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# Dibromido{2-[(4-nitrophenyl)iminomethyl]pyridine-$\kappa^2N,N'$}zinc(II)

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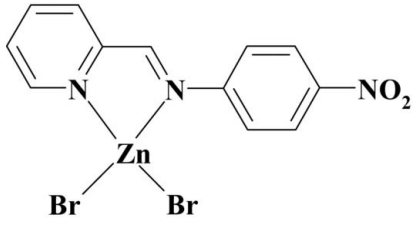
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(Br–Zn) = 0.007 Å; disorder in main residue; $R$ factor = 0.056; $wR$ factor = 0.140; data-to-parameter ratio = 13.7.

In the title compound, $[ZnBr_2(C_{12}H_9N_3O_2)]$, the $Zn^{II}$ ion is bonded to two Br ions and two N atoms of the diimine ligand in a distorted tetrahedral geometry. With the exception of the Br atoms, all other atoms are disordered over two sets of sites corresponding to a 180° rotation of the molecule along $[\bar{1}02]$. The refined occupancies of the components are 0.809 (2) and 0.191 (2). In addition, the crystal studied was a non-merohedral twin with a refined component ratio of 0.343 (2):0.657 (2).

## Related literature

For related structures, see: Khalaj *et al.* (2009). For background information on diimine complexes, see: Khalaj *et al.* (2010); Salehzadeh *et al.* (2011).




## Experimental

### Crystal data

$[ZnBr_2(C_{12}H_9N_3O_2)]$
$M_r$ = 452.41
Triclinic, $P\bar{1}$
$a$ = 7.2614 (5) Å
$b$ = 7.9228 (8) Å
$c$ = 13.6436 (15) Å
$\alpha$ = 87.724 (4)°
$\beta$ = 74.719 (6)°
$\gamma$ = 82.007 (6)°
$V$ = 749.81 (12) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 6.97 mm$^{-1}$
$T$ = 150 K
0.28 × 0.15 × 0.08 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min}$ = 0.417, $T_{max}$ = 0.588
5868 measured reflections
3252 independent reflections
2630 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.082

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.140
$S$ = 1.04
3252 reflections
237 parameters
48 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.24 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Br1—Zn1 | 2.3428 (14) | Zn1—N1 | 2.034 (9) |
| Br2—Zn1 | 2.3357 (16) | Zn1—N2 | 2.074 (7) |
| N1—Zn1—N2 | 81.2 (3) | N1—Zn1—Br1 | 112.3 (3) |
| N1—Zn1—Br2 | 116.1 (3) | N2—Zn1—Br1 | 111.5 (2) |
| N2—Zn1—Br2 | 118.0 (2) | Br2—Zn1—Br1 | 113.75 (5) |

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2406).

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# supporting information

*Acta Cryst.* (2011). E**67**, m1556 [doi:10.1107/S1600536811042231]

# Dibromido{2-[(4-nitrophenyl)iminomethyl]pyridine-$\kappa^2N,N'$}zinc(II)

**Sadegh Salehzadeh, Mehdi Khalaj, Saeed Dehghanpour and Isaac Tarmoradi**

## S1. Comment

In our ongoing studies on the synthesis, structural and spectroscopic characterization of transition metal complexes with diimine ligands Khalaj *et al.* (2010); Salehzadeh *et al.* (2011), we report herein the crystal structure of the title complex that was prepared by the reaction of $ZnBr_2$ with the bidentate ligand (4-nitrophenyl)-pyridine-2-ylmethylene-amine (Scheme I).

The molecluar structure of the title complex is shown in Fig. 1. The $Zn^{II}$ ion is in a distorted tetrahedral environment formed by the chelating ligand and two Br ions. A comparison of the dihedral angles between the planes of the pyridine, chelate and the benzene ring indicates that the ligand is distorted from planarity, with twist of 22.23 (24)° between the chelate (N1C5C6N2) and the benzene (C7C8C9C10C11C12) planes. The Zn—Br and Zn—N bond dimensions compare well with the values found in other tetrahedral diimine complexes of zinc bromide (Khalaj *et al.*, 2009).

