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Bis(*o*-chlorophenylbenzoylthiourea-*κS*)-diiodomercury(II)

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Molecules of the title compound, $[HgI_2(C_{14}H_{11}ClN_2OS)_2]$, are discrete and have crystallographic twofold rotation symmetry, with the Hg atom in a four-coordinate environment. The geometry of the central Hg atom is distorted tetrahedral with bond angles in the range 99.00 (8)–137.56 (3)°.

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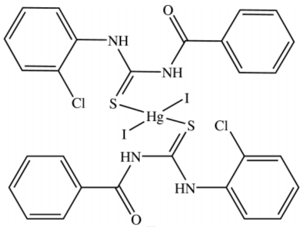
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.042
wR factor = 0.098
Data-to-parameter ratio = 20.1

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

Comment

Several mercury–thiourea complexes reported so far have mainly involved cyclothiourea ligands; examples are $Hg(C_8H_{16}N_4S_2)Cl_2$, $Hg(C_8H_{16}N_4S_2)Br_2$, $Hg(C_8H_{16}N_4S_2)I_2$, $Hg(C_8H_{16}N_4S_2)(SCN)_2$ and $Hg(C_8H_{16}N_4S_2)(CN)_2$ (Popovic *et al.*, 2000). Non-cyclothiourea mercury complexes are relatively scarce and, in fact, bis{μ-chloro-chloro[(*N*-diethylaminothiocarbonyl)benzimido-*O*-methyl ester-*S*]mercury(II)} was claimed to be the first chloro-bridged mercury–thiourea complex (Lebmann *et al.*, 2000). The title compound, (I), is probably the first mercury complex of a benzoylthiourea derivative and has twofold rotation symmetry.



(I)

The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are given in Table 1. The molecule is discrete and centrosymmetric about atom Hg1.

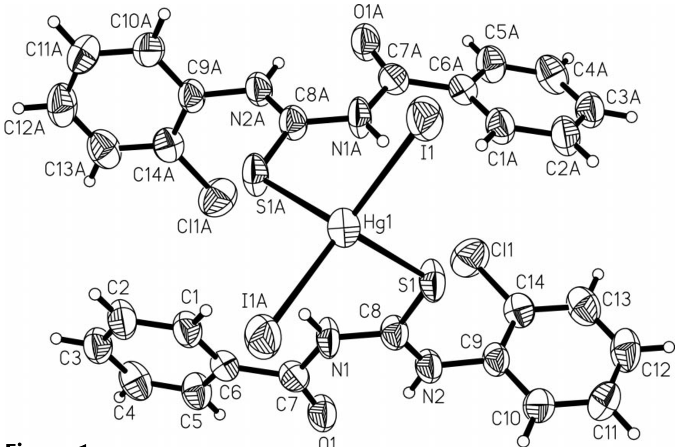


Figure 1
The molecular structure of the title compound, (I), drawn with 50% probability displacement ellipsoids. The suffix *A* corresponds to symmetry code (i) in Table 1.

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The geometry of the Hg atom is distorted tetrahedral, with bond angles ranging from 99.00 (8) to 137.56 (3)°. The Hg—I bond length of 2.6582 (6) Å is slightly shorter than that in the complex Hg($C_8H_{16}N_4S_2$)I_2 (Popovic *et al.*, 2000), where the corresponding bond is 2.7123 (5) Å; however, the Hg—S bond length of 2.6840 (16) Å is slightly longer [2.6119 (16) Å]. The structural dimensions of the ligand, in particular the C—S [1.690 (6) Å] and C(S)—N [1.366 (7) and 1.317 (7) Å] bond lengths, are normal and in agreement with values observed in other benzoylthiourea derivatives, such as *N*-benzoyl-*N*′-phenylthiourea [C—S = 1.6567 (15) Å, and C(S)—N = 1.393 (2) and 1.326 (2) Å] (Yamin & Yusof, 2003). The pseudo-six-membered ring (O1/C7/N1/C8/N2/H2*A*) in the ligand is maintained by the intramolecular interaction N2—H2*A*···O1 (Table 2).

Experimental

A solution of *o*-chlorophenylbenzoylthiourea (1.25 g, 4.3 mmol) in ethanol (50 ml) was added dropwise to 50 ml of an ethanol solution containing an equimolar amount of mercury(II) iodide in a two-neck round-bottomed flask. The solution was refluxed for about 2 h. The light-yellow solution was filtered and light-yellow crystals were obtained from the filtrate after evaporation for 3 d.

Crystal data

[$HgI_2(C_{14}H_{11}ClN_2OS)_2$]
M_r = 1035.91
Monoclinic, $C2/c$
a = 20.900 (4) Å
b = 8.850 (2) Å
c = 19.845 (4) Å
β = 118.26 (3)°
V = 3233.1 (1) Å^3
Z = 4
D_x = 2.128 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3229 reflections
θ = 2.2–27.6°
μ = 7.00 mm^{-1}
T = 293 (2) K
Slab, light yellow
0.24 × 0.11 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.269, $T_{\max}$ = 0.571
10 696 measured reflections
3734 independent reflections
2980 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.040
$\theta_{\max}$ = 27.6°
$h = -21 \rightarrow 27$
$k = -10 \rightarrow 11$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.098
S = 1.07
3734 reflections
186 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.7273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 1.33 e Å^{-3}
$\Delta\rho_{\min}$ = −0.67 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg1—I1	2.6582 (6)	O1—C7	1.213 (6)
Hg1—S1	2.6840 (16)	N1—C8	1.366 (7)
S1—C8	1.690 (6)	N2—C8	1.317 (7)
Cl1—C14	1.721 (6)		
I1—Hg1—I1^{i}	137.56 (3)	I1^{i}—Hg1—S1^{i}	99.55 (4)
I1—Hg1—S1^{i}	107.71 (4)	S1^{i}—Hg1—S1	99.00 (8)

Symmetry code: (i) $-x, y, \frac{1}{2} - z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	1.93	2.604 (7)	134

After checking their presence in Fourier difference maps, all the H atoms were positioned geometrically and allowed to ride on the parent C or N atoms, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C or N). The highest electron-density peak is located at 0.82 Å from I1.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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