

Table 2. Selected geometric parameters (Å, °)

Cd—N(9)	2.317 (1)	C(7)—N(8)	1.332 (2)
Cd—O(1)	2.253 (2)	N(8)—N(9)	1.376 (2)
Cd—O(11)	2.307 (2)	N(9)—C(4)	1.336 (2)
N(1)—C(2)	1.389 (2)	C(2)—O(2)	1.222 (2)
C(2)—N(3)	1.372 (2)	C(6)—O(6)	1.233 (2)
N(3)—C(4)	1.367 (2)	N(3)—N(9)	2.419 (2)
C(4)—C(5)	1.408 (2)	N(11)—O(11)	1.256 (2)
C(5)—C(6)	1.436 (2)	N(11)—O(12)	1.238 (2)
C(6)—N(1)	1.377 (2)	N(11)—O(13)	1.236 (2)
C(5)—C(7)	1.390 (3)		
N(9)—Cd—O(1)	89.65 (8)	C(7)—N(8)—N(9)	112.9 (2)
N(9)—Cd—O(1')	90.35 (8)	N(8)—N(9)—C(4)	104.4 (1)
N(9)—Cd—O(11)	85.40 (6)	N(9)—C(4)—C(5)	110.8 (2)
N(9)—Cd—O(11')	94.60 (6)	N(3)—C(4)—N(9)	126.9 (2)
O(1)—Cd—O(11)	90.96 (9)	C(6)—C(5)—C(7)	135.0 (2)
O(1)—Cd—O(11')	89.04 (9)	N(1)—C(2)—O(2)	120.7 (2)
C(6)—N(1)—C(2)	128.0 (2)	N(3)—C(2)—O(2)	123.2 (2)
N(1)—C(2)—N(3)	116.1 (2)	N(1)—C(6)—O(6)	120.9 (2)
C(2)—N(3)—C(4)	120.5 (2)	C(5)—C(6)—O(6)	125.6 (2)
N(3)—C(4)—C(5)	122.3 (1)	Cd—N(9)—N(8)	121.7 (1)
C(4)—C(5)—C(6)	119.4 (2)	Cd—N(9)—C(4)	133.9 (1)
C(5)—C(6)—N(1)	113.5 (1)	O(11)—N(11)—O(12)	117.9 (2)
C(4)—C(5)—C(7)	105.5 (1)	O(11)—N(11)—O(13)	120.7 (2)
C(5)—C(7)—N(8)	106.3 (2)	O(12)—N(11)—O(13)	121.4 (2)

Table 3. Hydrogen-bonding geometry (Å, °)

D	H	A	D—H	H...A	D...A	D—H...A
N(1)	H(1)	O(6)	0.78 (3)	2.08 (3)	2.856 (2)	175 (3)
N(3)	H(3)	O(11)	1.11 (4)	2.02 (4)	2.866 (3)	131 (3)
N(3)	H(3)	O(12)	1.11 (4)	2.20 (4)	3.288 (2)	166 (3)
N(8)	H(8)	O(11)	0.93 (3)	2.88 (3)	3.425 (3)	119 (2)
N(8)	H(8)	O(13)	0.93 (3)	1.94 (3)	2.859 (2)	166 (3)
O(1)	H(11)	O(2)	0.81 (4)	2.09 (4)	2.770 (3)	141 (4)
O(1)	H(12)	O(6)	0.84 (4)	2.18 (4)	2.857 (3)	138 (4)

The structure determination was started with the atomic coordinates of the non-H atoms of the isostructural Cu complex (Hänggi, Schmalte & Dubler, 1993); refinement was by full-matrix least-squares calculations applying the program *MolEN* (Fair, 1990). After anisotropic refinement, all H atoms could be located in the difference Fourier maps and were included in the refinement with variable positional and isotropic displacement parameters.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71589 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SH1062]

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n-Butyltris(2-pyrimidinethiolato-*N,S*)tin(IV)

