

# Crystal structure of (*N*<sup>1</sup>-benzyl-*N*<sup>1</sup>,*N*<sup>2</sup>,*N*<sup>2</sup>-trimethylethane-1,2-diamine- $\kappa^2$ *N,N'*)dichlorido-mercury(II)

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Received 27 June 2014

Accepted 30 July 2014

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Edited by M. Weil, Vienna University of Technology, Austria

**Keywords:** crystal structure; mercury complex; tertiary amine donors

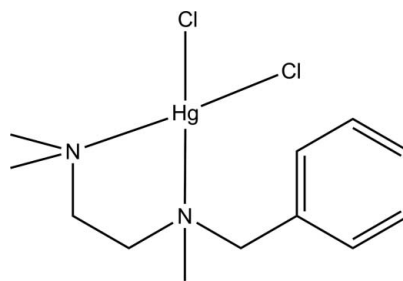
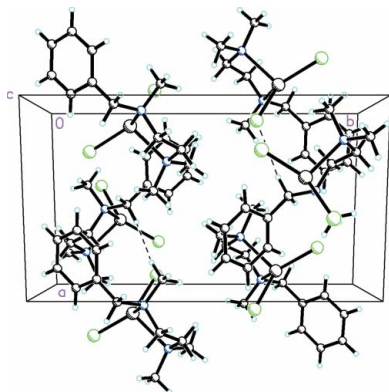
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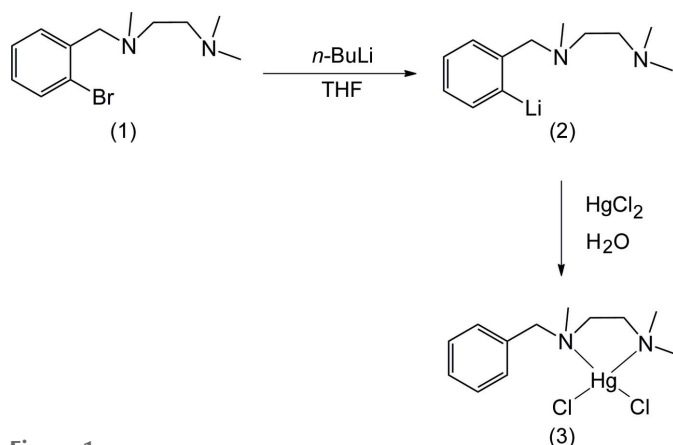
In the structure of the title compound, [HgCl<sub>2</sub>(C<sub>12</sub>H<sub>20</sub>N<sub>2</sub>)], the Hg<sup>II</sup> atom has a distorted tetrahedral coordination sphere defined by two tertiary amine N-atom donors, as well as two Cl<sup>-</sup> anions [the dihedral angle between the N–Hg–N and Cl–Hg–Cl planes is 82.80 (9)°]. The five-membered chelate ring adopts an envelope conformation, with puckering parameters of  $Q(2) = 0.446(6)$  Å and  $\varphi(2) = 88.8(6)$ °, with the two amine CH<sub>3</sub> substituents on opposite sides of the ring. In the crystal, the molecules are linked by C–H...Cl interactions into a zigzag chain parallel to [101].

## 1. Chemical context

The chemistry of mercuric compounds with multidentate amine ligands is of interest due to the low coordination number and geometry preferences of Hg<sup>II</sup>, which facilitates extraordinarily rapid exchange of simple ligands (Bebout *et al.*, 2013; Carra *et al.*, 2013). The enhanced binding thermodynamics of these multidentate ligands has been used to suppress intermolecular ligand-exchange rates for a variety of Hg<sup>II</sup> complexes in solution, greatly enhancing the meaningfulness of NMR characterization. Significantly, under conditions of slow intermolecular exchange the rates of intramolecular isomerization processes for Hg<sup>II</sup> can still exceed both the chemical shift and coupling constant time scale, particularly when bond cleavage is unnecessary and structures of these complexes have been determined (Bebout *et al.*, 2013; Carra *et al.*, 2013).



