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Bis(1,3-dibutylthiourea)dicyanido-mercury(II)

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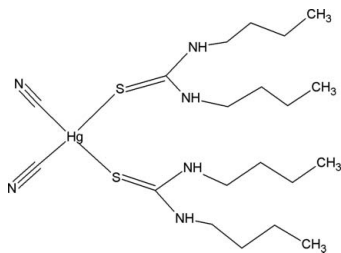
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.022; wR factor = 0.044; data-to-parameter ratio = 25.2.

In the title compound, $[\text{Hg}(\text{CN})_2(\text{C}_9\text{H}_{20}\text{N}_2\text{S})_2]$, the Hg atom lies on a twofold rotation axis. There is only half a molecule in the asymmetric unit. The Hg atom has a distorted tetrahedral coordination involving the S atoms of two 1-butyl-3-propylthiourea groups and the C atoms of the two CN^- anions. In the crystal packing, adjacent molecules are connected by intermolecular $\text{N}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds, forming infinite chains in three dimensions.

Related literature

For the coordination chemistry of thiourea-type ligands, see: Nadeem *et al.* (2009, 2008); Zoufalá *et al.* (2007); Khan *et al.* (2007); Hanif *et al.* (2007); Fuks *et al.* (2005); Moro *et al.* (2009); Matesanz & Souza (2007). For crystallographic reports about mercury(II) complexes containing thioamides, see: Popovic *et al.* (2000, 2002); Pavlović *et al.* (2000); Jiang *et al.* (2001); Wu *et al.* (2004). For the spectroscopy and structural chemistry of cyanide complexes of silver(I) and gold(I) with thiones, see: Hanif *et al.* (2007); Wu *et al.* (2004); Ahmad, Isab & Ashraf (2002); Ahmad, Isab & Perzanowski (2002); Ashraf *et al.* (2002); Ahmad & Isab (2001); Ahmad (2004).



Experimental

Crystal data

$[\text{Hg}(\text{CN})_2(\text{C}_9\text{H}_{20}\text{N}_2\text{S})_2]$
 $M_r = 629.31$
 Monoclinic, $C2/c$
 $a = 17.4692$ (3) Å
 $b = 9.5928$ (2) Å
 $c = 17.4699$ (4) Å
 $\beta = 111.540$ (1)°
 $V = 2723.12$ (10) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 5.82$ mm⁻¹
 $T = 296$ K
 $0.14 \times 0.15 \times 0.17$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
 Absorption correction: none
 15120 measured reflections
 3372 independent reflections
 2918 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.044$
 $S = 1.02$
 3372 reflections
 134 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.40$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.72$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N}2-\text{H}2\cdots\text{S}1^i$	0.86	2.68	3.479 (2)	155
$\text{N}3-\text{H}3\cdots\text{N}1^{\text{ii}}$	0.86	2.20	2.991 (3)	153
$\text{C}7-\text{H}7\text{B}\cdots\text{S}1$	0.97	2.67	3.070 (3)	105

Symmetry codes: (i) $-x + 2, y, -z + \frac{3}{2}$; (ii) $x + \frac{1}{2}, y + \frac{1}{2}, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5052).

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supplementary materials

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Bis(1,3-dibutylthiourea)dicyanidomercury(II)

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Comment

The coordination chemistry of thiourea type ligands has been the subject of several recent studies because of the relevance of their binding sites to those in living systems (Nadeem *et al.*, 2009; Nadeem *et al.*, 2008; Zoufalá *et al.*, 2007; Khan *et al.*, 2007; Hanif *et al.*, 2007; Fuks *et al.*, 2005; Moro *et al.*, 2009; Matesanz & Souza, 2007). Crystallographic reports about mercury (II) complexes containing thioamides establish that these ligands are coordinated *via* the sulfur atom (Popovic *et al.*, 2000, 2002; Pavlović, Popović, Soldin *et al.*, 2000; Jiang *et al.*, 2001; Wu *et al.*, 2004). We have been involved in investigating the spectral and structural chemistry of cyanido complexes of silver (I) and gold (I) with thiones with emphasis on ligand scrambling reactions (Hanif *et al.*, 2007; Wu *et al.*, 2004; Ahmad, Isab & Ashraf, 2002; Ahmad, Isab & Perzanowski, 2002; Ashraf *et al.*, 2002; Ahmad & Isab, 2001; Ahmad, 2004). As a part of extension of our work towards complexation of Hg (CN)₂ with thiones, we report here the crystal structures of [(*N,N'*-dibutylthiourea)₂Hg(CN)₂], (I).

