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# catena-Poly[[dibromidomercury(II)]- $\mu$ -3-(1-methylpyrrolidin-2-yl)pyridine- $\kappa^2$ N:N']

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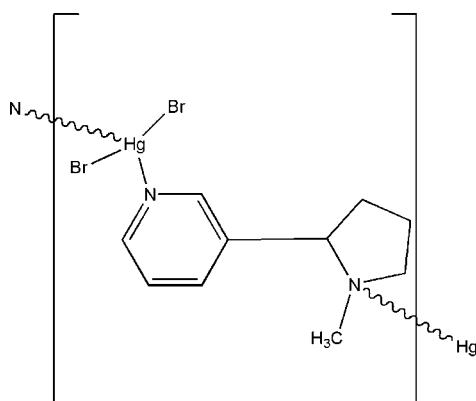
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.014$  Å;  $R$  factor = 0.038;  $wR$  factor = 0.076; data-to-parameter ratio = 19.0.

In the title polymeric complex,  $[\text{HgBr}_2(\text{C}_{10}\text{H}_{14}\text{N}_2)]_n$ , each nicotine molecule is bonded to two adjacent Hg atoms, one through the pyrrolidine N atom and the other through the pyridine N atom, forming zigzag chains along [010]. The coordination around mercury is completed by two bromido ligands resulting in a distorted tetrahedral arrangement.

## Related literature

For other nicotine complexes of copper and mercury, see: Meyer *et al.* (2006); Haendler (1990). For the isostructural dichlorido(nicotine)mercury(II) chain polymer complex, see: Udupa & Krebs (1980);



## Experimental

## Crystal data

$[\text{HgBr}_2(\text{C}_{10}\text{H}_{14}\text{N}_2)]$   
 $M_r = 522.64$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 7.6306$  (9) Å  
 $b = 11.2177$  (14) Å  
 $c = 15.443$  (2) Å

$V = 1321.9$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 17.66$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
 $0.20 \times 0.16 \times 0.12$  mm

## Data collection

Bruker SMART APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.062$ ,  $T_{\max} = 0.153$   
 (expected range = 0.049–0.120)

10476 measured reflections  
 2601 independent reflections  
 2137 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.057$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.076$   
 $S = 1.00$   
 2601 reflections  
 137 parameters  
 H-atom parameters constrained

$\Delta\rho_{\text{max}} = 1.44$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.03$  e Å<sup>-3</sup>  
 Absolute structure: Flack, (1983),  
 1083 Friedel pairs  
 Flack parameter:  $-0.006$  (16)

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXL97 (Sheldrick, 2008); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2110).

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**supplementary materials**

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***catena*-Poly[[dibromidomercury(II)]- $\mu$ -3-(1-methylpyrrolidin-2-yl)pyridine- $\kappa^2$ N:N']**

**Z. Jiang, G. Tang, Y. Zhang and J. Zhao**

**Comment**

Compounds containing nicotine [3-(1-methyl-2-pyrrolidinyl) pyridine] have been reported to form molecular and polynuclear complexes (Meyer *et al.*, 2006; Haendler, 1990). The crystal structure of the title compound appeared to be isostructural with the dichlorido(nicotine)mercury(II) chain polymer complex (Udupa & Krebs, 1980).

As illustrated in Fig. 1, each nicotine molecule in (I) is coordinated to two adjacent mercury atoms, one through the pyrrolidine nitrogen (Hg—N 2.400 (8) Å) and the other through the pyridine nitrogen (Hg—N 2.460 (8) Å), forming zig-zag polymeric chains along the *b* axis. The coordination around mercury is completed by two bromine ligands (Hg—Br 2.4760 (12) and 2.5034 (12) Å), resulting in a distorted tetrahedral arrangement. In addition, the absolute configurations of C6 and N2 can be given as *S* (*S*-nicotine was used as a starting material). No notable interactions were found between polymeric chains.

**Experimental**

HgBr<sub>2</sub> (360 mg, 1 mmol) was added to a solution of 4-cyanopyridine (104 mg, 1 mmol) in dmf (5 ml). The resulting mixture was stirred for about 10 min after which a white precipitate formed. *S*-Nicotine (3 ml) was then added dropwise to the reaction mixture and stirring was continued, during which time the precipitate changed its colour, giving a flesh colored precipitate. The precipitate was washed with ethanol and vacuum dried. Yield: 0.324 g, 62% (based on HgBr<sub>2</sub> used). The compound (100 mg) was dissolved in dmf (5 ml), the resulting solution filtered and the light-yellow filtrate transferred into a test tube and *i*-PrOH (10 ml) was carefully laid on the surface of the filtrate. Light-yellow block crystals were obtained after 15 days. Analysis: Found: C 23.12, H 2.82, N 5.26%; Calculated for C<sub>10</sub>H<sub>14</sub>HgBr<sub>2</sub>N<sub>2</sub>: C 22.98, H 2.70, N 5.36%.

