



Crystal structure of dichlorido[*N*¹-phenyl-*N*⁴-[(quinolin-2-yl- κ N)methylidene]benzene-1,4-diamine- κ *N*⁴]mercury(II)

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In the mononuclear title complex, [HgCl₂(C₂₂H₁₇N₃)], synthesized from the quinoline-derived Schiff base *N*¹-phenyl-*N*⁴-[(quinolin-2-yl)methylidene]benzene-1,4-diamine (PQMBD) and HgCl₂, the coordination sphere around the Hg²⁺ atom is distorted tetrahedral, comprising two Cl atoms [Hg—Cl = 2.3487 (14) and 2.4490 (15) Å] and two N atom donors from the PQMBD ligand, *viz.* the quinolyl and the imine N atom [Hg—N = 2.270 (4) and 2.346 (4) Å, respectively]. The dihedral angle between the two benzene rings attached to the amino group is 43.7 (3)°. In the crystal, N—H...Cl and C—H...Cl hydrogen bonds, as well as π – π stacking interactions between one phenyl ring and the pyridine ring of the quinoline moiety of an adjacent molecule [centroid-to-centroid separation = 3.617 (4) Å] are observed, resulting in a three-dimensional network.

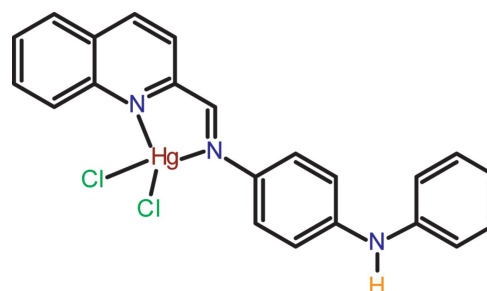
Keywords: crystal structure; Schiff base; mercury(II) complex; N—H...Cl and C—H...Cl hydrogen bonding; π – π stacking interactions.

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1. Related literature

For the hazards of mercury in organisms, see: Mandal *et al.* (2012). For reports of quinolyl derivatives of Schiff bases, see: Motswainyana *et al.* (2013); Das *et al.* (2013); Song *et al.* (2011); Jursic *et al.* (2002). For background to related Schiff base–metal complexes, see: Faizi & Hussain (2014); Faizi *et al.* (2014); Moroz *et al.* (2012). For related Hg-containing structures, see: Marjani *et al.* (2009); Faizi & Sen (2014), and for related Schiff base complexes, see: Penkova *et al.* (2009, 2010);

Strotmeyer *et al.* (2003); Petrusenko *et al.* (1997). The amino group of the title compound is separated from the chelating unit which makes this complex a possible precursor for further functionalization, eventually yielding binuclear compounds as reported by Fritsky *et al.* (1998, 2006) and Kanderl *et al.* (2005).



2. Experimental

2.1. Crystal data

[HgCl ₂ (C ₂₂ H ₁₇ N ₃)]	<i>V</i> = 4111.4 (12) Å ³
<i>M_r</i> = 594.88	<i>Z</i> = 8
Monoclinic, <i>C</i> 2/ <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 29.265 (5) Å	μ = 7.76 mm ⁻¹
<i>b</i> = 7.5671 (13) Å	<i>T</i> = 100 K
<i>c</i> = 18.811 (3) Å	0.18 × 0.15 × 0.10 mm
β = 99.271 (7)°	

2.2. Data collection

Bruker SMART APEX CCD diffractometer	22545 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2003)	5133 independent reflections
<i>T</i> _{min} = 0.336, <i>T</i> _{max} = 0.511	3182 reflections with <i>I</i> > 2σ(<i>I</i>)
	<i>R</i> _{int} = 0.059

2.3. Refinement

<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.038	253 parameters
<i>wR</i> (<i>F</i> ²) = 0.087	H-atom parameters constrained
<i>S</i> = 1.00	$\Delta\rho_{\max}$ = 0.99 e Å ⁻³
5133 reflections	$\Delta\rho_{\min}$ = -0.56 e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3A...Cl2 ⁱ	0.86	2.58	3.363 (4)	151
C10—H10...Cl2 ⁱⁱ	0.93	2.81	3.679 (7)	157
C20—H20...Cl1 ⁱⁱⁱ	0.93	2.80	3.692 (11)	160

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

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2015); molecular graphics: DIAMOND (Brandenburg & Putz, 2006) and Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5117).

