

# Dibromidobis(pyridine-3-carbonitrile- $\kappa N^1$ )mercury(II)

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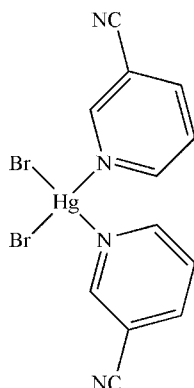
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Key indicators: single-crystal X-ray study;  $T = 120$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.030;  $wR$  factor = 0.084; data-to-parameter ratio = 23.1.

In the crystal structure of the title compound,  $[\text{HgBr}_2(\text{C}_6\text{H}_4\text{N}_2)_2]$ , the Hg atom is four coordinated by two pyridine N atoms and two  $\text{Br}^-$  anions in a considerably distorted tetrahedral environment.  $\pi$ - $\pi$  interactions between adjacent pyridine rings [centroid-centroid distance of 3.648 (3) Å] stabilize the crystal structure.

## Related literature

For related structures, see: Ghiasi (2011); Steffen & Palenik (1977); Li *et al.* (2004).



## Experimental

### Crystal data

$[\text{HgBr}_2(\text{C}_6\text{H}_4\text{N}_2)_2]$   
 $M_r = 568.61$   
Triclinic,  $P\bar{1}$   
 $a = 8.5823$  (6) Å  
 $b = 9.4069$  (6) Å  
 $c = 9.8562$  (7) Å  
 $\alpha = 81.935$  (5)°  
 $\beta = 71.435$  (6)°

$\gamma = 80.508$  (6)°  
 $V = 740.70$  (9) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 15.78$  mm<sup>-1</sup>  
 $T = 120$  K  
 $0.45 \times 0.22 \times 0.20$  mm

### Data collection

Bruker SMART CCD  
diffractometer  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 1998)  
 $T_{\min} = 0.033$ ,  $T_{\max} = 0.052$

8486 measured reflections  
3967 independent reflections  
3751 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.084$   
 $S = 1.18$   
3967 reflections

172 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 1.13$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -2.48$  e Å<sup>-3</sup>

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).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5511).

## References

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## supporting information

*Acta Cryst.* (2011). E67, m595 [https://doi.org/10.1107/S1600536811013274]

**Dibromidobis(pyridine-3-carbonitrile- $\kappa$ N<sup>1</sup>)mercury(II)****Reza Ghiasi****S1. Comment**

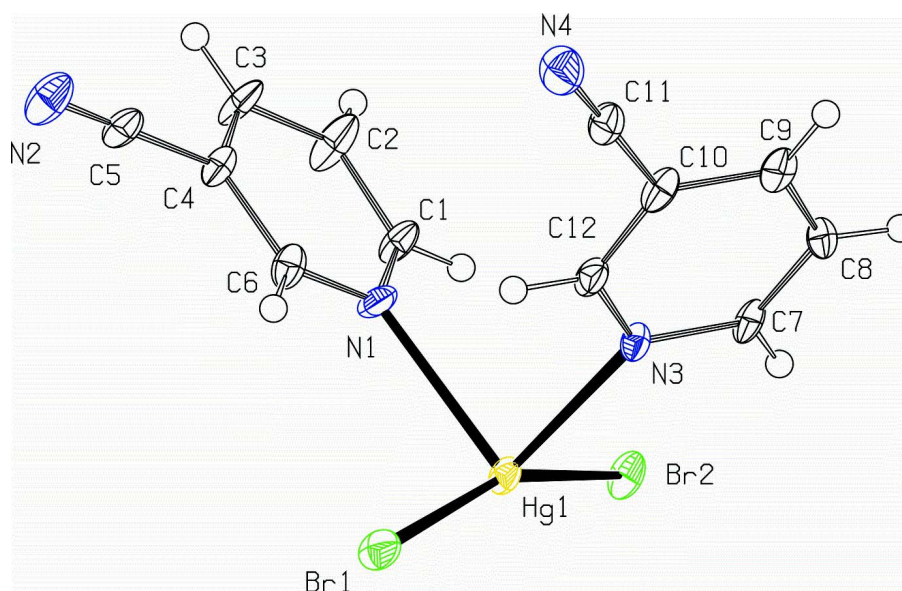
Recently, the crystal structure of dibromozinc(II)-di-3-pyridine-carbonitrile have been reported, (Ghiasi, 2011). On the other hand there are several complexes, with formula,  $[MX_2L_2]$ , such as  $[ZnCl_2(4\text{-cypy})_2]$ , (Steffen & Palenik, 1977),  $[CuBr_2(3\text{-Cypy})_2]$ , (Li *et al.* 2004), [where py is pyridine, 4-cypy is 4-cyanopyridine and 3-cypy is 3-cyanopyridine] have been synthesized and characterized by single-crystal X-ray diffraction methods. The molecular structure of the title compound is shown in Fig. 1. The Hg<sup>II</sup> atom is four-coordinated in a slightly distorted tetrahedral configuration by two N atoms from two pyridine rings and two Br<sup>-</sup> anions. The Hg—Br and Hg—N bond distances and angles (Table 1) are within normal ranges.  $\pi$ - $\pi$  interactions between adjacent pyridine rings [centroid...centroid distance of 3.648 (3) Å, symmetry code:  $-x, 1-y, 1-z$ ] stabilize the packing of the crystal structure.

