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catena-Poly[[dichloridomercury(II)]-μ-3,5-bis[2-(pyridin-4-yl)ethynyl]pyridine-κ^2N:N']

Peng Zhang, Qi Yang and Minjian Zhao*

Beijing Key Laboratory for Green Catalysis and Separation, Department of Chemistry and Chemical Engineering, College of Environmental and Energy Engineering, Beijing University of Technology, Beijing 100124, People's Republic of China. *Correspondence e-mail: wangbin_01@yeah.net

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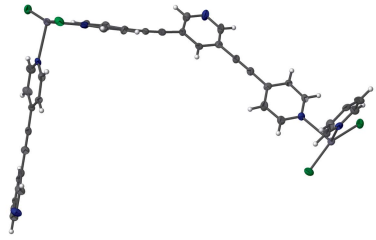
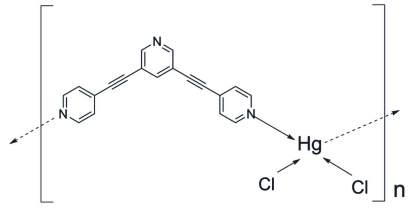
Structural data: full structural data are available from iucrdata.iucr.org

In the title coordination polymer, $[HgCl_2(C_{19}H_{11}N_3)]_n$, the Hg^{II} atom is coordinated by two N atoms of symmetry-related 3,5-bis(pyridin-4-ylethynyl)-pyridine ligands (*L*) and by two chloride ions in a distorted tetrahedral geometry. The dihedral angles between the coordinated pyridine rings and the central pyridine ring are 44.6 (3) and 14.2 (3)°, respectively, while the dihedral angle between the two coordinating pyridine rings is 56.1 (3)°. The ligand bridges the Hg^{II} atoms, forming a zigzag chain running parallel to the *b* axis. There are no other significant intermolecular interactions present in the crystal.

3D view



Chemical scheme



Structure description

Coordination polymers (CPs) have attracted much attention because of their fascinating architectures and intriguing topologies as well as their potential applications in catalysis, adsorption, separation, and luminescence. Pyridine-based ligands are widely used in the construction of CPs, most of which are constructed from linear ligands. However, CPs assembled from angular pyridyl-based ligands are relatively rare.

In this work, an angular pyridyl-based ligand, 3,5-bis(pyridin-4-ylethynyl)pyridine (*L*), was employed to react with $HgCl_2$ to afford the title coordination polymer, illustrated in Fig. 1. The Hg^{II} atom, Hg1, is coordinated by two N atoms, N1 and N3, of two symmetry-related *L* ligands and two chloride ions in a distorted tetrahedral geometry (Table 1 and Fig. 1). The τ_4 descriptor for fourfold coordination = 0.33 (extreme forms: 0.00 for square-planar and 1.00 for tetrahedral; Yang *et al.*, 2007)

The dihedral angles between the coordinated pyridine rings (N1/C1–C5 and N3/C15–C19) and the central pyridine ring (N2/C8–C12) are 44.6 (3) and 14.2 (3)°, respectively, and the dihedral angle between the two coordinating pyridine rings is 56.1 (3)°. The

Table 1
Selected geometric parameters (Å, °).

Hg1—Cl2	2.3508 (16)	Hg1—N3^{i}	2.420 (5)
Hg1—Cl1	2.3623 (16)	Hg1—N1	2.441 (5)
Cl2—Hg1—Cl1	156.83 (6)	Cl2—Hg1—N1	97.54 (13)
Cl2—Hg1—N3^{i}	99.51 (12)	Cl1—Hg1—N1	96.90 (13)
Cl1—Hg1—N3^{i}	97.04 (13)	N3^{i}—Hg1—N1	95.45 (16)

Symmetry code: (i) $-x-2, y+\frac{1}{2}, -z+\frac{3}{2}$.

