Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Di-μ-chlorido-bis({2-[(4-bromophenyl)-iminomethyl]pyridine-κ^2N,N'}chloridomercury(II))

Ali Mahmoudi,[a]* Saeed Dehghanpour,[b] Mehdi Khalaj[c] and Shabnam Pakravan[a]

[a]Department of Chemistry, Islamic Azad University, Karaj Branch, Karaj, Iran, [b]Department of Chemistry, Alzahra University, PO Box 1993891176, Vanak, Tehran, Iran, and [c]Department of Chemistry, Islamic Azad University, Buinzahra Branch, Qazvin, Iran
Correspondence e-mail: Mahmoudi_Ali@yahoo.com

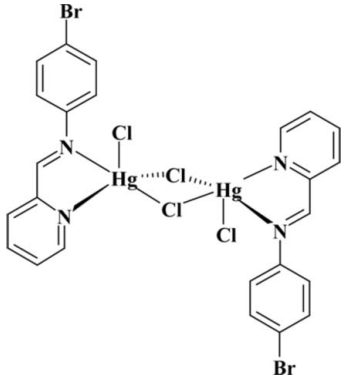
Received 11 June 2009; accepted 2 July 2009

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.019; wR factor = 0.041; data-to-parameter ratio = 24.8.

The unique Hg^{II} ion in the title centrosymmetric dinuclear complex, $[Hg_2Cl_4(C_{12}H_9BrN_2)_2]$, is in a distorted trigonal–bipyramidal coordination environment formed by the bis-chelating *N*-heterocyclic ligand, two bridging Cl atoms and one terminal Cl atom. One of the bridging Hg—Cl bonds is significantly longer than the other.

Related literature

For background information on diimine complexes, see: Dehghanpour & Mahmoudi (2007); Dehghanpour, Mahmoudi, Khalaj & Salmanpour (2007). For related crystal structures, see: Mahmoudi *et al.* (2009); Dehghanpour, Mahmoudi, Khalaj, Salmanpour & Adib (2007).



Experimental

Crystal data

$[Hg_2Cl_4(C_{12}H_9BrN_2)_2]$
M_r = 1065.22
Monoclinic, $P2_1/n$
a = 7.6697 (2) Å
b = 15.0247 (4) Å
c = 12.2129 (4) Å
β = 96.738 (1)°
V = 1397.63 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 14.24 mm^{-1}
T = 100 K
0.10 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.280, T_{max} = 0.491
17922 measured reflections
4047 independent reflections
3636 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.041
S = 1.01
4047 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −1.15 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg1—N2	2.318 (2)	Hg1—Cl2	2.4941 (7)
Hg1—Cl1	2.3799 (7)	Hg1—Cl2^{i}	2.8799 (6)
Hg1—N1	2.472 (2)		
N2—Hg1—Cl1	129.00 (6)	N2—Hg1—Cl2^{i}	88.36 (6)
N2—Hg1—N1	70.58 (7)	Cl1—Hg1—Cl2^{i}	90.07 (2)
Cl1—Hg1—N1	107.12 (5)	N1—Hg1—Cl2^{i}	158.28 (5)
N2—Hg1—Cl2	102.20 (6)	Cl2—Hg1—Cl2^{i}	88.926 (19)
Cl1—Hg1—Cl2	128.74 (3)	Hg1—Cl2—Hg1^{i}	91.074 (19)
N1—Hg1—Cl2	90.35 (5)		

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL*.

AM acknowledges the Islamic Azad University Research Council for partial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2844).

References

Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dehghanpour, S. & Mahmoudi, A. (2007). *Synth. React. Inorg. Met. Org. Chem.* **37**, 35–40.
Dehghanpour, S., Mahmoudi, A., Khalaj, M. & Salmanpour, S. (2007). *Acta Cryst.* E**63**, m2840.
Dehghanpour, S., Mahmoudi, A., Khalaj, M., Salmanpour, S. & Adib, M. (2007). *Acta Cryst.* E**63**, m2841.
Mahmoudi, A., Khalaj, M., Gao, S., Ng, S. W. & Mohammadgholiha, M. (2009). *Acta Cryst.* E**65**, m555.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2009). E**65**, m889 [doi:10.1107/S1600536809025641]

