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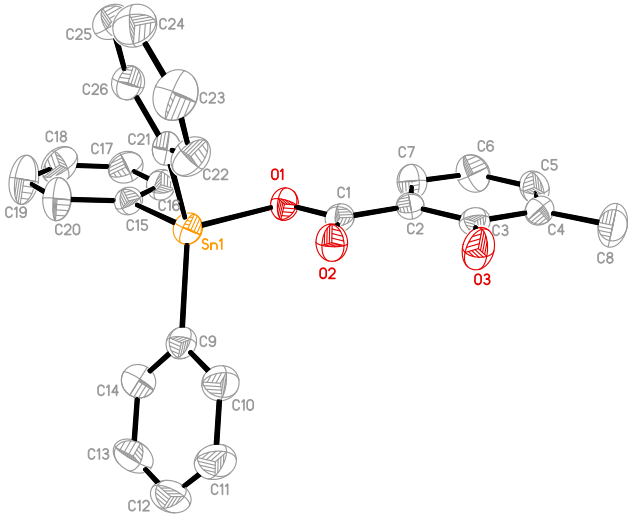
Crystal structure of [2-hydroxy-3-methyl-benzoato-k^1*O*-triphenyltin(IV)], $C_{26}H_{22}O_3Sn$



https://doi.org/10.1515/ncrs-2022-0420
Received August 20, 2022; accepted October 10, 2022;
published online November 1, 2022

Abstract

$C_{26}H_{22}O_3Sn$, triclinic, $P\bar{1}$ (no. 2), a = 10.8480(9) Å, b = 11.3511(11) Å, c = 11.4109(12) Å, α = 114.431(3)°, β = 96.994(2)°, γ = 108.207(3)°, V = 1162.94(19) Å^3, Z = 2, $R_{gt}(F)$ = 0.0357, $wR_{ref}(F^2)$ = 0.0667, T = 298 K.

CCDC no.: 2211954.

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	0.33 × 0.18 × 0.17 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.12 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5986, 4050, 0.026
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3222
$N(param)_{refined}$:	272
Programs:	Bruker programs [1], Shelx [2]

Source of materials

The reaction was carried out under a nitrogen atmosphere by use of standard Schlenk techniques. The 2-hydroxy-3-methylbenzoic acid (0.152 g, 1.0 mmol) was added to the solution of methanol (30 mL) together with sodium ethoxide (0.068 g, 1.0 mmol), and the mixture was stirred for 0.5 h. The triphenyltin chloride (0.385 g, 1.0 mmol) was added, the mixture was stirred at 318 K for 12 h and then filtered. The solvent was gradually removed by evaporation under reduced pressure until a white powder was obtained. The powder was then recrystallized from ether, and colorless crystals were recovered.

Experimental details

All hydrogen atomic positions were taken from a difference Fourier map. Hydrogen atoms were assigned with common isotropic displacement factors U_{iso} (H) = 1.2 times U_{eq} (C, phenyl ring and methylene carbon) and U_{iso} (H) = 1.5 times U_{eq} (C, methyl carbon). All the H atoms were refined as riding on their parent atom.

Comment

In recent years, organotin complexes have been attracting more and more attention due to their industrial applications and their biological activity [3–6]. Among these, the organotin carboxylates are the most intensively investigated [7]. Carboxylate ligands can offer a number of distinct advantages such as the coordination ability as either a multidentate or a bridging building block in structural assemblies. Meanwhile, some organotin carboxylates also have shown high biological activities in

