Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *catena*-Poly[[dichloridomercury(II)]-$\mu$-1,4-bis[2-(pyridin-4-yl)ethynyl]benzene-$\kappa^2N$:$N'$]

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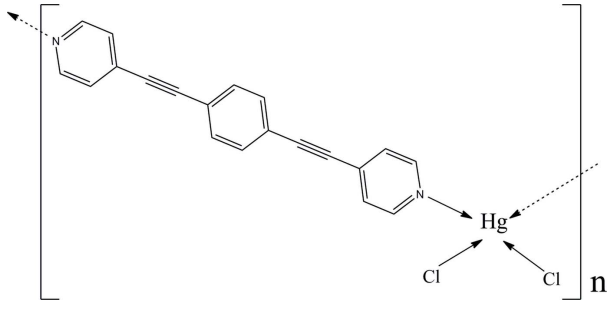
Received 5 May 2014; accepted 6 May 2014

Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.028; $wR$ factor = 0.070; data-to-parameter ratio = 13.9.

In the polymeric title compound, $[HgCl_2(C_{20}H_{12}N_2)]_n$, the $Hg^{II}$ atom is located on a twofold rotation axis and the benzene ring of the bidentate bridging 1,4-bis[2-(pyridin-4-yl)-ethynyl]benzene ($L$) ligand is located about a twofold rotation axis. The $Hg^{II}$ atom is coordinated by two N atoms of two different $L$ ligands and by two chloride ions in a distorted tetrahedral geometry. The dihedral angle between the coordinating pyridine and the benzene ring is 12.8 (2)°. The result of the bridging is the formation of a zigzag chain running parallel to [102]. The chains pack with no specific intermolecular interactions between them.

## Related literature

For examples of 1,4-bis[2-(pyridin-4-yl)ethynyl]benzene-containing polymers, see: Yamada *et al.* (2011). For examples of Hg-containing polymers, see: Xie & Wu (2007). For the synthesis of the ligand, see: Fasina *et al.* (2004).




## Experimental

### Crystal data

$[HgCl_2(C_{20}H_{12}N_2)]$
$M_r$ = 551.81
Monoclinic, $P2/c$
$a$ = 12.285 (3) Å
$b$ = 4.8482 (10) Å
$c$ = 15.271 (3) Å
$\beta$ = 98.00 (3)°
$V$ = 900.7 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 8.85 mm$^{-1}$
$T$ = 173 K
0.18 × 0.16 × 0.16 mm

### Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1995)
$T_{min}$ = 0.222, $T_{max}$ = 0.243
4238 measured reflections
1585 independent reflections
1512 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.070
$S$ = 0.92
1585 reflections
114 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.73 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Hg1—Cl1$^{i}$ | 2.3719 (12) | Hg1—N1$^{i}$ | 2.412 (3) |
| Hg1—Cl1 | 2.3719 (12) | Hg1—N1 | 2.412 (3) |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors achnowledge Qing Dao University of Science and Technology and Beijing University of Technology for supporting this work.

Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5312).

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# supporting information

*Acta Cryst.* (2014). E**70**, m208 [doi:10.1107/S1600536814010228]

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### S1. Structural commentary

Recently, a large number of coordination polymers assembled from pyridyl-based ligands have been extensively investigated. Most of these coordination polymers are constructed from 4,4′-bipyridyl but other examples of bridging ligands are known, such as with 1,4-bis(pyridin-4-ylethynyl)benzene (Yamada *et al.*, 2011). Mercury coordination polymers are known (Xie *et al.*, 2007)

In this work, an linear pyridyl-based ligand, 1,4-bis(pyridin-4-ylethynyl)benzene, was employed to react with $HgCl_2$ to afford the title complex, $[Hg(C_{20}H_{12}N_2)Cl_2]_n$ (I). In I, the Hg(II) center is coordinated by two N atoms of two different 1,4-bis(pyridin-4-ylethynyl)benzene ligands and two chloride ions in a distorted tetrahedral geometry (Fig. 1). The Hg(II) centers are linked by 1,4-bis(pyridin-4-ylethynyl)benzene ligands to form a one-dimensional zigzag chain and the chain is parallel to [102] (Fig. 2). The dihedral angles between coordinated pyridine rings and benzene ring are *ca.* 12.8 (2)°.