In the title compound (I), (Fig. 1), the Hg anion lies on a twofold rotation axes parallel to the *b* axis in space group *C2/c* and one half of the molecule to the other half are connected by this symmetry operation. The Hg atom has a distorted tetrahedral coordination by the S atoms of two *N,N'*-dibutylthiourea groups and the C atoms of the two CN groups. The bond distances Hg—S and Hg—C are 2.7424 (7) Å and 2.072 (3) Å, and the bond angles C—Hg—C, S—Hg—S and C—Hg—C are 150.51 (11)°, 95.55 (2)° and 100.45 (8)°. All bond lengths and bond angles in (I) are in the range of expected values.

In the crystal packing, the adjacent molecules are connected by intermolecular N—H⋯N and N—H⋯S hydrogen bonds (Table 1). In Fig. 2, the packing and hydrogen bonding of (I) are shown viewed down *b* axis.

Experimental

For the preparation of the title complex, Hg (CN)₂ was prepared first by the reaction of 1 mmol HgCl₂ in methanol with 2 mmole of KCN in water. Then 0.253 g (1 mmole) Hg (CN)₂ dissolved in 15 ml methanol was mixed with 2 equivalents of *N,N'*-dibutylthiourea in 15 methanol. After stirring for 15 minutes, the resulting mixture was filtered and filtrate was kept at room temperature. After 24 h white crystals were obtained.

Refinement

H atoms were located geometrically and treated as riding with C—H = 0.97 Å (methylene), C—H = 0.96 Å (methyl) and N—H = 0.86 Å with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C}, \text{N})$.

Figures

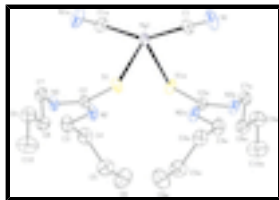


Fig. 1. The title molecule with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

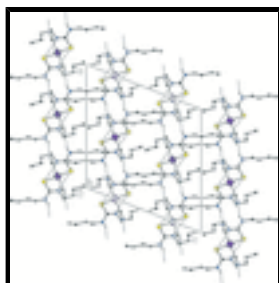


Fig. 2. The packing and hydrogen bonding of (I) viewed down *b* axis. Hydrogen atoms not involved in the showed interactions have been omitted for clarity.

Bis(1,3-dibutylthiourea)dicyanidomercury(II)

Crystal data

[Hg(CN)₂(C₉H₂₀N₂S)₂]

M_r = 629.31

Monoclinic, *C2/c*

Hall symbol: -*C* 2yc

a = 17.4692 (3) Å

b = 9.5928 (2) Å

c = 17.4699 (4) Å

β = 111.540 (1)°

V = 2723.12 (10) Å³

Z = 4

*F*₀₀₀ = 1256

D_x = 1.535 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 6609 reflections

θ = 2.5–27.2°

μ = 5.82 mm⁻¹

T = 296 K

Irregular, white

0.17 × 0.15 × 0.14 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer

Radiation source: sealed tube

Monochromator: graphite

T = 296 K

φ and ω scans

Absorption correction: none

15120 measured reflections

3372 independent reflections

2918 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.032

θ_{max} = 28.3°

θ_{min} = 2.5°

h = -23→23

k = -12→12

l = -20→23

Refinement

Refinement on *F*²

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.022$$

$$wR(F^2) = 0.044$$

$$S = 1.02$$

3372 reflections

134 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0211P)^2],$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.40 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.72 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	1.00000	0.20478 (1)	0.75000	0.0405 (1)
S1	1.08516 (3)	0.39691 (7)	0.86634 (4)	0.0414 (2)
N1	0.86048 (15)	0.1224 (3)	0.81955 (17)	0.0718 (10)
N2	1.11488 (12)	0.5094 (2)	0.74219 (12)	0.0422 (7)
N3	1.22801 (11)	0.4758 (2)	0.85840 (12)	0.0411 (7)
C1	0.91098 (16)	0.1498 (3)	0.79668 (17)	0.0475 (9)
C2	1.14750 (13)	0.4655 (2)	0.81878 (15)	0.0341 (7)
C3	1.16093 (17)	0.5591 (3)	0.69240 (17)	0.0548 (10)
C4	1.10347 (17)	0.6051 (3)	0.60900 (17)	0.0534 (10)
C5	1.0548 (2)	0.7334 (4)	0.6094 (2)	0.0633 (12)
C6	0.9979 (3)	0.7767 (4)	0.5243 (3)	0.0875 (17)
C7	1.27223 (15)	0.4387 (3)	0.94375 (16)	0.0441 (8)
C8	1.27906 (17)	0.5571 (3)	1.00242 (16)	0.0473 (9)
C9	1.3311 (2)	0.5232 (3)	1.09034 (17)	0.0586 (11)
C10	1.3434 (3)	0.6466 (4)	1.1477 (2)	0.0795 (14)
H2	1.06210	0.50880	0.71950	0.0510*
H3	1.25650	0.50710	0.83120	0.0490*
H3A	1.19600	0.48500	0.68630	0.0660*
H3B	1.19580	0.63660	0.72020	0.0660*
H4A	1.13530	0.62230	0.57470	0.0640*
H4B	1.06550	0.52970	0.58410	0.0640*
H5A	1.09240	0.80930	0.63420	0.0760*

