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The Bruker AXS SMART CCD*:* Technology Analysis Crystal Structure of Bis (Trimethyltin) Croconate $[(CH_3)_3Sn]_2C_5O\ 2H_2O$

Asrial[1], Haryanto[1], Asmiyunda[1]
[1] Department of Chemistry Education, Faculty of Teaching and Education, Universitas Jambi, Jambi, Indonesia

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ABSTRACT

Purpose of the study: This study aimed to synthesize and characterize a novel organotin oxocarbon complex, namely bis(trimethyltin) croconate dihydrate $[(CH_3)_3Sn]_2C_5O_5 \cdot 2H_2O$, and to investigate its molecular geometry, coordination behavior, supramolecular arrangement, and spectroscopic properties.

Methodology: The compound was synthesized through a solution reaction between sodium croconate and trimethyltin chloride under atmospheric conditions at room temperature. Structural characterization was conducted using single-crystal X-ray diffraction analysis with a Bruker AXS SMART CCD-System diffractometer and refined using the SHELXS-97 software package. Additional characterization techniques included FTIR spectroscopy, CHN elemental analysis, and ^{1}H- and ^{13}C-NMR spectroscopy.

Main Findings: The synthesized compound crystallized in the orthorhombic system with the Fddd space group and formed bright yellow needle-shaped crystals. Structural analysis revealed that the croconate dianion acts as a bidentate bridging ligand connecting two trimethyltin groups. Each tin atom exhibits pentacoordination with distorted trigonal bipyramidal geometry. Bond length analysis confirmed π-electron delocalization within the croconate ring, indicating aromatic character. Hydrogen bonding interactions between coordinated water molecules and croconate oxygen atoms generated an extended supramolecular network. FTIR and NMR spectra further supported the formation of the target complex, while elemental analysis confirmed agreement between theoretical and experimental compositions.

Novelty/Originality of this study: This study reports the successful synthesis and comprehensive crystallographic characterization of bis(trimethyltin) croconate dihydrate, a croconate-based organotin complex that has rarely been explored. The research provides new insights into the coordination behavior of croconate ligands toward trimethyltin centers, the formation of hydrogen-bonded supramolecular structures, and the role of π-electron delocalization in stabilizing organotin oxocarbon frameworks.

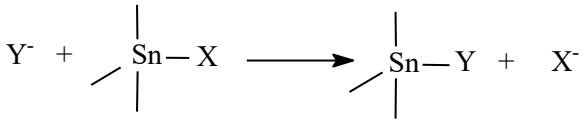
Corresponding Author:
Asrial,
Department of Chemistry Education, Faculty of Teaching and Education, Universitas Jambi,
Jl. Lintas Jambi-Ma.Bulian, Muaro Jambi, Jambi, 36361, Indonesia
Email: asrial@unja.ac.id

1. INTRODUCTION

Organotin compounds are a class of organometallic compounds characterized by the presence of one or more tin–carbon (Sn–C) bonds. These compounds are predominantly anthropogenic in origin, although certain species such as methyltin may also be naturally formed through environmental biomethylation processes [1]-[4].

In general, organotin compounds contain tin in the +4 oxidation state and can be represented by the formula RnSnXm, where *R* denotes alkyl or aryl groups (e.g., methyl, butyl, phenyl, or octyl), *X* represents an anionic ligand (e.g., Cl, OH, O, or other functional groups), and *n* ranges from 1 to 4 [5]-[9]. Due to their versatile chemical and physical properties, organotin compounds have been widely utilized in numerous industrial and agricultural applications, including as biocides, antifouling agents in marine paints, heat and light stabilizers for polyvinyl chloride (PVC), catalysts in polyurethane production, and protective agents for glass surfaces from chemical etching [10]-[13]. Their extensive applications have stimulated continuous interest in the synthesis and structural investigation of new organotin derivatives with unique coordination behavior and physicochemical properties [14]-[20].