### S2. Synthesis and crystallization

The ligand 1,4-bis(pyridin-4-ylethynyl)benzene (bpyb) was synthesized from the reaction between 4-(prop-1-yn-1-yl)pyridine and 1,4-diiodobenzene following the reported procedure (Fasina *et al.*, 2004). A methanol (3 ml) solution of $HgCl_2$ (0.1 mmol, 27 mg) was layered upon a chloroform solution (3 ml) of bpyp (0.2 mmol, 56 mg). After three days, colourless crystals of the title complex suitable for X-ray analysis were obtained.

### S3. Refinement

Hydrogen atoms were included in calculated positions and treated as riding on their parent C atoms with C—H = 0.95Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The maximum and minimum residual electron density peaks of 2.15 and 1.73 eÅ$^{-3}$, respectively, were located 0.93 Å and 1.00 Å from the Hg atom.

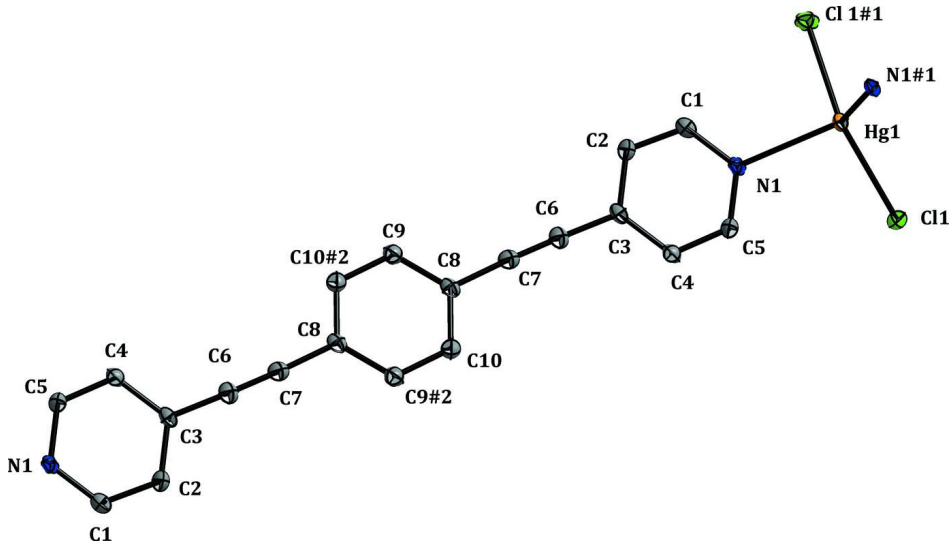


**Figure 1**

The coordination mode of the title complex, with displacement ellipsoids drawn at the 50% probability level. All H atoms have been omitted for clarity. [Symmetry codes: (#1) -x+1, y, -z+1/2; (#2) -x, -y+3, z+1.]

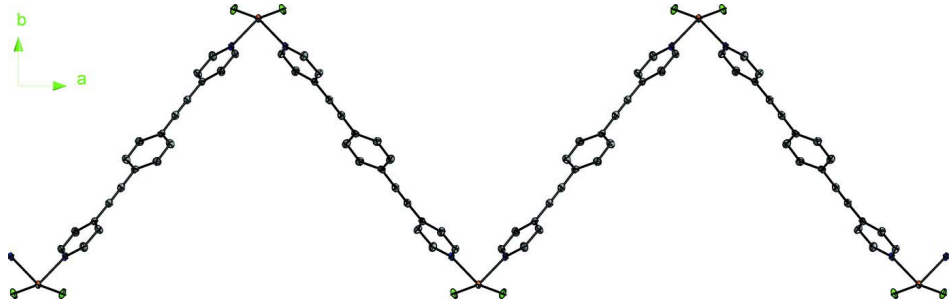


**Figure 2**

The zigzag chain of the complex. View down the *c axis*, with displacement ellipsoids drawn at the 50% probability level. All hydrogen atoms are omitted for clarity.

