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(2,2′-Dimethyl-4,4′-bi-1,3-thiazole-κ^2*N*,*N*′)bis(thiocyanato-κ*S*)mercury(II)

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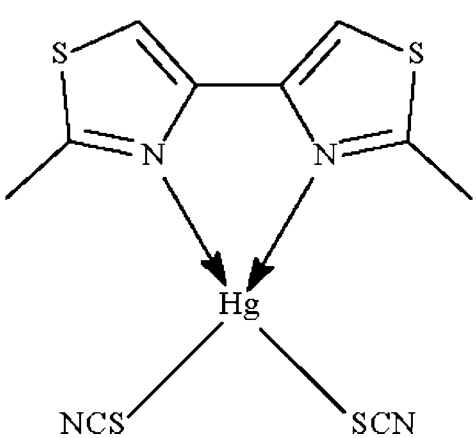
Key indicators: single-crystal X-ray study; *T* = 118 K; mean σ(C–C) = 0.005 Å; *R* factor = 0.022; *wR* factor = 0.054; data-to-parameter ratio = 19.1.

The Hg^{II} atom in the title compound, $[Hg(SCN)_2(C_8H_8N_2S_2)]$, is chelated by the bidentate heterocycle through the N atoms and is coordinated by the S atoms of two thiocyanate anions, resulting in a considerably distorted tetrahedral coordination geometry.

Related literature

There are several examples of mercuric thiocyanate–α,α′-dimine type of adducts which exist as four-coordinate, tetrahedral molecules. For the 4,4′,5,5′-tetramethyl-2,2′-biimidazole adduct, see: Mahjoub *et al.* (2003); Morsali (2006). For the 2,2′-diamino-4,4′-bithiazole adduct, see: Morsali *et al.* (2003). For the 2,2′-biquinoline adduct, see: Morsali *et al.* (2004); Ramazani *et al.* (2004). For the 2,2′-diphenyl-4,4′-bithiazole adduct, see: Mahjoub & Morsali (2003).



Experimental

Crystal data

$[Hg(NCS)_2(C_8H_8N_2S_2)]$
M_r = 513.03
Monoclinic, $P2_1/c$
a = 17.3764 (3) Å
b = 12.0534 (2) Å
c = 7.0601 (1) Å
β = 100.676 (1)°
V = 1453.10 (4) Å^3
Z = 4
Mo *K*α radiation
μ = 11.16 mm^{-1}
T = 118 K
0.22 × 0.06 × 0.04 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.274, T_{max} = 0.640
10030 measured reflections
3330 independent reflections
2982 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.054
S = 1.04
3330 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −1.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg1—S3	2.413 (1)	Hg1—N1	2.430 (3)
Hg1—S4	2.421 (1)	Hg1—N2	2.476 (3)
S3—Hg1—S4	149.25 (4)	S4—Hg1—N1	113.49 (8)
S3—Hg1—N1	95.66 (8)	S4—Hg1—N2	94.04 (8)
S3—Hg1—N2	105.84 (8)	N1—Hg1—N2	69.1 (1)

Data collection: *APEX2* (Bruker, 2008); cell refinement: *APEX2* (Bruker, 2008); data reduction: *SAINT*; 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, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2488).

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supporting information

Acta Cryst. (2009). E**65**, m372   [doi:10.1107/S1600536809006904]

(2,2′-Dimethyl-4,4′-bi-1,3-thiazole-κ^2*N*,*N*′)bis(thiocyanato-κ*S*)mercury(II)

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S1. Experimental

A solution of 2,2′-dimethyl-4,4′-bithiazole (0.13 g, 0.66 mmol) in methanol (10 ml) was added to a solution of mercuric thiocyanate (0.21 g, 0.66 mmol) in methanol (5 ml). Crystals were obtained by diffusing the methanol solution into DMSO for a week (yield: 80%; m.p. 456 K).

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95–0.98 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2–1.5U_{eq}(C).

The crystal diffracted strongly owing to the extremely heavy metal atom; however, its presence introduced severe absorption problems that could not be corrected analytically as the crystal did not have regular faces. The final difference Fourier map had a large peak/hole in the vicinity of the mercury atom.