Among the various organotin compounds, trimethyltin chloride, (CH3)3SnCl, has attracted considerable attention because of its high reactivity and ability to undergo nucleophilic substitution reactions. Structurally, trimethyltin chloride crystallizes in the C2 space group and adopts a geometry approaching trigonal bipyramidal coordination, in which the three methyl groups occupy the equatorial positions [21]. This compound appears as a white crystalline solid, is readily sublimed, and exhibits significant toxicity. The chloride ligand in trimethyltin chloride can be easily substituted by various nucleophilic species, including hydroxide, alkoxide, carboxylate, and other donor ligands, leading to the formation of diverse organotin complexes with distinct structural characteristics. This compound is a toxic, white crystalline substance that is easily sublimed and readily undergoes nucleophilic substitution according to equation (1) below, where Y is the anion HO, RO, R_2MO, R_3N, RCOO-, R, H and R_4Sn [21].



(1)

In particular, the chlorine atom can be displaced by oxygen-donor ligands or metal-containing species, facilitating the formation of stable coordination compounds with interesting molecular architectures and potential functional properties [22]. The ability of organotin compounds to form flexible coordination geometries has made them attractive for crystal engineering and coordination chemistry studies [23], [24].

Croconic acid (H2C5O5), first synthesized by Gmelin in 1825, is one of the most important members of the oxocarbon family. Its dianion, croconate (C5O52−), possesses remarkable aromatic character arising from its planar cyclic structure and extensive π-electron delocalization [25], [26]. The croconate ion belongs to the oxocarbon series consisting of deltate, squarate, croconate, and rhodizonate ions, which generally follow the formula CnO2n2− [27]. Structurally, the croconate dianion belongs to the D2h point group and exhibits strong infrared absorption bands around 1500 cm−1 due to the stretching vibration of the carbonyl groups [28]. Oxocarbon compounds have attracted increasing attention because of their unique electronic delocalization, coordination flexibility, and potential applications in supramolecular chemistry, nonlinear optical materials, and molecular electronics. In addition, the strong electron-accepting ability of croconate ligands enables the formation of coordination compounds with interesting structural and electronic properties [29].

Despite the growing interest in oxocarbon chemistry, studies concerning croconate-based organotin compounds remain relatively limited. Previous investigations have predominantly focused on deltate and squarate derivatives, while croconate complexes, particularly those involving trimethyltin moieties, have received far less attention in terms of synthesis, crystal structure analysis, and spectroscopic characterization [30].

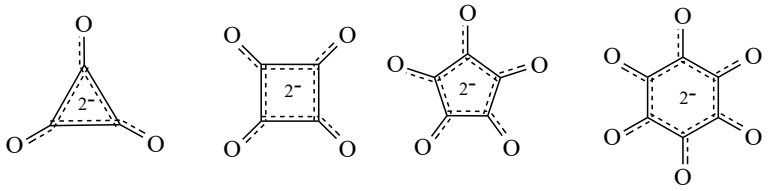


Figure 1. Oxocarbon anions (a) deltat, (b) squarate, (c) croconate and (d) rhodizonate

Since the first synthesis reported by Braga and co-workers, only a limited number of croconate derivatives have been described in the literature, indicating a significant research gap in understanding the coordination behavior and structural properties of croconate–organotin systems. Furthermore, detailed studies regarding the interaction between croconate ligands and trimethyltin groups, especially in hydrated crystalline forms, are still scarce. Most previous studies focused mainly on general oxocarbon coordination compounds without specifically examining the structural influence of trimethyltin substitution on croconate frameworks [31].