In view of this interest in the coordination chemistry of mercury with multidentate amine ligands, and the lack of such structures involving tertiary amine donors, we report here the structure of the HgCl<sub>2</sub> adduct of *N*<sup>1</sup>-benzyl-*N*<sup>1</sup>,*N*<sup>2</sup>,*N*<sup>2</sup>-trimethylethane-1,2-diamine. The *o*-diamine-substituted aryl bromide, *N*<sup>1</sup>-(2-bromobenzyl)-*N*<sup>1</sup>,*N*<sup>2</sup>,*N*<sup>2</sup>-trimethylethane-1,2-diamine, can be prepared by the reaction of *N*<sup>1</sup>,*N*<sup>1</sup>,*N*<sup>2</sup>-trimethylethane-1,2-diamine and *ortho*-bromobenzyl bromide. The ligand is moisture sensitive and is difficult to purify by

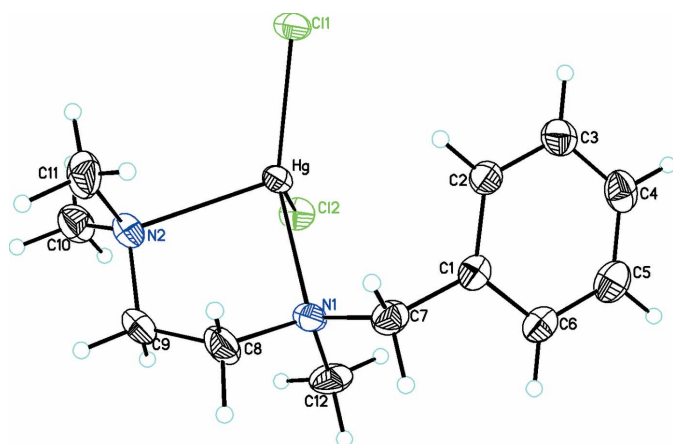


**Figure 1**  
Reaction scheme showing the synthesis of the title compound.

column chromatography. However, it could easily be purified by vacuum distillation. The moisture-sensitive ligand, when treated with *n*-BuLi in tetrahydrofuran (THF) and mercuric chloride, afforded the title compound,  $[\text{HgCl}_2(\text{C}_{12}\text{H}_{20}\text{N}_2)]$ , (3) (Fig. 1).

## 2. Structural commentary

In the structure of (3), the  $\text{Hg}^{\text{II}}$  atom is four-coordinated by two tertiary amine N-atom donors, as well as two  $\text{Cl}^-$  anions to give a distorted tetrahedral coordination environment (Fig. 2). The distortion from ideal values can be seen by the dihedral angle between the  $\text{N1}-\text{Hg}-\text{N2}$  and  $\text{Cl1}-\text{Hg}-\text{Cl2}$  planes of  $82.80(9)^\circ$ . The  $\text{Hg}-\text{N}$  and  $\text{Hg}-\text{Cl}$  bond lengths are in the normal ranges for such bonds (Allen, 2002). The five-membered chelate ring adopts an envelope conformation with puckering parameters of  $Q(2) = 0.446(6)\text{Å}$  and  $\varphi(2) = 88.8(6)^\circ$  (Cremer & Pople, 1975), with the two amine  $\text{CH}_3$  substituents on opposite sides of the ring. Of the two reported structures which contain  $\text{Hg}^{\text{II}}$  attached to tertiary N donors (Choi *et al.*, 2005; Niu *et al.*, 2004), only one has  $\text{Hg}^{\text{II}}$  in an  $\text{N}_2\text{Cl}_2$  coordination environment (Choi *et al.*, 2005) and thus provides the best comparison. The  $\text{Hg}-\text{Cl}$  [2.3875(14) and



**Figure 2**  
The molecular structure of  $[\text{HgCl}_2(\text{C}_{12}\text{H}_{20}\text{N}_2)]$ , showing the atom labelling and displacement ellipsoids at the 30% probability level.