supplementary materials

H5B	1.02240	0.71650	0.64330	0.0760*
H6A	1.02880	0.78550	0.48910	0.1310*
H6B	0.97300	0.86460	0.52750	0.1310*
H6C	0.95580	0.70750	0.50240	0.1310*
H7A	1.32710	0.40780	0.95010	0.0530*
H7B	1.24430	0.36120	0.95810	0.0530*
H8A	1.22430	0.58250	0.99950	0.0570*
H8B	1.30250	0.63730	0.98510	0.0570*
H9A	1.38450	0.49040	1.09270	0.0700*
H9B	1.30520	0.44820	1.10920	0.0700*
H10A	1.36760	0.72220	1.12850	0.1190*
H10B	1.37910	0.62040	1.20210	0.1190*
H10C	1.29110	0.67540	1.14870	0.1190*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0323 (1)	0.0459 (1)	0.0478 (1)	0.0000	0.0199 (1)	0.0000
S1	0.0359 (3)	0.0566 (4)	0.0340 (3)	-0.0115 (3)	0.0154 (3)	-0.0005 (3)
N1	0.0516 (14)	0.104 (2)	0.0668 (17)	-0.0297 (15)	0.0300 (13)	-0.0046 (17)
N2	0.0326 (10)	0.0594 (14)	0.0352 (12)	-0.0068 (9)	0.0133 (9)	0.0057 (11)
N3	0.0313 (10)	0.0545 (13)	0.0383 (12)	-0.0043 (9)	0.0136 (9)	0.0051 (10)
C1	0.0385 (13)	0.0553 (16)	0.0463 (16)	-0.0125 (12)	0.0126 (12)	-0.0037 (14)
C2	0.0330 (11)	0.0369 (13)	0.0340 (14)	-0.0030 (9)	0.0142 (10)	-0.0015 (11)
C3	0.0473 (15)	0.076 (2)	0.0491 (17)	-0.0018 (14)	0.0270 (14)	0.0144 (15)
C4	0.0563 (16)	0.069 (2)	0.0396 (16)	-0.0019 (14)	0.0232 (13)	0.0039 (15)
C5	0.076 (2)	0.066 (2)	0.052 (2)	0.0065 (17)	0.0285 (17)	0.0103 (16)
C6	0.084 (3)	0.101 (3)	0.074 (3)	0.026 (2)	0.025 (2)	0.020 (2)
C7	0.0353 (12)	0.0476 (15)	0.0446 (16)	0.0040 (11)	0.0089 (11)	0.0054 (13)
C8	0.0477 (14)	0.0466 (15)	0.0427 (16)	0.0038 (12)	0.0110 (12)	0.0064 (13)
C9	0.0665 (19)	0.0565 (19)	0.0433 (17)	0.0044 (15)	0.0090 (15)	0.0050 (15)
C10	0.107 (3)	0.066 (2)	0.051 (2)	-0.005 (2)	0.012 (2)	-0.0008 (19)

Geometric parameters (\AA , $^\circ$)

Hg1—S1	2.7424 (7)	C3—H3A	0.9700
Hg1—C1	2.072 (3)	C3—H3B	0.9700
Hg1—S1 ⁱ	2.7424 (7)	C4—H4A	0.9700
Hg1—C1 ⁱ	2.072 (3)	C4—H4B	0.9700
S1—C2	1.724 (2)	C5—H5A	0.9700
N1—C1	1.125 (4)	C5—H5B	0.9700
N2—C2	1.316 (3)	C6—H6A	0.9600
N2—C3	1.465 (4)	C6—H6B	0.9600
N3—C2	1.324 (3)	C6—H6C	0.9600
N3—C7	1.449 (3)	C7—H7A	0.9700
N2—H2	0.8600	C7—H7B	0.9700
N3—H3	0.8600	C8—H8A	0.9700
C3—C4	1.500 (4)	C8—H8B	0.9700