Di-μ-chlorido-bis({2-[(4-bromophenyl)iminomethyl]pyridine-κ^2N,N'}chloridomercury(II))

Ali Mahmoudi, Saeed Dehghanpour, Mehdi Khalaj and Shabnam Pakravan

S1. Comment

In our ongoing studies on the synthesis, structural and spectroscopic characterization of transition metal complexes with diimine ligands (Dehghanpour & Mahmoudi, 2007; Dehghanpour, Mahmoudi, Khalaj, Salmanpour & Adib (2007), we report herein the crystal structure of the title complex. The title compound was prepared by the reaction of $HgCl_2$ with (4-bromophenyl)pyridin-2-ylmethyleneamine.

The molecluar structure of the title complex (I) is shown in (Fig. 1). The unique Hg^{II} ion in is in a distorted trigonal-bipyramidal coordination environment formed by a bis-chelating ligand, two bridging Cl atoms and one terminal Cl atom. One of the bridging Hg-Cl bonds is significantly longer than the other.

S2. Experimental

The title complex was prepared by the reaction of $HgCl_2$ and (4-bromophenyl)pyridin-2-ylmethyleneamine (molar ratio 1:1) in acetonitrile at room temperature. The solution was then concentrated under vacuum, and diffusion of diethyl ether vapor into the concentrated solution gave yellow crystals of (I) in 69% yield. Calc. for $C_{12}H_9BrCl_2HgN_2$: C 27.06, H 1.70, N 5.26%; found: C 27.01, H 1.72, N 5.20%.

S3. Refinement

The H atom were placed in calcluated positions with C-H = 0.95Å and refined in a a riding-model approximation with U_{iso}(H) = 1.2 U_{eq}(C).

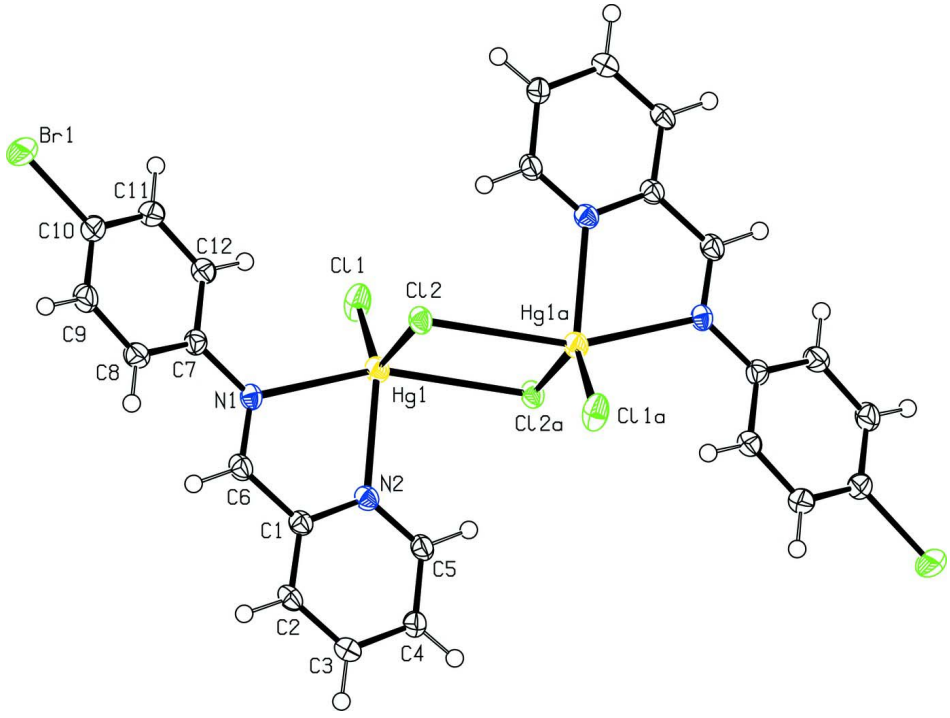


Figure 1

The molecular structure od the title complex, with displacement ellipsoids drawn at the 50% probability level. H atoms are represented as spheres of arbitrary radius [symmetry code: (a) -x, -y+1, -z].