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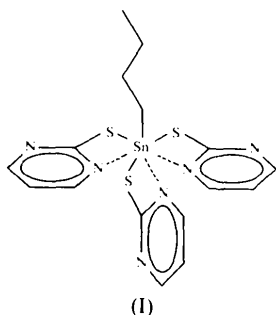
Abstract

The crystal structure of the title compound contains two crystallographically independent molecules. The 2-pyrimidinethiolato ligands (SPym) are bidentate. Sn—S bond distances range from 2.445 (4) to 2.561 (5) Å and Sn...N coordination is inferred from short Sn—N distances [2.470 (5)–2.622 (6) Å]. The coordination polyhedron around Sn in both molecules can be considered as a distorted pentagonal bipyramid. The pentagonal plane in each molecule is formed by two SPym ligands, with S atoms in *cis* positions, and the N atom of the third SPym ligand. The S atom of this ligand, which is arranged nearly perpendicular to the equatorial plane, and the C(*n*-butyl) atom occupy the axial positions. Intermolecular distances shorter than the sum of the van der Waals radii were not found.

Comment

In diorganotin(IV) complexes of 2-mercaptopyridine (HSPy) and 2-mercaptopyrimidine (HSPym), the ligands form four-membered bidentate chelate rings with strong intramolecular Sn—N coordination (Mullins, 1979; Schmiedgen, 1992). For monoorganotin(IV) complexes with the same ligands, e.g. *RSn*(SPym)₃ (*R* = methyl, *n*-butyl, phenyl), an analogous bonding behavior and a distorted pentagonal bipyramidal coordination polyhedron around Sn has

been inferred from IR and ¹¹⁹Sn Mössbauer data (Schmiedgen, 1992; Schmiedgen, Huber, Schürmann & Barbieri, 1994), and *p*-TolSn(SPy)₃ (*p*-Tol = 4-CH₃C₆H₄) was shown recently by X-ray structure determination to have such a molecular structure (Schürmann & Huber, 1994). We report here on the crystal structure determination of "BuSn(SPy)₃ (I), as a first example of the structure of a monoorganotrakis(2-pyrimidinethiolato)tin(IV) complex.



The title compound was prepared in chloroform from "BuSnCl₃, HSPym and equivalent amounts of NaOMe in MeOH. After evaporation of the solvent, the residue was redissolved in chloroform, NaCl was filtered off and petroleum ether (b.p. 313–333 K) was added to precipitate the crystals (m.p. 461 K).

A view of the two crystallographically independent molecules of the title compound with the atomic numbering scheme is shown in Fig. 1 and a stereoscopic view of the unit cell is shown in Fig. 2. The coordination polyhedron around tin can be described as a distorted pentagonal bipyramid. The pentagonal plane in both molecules is formed by two SPym ligands, with S atoms in *cis* positions, and the N atom of the third ligand. The S atom of this ligand, which is arranged nearly perpendicular to the pentagonal plane, and the C(*n*-butyl) atom occupy the axial positions.

Each of the three Sn—N bond distances in both molecules [Sn—N = 2.470 (5)–2.622 (6) Å] is appreciably shorter than the sum of the appropriate van der Waals radii (3.75 Å; Bondi, 1964) indicating the bidentate nature of all three SPym ligands. Similar distances are found in Ph₂Sn(SPy)₂ [Sn—N = 2.667 (4) Å; Schmiedgen, Huber & Preut, 1993], "Bu₂Sn(SPy-5-NO₂)₂ [Sn—N = 2.77 (1) Å; Domazetis, James, Mackay & Magee, 1979], *p*-TolSn(SPy)₃ [Sn—N = 2.444 (8)–2.487 (7) Å; Schürmann & Huber, 1994] and MeSn(SPy)₃ [Sn—N = 2.4159 (5)–2.5781 (4) Å; Schmiedgen, Huber & Schürmann, 1994]. The Sn—S bond distances [Sn—S = 2.445 (4)–2.561 (5) Å] are essentially the same as in MeSn(SPy)₃ [Sn—S = 2.4793 (5)–2.5857 (4) Å; Schmiedgen, Huber & Schürmann, 1994], *p*-TolSn(SPy)₃ [Sn—S = 2.486 (3)–2.571 (3) Å; Schürmann &