**S2. Experimental**

Mercury(II) bromide (0.72 gr, 2 mmol) was dissolved in methanol (12 ml) and the solution was mixed with a methanolic solution (10 ml) of 3-pyridinecarbonitrile (0.42 g, 4 mmol). This solution was left to evaporate slowly at room temperature. After one week, colorless prismatic crystals of the title compound were isolated (yield 0.64 g, 56.0%, m.p. < 570 K).

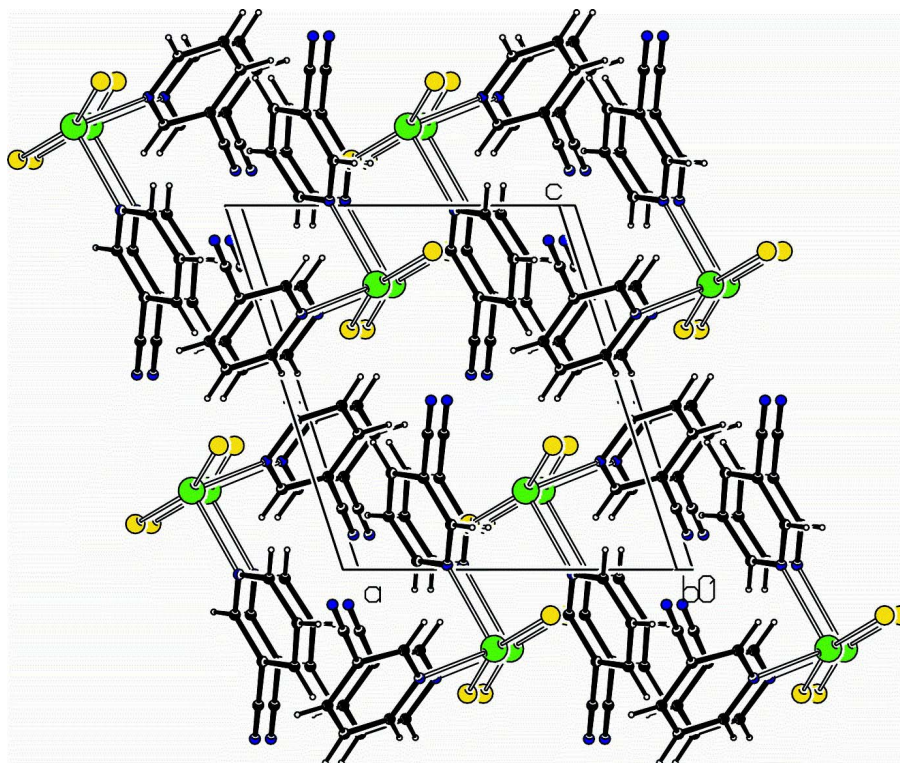
**S3. Refinement**

All H atoms were positioned geometrically, with C—H=0.96 Å aromatics hydrogen atoms and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}$ .



**Figure 1**

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



**Figure 2**

Unit-cell packing diagram for (I).