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Acta Cryst. (2015). E71, m46–m47 [doi:10.1107/S2056989015001620]

Crystal structure of dichlorido{*N*¹-phenyl-*N*⁴-[(quinolin-2-yl- κ N)methylidene]benzene-1,4-diamine- κ N⁴}mercury(II)

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S1. Experimental

The iminoquinolyl ligand *N*¹-phenyl-*N*⁴-[(quinolin-2-yl)methylidene]benzene-1,4-diamine (PQMBD) was prepared by reacting 2-quinolinecarboxaldehyde (0.085 g, 0.54 mmol) with one equivalent of *N*-phenyl-*p*-phenylenediamine (0.100 g, 0.54 mmol) and was obtained in 88% yield (0.15 g). The obtained compound was characterized by FT-IR, NMR and ESI-mass spectroscopy: IR (KBr, ν / cm^{-1}): 3417, 3052 (C-H arom), 1620 (C=N), 1515, 1313, 843, 756. ¹H NMR (400 MHz, CDCl₃, δ /p.p.m.): 8.85 (1H, s), 8.37 (1H, d), 8.23 (1H, d), 8.16 (1H, d), 7.86 (1H, d), 7.75 (1H, t), 7.58 (1H, t), 7.40 (2H, d), 7.30 (1H, t), 7.13 (5H, m), 6.51 (1H, t). ESI-MS *m/z*: 324 (M+1).

PQMBD (0.10 g, 0.31 mmol), mercury(II) chloride (0.08 g, 0.31 mmol) and ethanol (5 ml) were stirred vigorously for 1 h, after which the precipitate was filtered off and redissolved in dimethylformamide. Crystals of the title complex suitable for X-ray analysis was obtained within 3 days by slow evaporation of the DMF solvent.

S2. Refinement

The N-bound H-atom was located in a difference Fourier maps, and the positions restrained to N—H = 0.86 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. All other H-atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

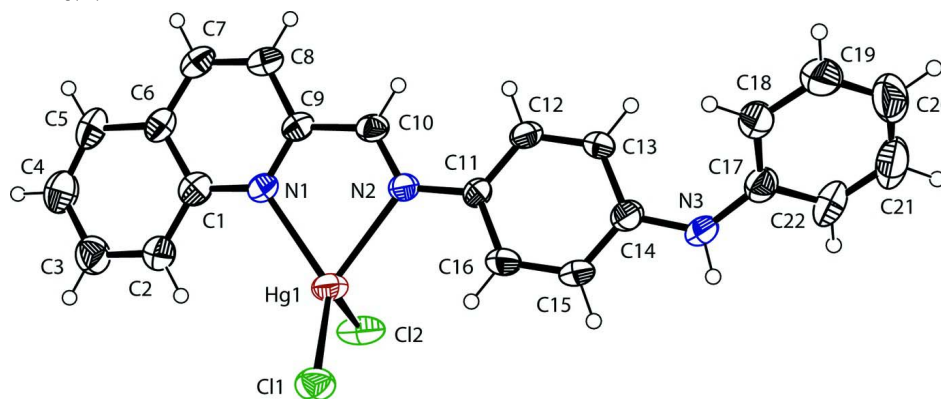


Figure 1

The molecular structure and the atom-numbering scheme of the title complex, with non-H atoms drawn as displacement ellipsoids at the 40% probability level.