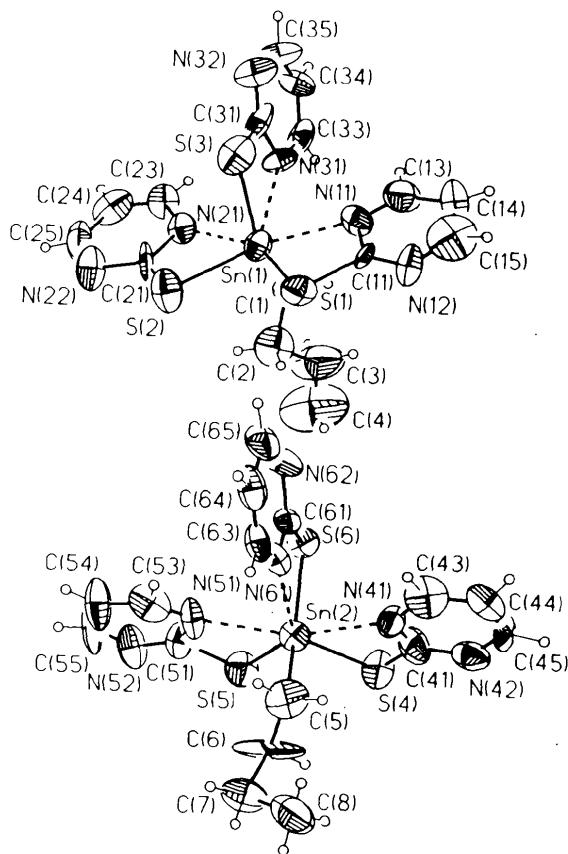


Fig. 1. View (*SHELXTL-Plus*; Sheldrick, 1987) of part of the crystal structure, showing the atom-numbering scheme.

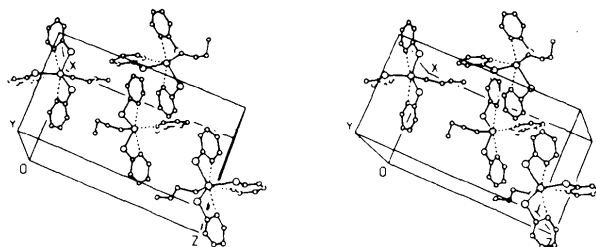


Fig. 2. Stereoscopic view (*SHELXTL-Plus*; Sheldrick, 1987) of the title structure. The alkyl H atoms are omitted for clarity.

Huber, 1994] and PhSn(pte)₃ (pte = 1-pyrrolothio-carboxylato) [Sn—S = 2.448 (1)–2.538 (1) Å; Srivastava, Gupta, Nöth & Rattay, 1988], and similar to those in "BuSn(S₂CNEt₂)₃ [Sn—S = 2.491 (7)–2.820 (7) Å; Morris & Schlemper, 1979].

The six SPym ligands (considering both molecules) differ distinctly from each other with regard to their Sn—N bond distances [2.470 (5)–2.622 (6) Å] and S—Sn—N bite angles [60.1 (2)–63.8 (2)°]. Appreciable differences in Sn—N distances and S—Sn—N

bite angles are also observed in MeSn(SPy)₃ (Schmiedgen, Huber & Schürmann, 1994). In contrast, in Ph₃Sn(SPy)₂ the appropriate values [Sn—N (mean) = 2.67 (4) Å, S—Sn—N = 60.7 (8) ; Schmiedgen, Huber & Preut, 1993] are almost identical. An obvious conclusion is to correlate the differences observed in the RSnX₃ compounds (X = SPy, SPym) with sterical crowding at Sn.