**Refinement**

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 - 0.98 Å and with  $U_{\text{iso}}(\text{H}) = 1.2$  (1.5 for methyl groups) times  $U_{\text{eq}}(\text{C})$ . The absolute structure parameter  $x$  (Flack, 1983) was refined to -0.006 (16) using 1083 measured Friedel pairs.

**Figures**

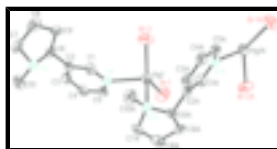


Fig. 1. Molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids. All H atoms have been omitted. Symmetry transformations: A is  $-x + 1/2, -y, z + 1/2$ .

# supplementary materials

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## catena-Poly[[dibromidomercury(II)]- $\mu$ -3-(1-methylpyrrolidin-2-yl)pyridine- $\kappa^2$ N:N']

### Crystal data

|   |   |
|---|---|
| [HgBr <sub>2</sub> (C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> )] | $F_{000} = 952$                           |
| $M_r = 522.64$  | $D_x = 2.626 \text{ Mg m}^{-3}$           |
| Orthorhombic, $P2_12_12_1$  | Mo $K\alpha$ radiation                    |
| Hall symbol: P 2ac 2ab  | $\lambda = 0.71073 \text{ \AA}$           |
| $a = 7.6306 (9) \text{ \AA}$  | Cell parameters from 3183 reflections     |
| $b = 11.2177 (14) \text{ \AA}$  | $\theta = 4.5\text{--}43.1^\circ$         |
| $c = 15.443 (2) \text{ \AA}$  | $\mu = 17.66 \text{ mm}^{-1}$             |
| $V = 1321.9 (3) \text{ \AA}^3$  | $T = 296 (2) \text{ K}$                   |
| $Z = 4$   | Block, light yellow                       |
|   | $0.20 \times 0.16 \times 0.12 \text{ mm}$ |

### Data collection

|  |  |
|--|--|
| Bruker SMART APEXII CCD diffractometer                   | 2601 independent reflections           |
| Radiation source: fine-focus sealed tube                 | 2137 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite                                  | $R_{\text{int}} = 0.057$               |
| $T = 296(2) \text{ K}$                                   | $\theta_{\text{max}} = 26.0^\circ$     |
| $\varphi$ and $\omega$ scans                             | $\theta_{\text{min}} = 2.2^\circ$      |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $h = -8 \rightarrow 9$                 |
| $T_{\text{min}} = 0.062$ , $T_{\text{max}} = 0.153$      | $k = -13 \rightarrow 13$               |
| 10476 measured reflections                               | $l = -19 \rightarrow 16$               |

### Refinement

|  |  |
|--|--|
| Refinement on $F^2$  | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full                                     | H-atom parameters constrained                            |
| $R[F^2 > 2\sigma(F^2)] = 0.039$                                | $w = 1/[\sigma^2(F_o^2) + (0.0314P)^2]$                  |
| $wR(F^2) = 0.076$  | where $P = (F_o^2 + 2F_c^2)/3$                           |
| $S = 1.00$   | $(\Delta/\sigma)_{\text{max}} = 0.001$                   |
| 2601 reflections   | $\Delta\rho_{\text{max}} = 1.44 \text{ e \AA}^{-3}$      |
| 137 parameters   | $\Delta\rho_{\text{min}} = -1.03 \text{ e \AA}^{-3}$     |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none                              |
| Secondary atom site location: difference Fourier map           | Absolute structure: Flack, (1983), 1083 Friedel pairs    |
|  | Flack parameter: $-0.006 (16)$                           |