Therefore, this study aims to synthesize and characterize a novel organotin croconate complex, namely bis(trimethyltin) croconate dihydrate, [(CH3)3Sn]2C5O5·2H2O. The novelty of this research lies in the successful preparation and comprehensive characterization of a trimethyltin-based croconate crystal, which has rarely been reported in previous studies. This research specifically addresses the existing gap related to the limited availability of structural and spectroscopic data on croconate-containing organotin complexes. Through synthesis and characterization analyses, this study contributes to expanding the understanding of organotin–oxocarbon coordination chemistry, particularly regarding molecular structure, ligand coordination behavior, and intermolecular interactions in hydrated organotin crystals. The findings are expected to provide new insights for the future development of functional organotin materials and enrich the existing literature on oxocarbon-derived coordination compounds.

2. RESEARCH METHOD

All chemicals used in this study were of analytical grade and employed without further purification. Distilled water was used as the reaction solvent throughout the synthesis process. The main reagents consisted of trimethyltin chloride, $(CH_3)_3SnCl$, and sodium croconate, $Na_2C_5O_5$.

The structural characterization of the synthesized bis(trimethyltin) croconate dihydrate, $[(CH_3)_3Sn]_2C_5O_5\cdot 2H_2O$, was carried out using single-crystal X-ray diffraction analysis with a Bruker AXS SMART CCD-System diffractometer at the Inorganic Chemistry Laboratory, Magdeburg University, Germany. The crystal structure solution and refinement were performed using the SHELXS-97 program package developed by Sheldrick [32]. The Bruker AXS SMART CCD-System diffractometer is an advanced single-crystal X-ray diffraction (SCXRD) instrument widely used for determining the three-dimensional molecular and crystal structures of crystalline materials with high precision [33], [34]. This instrument operates by directing monochromatic X-rays onto a single crystal sample and measuring the diffraction patterns generated when the X-rays interact with the electron density within the crystal lattice. The diffraction data obtained are subsequently processed computationally to determine atomic positions, bond lengths, bond angles, molecular geometry, crystal symmetry, and intermolecular interactions in the crystal structure. The Bruker AXS SMART system is equipped with a CCD (Charge-Coupled Device) detector, which enables rapid and highly sensitive collection of diffraction data [35]. Compared with conventional point detectors, CCD detectors are capable of simultaneously capturing a large number of diffraction spots, resulting in faster data acquisition, improved sensitivity, and higher structural resolution [36]-[39]. This capability is particularly important for organometallic compounds such as bis(trimethyltin) croconate because such compounds often exhibit complex coordination geometries and weak intermolecular interactions that require accurate structural determination. In this study, the Bruker AXS SMART CCD-System diffractometer was used to analyze the single crystals of bis(trimethyltin) croconate $[(CH_3)_3Sn]_2C_5O_5\cdot 2H_2O$ obtained from the crystallization process. The diffraction data generated by the instrument allowed determination of important crystallographic parameters, including the orthorhombic crystal system, the Fddd space group, unit cell dimensions, atomic coordinates, coordination geometry around the tin atom, and hydrogen-bonding interactions within the crystal structure.

Infrared (IR) spectra were recorded in KBr pellets using a Perkin-Elmer System 2000 FTIR spectrometer in order to identify the functional groups and coordination interactions within the compound. Elemental composition analyses for carbon, hydrogen, and nitrogen (CHN) were conducted using a LECO CHNS-932 Elemental Analyzer to verify the purity and empirical composition of the synthesized complex. The synthesis of bis(trimethyltin) croconate dihydrate was performed under normal atmospheric conditions at room temperature based on the reaction shown in Equation (2):

$$Na_2C_5O_5 + 2(CH_3)_3SnCl + 2H_2O \rightarrow [(CH_3)_3Sn]_2C_5O_5 \cdot 2H_2O + 2NaCl \qquad (2)$$

Initially, 2 mmol of sodium croconate ($Na_2C_5O_5$) were dissolved in distilled water under continuous stirring while gently heated to ensure complete dissolution. Subsequently, 4 mmol of trimethyltin chloride ($(CH_3)_3SnCl$), previously dissolved in water, were added dropwise into the hot sodium croconate solution while maintaining constant stirring. The resulting bright yellow solution was continuously heated and stirred for approximately 1 h to promote the formation of the organotin croconate complex.