C4—C5	1.497 (5)	C9—H9A	0.9700
C5—C6	1.512 (6)	C9—H9B	0.9700
C7—C8	1.505 (4)	C10—H10A	0.9600
C8—C9	1.505 (4)	C10—H10B	0.9600
C9—C10	1.514 (5)	C10—H10C	0.9600
S1…C1	3.693 (3)	H3A…N3	2.8500
S1…C8	3.684 (3)	H3A…H3	2.3700
S1…N2 ⁱ	3.479 (2)	H3A…H10C ^{vi}	2.5200
S1…H7B	2.6700	H3B…N3	2.7400
S1…H2 ⁱ	2.6800	H3B…H3	2.2200
S1…H6A ⁱⁱ	3.1900	H3B…H5A	2.5000
N1…N3 ⁱⁱⁱ	2.991 (3)	H3B…N1 ^{iv}	2.7600
N1…C3 ⁱⁱⁱ	3.431 (4)	H4A…H6A	2.4700
N2…S1 ⁱ	3.479 (2)	H4B…H2	2.4000
N3…N1 ^{iv}	2.991 (3)	H4B…H6C	2.5700
N1…H3B ⁱⁱⁱ	2.7600	H5A…H3B	2.5000
N1…H3 ⁱⁱⁱ	2.2000	H5A…H7A ^{vii}	2.5600
N2…H5B	2.7400	H5B…N2	2.7400
N3…H3A	2.8500	H5B…H2	2.3500
N3…H3B	2.7400	H6A…H4A	2.4700
C1…S1	3.693 (3)	H6A…S1 ^{vi}	3.1900
C1…C2 ⁱ	3.574 (4)	H6C…H4B	2.5700
C3…N1 ^{iv}	3.431 (4)	H7A…H9A	2.4500
C8…S1	3.684 (3)	H7A…H5A ^{viii}	2.5600
C1…H10B ^v	3.0100	H7B…S1	2.6700
C3…H3	2.4400	H7B…H9B	2.6000
C5…H2	2.8600	H7B…H7B ^{ix}	2.5500
H2…C5	2.8600	H8A…H10C	2.5900
H2…H4B	2.4000	H8B…H10A	2.4800
H2…H5B	2.3500	H9A…H7A	2.4500
H2…S1 ⁱ	2.6800	H9B…H7B	2.6000
H3…C3	2.4400	H10A…H8B	2.4800
H3…H3A	2.3700	H10B…C1 ^x	3.0100
H3…H3B	2.2200	H10C…H8A	2.5900
H3…N1 ^{iv}	2.2000	H10C…H3A ⁱⁱ	2.5200
S1—Hg1—C1	99.25 (8)	C4—C5—H5A	109.00
S1—Hg1—S1 ⁱ	95.55 (2)	C4—C5—H5B	109.00
S1—Hg1—C1 ⁱ	100.45 (8)	C6—C5—H5A	109.00
S1 ⁱ —Hg1—C1	100.45 (8)	C6—C5—H5B	109.00
C1—Hg1—C1 ⁱ	150.51 (11)	H5A—C5—H5B	108.00
S1 ⁱ —Hg1—C1 ⁱ	99.25 (8)	C5—C6—H6A	109.00
Hg1—S1—C2	99.56 (8)	C5—C6—H6B	109.00
C2—N2—C3	125.5 (2)	C5—C6—H6C	109.00
C2—N3—C7	125.6 (2)	H6A—C6—H6B	109.00

