

Dichlorido(6-methyl-2,2'-bipyridine- κ^2N,N')mercury(II)

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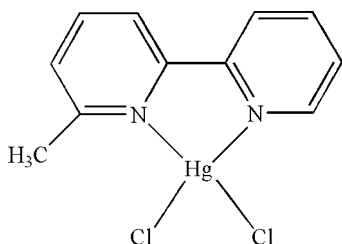
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(C-C) = 0.016$ Å; R factor = 0.092; wR factor = 0.197; data-to-parameter ratio = 22.2.

In the molecule of the title compound, $[HgCl_2(C_{11}H_{10}N_2)]$, the Hg^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from a 6-methyl-2,2'-bipyridine ligand and two Cl atoms. There is a $\pi-\pi$ contact between the pyridine rings [centroid-centroid distance = 3.9758 (5) Å].

Related literature

For related literature, see: Ahmadi, Kalateh, Ebadi *et al.* (2008); Ahmadi, Khalighi *et al.* (2008); Ahmadi, Kalateh, Abedi *et al.* (2008); Kalateh, Ahmadi *et al.* (2008); Kalateh, Ebadi *et al.* (2008); Khalighi *et al.* (2008); Khavasi *et al.* (2008); Tadayon Pour *et al.* (2008); Yousefi, Rashidi Vahid *et al.* (2008); Yousefi, Tadayon Pour *et al.* (2008); Yousefi, Khalighi *et al.* (2008). For related structures, see: Chen *et al.* (2006); Liu *et al.* (2004).



Experimental

Crystal data

$[HgCl_2(C_{11}H_{10}N_2)]$
 $M_r = 441.70$
 Monoclinic, $P2_1/c$
 $a = 9.4742$ (19) Å
 $b = 16.164$ (3) Å
 $c = 8.2107$ (16) Å
 $\beta = 105.70$ (3)°

$V = 1210.4$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 13.13$ mm⁻¹
 $T = 120$ (2) K
 $0.50 \times 0.15 \times 0.09$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: numerical *via* shape of crystal determined optically (*X-SHAPE* and

X-RED; Stoe & Cie, 2005)
 $T_{min} = 0.108$, $T_{max} = 0.307$
 14334 measured reflections
 3263 independent reflections
 2925 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.100$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.092$
 $wR(F^2) = 0.197$
 $S = 1.14$
 3263 reflections

147 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 1.39$ e Å⁻³
 $\Delta\rho_{min} = -1.12$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cl1—Hg1	2.438 (2)	N1—Hg1	2.394 (9)
Cl2—Hg1	2.423 (3)	N2—Hg1	2.297 (10)
Cl2—Hg1—Cl1	112.32 (10)	N2—Hg1—Cl1	132.8 (2)
N1—Hg1—Cl1	103.4 (2)	N2—Hg1—Cl2	109.8 (2)
N1—Hg1—Cl2	121.1 (2)	N2—Hg1—N1	71.0 (3)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2551).

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supplementary materials

Acta Cryst. (2008). E64, m1407 [doi:10.1107/S1600536808032777]