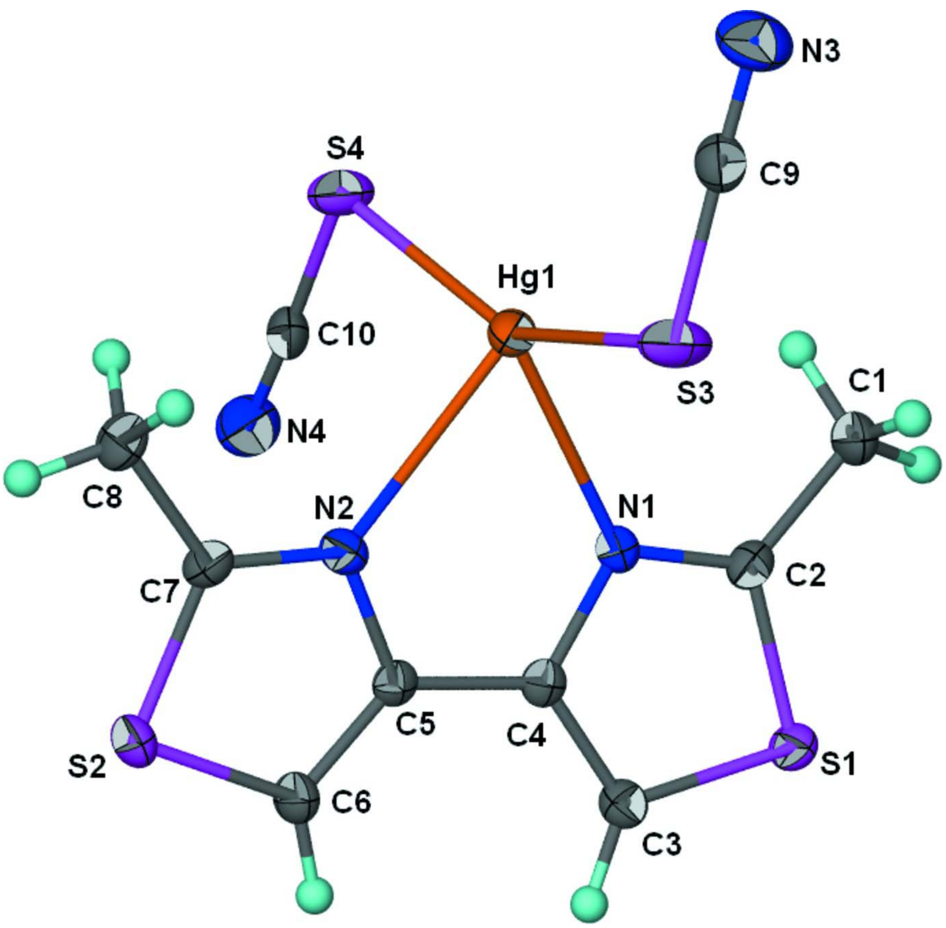

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Hg(SCN)_2(C_{10}H_8N_2S_2)$; ellipsoids are drawn at the 70% probability level and H atoms of arbitrary radius.

(2,2′-Dimethyl-4,4′-bi-1,3-thiazole- *κ*²*N*,*N*′)bis(thiocyanato-*κS*)mercury(II)

Crystal data

$[Hg(NCS)_2(C_8H_8N_2S_2)]$
M_r = 513.03
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 17.3764 (3) Å
b = 12.0534 (2) Å
c = 7.0601 (1) Å
β = 100.676 (1)°
V = 1453.10 (4) Å^3
Z = 4
$F(000)$ = 960
D_x = 2.345 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4390 reflections
θ = 2.4–28.3°
μ = 11.16 mm^{-1}
T = 118 K
Block, colorless
0.22 × 0.06 × 0.04 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.274, T_{max} = 0.640
10030 measured reflections
3330 independent reflections