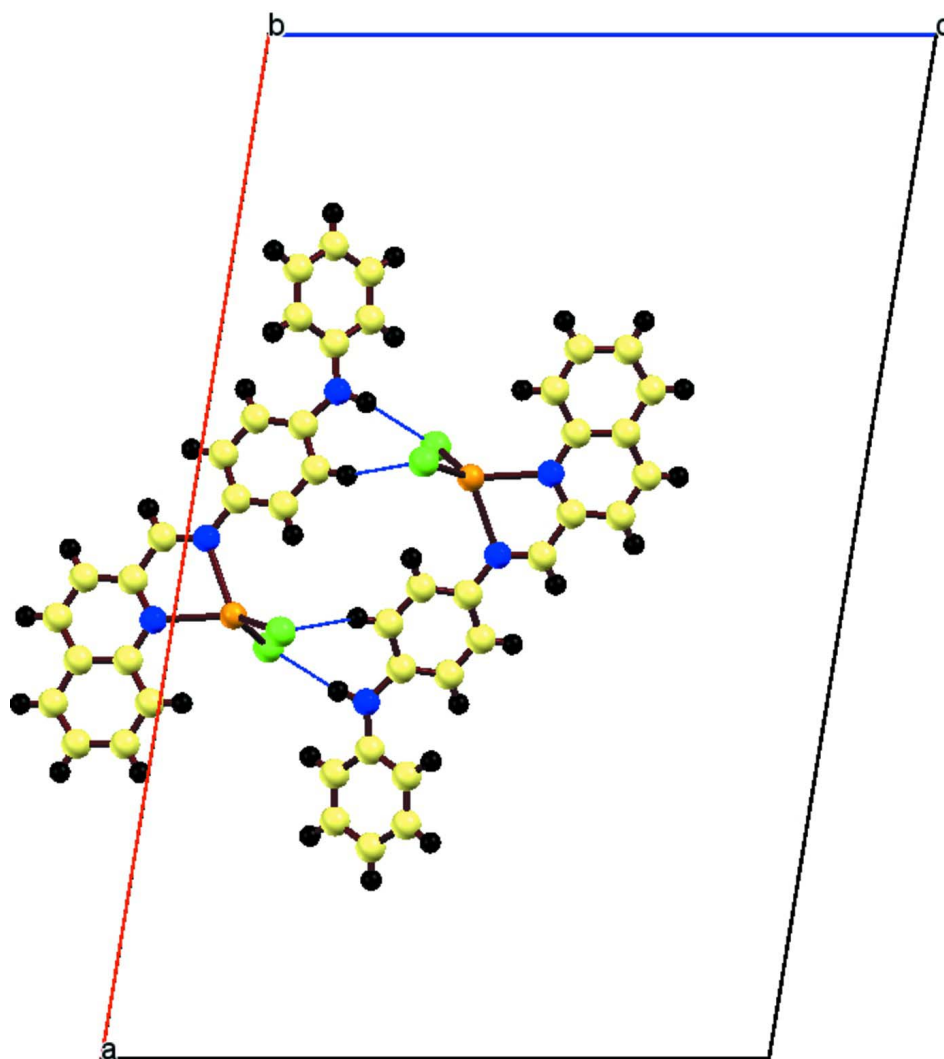


Figure 2

N—H \cdots Cl hydrogen bonds between adjacent molecules as viewed along [010].

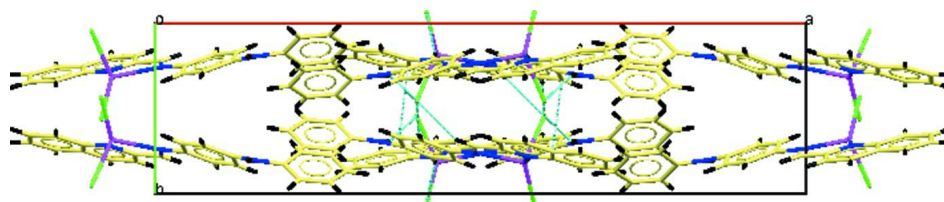


Figure 3

The packing of molecules in the title compound, showing intermolecular interactions as dashed lines.

Dichlorido[*N*¹-phenyl-*N*⁴-[(quinolin-2-yl- κ N)methylidene]benzene-1,4-diamine- κ N⁴]mercury(II)

Crystal data

[HgCl₂(C₂₂H₁₇N₃)]

M_r = 594.88

Monoclinic, *C*2/*c*

Hall symbol: -C 2yc

a = 29.265 (5) Å

b = 7.5671 (13) Å

$c = 18.811 (3) \text{ \AA}$
 $\beta = 99.271 (7)^\circ$
 $V = 4111.4 (12) \text{ \AA}^3$
 $Z = 8$
 $F(000) = 2272$
 $D_x = 1.922 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 7479 reflections
 $\theta = 2.8\text{--}24.6^\circ$
 $\mu = 7.76 \text{ mm}^{-1}$
 $T = 100 \text{ K}$
 Block, colourless
 $0.18 \times 0.15 \times 0.10 \text{ mm}$

