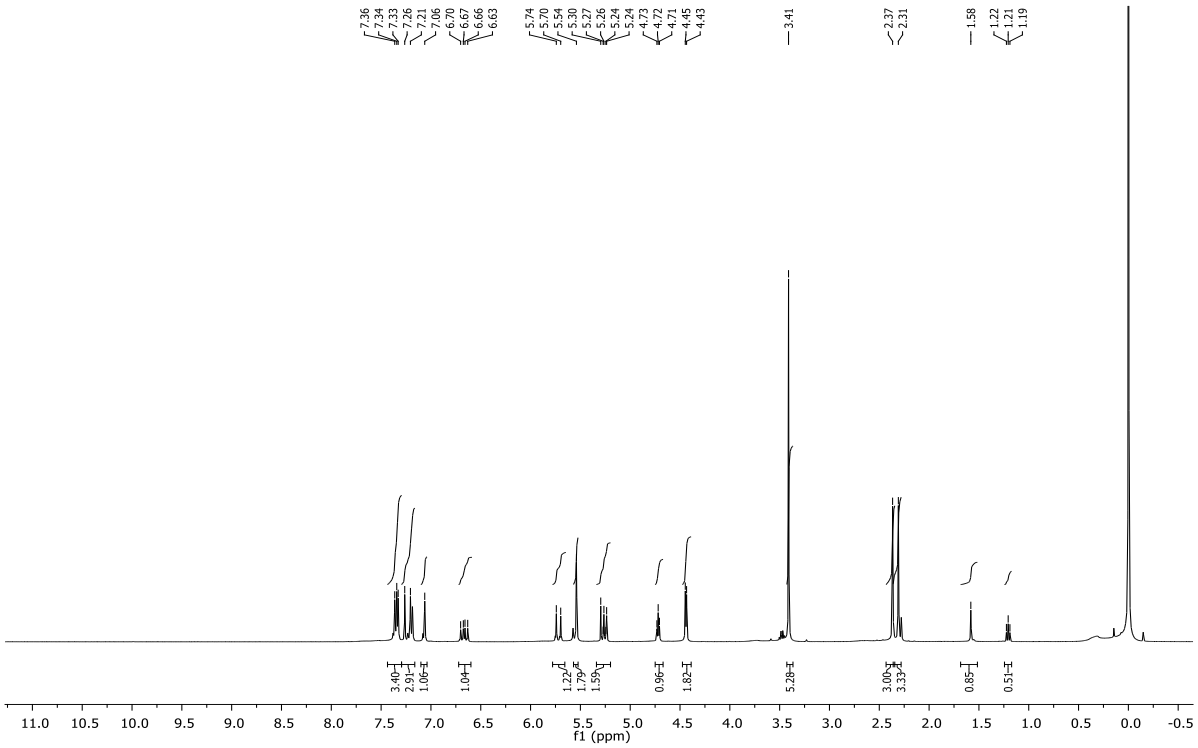
The benzimidazolium silver complex was isolated as white solids in very good yields and fully characterized by ^1H and ^{13}C NMR spectroscopy, and elemental analyses (see Experimental section). The ^1H NMR spectra of the silver complex further supported the assigned structures. in detail the materials and methods used when conducting the study. The citations you make from different sources must be given and referenced in references.



