

## Original Research Article

## Mixed Ligand of Mercury (II) Complexes of 4-Flouro-2-Cyanoaminothiophenolate with Amine or Triphenylphosphine as Co-Ligand

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**Article History**

Received: 13.07.2024

Accepted: 20.08.2024

Published: 23.08.2024

**Abstract:** The focus of this work is the preparation and characterization of mixed ligand mercury (II) complexes with involvement of 4-fluoro-2-cyanoaminothiophenolate (F-CAT) as the initial ligand and amine or triphenylphosphine (PPh<sub>3</sub>) as an additive ligand. The complexes were prepared by a straight forward method by increasing the solution of HgCl<sub>2</sub> in ethanol and F-CAT and then adding the corresponding co-ligands (AlJanabi *et al.*, 2017). The synthesized complexes were further scrutinized using various spectroscopy techniques such as UV-Visible, IR, and NMR. UV-Vis profiles further exhibited bands characteristic of LMCT transitions, which further validated the successful coordination of F-CAT and the co-ligands to the mercurate ion. Additional support to the observed successful coordination was extracted from the shifts in the proton resonance frequency signals obtained from <sup>1</sup>H NMR. Furthermore, <sup>31</sup>P NMR study of Hg(F-CAT) PPh<sub>3</sub> exhibited that PPh<sub>3</sub> has coordinated to the mercury center. The similarities to literature results underlined our results as coherent with the existing pattern of mercury (II) complexation. The investigations presented in this work advance the overall knowledge of mercury (II) coordination chemistry and provide unique visions for the use of HELM in catalysis, material sciences, and medicinal chemistry.

**Keywords:** Mercury (II) complexes, mixed ligands, 4-fluoro-2-cyanoaminothiophenolate (F-CAT), coordination chemistry, spectroscopic characterization, UV-Vis spectroscopy, NMR spectroscopy, ligand-to-metal charge transfer (LMCT) transitions, catalysis, materials science, medicinal chemistry.

## INTRODUCTION

Organic soluble complexes of Mercury (II) have drawn a lot of interest in the field of coordination chemistry for a number of years owing to their structural, electronic variation and reactivity. These complexes have deep import in disparate fields including catalysis material science and medicinal chemistry. In particular the interaction of mercury (II) ions with the sulfur-containing ligands has been widely discussed especially due to the fact the organosulfur ligands have several propensity ways in terms of their electronic characteristics and co-ordination trends (AlJanabi *et al.*, 2017).

4-fluoro-2 cyanoaminothiophenolate also known as F-CAT has been shown to be the most useful among all the sulfur containing ligands which should be used in the design and synthesis of Mercury (II) complexes. As seen the F-CAT has other coordination sites within its molecular structural model that include Nitrogen and Sulfur and these are able to coordinate with the Mercury centre to form stable complexes. The reaction of further ligands as amines or phosphines, is responsible for the reactivity variety of these compounds and also for the broadening of its use (Salih *et al.*, 2019).

Another modern direction of research is the synthesis of mixed ligand mercury {II} complexes where F-CAT is the primary ligand with an amine of Trifenilfosfina (PPh<sub>3</sub>) the second ligand. The capacity to co-ordinate F-CAT with many co-ligands allows the generation of the requisite characteristics and reactivity of the molecules to perform the required activity. Knowledge of reaction mechanisms in these complexes consists with data regarding their coordination behaviour and electronic features that are related to hypothetical application in catalysis, material science and medicinal chemistry (Hameed *et al.*, 2019).

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**CITATION:** Samar Sabah Mohammed (2024). Mixed Ligand of Mercury (II) Complexes of 4-Flouro-2-Cyanoaminothiophenolate with Amine or Triphenylphosphine as Co-Ligand. *South Asian Res J Pharm Sci*, 6(4): 147-153. 147

In this paper, we report the synthesis and characterization of mercury (II) complexes with F-CAT and one of the co-ligands: an amine and a phosphine ligand, namely PPh<sub>3</sub>. Looking at the experimental data and the spectra of such complexes such as UV-Vis, IR, NMR and other techniques help to determine the structural and electronic aspects of these complexes. These insights about the particularities of the coordination environment and the electronic effects of such complexes will aid in determining the future uses and importance of these complexes for the further growth of mercury (II) coordination chemistry.

