

Chemistry and applications of organotin (IV) complexes of Schiff bases emphasizing their structural and functional diversity

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Abstract

Organotin(IV) complexes of Schiff bases have emerged as a versatile class of compounds due to their structural diversity and broad functional applications, primarily facilitated by their ability to coordinate with metal centers in multiple oxidation states, which leads to distinctive geometric configurations, including tetrahedral, octahedral, and trigonal bipyramidal structures; these complexes demonstrate remarkable stability attributed to the electronic and steric factors of Schiff base ligands and exhibit significant biological activities such as antimicrobial, antitumor, and DNA-binding capabilities, with studies employing techniques like density functional theory (DFT) and molecular docking revealing detailed mechanistic insights into their electronic configuration, charge transfer properties, and interaction dynamics with biological macromolecules, while experimental evaluations underscore their reduced cytotoxicity compared to traditional chemotherapeutic agents like cisplatin and potential for enhanced therapeutic efficacy against drug-resistant strains, making them a promising frontier for innovative drug design and advanced material development

Keywords: Organotin (IV) complexes, Schiff bases, Structural diversity, Density functional theory (DFT), Biological activities, Therapeutic applications

Introduction

Organotin(IV) complexes of Schiff bases, derived from the condensation of primary amines with aldehydes or ketones, represent a unique intersection of synthetic chemistry and functional applications owing to their remarkable structural diversity spanning tetrahedral, octahedral, and trigonal bipyramidal geometries facilitated by the ligand's ability to coordinate through azomethine nitrogen, hydroxyl oxygen, or carboxylate groups, which not only stabilizes multiple oxidation states of tin but also imparts the complexes with exceptional versatility in fields such as catalysis, biomedicine, and materials science, as exemplified by their high catalytic efficiency in polymerization reactions and oxidative transformations (Nath & Saini, 2011), their potent antimicrobial and antitumor activities that often surpass conventional treatments like cisplatin due to lower cytotoxicity toward normal cells (Mansour et al., 2024), and their capacity to interact with biomolecules such as DNA and proteins via groove-binding or intercalative mechanisms, a property leveraged in molecular docking studies to explore anti-cancer and anti-microbial applications (Yang et al., 2016), while density functional theory (DFT) analyses have further illuminated the electronic and structural properties underpinning these complexes' reactivity and stability, paving the way for innovative developments in energy materials, such as dye-sensitized solar cells and conductive thermoelectric materials (Yusof et al., 2019), and contributing significantly to advancements in sustainable chemistry by utilizing environmentally benign synthetic routes and readily available starting materials, thus underscoring their potential as cost-effective, multifunctional agents in addressing global challenges spanning medical, industrial, and environmental domains (Kumar et al., 2024).

Statement of the research problem

The research regarding the organotin(IV) complexes with Schiff bases as ligands remained important within the inorganic and organometallic chemistry, because they can yield considerably diverse coordination geometries with a broad range of coordination energies (from trigonal bipyramidal to octahedral coordination modes), while the flexible donor site on the ligands (azomethine nitrogen, carboxylate oxygen, and phenolic oxygen) considerably affect their stabilization, reactivity, and electronic properties. Indeed, their biological activities such as anticancer, antibacterial and antifungal activities and the existing gaps in the theoretical understanding and mechanistic pathways behind their bioavailability, cytotoxicity, and environmental compatibility (Sirikci et al., 2015), (Yin et al., 2012) prompted the recent computational and experimental studies using advanced density functional theory (DFT) and molecular docking techniques that confirmed the presence of their imidazole-based ligands in the major biomolecular targets such as DNA/proteins, and simultaneously, allow to pinpoint the importance of the azomethine nitrogen in the oxidative-stress modulating properties and selective inhibition of various enzymes (Joshi et al., 2020), (Devi et al., 2021). In general, most of the tin complexes demonstrated high and potent pharmacological profiles, broad antimicrobial spectra and reduced environmental toxicity, but still presented an opportunity to develop palladium-free intermediate, that would allow the synthesis of substantial amounts of related ligands and organometallic compounds (Yin et al., 2012). However, other existing gaps are in their unique electronic and optical properties for sustainable development and medical innovation application, such as semiconductors, photovoltaic cells, and thermoelectrics - these all should also be addressed.

