Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dimethyl(1,10-phenanthroline-κ^2N,N')-bis(thiocyanato-κN)tin(IV)

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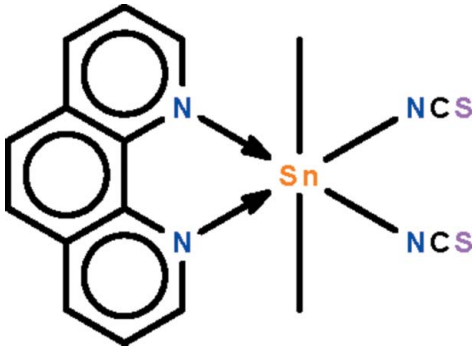
Received 17 November 2012; accepted 20 November 2012

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.010 Å; R factor = 0.039; wR factor = 0.106; data-to-parameter ratio = 20.0.

The Sn^{IV} atom in the title compound, $[Sn(CH_3)_2(NCS)_2(C_{12}H_8N_2)]$, is located on a twofold rotation axis in a distorted octahedral enviroment. The methyl groups are *trans* to each other [C—Sn—C = 175.7 (3)°], whereas the thiocyanate groups are *cis* to each other.

Related literature

For dimethyltin dithiothiocyanate, see: Britton (2006). For the 4,4′-bipyridine adduct, see: Najafi *et al.* (2011).



Experimental

Crystal data

$[Sn(CH_3)_2(NCS)_2(C_{12}H_8N_2)]$
M_r = 445.12
Orthorhombic, *Pccn*
a = 6.8218 (7) Å
b = 12.9272 (13) Å
c = 20.746 (2) Å
V = 1829.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.63 mm^{-1}
T = 295 K
0.30 × 0.15 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.641, T_{max} = 0.923
10262 measured reflections
2116 independent reflections
1368 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.01
2116 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Shahid Beheshti University and the Ministry of Higher Education of Malaysia (grant No. UM.C/HIR/MOHE/SC/12) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6862).

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supporting information

Acta Cryst. (2012). E**68**, m1544 [doi:10.1107/S1600536812047691]

Dimethyl(1,10-phenanthroline-κ^2N,N')bis(thiocyanato-κN)tin(IV)

Ezzatollah Najafi, Mostafa M. Amini and Seik Weng Ng

S1. Comment

Few amine adducts of dimethyltin dithiocyanate, which exists as a weakly bridged polymeric chain (Britton, 2006), have been reported. The 4,4′-bipyridine adduct is polymeric (Najafi *et al.*, 2011). In the 1,10-phenanthroline adduct (Scheme I, Fig. 1), the Sn^{IV} atom is located on a twofold rotation axis in an octahedral enviroment. The methyl groups are *trans* to each other whereas the thiocyanate groups are *cis* to each other.

S2. Experimental

Dimethyltin dithiocyanate (0.27 g, 1 mmol) and 1,10-phenanthroline hydrate (0.19 g, 1 mmol) were loaded into a convection tube; the tube was filled with ethyl alcohol and kept at 333 K. Colorless crystals were collected from the side arm after several days.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.93 to 0.96 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

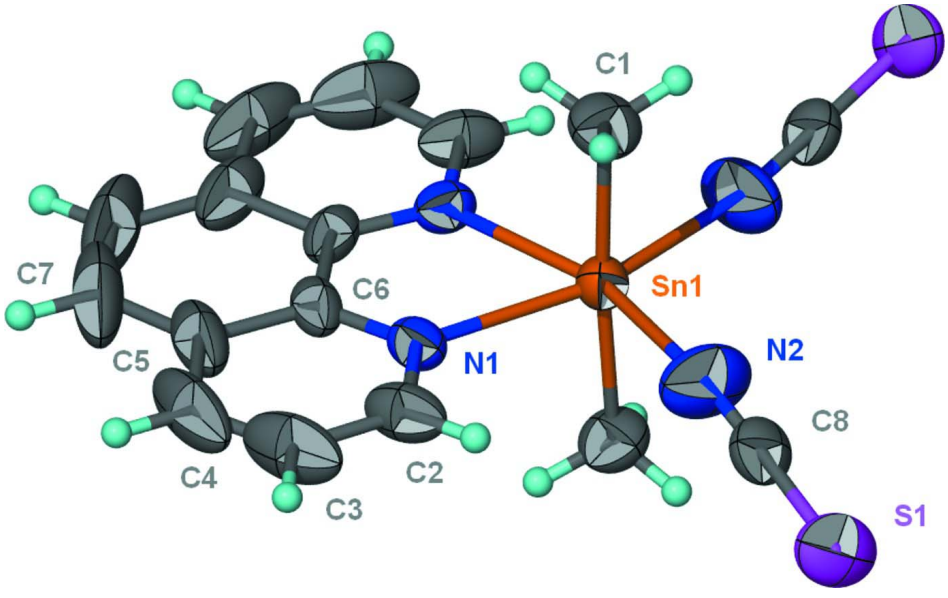

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $(CH_3)_2Sn(NCS)_2(C_{12}H_8N_2)$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Dimethyl(1,10-phenanthroline-κ^2N,N')bis(thiocyanato-κN)tin(IV)