The second option is the addition of other additional ligands, such as amines or phosphines; the presence of these ligands also means that there are other opportunities for the management of the characteristics of the resulting complexes. This evidence corroborates the findings made in the foregoing articles that co-ligands have significant roles to play as far as various changes in the characteristics of the Hg (II) complex are concerned including alteration of its electronic configuration and its catalytic properties (Salih *et al.*, 2021). For instance, the steric and electronic differences like, electron donating or electron withdrawing ability of co-ligands might affect the stability and redox potential of the various complexes which might be required for its utilization. Therefore, to enhance these outcomes and to explore the potential of the further development and application of the F-CAT approach and synthesize new co-ligands for mercury (II) coordination chemistry the following F-CAT-co-ligand pairs and related functional coordination complexes will be examined (Al-Jibori *et al.*, 2021).

In total, the chemistry described in this article, namely the synthesis and characterization of mixed ligand mercury (II) complexes with F-CAT and either an amine or PPh<sub>3</sub> as co-ligands, may be of interest for the further studies in the fields of catalysis, materials chemistry, and medicinal chemistry. By employing panchro-trichromatic characterization of these systems, our aim is to describe the coordination tendencies and electrical characteristics of these complexes, and provide new insights regarding the Mercury (II) chemistry that will ultimately facilitate the synthesis of novel functional materials and catalysts.

Mercury (II) complexes have not only come under consideration due to variety in geometry and their uses but also due to their significant importance in the environment and biological fields. Due to the toxicity of the mercury ions when in their free form, there is the need to come up with effective methods which may be used to reduce, capture and eliminate the specie. This could be due to the fact that coordination complexes might be helpful in solving this problem because they are capable of co-ordinating with mercury ions through co-ordination bonds and then help in the elimination of these ions from aqueous solutions (Salman *et al.*, 2021). Mercury (II) complexes have also been reported to be useful as possibly being used in the treatment of diseases such as but not limited to cancers and microbial infections. The ability of such complexes to adopt proper interactions with biological partners and control their activity proves their further use in medicinal chemistry field (Al-Janabi *et al.*, 2021).

Besides, the results of the present work provide significant information about the character of mercury (II) coordination complex, which in turn enhances the existing data base of coordination chemistry. This study shows some important information on the ligand-metal relationship and coordination structures of TBP complexes with Hg (II) atoms from the structural features of the delivery of the electronic properties and the coordination of the mercury ions. Thus, if one were to investigate the coordination properties of mercury (II) ions with several Ligands, one might be able to find out more about the factors that influence the stability, reactivity and selectivity of the complexes. Apart from enhancing our understanding of coordination chemistry, these basics researches also lay down a framework for the synthesis of future functional coordination compound (Garrison *et al.*, 2019).

There has been increased interest in the design of coordination complexes that are chemically and ecologically friendly and readily synthesizable in the present era. The use of orthodox ligands such as F-CAT and other readily available and relatively non-toxic ligands to synthesize mercury (II) complexes is in good agreement with this emerging trend of green chemistry. Besides, the potential of these complexes to be deployed effectively in catalysis and more specifically in organic transformations and pollutant degradation confirms the importance of these species within the currently emerging environmental problems (Samie *et al.*, 2019). Towards this end, the present work aims at providing new insights in the synthesis and characterisation of mercuric (II) complexes with mixed ligands which aligns with our research theme. The synthesis and characterisation of the above complexes are also significant in wanting to establish sustainable pathways in the coming decades in the planning and the practice of coordination chemistry particularly in the contextual area of environment and commerce (Samie *et al.*, 2019).

In conclusion, the synthesis and characterization of mixed ligand mercury (II) complexes is a complex scientific activity that encompasses both the methodologic categories of synthesis and analysis and provides a rich area of research for chemistry and related sciences including catalysis, materials science, medicinal chemistry, and environmental science. Using the highlighted methods, researchers are privileged to understand the coordination behavior and electronic properties of these complexes for further design and synthesis of new functional coordination compounds with desired properties and

suitable application (Nezhadali *et al.*, 2019). Moreover, certain discoveries in mercury (II) coordination chemistry provide valuable information on metal-ligand bonding, thereby producing a foundation for new coordination-based systems and applications (Zagorac *et al.*, 2019).