*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 ( $\text{\AA}^2$ )*

|      | <i>x</i>     | <i>y</i>     | <i>z</i>    | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|-------------|----------------------------------|
| Br1  | 0.09573 (17) | 1.16819 (12) | 0.93970 (8) | 0.0688 (4)                       |
| Br2  | 0.15737 (16) | 1.07721 (14) | 0.64794 (8) | 0.0622 (4)                       |
| C1   | 0.2197 (13)  | 0.7896 (8)   | 0.7769 (6)  | 0.035 (2)                        |
| H1   | 0.1843       | 0.8032       | 0.7201      | 0.042*                           |
| C2   | 0.3218 (11)  | 0.6891 (8)   | 0.7935 (6)  | 0.028 (2)                        |
| C3   | 0.3679 (13)  | 0.6710 (9)   | 0.8800 (7)  | 0.044 (3)                        |
| H3   | 0.4355       | 0.6053       | 0.8952      | 0.052*                           |
| C4   | 0.3143 (14)  | 0.7495 (9)   | 0.9428 (7)  | 0.045 (3)                        |
| H4   | 0.3438       | 0.7373       | 1.0005      | 0.054*                           |
| C5   | 0.2161 (14)  | 0.8467 (9)   | 0.9184 (6)  | 0.040 (3)                        |
| H5   | 0.1806       | 0.9003       | 0.9609      | 0.048*                           |
| C6   | 0.3777 (12)  | 0.6034 (8)   | 0.7256 (6)  | 0.034 (2)                        |
| H6   | 0.4914       | 0.5703       | 0.7427      | 0.041*                           |
| C7   | 0.3129 (14)  | 0.4423 (10)  | 0.6345 (7)  | 0.055 (3)                        |
| H7A  | 0.2193       | 0.3962       | 0.6084      | 0.066*                           |
| H7B  | 0.4103       | 0.3896       | 0.6470      | 0.066*                           |
| C8   | 0.3698 (16)  | 0.5418 (10)  | 0.5746 (7)  | 0.058 (3)                        |
| H8A  | 0.2811       | 0.5570       | 0.5310      | 0.070*                           |
| H8B  | 0.4789       | 0.5216       | 0.5459      | 0.070*                           |
| C9   | 0.3936 (14)  | 0.6494 (9)   | 0.6325 (6)  | 0.047 (3)                        |
| H9A  | 0.3041       | 0.7086       | 0.6207      | 0.057*                           |
| H9B  | 0.5078       | 0.6852       | 0.6231      | 0.057*                           |
| C10  | 0.2521 (15)  | 0.4153 (9)   | 0.7882 (7)  | 0.054 (3)                        |
| H10A | 0.1949       | 0.3428       | 0.7712      | 0.081*                           |
| H10B | 0.1910       | 0.4499       | 0.8365      | 0.081*                           |
| H10C | 0.3708       | 0.3983       | 0.8047      | 0.081*                           |
| Hg1  | 0.04788 (5)  | 1.06376 (4)  | 0.80044 (3) | 0.04142 (13)                     |
| N1   | 0.1699 (10)  | 0.8672 (7)   | 0.8373 (5)  | 0.036 (2)                        |
| N2   | 0.2514 (11)  | 0.5010 (7)   | 0.7140 (5)  | 0.040 (2)                        |

## supplementary materials

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### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$    | $U^{22}$    | $U^{33}$   | $U^{12}$   | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|------------|------------|-------------|-------------|
| Br1 | 0.0714 (10) | 0.0714 (9)  | 0.0635 (8) | 0.0005 (7) | -0.0093 (6) | -0.0279 (7) |
| Br2 | 0.0525 (7)  | 0.0861 (10) | 0.0481 (7) | 0.0000 (7) | 0.0091 (5)  | 0.0157 (7)  |
| C1  | 0.043 (6)   | 0.033 (6)   | 0.029 (6)  | 0.005 (5)  | -0.011 (4)  | -0.001 (4)  |
| C2  | 0.026 (5)   | 0.025 (5)   | 0.032 (5)  | 0.002 (4)  | -0.005 (4)  | -0.001 (4)  |
| C3  | 0.037 (6)   | 0.034 (6)   | 0.060 (7)  | 0.000 (5)  | 0.000 (5)   | 0.004 (5)   |
| C4  | 0.059 (8)   | 0.038 (6)   | 0.037 (6)  | -0.015 (5) | 0.006 (5)   | 0.000 (5)   |
| C5  | 0.050 (7)   | 0.037 (6)   | 0.032 (6)  | -0.011 (5) | 0.008 (5)   | -0.001 (5)  |
| C6  | 0.023 (5)   | 0.037 (6)   | 0.044 (6)  | 0.005 (4)  | 0.001 (4)   | -0.009 (4)  |
| C7  | 0.051 (7)   | 0.042 (7)   | 0.072 (8)  | 0.012 (6)  | 0.014 (6)   | -0.020 (7)  |
| C8  | 0.068 (8)   | 0.066 (9)   | 0.041 (7)  | 0.010 (7)  | 0.009 (6)   | -0.015 (6)  |
| C9  | 0.046 (7)   | 0.052 (7)   | 0.044 (7)  | -0.011 (5) | 0.023 (5)   | -0.003 (5)  |
| C10 | 0.052 (7)   | 0.039 (7)   | 0.072 (8)  | 0.007 (5)  | -0.007 (6)  | 0.021 (6)   |
| Hg1 | 0.0416 (2)  | 0.0400 (2)  | 0.0427 (2) | 0.0040 (2) | -0.0016 (2) | -0.0011 (2) |
| N1  | 0.038 (5)   | 0.037 (5)   | 0.032 (5)  | 0.002 (4)  | 0.000 (4)   | 0.003 (4)   |
| N2  | 0.030 (4)   | 0.035 (5)   | 0.054 (6)  | 0.006 (4)  | 0.001 (4)   | -0.002 (4)  |

