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Dichlorobis(1,10-phenanthroline)mercury(II)

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.007 Å
R factor = 0.037
wR factor = 0.090
Data-to-parameter ratio = 16.5

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

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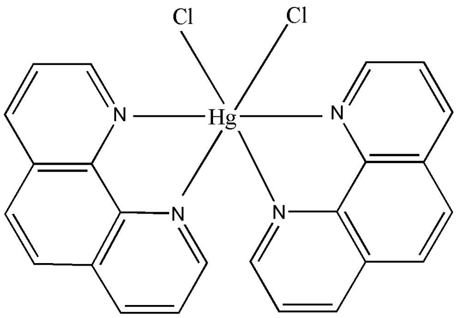
The title compound, $[HgCl_2(C_{12}H_8N_2)_2]$, is a six-coordinate complex with a distorted octahedral geometry around the Hg atom. There are some π–π stacking interactions in the crystal structure, with short distances between parallel aromatic rings.

Comment

We are interested in mercury complexes containing 1,10-phenanthroline or its derivatives. In a recent study, a neutral mercury complex, [Hg(ophen)$_2$] (Hophen is 1*H*-1,10-phenanthrolin-2-one) was synthesized (Zheng *et al.*, 2003), in which a derivative of 1,10-phenanthroline acts as a ligand. A mercury(II) complex with a mixed-donor 1,10-phenanthroline-containing macrocycle has also been reported (Aragoni *et al.*, 2002). As part of a study of mercury(II) halide complexes with N-donor organic ligands (Freire *et al.*, 1999), a four-coordinate complex, $[HgI_2(phen)]$, was synthesized and its crystal structure was determined. We report here the crystal structure of a six-coordinate complex of mercury(II), containing 1,10-phenanthroline as a ligand. The complex was prepared using a new adduct of 1,10-phenanthroline and pyridine-2,6-dicarboxylic acid (Moghimi *et al.*, 2005). We have previously reported some complexes with this adduct, in which both ligands were observed in the crystal structures of the complexes (Moghimi *et al.*, 2005). In the present work, only the 1,10-phenanthroline group acts as a ligand.



(I)

The title complex, (I) (Fig. 1), has a distorted octahedral geometry. The central Hg atom is coordinated by the two 1,10-phenanthroline ligands through the donor N atoms, as well as by two Cl atoms. The Hg—N bond lengths (Table 1) are similar to those of the four-coordinate Hg-phen complex reported previously (Freire *et al.*, 1999). Short distances between parallel aromatic rings in neighboring molecules indicate π–π stacking interactions (Fig. 2). The distance between the N1/N2/C1–C10 and N1*A*/N2*A*/C1*A*–C10*A* planes in Fig. 3 is 3.303 Å, and a distance of 3.371 Å is observed

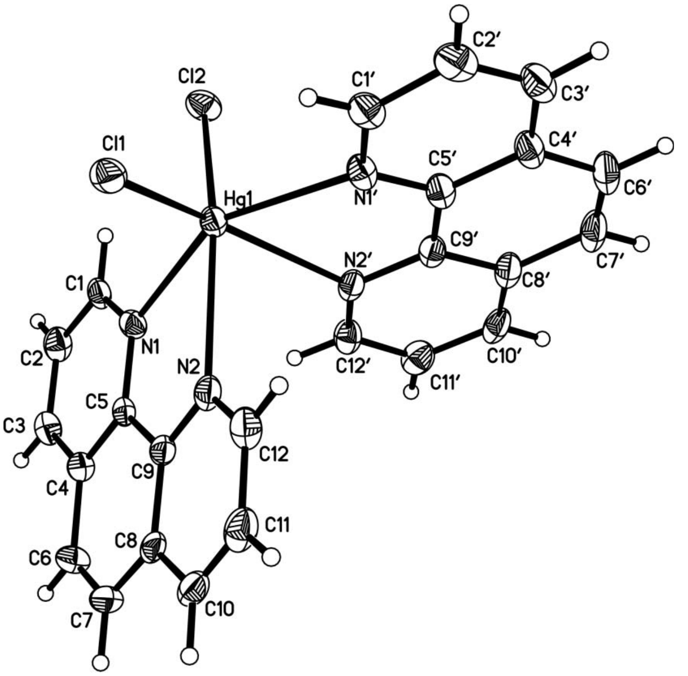


Figure 1
The molecular structure of the title complex, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

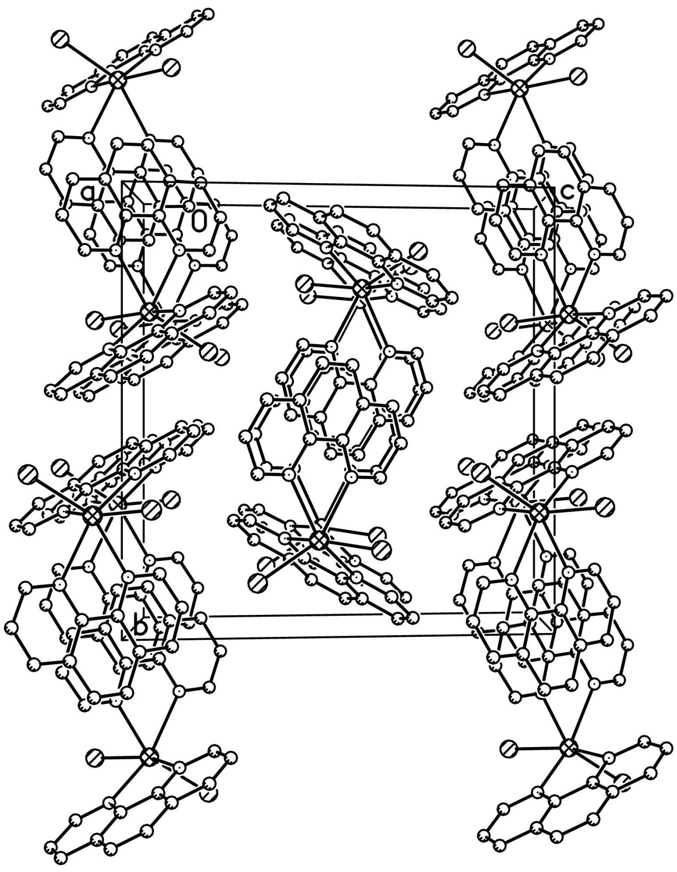


Figure 2
The crystal packing of the title complex. H atoms have been omitted.