**Table 1**  
Hydrogen-bond geometry ( $\text{Å}, ^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C7}-\text{H7A}\cdots\text{Cl2}^i$	0.99	2.78	3.748 (6)	165

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

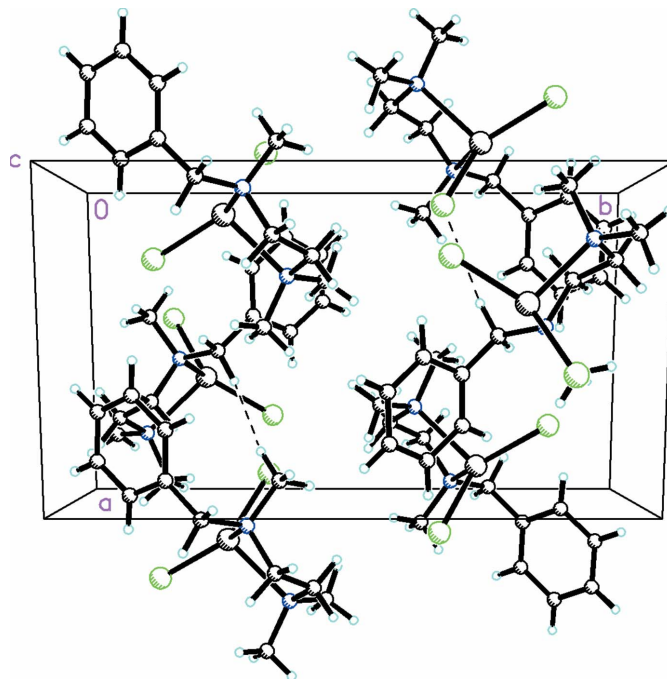
2.4397(13)  $\text{Å}$ ] and  $\text{Hg}-\text{N}$  bond lengths [2.355(4) and 2.411(4)  $\text{Å}$ ] in (3) agree well with those found in the previous example [ $\text{Hg}-\text{Cl} = 2.397(3)$  and 2.374(2)  $\text{Å}$ ;  $\text{Hg}-\text{N} = 2.353(7)$  and 2.391(6)  $\text{Å}$ ].

## 3. Supramolecular features

The molecular adducts are linked by  $\text{C}-\text{H}\cdots\text{Cl}$  interactions (Table 1 and Fig. 3) into a zigzag chain parallel to [101]. As a result of the bulky nature of the complex, with the two amine  $\text{CH}_3$  substituents on opposite sides of the chelate ring, there is no evidence of any  $\pi-\pi$  interactions.

## 4. Database survey

In view of the interest in the coordination chemistry of mercury, it is surprising that a search of the Cambridge Structural Database (Version 5.35, November 2013 with one update; Allen, 2002) for structures of  $\text{Hg}^{\text{II}}$  with an  $\text{N}_2\text{Cl}_2$  coordination sphere gave 96 hits, but the vast majority of these involved aromatic N donors such as pyridine and imidazole. There were only six hits involving aliphatic amine N-atom donors and only two (Choi *et al.*, 2005; Niu *et al.*, 2004) where the N atoms involved were both from tertiary amine functionalities.



**Figure 3**  
The molecular packing for  $[\text{HgCl}_2(\text{C}_{12}\text{H}_{20}\text{N}_2)]$  viewed along the  $c$  axis.  $\text{C}-\text{H}\cdots\text{Cl}$  interactions are shown as dashed lines.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	[HgCl <sub>2</sub> (C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> )]
<i>M<sub>r</sub></i>	463.79
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	200
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.0839 (3), 15.5367 (6), 11.3161 (5)
$\beta$ (°)	104.324 (4)
<i>V</i> (Å <sup>3</sup> )	1547.43 (10)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	10.27
Crystal size (mm)	0.79 × 0.23 × 0.05
Data collection	
Diffractometer	Agilent Xcalibur
Absorption correction	Analytical [ <i>CrysAlis PRO</i> (Agilent, 2014) using a multi-faceted crystal model based on expressions derived by Clark & Reid (1995)]
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.026, 0.339
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	13173, 5125, 3248
<i>R</i> <sub>int</sub>	0.067
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.758
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.044, 0.074, 0.96
No. of reflections	5125
No. of parameters	158
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	1.54, -1.61

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008), *WinGX* (Farrugia, 2012) and *pubCIF* (Westrip, 2010).