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Comment

Recently, we reported the syntheses and crystal structures of [Zn(5,5'-dmbpy)Cl₂], (II), (Khalighi *et al.*, 2008), [Zn(6-mbpy)Cl₂], (III), (Ahmadi, Kalateh, Ebadi *et al.*, 2008), [HgI₂(4,4'-dmbpy)], (IV), (Yousefi, Tadayon Pour *et al.*, 2008), [Cd(5,5'-dmbpy)(μ -Cl)₂]_n, (V), (Ahmadi, Khalighi *et al.*, 2008), [Hg(5,5'-dmbpy)I₂], (VI), (Tadayon Pour *et al.*, 2008), [Cu(5,5'-dcbpy)(en)(H₂O)₂].2.5H₂O, (VII), (Yousefi, Khalighi *et al.*, 2008), [Hg(dmphen)I₂], (VIII), (Yousefi, Rashidi Vahid *et al.*, 2008), [In(4,4'-dmbpy)Cl₃(DMSO)], (IX), (Ahmadi, Kalateh, Abedi *et al.*, 2008), [In(5,5'-dmbpy)Cl₃(MeOH)], (X), (Kalateh, Ahmadi *et al.*, 2008), {[HgCl(dm4bt)]₂(μ -Cl)₂}, (XI), (Khavasi *et al.*, 2008) and {[HgBr(4,4'-dmbpy)]₂(μ -Br)₂}, (XII), (Kalateh, Ebadi *et al.*, 2008) [where 5,5'-dmbpy is 5,5'-dimethyl-2,2'-bipyridine, 6-mbpy is 6-methyl-2,2'-bipyridine, 4,4'-dmbpy is 4,4'-dimethyl-2,2'-bipyridine, 5,5'-dcbpy is 2,2'-bipyridine-5,5'-dicarboxylate, en is ethylene-diamine, dmphen is 4,7-diphenyl-1,10-phenanthroline, DMSO is dimethyl sulfoxide and dm4bt is 2,2'-dimethyl-4,4'-bithiazole]. There are several Hg^{II} complexes, with formula, [HgCl₂(N—N)], such as [HgCl₂(bipy)], (XIII) and [HgCl₂(bipy)][HgCl₂], (XIV), (Chen *et al.*, 2006) and [HgCl₂(dpdmbip)].CH₂Cl₂, (XV), (Liu *et al.*, 2004) [where bipy is 2,2'-bipyridine and dpdmbip is 4,4'-diphenyl-6,6'-dimethyl-2,2'-bipyrimidine] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound, (I).

In the title compound, (I), (Fig. 1), the Hg^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from 6-methyl-2,2'-bipyridine and two Cl atoms. The Hg—Cl and Hg—N bond lengths and angles (Table 1) are within normal ranges, as in (XIV) and (XV).

In the crystal structure, the π - π contact (Fig. 2) between the pyridine rings, Cg2—Cg3ⁱ [symmetry code: (i) $x, 1/2 - y, -1/2 + z$, where Cg2 and Cg3 are centroids of the rings (N1/C2-C6) and (N2/C7-C11), respectively] may stabilize the structure, with centroid-centroid distance of 3.9758 (5) Å.

Experimental

For the preparation of the title compound, (I), a solution of 6-methyl-2,2'-bipyridine (0.15 g, 0.88 mmol) in methanol (10 ml) was added to a solution of HgCl₂ (0.24 g, 0.88 mmol) in acetonitrile (30 ml) and the resulting colorless solution was stirred for 20 min at 313 K. Then, it was left to evaporate slowly at room temperature. After one week, colorless needle crystals of the title compound were isolated (yield; 0.28 g, 72.03%).

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

Figures

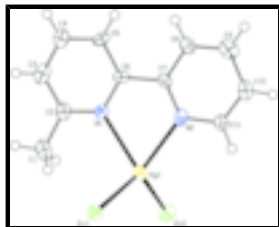


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

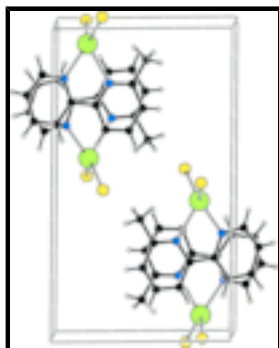


Fig. 2. A partial packing diagram of the title compound.

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Crystal data

[HgCl₂(C₁₁H₁₀N₂)]

$M_r = 441.70$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 9.4742$ (19) Å

$b = 16.164$ (3) Å

$c = 8.2107$ (16) Å

$\beta = 105.70$ (3)°

$V = 1210.4$ (4) Å³

$Z = 4$

$F_{000} = 816$

$D_x = 2.424$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 1234 reflections

$\theta = 2.2$ – 29.2°

$\mu = 13.13$ mm⁻¹

$T = 120$ (2) K

Needle, colorless

$0.50 \times 0.15 \times 0.09$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

3263 independent reflections

Radiation source: fine-focus sealed tube

2925 reflections with $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.100$

$T = 120$ (2) K

$\theta_{\text{max}} = 29.2^\circ$

φ and ω scans

$\theta_{\text{min}} = 2.2^\circ$

Absorption correction: numerical

via shape of crystal determined optically (*X-SHAPE* and *X-RED*; Stoe & Cie, 2005)