Di-μ-chlorido-bis({2-[(4-bromophenyl)iminomethyl]pyridine- κ^2N,N'}chloridomercury(II))

Crystal data

$[Hg_2Cl_4(C_{12}H_9BrN_2)_2]$
M_r = 1065.22
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 7.6697 (2) Å
b = 15.0247 (4) Å
c = 12.2129 (4) Å
β = 96.738 (1)°
V = 1397.63 (7) Å^3
Z = 2
$F(000)$ = 976
D_x = 2.531 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8129 reflections
θ = 2.2–29.7°
μ = 14.24 mm^{-1}
T = 100 K
Prism, yellow
0.10 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.280, T_{max} = 0.491
17922 measured reflections
4047 independent reflections
3636 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 30.0°, θ_{min} = 2.2°
h = −10→10
k = −21→20
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.041$
$S = 1.01$
4047 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.015P)^2 + 1.35P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.97$ e Å^{-3}
$\Delta\rho_{min} = -1.15$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.170956 (13)	0.446982 (7)	0.108289 (9)	0.02080 (3)
Br1	0.86964 (5)	0.10383 (2)	−0.01114 (3)	0.04340 (9)
Cl1	0.42148 (9)	0.53787 (4)	0.15929 (7)	0.03126 (16)
Cl2	0.04621 (9)	0.39647 (4)	−0.07921 (5)	0.02143 (12)
N1	0.2551 (3)	0.29234 (14)	0.15931 (18)	0.0183 (4)
N2	−0.0272 (3)	0.38863 (15)	0.21855 (18)	0.0192 (4)
C1	−0.0010 (3)	0.30362 (17)	0.2535 (2)	0.0192 (5)
C2	−0.1169 (4)	0.26078 (18)	0.3146 (2)	0.0207 (5)
H2A	−0.0974	0.2006	0.3366	0.025*
C3	−0.2618 (4)	0.30668 (18)	0.3433 (2)	0.0219 (5)
H3A	−0.3420	0.2788	0.3861	0.026*
C4	−0.2871 (4)	0.39390 (18)	0.3083 (2)	0.0218 (5)
H4A	−0.3842	0.4272	0.3275	0.026*
C5	−0.1679 (4)	0.43198 (18)	0.2445 (2)	0.0209 (5)
H5A	−0.1878	0.4911	0.2184	0.025*
C6	0.1522 (4)	0.25556 (18)	0.2214 (2)	0.0212 (5)
H6A	0.1752	0.1965	0.2471	0.025*
C7	0.3966 (3)	0.24488 (18)	0.1221 (2)	0.0194 (5)
C8	0.4078 (4)	0.15213 (19)	0.1228 (2)	0.0239 (5)
H8A	0.3193	0.1175	0.1508	0.029*
C9	0.5489 (4)	0.1107 (2)	0.0824 (2)	0.0270 (6)
H9A	0.5572	0.0476	0.0820	0.032*
C10	0.6778 (4)	0.1622 (2)	0.0425 (2)	0.0260 (6)
C11	0.6691 (4)	0.25420 (19)	0.0398 (2)	0.0230 (5)
H11A	0.7587	0.2884	0.0122	0.028*