## S2. Experimental

The title complex was prepared by the reaction of $ZnBr_2$ (22.5 mg, 0.1 mmol) and (4-nitrophenyl)pyridin-2-ylmethylene-amine (22.7 mg, 0.1 mmol) in 15 ml acetonitrile at room temperature. The solution was then concentrated under vacuum, and diffusion of diethyl ether vapor into the concentrated solution gave yellow crystals of the title compound in 60% yield.

## S3. Refinement

The H(C) atom positions were calculated and refined in isotropic approximation within riding model with the $U_{iso}$(H) parameters equal to 1.2 $U_{eq}$(C) where $U_{eq}$(C) is the equivalent thermal parameter of the carbon atoms to which corresponding H atoms are bonded. When the results of the initial refinements of the structure were examined for twinning the PLATON (Spek, 2009) software indicated that the crystal was a non-merohedral twin with twin matrix -1 0 0, 0 -1 0, -1 0 1. When refined using data generated by this twin matrix the ratio of the twin components refined to 0.342 (2): 0.658. Further to refinement of the twin components, residual electron density peaks were located in difference Fourier maps which indicated the structure was disordered. All atoms, except for the Br atoms were modeled as disordered corresponding to a rotation of approximately 180° (see Fig. 1). The Br atoms related by unit cell translations along the a axis are in sites which coordinate to both the major and minor components of disorder with an occupancy ratio of 0.809 (2):0.191 (2). The geometry of the twin components were constrained to be the same using the SAME instruction in SHELXL (Sheldrick, 2008) and the anisotropic displacement parameters of each individual major and minor atom site were constrained to be equal using the EADP instruction in SHELXL. The twin law corresponds to a 180° rotation about the [-1 0 2] direction and this direction is parallel to the rotation axis relating the two disordered sites of the molecule.

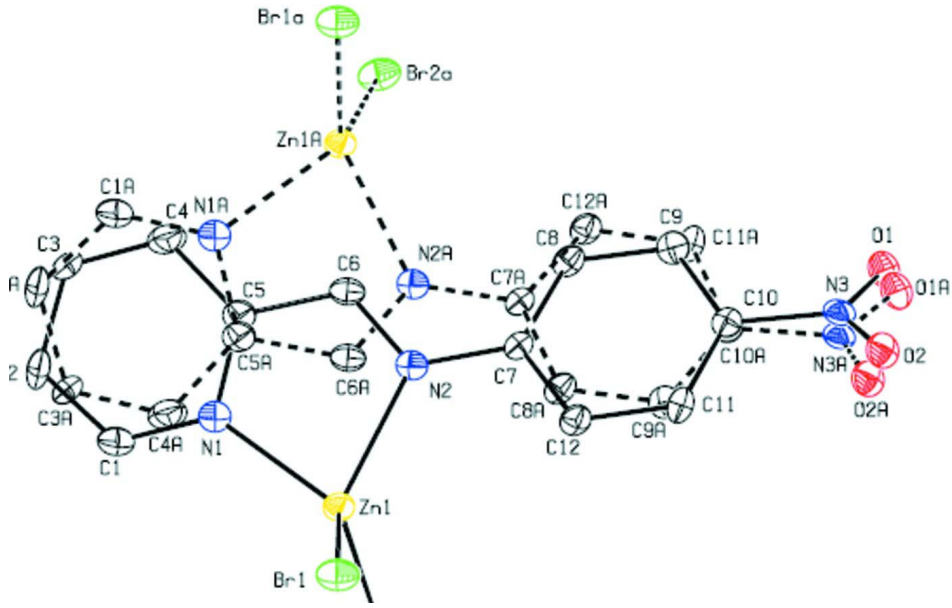


**Figure 1**

The molecular structure of the title compound showing both disordered components. The minor component is labeled with the suffix ′A′. The atoms Br1a and Br2a are related by the symmetry operation (x-1, y, x).