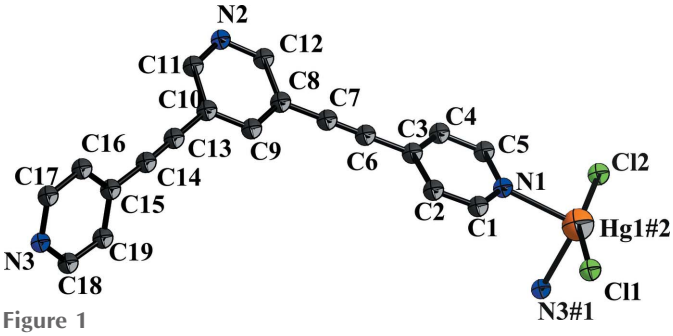


Figure 1
The coordination mode of the title complex, with the atom labelling [symmetry codes: (#1) $-x-2, y+\frac{1}{2}, -z+\frac{3}{2}$; (#2) $-x-2, y-\frac{1}{2}, -z+\frac{3}{2}$]. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

ligands bridge the mercury atoms, forming a zigzag chain running parallel to the *b* axis (Fig. 2). There are no other significant intermolecular interactions present in the crystal.

The linear pyridyl-based ligand, 1,4-bis(pyridin-4-ylethynyl)benzene, has also been used to form a similar zigzag coordination polymer with $HgCl_2$ (Wang *et al.*, 2014).

Synthesis and crystallization

The organic ligand 3,5-bis(pyridin-4-ylethynyl)pyridine (*L*) was synthesized from the reaction between 3,5-dibromopyridine and 4-ethynylpyridine hydrochloride following the reported procedure (Yamamoto *et al.*, 2003). To synthesise the title coordination polymer, a 3 ml methanol solution of $HgCl_2$ (0.1 mmol, 27 mg) was layered onto a 3 ml chloroform solution of *L* (0.2 mmol, 56 mg). After three days, colourless crystals of the title coordination polymer were obtained.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[HgCl_2(C_{19}H_{11}Cl_2N_3)]$
M_r	552.80
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	5.0941 (10), 22.946 (5), 15.831 (3)
β (°)	96.229 (4)
V (Å^3)	1839.5 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.66
Crystal size (mm)	0.18 × 0.16 × 0.16
Data collection	
Diffractometer	Bruker SMART 1000 CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 1998)
T_{min}, T_{max}	0.305, 0.338
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9673, 3224, 2631
R_{int}	0.044
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.079, 0.97
No. of reflections	3224
No. of parameters	226
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.81, −1.43

Computer programs: *SMART* and *SAINT* (Bruker, 1998), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The maximum and minimum

Figure 2
A view along the *b* axis of the zigzag chain structure of the title coordination polymer. Displacement ellipsoids are drawn at the 50% probability level, and H atoms have been omitted for clarity.

residual electron density peaks of 1.81 and −1.42 e Å^{-3}, respectively, are located at *ca* 1.00 Å from the Hg atom.

Acknowledgements

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full crystallographic data

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***catena*-Poly[[dichloridomercury(II)]-μ-3,5-bis[2-(pyridin-4-yl)ethynyl]pyridine-κ^2N:N']**