$h = -12 \rightarrow 11$

$T_{\text{min}} = 0.108$, $T_{\text{max}} = 0.307$

$k = -22 \rightarrow 22$

14334 measured reflections

$l = -9 \rightarrow 11$

Refinement

Refinement on F^2

Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.092$

$w = 1/[\sigma^2(F_o^2) + (0.1638P)^2 + 3.9978P]$
where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.197$

$(\Delta/\sigma)_{\max} = 0.005$

$S = 1.14$

$\Delta\rho_{\max} = 1.39 \text{ e } \text{\AA}^{-3}$

3263 reflections

$\Delta\rho_{\min} = -1.12 \text{ e } \text{\AA}^{-3}$

147 parameters

Extinction correction: SHELXTL (Sheldrick, 2008),

$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.020 (2)

Secondary atom site location: difference Fourier map

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.81647 (4)	0.05913 (2)	0.29276 (5)	0.0248 (3)
Cl1	0.8330 (3)	-0.00698 (17)	0.5642 (3)	0.0244 (5)
Cl2	0.7288 (3)	-0.03469 (19)	0.0569 (4)	0.0299 (6)
N1	0.6912 (9)	0.1861 (5)	0.3103 (11)	0.0187 (16)
N2	0.9427 (10)	0.1664 (6)	0.2138 (11)	0.0227 (18)
C1	0.4897 (12)	0.1134 (9)	0.3776 (14)	0.032 (2)
H1A	0.4493	0.0873	0.2700	0.048*
H1B	0.4123	0.1261	0.4285	0.048*
H1C	0.5585	0.0767	0.4500	0.048*
C2	0.5650 (11)	0.1903 (7)	0.3534 (13)	0.024 (2)
C3	0.5077 (11)	0.2686 (8)	0.3770 (14)	0.030 (2)
H3	0.4196	0.2725	0.4058	0.036*
C4	0.5820 (12)	0.3385 (8)	0.3573 (14)	0.029 (2)
H4	0.5457	0.3900	0.3764	0.034*
C5	0.7106 (11)	0.3335 (6)	0.3093 (15)	0.024 (2)

supplementary materials

H5	0.7601	0.3811	0.2924	0.028*
C6	0.7649 (11)	0.2543 (6)	0.2868 (11)	0.0175 (17)
C7	0.9018 (10)	0.2430 (6)	0.2327 (11)	0.0175 (17)
C8	0.9819 (11)	0.3114 (7)	0.2004 (15)	0.025 (2)
H8	0.9522	0.3648	0.2181	0.030*
C9	1.1063 (13)	0.2995 (8)	0.1417 (14)	0.031 (2)
H9	1.1609	0.3437	0.1191	0.037*
C10	1.1450 (11)	0.2146 (8)	0.1183 (13)	0.028 (2)
H10	1.2258	0.2029	0.0784	0.033*
C11	1.0615 (10)	0.1513 (7)	0.1553 (12)	0.0211 (19)
H11	1.0870	0.0969	0.1399	0.025*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0291 (4)	0.0223 (4)	0.0234 (4)	-0.00241 (12)	0.0075 (2)	-0.00050 (12)
Cl1	0.0251 (11)	0.0254 (12)	0.0226 (10)	0.0004 (9)	0.0061 (8)	0.0033 (9)
Cl2	0.0307 (13)	0.0297 (13)	0.0264 (12)	-0.0031 (11)	0.0032 (10)	-0.0077 (11)
N1	0.012 (3)	0.021 (4)	0.020 (4)	-0.001 (3)	0.000 (3)	-0.003 (3)
N2	0.022 (4)	0.032 (5)	0.014 (3)	0.001 (3)	0.004 (3)	-0.007 (3)
C1	0.019 (4)	0.050 (7)	0.023 (5)	-0.005 (5)	0.002 (4)	0.002 (5)
C2	0.014 (4)	0.034 (5)	0.023 (5)	0.002 (4)	0.001 (3)	0.002 (4)
C3	0.015 (4)	0.044 (7)	0.026 (5)	0.001 (4)	-0.003 (4)	-0.012 (5)
C4	0.025 (5)	0.039 (6)	0.020 (4)	0.005 (4)	0.003 (4)	-0.004 (4)
C5	0.018 (4)	0.018 (4)	0.031 (5)	0.003 (3)	0.000 (4)	-0.005 (4)
C6	0.025 (4)	0.014 (4)	0.008 (3)	0.000 (3)	-0.005 (3)	0.001 (3)
C7	0.018 (4)	0.023 (4)	0.009 (3)	-0.002 (3)	0.000 (3)	0.004 (3)
C8	0.018 (4)	0.030 (5)	0.025 (5)	-0.006 (4)	0.003 (3)	0.000 (4)
C9	0.025 (5)	0.042 (7)	0.018 (4)	0.004 (4)	-0.008 (4)	0.017 (5)
C10	0.017 (4)	0.045 (7)	0.019 (4)	0.004 (4)	0.001 (3)	0.004 (5)
C11	0.019 (4)	0.027 (5)	0.017 (4)	0.008 (4)	0.003 (3)	0.009 (4)