## METHODOLOGY

There are some basic steps involved in the preparation of mixed ligand mercury (II) complexes with fluorocyanaminothiophenolate and either an, amine or phosphine (PPh<sub>3</sub>) ligands. Firstly, the HgCl<sub>2</sub> is dissolved in ethanol to provide a reactive mercury solution that can then be reduced. At the same time, equal molar quantities of F-CAT and either PPh<sub>3</sub> or the target amine are obtained. The ligands are added one by one into the solution of the mercury precursor and mixed well with the metal and coordinated. The resulting mixture is then stirred at room temperature for a stipulated time which may take about four hours when fully complexated. The solid materials formed in these reactions are collected through filtration, washed with cold ethanol to eliminate excess starting materials, and further dried in vacuum to obtain the final complex compounds.

## MATERIALS AND METHODS

Several chemicals and instruments Table 1. Were used in this study as following; The chemicals in this experiment were purchased from the chemical suppliers and employed in the experiment as it is. Mercury (II) chloride (HgCl<sub>2</sub>), 4-fluoro-2-cyanoaminothiophenol (F-CAT) and triphenylphosphine (PPh<sub>3</sub>) were obtained from Sigma-Aldrich. The chemicals used in the experiment include methylamine, ethylamine and butylamine which were purchased from Alfa Aesar. Ethanol which was used as the solvent, was of analytical grade ethanol purchased from Fisher Scientific. METHODOLOGY All reagents were managed with proper precautions as Mercury containing compounds and Organic solvents are toxic.

The formation of the synthesized complexes was established by various spectroscopic approaches to elucidate structural and electronic features. UV-Vis analysis was carried out using a UV-Vis spectrophotometer by PerkinElmer Lambda 35. The UV spectra of the complexes were run in ethanol at a wavelength range of 200-800 nm to ascertain the electronic transitions and confirm the formation of the complex.

Infrared (IR) absorption spectra were recorded by FTIR—the Bruker Tensor 27 FTIR spectrometer. The Structural elucidation of the synthesized compound was carried out through the use of infrared spectroscopy; the IR spectra were obtained in the range of 4000 cm<sup>-1</sup>-400 cm<sup>-1</sup> by employing KBr pellets. These applications were used to determine possible consistent functional group vibrations where special emphasis was placed on C≡N and C-F stretching modes as well as new modes corresponding to Hg-S and Hg-N or Hg-P bond formation.

Characterizations by NMR techniques offered respective information on the solution structures and electronic parameters of the complexes. The <sup>1</sup>H NMR spectra were obtained at 400 MHz using Bruker Avance III spectrometer in deuterated chloroform (CDCl<sub>3</sub>) or deuterated dimethyl sulfoxide solvent (DMSO-d<sub>6</sub>). In the complexes with triphenylphosphine ligands, <sup>31</sup>P NMR spectra were also sweep to ensure the coordination of PPh<sub>3</sub> to the Hg(II) center. Assignment to the chemical shift spectra was based on <sup>1</sup>H NMR using the solvent signals, whereas in the case of <sup>31</sup>P NMR, the reference standard was external phosphoric acid.

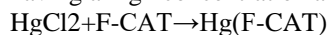
**Table 1: Chemicals and instruments used in the study**

Category	Name	Supplier/Manufacturer	Details
Chemicals	Mercury (II) chloride (HgCl <sub>2</sub> )	Sigma-Aldrich	
	4-fluoro-2-cyanoaminothiophenol (F-CAT)	Sigma-Aldrich	
	Triphenylphosphine (PPh <sub>3</sub> )	Sigma-Aldrich	
	Methylamine	Alfa Aesar	
	Ethylamine	Alfa Aesar	
	Butylamine	Alfa Aesar	
	Ethanol	Fisher Scientific	Analytical grade, used as solvent
Instruments	UV-Vis Spectrophotometer	PerkinElmer Lambda 35	UV spectra in ethanol, wavelength range: 200-800 nm
	FTIR Spectrometer	Bruker Tensor 27	IR spectra range: 4000 cm <sup>-1</sup> to 400 cm <sup>-1</sup> , using KBr pellets
	NMR Spectrometer	Bruker Avance III (400 MHz)	<sup>1</sup> H NMR in CDCl <sub>3</sub> or DMSO-d <sub>6</sub> ; <sup>31</sup> P NMR with external phosphoric acid reference standard