Crystal data

$[HgCl_2(C_{19}H_{11}N_3)]$
M_r = 552.80
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 5.0941 (10) Å
b = 22.946 (5) Å
c = 15.831 (3) Å
β = 96.229 (4)°
V = 1839.5 (6) Å^3
Z = 4
$F(000)$ = 1040
D_x = 1.996 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2134 reflections
θ = 3.6–25.0°
μ = 8.66 mm^{-1}
T = 173 K
Block, colourless
0.18 × 0.16 × 0.16 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and phi scans
Absorption correction: multi-scan (SADABS; Bruker, 1998)
T_{min} = 0.305, T_{max} = 0.338
9673 measured reflections
3224 independent reflections
2631 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 25.0°, θ_{min} = 1.6°
h = −5→6
k = −27→27
l = −18→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.079
S = 0.97
3224 reflections
226 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
$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.81 e Å^{-3}
$\Delta\rho_{min}$ = −1.43 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.44656 (4)	0.513510 (10)	0.762796 (15)	0.02213 (10)
Cl2	0.5910 (3)	0.44510 (7)	0.86826 (10)	0.0285 (4)
Cl1	0.4855 (3)	0.58105 (7)	0.65222 (10)	0.0289 (4)
N1	0.0952 (9)	0.4547 (2)	0.6882 (3)	0.0253 (12)
C5	0.0249 (12)	0.4028 (3)	0.7178 (4)	0.0283 (15)
H5	0.1159	0.3886	0.7677	0.034*
C14	−1.5891 (11)	0.1642 (3)	0.5383 (4)	0.0232 (14)
C16	−1.9249 (11)	0.0862 (3)	0.5394 (4)	0.0227 (13)
H16	−1.8960	0.0752	0.4847	0.027*
C8	−0.8904 (11)	0.2939 (2)	0.4708 (4)	0.0203 (13)
N3	−2.1573 (9)	0.0714 (2)	0.6592 (3)	0.0202 (11)
C13	−1.4324 (11)	0.1912 (3)	0.5042 (4)	0.0236 (14)
C12	−1.0721 (10)	0.2621 (2)	0.5116 (4)	0.0210 (13)
H12	−1.0797	0.2661	0.5697	0.025*
C1	−0.0400 (11)	0.4744 (3)	0.6168 (4)	0.0252 (14)
H1	0.0040	0.5106	0.5959	0.030*
C9	−0.8887 (12)	0.2864 (3)	0.3838 (4)	0.0283 (15)
H9	−0.7668	0.3077	0.3567	0.034*
N2	−1.0527 (10)	0.2503 (2)	0.3359 (3)	0.0338 (14)
C7	−0.6965 (11)	0.3303 (3)	0.5187 (4)	0.0262 (14)
C17	−2.1085 (11)	0.0572 (3)	0.5815 (4)	0.0234 (14)
H17	−2.2017	0.0265	0.5542	0.028*
C4	−0.1776 (12)	0.3696 (3)	0.6770 (4)	0.0294 (15)
H4	−0.2199	0.3337	0.6991	0.035*
C11	−1.2422 (11)	0.2241 (3)	0.4638 (4)	0.0215 (13)
C10	−1.2246 (12)	0.2200 (3)	0.3777 (4)	0.0324 (16)
H10	−1.3391	0.1945	0.3463	0.039*
C19	−1.8426 (12)	0.1472 (3)	0.6601 (4)	0.0302 (15)
H19	−1.7571	0.1784	0.6887	0.036*
C18	−2.0270 (12)	0.1161 (3)	0.6974 (4)	0.0283 (15)
H18	−2.0630	0.1266	0.7518	0.034*
C15	−1.7825 (11)	0.1325 (3)	0.5794 (4)	0.0211 (13)
C2	−0.2419 (12)	0.4432 (3)	0.5727 (4)	0.0290 (15)
H2	−0.3273	0.4582	0.5224	0.035*
C3	−0.3178 (11)	0.3903 (3)	0.6024 (4)	0.0240 (14)