Crystal data

$[Sn(CH_3)_2(NCS)_2(C_{12}H_8N_2)]$
$M_r = 445.12$
Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
$a = 6.8218$ (7) Å
$b = 12.9272$ (13) Å
$c = 20.746$ (2) Å
$V = 1829.5$ (3) Å^3
$Z = 4$
$F(000) = 880$
$D_x = 1.616$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1757 reflections
$\theta = 3.2$–$27.5°$
$\mu = 1.63$ mm^{-1}
$T = 295$ K
Prism, colorless
0.30 × 0.15 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.641$, $T_{max} = 0.923$
10262 measured reflections
2116 independent reflections
1368 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.2°$
$h = -6 \rightarrow 8$
$k = -16 \rightarrow 16$
$l = -27 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.106$
$S = 1.01$
2116 reflections
106 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.5974P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0024 (4)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.7500	0.2500	0.243352 (18)	0.04816 (19)
S1	0.3311 (2)	0.45584 (12)	0.09896 (7)	0.0957 (6)
N1	0.5798 (5)	0.3037 (3)	0.33508 (16)	0.0515 (8)
N2	0.5246 (7)	0.3231 (4)	0.1785 (2)	0.1073 (18)
C1	0.5903 (7)	0.1114 (4)	0.2395 (2)	0.0746 (14)
H1A	0.6337	0.0710	0.2034	0.112*
H1B	0.4533	0.1267	0.2349	0.112*
H1C	0.6109	0.0731	0.2786	0.112*
C2	0.4146 (7)	0.3576 (4)	0.3337 (3)	0.0736 (14)
H2	0.3600	0.3748	0.2941	0.088*
C3	0.3208 (10)	0.3891 (5)	0.3898 (4)	0.107 (2)
H3	0.2060	0.4276	0.3875	0.128*

C4	0.3969 (12)	0.3635 (6)	0.4470 (4)	0.115 (3)
H4	0.3327	0.3832	0.4846	0.138*
C5	0.5721 (10)	0.3073 (5)	0.4510 (3)	0.0882 (18)
C6	0.6600 (6)	0.2783 (3)	0.3924 (2)	0.0556 (11)
C7	0.6688 (15)	0.2767 (9)	0.5097 (3)	0.142 (5)
H7	0.6135	0.2956	0.5490	0.170*
C8	0.4443 (7)	0.3778 (4)	0.1449 (2)	0.0644 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0574 (3)	0.0459 (3)	0.0411 (3)	0.00503 (18)	0.000	0.000
S1	0.1188 (12)	0.0817 (11)	0.0866 (11)	0.0168 (9)	−0.0541 (9)	−0.0028 (8)
N1	0.056 (2)	0.043 (2)	0.055 (2)	0.0032 (17)	0.0090 (16)	−0.0054 (17)
N2	0.127 (4)	0.085 (4)	0.110 (4)	0.010 (3)	−0.058 (3)	0.019 (3)
C1	0.081 (4)	0.065 (3)	0.078 (4)	−0.010 (3)	−0.014 (2)	−0.009 (3)
C2	0.062 (3)	0.054 (3)	0.105 (4)	0.005 (2)	0.023 (3)	−0.010 (3)
C3	0.085 (4)	0.075 (4)	0.161 (7)	−0.002 (3)	0.061 (5)	−0.028 (5)
C4	0.137 (6)	0.096 (5)	0.113 (6)	−0.044 (5)	0.087 (5)	−0.050 (5)
C5	0.123 (5)	0.082 (4)	0.059 (3)	−0.039 (4)	0.038 (3)	−0.022 (3)
C6	0.071 (3)	0.052 (3)	0.044 (2)	−0.021 (2)	0.014 (2)	−0.008 (2)
C7	0.225 (15)	0.156 (12)	0.044 (3)	−0.092 (10)	0.035 (4)	−0.019 (4)
C8	0.071 (3)	0.068 (3)	0.054 (3)	−0.001 (3)	−0.015 (2)	−0.009 (2)

Geometric parameters (Å, º)

