Crystal structure of (*N*-*o*-tolylpyridine-2-carbaldimine)trichlorovinyltin(IV), $C_{15}H_{15}Cl_3N_2Sn$

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Source of material: The title compound was isolated from the 1/1 reaction of $\text{vinyl}_2\text{SnCl}_2$ and the ligand (generated in situ from 2-toluidine and 2-pyridinecarboxyaldehyde) in dichloromethane solution as a disproportionation product; pale-yellow crystals with mp 498 K.

Vinyl group was found to be disordered. Two sites were modelled for C(15) with 0.62/0.38 site occupancies. The C atoms were refined isotropically and H atoms not included. The max. residual peak ($0.68 \text{ e} \text{ \AA}^{-3}$) was found in this region. The tin atom exists in a distorted octahedral geometry defined by three chloride atoms, two nitrogen atoms of the chelating ligand and the α -carbon of the vinyl group; the major distortion occurs owing to the restricted bite distance of the chelate. There is a disparity in $d(\text{Sn}-\text{N})$ such that the shortest distance ($2.270(6) \text{ \AA}$) involves the N(1) atom *trans* to the vinyl group and the longer ($2.304(6) \text{ \AA}$) has N(2) opposite the more tightly bound Cl(2) atom ($2.410(2) \text{ \AA}$); the other Sn–Cl distances are $2.448(2) \text{ \AA}$ and $2.478(2) \text{ \AA}$, respectively. There is a twist in the C(6)–N(2)–C(7)–C(8) portion of the chelate (torsion angle $57(1)^\circ$). There are two closely related structures available for comparison. A similar arrangement of the $\text{Cl}_3\text{N}_2\text{C}$ donor set as in the title compound is found in the structure of $[\text{nBuSnCl}_3(4\text{-MeOC}_6\text{H}_4\text{N}=\text{C}(\text{H})\text{C}_5\text{H}_4\text{N}-2)]$ (see ref. 1) with a similar variation in $d(\text{Sn}-\text{Cl})$. By contrast, in the structure of $[\text{benzylSnCl}_3(1,10\text{-phenanthroline})]$ adduct (isolated as a 1/1 benzene solvate) a different arrangement of the donor atoms is found such that the tin-bound organic substituent is now *trans* to a chloride atom (see ref. 2).

$C_{15}H_{15}Cl_3N_2Sn$, monoclinic, $P12_1/c1$ (No. 14), $a=16.785(2) \text{ \AA}$, $b=7.172(3) \text{ \AA}$, $c=14.401(3) \text{ \AA}$, $\beta=99.21(1)^\circ$, $V=1711.3 \text{ \AA}^3$, $Z=4$, $R(F)=0.041$, $R_w(F)=0.039$.

Table 1. Parameters used for the X-ray data collection

Crystal:	pale-yellow block, size 0.08 x 0.16 x 0.16 mm
Wavelength:	Mo K_α radiation (0.7107 $\text{\AA}$)
μ :	19.55 cm^{-1}
Diffractometer:	AFC6R
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	1849
Criterion for F_o :	$F_o > 6 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	184
Program:	teXsan

Table 2. Final atomic coordinates and displacement parameters (in $\text{\AA}^2$)

Atom	Site	Occ.	x	y	z	U_{iso}
C(14)	4e		0.7276(7)	0.406(2)	0.2100(9)	0.094(3)
C(15)	4e	0.62	0.6793(9)	0.509(2)	0.203(1)	0.080(5)
C(15')	4e	0.38	0.724(2)	0.418(4)	0.145(2)	0.11(1)
H(1)	4e		0.9401	0.2933	0.5160	0.0675
H(2)	4e		0.9924	0.1093	0.6468	0.0786
H(3)	4e		0.9415	−0.1921	0.6609	0.0789
H(4)	4e		0.8349	−0.2992	0.5470	0.0752
H(6)	4e		0.7334	−0.2334	0.4032	0.0647
H(9a)	4e		0.5379	0.0030	0.4245	0.1072
H(9b)	4e		0.5593	−0.2122	0.4271	0.1072
H(9c)	4e		0.6291	−0.0619	0.4474	0.1072
H(10)	4e		0.4643	−0.1580	0.2620	0.0884
H(11)	4e		0.4672	−0.1359	0.1025	0.0970
H(12)	4e		0.5852	−0.0479	0.0470	0.0923
H(13)	4e		0.7041	0.0086	0.1563	0.0742

