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# Bis{$\mu$-2,5-bis[4-(2-pyridylmethylamino)-phenyl]-1,3,4-oxadiazole}bis[dichloridomercury(II)]

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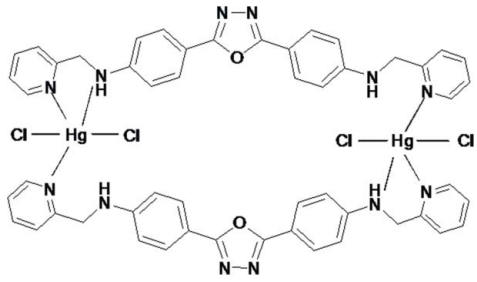
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.011 Å; $R$ factor = 0.045; $wR$ factor = 0.118; data-to-parameter ratio = 14.3.

In the title centrosymmetric compound, $[Hg_2Cl_4(C_{26}H_{22}N_6O)_2]$, each $Hg^{II}$ center adopts a distorted $HgN_3Cl_2$ trigonal bipyramidal coordination geometry, formed by two pyridine N atoms, one imine N atom and two chloride anions. Within the organic ligand, the oxadiazole ring is nearly coplanar with the two benzene rings [dihedral angles = 5.9 (4) and 6.5 (4)°] and nearly perpendicular to the two pyridine rings with the same dihedral angle of 77.4 (4)°. The two organic ligands bridge two $Hg^{II}$ ions to form the macrocyclic complex. Intermolecular N—H···Cl and N—H···N hydrogen bonding helps to stabilize the crystal structure.

## Related literature

For general background, see: Dong *et al.* (2003). For related structures, see: Gallagher *et al.* (1999); Grupce *et al.* (1999). For synthesis, see: Ren *et al.* (1995).



## Experimental

### Crystal data

$[Hg_2Cl_4(C_{26}H_{22}N_6O)_2]$
$M_r$ = 1411.98
Triclinic, $P\overline{1}$
$a$ = 8.5426 (19) Å
$b$ = 9.945 (2) Å
$c$ = 16.533 (4) Å
$\alpha$ = 83.773 (3)°
$\beta$ = 80.001 (3)°
$\gamma$ = 67.671 (2)°
$V$ = 1278.2 (5) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 6.26 mm$^{-1}$
$T$ = 298 (2) K
0.40 × 0.40 × 0.30 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min}$ = 0.113, $T_{max}$ = 0.153
6681 measured reflections
4652 independent reflections
3878 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
$S$ = 1.04
4652 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.84 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Hg1—Cl1 | 2.373 (2) | Hg1—N4 | 2.275 (6) |
| Hg1—Cl2 | 2.451 (2) | Hg1—N6$^{i}$ | 2.745 (7) |
| Hg1—N3 | 2.587 (6) | | |
| N4—Hg1—Cl1 | 145.19 (16) | Cl2—Hg1—N3 | 95.30 (13) |
| N4—Hg1—Cl2 | 99.31 (16) | N4—Hg1—N6$^{i}$ | 86.73 (19) |
| Cl1—Hg1—Cl2 | 114.87 (10) | Cl1—Hg1—N6$^{i}$ | 84.60 (15) |
| N4—Hg1—N3 | 70.81 (18) | Cl2—Hg1—N6$^{i}$ | 115.31 (15) |
| Cl1—Hg1—N3 | 98.44 (13) | N3—Hg1—N6$^{i}$ | 144.82 (18) |

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

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···N2$^{ii}$ | 0.91 | 2.36 | 3.191 (8) | 152 |
| N5—H5···Cl1$^{iii}$ | 0.86 | 2.68 | 3.517 (7) | 166 |

Symmetry codes: (ii) $x+1, y, z$; (iii) $-x+1, -y, -z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2406).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, m555 [ **doi:10.1107/S1600536808006788** ]

# Bis{$\mu$-2,5-bis[4-(2-pyridylmethylamino)phenyl]-1,3,4-oxadiazole}bis[dichloridomercury(II)]

**L.-L. Liu, G.-G. Hou, J.-P. Ma, R.-Q. Huang and Y.-B. Dong**

## Comment

Combining metal ions with oxadiazole-bridging organic ligands may result in coordination polymers with novel network connectivities (Dong *et al.*, 2003). Our interest in understanding the relationship between the metal coordination modes with such ligands and their extended structures led us to synthesize the title $Hg^{II}$ compound, (I).