## 5. Synthesis and crystallization

A stirred solution of *N*<sup>1</sup>-(2-bromobenzyl)-*N*<sup>1</sup>,*N*<sup>2</sup>,*N*<sup>2</sup>-trimethylethane-1,2-diamine, (1), (1.10 ml, 5.34 mmol) in dry THF (15 ml) was treated dropwise with a 1.6 *M* solution of *n*-BuLi in hexane (3.80 ml, 6.15 mmol) *via* syringe under N<sub>2</sub> at 273 K. On stirring the reaction mixture for 2 h at this temperature, the lithiated product (2) was obtained. Mercuric chloride (1.55 g, 5.70 mmol) was added to the reaction mixture under a brisk flow of N<sub>2</sub> gas and stirring was continued for an

additional 6 h at room temperature. The reaction mixture was then removed from the N<sub>2</sub> line and evaporated to dryness to give a colourless hygroscopic solid. The solid was extracted with dry chloroform. The organic phase was separated, dried over Na<sub>2</sub>SO<sub>4</sub>, and filtered. The filtrate was evaporated to dryness to give a colourless crystalline solid of the HgCl<sub>2</sub> adduct of *N*<sup>1</sup>-benzyl-*N*<sup>1</sup>,*N*<sup>2</sup>,*N*<sup>2</sup>-trimethylethane-1,2-diamine, (3) (yield 1.25 g, 51 %). The reaction scheme is shown in Fig. 1.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H distances of 0.95 (aromatic) and 0.99 Å (methylene), with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C), and C–H = 0.98 Å for methyl H atoms, with *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C).

## Acknowledgements

RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase an X-ray diffractometer.

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## supporting information

*Acta Cryst.* (2014). E70, 118-120 [doi:10.1107/S1600536814017516]

## Crystal structure of (*N*<sup>1</sup>-benzyl-*N*<sup>1</sup>,*N*<sup>2</sup>,*N*<sup>2</sup>-trimethylethane-1,2-diamine- $\kappa^2$ *N,N'*)dichloridomercury(II)

Sudesh T. Manjare, Harkesh B. Singh and Ray J. Butcher

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

### (*N*<sup>1</sup>-Benzyl-*N*<sup>1</sup>,*N*<sup>2</sup>,*N*<sup>2</sup>-trimethylethane-1,2-diamine- $\kappa^2$ *N,N'*)dichloridomercury(II)

#### Crystal data

[HgCl<sub>2</sub>(C<sub>12</sub>H<sub>20</sub>N<sub>2</sub>)]  
*M<sub>r</sub>* = 463.79  
 Monoclinic, *P*2<sub>1</sub>/*n*  
 Hall symbol: -*P* 2<sub>1</sub>*n*  
*a* = 9.0839 (3) Å  
*b* = 15.5367 (6) Å  
*c* = 11.3161 (5) Å  
 $\beta$  = 104.324 (4)°  
*V* = 1547.43 (10) Å<sup>3</sup>  
*Z* = 4

*F*(000) = 880  
*D<sub>x</sub>* = 1.991 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation,  $\lambda$  = 0.71073 Å  
 Cell parameters from 1518 reflections  
 $\theta$  = 5.3–30.8°  
 $\mu$  = 10.27 mm<sup>-1</sup>  
*T* = 200 K  
 Plate, colorless  
 0.79 × 0.23 × 0.05 mm

#### Data collection

Agilent Xcalibur  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution: 10.5081 pixels mm<sup>-1</sup>  
 $\omega$  scans  
 Absorption correction: analytical  
 [*CrysAlis PRO* (Agilent, 2014) using a multi-  
 faceted crystal model based on expressions  
 derived by Clark & Reid (1995)]

*T*<sub>min</sub> = 0.026, *T*<sub>max</sub> = 0.339  
 13173 measured reflections  
 5125 independent reflections  
 3248 reflections with *I* > 2 $\sigma$ (*I*)  
*R*<sub>int</sub> = 0.067  
 $\theta$ <sub>max</sub> = 32.6°,  $\theta$ <sub>min</sub> = 5.1°  
*h* = -13→11  
*k* = -16→23  
*l* = -16→16