**Dibromido{2-[(4-nitrophenyl)iminomethyl]pyridine- $\kappa^2N,N'$}zinc(II)**

*Crystal data*

$[ZnBr_2(C_{12}H_9N_3O_2)]$
$M_r = 452.41$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2614$ (5) Å
$b = 7.9228$ (8) Å
$c = 13.6436$ (15) Å
$\alpha = 87.724$ (4)°
$\beta = 74.719$ (6)°
$\gamma = 82.007$ (6)°
$V = 749.81$ (12) Å$^3$
$Z = 2$
$F(000) = 436$
$D_x = 2.004$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6572 reflections
$\theta = 2.6$–27.5°
$\mu = 6.97$ mm$^{-1}$
$T = 150$ K
Plate, colourless
0.28 × 0.15 × 0.08 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm$^{-1}$
$\varphi$ scans and $\omega$ scans with $\kappa$ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.417$, $T_{max} = 0.588$
5868 measured reflections
3252 independent reflections
2630 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.6°$
$h = -9\rightarrow9$
$k = -10\rightarrow10$
$l = -9\rightarrow17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.140$
$S = 1.04$
3252 reflections
237 parameters
48 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
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 2.802P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.70$ e Å$^{-3}$
$\Delta\rho_{min} = -1.24$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Br1 | 0.33600 (13) | 0.49862 (12) | 0.72990 (8) | 0.0358 (2) | |
| Br2 | 0.43682 (13) | −0.00007 (12) | 0.71961 (8) | 0.0366 (3) | |
| Zn1 | 0.20560 (17) | 0.24153 (16) | 0.74480 (11) | 0.0259 (3) | 0.809 (2) |
| O1 | 0.056 (2) | 0.137 (2) | 0.2086 (8) | 0.036 (3) | 0.809 (2) |
| O2 | 0.2084 (14) | 0.3589 (19) | 0.1962 (8) | 0.034 (3) | 0.809 (2) |
| N1 | −0.0223 (12) | 0.2369 (13) | 0.8687 (7) | 0.027 (2) | 0.809 (2) |
| N2 | −0.0123 (10) | 0.2536 (11) | 0.6714 (6) | 0.0235 (16) | 0.809 (2) |
| N3 | 0.1139 (15) | 0.2531 (18) | 0.2458 (5) | 0.027 (2) | 0.809 (2) |
| C1 | −0.0292 (14) | 0.2250 (15) | 0.9678 (9) | 0.032 (2) | 0.809 (2) |
| H1A | 0.0888 | 0.2123 | 0.9868 | 0.038* | 0.809 (2) |
| C2 | −0.2000 (15) | 0.2302 (17) | 1.0447 (9) | 0.036 (3) | 0.809 (2) |
| H2A | −0.1998 | 0.2239 | 1.1143 | 0.043* | 0.809 (2) |
| C3 | −0.3711 (15) | 0.245 (2) | 1.0150 (10) | 0.038 (3) | 0.809 (2) |
| H3A | −0.4906 | 0.2452 | 1.0647 | 0.046* | 0.809 (2) |
| C4 | −0.3672 (16) | 0.259 (2) | 0.9150 (10) | 0.042 (3) | 0.809 (2) |
| H4A | −0.4839 | 0.2762 | 0.8947 | 0.050* | 0.809 (2) |
| C5 | −0.1929 (19) | 0.249 (2) | 0.8435 (6) | 0.029 (2) | 0.809 (2) |
| C6 | −0.1789 (12) | 0.2637 (12) | 0.7350 (8) | 0.027 (2) | 0.809 (2) |
| H6A | −0.2922 | 0.2807 | 0.7115 | 0.032* | 0.809 (2) |
| C7 | 0.0079 (12) | 0.2568 (13) | 0.5649 (7) | 0.022 (2) | 0.809 (2) |
| C8 | −0.1213 (16) | 0.1964 (17) | 0.5189 (8) | 0.026 (2) | 0.809 (2) |
| H8A | −0.2320 | 0.1533 | 0.5603 | 0.032* | 0.809 (2) |
| C9 | −0.091 (2) | 0.198 (2) | 0.4148 (11) | 0.028 (3) | 0.809 (2) |
| H9A | −0.1801 | 0.1597 | 0.3837 | 0.033* | 0.809 (2) |
| C10 | 0.074 (3) | 0.259 (2) | 0.3573 (6) | 0.023 (3) | 0.809 (2) |