As shown in Fig. 1, there are five primary bonds to each $Hg^{II}$ center, three Hg—N bonds and two Hg—Cl bonds, resulting in a distorted trigonal bipyramid coordination geometry around the Hg center. Three Hg—N bond distances (Table 1) are significantly different, but all agree with those reported previously (Gallagher *et al.*, 1999; Grupce *et al.*, 1999). The bond angles at Hg1 atom rang from 70.81 (18)° [N4—Hg—N3] to 145.19 (16)° [N4—Hg1—Cl1]. While the ligand chelates to a Hg atom by a pyridine N and an imine N atoms, the other pyridine N atom bridges to another Hg atom to form the title binuclear macrocyclic complex with the Hg···Hg separation of 12.969 (2) Å. Within the ligand, the dihedral angles between the oxadiazole and N4-pyridine rings and between the oxadiazole and N6-pyridine rings are identical [77.4 (4)°]. Intermolecular N—H···Cl and N—H···N hydrogen bonding helps to stabilize the crystal structure (Table 2).

## Experimental

2,5-Bis(4-aminophenyl)-1,3,4-oxadiazole (L1) was prepared according to the literature method (Ren *et al.*, 1995). A solution of L1 (2.56 g, 10 mmol) and 2-pyridylaldehyde (4 ml) in anhydrous EtOH (20 ml) was refluxed for 24 h, with HCOOH as catalyzer. After the mixture was cooled to room temperature, the precipitated product was filtered off, washed with EtOH and dried, yielding a light-yellow power [2,5-bis(4-((2-pyridinyl)methyleneamino)phenyl) −1,3,4-oxadiazole] (L2). Then the L2 was deoxidized by $NaBH_4$ in anhydrous $CH_3OH$ (20 ml). The solvent was removed under reduced pressure, and the residue was washed with water to afford the ligand [2,5-bis(4-((2-pyridinylmethyl)amino)phenyl)-1,3,4-oxadiazole] (*L*) as a yellow solid. A solution of $HgCl_2$ (13.58 mg, 0.05 mmol) in EtOH (8 ml) was layered onto a solution of the ligand *L* (21.7 mg, 0.05 mmol) in $CH_2Cl_2$ (8 ml). Single yellow crystals of the title compound were obtained after 7 d at room temperature.

## Refinement

All H atoms were placed in calculated positions with C—H = 0.93 (aromatic), 0.97 Å (methylene) and N—H = 0.91 or 0.86 Å imine groups), and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C,*N*).

## Figures

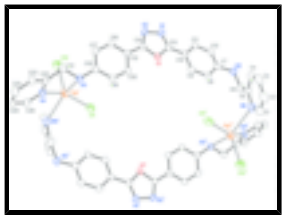


Fig. 1. The structure of (I), showing 30% displacement ellipsoids, hydrogen atoms have been omitted [symmetry code: (i) −*x* + 2,-*y*,-*z*].

## Bis{μ-2,5-bis[4-(2-pyridylmethylamino)phenyl]-1,3,4- oxadiazole}bis[dichloridomercury(II)]

### *Crystal data*

| | |
|---|---|
| $[Hg_2Cl_4(C_{26}H_{22}N_6O)_2]$ | $Z = 1$ |
| $M_r = 1411.98$ | $F_{000} = 684$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.834$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 8.5426$ (19) Å | Cell parameters from 2786 reflections |
| $b = 9.945$ (2) Å | $\theta = 2.5$–$25.6$º |
| $c = 16.533$ (4) Å | $\mu = 6.26$ mm$^{-1}$ |
| $\alpha = 83.773$ (3)º | $T = 298$ (2) K |
| $\beta = 80.001$ (3)º | Block, yellow |
| $\gamma = 67.671$ (2)º | 0.40 × 0.40 × 0.30 mm |
| $V = 1278.2$ (5) Å$^3$ | |