After completion of the reaction, the solution was filtered to remove any insoluble impurities. The filtrate was then stored in a dark environment for 24 h to minimize possible photodegradation and to facilitate initial crystallization. Following this period, an additional 4 mmol of trimethyltin chloride crystals were introduced into the filtrate, and the mixture was stirred continuously until all solids had completely dissolved. The resulting solution was filtered once again and allowed to stand undisturbed for several days. Bright yellow needle-shaped crystals gradually formed from the solution. To optimize crystal growth and obtain crystals suitable for single-crystal X-ray diffraction analysis, the crystallization vessel was maintained in a light-free environment for three days. The final product, bis(trimethyltin) croconate dihydrate, $[(CH_3)_3Sn]_2C_5O_5\cdot 2H_2O$, was successfully obtained

as bright yellow needle-like crystals with a yield of 0.28 g (28.70%). The synthesized compound was found to be soluble in water and exhibited a melting point of 256.00 °C.

The crystallographic data obtained from X-ray diffraction measurements were processed and refined using the SHELXS-97 software package (Sheldrick, 1997). Infrared spectral data were interpreted based on characteristic absorption bands associated with carbonyl groups, Sn–C vibrations, and ligand coordination modes. The CHN elemental analysis results were compared with theoretical values to confirm the molecular composition and purity of the synthesized compound.

3. RESULTS AND DISCUSSION

The successful growth of single crystals of bis(trimethyltin) croconate dihydrate, $[(CH_3)_3Sn]_2C_5O_5 \cdot 2H_2O$, indicates that the reaction between trimethyltin chloride and sodium croconate proceeded effectively and produced a thermodynamically stable coordination compound. The crystallization process carried out in a dark environment for three days at room temperature was essential for controlling the rate of nucleation and crystal growth. Slow crystallization under light-free conditions minimized structural defects and possible photochemical disturbances, thereby enabling the formation of high-quality single crystals suitable for X-ray diffraction analysis. The bright yellow transparent needle morphology observed in the obtained crystals also suggests a high degree of crystallinity and uniform molecular packing within the crystal lattice.

Table 1. Crystallographic data of bis(trimethyltin)croconate $[(CH_3)_3Sn]_2C_5O_5\ 2H_2O$

Crystal System	Ortorombik	
Space Group	Fddd	
Cell Parameters	a = 10,6209(10) Å	
	b = 24,2110(15) Å	α = β = γ
	c = 28,1090(2) Å	=90,00°
Cell Volume	7228,0(10) Å^3	
Crystal Size	0,64 Å x 0,43 Å x 0,36 Å	
Measurement Temperature	173(2),00 °K	

Based on the crystallographic data presented in Table 1, the synthesized compound crystallizes in the orthorhombic crystal system with the Fddd space group. The orthorhombic symmetry indicates a highly ordered arrangement of molecules within the crystal lattice. The relatively large unit cell volume of 7228.0(10) Å³ suggests that the crystal packing is influenced not only by coordination interactions between tin and croconate ligands but also by intermolecular interactions, particularly hydrogen bonding involving coordinated water molecules. The presence of the Fddd space group further demonstrates that the compound possesses a high degree of symmetry and regular molecular repetition throughout the crystal structure, contributing significantly to crystal stability.

The molecular structure shown in Figure 2 reveals that the croconate dianion acts as a bridging bidentate ligand connecting two trimethyltin fragments. The two trimethyltin groups occupy opposite sides of the croconate ring, forming a dinuclear organotin complex. This coordination mode confirms the ability of the croconate ion to function as an electron-delocalized oxygen donor ligand capable of stabilizing organotin centers. Such bridging coordination behavior generally contributes to enhanced structural rigidity and promotes the formation of extended supramolecular architectures in organometallic systems.