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.73573 (3)	0.44222 (3)	0.11642 (3)	0.05462 (11)
O1	0.5917 (2)	0.4799 (3)	0.2110 (2)	0.0571 (6)
O2	0.7714 (3)	0.6196 (3)	0.3887 (3)	0.0635 (7)
O3	0.7399 (3)	0.7707 (3)	0.6184 (3)	0.0778 (8)
H3	0.7810	0.7402	0.5655	0.117*
C1	0.6461 (4)	0.5700 (4)	0.3383 (4)	0.0523 (9)
C2	0.5545 (4)	0.6118 (4)	0.4175 (4)	0.0471 (9)
C3	0.6062 (4)	0.7108 (4)	0.5534 (4)	0.0530 (9)
C4	0.5204 (4)	0.7511 (4)	0.6285 (4)	0.0625 (11)
C5	0.3850 (5)	0.6936 (5)	0.5633 (5)	0.0709 (12)
H5	0.3269	0.7213	0.6116	0.085*
C6	0.3316 (4)	0.5958 (5)	0.4287 (5)	0.0792 (13)
H6	0.2389	0.5584	0.3874	0.095*
C7	0.4163 (4)	0.5537 (4)	0.3555 (4)	0.0664 (11)
H7	0.3808	0.4867	0.2649	0.080*
C8	0.5785 (5)	0.8542 (5)	0.7770 (4)	0.0998 (16)
H8A	0.6145	0.8122	0.8226	0.150*
H8B	0.5085	0.8775	0.8123	0.150*
H8C	0.6497	0.9386	0.7907	0.150*
C9	0.8689 (4)	0.6306 (4)	0.1263 (4)	0.0595 (10)
C10	0.9660 (4)	0.7441 (4)	0.2423 (5)	0.0751 (12)
H10	0.9783	0.7385	0.3216	0.090*
C11	1.0448 (5)	0.8654 (5)	0.2410 (6)	0.0933 (16)
H11	1.1083	0.9414	0.3199	0.112*
C12	1.0304 (5)	0.8745 (6)	0.1258 (7)	0.0998 (18)
H12	1.0845	0.9563	0.1259	0.120*
C13	0.9371 (6)	0.7642 (6)	0.0099 (6)	0.0983 (17)
H13	0.9277	0.7706	−0.0691	0.118*
C14	0.8558 (4)	0.6421 (5)	0.0098 (5)	0.0782 (13)
H14	0.7918	0.5673	−0.0695	0.094*
C15	0.5959 (4)	0.3020 (4)	−0.0796 (4)	0.0532 (9)
C16	0.4600 (4)	0.2799 (4)	−0.1049 (4)	0.0644 (11)
H16	0.4294	0.3299	−0.0357	0.077*
C17	0.3697 (5)	0.1857 (5)	−0.2301 (5)	0.0767 (12)
H17	0.2788	0.1718	−0.2448	0.092*
C18	0.4127 (6)	0.1133 (5)	−0.3320 (5)	0.0913 (15)
H18	0.3518	0.0497	−0.4170	0.110*
C19	0.5463 (6)	0.1339 (6)	−0.3093 (5)	0.1081 (18)
H19	0.5757	0.0833	−0.3792	0.130*
C20	0.6380 (5)	0.2289 (5)	−0.1843 (4)	0.0833 (13)
H20	0.7289	0.2434	−0.1710	0.100*
C21	0.8147 (4)	0.3260 (4)	0.1859 (4)	0.0507 (9)
C22	0.9232 (4)	0.3904 (4)	0.2995 (4)	0.0713 (12)
H22	0.9656	0.4885	0.3478	0.086*
C23	0.9689 (5)	0.3101 (6)	0.3418 (5)	0.0888 (14)
H23	1.0421	0.3544	0.4183	0.107*
C24	0.9078 (5)	0.1661 (6)	0.2725 (5)	0.0863 (14)
H24	0.9391	0.1128	0.3020	0.104*
C25	0.8001 (5)	0.1003 (5)	0.1593 (5)	0.0776 (13)
H25	0.7583	0.0022	0.1114	0.093*
C26	0.7543 (4)	0.1804 (4)	0.1168 (4)	0.0633 (11)
H26	0.6811	0.1354	0.0401	0.076*

terms of their antitumor, antibacterial, antileishmanial and antifungal efficacies [8]. As a part of our current research on the exploration of the biological activity of the organotin complexes, we report a new organotin carboxylate.

The asymmetry unit consists of one $[(Ph)_3Sn]^+$ unit and one deprotonation of 2-hydroxy-3-methylbenzoic acid. The Sn(IV) center in the title compound is in a slightly distorted tetrahedron environment with four coordinated atoms, three C atoms are from $[(Ph)_3Sn]$ unit with the remaining one O atom from the carboxyl group (see the figure). The Sn–C distances (Sn(1)–C(9) 2.122(4) Å, Sn(1)–C(15) 2.135(4) Å, Sn(1)–C(21) 2.124(3) Å) are within the normal range [8]. The Sn–O bond length (Sn(1)–O(1) 2.058(2) Å) is close to the covalent radii of Sn and O 2.13 Å.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This study was funded by Liaocheng University Doctoral Foundation (318051514).

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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