### *Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD diffractometer | 4652 independent reflections |
| Radiation source: fine-focus sealed tube | 3878 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.023$ |
| $T = 298(2)$ K | $\theta_{max} = 25.5$º |
| φ and ω scans | $\theta_{min} = 1.3$º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2002) | $h = -10 \rightarrow 10$ |
| $T_{min} = 0.113$, $T_{max} = 0.153$ | $k = -12 \rightarrow 11$ |
| 6681 measured reflections | $l = -20 \rightarrow 12$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | H-atom parameters constrained |
| $wR(F^2) = 0.118$ | $w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 1.1058P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|---|---|
| $S$ = 1.04 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 4652 reflections | $\Delta\rho_{max}$ = 2.20 e Å$^{-3}$ |
| 325 parameters | $\Delta\rho_{min}$ = −0.84 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N6 | 0.7661 (9) | −0.1644 (7) | −0.4018 (4) | 0.0529 (16) |
| C5 | 0.6054 (9) | −0.1027 (8) | −0.3635 (4) | 0.0418 (16) |
| C6 | 0.5468 (11) | −0.2001 (8) | −0.2981 (4) | 0.0516 (19) |
| H6A | 0.5341 | −0.2764 | −0.3251 | 0.062* |
| H6B | 0.6356 | −0.2462 | −0.2636 | 0.062* |
| N5 | 0.3889 (8) | −0.1271 (7) | −0.2465 (4) | 0.0495 (15) |
| H5 | 0.2971 | −0.1354 | −0.2559 | 0.059* |
| C7 | 0.3785 (9) | −0.0447 (7) | −0.1829 (4) | 0.0399 (15) |
| Hg1 | 0.95952 (4) | 0.33183 (3) | 0.324081 (19) | 0.05155 (14) |
| Cl1 | 1.0242 (3) | 0.1191 (2) | 0.25208 (17) | 0.0723 (6) |
| Cl2 | 0.6820 (3) | 0.4107 (3) | 0.41247 (15) | 0.0854 (8) |
| O1 | 0.4543 (5) | 0.2726 (5) | 0.0143 (3) | 0.0354 (10) |
| N3 | 0.8599 (7) | 0.5232 (6) | 0.2061 (3) | 0.0371 (12) |
| H3 | 0.9511 | 0.5157 | 0.1666 | 0.045* |
| C19 | 0.7868 (8) | 0.4113 (8) | 0.1043 (4) | 0.0413 (16) |
| H19 | 0.9008 | 0.3795 | 0.0803 | 0.050* |
| C13 | 0.3210 (8) | 0.2390 (7) | 0.0028 (4) | 0.0380 (15) |
| C14 | 0.3883 (8) | 0.3660 (7) | 0.0762 (4) | 0.0356 (14) |
| C18 | 0.7341 (8) | 0.4991 (7) | 0.1714 (4) | 0.0363 (14) |
| C9 | 0.4933 (9) | 0.0866 (8) | −0.1119 (4) | 0.0419 (16) |
| H9 | 0.5837 | 0.1135 | −0.1062 | 0.050* |
| C11 | 0.2122 (8) | 0.0950 (8) | −0.0669 (4) | 0.0421 (16) |
| H11 | 0.1104 | 0.1278 | −0.0308 | 0.051* |
| C10 | 0.3426 (8) | 0.1393 (8) | −0.0594 (4) | 0.0368 (14) |
| N2 | 0.2294 (7) | 0.3897 (7) | 0.1005 (4) | 0.0472 (15) |
| C15 | 0.5034 (8) | 0.4177 (7) | 0.1072 (4) | 0.0347 (14) |
| C16 | 0.4485 (8) | 0.5123 (8) | 0.1708 (4) | 0.0412 (16) |