C12	0.5255 (3)	0.29538 (18)	0.0786 (2)	0.0206 (5)
H12A	0.5151	0.3584	0.0756	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.02163 (5)	0.01490 (5)	0.02590 (6)	−0.00157 (4)	0.00290 (4)	0.00198 (4)
Br1	0.04489 (19)	0.03626 (17)	0.0548 (2)	0.01823 (15)	0.03004 (17)	0.01083 (16)
Cl1	0.0233 (3)	0.0157 (3)	0.0531 (5)	−0.0016 (2)	−0.0027 (3)	−0.0017 (3)
Cl2	0.0274 (3)	0.0159 (3)	0.0210 (3)	0.0040 (2)	0.0029 (2)	0.0000 (2)
N1	0.0210 (10)	0.0147 (10)	0.0187 (10)	0.0018 (8)	0.0009 (8)	−0.0002 (8)
N2	0.0221 (10)	0.0163 (10)	0.0194 (10)	−0.0008 (8)	0.0028 (8)	0.0005 (8)
C1	0.0227 (12)	0.0171 (12)	0.0179 (12)	0.0002 (9)	0.0025 (10)	0.0003 (9)
C2	0.0278 (13)	0.0152 (12)	0.0189 (12)	−0.0014 (10)	0.0027 (10)	0.0027 (9)
C3	0.0248 (13)	0.0226 (13)	0.0188 (12)	−0.0017 (10)	0.0043 (10)	0.0028 (10)
C4	0.0234 (12)	0.0201 (12)	0.0221 (13)	0.0042 (10)	0.0034 (10)	0.0019 (10)
C5	0.0256 (13)	0.0170 (12)	0.0203 (12)	0.0028 (10)	0.0030 (10)	0.0031 (10)
C6	0.0271 (13)	0.0162 (12)	0.0202 (12)	0.0018 (10)	0.0030 (10)	0.0014 (10)
C7	0.0201 (11)	0.0202 (12)	0.0175 (12)	0.0025 (10)	0.0004 (9)	0.0005 (10)
C8	0.0281 (13)	0.0203 (13)	0.0244 (13)	0.0015 (11)	0.0071 (11)	0.0030 (11)
C9	0.0365 (15)	0.0199 (13)	0.0258 (14)	0.0089 (11)	0.0086 (12)	0.0027 (11)
C10	0.0283 (13)	0.0273 (14)	0.0236 (13)	0.0088 (11)	0.0077 (11)	0.0036 (11)
C11	0.0231 (12)	0.0252 (13)	0.0209 (12)	0.0008 (11)	0.0038 (10)	0.0014 (11)
C12	0.0225 (12)	0.0204 (12)	0.0187 (12)	0.0003 (10)	0.0017 (10)	0.0011 (10)

Geometric parameters (Å, º)

Hg1—N2	2.318 (2)	C3—H3A	0.9500
Hg1—Cl1	2.3799 (7)	C4—C5	1.392 (4)
Hg1—N1	2.472 (2)	C4—H4A	0.9500
Hg1—Cl2	2.4941 (7)	C5—H5A	0.9500
Hg1—Cl2^{i}	2.8799 (6)	C6—H6A	0.9500
Br1—C10	1.894 (3)	C7—C8	1.396 (4)
Cl2—Hg1^{i}	2.8799 (6)	C7—C12	1.399 (4)
N1—C6	1.282 (3)	C8—C9	1.389 (4)
N1—C7	1.418 (3)	C8—H8A	0.9500
N2—C5	1.330 (3)	C9—C10	1.388 (4)
N2—C1	1.354 (3)	C9—H9A	0.9500
C1—C2	1.384 (4)	C10—C11	1.385 (4)
C1—C6	1.471 (4)	C11—C12	1.394 (4)
C2—C3	1.387 (4)	C11—H11A	0.9500
C2—H2A	0.9500	C12—H12A	0.9500
C3—C4	1.385 (4)		
N2—Hg1—Cl1	129.00 (6)	C3—C4—H4A	120.5
N2—Hg1—N1	70.58 (7)	C5—C4—H4A	120.5
Cl1—Hg1—N1	107.12 (5)	N2—C5—C4	122.4 (2)
N2—Hg1—Cl2	102.20 (6)	N2—C5—H5A	118.8