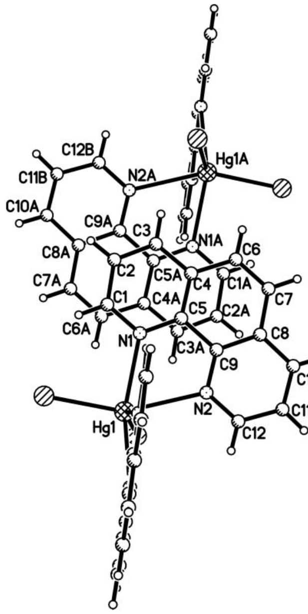


Figure 3
Parallel planes of the aromatic ligands with a distance of 3.303 Å. [Symmetry code: (*A*) $2 - x, -y, 1 - z$.]

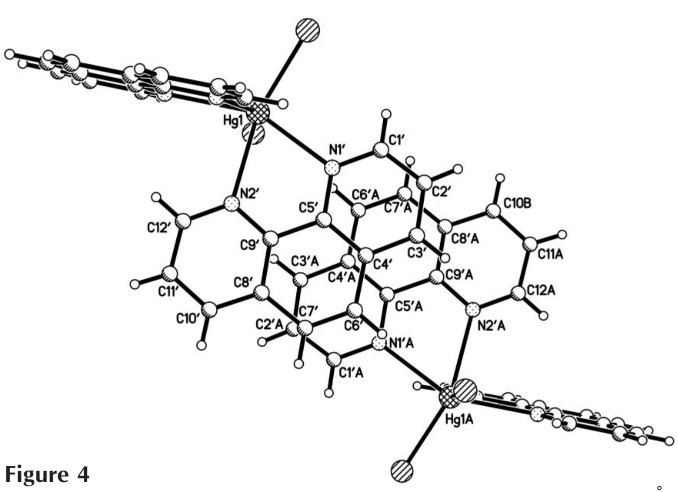


Figure 4
Parallel planes of the aromatic ligands with a distance of 3.371 Å. [Symmetry code: (*A*) $1 - x, 1 - y, 1 - z$.]

between the N1′/N2′/C1′–C10′ and N1′*A*/N2′*A*/C1′*A*–C10′*A* planes, as shown in Fig. 4. These values are close to the distance between the layers in the structure of graphite.

Experimental

A solution of $HgCl_2$ in dimethylsulfoxide (DMSO) was added to a solution of an adduct of 1,10-phenanthroline and pyridine-2,6-dicarboxylic acid in DMSO in a 1:2 molar ratio. Colorless crystals of the complex were obtained after two weeks.

Crystal data

$[HgCl_2(C_{12}H_8N_2)_2]$
$M_r = 631.90$
Monoclinic, $P2_1/c$
$a = 9.5847\ (17)$ Å
$b = 14.953\ (3)$ Å
$c = 14.508\ (3)$ Å
$\beta = 99.694\ (4)°$
$V = 2049.6\ (7)$ Å^3
$Z = 4$

$D_x = 2.048$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1024 reflections
$\theta = 2.2–26.5°$
$\mu = 7.79$ mm^{-1}
$T = 120\ (2)$ K
Prism, colorless
$0.35 \times 0.20 \times 0.20$ mm

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Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{\min} = 0.158$, $T_{\max} = 0.201$
13731 measured reflections
4621 independent reflections
4229 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.046$
$\theta_{\max} = 27.5°$
$h = -12 \rightarrow 11$
$k = -19 \rightarrow 19$
$l = -14 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.090$
$S = 1.06$
4621 reflections
280 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 8P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 2.27$ e Å^{-3}
$\Delta\rho_{\min} = -2.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg1—N1	2.449 (4)	Hg1—N2′	2.502 (4)
Hg1—N1′	2.463 (4)	Hg1—Cl2	2.5285 (12)
Hg1—Cl1	2.4937 (12)	Hg1—N2	2.582 (4)
N1—Hg1—N1′	150.46 (13)	Cl1—Hg1—Cl2	110.78 (4)
N1—Hg1—Cl1	109.58 (9)	N2′—Hg1—Cl2	90.89 (9)
N1′—Hg1—Cl1	92.75 (10)	N1—Hg1—N2	65.84 (13)
N1—Hg1—N2′	85.47 (13)	N1′—Hg1—N2	97.60 (12)
N1′—Hg1—N2′	66.87 (14)	Cl1—Hg1—N2	86.60 (10)
Cl1—Hg1—N2′	153.09 (10)	N2′—Hg1—N2	79.33 (12)
N1—Hg1—Cl2	89.59 (9)	Cl2—Hg1—N2	154.00 (11)
N1′—Hg1—Cl2	100.58 (9)		

The largest peak and hole of the final difference map both lie about 0.8 Å from the Hg atom and are principally due to considerable absorption effects which could not be completely corrected. H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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