| | | | | |
|---|---|---|---|---|
| H16 | 0.3331 | 0.5495 | 0.1924 | 0.049* |
| C12 | 0.2300 (9) | 0.0027 (8) | −0.1270 (4) | 0.0436 (16) |
| H12 | 0.1413 | −0.0282 | −0.1301 | 0.052* |
| C21 | 0.8165 (10) | 0.6524 (7) | 0.2504 (5) | 0.0481 (18) |
| H21A | 0.7151 | 0.6637 | 0.2903 | 0.058* |
| H21B | 0.7898 | 0.7365 | 0.2123 | 0.058* |
| N1 | 0.1858 (7) | 0.3049 (8) | 0.0520 (4) | 0.0508 (16) |
| C23 | 1.0048 (10) | 0.7665 (8) | 0.2940 (5) | 0.0516 (19) |
| H23 | 0.9519 | 0.8514 | 0.2637 | 0.062* |
| C20 | 0.6746 (8) | 0.3714 (8) | 0.0733 (4) | 0.0404 (15) |
| H20 | 0.7131 | 0.3121 | 0.0286 | 0.048* |
| C4 | 0.5020 (11) | 0.0367 (9) | −0.3836 (5) | 0.0547 (19) |
| H4 | 0.3909 | 0.0769 | −0.3564 | 0.066* |
| N4 | 1.0367 (7) | 0.5233 (6) | 0.3357 (3) | 0.0420 (13) |
| C22 | 0.9585 (9) | 0.6475 (7) | 0.2942 (4) | 0.0401 (15) |
| C25 | 1.2047 (10) | 0.6336 (9) | 0.3837 (5) | 0.055 (2) |
| H25 | 1.2881 | 0.6265 | 0.4151 | 0.066* |
| C17 | 0.5620 (9) | 0.5517 (8) | 0.2022 (4) | 0.0432 (16) |
| H17 | 0.5226 | 0.6150 | 0.2451 | 0.052* |
| C3 | 0.5663 (14) | 0.1169 (10) | −0.4453 (6) | 0.067 (2) |
| H3A | 0.5009 | 0.2133 | −0.4581 | 0.080* |
| C8 | 0.5139 (8) | −0.0050 (8) | −0.1727 (4) | 0.0415 (16) |
| H8 | 0.6178 | −0.0405 | −0.2071 | 0.050* |
| C1 | 0.8213 (13) | −0.0863 (11) | −0.4622 (6) | 0.069 (2) |
| H1 | 0.9318 | −0.1286 | −0.4897 | 0.083* |
| C24 | 1.1299 (11) | 0.7583 (9) | 0.3391 (5) | 0.058 (2) |
| H24 | 1.1628 | 0.8373 | 0.3391 | 0.069* |
| C26 | 1.1544 (9) | 0.5180 (8) | 0.3812 (4) | 0.0481 (17) |
| H26 | 1.2039 | 0.4332 | 0.4124 | 0.058* |
| C2 | 0.7255 (14) | 0.0522 (11) | −0.4864 (6) | 0.070 (3) |
| H2 | 0.7688 | 0.1012 | −0.5302 | 0.084* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N6 | 0.064 (4) | 0.042 (4) | 0.052 (4) | −0.020 (3) | −0.011 (3) | 0.011 (3) |
| C5 | 0.052 (4) | 0.034 (4) | 0.043 (4) | −0.017 (3) | −0.012 (3) | −0.006 (3) |
| C6 | 0.071 (5) | 0.036 (4) | 0.045 (4) | −0.019 (4) | −0.001 (4) | −0.003 (3) |
| N5 | 0.053 (4) | 0.051 (4) | 0.048 (4) | −0.023 (3) | −0.006 (3) | −0.012 (3) |
| C7 | 0.047 (4) | 0.024 (3) | 0.048 (4) | −0.013 (3) | −0.011 (3) | 0.004 (3) |
| Hg1 | 0.0623 (2) | 0.03300 (18) | 0.0642 (2) | −0.02039 (14) | −0.02216 (14) | 0.00926 (13) |
| Cl1 | 0.0659 (13) | 0.0379 (11) | 0.122 (2) | −0.0203 (10) | −0.0315 (12) | −0.0090 (11) |
| Cl2 | 0.0705 (14) | 0.104 (2) | 0.0654 (15) | −0.0260 (14) | −0.0016 (11) | 0.0254 (13) |
| O1 | 0.030 (2) | 0.039 (3) | 0.039 (3) | −0.0149 (19) | −0.0056 (18) | −0.0019 (19) |
| N3 | 0.040 (3) | 0.035 (3) | 0.038 (3) | −0.016 (2) | −0.007 (2) | −0.001 (2) |
| C19 | 0.030 (3) | 0.046 (4) | 0.042 (4) | −0.009 (3) | 0.000 (3) | −0.005 (3) |
| C13 | 0.036 (3) | 0.039 (4) | 0.041 (4) | −0.015 (3) | −0.011 (3) | 0.004 (3) |
| C14 | 0.034 (3) | 0.036 (4) | 0.034 (4) | −0.010 (3) | −0.002 (3) | 0.000 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C18 | 0.041 (4) | 0.034 (4) | 0.036 (4) | −0.016 (3) | −0.008 (3) | 0.004 (3) |