Data collection

Bruker SMART APEX CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2003)
 $T_{\min} = 0.336, T_{\max} = 0.511$

22545 measured reflections
 5133 independent reflections
 3182 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.059$
 $\theta_{\max} = 28.4^\circ, \theta_{\min} = 2.8^\circ$
 $h = -38 \rightarrow 38$
 $k = -10 \rightarrow 9$
 $l = -25 \rightarrow 25$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.087$
 $S = 1.00$
 5133 reflections
 253 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
 $w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 1.5818P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.99 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.56 \text{ e \AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.42861 (15)	0.2191 (5)	0.5298 (2)	0.0396 (10)
N2	0.50810 (14)	0.2420 (6)	0.4703 (2)	0.0389 (10)
N3	0.65162 (17)	0.3036 (7)	0.3095 (2)	0.0603 (14)
H3A	0.6410	0.3037	0.2641	0.072*
C11	0.54666 (17)	0.2526 (7)	0.4348 (2)	0.0373 (12)
C10	0.50915 (18)	0.2791 (7)	0.5369 (3)	0.0422 (13)
H10	0.5369	0.3144	0.5644	0.051*
C17	0.6984 (2)	0.3274 (7)	0.3265 (3)	0.0507 (14)
C12	0.59004 (18)	0.3146 (7)	0.4656 (2)	0.0431 (13)
H12	0.5952	0.3467	0.5140	0.052*

C1	0.3891 (2)	0.2106 (7)	0.5581 (3)	0.0475 (14)
C16	0.5400 (2)	0.2029 (7)	0.3633 (3)	0.0509 (15)
H16	0.5115	0.1588	0.3418	0.061*
C9	0.46781 (18)	0.2673 (7)	0.5702 (3)	0.0392 (12)
C15	0.5752 (2)	0.2181 (8)	0.3236 (3)	0.0572 (16)
H15	0.5697	0.1861	0.2753	0.069*
C13	0.62510 (18)	0.3293 (7)	0.4263 (3)	0.0447 (13)
H13	0.6537	0.3729	0.4481	0.054*
C6	0.3892 (2)	0.2468 (8)	0.6324 (3)	0.0479 (14)
C7	0.4309 (2)	0.2985 (7)	0.6737 (3)	0.0543 (15)
H7	0.4319	0.3271	0.7220	0.065*
C8	0.4699 (2)	0.3076 (8)	0.6443 (3)	0.0559 (16)
H8	0.4978	0.3400	0.6722	0.067*
C14	0.61872 (19)	0.2795 (7)	0.3533 (3)	0.0469 (14)
Hg1	0.432753 (8)	0.18401 (3)	0.411137 (10)	0.05198 (10)
Cl2	0.40186 (6)	0.4552 (2)	0.35050 (7)	0.0702 (5)
Cl1	0.41693 (5)	-0.0647 (2)	0.33652 (7)	0.0593 (4)
C2	0.3473 (2)	0.1623 (7)	0.5149 (3)	0.0553 (15)
H2	0.3471	0.1343	0.4667	0.066*
C4	0.3076 (2)	0.1986 (8)	0.6148 (4)	0.0699 (19)
H4	0.2798	0.1988	0.6327	0.084*
C3	0.3070 (2)	0.1557 (8)	0.5420 (3)	0.0656 (18)
H3	0.2795	0.1233	0.5129	0.079*
C5	0.3471 (2)	0.2397 (9)	0.6601 (3)	0.0624 (17)
H5	0.3465	0.2628	0.7085	0.075*
C18	0.7240 (2)	0.2570 (9)	0.3877 (3)	0.0632 (17)
H18	0.7096	0.1968	0.4210	0.076*
C19	0.7715 (3)	0.2770 (13)	0.3989 (4)	0.098 (3)
H19	0.7890	0.2272	0.4396	0.118*
C22	0.7218 (3)	0.4179 (9)	0.2794 (3)	0.0700 (19)
H22	0.7050	0.4696	0.2384	0.084*
C21	0.7680 (3)	0.4324 (11)	0.2915 (5)	0.091 (3)
H21	0.7826	0.4886	0.2573	0.110*
C20	0.7937 (3)	0.3686 (15)	0.3512 (5)	0.115 (4)
H20	0.8256	0.3856	0.3602	0.138*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.046 (3)	0.040 (3)	0.033 (2)	0.002 (2)	0.0060 (19)	0.0038 (18)
N2	0.043 (3)	0.040 (2)	0.033 (2)	-0.003 (2)	0.0032 (18)	-0.0005 (18)
N3	0.050 (3)	0.101 (4)	0.030 (2)	0.000 (3)	0.007 (2)	0.001 (2)
C11	0.039 (3)	0.041 (3)	0.034 (3)	0.001 (2)	0.011 (2)	-0.006 (2)
C10	0.045 (3)	0.044 (3)	0.034 (3)	0.003 (2)	-0.002 (2)	0.007 (2)
C17	0.053 (4)	0.056 (4)	0.046 (3)	0.003 (3)	0.015 (3)	-0.004 (3)
C12	0.050 (3)	0.050 (3)	0.029 (2)	-0.002 (3)	0.003 (2)	-0.002 (2)
C1	0.055 (4)	0.040 (3)	0.047 (3)	0.009 (3)	0.008 (3)	0.008 (2)
C16	0.048 (3)	0.064 (4)	0.039 (3)	-0.007 (3)	0.000 (2)	-0.014 (3)