| | | | | | |
|---|---|---|---|---|---|
| C11 | 0.2013 (19) | 0.3242 (17) | 0.3996 (9) | 0.024 (3) | 0.809 (2) |
| H11A | 0.3071 | 0.3731 | 0.3575 | 0.029* | 0.809 (2) |
| C12 | 0.1737 (16) | 0.3183 (16) | 0.5044 (8) | 0.027 (2) | 0.809 (2) |
| H12A | 0.2651 | 0.3551 | 0.5345 | 0.032* | 0.809 (2) |
| Zn1A | −0.4500 (7) | 0.2540 (7) | 0.7425 (4) | 0.0259 (3) | 0.191 (2) |
| O1A | 0.101 (12) | 0.141 (12) | 0.196 (3) | 0.036 (3) | 0.191 (2) |
| O2A | 0.252 (8) | 0.354 (10) | 0.211 (3) | 0.034 (3) | 0.191 (2) |
| N1A | −0.349 (2) | 0.259 (6) | 0.8676 (10) | 0.027 (2) | 0.191 (2) |
| N2A | −0.1587 (13) | 0.243 (4) | 0.6709 (11) | 0.0235 (16) | 0.191 (2) |
| N3A | 0.156 (7) | 0.240 (8) | 0.2468 (11) | 0.027 (2) | 0.191 (2) |
| C1A | −0.441 (3) | 0.265 (6) | 0.9666 (11) | 0.032 (2) | 0.191 (2) |
| H1AA | −0.5778 | 0.2718 | 0.9850 | 0.038* | 0.191 (2) |
| C2A | −0.348 (4) | 0.262 (8) | 1.0440 (14) | 0.036 (3) | 0.191 (2) |
| H2AA | −0.4183 | 0.2797 | 1.1130 | 0.043* | 0.191 (2) |
| C3A | −0.147 (4) | 0.233 (9) | 1.0156 (16) | 0.038 (3) | 0.191 (2) |
| H3AA | −0.0783 | 0.2113 | 1.0660 | 0.046* | 0.191 (2) |
| C4A | −0.051 (3) | 0.234 (10) | 0.916 (2) | 0.042 (3) | 0.191 (2) |
| H4AA | 0.0856 | 0.2229 | 0.8961 | 0.050* | 0.191 (2) |
| C5A | −0.154 (3) | 0.252 (7) | 0.8437 (12) | 0.029 (2) | 0.191 (2) |
| C6A | −0.0591 (17) | 0.252 (5) | 0.7351 (15) | 0.027 (2) | 0.191 (2) |
| H6AA | 0.0752 | 0.2576 | 0.7121 | 0.032* | 0.191 (2) |
| C7A | −0.072 (2) | 0.246 (4) | 0.5645 (11) | 0.022 (2) | 0.191 (2) |
| C8A | 0.108 (4) | 0.298 (7) | 0.5209 (16) | 0.026 (2) | 0.191 (2) |
| H8AA | 0.1774 | 0.3375 | 0.5635 | 0.032* | 0.191 (2) |
| C9A | 0.187 (6) | 0.292 (10) | 0.4172 (18) | 0.028 (3) | 0.191 (2) |
| H9AA | 0.3085 | 0.3294 | 0.3875 | 0.033* | 0.191 (2) |
| C10A | 0.083 (8) | 0.231 (11) | 0.3581 (11) | 0.023 (3) | 0.191 (2) |
| C11A | −0.090 (8) | 0.169 (11) | 0.3986 (17) | 0.024 (3) | 0.191 (2) |
| H11B | −0.1520 | 0.1210 | 0.3556 | 0.029* | 0.191 (2) |
| C12A | −0.171 (5) | 0.178 (8) | 0.5029 (14) | 0.027 (2) | 0.191 (2) |