#### Refinement

Refinement on *F*<sup>2</sup>  
 Least-squares matrix: full  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.044  
*wR*(*F*<sup>2</sup>) = 0.074  
*S* = 0.96  
 5125 reflections  
 158 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

$$w = 1/[\sigma^2(F_o^2) + (0.0132P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.54 \text{ e } \text{\AA}^{-3}$

$$\Delta\rho_{\min} = -1.61 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 2008),  $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.00248 (16)

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness 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 threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg	0.11248 (2)	0.279066 (14)	0.55937 (2)	0.03718 (9)
Cl1	0.24245 (15)	0.15445 (9)	0.51432 (13)	0.0476 (4)
Cl2	-0.08589 (15)	0.34782 (10)	0.40263 (13)	0.0502 (4)
N1	0.0504 (5)	0.3190 (3)	0.7420 (4)	0.0402 (11)
N2	0.2991 (5)	0.3891 (3)	0.6352 (4)	0.0423 (11)
C1	-0.0894 (5)	0.1816 (4)	0.7510 (5)	0.0368 (13)
C2	-0.0412 (6)	0.1163 (4)	0.6876 (5)	0.0431 (14)
H2A	0.0635	0.1125	0.6885	0.052*
C3	-0.1412 (7)	0.0563 (4)	0.6228 (5)	0.0511 (16)
H3A	-0.1059	0.0123	0.5784	0.061*
C4	-0.2928 (7)	0.0605 (4)	0.6231 (5)	0.0531 (16)
H4A	-0.3624	0.0194	0.5788	0.064*
C5	-0.3428 (6)	0.1239 (4)	0.6871 (6)	0.0552 (17)
H5A	-0.4470	0.1263	0.6879	0.066*
C6	-0.2417 (6)	0.1853 (4)	0.7516 (5)	0.0481 (15)
H6A	-0.2773	0.2294	0.7957	0.058*
C7	0.0218 (6)	0.2459 (4)	0.8187 (5)	0.0455 (14)
H7A	0.1193	0.2163	0.8541	0.055*
H7B	-0.0163	0.2691	0.8870	0.055*
C8	0.1829 (7)	0.3687 (4)	0.8088 (6)	0.0572 (18)
H8A	0.2647	0.3280	0.8471	0.069*
H8B	0.1540	0.4009	0.8752	0.069*
C9	0.2449 (7)	0.4314 (4)	0.7321 (6)	0.0574 (17)
H9A	0.1644	0.4732	0.6950	0.069*
H9B	0.3298	0.4638	0.7852	0.069*
C10	0.3076 (7)	0.4511 (4)	0.5401 (6)	0.0597 (18)
H10A	0.3811	0.4962	0.5747	0.090*
H10B	0.2074	0.4770	0.5077	0.090*
H10C	0.3401	0.4216	0.4743	0.090*
C11	0.4498 (6)	0.3478 (4)	0.6837 (7)	0.064 (2)
H11A	0.5219	0.3906	0.7281	0.095*

