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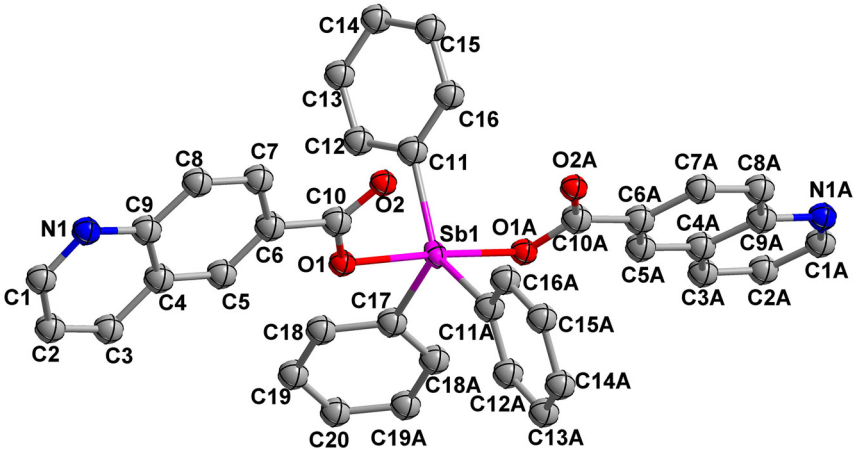
Crystal structure of (((oxido(quinolin-6-yl) methoxy)triphenyl-λ^5-stibanyl)oxy)(quinolin-7-yl) methanolate



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Abstract

$C_{38}H_{27}N_2O_4Sb$, orthorhombic, *Fdd*2 (no. 43), a = 15.5651(14) Å, b = 20.0031(18) Å, c = 20.0035(18) Å, V = 6,228.1(10) Å^3, Z = 8, $R_{gt}(F)$ = 0.0356, $wR_{ref}(F^2)$ = 0.0881, T = 298(2) K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.30 × 0.28 × 0.20 mm
Wavelength:	Mo*K*α radiation (0.71073 Å)
μ:	0.93 mm^{-1}
Diffractometer, scan mode:	Bruker APEX2, φ and ω scans
θ_{max}, completeness:	25.0°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6,942, 2,519, 0.055
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2,188
$N(param)_{refined}$:	205
Programs:	Bruker,[1] SHELX,[2,3] Olex2[4]

1 Source of material

A mixture of 6-quinolinecarboxylic acid (0.069 g, 0.4 mmol) and sodium ethoxide (0.0224 g, 0.4 mmol) was stirred in toluene (10 mL) at room temperature for 30 min. Subsequently, triphenylantimony dichloride (0.0848 g, 0.2 mmol) was added to the reaction mixture, which was heated at reflux for 12 h under continuous stirring. Upon completion, the solvent was removed under reduced pressure. The crude product was purified by recrystallization from a dichloromethane/petroleum ether mixture, yielding colorless, transparent block-crystals with a 68 % yield.

2 Experimental details

The structure was solved by Direct Methods with the SHELXS program and refined with SHELXL. Hydrogen atoms were positioned geometrically (C–H = 0.93–0.98 Å). Their U_{iso} values were set to 1.2U_{eq} or 1.5U_{eq} of the parent atoms.

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3 Comment

Organoantimony compounds represent a class of functional molecules formed through covalent bonding between antimony atoms and organic moieties (such as alkyl, aryl, or carboxyl groups).[5–8] Owing to their distinctive electronic configurations and reactive characteristics, these compounds have attracted considerable research interest across interdisciplinary fields including materials science, organic synthesis, and biomedical applications. Particularly, organoantimony carboxylate derivatives have emerged as a focal point in contemporary research due to their remarkable structural diversity and unique physicochemical properties.[9–11] In this study, employing coordination chemistry principles, we successfully synthesized a organoantimony carboxylate complex using 6-quinolinecarboxylic acid and triphenylantimony dichloride. The title complex adopts a monomeric structure featuring two deprotonated carboxylic acid ligands and a Ph_3Sb unit, where the central antimony (Sb) atom exhibits a five-coordinate trigonal bipyramidal geometry. The observed Sb1–O1 bond length of 2.101(4) Å, indicates a strong coordination interaction between these atoms. The axial O1–Sb1–O1A bond angle of 174.2(3)° reveals a slight deviation from the ideal trigonal bipyramidal configuration, suggesting minor structural distortion. These results correlate well with crystallographic parameters documented in structurally related Sb(V) complexes, reaffirming the characteristic bonding features of hypervalent antimony species.[12]

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

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