Dibromidobis(pyridine-3-carbonitrile- $\kappa N^1$ )mercury(II)

## Crystal data

[HgBr<sub>2</sub>(C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>)<sub>2</sub>] $M_r = 568.61$ Triclinic,  $P\bar{1}$ 

Hall symbol: -P 1

 $a = 8.5823$  (6) Å $b = 9.4069$  (6) Å $c = 9.8562$  (7) Å $\alpha = 81.935$  (5)° $\beta = 71.435$  (6)° $\gamma = 80.508$  (6)° $V = 740.70$  (9) Å<sup>3</sup> $Z = 2$  $F(000) = 516$  $D_x = 2.549$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 8405 reflections

 $\theta = 2.2$ – $29.2^\circ$  $\mu = 15.78$  mm<sup>-1</sup> $T = 120$  K

Prism, colorless

 $0.45 \times 0.22 \times 0.2$  mm

## Data collection

Bruker SMART CCD

diffractometer

Graphite monochromator

 $\phi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 1998)

 $T_{\min} = 0.033$ ,  $T_{\max} = 0.052$ 

8486 measured reflections

3967 independent reflections

3751 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.043$  $\theta_{\max} = 29.2^\circ$ ,  $\theta_{\min} = 2.2^\circ$  $h = -11 \rightarrow 11$  $k = -12 \rightarrow 12$  $l = -13 \rightarrow 13$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.030$  $wR(F^2) = 0.084$  $S = 1.18$ 

3967 reflections

172 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

 $w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.8751P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.013$  $\Delta\rho_{\max} = 1.13$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -2.48$  e Å<sup>-3</sup>

## 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<sup>2</sup>)

|    | $x$         | $y$        | $z$        | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|-------------|------------|------------|----------------------------------|
| C1 | 0.0093 (6)  | 0.7134 (5) | 0.4103 (5) | 0.0225 (9)                       |
| H1 | 0.0187      | 0.784      | 0.4635     | 0.027*                           |
| C2 | -0.1379 (6) | 0.6544 (5) | 0.4499 (6) | 0.0239 (9)                       |
| H2 | -0.2248     | 0.6851     | 0.5286     | 0.029*                           |