The pyrimidine rings are nearly planar, but the equatorial planes formed by Sn(1), S(1), S(2), N(11), N(21), N(31) and Sn(2), S(4), S(5), N(41), N(51), N(61) deviate significantly from planarity; both N(31) and N(61) are located more than 0.45 Å below their associated calculated plane. The conspicuous deviations of the C(1)—C(2)—C(3) [98.3 (5)] and C(5)—C(6)—C(7) [128.9 (7)] angles from the ideal angle of 109.5° are probably caused by lattice effects. Intermolecular distances shorter than the sum of the van der Waals radii were not found.

Experimental

Crystal data

[Sn(C₄H₃N₂S)₃(C₄H₉)]

M_r = 509.23

Monoclinic

*P*2₁

a = 9.523 (2) Å

b = 12.849 (3) Å

c = 17.079 (3) Å

β = 92.67 (3)°

V = 2087.5 (8) Å³

Z = 4

D_x = 1.620 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 50 reflections

θ = 7.8–15.1°

μ = 1.528 mm⁻¹

T = 291 (1) K

Block

0.34 × 0.28 × 0.20 mm

Colorless

Data collection

Nicolet *R3m/V* diffractometer

ω/2θ scans (3.0–15.0° min⁻¹ in θ)

Absorption correction: empirical

T_{min} = 0.925, *T_{max}* = 0.961

6035 measured reflections

3889 independent reflections

2664 observed reflections [*F* ≥ 1.5σ(*F*)]

R_{int} = 0.018

θ_{max} = 25°

h = -11 → 4

k = 0 → 13

l = -20 → 20

6 standard reflections

frequency: 150 min

intensity variation: none

Refinement

Refinement on *F*

R = 0.0293

wR = 0.0231

S = 0.75

2664 reflections

471 parameters

Only H-atom *U*'s refined

w = 1/[σ²(*F*) + 0.0002*F*²]

(Δ/σ)_{max} = 0.079

Δρ_{max} = 0.28 e Å⁻³

Δρ_{min} = -0.27 e Å⁻³

Atomic scattering factors

from *International Tables*

for *X-ray Crystallography*

(1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

$$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^* \cdot \mathbf{a}_i \cdot \mathbf{a}_j$$

Molecule A	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{eq}</i>
Sn(1)	0.2077 (2)	0	-0.03164 (9)	0.0503 (2)
S(1)	0.0077 (4)	0.1291 (3)	-0.0529 (3)	0.0612 (3)
S(2)	0.3377 (4)	0.1014 (3)	-0.1303 (3)	0.0773 (4)
S(3)	0.3176 (4)	0.0828 (3)	0.0846 (3)	0.0742 (4)
C(11)	-0.0864 (5)	0.0654 (4)	0.0208 (4)	0.0330 (4)
N(11)	-0.0019 (5)	-0.0090 (4)	0.0559 (4)	0.0579 (4)
C(13)	-0.0625 (6)	-0.0654 (5)	0.1081 (5)	0.0813 (4)
C(14)	-0.1979 (6)	-0.0521 (5)	0.1294 (5)	0.0832 (4)
C(15)	-0.2642 (6)	0.0476 (5)	0.0892 (5)	0.1075 (4)
N(12)	-0.2138 (5)	0.1018 (4)	0.0354 (4)	0.0611 (4)
C(21)	0.4624 (5)	0.0146 (5)	-0.1153 (4)	0.0646 (4)
N(21)	0.4458 (5)	-0.0629 (4)	-0.0585 (4)	0.0541 (4)
C(23)	0.5583 (5)	-0.1305 (4)	-0.0387 (4)	0.0545 (4)
C(24)	0.6811 (6)	-0.1273 (5)	-0.0772 (5)	0.0760 (4)
C(25)	0.6873 (6)	-0.0487 (5)	-0.1345 (5)	0.0917 (4)
N(22)	0.5867 (5)	0.0284 (4)	-0.1549 (4)	0.0750 (4)
C(31)	0.3522 (5)	-0.0345 (5)	0.1296 (5)	0.0646 (4)
N(31)	0.2977 (5)	-0.1159 (5)	0.0864 (4)	0.0541 (4)
C(33)	0.3127 (6)	-0.2131 (5)	0.1217 (5)	0.0722 (4)
C(34)	0.3848 (6)	-0.2201 (5)	0.1927 (4)	0.0647 (4)
C(35)	0.4198 (6)	-0.1345 (5)	0.2241 (5)	0.0881 (4)
N(32)	0.4135 (5)	-0.0382 (4)	0.1936 (4)	0.0697 (4)
C(1)	0.1484 (5)	-0.1455 (4)	-0.0831 (4)	0.0543 (4)
C(2)	0.1195 (6)	-0.1405 (5)	-0.1745 (5)	0.0889 (4)
C(3)	0.0386 (6)	-0.2633 (5)	-0.1875 (5)	0.1570 (4)
C(4)	-0.0009 (6)	-0.2692 (6)	-0.2545 (5)	0.2042 (4)