Cl1—Hg1—Cl2	128.74 (3)	C4—C5—H5A	118.8
N1—Hg1—Cl2	90.35 (5)	N1—C6—C1	120.8 (2)
N2—Hg1—Cl2^{i}	88.36 (6)	N1—C6—H6A	119.6
Cl1—Hg1—Cl2^{i}	90.07 (2)	C1—C6—H6A	119.6
N1—Hg1—Cl2^{i}	158.28 (5)	C8—C7—C12	119.9 (2)
Cl2—Hg1—Cl2^{i}	88.926 (19)	C8—C7—N1	123.3 (2)
Hg1—Cl2—Hg1^{i}	91.074 (19)	C12—C7—N1	116.8 (2)
C6—N1—C7	121.4 (2)	C9—C8—C7	119.7 (3)
C6—N1—Hg1	113.18 (17)	C9—C8—H8A	120.2
C7—N1—Hg1	125.39 (17)	C7—C8—H8A	120.2
C5—N2—C1	118.8 (2)	C10—C9—C8	119.4 (3)
C5—N2—Hg1	123.96 (18)	C10—C9—H9A	120.3
C1—N2—Hg1	117.19 (17)	C8—C9—H9A	120.3
N2—C1—C2	121.8 (2)	C11—C10—C9	122.1 (3)
N2—C1—C6	118.2 (2)	C11—C10—Br1	119.4 (2)
C2—C1—C6	119.9 (2)	C9—C10—Br1	118.5 (2)
C1—C2—C3	119.3 (2)	C10—C11—C12	118.2 (3)
C1—C2—H2A	120.4	C10—C11—H11A	120.9
C3—C2—H2A	120.4	C12—C11—H11A	120.9
C4—C3—C2	118.6 (2)	C11—C12—C7	120.7 (3)
C4—C3—H3A	120.7	C11—C12—H12A	119.7
C2—C3—H3A	120.7	C7—C12—H12A	119.7
C3—C4—C5	119.0 (2)		

N2—Hg1—Cl2—Hg1^{i}	88.09 (6)	C6—C1—C2—C3	−179.4 (2)
Cl1—Hg1—Cl2—Hg1^{i}	−89.22 (3)	C1—C2—C3—C4	0.9 (4)
N1—Hg1—Cl2—Hg1^{i}	158.29 (5)	C2—C3—C4—C5	0.8 (4)
Cl2^{i}—Hg1—Cl2—Hg1^{i}	0.0	C1—N2—C5—C4	1.5 (4)
N2—Hg1—N1—C6	−0.60 (18)	Hg1—N2—C5—C4	178.0 (2)
Cl1—Hg1—N1—C6	125.53 (18)	C3—C4—C5—N2	−2.1 (4)
Cl2—Hg1—N1—C6	−103.42 (18)	C7—N1—C6—C1	−175.9 (2)
Cl2^{i}—Hg1—N1—C6	−15.4 (3)	Hg1—N1—C6—C1	1.6 (3)
N2—Hg1—N1—C7	176.8 (2)	N2—C1—C6—N1	−2.1 (4)
Cl1—Hg1—N1—C7	−57.1 (2)	C2—C1—C6—N1	175.8 (3)
Cl2—Hg1—N1—C7	73.94 (19)	C6—N1—C7—C8	18.2 (4)
Cl2^{i}—Hg1—N1—C7	161.92 (14)	Hg1—N1—C7—C8	−159.0 (2)
Cl1—Hg1—N2—C5	86.3 (2)	C6—N1—C7—C12	−164.6 (2)
N1—Hg1—N2—C5	−177.1 (2)	Hg1—N1—C7—C12	18.3 (3)
Cl2—Hg1—N2—C5	−91.0 (2)	C12—C7—C8—C9	1.3 (4)
Cl2^{i}—Hg1—N2—C5	−2.5 (2)	N1—C7—C8—C9	178.5 (3)
Cl1—Hg1—N2—C1	−97.14 (19)	C7—C8—C9—C10	0.5 (4)
N1—Hg1—N2—C1	−0.46 (18)	C8—C9—C10—C11	−1.1 (5)
Cl2—Hg1—N2—C1	85.56 (18)	C8—C9—C10—Br1	179.6 (2)
Cl2^{i}—Hg1—N2—C1	174.10 (18)	C9—C10—C11—C12	0.0 (4)
C5—N2—C1—C2	0.4 (4)	Br1—C10—C11—C12	179.3 (2)
Hg1—N2—C1—C2	−176.4 (2)	C10—C11—C12—C7	1.8 (4)
C5—N2—C1—C6	178.2 (2)	C8—C7—C12—C11	−2.5 (4)

Hg1—N2—C1—C6	1.4 (3)	N1—C7—C12—C11	−179.8 (2)
N2—C1—C2—C3	−1.6 (4)		

Symmetry code: (i) −*x*, −*y*+1, −*z*.