| C9 | 0.037 (4) | 0.041 (4) | 0.049 (4) | −0.016 (3) | −0.012 (3) | 0.005 (3) |
| C11 | 0.034 (3) | 0.048 (4) | 0.043 (4) | −0.014 (3) | −0.005 (3) | −0.001 (3) |
| C10 | 0.035 (3) | 0.042 (4) | 0.036 (4) | −0.017 (3) | −0.012 (3) | 0.004 (3) |
| N2 | 0.040 (3) | 0.055 (4) | 0.050 (4) | −0.020 (3) | 0.002 (3) | −0.019 (3) |
| C15 | 0.031 (3) | 0.037 (4) | 0.035 (3) | −0.012 (3) | −0.007 (3) | 0.006 (3) |
| C16 | 0.035 (3) | 0.045 (4) | 0.039 (4) | −0.011 (3) | −0.004 (3) | −0.004 (3) |
| C12 | 0.039 (4) | 0.046 (4) | 0.050 (4) | −0.021 (3) | −0.008 (3) | −0.002 (3) |
| C21 | 0.057 (4) | 0.027 (4) | 0.065 (5) | −0.013 (3) | −0.031 (4) | 0.005 (3) |
| N1 | 0.035 (3) | 0.070 (5) | 0.055 (4) | −0.026 (3) | 0.000 (3) | −0.022 (3) |
| C23 | 0.065 (5) | 0.029 (4) | 0.065 (5) | −0.014 (3) | −0.027 (4) | −0.001 (3) |
| C20 | 0.042 (4) | 0.039 (4) | 0.041 (4) | −0.015 (3) | −0.007 (3) | −0.005 (3) |
| C4 | 0.071 (5) | 0.045 (5) | 0.053 (5) | −0.022 (4) | −0.021 (4) | −0.001 (4) |
| N4 | 0.045 (3) | 0.039 (3) | 0.044 (3) | −0.013 (3) | −0.017 (3) | 0.000 (3) |
| C22 | 0.049 (4) | 0.029 (3) | 0.040 (4) | −0.011 (3) | −0.011 (3) | −0.001 (3) |
| C25 | 0.057 (5) | 0.055 (5) | 0.059 (5) | −0.017 (4) | −0.027 (4) | −0.011 (4) |
| C17 | 0.045 (4) | 0.041 (4) | 0.042 (4) | −0.014 (3) | −0.003 (3) | −0.009 (3) |
| C3 | 0.094 (7) | 0.042 (5) | 0.071 (6) | −0.025 (5) | −0.040 (5) | 0.017 (4) |
| C8 | 0.035 (3) | 0.044 (4) | 0.043 (4) | −0.010 (3) | −0.011 (3) | 0.001 (3) |
| C1 | 0.072 (6) | 0.076 (7) | 0.062 (6) | −0.034 (5) | −0.014 (4) | 0.014 (5) |
| C24 | 0.068 (5) | 0.042 (5) | 0.072 (5) | −0.023 (4) | −0.025 (4) | −0.009 (4) |
| C26 | 0.055 (4) | 0.034 (4) | 0.050 (4) | −0.006 (3) | −0.019 (3) | 0.000 (3) |
| C2 | 0.096 (7) | 0.077 (7) | 0.060 (5) | −0.057 (6) | −0.032 (5) | 0.028 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N6—C1 | 1.330 (11) | C11—C10 | 1.373 (9) |
| N6—C5 | 1.343 (10) | C11—C12 | 1.375 (10) |
| C5—C4 | 1.372 (11) | C11—H11 | 0.9300 |
| C5—C6 | 1.520 (10) | N2—N1 | 1.407 (8) |
| C6—N5 | 1.437 (10) | C15—C16 | 1.385 (9) |
| C6—H6A | 0.9700 | C15—C20 | 1.388 (9) |
| C6—H6B | 0.9700 | C16—C17 | 1.368 (10) |
| N5—C7 | 1.373 (9) | C16—H16 | 0.9300 |
| N5—H5 | 0.8600 | C12—H12 | 0.9300 |
| C7—C12 | 1.385 (10) | C21—C22 | 1.500 (10) |
| C7—C8 | 1.397 (9) | C21—H21A | 0.9700 |
| Hg1—Cl1 | 2.373 (2) | C21—H21B | 0.9700 |
| Hg1—Cl2 | 2.451 (2) | C23—C24 | 1.379 (11) |
| Hg1—N3 | 2.587 (6) | C23—C22 | 1.383 (10) |
| Hg1—N4 | 2.275 (6) | C23—H23 | 0.9300 |
| Hg1—N6$^{i}$ | 2.745 (7) | C20—H20 | 0.9300 |
| O1—C13 | 1.350 (7) | C4—C3 | 1.394 (12) |
| O1—C14 | 1.355 (7) | C4—H4 | 0.9300 |
| N3—C18 | 1.408 (8) | N4—C22 | 1.338 (9) |
| N3—C21 | 1.440 (9) | N4—C26 | 1.340 (9) |
| N3—H3 | 0.9100 | C25—C24 | 1.361 (12) |
| C19—C20 | 1.358 (9) | C25—C26 | 1.378 (11) |
| C19—C18 | 1.390 (9) | C25—H25 | 0.9300 |