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Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Sn	4e	0.79972(3)	0.27516(7)	0.33147(4)	0.0485(3)	0.0484(3)	0.0494(3)	−0.0028(3)	0.0065(2)	0.0068(3)
Cl(1)	4e	0.8793(1)	0.0834(3)	0.2395(2)	0.068(1)	0.090(2)	0.053(1)	0.001(1)	0.017(1)	−0.003(1)
Cl(2)	4e	0.9028(1)	0.5103(3)	0.3660(2)	0.078(2)	0.075(2)	0.083(2)	−0.022(1)	0.011(1)	0.002(1)
Cl(3)	4e	0.7173(1)	0.3955(3)	0.4466(2)	0.069(1)	0.058(1)	0.091(2)	0.007(1)	0.028(1)	0.000(1)
N(1)	4e	0.8580(4)	0.1091(8)	0.4586(4)	0.052(4)	0.051(4)	0.039(4)	0.006(3)	0.011(3)	−0.007(3)
N(2)	4e	0.7266(3)	0.0048(8)	0.3376(4)	0.049(4)	0.050(4)	0.041(4)	−0.006(3)	0.011(3)	−0.003(3)
C(1)	4e	0.9179(5)	0.170(1)	0.5229(6)	0.056(5)	0.059(5)	0.052(6)	0.008(4)	0.005(4)	−0.009(4)
C(2)	4e	0.9494(5)	0.062(1)	0.5997(6)	0.059(6)	0.083(6)	0.051(6)	0.016(5)	−0.001(5)	−0.013(5)
C(3)	4e	0.9193(5)	−0.113(1)	0.6084(6)	0.067(6)	0.085(7)	0.043(5)	0.023(5)	0.001(5)	0.006(5)
C(4)	4e	0.8573(5)	−0.176(1)	0.5421(6)	0.075(6)	0.061(5)	0.053(6)	0.010(5)	0.011(5)	0.007(4)
C(5)	4e	0.8271(5)	−0.060(1)	0.4684(5)	0.061(5)	0.051(5)	0.044(5)	0.005(4)	0.007(4)	0.000(4)
C(6)	4e	0.7572(5)	−0.111(1)	0.4006(6)	0.064(5)	0.044(5)	0.054(5)	−0.001(4)	0.010(4)	0.006(4)
C(7)	4e	0.6532(5)	−0.039(1)	0.2739(5)	0.058(5)	0.042(4)	0.043(5)	0.001(4)	0.005(4)	0.000(4)
C(8)	4e	0.5825(5)	−0.083(1)	0.3090(6)	0.059(6)	0.051(5)	0.073(7)	0.004(4)	0.013(5)	0.009(5)
C(9)	4e	0.5767(6)	−0.089(1)	0.4108(7)	0.079(7)	0.116(8)	0.082(8)	0.004(6)	0.039(6)	0.020(7)
C(10)	4e	0.5141(5)	−0.122(1)	0.2411(8)	0.048(6)	0.070(6)	0.101(8)	−0.011(5)	0.006(6)	0.003(6)
C(11)	4e	0.5157(6)	−0.109(1)	0.1468(8)	0.068(7)	0.083(7)	0.085(8)	−0.019(6)	−0.008(6)	−0.005(6)
C(12)	4e	0.5847(6)	−0.059(1)	0.1141(6)	0.092(7)	0.084(7)	0.047(6)	−0.008(6)	−0.011(6)	−0.004(5)
C(13)	4e	0.6545(5)	−0.025(1)	0.1786(6)	0.061(6)	0.068(6)	0.057(6)	−0.013(5)	0.013(5)	−0.002(5)

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