Geometric parameters (\AA , $^\circ$)

Cl1—Hg1	2.438 (2)	C5—C6	1.410 (13)
Cl2—Hg1	2.423 (3)	C5—H5	0.9300
N1—Hg1	2.394 (9)	C6—N1	1.347 (13)
N2—Hg1	2.297 (10)	C6—C7	1.492 (14)
C1—C2	1.473 (17)	C7—N2	1.319 (14)
C1—H1A	0.9600	C7—C8	1.406 (14)
C1—H1B	0.9600	C8—C9	1.402 (17)
C1—H1C	0.9600	C8—H8	0.9300
C2—N1	1.338 (13)	C9—C10	1.446 (18)
C2—C3	1.411 (17)	C9—H9	0.9300
C3—C4	1.363 (18)	C10—C11	1.377 (16)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.381 (16)	C11—N2	1.360 (13)
C4—H4	0.9300	C11—H11	0.9300

C12—Hg1—C11	112.32 (10)	C3—C4—C5	120.6 (11)
N1—Hg1—C11	103.4 (2)	C3—C4—H4	119.7
N1—Hg1—C12	121.1 (2)	C5—C4—H4	119.7
N2—Hg1—C11	132.8 (2)	C4—C5—C6	118.1 (10)
N2—Hg1—C12	109.8 (2)	C4—C5—H5	121.0
N2—Hg1—N1	71.0 (3)	C6—C5—H5	121.0
C2—N1—Hg1	123.6 (7)	N1—C6—C5	120.3 (10)
C2—N1—C6	122.1 (9)	N1—C6—C7	117.9 (9)
C6—N1—Hg1	114.1 (6)	C5—C6—C7	121.8 (9)
C7—N2—Hg1	118.9 (7)	N2—C7—C8	121.7 (9)
C7—N2—C11	120.4 (10)	N2—C7—C6	117.2 (9)
C11—N2—Hg1	120.6 (8)	C8—C7—C6	121.1 (9)
C2—C1—H1A	109.5	C9—C8—C7	120.2 (11)
C2—C1—H1B	109.5	C9—C8—H8	119.9
H1A—C1—H1B	109.5	C7—C8—H8	119.9
C2—C1—H1C	109.5	C8—C9—C10	116.3 (11)
H1A—C1—H1C	109.5	C8—C9—H9	121.8
H1B—C1—H1C	109.5	C10—C9—H9	121.8
N1—C2—C3	119.1 (10)	C11—C10—C9	119.6 (10)
N1—C2—C1	119.5 (10)	C11—C10—H10	120.2
C3—C2—C1	121.3 (10)	C9—C10—H10	120.2
C4—C3—C2	119.8 (11)	N2—C11—C10	121.7 (10)
C4—C3—H3	120.1	N2—C11—H11	119.2
C2—C3—H3	120.1	C10—C11—H11	119.2
C2—N1—Hg1—C11	-51.3 (8)	C5—C6—C7—C8	-0.5 (13)
C2—N1—Hg1—C12	75.5 (8)	N2—C7—C8—C9	2.0 (15)
C2—N1—Hg1—N2	177.6 (8)	C6—C7—C8—C9	-176.9 (9)
C6—N1—Hg1—C11	123.3 (6)	C7—C8—C9—C10	-0.2 (14)
C6—N1—Hg1—C12	-109.9 (6)	C8—C9—C10—C11	-0.7 (14)
C6—N1—Hg1—N2	-7.7 (6)	C9—C10—C11—N2	0.0 (15)
C7—N2—Hg1—C11	-83.2 (8)	C3—C2—N1—C6	-0.7 (14)
C7—N2—Hg1—C12	124.8 (7)	C1—C2—N1—C6	-179.9 (9)
C7—N2—Hg1—N1	7.6 (7)	C3—C2—N1—Hg1	173.6 (7)
C11—N2—Hg1—C11	94.0 (7)	C1—C2—N1—Hg1	-5.7 (13)
C11—N2—Hg1—C12	-58.0 (7)	C5—C6—N1—C2	0.7 (14)
C11—N2—Hg1—N1	-175.2 (8)	C7—C6—N1—C2	-177.8 (8)
N1—C2—C3—C4	-0.7 (16)	C5—C6—N1—Hg1	-174.0 (7)
C1—C2—C3—C4	178.5 (10)	C7—C6—N1—Hg1	7.5 (10)
C2—C3—C4—C5	2.0 (16)	C8—C7—N2—C11	-2.7 (14)
C3—C4—C5—C6	-2.0 (16)	C6—C7—N2—C11	176.2 (8)
C4—C5—C6—N1	0.6 (14)	C8—C7—N2—Hg1	174.5 (7)
C4—C5—C6—C7	179.1 (9)	C6—C7—N2—Hg1	-6.6 (11)
N1—C6—C7—N2	-1.0 (12)	C10—C11—N2—C7	1.7 (14)
C5—C6—C7—N2	-179.4 (9)	C10—C11—N2—Hg1	-175.4 (7)
N1—C6—C7—C8	177.9 (9)		