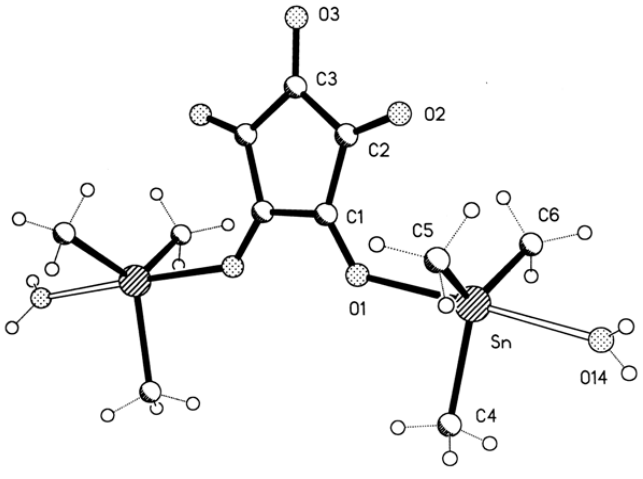


Figure 2. Crystal structure of the compound bis(trimethyltin)croconate $[(CH_3)_3Sn]_2C_5O_5\ 2H_2O$

As illustrated in Figure 2, each tin atom exhibits a coordination number of five and adopts a trigonal bipyramidal geometry. Three methyl carbon atoms occupy the equatorial positions, while two oxygen atoms, namely one oxygen atom from the croconate ligand and one oxygen atom from a coordinated water molecule, occupy the axial positions. The almost linear O1–Sn–O14 bond angle of 178.43(7)°, as listed in Table 2, strongly confirms the axial arrangement characteristic of trigonal bipyramidal geometry. This geometry is commonly observed in pentacoordinated organotin (IV) compounds and reflects the electronic and steric preferences of the Sn (IV) center. The nearly planar arrangement of the trimethyltin group also indicates minimal steric distortion around the tin atom, contributing to overall molecular stability.

Table 2. Selected bond lengths and angles of the bis(trimethyltin) croconate [(CH3)3Sn]2C5O5·2H2O compound

Bond Length (Å)		Bond Angle (º)	
O1-C1	1.253(2)	C5-Sn-C6	128.47(11)
O2-C2	1.237(3)	C5-Sn-C4	115.39(12)
O3-C3	2.248(4)	C6-Sn-C4	116.00(12)
C1-C1#	1.457(4)	C5-Sn-O1	93.50(8)
C1-C2	1468(3)	C6-Sn-O1	91.54(9)
C2-C3	1.474(3)	C4-Sn-O1	88.33(8)
Sn-O1	2.203	O1-Sn-O14	178.43(7)
Sn-O14	2.263		

The selected bond lengths presented in Table 2 provide important insight into the electronic structure of the croconate ligand. The C–C bond lengths within the croconate ring, namely C1–C1# = 1.457(4) Å, C1–C2 = 1.468(3) Å, and C2–C3 = 1.474(3) Å, are intermediate between normal single and double carbon–carbon bonds. These values strongly support the existence of π-electron delocalization throughout the croconate ring, confirming its aromatic character. Aromaticity in oxocarbon ions such as croconate arises from resonance stabilization, where electron density is distributed over the cyclic framework. The slightly shorter C1–C1# bond compared with the other C–C bonds indicates that electron delocalization is somewhat influenced by the coordination of oxygen atoms to the tin center. This observation is consistent, coordination interactions can alter electron density distribution in aromatic oxocarbon systems [40]-[42].

The C–O bond lengths listed in Table 2 also support the delocalized electronic nature of the croconate ion. The O1–C1 and O2–C2 bond lengths of approximately 1.24–1.25 Å are characteristic of partially delocalized carbonyl bonds rather than localized C=O double bonds. In contrast, the longer O3–C3 distance reflects a different electronic environment for the oxygen atom located at the apex position of the croconate ring. This elongation likely occurs because the O3 atom does not directly coordinate to the tin atom but instead participates in intermolecular hydrogen bonding interactions. Consequently, the electron density surrounding O3 differs from that of the coordinated oxygen atoms, resulting in variations in bond strength and bond length.