| | | | |
|---|---|---|---|
| C19—H19 | 0.9300 | C17—H17 | 0.9300 |
| C13—N1 | 1.280 (9) | C3—C2 | 1.354 (14) |
| C13—C10 | 1.446 (9) | C3—H3A | 0.9300 |
| C14—N2 | 1.284 (8) | C8—H8 | 0.9300 |
| C14—C15 | 1.452 (9) | C1—C2 | 1.365 (14) |
| C18—C17 | 1.381 (10) | C1—H1 | 0.9300 |
| C9—C10 | 1.373 (10) | C24—H24 | 0.9300 |
| C9—C8 | 1.374 (10) | C26—H26 | 0.9300 |
| C9—H9 | 0.9300 | C2—H2 | 0.9300 |
| C1—N6—C5 | 117.3 (7) | C16—C15—C20 | 117.9 (6) |
| N6—C5—C4 | 122.1 (7) | C16—C15—C14 | 122.2 (6) |
| N6—C5—C6 | 114.8 (6) | C20—C15—C14 | 119.9 (6) |
| C4—C5—C6 | 123.0 (7) | C17—C16—C15 | 120.8 (6) |
| N5—C6—C5 | 114.9 (6) | C17—C16—H16 | 119.6 |
| N5—C6—H6A | 108.5 | C15—C16—H16 | 119.6 |
| C5—C6—H6A | 108.5 | C11—C12—C7 | 120.7 (6) |
| N5—C6—H6B | 108.5 | C11—C12—H12 | 119.6 |
| C5—C6—H6B | 108.5 | C7—C12—H12 | 119.6 |
| H6A—C6—H6B | 107.5 | N3—C21—C22 | 112.4 (6) |
| C7—N5—C6 | 122.8 (6) | N3—C21—H21A | 109.1 |
| C7—N5—H5 | 118.6 | C22—C21—H21A | 109.1 |
| C6—N5—H5 | 118.6 | N3—C21—H21B | 109.1 |
| N5—C7—C12 | 120.0 (6) | C22—C21—H21B | 109.1 |
| N5—C7—C8 | 121.8 (6) | H21A—C21—H21B | 107.9 |
| C12—C7—C8 | 118.1 (6) | C13—N1—N2 | 106.8 (5) |
| N4—Hg1—Cl1 | 145.19 (16) | C24—C23—C22 | 119.5 (7) |
| N4—Hg1—Cl2 | 99.31 (16) | C24—C23—H23 | 120.3 |
| Cl1—Hg1—Cl2 | 114.87 (10) | C22—C23—H23 | 120.3 |
| N4—Hg1—N3 | 70.81 (18) | C19—C20—C15 | 121.1 (6) |
| Cl1—Hg1—N3 | 98.44 (13) | C19—C20—H20 | 119.5 |
| Cl2—Hg1—N3 | 95.30 (13) | C15—C20—H20 | 119.5 |
| N4—Hg1—N6$^{i}$ | 86.73 (19) | C5—C4—C3 | 118.9 (8) |
| Cl1—Hg1—N6$^{i}$ | 84.60 (15) | C5—C4—H4 | 120.6 |
| Cl2—Hg1—N6$^{i}$ | 115.31 (15) | C3—C4—H4 | 120.6 |
| N3—Hg1—N6$^{i}$ | 144.82 (18) | C22—N4—C26 | 119.0 (6) |
| C13—O1—C14 | 103.7 (5) | C22—N4—Hg1 | 117.2 (4) |
| C18—N3—C21 | 120.2 (5) | C26—N4—Hg1 | 123.8 (5) |
| C18—N3—Hg1 | 110.2 (4) | N4—C22—C23 | 120.9 (7) |
| C21—N3—Hg1 | 98.4 (4) | N4—C22—C21 | 117.1 (6) |
| C18—N3—H3 | 109.1 | C23—C22—C21 | 122.0 (6) |
| C21—N3—H3 | 109.1 | C24—C25—C26 | 118.6 (7) |
| Hg1—N3—H3 | 109.1 | C24—C25—H25 | 120.7 |
| C20—C19—C18 | 121.1 (6) | C26—C25—H25 | 120.7 |
| C20—C19—H19 | 119.5 | C16—C17—C18 | 121.2 (6) |
| C18—C19—H19 | 119.5 | C16—C17—H17 | 119.4 |
| N1—C13—O1 | 111.7 (6) | C18—C17—H17 | 119.4 |
| N1—C13—C10 | 128.3 (6) | C2—C3—C4 | 118.9 (8) |
| O1—C13—C10 | 120.0 (6) | C2—C3—H3A | 120.6 |

