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The crystal structure of (*E*)-2-(((5-((triphenylstannyl)thio)-1,3,4-thiadiazol-2-yl)imino)methyl)phenol, C₂₇H₂₁N₃OS₂Sn

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Abstract

C₂₇H₂₁N₃OS₂Sn, triclinic, *P* $\bar{1}$ (no. 2), *a* = 11.064(3) Å, *b* = 11.538(3) Å, *c* = 12.257(3) Å, *V* = 1258.2(6) Å³, *Z* = 2, *R*_{gt}(*F*) = 0.0316, *wR*_{ref}(*F*²) = 0.0664, *T* = 298 K.

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The molecular structure is shown in Figure. 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:	Yellow block
Size:	0.43 × 0.35 × 0.30 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	1.21 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART APEX II, ω
θ _{max} , completeness:	25.0°, 98%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	6580, 4357, 0.020
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2σ(<i>I</i> _{obs}), 3568
<i>N</i> (<i>param</i>) _{refined} :	307
Programs:	Bruker [1], SHELX [2]

calc. for C₂₇H₂₁N₃OS₂Sn: C 55.31, H 3.61, N 7.17; found: C 55.52, H 3.28, N 7.02.

Source of material

The title complex was obtained in a one-pot reaction, refluxing alicylaldehyde, 5-amino-1,3,4-thiadiazole-2-thiol and triphenyltin chloride in ethanol/benzene with a ratio of 2:3 for 4 h. The orange yellow solution was cooled and filtered. The clear solution was distilled and recrystallized from an ethanol/benzene mixture (v/v = 1:2). The block-shaped yellow crystals of the title compound were obtained. Yield: 76% (base on Sn element), and elemental analysis:

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Experimental details

All hydrogen atomic positions were added using a riding model. Their *U*_{iso} values were assigned with common isotropic displacement factors *U*_{iso} (H) = 1.2 times *U*_{eq} (C, benzene ring and methylene) and 1.5 times *U*_{eq} (O, phenolic hydroxyl).

Comment

Among organotin(IV) complexes, Sn(IV) thiolates are the most extensively used, with commercial applications [3, 4] in physical and chemical properties that are promising for

