Crystal structure of dichlorodicyanoethyl(1,10-phenanthroline)tin, [(NCCH₂CH₂)₂Sn(phen)Cl₂]

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Source of material: Crystals were obtained from the reaction of [(NCCH₂CH₂)₂SnCl₂] (a gift from Prof. K. Jurkschat, Dortmund) and 1,10-phenanthroline in an acetonitrile/chloroform solution (9/1 v/v).

The $d(\text{Sn}-\text{Cl})$ and $d(\text{Sn}-\text{N})$ distances of 2.509(1) Å, 2.549(1) Å, 2.355(2) Å and 2.352(2) Å are comparable with the 2,2'-bipyridyl analogue (see ref. 1), consistent with the similar coordinating potential of the two diimine bases.

$\text{C}_{18}\text{H}_{16}\text{Cl}_2\text{N}_4\text{Sn}$, triclinic, $P\bar{1}$ (No. 2), $a=10.237(1)$ Å, $b=12.194(2)$ Å, $c=8.235(3)$ Å, $\alpha=97.18(2)^\circ$, $\beta=107.87(2)^\circ$, $\gamma=77.02(1)^\circ$, $V=951.6$ Å³, $Z=2$, $R(F)=0.027$, $R_w(F)=0.030$.

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

Crystal:	colorless, block, size 0.15 x 0.19 x 0.29 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ :	16.31 cm ⁻¹
Diffractometer:	Rigaku AFC6R
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	3602
Criterion for I_o :	$I_o > 3 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	226
Programs:	SHELXS-86, TEXSAN

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(1a)	2i	-0.0235	-0.4237	0.2045	0.056
H(1b)	2i	0.1214	-0.3912	0.2197	0.056
H(2a)	2i	0.1138	-0.2935	0.4854	0.069
H(2b)	2i	-0.0209	-0.3415	0.4714	0.069
H(5a)	2i	-0.2728	-0.0676	-0.0658	0.059
H(5b)	2i	-0.1271	-0.0388	-0.0558	0.059
H(6a)	2i	-0.1364	0.0385	0.2367	0.077
H(6b)	2i	-0.2087	0.1133	0.0769	0.077
H(9)	2i	-0.1283	-0.1017	0.4920	0.063
H(10)	2i	-0.2982	-0.0715	0.6413	0.082
H(11)	2i	-0.5022	-0.1433	0.5225	0.081
H(14)	2i	-0.648	-0.2554	0.2786	0.086
H(15)	2i	-0.6713	-0.3570	0.0214	0.086
H(18)	2i	-0.5826	-0.4258	-0.2368	0.083
H(19)	2i	-0.4115	-0.4367	-0.3715	0.084
H(20)	2i	-0.2170	-0.3558	-0.2372	0.068

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn	2i	-0.07613(2)	-0.21372(2)	0.12320(3)	0.0336(1)	0.0340(1)	0.0345(1)	-0.00620(7)	0.01007(7)	0.00274(7)
Cl(1)	2i	0.0265(1)	-0.27918(9)	-0.1208(1)	0.0572(5)	0.0823(7)	0.0511(5)	-0.0122(5)	0.0290(4)	-0.0036(5)
Cl(2)	2i	0.10525(9)	-0.11180(7)	0.3322(1)	0.0478(4)	0.0483(5)	0.0651(6)	-0.0172(4)	0.0052(4)	-0.0035(4)
N(1)	2i	-0.2317(3)	-0.1872(2)	0.2906(3)	0.047(1)	0.033(1)	0.039(1)	-0.002(1)	0.018(1)	0.005(1)
N(2)	2i	-0.2678(3)	-0.2989(2)	-0.0235(3)	0.040(1)	0.038(1)	0.040(1)	-0.010(1)	0.007(1)	0.001(1)
N(4)	2i	0.2256(4)	-0.5374(3)	0.5798(5)	0.079(2)	0.062(2)	0.083(3)	0.005(2)	-0.003(2)	0.029(2)
N(8)	2i	-0.4477(4)	0.0784(3)	0.1957(5)	0.083(3)	0.082(3)	0.068(2)	0.016(2)	0.029(2)	0.014(2)
C(1)	2i	0.0336(3)	-0.3669(3)	0.2480(4)	0.050(2)	0.035(2)	0.048(2)	-0.003(1)	0.006(1)	0.005(1)
C(2)	2i	0.0662(4)	-0.3561(3)	0.4415(5)	0.071(2)	0.046(2)	0.049(2)	-0.001(2)	0.009(2)	0.012(2)
C(3)	2i	0.1556(4)	-0.4589(3)	0.5198(5)	0.060(2)	0.054(2)	0.053(2)	-0.010(2)	0.006(2)	0.010(2)
C(5)	2i	-0.1829(3)	-0.0563(3)	0.0102(5)	0.050(2)	0.048(2)	0.052(2)	-0.005(1)	0.013(2)	0.021(2)
C(6)	2i	-0.2106(4)	0.0471(3)	0.1297(6)	0.061(2)	0.034(2)	0.092(3)	-0.003(2)	0.015(2)	0.013(2)
C(7)	2i	-0.3437(4)	0.0644(3)	0.1672(5)	0.067(2)	0.043(2)	0.056(2)	0.006(2)	0.008(2)	0.007(2)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(9)	2i	−0.2134(4)	−0.1312(3)	0.4415(4)	0.071(2)	0.046(2)	0.040(2)	0.000(2)	0.020(2)	0.002(1)
C(10)	2i	−0.3133(5)	−0.1134(4)	0.5313(5)	0.107(4)	0.061(3)	0.051(2)	0.015(2)	0.041(2)	0.010(2)
C(11)	2i	−0.4314(5)	−0.1559(4)	0.4625(6)	0.093(3)	0.061(3)	0.090(3)	0.021(2)	0.067(3)	0.029(2)
C(12)	2i	−0.4531(4)	−0.2171(3)	0.3041(5)	0.051(2)	0.049(2)	0.080(3)	0.010(2)	0.035(2)	0.027(2)
C(13)	2i	−0.3493(3)	−0.2296(2)	0.2210(4)	0.037(2)	0.035(2)	0.054(2)	0.005(1)	0.017(1)	0.019(1)
C(14)	2i	−0.5750(4)	−0.2653(4)	0.2219(8)	0.048(2)	0.072(3)	0.144(5)	0.007(2)	0.054(3)	0.043(3)
C(15)	2i	−0.5895(4)	−0.3237(4)	0.0707(8)	0.040(2)	0.063(3)	0.146(5)	−0.005(2)	0.025(3)	0.036(3)
C(16)	2i	−0.3677(3)	−0.2901(2)	0.0565(4)	0.033(1)	0.031(1)	0.058(2)	−0.002(1)	0.008(1)	0.014(1)
C(17)	2i	−0.4873(4)	−0.3376(3)	−0.0189(6)	0.041(2)	0.046(2)	0.086(3)	−0.010(2)	0.005(2)	0.023(2)
C(18)	2i	−0.5010(4)	−0.3929(4)	−0.1805(7)	0.055(2)	0.057(2)	0.098(4)	−0.025(2)	−0.015(2)	0.007(2)
C(19)	2i	−0.4024(5)	−0.3987(4)	−0.2589(6)	0.078(3)	0.068(3)	0.064(3)	−0.029(2)	−0.005(2)	−0.011(2)
C(20)	2i	−0.2869(4)	−0.3509(3)	−0.1782(5)	0.058(2)	0.053(2)	0.051(2)	−0.016(2)	0.004(2)	−0.005(2)

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