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Synthesis and Characterization of Triethanolaminate Derivatives of Tributyltin

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Abstract

Triethanolaminate derivatives of tributyltin are an important group of organotin compounds, known for their diverse chemical properties, structural integrity, and wide-ranging applications. This review focuses on how these compounds are synthesized through coordination reactions involving tributyltin precursors and triethanolamine, leading to the formation of Sn–O–N bonded complexes with distinct geometries. By employing various spectroscopic, thermal, and elemental techniques for characterization, we gain valuable insights into their bonding environments and molecular structures. These derivatives are recognized for their significant biological activities, such as antimicrobial and cytotoxic effects, which stem from the reactivity of the tin center and the chelating properties of triethanolamine. Moreover, their contributions to material science especially as catalysts, stabilizers, and surface-active agents highlight their importance in industrial applications. However, there are ongoing concerns about their environmental persistence, potential for bioaccumulation, and toxicological effects, which align with the broader challenges associated with organotin compounds. The review stresses the importance of responsible use, the need for better synthetic methods, and the development of less toxic alternatives to promote safer and more sustainable practices.

Keywords*:* Tributyltin derivatives, Triethanolamine complexe, Organotin chemistry; Synthesis and characterization, Environmental toxicity.

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Introduction

Tributyltin (TBT) derivatives, a type of organotin compound, have been recognized for their various applications across industrial, agricultural, and biomedical sectors, largely due to their strong Lewis acidity and their ability to create stable bonds with heteroatoms (Goswami & Singh, 2017). Yet, the traditional use of TBT compounds has raised serious environmental and toxicological issues, including endocrine disruption, bioaccumulation, and harm to aquatic ecosystems. This has prompted scientists to look for safer, ligand-modified alternatives (Antizar-Ladislao, 2008). One promising method involves pairing tributyltin with multidentate ligands like triethanolamine (TEA), which can help mitigate toxicity while still ensuring effective functionality. Triethanolamine is a flexible chelating ligand that includes both nitrogen and oxygen donor atoms, allowing it to coordinate in bi-, tri-, or tetradentate modes. This capability leads to the formation of stable organotin complexes (Pellerito & Nagy, 2002). When it reacts with tributyltin halides or oxides, it generates triethanolaminate derivatives of tributyltin, which often show enhanced thermal stability, different reactivity, and better solubility than their original compounds (Tiekink, 2008). The synthesis usually involves ligand substitution, condensation, or alcoholysis reactions under mild conditions, which helps in creating the Sn–O and Sn–N bonds that are key to these complexes. The characterization of tributyltin–triethanolaminate derivatives is based on a blend of spectroscopic and analytical techniques. Fourier Transform Infrared (FTIR) spectroscopy is particularly useful for identifying Sn–O and Sn–N stretching vibrations. Meanwhile, ^1H, ^13C, and notably ^119Sn NMR spectroscopy offer valuable insights into the electronic environment of the tin center (Gielen & Tiekink, 2005). To confirm the molecular composition and purity, mass spectrometry and elemental analysis are employed. Additionally, X-ray crystallography can sometimes provide detailed structural information, including coordination geometry and the formation of chelate rings. There's been a surge of interest in organotin chemistry lately, especially regarding how ligand design can shape the structural, electronic, and biological behavior of tin complexes. Triethanolaminate derivatives of tributyltin have become a hot topic because the flexible, multidentate ligand TEA can really change the coordination geometry and reactivity of the organotin center (Gielen *et al*., 2008). The stable Sn–O and Sn–N bonds that form in these complexes not only enhance their thermal and hydrolytic stability but also affect how they interact with biomolecules, which is why they're so relevant in the realm of medicinal organometallic chemistry (Tiekink, 2012). Additionally, ligand-modified tributyltin compounds have emerged as promising controlled antimicrobial agents. By carefully adjusting the ligand environment, we can lower nonspecific toxicity while still maintaining the desired biological activity (Bokhari *et al*., 2019). These compounds are also being investigated for their catalytic potential in processes like esterification, transesterification, and polymerization reactions, where TEA coordination boosts both the robustness and recyclability of the catalyst (Amaral *et al*., 2010). Moreover, advancements in computational chemistry have provided valuable insights into the electronic structure, ligand binding energies, and preferred coordination motifs of tributyltin–TEA complexes (Alaghaz *et al*., 2014). The study and development of triethanolaminate derivatives of tributyltin is becoming an exciting field in organometallic research. This growth is fueled by the demand for organotin compounds that are not only structurally adaptable and functionally diverse but also more environmentally friendly.