Molecule B	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{eq}</i>
Sn(2)	-0.2921 (2)	-0.01559 (4)	-0.53128 (8)	0.0534 (3)
S(4)	-0.4924 (4)	-0.1451 (3)	-0.5519 (3)	0.0732 (4)
S(5)	-0.1637 (4)	-0.1170 (4)	-0.6353 (3)	0.0760 (4)
S(6)	-0.1819 (4)	-0.1024 (3)	-0.4169 (3)	0.0550 (3)
C(41)	-0.5716 (6)	-0.0755 (6)	-0.4815 (5)	0.0891 (4)
N(41)	-0.5130 (5)	0.0062 (5)	-0.4467 (4)	0.0596 (4)
C(43)	-0.5776 (6)	0.0481 (5)	-0.3849 (5)	0.0831 (4)
C(44)	-0.7088 (6)	0.0132 (5)	-0.3638 (4)	0.0753 (4)
C(45)	-0.7689 (5)	-0.0504 (5)	-0.4039 (4)	0.0594 (4)
N(42)	-0.7076 (6)	-0.0977 (4)	-0.4644 (4)	0.0769 (4)
C(51)	-0.0075 (5)	-0.0327 (4)	-0.6173 (5)	0.0585 (4)
N(51)	-0.0420 (5)	0.0346 (4)	-0.5627 (4)	0.0650 (4)
C(53)	0.0505 (6)	0.1040 (5)	-0.5533 (5)	0.0832 (4)
C(54)	0.1754 (6)	0.1038 (5)	-0.5883 (5)	0.0940 (4)
C(55)	0.1983 (6)	0.0304 (4)	-0.6414 (5)	0.0875 (4)
N(52)	0.1032 (5)	-0.0318 (5)	-0.6575 (4)	0.0785 (4)
C(61)	-0.1637 (5)	0.0232 (5)	-0.3738 (4)	0.0411 (4)
N(61)	-0.2065 (5)	0.1033 (5)	-0.4148 (4)	0.0528 (4)
C(63)	-0.1794 (5)	0.1963 (5)	-0.3871 (4)	0.0539 (4)
C(64)	-0.1167 (6)	0.2126 (5)	-0.3186 (5)	0.0691 (4)
C(65)	-0.0605 (6)	0.1219 (5)	-0.2709 (4)	0.0803 (4)
N(62)	-0.0897 (6)	0.0282 (5)	-0.2987 (4)	0.0820 (4)
C(5)	-0.3845 (6)	0.1191 (5)	-0.5886 (5)	0.0850 (4)
C(6)	-0.3971 (6)	0.1217 (5)	-0.6664 (5)	0.1646 (4)
C(7)	-0.4170 (6)	0.2127 (4)	-0.7189 (4)	0.0832 (4)
C(8)	-0.5574 (6)	0.2500 (5)	-0.7012 (4)	0.1177 (4)