Sn1—C1	2.098 (5)	C1—H1C	0.9600
Sn1—C1^{i}	2.098 (5)	C2—C3	1.388 (8)
Sn1—N2^{i}	2.251 (4)	C2—H2	0.9300
Sn1—N2	2.251 (4)	C3—C4	1.337 (10)
Sn1—N1	2.335 (3)	C3—H3	0.9300
Sn1—N1^{i}	2.335 (3)	C4—C5	1.401 (9)
S1—C8	1.588 (5)	C4—H4	0.9300
N1—C2	1.326 (5)	C5—C6	1.405 (6)
N1—C6	1.350 (5)	C5—C7	1.442 (9)
N2—C8	1.134 (5)	C6—C6^{i}	1.430 (9)
C1—H1A	0.9600	C7—C7^{i}	1.31 (2)
C1—H1B	0.9600	C7—H7	0.9300
C1—Sn1—C1^{i}	175.7 (3)	Sn1—C1—H1C	109.5
C1—Sn1—N2^{i}	88.48 (19)	H1A—C1—H1C	109.5
C1^{i}—Sn1—N2^{i}	88.94 (18)	H1B—C1—H1C	109.5
C1—Sn1—N2	88.94 (18)	N1—C2—C3	121.9 (6)
C1^{i}—Sn1—N2	88.48 (19)	N1—C2—H2	119.1
N2^{i}—Sn1—N2	106.6 (3)	C3—C2—H2	119.1
C1—Sn1—N1	91.51 (16)	C4—C3—C2	119.5 (7)
C1^{i}—Sn1—N1	92.01 (15)	C4—C3—H3	120.2
N2^{i}—Sn1—N1	162.09 (16)	C2—C3—H3	120.2

N2—Sn1—N1	91.30 (17)	C3—C4—C5	120.7 (6)
C1—Sn1—N1^{i}	92.01 (15)	C3—C4—H4	119.6
C1^{i}—Sn1—N1^{i}	91.51 (16)	C5—C4—H4	119.6
N2^{i}—Sn1—N1^{i}	91.30 (17)	C4—C5—C6	116.9 (6)
N2—Sn1—N1^{i}	162.09 (16)	C4—C5—C7	125.6 (6)
N1—Sn1—N1^{i}	70.80 (18)	C6—C5—C7	117.6 (7)
C2—N1—C6	119.4 (4)	N1—C6—C5	121.6 (5)
C2—N1—Sn1	124.2 (3)	N1—C6—C6^{i}	118.2 (2)
C6—N1—Sn1	116.4 (3)	C5—C6—C6^{i}	120.2 (4)
C8—N2—Sn1	163.6 (5)	C7^{i}—C7—C5	122.2 (4)
Sn1—C1—H1A	109.5	C7^{i}—C7—H7	118.9
Sn1—C1—H1B	109.5	C5—C7—H7	118.9
H1A—C1—H1B	109.5	N2—C8—S1	178.8 (5)

C1—Sn1—N1—C2	−89.4 (4)	Sn1—N1—C2—C3	−178.9 (4)
C1^{i}—Sn1—N1—C2	88.1 (4)	N1—C2—C3—C4	−0.9 (9)
N2^{i}—Sn1—N1—C2	−179.2 (5)	C2—C3—C4—C5	1.4 (10)
N2—Sn1—N1—C2	−0.5 (4)	C3—C4—C5—C6	−1.1 (9)
N1^{i}—Sn1—N1—C2	179.0 (4)	C3—C4—C5—C7	179.2 (8)
C1—Sn1—N1—C6	91.6 (3)	C2—N1—C6—C5	0.2 (6)
C1^{i}—Sn1—N1—C6	−90.9 (3)	Sn1—N1—C6—C5	179.3 (3)
N2^{i}—Sn1—N1—C6	1.8 (6)	C2—N1—C6—C6^{i}	−178.9 (4)
N2—Sn1—N1—C6	−179.5 (3)	Sn1—N1—C6—C6^{i}	0.1 (6)
N1^{i}—Sn1—N1—C6	0.0 (2)	C4—C5—C6—N1	0.3 (7)
C1—Sn1—N2—C8	−167.4 (17)	C7—C5—C6—N1	−180.0 (6)
C1^{i}—Sn1—N2—C8	9.2 (17)	C4—C5—C6—C6^{i}	179.4 (5)
N2^{i}—Sn1—N2—C8	−79.3 (17)	C7—C5—C6—C6^{i}	−0.8 (9)
N1—Sn1—N2—C8	101.1 (17)	C4—C5—C7—C7^{i}	179.3 (13)
N1^{i}—Sn1—N2—C8	99.4 (17)	C6—C5—C7—C7^{i}	−0.5 (19)
C6—N1—C2—C3	0.0 (7)		

Symmetry code: (i) −*x*+3/2, −*y*+1/2, *z*.