2982 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.2°$
$h = -22 \rightarrow 22$
$k = -15 \rightarrow 15$
$l = -8 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.054$
$S = 1.04$
3330 reflections
174 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
$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 2.1611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.17$ e Å^{-3}
$\Delta\rho_{min} = -1.32$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Hg1	0.272849 (8)	0.578858 (12)	0.74895 (2)	0.01665 (6)
S1	0.37984 (5)	0.20867 (8)	0.65772 (15)	0.0156 (2)
S2	0.03250 (6)	0.34937 (8)	0.73374 (16)	0.0192 (2)
S3	0.34553 (7)	0.58014 (9)	1.07522 (18)	0.0287 (3)
S4	0.20772 (7)	0.68035 (9)	0.46884 (17)	0.0241 (2)
N1	0.30803 (18)	0.3905 (3)	0.6768 (5)	0.0132 (7)
N2	0.16170 (18)	0.4504 (3)	0.7495 (5)	0.0147 (7)
N3	0.4178 (2)	0.7908 (3)	1.1095 (6)	0.0317 (9)
N4	0.1421 (2)	0.4986 (3)	0.2409 (6)	0.0270 (8)
C1	0.4453 (2)	0.4223 (3)	0.6435 (7)	0.0221 (9)
H1A	0.4274	0.4900	0.5719	0.033*
H1B	0.4807	0.3815	0.5755	0.033*
H1C	0.4730	0.4421	0.7729	0.033*
C2	0.3765 (2)	0.3514 (3)	0.6592 (6)	0.0149 (8)
C3	0.2837 (2)	0.2028 (3)	0.6837 (6)	0.0148 (8)
H3	0.2549	0.1364	0.6912	0.018*
C4	0.2545 (2)	0.3082 (3)	0.6921 (6)	0.0128 (8)
C5	0.1758 (2)	0.3395 (3)	0.7151 (5)	0.0124 (7)
C6	0.1123 (2)	0.2727 (3)	0.7042 (6)	0.0163 (8)
H6	0.1121	0.1949	0.6834	0.020*
C7	0.0890 (2)	0.4686 (3)	0.7608 (6)	0.0158 (8)
C8	0.0558 (2)	0.5793 (3)	0.7950 (7)	0.0207 (9)
H8A	0.0831	0.6090	0.9186	0.031*
H8B	−0.0001	0.5716	0.7980	0.031*
H8C	0.0626	0.6301	0.6910	0.031*
C9	0.3879 (2)	0.7054 (3)	1.0890 (6)	0.0201 (9)
C10	0.1696 (2)	0.5709 (3)	0.3354 (6)	0.0188 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.01515 (8)	0.01369 (8)	0.01971 (10)	−0.00045 (5)	−0.00039 (6)	−0.00147 (6)
S1	0.0154 (5)	0.0132 (4)	0.0188 (5)	0.0017 (3)	0.0049 (4)	−0.0005 (4)
S2	0.0120 (5)	0.0188 (5)	0.0271 (6)	−0.0016 (4)	0.0043 (4)	0.0004 (4)
S3	0.0367 (6)	0.0183 (5)	0.0249 (6)	−0.0089 (4)	−0.0108 (5)	0.0058 (5)
S4	0.0294 (6)	0.0140 (5)	0.0254 (6)	−0.0040 (4)	−0.0044 (5)	0.0029 (4)
N1	0.0118 (16)	0.0143 (15)	0.0133 (17)	−0.0004 (12)	0.0023 (12)	−0.0001 (13)
N2	0.0144 (16)	0.0150 (16)	0.0147 (18)	−0.0021 (12)	0.0029 (13)	0.0006 (13)
N3	0.036 (2)	0.025 (2)	0.031 (2)	−0.0093 (17)	−0.0018 (18)	−0.0027 (18)
N4	0.028 (2)	0.0228 (19)	0.027 (2)	−0.0006 (16)	−0.0031 (16)	−0.0014 (17)
C1	0.0134 (19)	0.018 (2)	0.035 (3)	0.0010 (15)	0.0055 (18)	0.0017 (19)
C2	0.0156 (19)	0.0140 (18)	0.014 (2)	0.0022 (14)	0.0011 (15)	−0.0001 (16)
C3	0.0145 (19)	0.0154 (19)	0.015 (2)	−0.0006 (14)	0.0037 (15)	−0.0014 (16)
C4	0.0134 (18)	0.0146 (18)	0.0099 (19)	0.0005 (14)	0.0013 (14)	0.0004 (15)
C5	0.0137 (18)	0.0140 (18)	0.0092 (19)	0.0008 (14)	0.0010 (14)	0.0022 (15)
C6	0.0129 (18)	0.0169 (19)	0.020 (2)	0.0005 (14)	0.0050 (15)	−0.0002 (17)
C7	0.0174 (19)	0.0133 (18)	0.017 (2)	0.0022 (15)	0.0037 (15)	0.0009 (16)
C8	0.018 (2)	0.018 (2)	0.027 (2)	0.0052 (16)	0.0064 (17)	−0.0023 (18)
C9	0.017 (2)	0.021 (2)	0.022 (2)	0.0007 (16)	0.0020 (16)	−0.0014 (18)
C10	0.0113 (19)	0.019 (2)	0.026 (2)	0.0012 (15)	0.0019 (16)	0.0042 (18)

Geometric parameters (Å, º)

Hg1—S3	2.413 (1)	N4—C10	1.146 (6)
Hg1—S4	2.421 (1)	C1—C2	1.490 (5)
Hg1—N1	2.430 (3)	C1—H1A	0.9800
Hg1—N2	2.476 (3)	C1—H1B	0.9800
S1—C2	1.721 (4)	C1—H1C	0.9800
S1—C3	1.716 (4)	C3—C4	1.374 (5)
S2—C6	1.711 (4)	C3—H3	0.9500
S2—C7	1.731 (4)	C4—C5	1.455 (5)
S3—C9	1.675 (4)	C5—C6	1.356 (5)
S4—C10	1.684 (4)	C6—H6	0.9500
N1—C2	1.308 (5)	C7—C8	1.491 (5)
N1—C4	1.379 (5)	C8—H8A	0.9800
N2—C7	1.299 (5)	C8—H8B	0.9800
N2—C5	1.389 (5)	C8—H8C	0.9800
N3—C9	1.150 (5)		
S3—Hg1—S4	149.25 (4)	C1—C2—S1	123.0 (3)
S3—Hg1—N1	95.66 (8)	C4—C3—S1	110.0 (3)
S3—Hg1—N2	105.84 (8)	C4—C3—H3	125.0
S4—Hg1—N1	113.49 (8)	S1—C3—H3	125.0
S4—Hg1—N2	94.04 (8)	C3—C4—N1	113.7 (3)
N1—Hg1—N2	69.1 (1)	C3—C4—C5	127.4 (3)
C2—S1—C3	90.37 (19)	N1—C4—C5	118.9 (3)