Table 2. Selected geometric parameters (Å, °)

Molecule A	Value	Molecule B	Value
Sn(1)—S(1)	2.539 (4)	Sn(2)—S(4)	2.543 (4)
Sn(1)—S(2)	2.503 (5)	Sn(2)—S(5)	2.561 (5)
Sn(1)—S(3)	2.446 (5)	Sn(2)—S(6)	2.445 (4)
Sn(1)—N(11)	2.552 (6)	Sn(2)—N(41)	2.622 (6)
Sn(1)—N(21)	2.470 (5)	Sn(2)—N(51)	2.549 (5)
Sn(1)—N(31)	2.619 (7)	Sn(2)—N(61)	2.611 (7)
Sn(1)—C(1)	2.131 (6)	Sn(2)—C(5)	2.156 (7)
S(1)—C(11)	1.778 (7)	S(4)—C(41)	1.702 (9)
S(2)—C(21)	1.641 (7)	S(5)—C(51)	1.855 (7)
S(3)—C(31)	1.717 (8)	S(6)—C(61)	1.779 (7)

C(11)—N(11)	1.370 (8)	C(41)—N(41)	1.318 (9)
C(11)—N(12)	1.335 (7)	C(41)—N(42)	1.371 (8)
N(11)—C(13)	1.306 (9)	N(41)—C(43)	1.36 (1)
C(15)—N(12)	1.27 (1)	C(45)—N(42)	1.356 (9)
C(21)—N(21)	1.405 (9)	C(51)—N(51)	1.32 (1)
C(21)—N(22)	1.402 (8)	C(51)—N(52)	1.284 (9)
N(21)—C(23)	1.407 (7)	N(51)—C(53)	1.258 (8)
C(25)—N(22)	1.411 (8)	C(55)—N(52)	1.229 (8)
C(31)—N(31)	1.369 (9)	C(61)—N(61)	1.300 (9)
C(31)—N(32)	1.22 (1)	C(61)—N(62)	1.437 (9)
N(31)—C(33)	1.391 (9)	N(61)—C(63)	1.306 (9)
C(35)—N(32)	1.344 (9)	C(65)—N(62)	1.319 (9)
N(31)—Sn(1)—C(1)	83.7 (2)	N(61)—Sn(2)—C(5)	89.1 (2)
N(21)—Sn(1)—C(1)	82.2 (2)	N(51)—Sn(2)—C(5)	93.8 (2)
N(21)—Sn(1)—N(31)	71.8 (2)	N(51)—Sn(2)—N(61)	75.6 (2)
N(11)—Sn(1)—C(1)	90.2 (2)	N(41)—Sn(2)—C(5)	81.1 (2)
N(11)—Sn(1)—N(31)	76.1 (2)	N(41)—Sn(2)—N(61)	75.3 (2)
N(11)—Sn(1)—N(21)	147.6 (2)	N(41)—Sn(2)—N(51)	150.6 (2)
S(3)—Sn(1)—C(1)	144.3 (2)	S(6)—Sn(2)—C(5)	151.7 (2)
S(3)—Sn(1)—N(31)	60.6 (2)	S(6)—Sn(2)—N(61)	63.2 (2)
S(3)—Sn(1)—N(21)	86.1 (2)	S(6)—Sn(2)—N(51)	85.0 (2)
S(3)—Sn(1)—N(11)	81.9 (2)	S(6)—Sn(2)—N(41)	86.2 (2)
S(2)—Sn(1)—C(1)	107.9 (2)	S(5)—Sn(2)—C(5)	106.9 (2)
S(2)—Sn(1)—N(31)	131.3 (2)	S(5)—Sn(2)—N(61)	133.3 (2)
S(2)—Sn(1)—N(21)	63.8 (2)	S(5)—Sn(2)—N(51)	60.1 (2)
S(2)—Sn(1)—N(11)	147.5 (2)	S(5)—Sn(2)—N(41)	149.1 (2)
S(2)—Sn(1)—S(3)	96.6 (2)	S(5)—Sn(2)—S(6)	97.0 (1)
S(1)—Sn(1)—C(1)	109.4 (2)	S(4)—Sn(2)—C(5)	100.2 (2)
S(1)—Sn(1)—N(31)	134.2 (2)	S(4)—Sn(2)—N(61)	133.9 (2)
S(1)—Sn(1)—N(21)	151.2 (2)	S(4)—Sn(2)—N(51)	147.0 (2)
S(1)—Sn(1)—N(11)	60.8 (2)	S(4)—Sn(2)—N(41)	62.0 (2)
S(1)—Sn(1)—S(3)	97.0 (2)	S(4)—Sn(2)—S(6)	95.9 (2)
S(1)—Sn(1)—S(2)	87.4 (1)	S(4)—Sn(2)—S(5)	87.2 (2)
Sn(1)—S(1)—C(11)	89.9 (3)	Sn(2)—S(4)—C(41)	85.0 (3)
Sn(1)—S(2)—C(21)	85.3 (3)	Sn(2)—S(5)—C(51)	89.6 (3)
Sn(1)—S(3)—C(31)	92.7 (3)	Sn(2)—S(6)—C(61)	87.0 (3)
Sn(1)—N(11)—C(11)	99.9 (4)	Sn(2)—N(41)—C(41)	90.0 (4)
Sn(1)—N(11)—C(13)	144.0 (5)	Sn(2)—N(41)—C(43)	151.1 (4)
Sn(1)—N(21)—C(21)	91.7 (4)	Sn(2)—N(51)—C(51)	104.4 (4)
Sn(1)—N(21)—C(23)	148.4 (5)	Sn(2)—N(51)—C(53)	143.9 (5)
Sn(1)—N(31)—C(31)	94.8 (4)	Sn(2)—N(61)—C(61)	91.5 (4)
Sn(1)—N(31)—C(33)	150.2 (5)	Sn(2)—N(61)—C(63)	149.5 (5)
Sn(1)—C(1)—C(2)	113.9 (4)	Sn(2)—C(5)—C(6)	119.3 (5)