Fig. 1

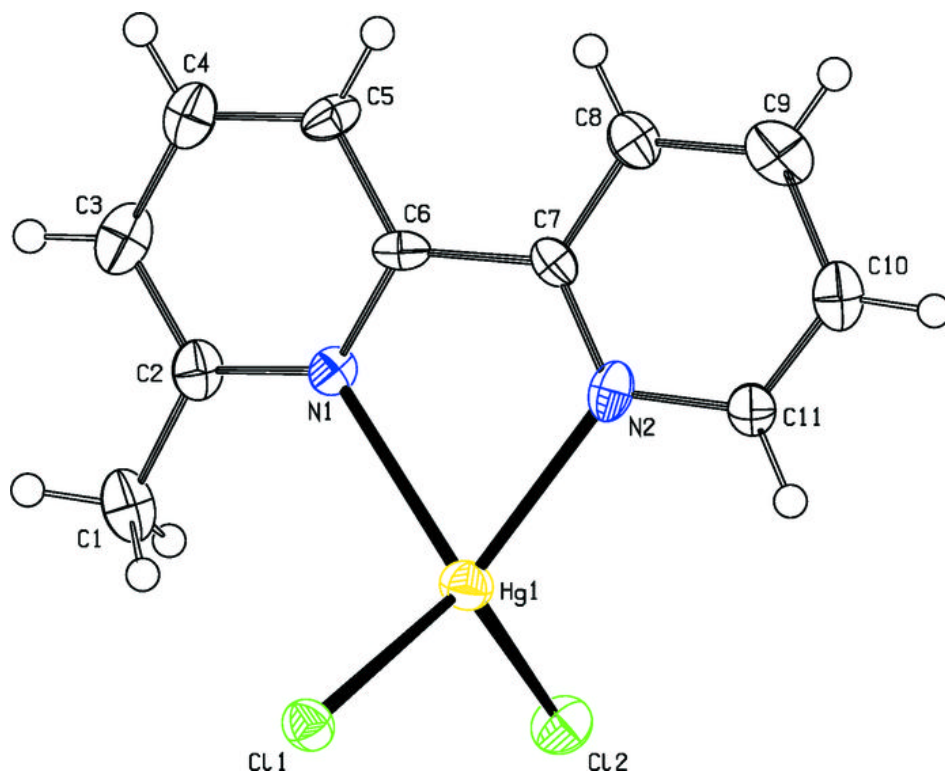


Fig. 2