H11B	0.4871	0.3247	0.6158	0.095*
H11C	0.4398	0.3008	0.7390	0.095*
C12	-0.0886 (6)	0.3744 (4)	0.7088 (6)	0.0575 (17)
H12A	-0.1164	0.3928	0.7833	0.086*
H12B	-0.1725	0.3415	0.6575	0.086*
H12C	-0.0679	0.4251	0.6641	0.086*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Hg	0.03850 (13)	0.03097 (13)	0.04205 (14)	-0.00121 (10)	0.00990 (8)	-0.00793 (11)
C11	0.0585 (9)	0.0360 (8)	0.0541 (9)	0.0049 (7)	0.0249 (7)	-0.0088 (7)
C12	0.0470 (8)	0.0549 (10)	0.0448 (9)	0.0077 (7)	0.0037 (6)	-0.0001 (8)
N1	0.050 (3)	0.032 (3)	0.041 (3)	-0.001 (2)	0.017 (2)	-0.006 (2)
N2	0.047 (3)	0.031 (3)	0.046 (3)	-0.004 (2)	0.007 (2)	-0.001 (2)
C1	0.034 (3)	0.039 (3)	0.037 (3)	0.007 (2)	0.008 (2)	0.012 (3)
C2	0.044 (3)	0.033 (3)	0.057 (4)	0.008 (3)	0.021 (3)	0.010 (3)
C3	0.069 (4)	0.040 (4)	0.048 (4)	0.003 (3)	0.022 (3)	0.009 (3)
C4	0.068 (4)	0.050 (4)	0.039 (4)	-0.013 (3)	0.009 (3)	0.009 (3)
C5	0.038 (3)	0.072 (5)	0.055 (4)	0.002 (3)	0.009 (3)	0.010 (4)
C6	0.046 (3)	0.055 (4)	0.047 (4)	0.003 (3)	0.018 (3)	0.006 (3)
C7	0.051 (3)	0.045 (4)	0.045 (4)	0.006 (3)	0.020 (3)	0.006 (3)
C8	0.076 (4)	0.050 (4)	0.046 (4)	-0.023 (3)	0.015 (3)	-0.018 (3)
C9	0.068 (4)	0.042 (4)	0.064 (4)	-0.018 (3)	0.020 (3)	-0.021 (3)
C10	0.075 (4)	0.043 (4)	0.061 (4)	-0.008 (3)	0.018 (3)	-0.001 (3)
C11	0.035 (3)	0.058 (5)	0.089 (5)	-0.006 (3)	-0.001 (3)	0.000 (4)
C12	0.062 (4)	0.048 (4)	0.069 (5)	0.026 (3)	0.029 (3)	0.003 (3)

*Geometric parameters (Å, °)*

Hg—N1	2.355 (4)	C5—C6	1.398 (8)
Hg—C11	2.3875 (14)	C5—H5A	0.9500
Hg—N2	2.411 (4)	C6—H6A	0.9500
Hg—C12	2.4397 (13)	C7—H7A	0.9900
N1—C8	1.472 (6)	C7—H7B	0.9900
N1—C7	1.491 (7)	C8—C9	1.503 (9)
N1—C12	1.497 (6)	C8—H8A	0.9900
N2—C10	1.460 (7)	C8—H8B	0.9900
N2—C9	1.465 (8)	C9—H9A	0.9900
N2—C11	1.489 (7)	C9—H9B	0.9900
C1—C2	1.375 (7)	C10—H10A	0.9800
C1—C6	1.386 (7)	C10—H10B	0.9800
C1—C7	1.491 (8)	C10—H10C	0.9800
C2—C3	1.379 (8)	C11—H11A	0.9800
C2—H2A	0.9500	C11—H11B	0.9800
C3—C4	1.380 (8)	C11—H11C	0.9800
C3—H3A	0.9500	C12—H12A	0.9800
C4—C5	1.364 (8)	C12—H12B	0.9800