The Sn–O bond distances shown in Table 2 provide additional evidence regarding the coordination environment of the tin center. The Sn–O(croconate) bond length of 2.203 Å is shorter than the Sn–O(water) bond length of 2.263 Å, indicating that the croconate oxygen atom forms a stronger coordination bond with the tin atom than the coordinated water molecule. This difference can be attributed to the stronger donor ability and higher electron density of the negatively charged croconate oxygen compared with the neutral water ligand. Therefore, the coordinated water molecules mainly function as stabilizing ligands and hydrogen-bond donors rather than strong coordinating ligands.

The bond angle data summarized in Table 2 further confirm the distorted trigonal bipyramidal geometry around the tin center. The relatively large C5–Sn–C6 bond angle of 128.47(11)° indicates steric repulsion between methyl groups in the equatorial plane. Meanwhile, the smaller C4–Sn–O1 bond angle of 88.33(8)° reflects structural adjustment due to axial coordination by oxygen donor atoms. Such deviations from ideal trigonal bipyramidal geometry are commonly observed in organotin complexes because of the combined effects of steric hindrance, ligand electronic properties, and crystal packing interactions.

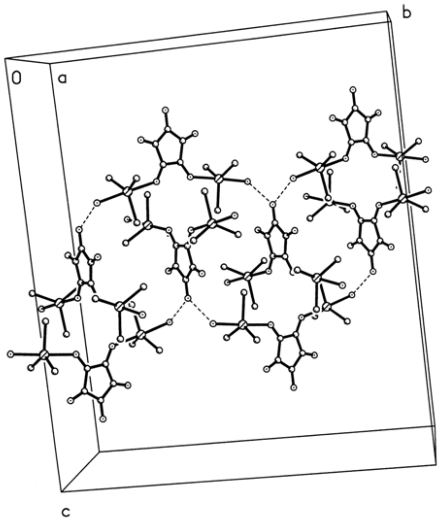


Figure 3. Crystal structure arrangement of the bis(trimethyltin) croconate $[(CH_3)_3Sn]_2C_5O_5\ 2H_2O$ compound

The supramolecular arrangement displayed in Figure 3 demonstrates that individual monomeric units are interconnected through intermolecular hydrogen bonds involving hydrogen atoms from coordinated water molecules and oxygen atoms at the O3 position of neighboring croconate ions. These hydrogen-bonding interactions generate an extended macromolecular network throughout the crystal lattice. Thus, the coordinated water molecules not only participate in coordination with the tin atom but also play an essential role in stabilizing the three-dimensional crystal packing. The hydrogen bonding involving the O3 oxygen atom represents a characteristic structural feature frequently observed in croconic acid and croconate derivatives [43]-[46]. The formation of this hydrogen-bonded network contributes significantly to the thermal and structural stability of the crystal.

Table 3. Analysis results of compound elements (Trimethyl tin) croconate $[(CH_3)_3Sn]_2C_5O_5\ 2H_2O$

	C(%)	H(%)	n(C) : n(H)
Calculation	26.23	4.40	1 : 2.00
Obtained	25.83	4.49	1 : 2.07

The elemental analysis results presented in Table 3 show good agreement between theoretical and experimental values. The calculated carbon and hydrogen contents were 26.23% and 4.40%, respectively, whereas the experimentally obtained values were 25.83% and 4.49%. The close correspondence between these values confirms the successful synthesis of the proposed compound with relatively high purity. Furthermore, the experimentally obtained carbon-to-hydrogen molar ratio of 1:2.07 closely matches the theoretical ratio of 1:2.00, thereby supporting the validity of the molecular formula $[(CH_3)_3Sn]_2C_5O_5 \cdot 2H_2O$.