Statement of the research problem

As organotin(IV) complexes with Schiff base ligands that are well known for the coordination at the diverse donor atoms such as nitrogen, sulfur, and oxygen to produce very stable and geometrically versatile frameworks, their studies are significantly important in helping to provide insight into the electronic structures and geometric functional features related to the diversity in their applications in catalysis (Bhanuka et al., 2020), antimicrobial (Joshi et al., 2020), and anticancer (Yang et al., 2016) activities via interactions with biological targets such as DNA and proteins through groove-binding, intercalation, and covalent attachment mechanisms, however, there are still many combined synthetic challenges in producing them and problems with predicting their reactivity characterizations and aimed selectivity to specific biological targets accompanied by undesired cytotoxicities, this represents not only a fundamental challenge for the establishing of synthetic principles having generality but also for obtaining a broad psychobiological activity spectrum for them (Xiao et al., 2022) upon gaining this recent success by utilizing computational tools such as density functional theory (DFT) (Bhanuka et al., 2020) and molecular docking analyses (Joshi et al., 2020).

Review of relevant literature related to the study

Recent studies on organotin(IV) complexes of Schiff bases have extensively explored their structural and functional diversity, as Schiff base ligands formed by the condensation of aldehydes or ketones with primary amines act as versatile chelating agents capable of coordinating through donor atoms such as nitrogen, oxygen, and sulfur, resulting in stable frameworks with diverse geometries including tetrahedral, octahedral, and trigonal bipyramidal configurations that have been characterized through advanced spectroscopic techniques like IR, NMR, and X-ray diffraction, while density functional theory (DFT) analyses have significantly contributed to understanding their electronic configurations and reactivity, as evidenced by the synthesis of organotin complexes with quinazoline Schiff bases showing remarkable antimicrobial and anticancer properties owing to their ability to interact with biomolecules via groove-binding and partial intercalation mechanisms (Mansour et al., 2024), (Bhanuka et al., 2020); furthermore, theoretical studies of ONO-donor Schiff bases reveal that such complexes possess distinctive chemical reactivity descriptors and polarizabilities, which are key to tailoring their bioactivity, as demonstrated in studies utilizing Schiff base derivatives to create organotin complexes with significant antibacterial and antifungal effects against multidrug-resistant pathogens (Sirikci et al., 2015); additional investigations into organotin complexes derived from chromone Schiff bases indicate strong DNA-binding affinities, verified through molecular docking and gel electrophoresis, showcasing their potential as DNA-targeting therapeutic agents (Arjmand & Yousuf, 2013); studies on diorganotin (IV) Schiff base derivatives also highlight their distinct electronic and molecular configurations, enabling selective interaction with microbial enzymes and enhanced antiproliferative effects against cancer cells, which surpass traditional treatments like cisplatin in terms of efficacy and reduced cytotoxicity (Hong et al., 2014); similarly, research on Schiff bases containing pyridine rings has established their role in stabilizing trigonal bipyramidal and octahedral geometries in organotin complexes, which exhibit broad-spectrum antimicrobial activity and potential as eco-friendly

antifungal agents (Sedaghat et al., 2012); these findings collectively underscore the immense promise of organotin(IV) complexes as multifunctional agents in drug development, environmental remediation, and advanced materials, while emphasizing the need for continued research to address challenges related to synthetic scalability, biocompatibility, and targeted functionalization.

Research Gap related to the study

Recent structures of organotin(IV) complexes of Schiff bases have shown significant advances in their syntheses and characterizations at molecular scales, but considerable knowledge gaps remain in understanding the detailed mechanisms of their biological actions (i.e., DNA-binding, protein inhibition, and low cytotoxicity) and pharmacokinetics, including gender dependence in rodents; while Schiff base complexes are known for having high microbial, anticancer, and antioxidant properties their environmental studies have not progressed to the same standards in regards to structural stabilities in biological compartments, bioethics, and rapid molecular applications (Bhanuka et al., 2020; Mansour et al., 2024; Şirikci et al., 2015); such designs depend on greater integration of their unique structural fingerprints into multifunctional agents for advanced catalysis and energy materials (Yusof et al., 2019) as most in vitro and in vivo studies are irrational, with undesired or mischaracterized behavior of the organometallic catalyst, leading to ineffective generalizations; thus, the quest for understanding the environmental fate of organotin(IV)Schiff-br cation complexes is herein emphasized on slow and zero-speed release (poor solubility) of biocatalytic function and purity from chemical cooking.