C6	−0.5281 (11)	0.3577 (3)	0.5586 (4)	0.0253 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.02305 (14)	0.02195 (16)	0.02119 (16)	−0.00100 (10)	0.00146 (9)	−0.00379 (10)
Cl2	0.0322 (8)	0.0272 (8)	0.0249 (9)	0.0067 (6)	−0.0021 (6)	−0.0016 (7)
Cl1	0.0368 (8)	0.0263 (8)	0.0238 (9)	−0.0080 (7)	0.0041 (6)	0.0005 (7)
N1	0.022 (3)	0.029 (3)	0.027 (3)	0.002 (2)	0.008 (2)	−0.004 (2)
C5	0.034 (4)	0.029 (4)	0.021 (4)	−0.002 (3)	0.001 (3)	−0.002 (3)
C14	0.020 (3)	0.020 (3)	0.029 (4)	0.003 (3)	−0.002 (3)	0.003 (3)
C16	0.026 (3)	0.020 (3)	0.024 (4)	0.000 (3)	0.009 (3)	−0.001 (3)
C8	0.018 (3)	0.017 (3)	0.026 (4)	0.002 (2)	0.000 (2)	0.003 (3)
N3	0.023 (3)	0.017 (3)	0.019 (3)	0.002 (2)	−0.001 (2)	0.006 (2)
C13	0.022 (3)	0.025 (3)	0.023 (4)	−0.004 (3)	−0.001 (3)	0.000 (3)
C12	0.022 (3)	0.018 (3)	0.023 (4)	0.007 (3)	0.003 (2)	0.002 (3)
C1	0.020 (3)	0.022 (3)	0.033 (4)	0.001 (2)	0.003 (3)	0.006 (3)
C9	0.026 (3)	0.029 (4)	0.030 (4)	−0.004 (3)	−0.001 (3)	0.004 (3)
N2	0.039 (3)	0.035 (3)	0.027 (4)	−0.015 (3)	−0.001 (2)	0.004 (3)
C7	0.022 (3)	0.023 (3)	0.034 (4)	0.004 (3)	0.006 (3)	−0.003 (3)
C17	0.025 (3)	0.019 (3)	0.026 (4)	0.000 (2)	−0.001 (3)	−0.001 (3)
C4	0.033 (4)	0.029 (4)	0.028 (4)	−0.011 (3)	0.009 (3)	−0.003 (3)
C11	0.019 (3)	0.020 (3)	0.025 (4)	0.005 (2)	0.001 (2)	0.002 (3)
C10	0.033 (4)	0.030 (4)	0.031 (4)	−0.012 (3)	−0.006 (3)	0.001 (3)
C19	0.035 (4)	0.032 (4)	0.023 (4)	−0.010 (3)	−0.003 (3)	0.001 (3)
C18	0.035 (4)	0.030 (4)	0.019 (4)	−0.004 (3)	0.000 (3)	0.000 (3)
C15	0.017 (3)	0.025 (3)	0.021 (4)	0.004 (2)	−0.001 (2)	0.009 (3)
C2	0.027 (3)	0.030 (4)	0.028 (4)	0.002 (3)	−0.006 (3)	−0.001 (3)
C3	0.021 (3)	0.023 (3)	0.029 (4)	−0.004 (3)	0.010 (2)	−0.009 (3)
C6	0.023 (3)	0.025 (4)	0.029 (4)	−0.004 (3)	0.009 (3)	−0.009 (3)

Geometric parameters (Å, º)

Hg1—Cl2	2.3508 (16)	N3—C18	1.332 (8)
Hg1—Cl1	2.3623 (16)	N3—Hg1^{ii}	2.420 (5)
Hg1—N3^{i}	2.420 (5)	C13—C11	1.433 (8)
Hg1—N1	2.441 (5)	C12—C11	1.392 (8)
N1—C1	1.338 (8)	C1—C2	1.379 (8)
N1—C5	1.343 (8)	C9—N2	1.350 (8)
C5—C4	1.385 (8)	N2—C10	1.346 (8)
C14—C13	1.185 (9)	C7—C6	1.188 (8)
C14—C15	1.437 (9)	C4—C3	1.395 (9)
C16—C17	1.377 (8)	C11—C10	1.380 (9)
C16—C15	1.397 (8)	C19—C18	1.364 (9)
C8—C9	1.389 (9)	C19—C15	1.387 (9)
C8—C12	1.391 (9)	C2—C3	1.373 (9)
C8—C7	1.445 (8)	C3—C6	1.424 (8)
N3—C17	1.323 (8)		