Chemical Background

Organotin compounds are a significant part of organometallic chemistry, where tin (Sn) atoms are bonded to one or more organic groups. Their general formula, R_nSnX_{4-n}, indicates how many organic substituents (R) and inorganic or organic anions (X) are attached to the tin atom (Gielen & Tiekink, 2005). A notable example is tributyltin (TBT) derivatives, which have three butyl groups linked to tin. These compounds show unique chemical properties because of their strong Lewis acidity, varying coordination geometry, and ability to interact with different donor atoms like oxygen, nitrogen, and sulfur (Pellerito & Nagy, 2002). The electrophilic nature of the tin center allows tributyltin compounds to create stable complexes with multidentate ligands, which affects their structural, thermal, and biological properties. The coordination chemistry of organotin compounds is determined by the hybridization state of tin and the electronic demands posed by the ligands. TBT species often adopt geometries that are four-, five-, or six-coordinate, including arrangements like trigonal bipyramidal and octahedral, which depend on the denticity of the ligands and any steric constraints (Tiekink, 2008). This versatility in coordination gives organotin compounds a wide range of reactivity, making them valuable in catalysis, materials chemistry, and biomedical research. Triethanolamine (TEA) is a widely recognized chelating ligand, featuring three hydroxyl groups and a tertiary amine. This composition allows it to function as a bi-, tri-, or tetradentate ligand (Pellerito *et al*., 2006). One of the key advantages of TEA is its capacity to form five- or six-membered chelate rings, which enhances stability when it coordinates with metal centers. When TEA interacts with tributyltin moieties, the resulting complexes often display Sn–O and Sn–N bonds. These bonds modify the electronic environment of the tin atom, which can influence the physicochemical and biological properties of the derivatives (Alaghaz *et al*., 2014).

Synthesis of Triethanolaminate Derivatives of Tributyltin

The synthesis of triethanolaminate derivatives from tributyltin generally takes place via ligand-substitution or alcoholysis reactions that utilize tributyltin chloride (Bu_3SnCl) or tributyltin oxide (Bu_3Sn_2O). Triethanolamine (TEA), which has three hydroxyl groups and one tertiary nitrogen, reacts quite easily with tributyltin precursors when heated gently, forming stable Sn–O and Sn–N coordinated complexes (Pellerito & Nagy, 2002).

•General Reaction Pathway

1. from Tributyltin Chloride:

$$Bu_3SnCl + H_3\,TEA \xrightarrow[\text{Heat}]{\text{Base}} Bu_3Sn\,(TEAH_2) + HCl$$

Often, a base like pyridine or triethylamine is added to neutralize the HCl that's released and help the reaction reach completion.

2. From Tributyltin Oxide:

$$(Bu_3Sn)_2O + 2H_3TEA \xrightarrow{\Delta} 2Bu_3Sn\,(TEAH_2) + H_2O$$

This alcoholysis method is favored because it produces fewer by-products and achieves higher yields (Tiekink, 2008).

The reaction typically takes place in refluxing toluene, ethanol, or benzene, where TEA coordinates through its oxygen and nitrogen donor atoms to create chelated structures (Gielen *et al*., 2008). The resulting complexes can show either bidentate or tridentate coordination, which depends on the stoichiometry and the specific reaction conditions. The formation of Sn–O and Sn–N bonds enhances stability and alters the steric and electronic environment around the tin center (Alaghaz *et al*., 2014).

Characterization of Tributyltin–Triethanolaminate Derivatives

It's crucial to verify ligand coordination, structural geometry, purity, and bonding modes. To get a clear picture of the Sn–O and Sn–N interactions that occur during complexation, a mix of spectroscopic, analytical, and structural techniques is typically used.

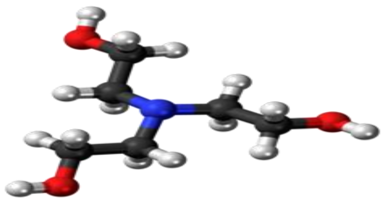
A.Fourier Transform Infrared (FTIR) spectroscopy: The first sign of coordination can be seen through changes in the stretching frequencies of O–H, C–O, and C–N groups. The emergence of specific bands in the 400–650 cm^{-1} range, which relate to Sn–O and Sn–N vibrations, confirms that triethanolamine has chelated to the tributyltin center (Pellerito & Nagy, 2002). If the free O–H stretching band reduces or disappears, it suggests deprotonation has occurred, leading to the formation of the Sn–O bond (Tiekink, 2008).

B.Nuclear Magnetic Resonance (NMR) spectroscopy: Discover the ultimate tool for understanding tin coordination environments! The ^1H and ^13C NMR spectra reveal shifts in the chemical signals of TEA's hydroxyl and methylene groups when they form complexes, suggesting changes in their electronic surroundings (Gielen & Tiekink, 2005). The ^119Sn NMR chemical shift is especially telling: its broad sensitivity range makes it possible to accurately identify the tin coordination number. Generally, four-coordinated tin shows up between –60 to –200 ppm, while five- or six-coordinated species can be found in the range of –200 to –400 ppm (Alaghaz *et al*., 2014).

C.Mass spectrometry (MS): We can confirm the molecular structure, fragmentation patterns, and ligand binding by looking at identifiable peaks that relate to tributyltin–TEA units. Additionally, elemental analysis is key to ensuring the purity of the compounds and checking the stoichiometric ratios of carbon, hydrogen, nitrogen, and tin in the complexes.