Research Methodology

The methodology for investigating organotin(IV) complexes of Schiff bases involves a multifaceted approach encompassing the synthesis of these complexes through standard condensation reactions of Schiff base ligands—typically derived from aldehydes or ketones and primary amines—with organotin precursors under controlled reaction conditions, followed by detailed structural characterization using spectroscopic techniques such as FT-IR, NMR (¹H, ¹³C, ¹¹⁹Sn), and X-ray crystallography to elucidate their molecular geometries, coordination modes, and electronic configurations; subsequent theoretical analysis employs density functional theory (DFT) with advanced functionals like B3LYP and wB97XD, incorporating empirical dispersion corrections and polarizable continuum models to simulate solvent effects and calculate key molecular properties such as chemical reactivity descriptors, band gaps, and vibrational frequencies, with results corroborated by experimental data to validate computational models, while biological evaluation entails in vitro assays to determine antimicrobial, anticancer, and antioxidant activities against target organisms or cell lines such as *Staphylococcus aureus*, *Escherichia coli*, and MCF-7, often combined with molecular docking studies to explore interactions with biological macromolecules like DNA and proteins, revealing mechanisms such as intercalative binding and groove interactions, as demonstrated in the studies of Schiff base complexes with quinazoline ligands (Mansour et al., 2024), and further augmented by advanced techniques like Mössbauer spectroscopy and thermogravimetric analysis to assess their thermal stability and electronic configurations, while addressing gaps in environmental compatibility and synthetic scalability through iterative experimental optimizations and computational predictions (Bhanuka et al., 2020), ultimately aiming to establish robust structure-function correlations for the development of multifunctional organotin complexes suitable for biomedical and industrial applications (Devi et al., 2021).

Major objectives of the study

1. To synthesize organotin (IV) complexes using Schiff base ligands derived from aldehydes or ketones and primary amines, and to characterize their structural properties through advanced spectroscopic techniques (e.g., FT-IR, NMR, and X-ray crystallography) to elucidate their molecular geometries, coordination patterns, and electronic configurations.
2. To employ computational approaches such as density functional theory (DFT) with various functionals and solvent models for predicting chemical reactivity descriptors, molecular interactions, and vibrational frequencies, validating these theoretical insights through experimental observations.
3. To investigate the antimicrobial, anticancer, and antioxidant potentials of the synthesized organotin (IV) complexes via in vitro assays, molecular docking studies, and DNA/protein interaction analysis, with a focus on elucidating the mechanisms of biological activity, including intercalative and groove-binding interactions.
4. To establish correlations between the structural features of organotin (IV) complexes and their functional properties, aiming to optimize their applications in biomedical fields such as drug development, as well as in

industrial applications like catalysis and material science, while addressing challenges related to environmental impact and synthetic scalability.

Synthesize organotin (IV) complexes using Schiff base ligands derived from aldehydes or ketones and primary amines, and to characterize their structural properties through advanced spectroscopic techniques (e.g., FT-IR, NMR, and X-ray crystallography) to elucidate their molecular geometries, coordination patterns, and electronic configurations

The preparation of organotin(IV) complexes with Schiff base ligands involving the condensation of an aldehyde or ketone with a primary amine can be assumed to give either bidentate or tridentate coordination by donor atoms such as nitrogen and oxygen with their structural characterization accomplishment via inductively coupled plasma-optical emission spectrometry (ICP-OES) for their relative stabilities, FT-IR for bonding modes (Sn–O and Sn–N vibrations), DFT calculations predicting optimized geometries, and nuclear magnetic resonance (NMR) for their chemical environments (Abbas et al., 2024), X-ray diffraction for their bond distances delivering LUMO and HOMO within the extremes of the wall-to-wall distance or axial separations of the two bulky substituents that related preferred modes between structural configuration and the expectation of innate reactivity (Vinayak et al., 2018) that consistently supported electronic and steric interactions that showed DNA groove-binding for their respective selective antibacterial actions through ultra-high liquid sobitum (Yin et al., 2012); furthermore, their direct interactions with the bacterial cell wall have been shown to potentiate the antibacterial actions of these complexes with a significant mode of action inducing the structurally varied biomolecules (Hong et al., 2014) and their antimicrobial activity was also determined experimentally observing about an 86% growth inhibition of colon, stomach, and human breast and epidermoid carcinoma demonstrated B3LYP method use as in a shape selected site of twisted junks of concentrated reaction phenazines (Zhang et al., 2022) and comparison with and incorporation with phenazine or hydroxyl or hydroxy-chlorobenzaldehyde gave a similar indication towards potentiation unable to discover behavior of the ligand.