| | | | |
|---|---|---|---|
| N2—C14—O1 | 112.0 (6) | C4—C3—H3A | 120.6 |
| N2—C14—C15 | 130.1 (6) | C9—C8—C7 | 119.8 (6) |
| O1—C14—C15 | 117.8 (5) | C9—C8—H8 | 120.1 |
| C17—C18—C19 | 117.8 (6) | C7—C8—H8 | 120.1 |
| C17—C18—N3 | 124.0 (6) | N6—C1—C2 | 124.0 (9) |
| C19—C18—N3 | 118.1 (6) | N6—C1—H1 | 118.0 |
| C10—C9—C8 | 121.6 (6) | C2—C1—H1 | 118.0 |
| C10—C9—H9 | 119.2 | C25—C24—C23 | 119.4 (7) |
| C8—C9—H9 | 119.2 | C25—C24—H24 | 120.3 |
| C10—C11—C12 | 120.9 (6) | C23—C24—H24 | 120.3 |
| C10—C11—H11 | 119.5 | N4—C26—C25 | 122.4 (7) |
| C12—C11—H11 | 119.5 | N4—C26—H26 | 118.8 |
| C11—C10—C9 | 118.5 (6) | C25—C26—H26 | 118.8 |
| C11—C10—C13 | 120.4 (6) | C3—C2—C1 | 118.7 (9) |
| C9—C10—C13 | 121.0 (6) | C3—C2—H2 | 120.6 |
| C14—N2—N1 | 105.8 (5) | C1—C2—H2 | 120.6 |
| C1—N6—C5—C4 | −1.7 (11) | C8—C7—C12—C11 | 4.7 (11) |
| C1—N6—C5—C6 | 177.0 (7) | C18—N3—C21—C22 | 170.7 (6) |
| N6—C5—C6—N5 | 168.7 (6) | Hg1—N3—C21—C22 | 51.3 (6) |
| C4—C5—C6—N5 | −12.7 (11) | O1—C13—N1—N2 | 0.0 (8) |
| C5—C6—N5—C7 | −77.9 (9) | C10—C13—N1—N2 | −179.9 (7) |
| C6—N5—C7—C12 | −169.2 (7) | C14—N2—N1—C13 | −0.4 (8) |
| C6—N5—C7—C8 | 11.5 (11) | C18—C19—C20—C15 | 0.4 (11) |
| N4—Hg1—N3—C18 | −162.2 (4) | C16—C15—C20—C19 | 3.5 (10) |
| Cl1—Hg1—N3—C18 | 52.0 (4) | C14—C15—C20—C19 | −176.2 (6) |
| Cl2—Hg1—N3—C18 | −64.2 (4) | N6—C5—C4—C3 | −0.4 (11) |
| N6$^{i}$—Hg1—N3—C18 | 144.6 (4) | C6—C5—C4—C3 | −179.0 (7) |
| N4—Hg1—N3—C21 | −35.6 (4) | Cl1—Hg1—N4—C22 | 93.9 (5) |
| Cl1—Hg1—N3—C21 | 178.6 (4) | Cl2—Hg1—N4—C22 | −75.3 (5) |
| Cl2—Hg1—N3—C21 | 62.4 (4) | N3—Hg1—N4—C22 | 17.1 (5) |
| N6$^{i}$—Hg1—N3—C21 | −88.8 (5) | N6$^{i}$—Hg1—N4—C22 | 169.6 (5) |
| C14—O1—C13—N1 | 0.3 (8) | Cl1—Hg1—N4—C26 | −86.1 (6) |
| C14—O1—C13—C10 | −179.8 (6) | Cl2—Hg1—N4—C26 | 104.7 (5) |
| C13—O1—C14—N2 | −0.6 (7) | N3—Hg1—N4—C26 | −162.9 (6) |
| C13—O1—C14—C15 | 176.6 (6) | N6$^{i}$—Hg1—N4—C26 | −10.5 (6) |
| C20—C19—C18—C17 | −3.9 (11) | C26—N4—C22—C23 | 3.9 (10) |
| C20—C19—C18—N3 | 173.1 (6) | Hg1—N4—C22—C23 | −176.2 (5) |
| C21—N3—C18—C17 | −28.4 (10) | C26—N4—C22—C21 | −174.5 (6) |
| Hg1—N3—C18—C17 | 84.8 (7) | Hg1—N4—C22—C21 | 5.4 (8) |
| C21—N3—C18—C19 | 154.7 (7) | C24—C23—C22—N4 | −1.9 (11) |
| Hg1—N3—C18—C19 | −92.1 (6) | C24—C23—C22—C21 | 176.4 (7) |
| C12—C11—C10—C9 | −1.6 (11) | N3—C21—C22—N4 | −44.7 (9) |
| C12—C11—C10—C13 | 178.6 (7) | N3—C21—C22—C23 | 136.9 (7) |
| C8—C9—C10—C11 | 2.0 (11) | C15—C16—C17—C18 | 0.3 (11) |
| C8—C9—C10—C13 | −178.2 (6) | C19—C18—C17—C16 | 3.6 (11) |
| N1—C13—C10—C11 | −5.6 (12) | N3—C18—C17—C16 | −173.3 (6) |
| O1—C13—C10—C11 | 174.5 (6) | C5—C4—C3—C2 | 3.3 (12) |
| N1—C13—C10—C9 | 174.6 (8) | C10—C9—C8—C7 | 0.9 (11) |

