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# Tetrachloro(1,10-phenanthroline-$\kappa^2N,N'$)tin(IV)

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**Key indicators**

Single-crystal X-ray study
$T$ = 295 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.024
$wR$ factor = 0.066
Data-to-parameter ratio = 19.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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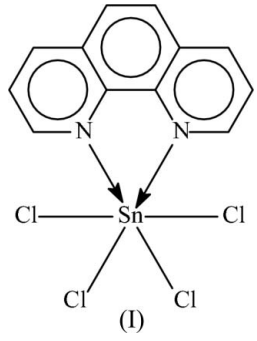
The tin(IV) atom in the title compound, $[SnCl_4(C_{12}H_8N_2)]$, is six-coordinate in an octahedral geometry.

## Comment

The 1,10-phenanthroline adduct of Lewis-acidic stannic chloride was synthesized many years ago (Beattie *et al.*, 1963; Clark *et al.*, 1968; Ohkaku & Nakamoto, 1973; Smith & Wassef, 1975); the adduct has recently been studied theoretically (Davydova *et al.*, 2006). It has been characterized by X-ray crystallography as a 1/4 benzene solvate (Hall & Tiekink, 1996) in which the chelated Sn atom is in an octahedral environment. The title compound adopts a similar structure (Fig. 1), and its geometric parameters are similar to those reported for the benzene solvate.




(I)

## Experimental

Stannic chloride (1.41 g, 4.0 mmol), copper(II) sulfate pentahydrate (0.43 g, 1.7 mmol), 1,10-phenanthroline (0.23 g, 1.15 mmol) and water (10 ml) were placed in a 20-ml Teflon-lined Parr bomb. The bomb was heated to 433 K for 6 d. Colorless block-shaped crystals were isolated from the cool solution.

### *Crystal data*

$[SnCl_4(C_{12}H_8N_2)]$
$M_r$ = 440.69
Monoclinic, $P2_1/c$
$a$ = 7.5183 (4) Å
$b$ = 19.5789 (9) Å
$c$ = 10.5220 (5) Å
$\beta$ = 108.556 (1)°
$V$ = 1468.3 (1) Å$^3$
$Z$ = 4
$D_x$ = 1.994 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 2.45 mm$^{-1}$
$T$ = 295 (2) K
Block, colorless
0.24 × 0.16 × 0.14 mm

### *Data collection*

Bruker APEX-II area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.591, $T_{max}$ = 0.725
10809 measured reflections
3346 independent reflections
2930 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.017
$\theta_{max}$ = 27.5°

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 0.9593P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.024$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $wR(F^2) = 0.066$ | $\Delta\rho_{max} = 0.65$ e Å$^{-3}$ |
| $S = 1.02$ | $\Delta\rho_{min} = -0.67$ e Å$^{-3}$ |
| 3346 reflections | |
| 172 parameters | |
| H-atom parameters constrained | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Sn1—N1 | 2.234 (2) | Sn1—Cl2 | 2.3498 (8) |
| Sn1—N2 | 2.241 (2) | Sn1—Cl3 | 2.3779 (8) |
| Sn1—Cl1 | 2.3707 (7) | Sn1—Cl4 | 2.3970 (8) |
| | | | |
| N1—Sn1—N2 | 74.56 (8) | N2—Sn1—Cl4 | 87.26 (6) |
| N1—Sn1—Cl1 | 93.41 (6) | Cl1—Sn1—Cl2 | 99.40 (3) |
| N1—Sn1—Cl2 | 167.12 (6) | Cl1—Sn1—Cl3 | 91.32 (3) |
| N1—Sn1—Cl3 | 86.45 (6) | Cl1—Sn1—Cl4 | 93.48 (3) |
| N1—Sn1—Cl4 | 86.59 (6) | Cl2—Sn1—Cl3 | 91.86 (3) |
| N2—Sn1—Cl1 | 167.89 (6) | Cl2—Sn1—Cl4 | 93.95 (3) |
| N2—Sn1—Cl2 | 92.59 (6) | Cl3—Sn1—Cl4 | 171.76 (3) |
| N2—Sn1—Cl3 | 86.64 (6) | | |

H atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with $U_{iso}$(H)= 1.2$U_{eq}$(C).

Data collection: *APEX-II Software* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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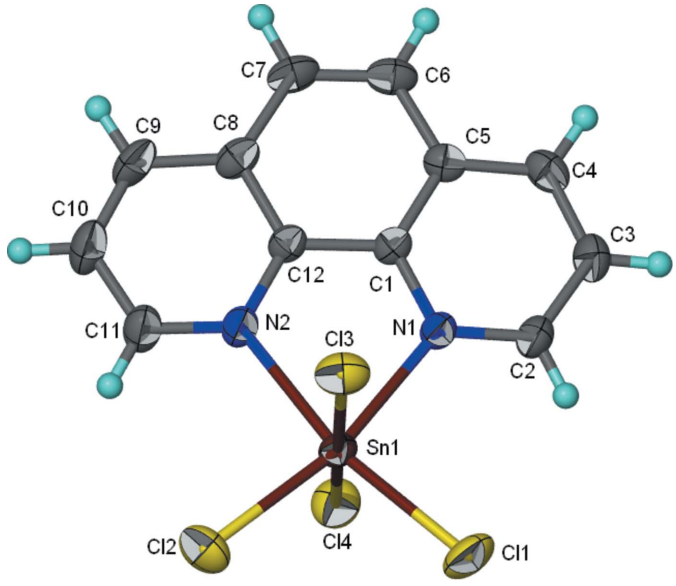


**Figure 1**
**Fig. 1**. The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level; H atoms are shown as spheres of arbitrary radius.

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