Employ computational approaches such as density functional theory (DFT) with various functionals and solvent models for predicting chemical reactivity descriptors, molecular interactions, and vibrational frequencies, validating these theoretical insights through experimental observations

Density functional theory (DFT) was used in the analysis of organotin(IV) derivatives evolving from schiff bases employing the advanced means of quantum chemical calculations at B3LYP/6-31G(d,p) or Def2-SVP levels of theory leading to molecular equilibration, electronic properties such as HOMO-LUMO energy gaps and chemical reactivity descriptors including chemical hardness, electronegativity, and global electrophilicity where time-dependent DFT (TD-DFT) analyses elucidated electronic transitions revealed in UV-visible spectroscopy and further validation through spectroscopic data such as FT-IR, NMR and X-ray diffraction techniques ensuring theoretical accurateness and thus validating the alignment with observed vibrational frequencies and structural parameters (Joshi et al., 2020), (Kaur et al., 2019) as recently presented where natural bond orbital (NBO) and molecular electrostatic potential (MEP) analyses identified the active of nucleophilic and electrophilic sites in favorable biological interactions including groove-binding and intercalative mechanism with DNA linking computational insights to biological efficacy where these tools advanced their applications in antimicrobial and anticancer therapy (Joshi et al., 2020), (Kaur et al., 2019) further allowing the interpretation of ligand-metal bonding in terms of AIM and NBO parameters with DFT affording an avenue to undertake a detailed exploration of trimethyltin and triethyltin-ligand interactions with experimental findings supported by AIM theoretical analysis (Butt et al., 2019).

The antimicrobial, anticancer, and antioxidant potentials of the synthesized organotin (IV) complexes via in vitro assays, molecular docking studies, and DNA/protein interaction analysis, with a focus on elucidating the mechanisms of biological activity, including intercalative and groove-binding interactions

The antimicrobial, anticancer, and antioxidant potentials of synthesized organotin(IV) complexes are primarily assessed through in vitro assays targeting bacterial and fungal strains, such as *Staphylococcus aureus*, *Escherichia coli*, and *Candida albicans*, and cancer cell lines like MCF-7 and HeLa, employing molecular docking studies to confirm binding modes—intercalative or groove-binding interactions with DNA—and experimental techniques like UV-Vis, fluorescence spectroscopy, and gel electrophoresis for DNA interaction studies, which consistently reveal that Schiff base-derived complexes exhibit enhanced biological activities compared to free ligands due to the stabilization of reactive intermediates by organotin moieties, as evidenced by the superior antibacterial efficacy and DNA-binding constants of complexes coordinated through azomethine nitrogen and phenolic oxygen, particularly in diorganotin(IV) compounds that display potent anticancer activity against breast and cervical cancer cells while demonstrating significant antioxidant properties via DPPH radical scavenging assays, further supported by

computational data correlating molecular structure to reactivity indices (Adeyemi et al., 2018), (Palanimurugan & Kulandaisamy, 2018), and (Arjmand & Yousuf, 2013).

Correlations between the structural features of organotin (IV) complexes and their functional properties, aiming to optimize their applications in biomedical fields such as drug development, as well as in industrial applications like catalysis and material science, while addressing challenges related to environmental impact and synthetic scalability

The structural features of organotin(IV) complexes, determined by their Schiff base ligands' coordination modes through nitrogen, oxygen, and sulfur donor atoms, directly influence their functional properties, as evidenced by their diverse geometries—ranging from trigonal bipyramidal to octahedral—and their strong correlation with biological activity, including antimicrobial, anticancer, and antioxidant effects, which are enhanced by electronic properties such as HOMO-LUMO energy gaps and steric stability derived from Schiff base chelation, while computational studies like DFT reveal key molecular interactions and charge transfer characteristics that explain experimental results; for instance, studies on triorganotin(IV) complexes exhibit superior antifungal activity due to optimized ligand-metal interactions (Joshi et al., 2020), while organotin complexes of hydrazone Schiff bases demonstrate significant cytotoxicity through intercalative and groove-binding interactions with DNA (Liu et al., 2017); similarly, the catalytic efficacy of these complexes in polymerization reactions is linked to their electronic configurations, making them viable in industrial and biomedical fields, yet challenges such as synthetic scalability, environmental impact, and fine-tuning of specific functional properties persist, emphasizing the need for integrated experimental and computational approaches to optimize their structural and functional capabilities for applications ranging from drug development to material science (Bhanuka et al., 2020), (Devi et al., 2021).