| H12B | −0.2923 | 0.1394 | 0.5319 | 0.032* | 0.191 (2) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0307 (5) | 0.0262 (4) | 0.0540 (6) | −0.0087 (3) | −0.0146 (5) | −0.0002 (5) |
| Br2 | 0.0281 (4) | 0.0272 (4) | 0.0537 (7) | −0.0054 (3) | −0.0079 (5) | −0.0030 (5) |
| Zn1 | 0.0226 (5) | 0.0275 (5) | 0.0292 (6) | −0.0083 (4) | −0.0068 (5) | −0.0006 (6) |
| O1 | 0.041 (9) | 0.039 (4) | 0.031 (5) | −0.007 (6) | −0.013 (4) | −0.010 (4) |
| O2 | 0.037 (7) | 0.035 (4) | 0.029 (5) | −0.010 (5) | −0.009 (4) | 0.009 (4) |
| N1 | 0.028 (4) | 0.024 (4) | 0.031 (5) | −0.005 (3) | −0.008 (4) | 0.001 (5) |
| N2 | 0.026 (4) | 0.016 (4) | 0.031 (4) | −0.004 (3) | −0.009 (4) | −0.004 (4) |
| N3 | 0.023 (6) | 0.029 (4) | 0.031 (4) | 0.006 (5) | −0.013 (4) | −0.003 (5) |
| C1 | 0.026 (5) | 0.032 (5) | 0.040 (7) | −0.001 (4) | −0.013 (5) | 0.003 (6) |
| C2 | 0.042 (6) | 0.043 (7) | 0.017 (5) | −0.007 (6) | 0.003 (5) | −0.006 (6) |
| C3 | 0.018 (5) | 0.065 (9) | 0.028 (7) | −0.005 (5) | 0.002 (5) | −0.008 (7) |
| C4 | 0.023 (5) | 0.060 (8) | 0.042 (8) | −0.010 (5) | −0.006 (6) | 0.012 (8) |
| C5 | 0.026 (6) | 0.029 (4) | 0.034 (5) | −0.009 (5) | −0.008 (5) | −0.009 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.023 (4) | 0.023 (5) | 0.037 (6) | −0.006 (4) | −0.011 (5) | 0.001 (5) |
| C7 | 0.020 (6) | 0.020 (4) | 0.024 (4) | −0.002 (5) | −0.002 (4) | 0.001 (4) |
| C8 | 0.025 (6) | 0.022 (5) | 0.030 (6) | −0.009 (4) | −0.001 (5) | 0.000 (5) |
| C9 | 0.031 (6) | 0.019 (8) | 0.033 (7) | −0.004 (5) | −0.008 (5) | −0.007 (5) |
| C10 | 0.025 (4) | 0.015 (8) | 0.027 (4) | 0.003 (4) | −0.006 (4) | 0.001 (4) |
| C11 | 0.033 (6) | 0.014 (6) | 0.021 (6) | −0.005 (4) | 0.001 (5) | 0.002 (4) |
| C12 | 0.025 (6) | 0.027 (5) | 0.029 (6) | −0.011 (5) | −0.003 (4) | −0.001 (5) |
| Zn1A | 0.0226 (5) | 0.0275 (5) | 0.0292 (6) | −0.0083 (4) | −0.0068 (5) | −0.0006 (6) |
| O1A | 0.041 (9) | 0.039 (4) | 0.031 (5) | −0.007 (6) | −0.013 (4) | −0.010 (4) |
| O2A | 0.037 (7) | 0.035 (4) | 0.029 (5) | −0.010 (5) | −0.009 (4) | 0.009 (4) |
| N1A | 0.028 (4) | 0.024 (4) | 0.031 (5) | −0.005 (3) | −0.008 (4) | 0.001 (5) |