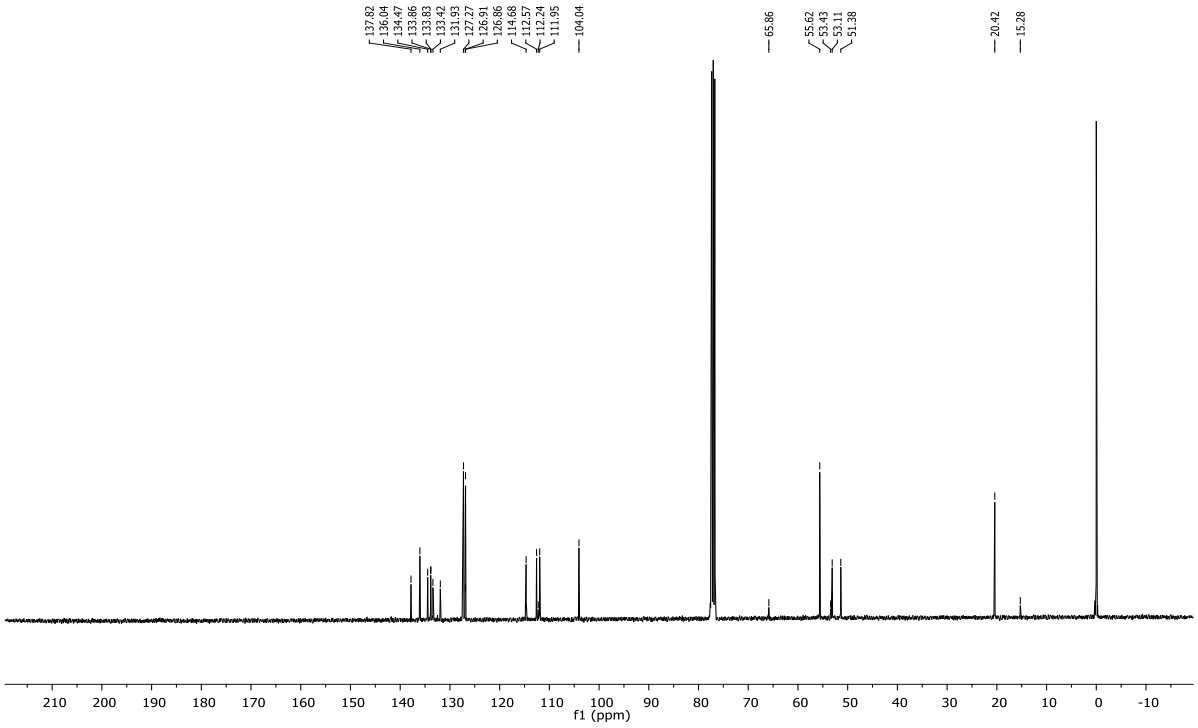
Chloro[1-(4-Vinylbenzyl)-3-(2,2-dimethoxyethyl)-5,6-dimethylbenzimidazole-2-ylidene]silver(I), 1

Yield: 80 %. FT-IR ν(CN): 1560 cm^{-1}; ^1H NMR (399.9 MHz, $CDCl_3$, 25 °C): δ = 2.31 and 2.37 (s, 6H, 5,6-$(CH_3)_2$-C_6H_2), 3.41 [s, 6H, $NCH_2CH(OCH_3)_2$], 4.46 [s, 2H, $NCH_2CH(OCH_3)_2$], 5.24 and 5.70 (d, 2H, J = 8, $NCH_2C_6H_4CH=CH_2$-4), 5.54 [s, 1H, $NCH_2CH(OCH_3)_2$], 5.84 (s, 2H, $NCH_2C_6H_4CH=CH_2$-4), 6.67 (dd, 1H, J = 12.2 and 10.8 Hz, $NCH_2C_6H_4CH=CH_2$-4), 7.06- 7.36 (m, 6H, $NCH_2C_6H_4CH=CH_2$-4 and 5,6-$(CH_3)_2$-C_6H_2). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ = 20.4 (5,6-$(CH_3)_2$-C_6H_2), 51.4

($NCH_2C_6H_4CH=CH_2$-4), 53.4 [$NCH_2CH(OCH_3)_2$], 55.6 [$NCH_2CH(OCH_3)_2$], 104.4 [$NCH_2CH(OCH_3)_2$], 111.9 ($NCH_2C_6H_4CH=CH_2$-4), 126.8 ($NCH_2C_6H_4CH=CH_2$-4), 112.2, 112.6, 114.7, 126.9, 127.8, 136.0 and 137.8 [$NCH_2C_6H_4CH=CH_2$-4 and 5,6-$(CH_3)_2$-C_6H_2)].



^{1}H NMR Spectrum of compound 1



^{13}C NMR Spectrum of compound 1

III. DISCUSSION

The benzimidazolium silver complex was isolated as white solids in very good yields and fully characterized by ^{1}H and ^{13}C NMR spectroscopy, and elemental analyses (see Experimental section). The ^{1}H NMR spectra of the silver complex further supported the assigned structures.

IV. CONCLUSION

Consequently, we synthesized a vinyl functionalized 5,6-dimethylbenzimidazolium Ag-NHC. These complex have been characterized by using elemental analyses, ^{1}H-NMR, ^{13}C-NMR,and IR spectroscopy techniques.

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