Discussion related to the study

The environmental impact and synthetic scalability of organotin(IV) complexes are critical considerations in their development for biomedical and industrial applications, as these complexes, synthesized from Schiff base ligands, often require environmentally sensitive reagents and solvents, with concerns about the toxicity of tin derivatives and their persistence in ecosystems due to the slow degradation rates of organotin compounds, necessitating the exploration of greener synthetic routes that utilize biocompatible ligands and non-toxic reaction conditions, as exemplified by studies where Schiff base ligands derived from amino acids and naturally occurring aldehydes significantly reduced the environmental footprint while retaining high catalytic and biological activity (Bhanuka et al., 2020); furthermore, efforts to enhance synthetic scalability include the use of microwave-assisted synthesis and flow chemistry techniques, which not only increase yield but also reduce energy consumption and reaction times, as demonstrated in the production of triorganotin(IV) complexes exhibiting superior antifungal properties (Joshi et al., 2020); however, the safe disposal and recycling of by-products, including tin oxides, remain a challenge that requires innovative approaches, such as ligand modifications that enable selective degradation of the complexes into less harmful derivatives, as highlighted in recent research where Schiff base hydrazones facilitated the complete mineralization of tin-containing residues (Devi et al., 2021); additionally, the development of water-soluble organotin complexes offers a promising avenue for reducing bioaccumulation and enhancing the environmental compatibility of these compounds, paving the way for their broader application in areas such as drug delivery and green catalysis (Liu et al., 2017).

Chemical implication associated with the study

The chemical implications of organotin(IV) complexes derived from Schiff bases encompass their unique coordination chemistry, which allows for versatile bonding modes, including bidentate and tridentate interactions through nitrogen, oxygen, and sulfur donor atoms, resulting in diverse geometries such as trigonal bipyramidal and distorted octahedral structures, and these configurations significantly influence their electronic properties, reactivity, and stability, as evidenced by density functional theory (DFT) studies that reveal the relationships between their molecular orbitals, polarizabilities, and chemical reactivity descriptors like global electrophilicity and hardness, thereby providing insights into their catalytic, biological, and material science applications (Bhanuka et al., 2020); furthermore, the

electron-rich environments created by the Schiff base ligands enhance the metal-ligand charge transfer properties, which are critical in photocatalysis and electronic applications, while the complexes exhibit strong DNA-binding affinities via intercalative and groove-binding mechanisms, underscoring their potential as anticancer agents, as demonstrated in studies where specific organotin(IV) derivatives exhibited potent cytotoxicity against drug-resistant tumor cells (Joshi et al., 2020); additionally, the synthetic scalability and environmental impact of these complexes remain a challenge, as traditional synthesis routes often rely on halogenated solvents and metal precursors that produce persistent byproducts, prompting the exploration of greener synthetic methods, including solvent-free reactions and the use of bio-derived ligands, which have successfully reduced toxicity without compromising the structural integrity or reactivity of the complexes, as seen in studies utilizing amino acid-derived Schiff bases (Devi et al., 2021); lastly, the ability of these complexes to exhibit tunable properties through ligand modification highlights their applicability in fields ranging from catalysis, where they accelerate polymerization reactions, to optoelectronic devices, where their narrow bandgaps and high electron delocalization enable enhanced performance in energy materials and sensors (Sánchez-Vergara et al., 2021).

Conclusion

The conclusion emphasizes that organotin(IV) complexes derived from Schiff bases exhibit remarkable structural and functional diversity due to their versatile coordination modes involving nitrogen, oxygen, and sulfur donor atoms, enabling the formation of diverse geometries such as trigonal bipyramidal and distorted octahedral structures that significantly influence their electronic, biological, and catalytic properties, as these complexes demonstrate strong antimicrobial, anticancer, and antioxidant activities through mechanisms like DNA intercalation and groove-binding interactions, while advanced computational studies such as density functional theory (DFT) reveal their electronic configurations, reactivity indices, and molecular interactions that correlate with experimental observations, thereby advancing their application potential in fields such as drug development, polymerization catalysis, and optoelectronics, yet challenges remain in optimizing synthetic scalability, reducing environmental impact, and tailoring specific functional properties, which underscores the need for continued research integrating innovative synthetic methods, eco-friendly practices, and multidisciplinary approaches to fully harness their potential in both biomedical and industrial domains.

Scope for further research and limitations of the study

The scope for further research on organotin(IV) complexes of Schiff bases lies in exploring their untapped potential in advanced biomedical applications, such as targeted drug delivery systems and photodynamic therapy, as well as in industrial sectors like green catalysis and energy storage, while addressing the limitations of the study, including the narrow range of Schiff base ligands used, the need for more comprehensive investigations into their long-term environmental impact and bioaccumulation, and the challenges in achieving synthetic scalability with eco-friendly methods, which require the development of novel ligands with enhanced stability, biocompatibility, and specificity for desired applications, alongside more robust computational models and experimental techniques to predict and verify their interactions, reactivity, and structural adaptability under diverse conditions, thereby paving the way for multidisciplinary advancements that integrate chemistry, biology, and materials science to overcome these limitations and fully utilize the structural and functional diversity of these complexes.

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