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*Crystal data*

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$c$ = 15.271 (3) Å
$\beta$ = 98.00 (3)°
$V$ = 900.7 (3) Å$^3$
$Z$ = 2
$F(000)$ = 520
$D_x$ = 2.035 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
$\mu$ = 8.85 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
$\omega$ and phi scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1995)
$T_{min}$ = 0.222, $T_{max}$ = 0.243

4238 measured reflections
1585 independent reflections
1512 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -11 \rightarrow 14$
$k = -5 \rightarrow 5$
$l = -18 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.070$
$S = 0.92$
1585 reflections
114 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
$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 2.093P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.15$ e Å$^{-3}$
$\Delta\rho_{min} = -1.73$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Hg1 | 0.5000 | −0.01536 (4) | 0.2500 | 0.01426 (13) |
| Cl1 | 0.61049 (9) | −0.1178 (2) | 0.38614 (6) | 0.0215 (3) |
| C6 | 0.1775 (4) | 0.9118 (11) | 0.3998 (3) | 0.0188 (9) |
| C5 | 0.3948 (4) | 0.3872 (9) | 0.3923 (3) | 0.0178 (9) |
| H5 | 0.4536 | 0.3071 | 0.4310 | 0.021* |
| C3 | 0.2446 (3) | 0.7051 (9) | 0.3688 (3) | 0.0161 (9) |
| C2 | 0.2249 (4) | 0.6136 (9) | 0.2821 (3) | 0.0193 (9) |
| H2 | 0.1656 | 0.6871 | 0.2425 | 0.023* |
| C7 | 0.1230 (4) | 1.0887 (10) | 0.4276 (3) | 0.0179 (9) |
| C8 | 0.0599 (3) | 1.2960 (8) | 0.4641 (3) | 0.0156 (8) |
| C4 | 0.3310 (4) | 0.5860 (11) | 0.4251 (3) | 0.0196 (9) |
| H4 | 0.3457 | 0.6411 | 0.4853 | 0.024* |
| C1 | 0.2929 (4) | 0.4134 (11) | 0.2537 (3) | 0.0197 (9) |
| H1 | 0.2795 | 0.3527 | 0.1940 | 0.024* |
| C10 | 0.1000 (4) | 1.4112 (11) | 0.5461 (3) | 0.0205 (9) |
| H10 | 0.1682 | 1.3511 | 0.5772 | 0.025* |
| C9 | −0.0398 (4) | 1.3864 (10) | 0.4180 (3) | 0.0197 (9) |
| H9 | −0.0665 | 1.3092 | 0.3619 | 0.024* |
| N1 | 0.3772 (3) | 0.3030 (7) | 0.3080 (2) | 0.0141 (7) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Hg1 | 0.01265 (19) | 0.01679 (18) | 0.01374 (17) | 0.000 | 0.00326 (11) | 0.000 |
| Cl1 | 0.0189 (6) | 0.0284 (7) | 0.0167 (5) | 0.0057 (4) | 0.0013 (4) | 0.0040 (4) |
| C6 | 0.018 (3) | 0.019 (2) | 0.020 (2) | −0.001 (2) | 0.0039 (19) | 0.0006 (19) |
| C5 | 0.014 (2) | 0.020 (2) | 0.018 (2) | 0.0032 (18) | 0.0009 (17) | −0.0011 (17) |
| C3 | 0.016 (2) | 0.015 (2) | 0.018 (2) | −0.0011 (17) | 0.0063 (16) | −0.0011 (16) |
| C2 | 0.018 (2) | 0.020 (3) | 0.019 (2) | 0.0059 (19) | 0.0012 (18) | 0.0001 (18) |
| C7 | 0.018 (3) | 0.020 (2) | 0.016 (2) | −0.002 (2) | 0.0014 (18) | 0.0005 (19) |
| C8 | 0.017 (2) | 0.015 (2) | 0.0162 (19) | −0.0015 (17) | 0.0068 (16) | 0.0019 (16) |
| C4 | 0.018 (3) | 0.023 (2) | 0.018 (2) | 0.001 (2) | 0.0053 (18) | −0.005 (2) |
| C1 | 0.020 (3) | 0.024 (2) | 0.017 (2) | 0.002 (2) | 0.0060 (19) | −0.0011 (19) |
| C10 | 0.019 (3) | 0.022 (2) | 0.020 (2) | 0.004 (2) | 0.0039 (19) | 0.002 (2) |
| C9 | 0.020 (2) | 0.021 (2) | 0.018 (2) | 0.0003 (19) | 0.0041 (18) | −0.0036 (18) |
| N1 | 0.0115 (18) | 0.0172 (18) | 0.0145 (16) | −0.0012 (14) | 0.0053 (13) | −0.0004 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Hg1—Cl1$^{i}$ | 2.3719 (12) | C2—H2 | 0.9500 |
| Hg1—Cl1 | 2.3719 (12) | C7—C8 | 1.428 (6) |
| Hg1—N1$^{i}$ | 2.412 (3) | C8—C9 | 1.396 (6) |
| Hg1—N1 | 2.412 (3) | C8—C10 | 1.397 (6) |
| C6—C7 | 1.202 (8) | C4—H4 | 0.9500 |
| C6—C3 | 1.420 (6) | C1—N1 | 1.344 (6) |
| C5—N1 | 1.339 (5) | C1—H1 | 0.9500 |
| C5—C4 | 1.380 (7) | C10—C9$^{ii}$ | 1.386 (7) |
| C5—H5 | 0.9500 | C10—H10 | 0.9500 |
| C3—C2 | 1.385 (6) | C9—C10$^{ii}$ | 1.386 (7) |
| C3—C4 | 1.395 (6) | C9—H9 | 0.9500 |
| C2—C1 | 1.389 (7) | | |
| | | | |
| Cl1$^{i}$—Hg1—Cl1 | 155.82 (6) | C9—C8—C7 | 120.7 (4) |
| Cl1$^{i}$—Hg1—N1$^{i}$ | 97.08 (8) | C10—C8—C7 | 119.2 (4) |
| Cl1—Hg1—N1$^{i}$ | 98.33 (8) | C5—C4—C3 | 119.1 (4) |
| Cl1$^{i}$—Hg1—N1 | 98.33 (8) | C5—C4—H4 | 120.4 |
| Cl1—Hg1—N1 | 97.08 (8) | C3—C4—H4 | 120.4 |
| N1$^{i}$—Hg1—N1 | 100.42 (16) | N1—C1—C2 | 122.1 (4) |
| C7—C6—C3 | 178.3 (5) | N1—C1—H1 | 119.0 |
| N1—C5—C4 | 122.5 (4) | C2—C1—H1 | 119.0 |
| N1—C5—H5 | 118.7 | C9$^{ii}$—C10—C8 | 119.8 (4) |
| C4—C5—H5 | 118.7 | C9$^{ii}$—C10—H10 | 120.1 |
| C2—C3—C4 | 118.3 (4) | C8—C10—H10 | 120.1 |
| C2—C3—C6 | 120.8 (4) | C10$^{ii}$—C9—C8 | 120.1 (4) |
| C4—C3—C6 | 120.9 (4) | C10$^{ii}$—C9—H9 | 120.0 |
| C3—C2—C1 | 119.3 (4) | C8—C9—H9 | 120.0 |
| C3—C2—H2 | 120.3 | C5—N1—C1 | 118.6 (4) |
| C1—C2—H2 | 120.3 | C5—N1—Hg1 | 121.5 (3) |