The NMR spectral data further support the successful formation of the target complex. The ^{1}H-NMR spectrum exhibits a single resonance signal at δ 2.5 ppm, indicating that all methyl groups attached to the tin atom are chemically equivalent and experience a symmetrical electronic environment. Meanwhile, the ^{13}C-NMR spectrum displays a signal at δ 13.08 ppm corresponding to methyl carbon atoms bonded to tin, while the resonance at δ 183.00 ppm is characteristic of the croconate carbon atoms. The downfield chemical shift of the croconate carbon signal reflects the strong electron-withdrawing effect of oxygen atoms and extensive π-electron delocalization within the aromatic oxocarbon ring [47]-[50].

Table 4. Infrared Spectrum (in cm^{-1}) of bis(trimethyltin) croconate $[(CH_3)_3Sn]_2C_5O_5 \cdot 2H_2O$

Spectrum	Description
3419 (m, br)	vO - H water
1548 (vs, br)	vC - O croconate ion

Note: vs= very strong; m = medium; br = broad

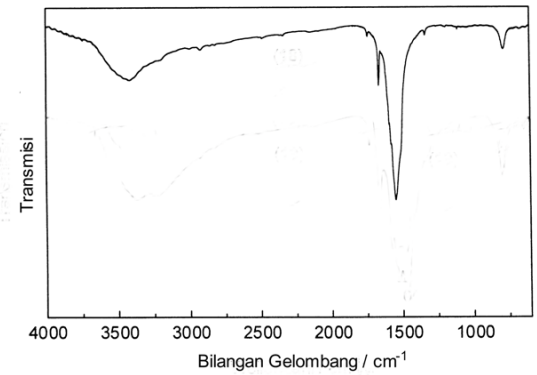


Figure 4. Infrared spectrum of the bis(trimethyltin) croconate $[(CH_3)_3Sn]_2C_5O_5\ 2H_2O$ compound

The FTIR spectrum shown in Figure 4 and summarized in Table 4 provides additional confirmation of the molecular structure. The medium broad absorption band at 3419 cm^{-1} corresponds to O–H stretching vibrations of coordinated water molecules, confirming the hydrated nature of the crystal structure. Meanwhile, the very strong broad absorption band at 1548 cm^{-1} is attributed to the C–O stretching vibration of the croconate ion. The intensity and broadness of this band are characteristic of conjugated oxocarbon systems containing delocalized π electrons. The broad nature of both absorption bands further indicates the presence of extensive hydrogen bonding interactions within the crystal lattice, consistent with the supramolecular arrangement observed in Figure 3.

Overall, the crystallographic, spectroscopic, and elemental analyses presented in Figures 2–4 and Tables 1–4 conclusively demonstrate the successful synthesis of a pentacoordinated organotin croconate complex possessing trigonal bipyramidal geometry and an extended hydrogen-bonded supramolecular framework. The study confirms that the croconate ligand acts as an aromatic bidentate bridging ligand capable of stabilizing organotin centers while simultaneously facilitating intermolecular assembly through hydrogen-bonding interactions.

The novelty of this study lies in the successful synthesis and comprehensive structural characterization of a rare croconate-based organotin complex, bis(trimethyltin) croconate dihydrate $[(CH_3)_3Sn]_2C_5O_5\cdot 2H_2O$. Unlike previous studies that mainly focused on squarate and deltate derivatives, this research specifically investigates the coordination behavior of the croconate ligand toward trimethyltin centers using single-crystal X-ray diffraction analysis. The study also reveals the formation of a pentacoordinated trigonal bipyramidal geometry and an extended supramolecular hydrogen-bonding network stabilized by coordinated water molecules. Furthermore, this work provides new evidence regarding π-electron delocalization within the croconate ring and its influence on molecular stability and crystal packing in organotin oxocarbon systems. The findings of this study contribute significantly to the development of organotin and oxocarbon coordination chemistry, particularly in understanding the interaction between croconate ligands and organotin centers. The structural information obtained from this research may serve as a valuable reference for the design of new organometallic materials with potential applications in supramolecular chemistry, molecular electronics, nonlinear optical materials, and functional coordination compounds. In addition, the identification of hydrogen-bonded supramolecular frameworks and aromatic electron delocalization broadens the understanding of crystal engineering strategies involving oxocarbon ligands. The study also demonstrates the effectiveness of single-crystal X-ray diffraction analysis in elucidating detailed structural properties of complex organometallic compounds.