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

|          |             |                      |            |
|----------|-------------|----------------------|------------|
| Br1—Hg1  | 2.4760 (12) | C7—N2                | 1.470 (12) |
| Br2—Hg1  | 2.5034 (12) | C7—C8                | 1.512 (15) |
| C1—N1    | 1.332 (11)  | C7—H7A               | 0.9700     |
| C1—C2    | 1.394 (12)  | C7—H7B               | 0.9700     |
| C1—H1    | 0.9300      | C8—C9                | 1.512 (14) |
| C2—C3    | 1.396 (14)  | C8—H8A               | 0.9700     |
| C2—C6    | 1.485 (12)  | C8—H8B               | 0.9700     |
| C3—C4    | 1.372 (14)  | C9—H9A               | 0.9700     |
| C3—H3    | 0.9300      | C9—H9B               | 0.9700     |
| C4—C5    | 1.376 (14)  | C10—N2               | 1.496 (12) |
| C4—H4    | 0.9300      | C10—H10A             | 0.9600     |
| C5—N1    | 1.321 (12)  | C10—H10B             | 0.9600     |
| C5—H5    | 0.9300      | C10—H10C             | 0.9600     |
| C6—N2    | 1.510 (12)  | Hg1—N2 <sup>i</sup>  | 2.400 (8)  |
| C6—C9    | 1.532 (13)  | Hg1—N1               | 2.460 (8)  |
| C6—H6    | 0.9800      | N2—Hg1 <sup>ii</sup> | 2.400 (8)  |
| N1—C1—C2 | 124.0 (9)   | C7—C8—H8B            | 110.7      |
| N1—C1—H1 | 118.0       | C9—C8—H8B            | 110.7      |
| C2—C1—H1 | 118.0       | H8A—C8—H8B           | 108.8      |
| C1—C2—C3 | 115.8 (9)   | C8—C9—C6             | 106.0 (8)  |
| C1—C2—C6 | 123.6 (9)   | C8—C9—H9A            | 110.5      |
| C3—C2—C6 | 120.6 (8)   | C6—C9—H9A            | 110.5      |
| C4—C3—C2 | 120.5 (10)  | C8—C9—H9B            | 110.5      |
| C4—C3—H3 | 119.7       | C6—C9—H9B            | 110.5      |
| C2—C3—H3 | 119.7       | H9A—C9—H9B           | 108.7      |
| C3—C4—C5 | 118.5 (10)  | N2—C10—H10A          | 109.5      |

|            |            |                          |            |
|------------|------------|--------------------------|------------|
| C3—C4—H4   | 120.7      | N2—C10—H10B              | 109.5      |
| C5—C4—H4   | 120.7      | H10A—C10—H10B            | 109.5      |
| N1—C5—C4   | 122.9 (10) | N2—C10—H10C              | 109.5      |
| N1—C5—H5   | 118.6      | H10A—C10—H10C            | 109.5      |
| C4—C5—H5   | 118.6      | H10B—C10—H10C            | 109.5      |
| C2—C6—N2   | 113.1 (8)  | N2 <sup>i</sup> —Hg1—N1  | 96.8 (3)   |
| C2—C6—C9   | 117.9 (8)  | N2 <sup>i</sup> —Hg1—Br1 | 111.1 (2)  |
| N2—C6—C9   | 101.3 (7)  | N1—Hg1—Br1               | 99.6 (2)   |
| C2—C6—H6   | 108.0      | N2 <sup>i</sup> —Hg1—Br2 | 104.3 (2)  |
| N2—C6—H6   | 108.0      | N1—Hg1—Br2               | 98.36 (19) |
| C9—C6—H6   | 108.0      | Br1—Hg1—Br2              | 137.68 (5) |
| N2—C7—C8   | 105.8 (8)  | C5—N1—C1                 | 118.3 (8)  |
| N2—C7—H7A  | 110.6      | C5—N1—Hg1                | 118.5 (7)  |
| C8—C7—H7A  | 110.6      | C1—N1—Hg1                | 122.2 (6)  |
| N2—C7—H7B  | 110.6      | C7—N2—C10                | 110.6 (8)  |
| C8—C7—H7B  | 110.6      | C7—N2—C6                 | 103.7 (8)  |
| H7A—C7—H7B | 108.7      | C10—N2—C6                | 113.3 (8)  |
| C7—C8—C9   | 105.2 (8)  | C7—N2—Hg1 <sup>ii</sup>  | 110.9 (6)  |
| C7—C8—H8A  | 110.7      | C10—N2—Hg1 <sup>ii</sup> | 105.2 (6)  |
| C9—C8—H8A  | 110.7      | C6—N2—Hg1 <sup>ii</sup>  | 113.3 (6)  |

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

Fig. 1