| | | | |
|---|---|---|---|
| O1—C13—C10—C9 | −5.3 (10) | N5—C7—C8—C9 | 175.1 (7) |
| O1—C14—N2—N1 | 0.6 (8) | C12—C7—C8—C9 | −4.3 (10) |
| C15—C14—N2—N1 | −176.1 (7) | C5—N6—C1—C2 | 0.9 (13) |
| N2—C14—C15—C16 | −2.9 (12) | C26—C25—C24—C23 | 0.9 (13) |
| O1—C14—C15—C16 | −179.4 (6) | C22—C23—C24—C25 | −0.6 (12) |
| N2—C14—C15—C20 | 176.7 (7) | C22—N4—C26—C25 | −3.5 (11) |
| O1—C14—C15—C20 | 0.2 (9) | Hg1—N4—C26—C25 | 176.6 (6) |
| C20—C15—C16—C17 | −3.8 (10) | C24—C25—C26—N4 | 1.1 (12) |
| C14—C15—C16—C17 | 175.8 (7) | C4—C3—C2—C1 | −4.1 (13) |
| C10—C11—C12—C7 | −1.8 (11) | N6—C1—C2—C3 | 2.0 (15) |
| N5—C7—C12—C11 | −174.7 (7) | | |

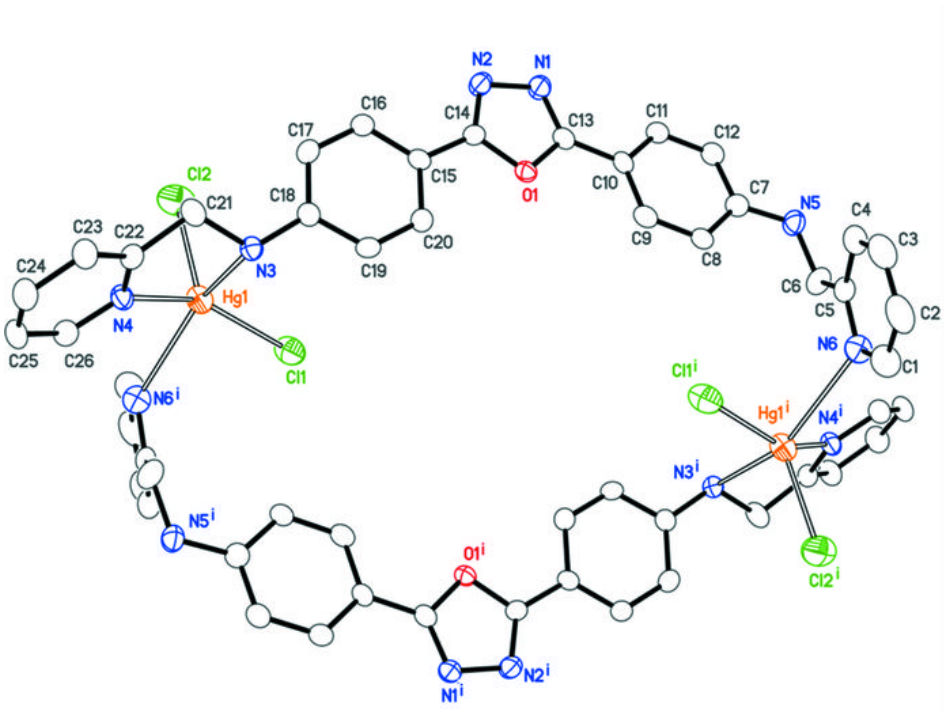
Symmetry codes: (i) −*x*+2, −*y*, −*z*.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···N2$^{ii}$ | 0.91 | 2.36 | 3.191 (8) | 152 |
| N5—H5···Cl1$^{iii}$ | 0.86 | 2.68 | 3.517 (7) | 166 |

Symmetry codes: (ii) *x*+1, *y*, *z*; (iii) −*x*+1, −*y*, −*z*.

**Fig. 1**


N2
N1
C16
C14
C17
C13
C11
C12
Cl2
C15
O1
C10
C7
N5
C18
C21
C4
C23
C22
C20
C9
C3
C24
N3
C19
C8
C6
Hg1
C5
C2
N4
N6
C25
C26
Cl1
C1
Cl1i
N6i
Hg1i
N4i
N3i
N5i
O1i
Cl2i
N2i
N1i