|     |             |               |               |              |
|-----|-------------|---------------|---------------|--------------|
| C3  | −0.1559 (7) | 0.5491 (5)    | 0.3719 (5)    | 0.0241 (9)   |
| H3  | −0.2534     | 0.5073        | 0.3971        | 0.029*       |
| C4  | −0.0218 (6) | 0.5089 (5)    | 0.2548 (5)    | 0.0224 (9)   |
| C5  | −0.0290 (6) | 0.4010 (5)    | 0.1668 (6)    | 0.0241 (9)   |
| C6  | 0.1248 (7)  | 0.5712 (5)    | 0.2222 (5)    | 0.0227 (9)   |
| H6  | 0.2146      | 0.5409        | 0.1454        | 0.027*       |
| C7  | 0.2284 (7)  | 1.0208 (6)    | −0.0244 (6)   | 0.0277 (10)  |
| H7  | 0.1906      | 1.0754        | 0.0541        | 0.033*       |
| C8  | 0.1848 (9)  | 1.0747 (6)    | −0.1468 (6)   | 0.0355 (13)  |
| H8  | 0.1204      | 1.1641        | −0.1508       | 0.043*       |
| C9  | 0.2387 (8)  | 0.9933 (6)    | −0.2636 (6)   | 0.0308 (11)  |
| H9  | 0.2099      | 1.0259        | −0.347        | 0.037*       |
| C10 | 0.3368 (6)  | 0.8616 (5)    | −0.2530 (5)   | 0.0221 (9)   |
| C11 | 0.3959 (7)  | 0.7725 (6)    | −0.3706 (6)   | 0.0265 (10)  |
| C12 | 0.3758 (7)  | 0.8154 (5)    | −0.1251 (5)   | 0.0237 (9)   |
| H12 | 0.4413      | 0.7271        | −0.118        | 0.028*       |
| Br1 | 0.59621 (7) | 0.60216 (6)   | 0.12550 (6)   | 0.02802 (12) |
| Br2 | 0.25093 (7) | 1.02533 (5)   | 0.34027 (6)   | 0.02714 (12) |
| Hg1 | 0.38539 (2) | 0.805335 (18) | 0.216864 (18) | 0.02106 (7)  |
| N1  | 0.1397 (5)  | 0.6727 (5)    | 0.2979 (4)    | 0.0223 (8)   |
| N2  | −0.0327 (6) | 0.3162 (5)    | 0.0956 (6)    | 0.0311 (10)  |
| N3  | 0.3219 (6)  | 0.8943 (5)    | −0.0129 (5)   | 0.0238 (8)   |
| N4  | 0.4417 (7)  | 0.7012 (5)    | −0.4646 (6)   | 0.0351 (11)  |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$      |
|-----|--------------|--------------|--------------|--------------|--------------|---------------|
| C1  | 0.027 (2)    | 0.019 (2)    | 0.022 (2)    | 0.0020 (17)  | −0.0076 (19) | −0.0081 (17)  |
| C2  | 0.020 (2)    | 0.025 (2)    | 0.024 (2)    | 0.0023 (17)  | −0.0048 (18) | −0.0038 (18)  |
| C3  | 0.027 (2)    | 0.022 (2)    | 0.021 (2)    | −0.0032 (18) | −0.0052 (19) | 0.0010 (18)   |
| C4  | 0.025 (2)    | 0.022 (2)    | 0.021 (2)    | −0.0013 (18) | −0.0076 (18) | −0.0055 (17)  |
| C5  | 0.024 (2)    | 0.024 (2)    | 0.025 (2)    | −0.0017 (18) | −0.0073 (19) | −0.0041 (18)  |
| C6  | 0.025 (2)    | 0.022 (2)    | 0.020 (2)    | −0.0005 (17) | −0.0043 (18) | −0.0075 (17)  |
| C7  | 0.035 (3)    | 0.024 (2)    | 0.025 (2)    | 0.002 (2)    | −0.010 (2)   | −0.0065 (19)  |
| C8  | 0.055 (4)    | 0.025 (2)    | 0.026 (3)    | 0.010 (2)    | −0.017 (3)   | −0.007 (2)    |
| C9  | 0.043 (3)    | 0.025 (2)    | 0.026 (2)    | 0.004 (2)    | −0.016 (2)   | −0.005 (2)    |
| C10 | 0.025 (2)    | 0.021 (2)    | 0.020 (2)    | −0.0017 (17) | −0.0062 (18) | −0.0037 (17)  |
| C11 | 0.031 (3)    | 0.025 (2)    | 0.024 (2)    | 0.0001 (19)  | −0.011 (2)   | −0.0036 (19)  |
| C12 | 0.027 (2)    | 0.021 (2)    | 0.024 (2)    | −0.0018 (18) | −0.010 (2)   | −0.0032 (18)  |
| Br1 | 0.0268 (2)   | 0.0291 (2)   | 0.0289 (3)   | 0.00759 (19) | −0.0111 (2)  | −0.01227 (19) |
| Br2 | 0.0334 (3)   | 0.0236 (2)   | 0.0239 (2)   | 0.00029 (19) | −0.0065 (2)  | −0.01056 (18) |
| Hg1 | 0.02188 (10) | 0.02100 (10) | 0.02036 (10) | 0.00031 (7)  | −0.00584 (7) | −0.00698 (7)  |
| N1  | 0.024 (2)    | 0.0245 (19)  | 0.0182 (18)  | −0.0005 (15) | −0.0058 (16) | −0.0068 (15)  |
| N2  | 0.030 (2)    | 0.029 (2)    | 0.034 (2)    | −0.0031 (18) | −0.007 (2)   | −0.0104 (19)  |
| N3  | 0.023 (2)    | 0.0250 (19)  | 0.022 (2)    | 0.0014 (16)  | −0.0068 (16) | −0.0052 (16)  |
| N4  | 0.044 (3)    | 0.031 (2)    | 0.031 (2)    | −0.001 (2)   | −0.010 (2)   | −0.009 (2)    |