supplementary materials

C2—N2—H2	117.00	H6A—C6—H6C	110.00
C3—N2—H2	117.00	H6B—C6—H6C	109.00
C2—N3—H3	117.00	N3—C7—H7A	109.00
C7—N3—H3	117.00	N3—C7—H7B	109.00
Hg1—C1—N1	177.4 (3)	C8—C7—H7A	109.00
S1—C2—N2	119.84 (19)	C8—C7—H7B	109.00
S1—C2—N3	120.95 (18)	H7A—C7—H7B	108.00
N2—C2—N3	119.2 (2)	C7—C8—H8A	109.00
N2—C3—C4	110.8 (2)	C7—C8—H8B	109.00
C3—C4—C5	114.6 (2)	C9—C8—H8A	109.00
C4—C5—C6	113.0 (3)	C9—C8—H8B	109.00
N3—C7—C8	113.2 (2)	H8A—C8—H8B	108.00
C7—C8—C9	113.5 (2)	C8—C9—H9A	109.00
C8—C9—C10	113.1 (3)	C8—C9—H9B	109.00
N2—C3—H3A	109.00	C10—C9—H9A	109.00
N2—C3—H3B	109.00	C10—C9—H9B	109.00
C4—C3—H3A	109.00	H9A—C9—H9B	108.00
C4—C3—H3B	109.00	C9—C10—H10A	109.00
H3A—C3—H3B	108.00	C9—C10—H10B	109.00
C3—C4—H4A	109.00	C9—C10—H10C	109.00
C3—C4—H4B	109.00	H10A—C10—H10B	110.00
C5—C4—H4A	109.00	H10A—C10—H10C	109.00
C5—C4—H4B	109.00	H10B—C10—H10C	110.00
H4A—C4—H4B	108.00		
C1—Hg1—S1—C2	-169.87 (11)	C7—N3—C2—S1	-2.8 (3)
S1 ⁱ —Hg1—S1—C2	-68.30 (8)	C7—N3—C2—N2	176.7 (2)
C1 ⁱ —Hg1—S1—C2	32.19 (11)	C2—N3—C7—C8	-88.9 (3)
Hg1—S1—C2—N2	51.24 (18)	N2—C3—C4—C5	67.9 (3)
Hg1—S1—C2—N3	-129.28 (17)	C3—C4—C5—C6	179.8 (3)
C3—N2—C2—S1	-174.74 (19)	N3—C7—C8—C9	-175.0 (2)
C3—N2—C2—N3	5.8 (3)	C7—C8—C9—C10	175.2 (3)
C2—N2—C3—C4	-178.1 (2)		

Symmetry codes: (i) $-x+2, y, -z+3/2$; (ii) $x, -y+1, z+1/2$; (iii) $x-1/2, y-1/2, z$; (iv) $x+1/2, y+1/2, z$; (v) $x-1/2, -y+1/2, z-1/2$; (vi) $x, -y+1, z-1/2$; (vii) $-x+5/2, y+1/2, -z+3/2$; (viii) $-x+5/2, y-1/2, -z+3/2$; (ix) $-x+5/2, -y+1/2, -z+2$; (x) $x+1/2, -y+1/2, z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 \cdots S1 ⁱ	0.86	2.68	3.479 (2)	155
N3—H3 \cdots N1 ^{iv}	0.86	2.20	2.991 (3)	153
C7—H7B \cdots S1	0.97	2.67	3.070 (3)	105

Symmetry codes: (i) $-x+2, y, -z+3/2$; (iv) $x+1/2, y+1/2, z$.

Fig. 1

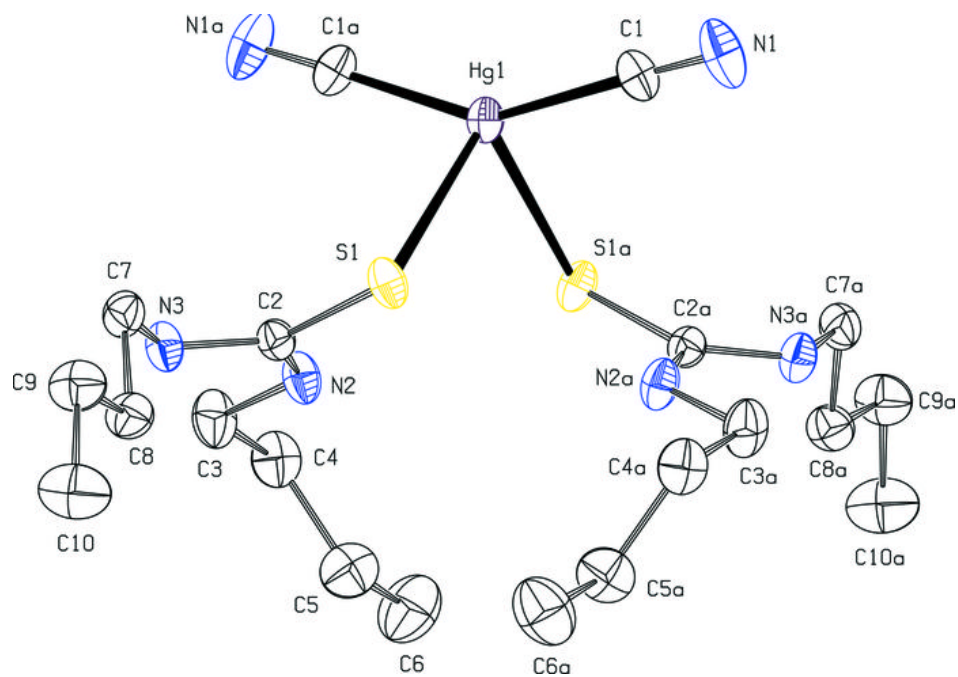


Fig. 2