| N2A | 0.026 (4) | 0.016 (4) | 0.031 (4) | −0.004 (3) | −0.009 (4) | −0.004 (4) |
| N3A | 0.023 (6) | 0.029 (4) | 0.031 (4) | 0.006 (5) | −0.013 (4) | −0.003 (5) |
| C1A | 0.026 (5) | 0.032 (5) | 0.040 (7) | −0.001 (4) | −0.013 (5) | 0.003 (6) |
| C2A | 0.042 (6) | 0.043 (7) | 0.017 (5) | −0.007 (6) | 0.003 (5) | −0.006 (6) |
| C3A | 0.018 (5) | 0.065 (9) | 0.028 (7) | −0.005 (5) | 0.002 (5) | −0.008 (7) |
| C4A | 0.023 (5) | 0.060 (8) | 0.042 (8) | −0.010 (5) | −0.006 (6) | 0.012 (8) |
| C5A | 0.026 (6) | 0.029 (4) | 0.034 (5) | −0.009 (5) | −0.008 (5) | −0.009 (5) |
| C6A | 0.023 (4) | 0.023 (5) | 0.037 (6) | −0.006 (4) | −0.011 (5) | 0.001 (5) |
| C7A | 0.020 (6) | 0.020 (4) | 0.024 (4) | −0.002 (5) | −0.002 (4) | 0.001 (4) |
| C8A | 0.025 (6) | 0.022 (5) | 0.030 (6) | −0.009 (4) | −0.001 (5) | 0.000 (5) |
| C9A | 0.031 (6) | 0.019 (8) | 0.033 (7) | −0.004 (5) | −0.008 (5) | −0.007 (5) |
| C10A | 0.025 (4) | 0.015 (8) | 0.027 (4) | 0.003 (4) | −0.006 (4) | 0.001 (4) |
| C11A | 0.033 (6) | 0.014 (6) | 0.021 (6) | −0.005 (4) | 0.001 (5) | 0.002 (4) |
| C12A | 0.025 (6) | 0.027 (5) | 0.029 (6) | −0.011 (5) | −0.003 (4) | −0.001 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—Zn1A$^{i}$ | 2.340 (5) | C12—H12A | 0.9500 |
| Br1—Zn1 | 2.3428 (14) | Zn1A—N1A | 2.033 (9) |
| Br2—Zn1 | 2.3357 (16) | Zn1A—N2A | 2.074 (8) |
| Br2—Zn1A$^{i}$ | 2.339 (5) | Zn1A—Br2$^{ii}$ | 2.339 (5) |
| Zn1—N1 | 2.034 (9) | Zn1A—Br1$^{ii}$ | 2.340 (5) |
| Zn1—N2 | 2.074 (7) | O1A—N3A | 1.239 (10) |
| O1—N3 | 1.239 (10) | O2A—N3A | 1.226 (10) |
| O2—N3 | 1.226 (10) | N1A—C1A | 1.340 (14) |
| N1—C1 | 1.340 (14) | N1A—C5A | 1.361 (16) |
| N1—C5 | 1.361 (16) | N2A—C6A | 1.284 (11) |
| N2—C6 | 1.284 (11) | N2A—C7A | 1.422 (12) |
| N2—C7 | 1.421 (12) | N3A—C10A | 1.472 (10) |
| N3—C10 | 1.472 (10) | C1A—C2A | 1.394 (14) |
| C1—C2 | 1.394 (14) | C1A—H1AA | 0.9500 |
| C1—H1A | 0.9500 | C2A—C3A | 1.394 (15) |
| C2—C3 | 1.394 (15) | C2A—H2AA | 0.9500 |
| C2—H2A | 0.9500 | C3A—C4A | 1.357 (18) |
| C3—C4 | 1.357 (18) | C3A—H3AA | 0.9500 |
| C3—H3A | 0.9500 | C4A—C5A | 1.373 (16) |
| C4—C5 | 1.373 (16) | C4A—H4AA | 0.9500 |