*Geometric parameters (Å, °)*

|             |            |               |            |
|-------------|------------|---------------|------------|
| C1—N1       | 1.347 (6)  | C7—H7         | 0.93       |
| C1—C2       | 1.384 (7)  | C8—C9         | 1.385 (8)  |
| C1—H1       | 0.93       | C8—H8         | 0.93       |
| C2—C3       | 1.391 (7)  | C9—C10        | 1.389 (7)  |
| C2—H2       | 0.93       | C9—H9         | 0.93       |
| C3—C4       | 1.390 (7)  | C10—C12       | 1.399 (7)  |
| C3—H3       | 0.93       | C10—C11       | 1.436 (7)  |
| C4—C6       | 1.401 (7)  | C11—N4        | 1.148 (7)  |
| C4—C5       | 1.446 (7)  | C12—N3        | 1.334 (7)  |
| C5—N2       | 1.144 (7)  | C12—H12       | 0.93       |
| C6—N1       | 1.337 (6)  | Br1—Hg1       | 2.4581 (5) |
| C6—H6       | 0.93       | Br2—Hg1       | 2.4736 (5) |
| C7—N3       | 1.333 (7)  | Hg1—N1        | 2.481 (4)  |
| C7—C8       | 1.381 (8)  | Hg1—N3        | 2.496 (4)  |
| N1—C1—C2    | 122.7 (5)  | C8—C9—C10     | 118.4 (5)  |
| N1—C1—H1    | 118.7      | C8—C9—H9      | 120.8      |
| C2—C1—H1    | 118.7      | C10—C9—H9     | 120.8      |
| C1—C2—C3    | 120.0 (5)  | C9—C10—C12    | 119.1 (5)  |
| C1—C2—H2    | 120        | C9—C10—C11    | 120.7 (5)  |
| C3—C2—H2    | 120        | C12—C10—C11   | 120.1 (4)  |
| C4—C3—C2    | 117.1 (5)  | N4—C11—C10    | 179.3 (6)  |
| C4—C3—H3    | 121.4      | N3—C12—C10    | 121.9 (5)  |
| C2—C3—H3    | 121.4      | N3—C12—H12    | 119        |
| C3—C4—C6    | 120.0 (5)  | C10—C12—H12   | 119        |
| C3—C4—C5    | 121.2 (5)  | Br1—Hg1—Br2   | 159.99 (2) |
| C6—C4—C5    | 118.8 (5)  | Br1—Hg1—N1    | 98.01 (10) |
| N2—C5—C4    | 179.0 (6)  | Br2—Hg1—N1    | 97.02 (10) |
| N1—C6—C4    | 122.1 (5)  | Br1—Hg1—N3    | 97.22 (10) |
| N1—C6—H6    | 119        | Br2—Hg1—N3    | 95.88 (10) |
| C4—C6—H6    | 119        | N1—Hg1—N3     | 90.10 (14) |
| N3—C7—C8    | 123.4 (5)  | C6—N1—C1      | 118.1 (4)  |
| N3—C7—H7    | 118.3      | C6—N1—Hg1     | 121.2 (3)  |
| C8—C7—H7    | 118.3      | C1—N1—Hg1     | 120.3 (3)  |
| C7—C8—C9    | 118.7 (5)  | C7—N3—C12     | 118.5 (5)  |
| C7—C8—H8    | 120.6      | C7—N3—Hg1     | 120.3 (3)  |
| C9—C8—H8    | 120.6      | C12—N3—Hg1    | 121.2 (3)  |
| N1—C1—C2—C3 | −0.3 (8)   | C2—C1—N1—C6   | 0.0 (7)    |
| C1—C2—C3—C4 | −0.5 (7)   | C2—C1—N1—Hg1  | 172.5 (4)  |
| C2—C3—C4—C6 | 1.7 (7)    | Br1—Hg1—N1—C6 | −38.3 (4)  |
| C2—C3—C4—C5 | −179.7 (5) | Br2—Hg1—N1—C6 | 155.0 (4)  |
| C3—C4—C5—N2 | 16E1 (4)   | N3—Hg1—N1—C6  | 59.0 (4)   |
| C6—C4—C5—N2 | −2E1 (4)   | Br1—Hg1—N1—C1 | 149.5 (4)  |
| C3—C4—C6—N1 | −2.1 (8)   | Br2—Hg1—N1—C1 | −17.2 (4)  |
| C5—C4—C6—N1 | 179.3 (5)  | N3—Hg1—N1—C1  | −113.2 (4) |

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|                |            |                |            |
|----------------|------------|----------------|------------|
| N3—C7—C8—C9    | 0.8 (10)   | C8—C7—N3—C12   | −0.2 (9)   |
| C7—C8—C9—C10   | −1.0 (10)  | C8—C7—N3—Hg1   | −178.2 (5) |
| C8—C9—C10—C12  | 0.7 (9)    | C10—C12—N3—C7  | −0.1 (8)   |
| C8—C9—C10—C11  | 179.9 (6)  | C10—C12—N3—Hg1 | 177.9 (4)  |
| C9—C10—C11—N4  | −6E1 (5)   | Br1—Hg1—N3—C7  | −169.9 (4) |
| C12—C10—C11—N4 | 12E1 (5)   | Br2—Hg1—N3—C7  | −5.0 (4)   |
| C9—C10—C12—N3  | −0.2 (8)   | N1—Hg1—N3—C7   | 92.1 (4)   |
| C11—C10—C12—N3 | −179.3 (5) | Br1—Hg1—N3—C12 | 12.2 (4)   |
| C4—C6—N1—C1    | 1.2 (7)    | Br2—Hg1—N3—C12 | 177.1 (4)  |
| C4—C6—N1—Hg1   | −171.2 (4) | N1—Hg1—N3—C12  | −85.9 (4)  |

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