C6—S2—C7	90.33 (19)	C6—C5—N2	114.4 (3)
C9—S3—Hg1	102.01 (16)	C6—C5—C4	127.7 (4)
C10—S4—Hg1	97.89 (15)	N2—C5—C4	117.9 (3)
C2—N1—C4	112.8 (3)	C5—C6—S2	110.0 (3)
C2—N1—Hg1	128.7 (3)	C5—C6—H6	125.0
C4—N1—Hg1	117.1 (2)	S2—C6—H6	125.0
C7—N2—C5	112.2 (3)	N2—C7—C8	124.8 (4)
C7—N2—Hg1	131.5 (3)	N2—C7—S2	113.0 (3)
C5—N2—Hg1	116.0 (2)	C8—C7—S2	122.2 (3)
C2—C1—H1A	109.5	C7—C8—H8A	109.5
C2—C1—H1B	109.5	C7—C8—H8B	109.5
H1A—C1—H1B	109.5	H8A—C8—H8B	109.5
C2—C1—H1C	109.5	C7—C8—H8C	109.5
H1A—C1—H1C	109.5	H8A—C8—H8C	109.5
H1B—C1—H1C	109.5	H8B—C8—H8C	109.5
N1—C2—C1	123.8 (3)	N3—C9—S3	176.2 (4)
N1—C2—S1	113.1 (3)	N4—C10—S4	177.9 (4)

S4—Hg1—S3—C9	−25.10 (19)	C2—S1—C3—C4	0.0 (3)
N1—Hg1—S3—C9	136.75 (17)	S1—C3—C4—N1	0.4 (4)
N2—Hg1—S3—C9	−153.45 (17)	S1—C3—C4—C5	−179.5 (3)
S3—Hg1—S4—C10	−173.66 (15)	C2—N1—C4—C3	−0.7 (5)
N1—Hg1—S4—C10	26.10 (17)	Hg1—N1—C4—C3	−168.8 (3)
N2—Hg1—S4—C10	−42.80 (16)	C2—N1—C4—C5	179.2 (3)
S3—Hg1—N1—C2	−67.8 (3)	Hg1—N1—C4—C5	11.1 (4)
S4—Hg1—N1—C2	102.2 (3)	C7—N2—C5—C6	−1.3 (5)
N2—Hg1—N1—C2	−172.6 (4)	Hg1—N2—C5—C6	−176.0 (3)
S3—Hg1—N1—C4	98.2 (3)	C7—N2—C5—C4	177.8 (3)
S4—Hg1—N1—C4	−91.8 (3)	Hg1—N2—C5—C4	3.1 (4)
N2—Hg1—N1—C4	−6.6 (3)	C3—C4—C5—C6	−10.6 (7)
S3—Hg1—N2—C7	98.2 (4)	N1—C4—C5—C6	169.5 (4)
S4—Hg1—N2—C7	−58.1 (4)	C3—C4—C5—N2	170.4 (4)
N1—Hg1—N2—C7	−171.8 (4)	N1—C4—C5—N2	−9.5 (5)
S3—Hg1—N2—C5	−88.4 (3)	N2—C5—C6—S2	0.9 (4)
S4—Hg1—N2—C5	115.3 (3)	C4—C5—C6—S2	−178.1 (3)
N1—Hg1—N2—C5	1.7 (2)	C7—S2—C6—C5	−0.3 (3)
C4—N1—C2—C1	−178.9 (4)	C5—N2—C7—C8	−179.5 (4)
Hg1—N1—C2—C1	−12.4 (6)	Hg1—N2—C7—C8	−5.8 (6)
C4—N1—C2—S1	0.6 (4)	C5—N2—C7—S2	1.0 (4)
Hg1—N1—C2—S1	167.11 (18)	Hg1—N2—C7—S2	174.69 (19)
C3—S1—C2—N1	−0.3 (3)	C6—S2—C7—N2	−0.4 (3)
C3—S1—C2—C1	179.2 (4)	C6—S2—C7—C8	−179.9 (4)