D.Single-Crystal X-Ray Diffraction (Scxrd): This provides a three-dimensional perspective of the molecular structure. It highlights the coordination geometry, bond lengths, the formation of chelate rings, and intermolecular interactions, giving a clear confirmation of the structure (Tiekink, 2012).

Structural Feature



Tributyltin–triethanolaminate derivatives showcase some distinctive structural traits that stem from the interaction between the organotin center and the multidentate triethanolaminate (TEA) ligand. Triethanolamine usually serves as a tridentate or tetradentate ligand, coordinating through its nitrogen atom along with one or more oxygen atoms from hydroxyl groups. This setup stabilizes the organotin part through chelation (Gielen & Tacke, 2019). In these derivatives, the tin atom typically has a coordination environment that is either five- or six-coordinate, influenced by the extent of ligand substitution and the steric hindrance from the butyl groups (Tacke & Böhme, 2017). The Sn–O and Sn–N bond lengths are crucial for determining the molecular geometry, often resulting in distorted trigonal bipyramidal or octahedral configurations (Pellerito & Nagy, 2002). When three butyl substituents are attached to the tin center, they bring about a notable increase in hydrophobicity and steric bulk, which significantly affect both the reactivity and the overall molecular shape. Infrared and NMR spectroscopic studies usually validate coordination by observing shifts in the ν(Sn–O) and ν(Sn–N) bands, along with specific ^119Sn NMR signals that suggest changes in coordination number (Gielen *et al*., 2008). These coordinated structural characteristics are essential in determining the chemical behavior, stability, and possible biological activity of the resulting organotin–TEA complexes.

Biological and Material Applications

Tributyltin–triethanolaminate derivatives are fascinating compounds that have a wide range of biological and material applications, thanks to their unique organometallic structure and impressive coordination stability. On the biological front, these complexes have shown strong antimicrobial and antifungal properties. This effectiveness comes from the way organotin centers can interfere with cellular metabolism and disrupt membrane integrity (Gielen & Tiekink, 2005). Their ability to interact with biomolecules like proteins and enzymes boosts their cytotoxic effects, positioning them as promising candidates for anticancer research (Nagy & Pellerito, 2005). Tributyltin derivatives hold a valued place in materials science due to their durable thermal stability and their ability to create long-lasting polymeric networks. They act as catalysts and stabilizers in the processing of PVC, enhancing its resistance to degradation and improving its mechanical properties (Tacke & Böhme, 2017). Additionally, their strong Sn–O bonding capability makes them ideal for use in surface coatings and anticorrosive formulations, where durability over time is crucial (Gielen & Tacke, 2019). This unique blend of biological and material properties expands their significance across both industrial and scientific sectors.

Environmental and Toxicological Considerations

Tributyltin–triethanolaminate derivatives, much like other organotin compounds, raise serious environmental and health concerns because they stick around for a long time, accumulate in living organisms, and are highly reactive biologically. These organotin compounds have a tendency to cling to sediments and organic matter in water, which means they can linger in the environment and build up in aquatic food chains (Antizar-Ladislao, 2008). Tributyltin (TBT), in particular, is linked to endocrine-disrupting effects, especially causing imposex in mollusks, prompting global regulatory measures (Gibbs & Bryan, 1996). While modifying it with triethanolamine might change its solubility and reactivity, the tin component still remains toxic. Toxicological studies show that organotin complexes can mess with mitochondrial function, disrupt oxidative balance, and throw off cytokine regulation, which can lead to immunotoxicity and neurotoxicity (Sousa *et al*., 2020). In mammals, being exposed to tributyltin derivatives has been associated with liver damage, reproductive issues, and metabolic problems due to the activation of nuclear receptors like PPARγ (Grün, 2014). The environmental breakdown of these compounds can be quite slow, raising worries about long-term contamination, particularly in aquatic ecosystems.

Conclusion

Tributyltin–triethanolaminate derivatives are an essential category of organotin complexes that have notable chemical, structural, and functional significance. Their creation involves coordinating tributyltin with triethanolamine, resulting in stable Sn–O–N frameworks that improve both their reactivity and practical applications. Characterization studies using various spectroscopic and analytical techniques have validated their unique bonding patterns and coordination geometries. These derivatives have exhibited promising biological activities, including antimicrobial and cytotoxic properties, as well as valuable uses in catalysis and polymer stabilization. However, the potential benefits are tempered by serious environmental and toxicological concerns, particularly due to the persistence and bioaccumulation of organotin compounds. Thus, it’s vital to handle them with care, use them in a regulated manner, and explore safer alternatives. Future research should concentrate on refining synthesis processes, reducing toxicity, and looking into greener alternatives to ensure a balance between functionality and environmental safety. In summary, these derivatives are scientifically significant but need to be applied thoughtfully and studied further.

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