C9	0.048 (3)	0.038 (3)	0.033 (3)	0.007 (2)	0.007 (2)	0.000 (2)
C15	0.055 (4)	0.085 (5)	0.030 (3)	-0.009 (3)	0.002 (3)	-0.013 (3)
C13	0.037 (3)	0.058 (4)	0.037 (3)	-0.005 (3)	0.000 (2)	-0.007 (3)
C6	0.057 (4)	0.048 (3)	0.042 (3)	0.006 (3)	0.015 (3)	0.009 (3)
C7	0.070 (4)	0.061 (4)	0.034 (3)	0.002 (3)	0.015 (3)	-0.003 (3)
C8	0.060 (4)	0.071 (4)	0.034 (3)	-0.001 (3)	0.000 (3)	0.003 (3)
C14	0.046 (3)	0.058 (4)	0.037 (3)	0.005 (3)	0.007 (2)	0.000 (3)
Hg1	0.05736 (16)	0.05833 (16)	0.03782 (13)	-0.00317 (12)	0.00037 (9)	-0.00853 (11)
Cl2	0.1027 (13)	0.0504 (9)	0.0476 (8)	0.0032 (9)	-0.0178 (8)	-0.0030 (7)
Cl1	0.0732 (10)	0.0508 (9)	0.0524 (8)	-0.0083 (8)	0.0053 (7)	-0.0122 (7)
C2	0.052 (4)	0.064 (4)	0.052 (3)	-0.002 (3)	0.012 (3)	0.000 (3)
C4	0.066 (4)	0.078 (5)	0.073 (5)	0.007 (4)	0.032 (4)	-0.001 (4)
C3	0.049 (4)	0.078 (5)	0.070 (4)	0.003 (3)	0.011 (3)	0.007 (4)
C5	0.069 (5)	0.068 (4)	0.058 (4)	0.009 (4)	0.034 (4)	0.010 (3)
C18	0.051 (4)	0.087 (5)	0.052 (4)	0.003 (4)	0.010 (3)	0.009 (3)
C19	0.057 (5)	0.174 (9)	0.062 (4)	0.006 (5)	0.006 (4)	-0.022 (5)
C22	0.082 (5)	0.076 (5)	0.061 (4)	0.009 (4)	0.040 (4)	0.008 (4)
C21	0.094 (6)	0.097 (6)	0.098 (6)	-0.031 (5)	0.061 (5)	-0.025 (5)
C20	0.069 (6)	0.179 (10)	0.107 (7)	-0.036 (6)	0.045 (5)	-0.069 (7)

Geometric parameters (Å, °)