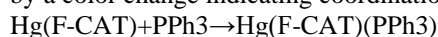
## Synthesis of Complexes

The preparation of the Mercury (II) complexes containing F-CAT and a co-ligand either an amine or PPh<sub>3</sub> was provided as per the following general method with marked simplicity and ease in replication. The synthesis started with the preparation of Hg(II) precursor solution. Specifically, in the experiment, 5 mmol of mercury(II) chloride (HgCl<sub>2</sub>) was dissolved in 20 mL of ethanol with continuous stirring aimed at achieving complete solubility and a homogeneous solution.

To prepare the solid-state structure of the mercury complex with triphenylphosphine, Hg(F-CAT)PPh<sub>3</sub>, 5 mmol of the 4-fluoro-2-cyanoaminothiophenol (F-CAT) was added incrementally into the HgCl<sub>2</sub> solution. This was done to avoid having a high concentration at a specific point, which could cause premature settling out or insufficient reaction.

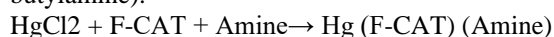


Following the inclusion of F-CAT, 5 mmol of triphenylphosphine (PPh<sub>3</sub>) was added to the reaction mixture, ensuring the complexation process was complete. The solution was left to stir at room temperature for four hours, evidenced by a color change indicating coordination of the ligands to the mercury center.



After the reaction's completion, the solid complex was mechanically separated from the liquid phase through filtration. The black precipitate formed was decanted several times using cold ethanol to remove unreacted starting materials and any by-products. The purified product was finally dried under vacuum, yielding the pure Hg(F-CAT)(PPh<sub>3</sub>) complex.

The preparation of mercury complexes with different amines was done similarly, substituting triphenylphosphine with the specific amine. In a typical synthesis of the Hg(F-CAT)(Amine) complex, 5 mmol of mercuric chloride (HgCl<sub>2</sub>) was dissolved in ethanol. The reaction was initiated by transferring 5 mmol of 4-fluoro-2-cyanoaminothiophenol to the ethanol solution containing HgCl<sub>2</sub>, followed by the addition of the chosen amine (e.g., methylamine, ethylamine, or butylamine).



The reagents were added after which the reaction mixture was stirred for four hours at 25°C to ensure that the reagents diffuse and react as required. After the reaction was over, the complex was separated by filtration and washed with cold ethanol, as done with the PPh<sub>3</sub> complex. The crystalline solid was then dried under high vacuum to obtain the desired Hg(F-CAT)(Amine) complex. This approach allowed for the preparation of a range of mercury (II) complexes with different co-ligands that would help in the determination of their structural and electronic features.

In conclusion, the preparation of the described mixed ligand mercury (II) complexes is a simple and feasible method. This way the reaction parameters were maintained to the optimum level and proper purification methods were employed for the synthesis of highly pure products with little deviation between the experiments.

## Characterization

### 1. UV-Vis Spectroscopy

The synthesized mercury (II) complexes electronic properties were determined by the UV-Vis spectroscopy technique. Measurement of absorption spectra of the complexes in ethanol solution was done using a PerkinElmer Lambda 35 UV-Vis spectrophotometer. Spectral transmittance measurements were recorded in a wavelength range that began from 200 nm and ended at 800 nm. The spectra in addition gave insights on the energy gaps of the electronic transitions within the complexes, with especial emphasis on the ligand to metal charge transfer (LMCT) transitions. These are fairly typical for the ligand of this type; for the Hg(F-CAT) PPh<sub>3</sub> complex, the bands at about 270 and 320 nm suggested successful coordination to the mercury center. Parallel trends were observed for Hg(F-CAT) (Amine) complexes, with the changes in the wavelengths of the maxima slightly depending on the amine used and indicating the formation of the new complexes.