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} */U _{eq}
Sn1	0.37098 (2)	0.51672 (2)	0.21212 (2)	0.03682 (9)
N1	0.3022 (3)	0.3013 (3)	0.3100 (2)	0.0427 (7)
N2	0.2684 (3)	0.1746 (3)	0.3196 (3)	0.0465 (7)
N3	0.2050 (3)	0.0538 (3)	0.4456 (3)	0.0476 (7)
O1	0.1597 (3)	−0.2056 (3)	0.4026 (3)	0.0813 (9)
H1	0.1778	−0.1349	0.3886	0.122*
S1	0.25398 (10)	0.32846 (10)	0.51139 (8)	0.0444 (2)
S2	0.34326 (10)	0.56086 (10)	0.41536 (8)	0.0482 (2)
C1	0.3010 (3)	0.3924 (4)	0.4036 (3)	0.0399 (8)
C2	0.2409 (3)	0.1733 (3)	0.4194 (3)	0.0394 (8)
C3	0.1784 (4)	0.0541 (4)	0.5451 (4)	0.0507 (9)
H3	0.1829	0.1345	0.5966	0.061*
C4	0.1419 (4)	−0.0640 (4)	0.5813 (3)	0.0477 (9)
C5	0.1348 (4)	−0.1877 (4)	0.5096 (4)	0.0571 (11)
C6	0.1031 (4)	−0.2954 (5)	0.5489 (5)	0.0721 (13)
H6	0.1000	−0.3773	0.5024	0.086*
C7	0.0759 (4)	−0.2821 (5)	0.6567 (5)	0.0733 (14)
H7	0.0526	−0.3567	0.6816	0.088*
C8	0.0823 (4)	−0.1610 (5)	0.7295 (4)	0.0657 (12)
H8	0.0636	−0.1533	0.8025	0.079*
C9	0.1167 (4)	−0.0533 (4)	0.6913 (4)	0.0599 (11)
H9	0.1236	0.0298	0.7401	0.072*
C10	0.1648 (3)	0.3571 (3)	0.0875 (3)	0.0363 (8)
C11	0.0620 (4)	0.3904 (4)	0.0691 (3)	0.0500 (9)
H11	0.0834	0.4823	0.1125	0.060*
C12	−0.0725 (4)	0.2895 (4)	−0.0128 (4)	0.0626 (11)
H12	−0.1414	0.3133	−0.0230	0.075*
C13	−0.1048 (4)	0.1550 (4)	−0.0786 (4)	0.0584 (11)
H13	−0.1949	0.0877	−0.1347	0.070*
C14	−0.0042 (4)	0.1196 (4)	−0.0620 (3)	0.0522 (10)
H14	−0.0264	0.0276	−0.1063	0.063*
C15	0.1305 (4)	0.2198 (4)	0.0203 (3)	0.0446 (9)
H15	0.1986	0.1950	0.0307	0.053*
C16	0.5506 (3)	0.4951 (3)	0.1963 (3)	0.0344 (7)
C17	0.5643 (4)	0.3863 (4)	0.2110 (3)	0.0454 (9)
H17	0.4870	0.3105	0.2179	0.055*
C18	0.6912 (4)	0.3894 (4)	0.2156 (4)	0.0578 (11)
H18	0.6986	0.3155	0.2245	0.069*
C19	0.8066 (4)	0.5022 (4)	0.2070 (4)	0.0558 (10)
H19	0.8935	0.5067	0.2137	0.067*
C20	0.7936 (4)	0.6078 (4)	0.1885 (3)	0.0500 (10)
H20	0.8703	0.6817	0.1792	0.060*
C21	0.6672 (3)	0.6048 (4)	0.1837 (3)	0.0411 (8)
H21	0.6597	0.6775	0.1719	0.049*
C22	0.4272 (3)	0.7214 (3)	0.2121 (3)	0.0412 (8)
C23	0.4406 (4)	0.8290 (4)	0.3099 (4)	0.0609 (11)
H23	0.4247	0.8124	0.3781	0.073*
C24	0.4767 (5)	0.9600 (4)	0.3090 (5)	0.0834 (15)
H24	0.4842	1.0306	0.3757	0.100*
C25	0.5015 (5)	0.9858 (5)	0.2096 (6)	0.0828 (16)
H25	0.5260	1.0742	0.2084	0.099*
C26	0.4902 (5)	0.8814 (5)	0.1114 (5)	0.0819 (15)
H26	0.5074	0.8990	0.0438	0.098*
C27	0.4536 (4)	0.7509 (4)	0.1132 (4)	0.0588 (11)
H27	0.4465	0.6808	0.0464	0.071*

the creation of new biologicals and anti-cancer-activity [5]. The investigation of organotin(IV) complexes have been focused on acquiring well-defined Schiff base organotin complexes, which have potential applications in catalysis and biological activity [6]. To the best of our knowledge, thiolates that contain the following two structural units HS–C–N–N or S=C–N–N can coordinate to metal ions through S or N or both atoms [7, 8]. As a result of our continuing interest in the coordination of organotin with S, N ligands we here report the synthesis and crystal structure of the title compound.

In the title structure, the Sn atom centre exhibits a four-coordinated tetrahedral geometry with three phenyl C and one S atom from the Schiff-base moiety. The bond angles of C–Sn–S (107.14(9), 113.62(8) and 97.79(10) Å) are unequal, so the tetrahedral geometry is distorted. The Schiff-base ligand coordinates to the Sn atom as a monodentate mode. The bond length of Sn–S is 2.478(3) Å, which is comparable with those reported in the literature [9, 10]. The intra-molecular hydrogen bonding occur by a typical O–H⋯O interaction.

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