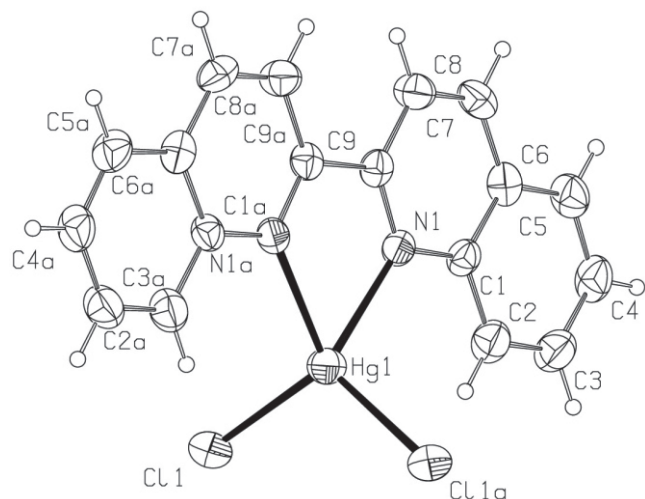


Crystal structure of 2,2'-biquinoline- κ^2N,N' dichloromercury(II), $C_{18}H_{12}Cl_2HgN_2$

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Abstract

$C_{18}H_{12}Cl_2HgN_2$, monoclinic, $C2/c$ (no. 15), $a = 13.442(1)$ Å, $b = 16.094(1)$ Å, $c = 7.585(1)$ Å, $\beta = 96.26(1)^\circ$, $V = 1631.1$ Å³, $Z = 4$, $R_g(F) = 0.0458$, $wR_{ref}(F^2) = 0.0813$, $T = 298$ K.

Table 1. Data collection and handling.

Crystal:	yellow needles, size 0.03×0.05×0.60 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	97.63 cm ⁻¹
Diffractometer, scan mode:	Bruker APEX II CCD area detector, ω
$2\theta_{max}$:	55.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8190, 1971
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1186
$N(param)_{refined}$:	105
Programs:	SHELX [8]

Source of material

A solution of 2,2'-biquinoline (0.20 g, 0.78 mmol) in methanol (5 ml) and chloroform (5 ml) was added to a solution of $HgCl_2$ (0.21, 0.78 mmol) in methanol (5 ml) and the resulting light yellow solution was stirred for 30 minutes at room temperature. This solution was left to evaporate slowly at room temperature. After three weeks, needle-shaped yellow crystals were isolated (yield: 0.27 g, 65.9%).

Discussion

Due to their strong luminescence properties, the 2,2'-biquinoline ligand and its derivatives are widely used in various thin film application devices to mimic photosynthetic light harvesting [1]. The coordination chemistry of nitrogen donor ligands such as 2,2'-biquinoline has been extensively studied and is mostly related to their relevance to biological systems [2]. In this study, we

report the structure of a new mercury(II) complex with 2,2'-biquinoline under the formula $[HgCl_2(2,2'-biquinoline)]$. Although there is only one report on the coordination of this ligand to Hg ($Hg(SCN)_2(2,2'-biquinoline)$ [3]. Five complexes with other metal centers with the general formula of $[MCl_2(2,2'-biquinoline)]$ including $[CoCl_2(2,2'-biquinoline)]$ [4], $[FeCl_2(2,2'-biquinoline)]$ [5], $[PtCl_2(2,2'-biquinoline)]$ [6], $[ZnCl_2(2,2'-biquinoline)]$, $[CuCl_2(2,2'-biquinoline)]$ and $[PdCl_2(2,2'-biquinoline)]$ [7], have been reported. The asymmetric unit of the title compound contains a half of the title complex. The title structure includes a mononuclear mercury(II) complex in which the four-coordinated Hg(II) ion has a distorted tetrahedral environment, surrounded by two nitrogen atoms from 2,2'-biquinoline ligand and two terminal chlorine atoms. The Hg–N bond length is 2.329(5) Å, which is shorter than to those reported in the literature (2.369(2) and 2.353(3) Å) for $[Hg(SCN)_2(2,2'-biquinoline)]$ [3]. The Hg–Cl bond length of 2.403(2) Å is within the normal range. The bond angles around the Hg(II) centre show notable deviations from ideal tetrahedral geometry. The biquinoline ligands form π - π bonded stacks in which each biquinoline ligand lies between two similar ligands of adjacent Hg complexes to generate a linear chains. The close contact distance between adjacent aromatic rings is 3.796 Å.

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(2)	8f	0.7043	0.3041	0.1693	0.082
H(3)	8f	0.8650	0.2980	0.0946	0.088
H(4)	8f	0.9508	0.4182	0.0439	0.088
H(5)	8f	0.8795	0.5451	0.0677	0.085
H(7)	8f	0.7300	0.6281	0.1346	0.078
H(8)	8f	0.5697	0.6311	0.2134	0.076

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(1)	8 <i>f</i>	0.6916(4)	0.4296(4)	0.1619(9)	0.048(4)	0.053(5)	0.052(4)	0.000(3)	0.007(3)	0.010(4)
C(2)	8 <i>f</i>	0.7383(5)	0.3528(5)	0.148(1)	0.053(4)	0.069(5)	0.085(6)	0.004(4)	0.014(4)	0.014(5)
C(3)	8 <i>f</i>	0.8341(5)	0.3492(5)	0.104(1)	0.060(4)	0.066(5)	0.095(6)	0.009(4)	0.015(4)	0.012(5)
C(4)	8 <i>f</i>	0.8858(5)	0.4218(6)	0.074(1)	0.048(4)	0.091(7)	0.083(6)	0.003(4)	0.015(4)	0.010(5)
C(5)	8 <i>f</i>	0.8439(5)	0.4972(6)	0.088(1)	0.057(4)	0.072(6)	0.085(6)	−0.013(4)	0.018(4)	0.007(5)
C(6)	8 <i>f</i>	0.7449(5)	0.5024(5)	0.1343(9)	0.051(4)	0.065(5)	0.050(4)	−0.005(3)	0.005(3)	0.004(4)
C(7)	8 <i>f</i>	0.6968(5)	0.5787(5)	0.153(1)	0.068(5)	0.053(5)	0.072(5)	−0.018(4)	0.008(4)	0.002(4)
C(8)	8 <i>f</i>	0.6017(5)	0.5806(5)	0.199(1)	0.067(4)	0.049(5)	0.075(5)	−0.002(4)	0.017(4)	0.000(4)
C(9)	8 <i>f</i>	0.5524(5)	0.5052(4)	0.2251(9)	0.049(3)	0.049(4)	0.042(4)	−0.003(3)	0.005(3)	0.008(3)
N(1)	8 <i>f</i>	0.5952(3)	0.4330(3)	0.2053(7)	0.043(3)	0.046(3)	0.059(4)	0.001(2)	0.006(2)	0.003(3)
Hg(1)	4 <i>e</i>	½	0.31545(3)	¼	0.0572(2)	0.0471(2)	0.0904(3)	0	0.0141(2)	0
Cl(1)	8 <i>f</i>	0.4190(2)	0.2302(1)	0.0168(3)	0.087(1)	0.053(1)	0.108(2)	−0.003(1)	−0.006(1)	−0.012(1)

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