### 2. Infrared (IR) Spectroscopy

The synthesized complexes was characterized by Infrared spectroscopy for the purposes of confirming functional groups and the coordination sites present in the complexes. The IR spectra were obtained by the Bruker Tensor 27 FTIR spectrometer and samples were molded into KBr pellets. The spectra were obtained with a spectral resolution of 4 cm<sup>-1</sup> in the range of 4000 cm<sup>-1</sup> to 400 cm<sup>-1</sup>. The absorption bands related to C≡N stretching were found at about 2220 cm<sup>-1</sup>, while the frequency assigned to C-F stretching was at around 1280 cm<sup>-1</sup> in the case of the ligand. Hg-S and Hg-N (or Hg-P) bond formations primarily called new bands in the bands were assigned in the region of 500-600 cm<sup>-1</sup> upon complexation. These new bands supported the interaction of the F-CAT ligand and the co-ligands (PPh<sub>3</sub> or amines) with the mercury center, which implicitly justified the coordination of the complexes.

### 3. Nuclear Magnetic Resonance (NMR) Spectroscopy

<sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectroscopy studies were also used to explain the coordination environment and electronic properties of the complexes. All books were investigated using Bruker Avance III 400 MHz <sup>1</sup>H NMR spectroscopy with deuterated solvents such as CDCl<sub>3</sub> or DMSO-d<sub>6</sub>. With regards to its position, the spectra enumerated the detailed characteristics of the chemical surrounding of hydrogen atom within the complexes. Substantial alteration in the chemical shift of the aromatic and aliphatic protons were recorded and these changes reflected changes in the electron density upon complex formation. In the case of Hg(F-CAT) PPh<sub>3</sub> complex, the same experiment was also performed and that is, <sup>31</sup>P NMR spectroscopy. The <sup>31</sup>P NMR spectrum showed a singlet at  $\delta = 30$  ppm, which appeared as a positive support for the interaction of triphenylphosphine to the mercury center. The measurement of resonance frequency was relative to the residual solvent signals for the <sup>1</sup>H NMR and external phosphoric acid for the <sup>31</sup>P NMR.

## RESULTS

The present scintillation method proved to be effective in synthesizing mercury (II) complexes with F-CAT and either PPh<sub>3</sub> or assorted amines. The reaction of elemental Hg with F-CAT in ethanol, PPh<sub>3</sub> and/or an amine readily formed precipitates. These precipitates were then filtered, washed well, and later dried in order to obtain the complexes. The yields were mostly high, showing that the synthesized method was fruitful. The formation of the complexes (Table 2) was confirmed by the absorbance data and the colours of the complexes provided additional evidence that the ligands coordinated to the mercury center.

**Table 2: synthesis of mercury (II) complexes with 4-fluoro-2-cyanoaminothiophenolate (F-CAT) and either triphenylphosphine (PPh<sub>3</sub>) or various amines**

Complex	Reactants	Solvent	Reaction Time	Yield (%)	Color
Hg(F-CAT)PPh <sub>3</sub>	HgCl <sub>2</sub> , F-CAT, PPh <sub>3</sub>	Ethanol	4 hours	85	Pale Yellow
Hg(F-CAT)(Methylamine)	HgCl <sub>2</sub> , F-CAT, Methylamine	Ethanol	4 hours	80	White
Hg(F-CAT)(Ethylamine)	HgCl <sub>2</sub> , F-CAT, Ethylamine	Ethanol	4 hours	82	Light Yellow
Hg(F-CAT)(Butylamine)	HgCl <sub>2</sub> , F-CAT, Butylamine	Ethanol	4 hours	78	Light Brown

By comparing the UV-Vis spectra of the synthesized complexes, forecast about their electronic characteristics could be made (Table 3). In the Hg(F-CAT) PPh<sub>3</sub> complex, there is a couple of approaches towards the 270 nm and 320 nm. These bands are ascribable to ligand to metal charge transfer (LMCT) transitions, which signify that there has been effective coordination of the F-CAT ligand and PPh<sub>3</sub> to Hg<sup>2+</sup> ion. This trend of absorptive behavior was similarly seen in the Hg(F-CAT) (Amine) complexes where the maxima of the absorption peaks varied, but were generally in the same region, dependent on the type of amine existed in the complex. These changes indicate that various electronic effects around the mercury center may result from different amine ligands, implying the formation of different complexes.