C4—H4A	0.9500	C12—H12C	0.9800
N1—Hg—C11	129.73 (12)	C1—C7—N1	113.9 (5)
N1—Hg—N2	78.51 (16)	C1—C7—H7A	108.8
C11—Hg—N2	108.04 (12)	N1—C7—H7A	108.8
N1—Hg—C12	103.21 (11)	C1—C7—H7B	108.8
C11—Hg—C12	121.01 (5)	N1—C7—H7B	108.8
N2—Hg—C12	106.03 (11)	H7A—C7—H7B	107.7
C8—N1—C7	109.8 (4)	N1—C8—C9	114.7 (5)
C8—N1—C12	111.0 (5)	N1—C8—H8A	108.6
C7—N1—C12	109.0 (4)	C9—C8—H8A	108.6
C8—N1—Hg	104.3 (3)	N1—C8—H8B	108.6
C7—N1—Hg	115.1 (3)	C9—C8—H8B	108.6
C12—N1—Hg	107.6 (3)	H8A—C8—H8B	107.6
C10—N2—C9	110.1 (5)	N2—C9—C8	112.6 (5)
C10—N2—C11	110.1 (5)	N2—C9—H9A	109.1
C9—N2—C11	111.5 (5)	C8—C9—H9A	109.1
C10—N2—Hg	111.5 (3)	N2—C9—H9B	109.1
C9—N2—Hg	104.4 (3)	C8—C9—H9B	109.1
C11—N2—Hg	109.1 (3)	H9A—C9—H9B	107.8
C2—C1—C6	118.7 (5)	N2—C10—H10A	109.5
C2—C1—C7	119.9 (5)	N2—C10—H10B	109.5
C6—C1—C7	121.3 (5)	H10A—C10—H10B	109.5
C1—C2—C3	121.5 (5)	N2—C10—H10C	109.5
C1—C2—H2A	119.2	H10A—C10—H10C	109.5
C3—C2—H2A	119.2	H10B—C10—H10C	109.5
C2—C3—C4	119.5 (6)	N2—C11—H11A	109.5
C2—C3—H3A	120.2	N2—C11—H11B	109.5
C4—C3—H3A	120.2	H11A—C11—H11B	109.5
C5—C4—C3	119.9 (6)	N2—C11—H11C	109.5
C5—C4—H4A	120.0	H11A—C11—H11C	109.5
C3—C4—H4A	120.0	H11B—C11—H11C	109.5
C4—C5—C6	120.5 (6)	N1—C12—H12A	109.5
C4—C5—H5A	119.7	N1—C12—H12B	109.5
C6—C5—H5A	119.7	H12A—C12—H12B	109.5
C1—C6—C5	119.8 (6)	N1—C12—H12C	109.5
C1—C6—H6A	120.1	H12A—C12—H12C	109.5
C5—C6—H6A	120.1	H12B—C12—H12C	109.5
C11—Hg—N1—C8	89.5 (4)	C7—C1—C2—C3	-179.3 (5)
N2—Hg—N1—C8	-14.5 (4)	C1—C2—C3—C4	-1.2 (9)
C12—Hg—N1—C8	-118.5 (3)	C2—C3—C4—C5	0.0 (9)
C11—Hg—N1—C7	-30.9 (4)	C3—C4—C5—C6	0.7 (9)
N2—Hg—N1—C7	-134.9 (4)	C2—C1—C6—C5	-0.9 (8)
C12—Hg—N1—C7	121.2 (3)	C7—C1—C6—C5	-179.9 (5)
C11—Hg—N1—C12	-152.6 (3)	C4—C5—C6—C1	-0.3 (9)
N2—Hg—N1—C12	103.4 (4)	C2—C1—C7—N1	85.1 (6)
C12—Hg—N1—C12	-0.6 (4)	C6—C1—C7—N1	-95.8 (6)

N1—Hg—N2—C10	-132.3 (4)	C8—N1—C7—C1	-168.4 (5)
Cl1—Hg—N2—C10	99.4 (4)	C12—N1—C7—C1	69.8 (6)
Cl2—Hg—N2—C10	-31.7 (4)	Hg—N1—C7—C1	-51.1 (5)
N1—Hg—N2—C9	-13.4 (4)	C7—N1—C8—C9	166.8 (5)
Cl1—Hg—N2—C9	-141.7 (3)	C12—N1—C8—C9	-72.6 (7)
Cl2—Hg—N2—C9	87.2 (4)	Hg—N1—C8—C9	43.0 (6)
N1—Hg—N2—C11	105.9 (4)	C10—N2—C9—C8	160.3 (5)
Cl1—Hg—N2—C11	-22.4 (4)	C11—N2—C9—C8	-77.1 (6)
Cl2—Hg—N2—C11	-153.5 (4)	Hg—N2—C9—C8	40.5 (6)
C6—C1—C2—C3	1.6 (8)	N1—C8—C9—N2	-61.6 (7)

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C7—H7A...Cl2 <sup>i</sup>	0.99	2.78	3.748 (6)	165

Symmetry code: (i)  $x+1/2, -y+1/2, z+1/2$ .