| | | | |
|---|---|---|---|
| C6—C7—C8 | 177.8 (5) | C1—N1—Hg1 | 119.7 (3) |
| C9—C8—C10 | 120.1 (4) | | |
| | | | |
| C4—C3—C2—C1 | −1.6 (7) | C4—C5—N1—C1 | −1.0 (7) |
| C6—C3—C2—C1 | 179.3 (5) | C4—C5—N1—Hg1 | 174.6 (4) |
| N1—C5—C4—C3 | −0.1 (8) | C2—C1—N1—C5 | 0.8 (7) |
| C2—C3—C4—C5 | 1.4 (7) | C2—C1—N1—Hg1 | −174.9 (4) |
| C6—C3—C4—C5 | −179.5 (5) | Cl1$^{i}$—Hg1—N1—C5 | 168.6 (3) |
| C3—C2—C1—N1 | 0.6 (8) | Cl1—Hg1—N1—C5 | 7.3 (3) |
| C9—C8—C10—C9$^{ii}$ | 0.7 (8) | N1$^{i}$—Hg1—N1—C5 | −92.5 (3) |
| C7—C8—C10—C9$^{ii}$ | 179.7 (5) | Cl1$^{i}$—Hg1—N1—C1 | −15.8 (3) |
| C10—C8—C9—C10$^{ii}$ | −0.7 (8) | Cl1—Hg1—N1—C1 | −177.1 (3) |
| C7—C8—C9—C10$^{ii}$ | −179.7 (5) | N1$^{i}$—Hg1—N1—C1 | 83.0 (3) |

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