Cl2—Hg1—Cl1	156.83 (6)	N1—C1—C2	122.7 (6)
Cl2—Hg1—N3^{i}	99.51 (12)	N2—C9—C8	124.2 (6)
Cl1—Hg1—N3^{i}	97.04 (13)	C10—N2—C9	116.0 (6)
Cl2—Hg1—N1	97.54 (13)	C6—C7—C8	176.4 (6)
Cl1—Hg1—N1	96.90 (13)	N3—C17—C16	122.4 (6)
N3^{i}—Hg1—N1	95.45 (16)	C5—C4—C3	119.6 (6)
C1—N1—C5	117.5 (5)	C10—C11—C12	118.4 (6)
C1—N1—Hg1	120.4 (4)	C10—C11—C13	121.6 (5)
C5—N1—Hg1	122.1 (4)	C12—C11—C13	120.0 (6)
N1—C5—C4	122.6 (6)	N2—C10—C11	124.4 (6)
C13—C14—C15	178.9 (7)	C18—C19—C15	120.2 (6)
C17—C16—C15	119.7 (6)	N3—C18—C19	122.6 (7)
C9—C8—C12	118.1 (5)	C19—C15—C16	116.6 (6)
C9—C8—C7	121.0 (6)	C19—C15—C14	121.6 (6)
C12—C8—C7	120.7 (6)	C16—C15—C14	121.8 (6)
C17—N3—C18	118.6 (6)	C3—C2—C1	120.5 (6)
C17—N3—Hg1^{ii}	121.7 (4)	C2—C3—C4	117.0 (5)
C18—N3—Hg1^{ii}	119.5 (4)	C2—C3—C6	121.5 (6)
C14—C13—C11	179.3 (7)	C4—C3—C6	121.5 (6)
C8—C12—C11	118.8 (6)	C7—C6—C3	176.8 (7)

Cl2—Hg1—N1—C1	−175.5 (5)	C8—C12—C11—C13	−179.6 (5)
Cl1—Hg1—N1—C1	−13.7 (5)	C14—C13—C11—C10	−171 (100)
N3^{i}—Hg1—N1—C1	84.1 (5)	C14—C13—C11—C12	8 (66)
Cl2—Hg1—N1—C5	6.4 (5)	C9—N2—C10—C11	0.5 (10)
Cl1—Hg1—N1—C5	168.2 (5)	C12—C11—C10—N2	0.0 (10)
N3^{i}—Hg1—N1—C5	−94.0 (5)	C13—C11—C10—N2	179.2 (6)
C1—N1—C5—C4	0.5 (10)	C17—N3—C18—C19	−1.0 (9)
Hg1—N1—C5—C4	178.7 (5)	Hg1^{ii}—N3—C18—C19	173.8 (5)
C15—C14—C13—C11	77 (79)	C15—C19—C18—N3	−0.6 (10)
C9—C8—C12—C11	0.4 (8)	C18—C19—C15—C16	1.9 (9)
C7—C8—C12—C11	−175.2 (5)	C18—C19—C15—C14	−179.9 (6)
C5—N1—C1—C2	−1.1 (10)	C17—C16—C15—C19	−1.7 (8)
Hg1—N1—C1—C2	−179.4 (5)	C17—C16—C15—C14	−179.9 (5)
C12—C8—C9—N2	0.1 (9)	C13—C14—C15—C19	−71 (37)
C7—C8—C9—N2	175.6 (6)	C13—C14—C15—C16	107 (37)
C8—C9—N2—C10	−0.5 (9)	N1—C1—C2—C3	1.7 (11)
C9—C8—C7—C6	−86 (12)	C1—C2—C3—C4	−1.6 (10)
C12—C8—C7—C6	89 (12)	C1—C2—C3—C6	179.1 (6)
C18—N3—C17—C16	1.2 (9)	C5—C4—C3—C2	1.0 (9)
Hg1^{ii}—N3—C17—C16	−173.5 (4)	C5—C4—C3—C6	−179.7 (6)
C15—C16—C17—N3	0.2 (9)	C8—C7—C6—C3	70 (19)
N1—C5—C4—C3	−0.4 (10)	C2—C3—C6—C7	62 (12)
C8—C12—C11—C10	−0.4 (8)	C4—C3—C6—C7	−117 (12)

Symmetry codes: (i) −*x*−2, *y*+1/2, −*z*+3/2; (ii) −*x*−2, *y*−1/2, −*z*+3/2.