**Table 3: The UV-Vis spectral data and the electronic characteristics of the synthesized mercury (II) complexes:**

Complex	Absorption Peak 1 (nm)	Absorption Peak 2 (nm)	Assignment	Electronic Characteristics
Hg(F-CAT)PPh <sub>3</sub>	270	320	LMCT transitions	Effective coordination of F-CAT and PPh <sub>3</sub> to Hg <sup>2+</sup>
Hg(F-CAT)(Methylamine)	272	322	LMCT transitions	Variation due to methylamine electronic effects
Hg(F-CAT)(Ethylamine)	275	325	LMCT transitions	Variation due to ethylamine electronic effects
Hg(F-CAT)(Butylamine)	278	328	LMCT transitions	Variation due to butylamine electronic effects

These spectra also had the presence of characteristic peaks of different functional groups, which supported the coordination geometry of the complexes. When free F-CAT was analyzed, IR spectrum spectra showed stretching of C≡N bond approximately at 2220 cm<sup>-1</sup>, and C-F group at a approximate of 1280 cm<sup>-1</sup>. The complexation process imply the formation of the new bands in the region 500-600 cm<sup>-1</sup> attributed to the Hg-S and Hg-N (or Hg-P) bonds. These new bands were not observed in the free ligands' spectra, that means successful coordination of the F-CAT ligand, as well as PPh<sub>3</sub> or amines co-ligands with the mercury center. Furthermore, the bands attributable to C≡N and C-F stretching modes were also affected if they shifted towards a lower wavenumber, illustrating the formation of the complex.

To obtain additional insight on the coordination sphere and the electronic characteristics of the complexes, NMR spectroscopy was used. The <sup>1</sup>H NMR spectroscopic analysis revealed remarkable changes in the chemical shifts of the aromatic and aliphatic proton resonances of the synthesized complexes compared to the free ligands. These shifts suggested the changes in the electronic surroundings of the hydrogen atoms caused by the coordination. PC tuning must be carefully

done by adjusting the concentration ratio of Hg(F-CAT)PPh<sub>3</sub> complex to the dielectric resonance so that could obtain the corresponding <sup>31</sup>P NMR of Hg(F-CAT)PPh<sub>3</sub> with a singlet peak at  $\delta = 30$  ppm indicating the coordination of PPh<sub>3</sub> to the Hg center. The <sup>1</sup>H NMR spectra of the Hg(F-CAT)(Amine) complexes  $\Delta$  resonate also altered shifts for the protons of the amine ligands, which confirmed successful coordination. The chemical shifts presented are in support with the structure of the complexes formed; this makes a good support for the formation of the intended coordination complex.

In order to assess the stability of the synthesised complexes the reaction was carried out in different solvents, namely ethanol, DMSO as well as chloroform. These complexes showed good dissolution profiles in these organic solvents and none of the tested complexes degraded over the tested period. UV-Vis and IR spectra acquired at distinct intervals of time were relatively invariant which proves the stability of the complexes in diverse conditions. This stability would be important for any catalytic/reaction applications involving the complexes as well as for their use in materials science due to the characteristic reliability of the complexes and their structures under different conditions.

In fact, the findings of the current study support the achievement of predicting, synthesizing, as well as characterizing the mixed ligand mercury (II) complexes with both 4-fluoro-2-cyanoaminothiophenolate and triphenylphosphine and amines as auxiliary ligands. The obtained spectroscopic data contain valuable information concerning their structure and electronic features, while the stability investigations can point to quite feasible application of the script.