N1—C9	1.322 (6)	C13—H13	0.9300
N1—C1	1.349 (7)	C6—C7	1.394 (8)
N1—Hg1	2.270 (4)	C6—C5	1.413 (8)
N2—C10	1.279 (6)	C7—C8	1.347 (8)
N2—C11	1.402 (6)	C7—H7	0.9300
N2—Hg1	2.346 (4)	C8—H8	0.9300
N3—C17	1.367 (7)	Hg1—Cl1	2.3487 (14)
N3—C14	1.377 (7)	Hg1—Cl2	2.4490 (15)
N3—H3A	0.8600	C2—C3	1.359 (8)
C11—C16	1.380 (6)	C2—H2	0.9300
C11—C12	1.389 (7)	C4—C5	1.358 (9)
C10—C9	1.453 (7)	C4—C3	1.403 (8)
C10—H10	0.9300	C4—H4	0.9300
C17—C22	1.385 (8)	C3—H3	0.9300
C17—C18	1.375 (8)	C5—H5	0.9300
C12—C13	1.362 (7)	C18—C19	1.381 (9)
C12—H12	0.9300	C18—H18	0.9300
C1—C2	1.404 (8)	C19—C20	1.375 (12)
C1—C6	1.425 (7)	C19—H19	0.9300
C16—C15	1.370 (8)	C22—C21	1.340 (9)
C16—H16	0.9300	C22—H22	0.9300
C9—C8	1.418 (7)	C21—C20	1.338 (11)
C15—C14	1.385 (7)	C21—H21	0.9300
C15—H15	0.9300	C20—H20	0.9300
C13—C14	1.409 (7)		

C9—N1—C1	120.4 (4)	C6—C7—H7	119.7
C9—N1—Hg1	114.8 (3)	C7—C8—C9	119.1 (5)
C1—N1—Hg1	124.5 (4)	C7—C8—H8	120.4
C10—N2—C11	124.0 (4)	C9—C8—H8	120.4
C10—N2—Hg1	112.2 (3)	C15—C14—N3	119.3 (5)
C11—N2—Hg1	123.5 (3)	C15—C14—C13	116.8 (5)
C17—N3—C14	130.3 (5)	N3—C14—C13	123.6 (5)
C17—N3—H3A	114.8	N1—Hg1—N2	72.96 (15)
C14—N3—H3A	114.8	N1—Hg1—C11	130.14 (11)
C16—C11—C12	118.3 (5)	N2—Hg1—C11	120.86 (11)
C16—C11—N2	116.8 (5)	N1—Hg1—C12	106.60 (11)
C12—C11—N2	124.9 (4)	N2—Hg1—C12	108.21 (11)
N2—C10—C9	121.3 (5)	C11—Hg1—C12	111.75 (5)
N2—C10—H10	119.4	C3—C2—C1	121.4 (6)
C9—C10—H10	119.4	C3—C2—H2	119.3
N3—C17—C22	119.6 (5)	C1—C2—H2	119.3
N3—C17—C18	122.4 (5)	C5—C4—C3	122.7 (6)
C22—C17—C18	118.0 (6)	C5—C4—H4	118.7
C13—C12—C11	121.2 (4)	C3—C4—H4	118.7
C13—C12—H12	119.4	C2—C3—C4	118.9 (6)
C11—C12—H12	119.4	C2—C3—H3	120.6
N1—C1—C2	120.5 (5)	C4—C3—H3	120.6
N1—C1—C6	120.8 (5)	C4—C5—C6	118.8 (6)
C2—C1—C6	118.7 (5)	C4—C5—H5	120.6
C15—C16—C11	120.5 (5)	C6—C5—H5	120.6
C15—C16—H16	119.7	C19—C18—C17	119.0 (6)
C11—C16—H16	119.7	C19—C18—H18	120.5
N1—C9—C8	121.4 (5)	C17—C18—H18	120.5
N1—C9—C10	118.3 (4)	C18—C19—C20	121.7 (8)
C8—C9—C10	120.3 (5)	C18—C19—H19	119.2
C16—C15—C14	122.1 (5)	C20—C19—H19	119.2
C16—C15—H15	118.9	C21—C22—C17	121.4 (7)
C14—C15—H15	118.9	C21—C22—H22	119.3
C12—C13—C14	121.0 (5)	C17—C22—H22	119.3
C12—C13—H13	119.5	C22—C21—C20	121.9 (7)
C14—C13—H13	119.5	C22—C21—H21	119.0
C7—C6—C5	122.9 (5)	C20—C21—H21	119.0
C7—C6—C1	117.6 (5)	C21—C20—C19	118.0 (8)
C5—C6—C1	119.4 (6)	C21—C20—H20	121.0
C8—C7—C6	120.6 (5)	C19—C20—H20	121.0
C8—C7—H7	119.7		
C10—N2—C11—C16	178.2 (5)	C16—C15—C14—N3	-175.4 (6)
Hg1—N2—C11—C16	-8.8 (7)	C16—C15—C14—C13	-1.1 (9)
C10—N2—C11—C12	-4.2 (8)	C17—N3—C14—C15	-165.2 (6)
Hg1—N2—C11—C12	168.9 (4)	C17—N3—C14—C13	20.9 (10)
C11—N2—C10—C9	179.3 (5)	C12—C13—C14—C15	0.9 (8)
Hg1—N2—C10—C9	5.6 (6)	C12—C13—C14—N3	174.9 (5)