Systematic absences ($h0l$) $h + l = 2n + 1$, ($00l$) $l = 2n + 1$, ($h00$) $h = 2n + 1$ and ($0k0$) $k = 2n + 1$ were detected. The space group $P2_1/n$, at first suggested by *SHELXTL-Plus* (Sheldrick, 1987), had to be dismissed as the structure could not be solved in this space group, but was instead solved by examination of the Patterson function and by trial-and-error testing, coupled with electron-density and least-squares calculations. The structure was solved by standard Patterson and difference Fourier methods and refined satisfactorily in space group $P2_1$ (No.4) by full-matrix least-squares calculations employing *SHELXTL-Plus*. The H atoms were placed in geometrically calculated positions and refined with common isotropic displacement parameters for different C—H types (aryl H, alkyl H). The programs used were *SHELXTL-Plus*, *PARST* (Nardelli, 1983), *PLATON* (Spek, 1982) and *MISSYM* (Le Page, 1987).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71555 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SE1034]

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(2,2'-Biquinoline- $\kappa^2 N, N'$)chloro-(2,2':6',2''-terpyridine- $\kappa^3 N, N', N''$)-ruthenium(II) Hexafluorophosphate, [RuCl(C₁₈H₁₂N₂)(C₁₅H₁₁N₃)] [PF₆]

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Abstract

The coordination geometry about Ru^{II}, involving one Cl and five N atoms, is distorted octahedral and shows several signs of interligand steric interactions. Ru—N distances are in the range 1.970 (7)–2.103 (6) Å and the Ru—Cl distance is 2.378 (2) Å.

Comment

The title compound (I) was synthesized and isolated as part of a program aimed at the development of new ruthenium complexes.