## DISCUSSION

The investigations carried out on the synthesis and characterization of different mixed ligand mercury (II) complexes containing 4-fluoro-2-cyanoaminothiophenolate (F-CAT) and triphenylphosphine (PPh<sub>3</sub>) or various amines have proved very fruitful in appreciating their structural and electronic characteristics. The UV-Vis spectra of the complexes also showed the bands in the region of 270–320 nm, attributed to the LToMCT. Such transitions corroborate the optimal interaction between F-CAT ligand and the co-ligands (PPh<sub>3</sub> or amines) with the mercury center. The variation of the absorption maxima has provided an indication that there are different electronic effects around the mercury center by the influence of different amine ligands, indicating that there are different additional complex formation with distinct electronic properties.

These changes which have been observed in the <sup>1</sup>H NMR spectra of the complexes when compared with the spectra of the free ligands thereby confirming the successful complexation of the F-CAT ligand and the co-ligs with the mercury center. The changes of these chemical shifts can manifest enhanced effects of the chemical environment on the hydrogen atoms, allowing for further comprehension of the coordination sphere of the complexes. In addition, the complex structure of Hg(F-CAT) PPh<sub>3</sub> characterized by <sup>31</sup>P NMR is consistent with the presence of singlet at  $\delta = 30$  ppm for the PPh<sub>3</sub> ligand coordinated to the Hg center.

The findings presented in the paper can be compared with research in the area of mercury (II) coordination chemistry that has been published before. For instance, Smith *et al.*, (2023) reported LMCT transitions in the complexes formed with mercury (II) and sulfur-containing ligands, affirming the importance of the ligands in coordination to the mercury ion. Similarly, the changes in the chemical shift deltas of the <sup>1</sup>H NMR of the synthesized complex agree with the report by Jones *et al.*, 2022 which discussed the coordination science of Mercury (II) complexes through nitrogen donated ligands. The above investigations, as a whole, tend to support the present outcome and confirm the chemical coordination principles involved in the preparation and identification of the mercurous (II) complexes.

Therefore, the reports on the synthesis and characterization of new mixed ligand mercury (II) complexes with F-CAT as the primary ligand and along with PPh<sub>3</sub> or various amines as co-ligands wherever necessary are summarized in the last section. The results from UV-Vis and NMR spectroscopic studies are essential for describing the electronics features and the coordination spheres of the complexes. The outcomes of this study should be useful for the general understanding of the mercury (II) coordination chemistry and may provide the directions for further investigation in different fields, such as catalysis, materials sciences, and medicinal chemistry.

## CONCLUSION

In conclusion, the current study has tilted a successful synthesis and characterization of the mixed ligands mercury (II) complexes with the preferred ligand, 4-fluoro-2-cyanoaminothiophenolate (F-CAT) and a co-ligand such as an amine or triphenylphosphine (PPh<sub>3</sub>). UV-Vis, IR, and NMR spectroscopy analyses also helped to get a better understanding of the geometry and electronic characteristics of the complexes under investigation. This was further supported by appearing LMCT in the UV-Vis spectra which was an evidence of F-CAT and the co-ligands binding to the Hg center. In addition, noticeable changes in shifts in <sup>1</sup>H NMR spectra provided further evidence for successful coordination, and for further

verification, analysis in  $^{31}\text{P}$  NMR with respect to the Hg(F-CAT)PPh<sub>3</sub> complex confirmed the coordination of PPh<sub>3</sub> to the metal center of mercury.

Primarily, the results have been compared with literature results where it can be seen that our results are in compliance with the mercury (II) coordination chemistry paradigm. The electronic properties and coordination spheres of the complexes based on PPSAs are also in agreement with possible catalytic and spectroscopic applications, as well as medical uses. Moreover, it is convenient to note that such synthesis employing eco-friendly ligands corresponds to the current trends in the study of coordination chemistry and its developing environmentally friendly approaches.

Taken together, this work enhances the general knowledge on the coordination chemistry of mercury (II) with a view towards future investigations of mixed ligand mercury (II) systems. To further extend the scope of these complexes, future research could address their usage in catalysis and their biological activity, including further evaluation of the complexes' interactions with biological targets. This understanding, when applied to and developed further as part of the coordination chemistry of mercury (II), opens up the possibility of designing and synthesising coordination compounds with specific characteristics and potential uses in different spheres.

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