This study primarily focused on the synthesis and structural characterization of bis(trimethyltin) croconate dihydrate and did not investigate its physical, electronic, thermal, or biological properties in detail. The characterization techniques were limited to crystallographic, spectroscopic, and elemental analyses without including computational modeling, thermal stability analysis, conductivity measurements, or reactivity studies. Furthermore, only one type of organotin derivative was synthesized, limiting broader comparisons regarding the influence of different organotin substituents on croconate coordination behavior and crystal architecture. Future studies are recommended to explore the thermal, optical, electronic, and biological properties of croconate-based organotin complexes in order to evaluate their potential applications in advanced functional materials. Further research may also investigate the synthesis of analogous croconate complexes using different organotin substituents such as tributyltin, triphenyltin, or dimethyltin to better understand substituent effects on molecular geometry and supramolecular interactions. In addition, computational chemistry approaches such as density functional theory (DFT) calculations are recommended to provide deeper insights into electron delocalization, bonding characteristics, and molecular stability. Thermal analysis techniques such as TGA and DSC could also be employed to examine the thermal behavior and decomposition patterns of the synthesized complexes.

4. CONCLUSION

This study successfully synthesized and characterized the organotin oxocarbon compound bis(trimethyltin) croconate dihydrate, $[(CH_3)_3Sn]_2C_5O_5 \cdot 2H_2O$, through the reaction between sodium croconate and trimethyltin chloride under atmospheric conditions. Single-crystal X-ray diffraction analysis revealed that the compound crystallizes in the orthorhombic crystal system with the Fddd space group and forms a highly ordered supramolecular structure. The croconate dianion acts as a bidentate bridging ligand connecting two trimethyltin groups, while each tin atom adopts a pentacoordinated distorted trigonal bipyramidal geometry. Bond length and bond angle analyses confirmed the presence of π-electron delocalization within the croconate ring, indicating aromatic character and contributing to structural stability. The crystal packing is further stabilized through intermolecular hydrogen bonding involving coordinated water molecules and croconate oxygen atoms, forming an extended macromolecular network. The FTIR, NMR, and elemental analysis results strongly supported the successful formation and purity of the synthesized complex. Overall, this research expands current understanding of croconate-based organotin coordination chemistry and provides valuable structural information regarding the interaction between organotin centers and aromatic oxocarbon ligands. The findings also highlight the potential of croconate ligands in the development of novel supramolecular and functional organometallic materials for future applications in coordination chemistry and material science. Future studies are recommended to investigate the thermal, electronic, optical, and potential biological activities of croconate-based organotin complexes using both experimental and computational approaches to further explore their applicability as advanced functional materials.

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AUTHOR CONTRIBUTIONS

The author was solely responsible for the conceptualization and design of the study, data collection, implementation of the narrative counseling intervention, data analysis, and interpretation of the results. The author also prepared the original draft of the manuscript, revised the content critically, and approved the final version for publication.

CONFLICTS OF INTEREST

The author(s) declare no conflict of interest.

USE OF ARTIFICIAL INTELLIGENCE (AI)-ASSISTED TECHNOLOGY

The authors declare that no artificial intelligence (AI) tools were used in the generation, analysis, or writing of this manuscript. All aspects of the research, including data collection, interpretation, and manuscript preparation, were carried out entirely by the authors without the assistance of AI-based technologies.

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