C14—N3—C17—C22	-153.7 (6)	C9—N1—Hg1—N2	5.3 (3)
C14—N3—C17—C18	29.6 (10)	C1—N1—Hg1—N2	178.8 (4)
C16—C11—C12—C13	1.1 (8)	C9—N1—Hg1—C11	121.6 (3)
N2—C11—C12—C13	-176.5 (5)	C1—N1—Hg1—C11	-64.9 (4)
C9—N1—C1—C2	178.9 (5)	C9—N1—Hg1—C12	-99.2 (3)
Hg1—N1—C1—C2	5.8 (7)	C1—N1—Hg1—C12	74.3 (4)
C9—N1—C1—C6	-2.3 (8)	C10—N2—Hg1—N1	-5.6 (3)
Hg1—N1—C1—C6	-175.5 (4)	C11—N2—Hg1—N1	-179.4 (4)
C12—C11—C16—C15	-1.3 (8)	C10—N2—Hg1—C11	-132.7 (3)
N2—C11—C16—C15	176.6 (5)	C11—N2—Hg1—C11	53.5 (4)
C1—N1—C9—C8	1.3 (7)	C10—N2—Hg1—C12	96.7 (4)
Hg1—N1—C9—C8	175.1 (4)	C11—N2—Hg1—C12	-77.1 (4)
C1—N1—C9—C10	-178.3 (5)	N1—C1—C2—C3	-178.9 (5)
Hg1—N1—C9—C10	-4.6 (6)	C6—C1—C2—C3	2.3 (8)
N2—C10—C9—N1	-0.9 (8)	C1—C2—C3—C4	0.1 (9)
N2—C10—C9—C8	179.5 (5)	C5—C4—C3—C2	-2.7 (10)
C11—C16—C15—C14	1.3 (10)	C3—C4—C5—C6	2.7 (10)
C11—C12—C13—C14	-1.0 (8)	C7—C6—C5—C4	175.9 (6)
N1—C1—C6—C7	2.8 (8)	C1—C6—C5—C4	-0.1 (9)
C2—C1—C6—C7	-178.5 (5)	N3—C17—C18—C19	175.8 (6)
N1—C1—C6—C5	178.9 (5)	C22—C17—C18—C19	-0.9 (10)
C2—C1—C6—C5	-2.3 (8)	C17—C18—C19—C20	1.4 (12)
C5—C6—C7—C8	-178.2 (6)	N3—C17—C22—C21	-174.9 (6)
C1—C6—C7—C8	-2.2 (9)	C18—C17—C22—C21	1.9 (10)
C6—C7—C8—C9	1.3 (9)	C17—C22—C21—C20	-3.5 (13)
N1—C9—C8—C7	-0.8 (8)	C22—C21—C20—C19	3.8 (14)
C10—C9—C8—C7	178.9 (5)	C18—C19—C20—C21	-2.8 (14)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3 <i>A</i> ...C12 ⁱ	0.86	2.58	3.363 (4)	151
C10—H10...C12 ⁱⁱ	0.93	2.81	3.679 (7)	157
C20—H20...C11 ⁱⁱⁱ	0.93	2.80	3.692 (11)	160

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