| | | | |
|---|---|---|---|
| C4—H4A | 0.9500 | C5A—C6A | 1.459 (14) |
| C5—C6 | 1.459 (14) | C6A—H6AA | 0.9500 |
| C6—H6A | 0.9500 | C7A—C8A | 1.400 (14) |
| C7—C8 | 1.400 (14) | C7A—C12A | 1.406 (12) |
| C7—C12 | 1.405 (12) | C8A—C9A | 1.379 (18) |
| C8—C9 | 1.379 (18) | C8A—H8AA | 0.9500 |
| C8—H8A | 0.9500 | C9A—C10A | 1.381 (18) |
| C9—C10 | 1.381 (18) | C9A—H9AA | 0.9500 |
| C9—H9A | 0.9500 | C10A—C11A | 1.380 (19) |
| C10—C11 | 1.380 (19) | C11A—C12A | 1.390 (16) |
| C11—C12 | 1.390 (16) | C11A—H11B | 0.9500 |
| C11—H11A | 0.9500 | C12A—H12B | 0.9500 |

| | | | |
|---|---|---|---|
| Zn1A$^{i}$—Br1—Zn1 | 64.77 (11) | C7—C12—H12A | 120.6 |
| Zn1—Br2—Zn1A$^{i}$ | 64.90 (12) | N1A—Zn1A—N2A | 81.2 (3) |
| N1—Zn1—N2 | 81.2 (3) | N1A—Zn1A—Br2$^{ii}$ | 114.8 (13) |
| N1—Zn1—Br2 | 116.1 (3) | N2A—Zn1A—Br2$^{ii}$ | 110.8 (8) |
| N2—Zn1—Br2 | 118.0 (2) | N1A—Zn1A—Br1$^{ii}$ | 111.9 (12) |
| N1—Zn1—Br1 | 112.3 (3) | N2A—Zn1A—Br1$^{ii}$ | 120.6 (8) |
| N2—Zn1—Br1 | 111.5 (2) | Br2$^{ii}$—Zn1A—Br1$^{ii}$ | 113.73 (19) |
| Br2—Zn1—Br1 | 113.75 (5) | C1A—N1A—C5A | 116.9 (9) |
| C1—N1—C5 | 117.0 (8) | C1A—N1A—Zn1A | 130.7 (7) |
| C1—N1—Zn1 | 130.6 (7) | C5A—N1A—Zn1A | 112.4 (7) |
| C5—N1—Zn1 | 112.4 (7) | C6A—N2A—C7A | 121.1 (8) |
| C6—N2—C7 | 121.2 (7) | C6A—N2A—Zn1A | 111.5 (6) |
| C6—N2—Zn1 | 111.5 (6) | C7A—N2A—Zn1A | 127.0 (6) |
| C7—N2—Zn1 | 127.2 (5) | O2A—N3A—O1A | 124.4 (8) |
| O2—N3—O1 | 124.5 (7) | O2A—N3A—C10A | 117.9 (9) |
| O2—N3—C10 | 118.0 (9) | O1A—N3A—C10A | 117.4 (9) |
| O1—N3—C10 | 117.5 (9) | N1A—C1A—C2A | 123.4 (10) |
| N1—C1—C2 | 123.6 (10) | N1A—C1A—H1AA | 118.3 |
| N1—C1—H1A | 118.2 | C2A—C1A—H1AA | 118.3 |
| C2—C1—H1A | 118.2 | C1A—C2A—C3A | 117.0 (12) |
| C1—C2—C3 | 117.2 (12) | C1A—C2A—H2AA | 121.5 |
| C1—C2—H2A | 121.4 | C3A—C2A—H2AA | 121.5 |
| C3—C2—H2A | 121.4 | C4A—C3A—C2A | 119.8 (12) |
| C4—C3—C2 | 120.0 (11) | C4A—C3A—H3AA | 120.1 |
| C4—C3—H3A | 120.0 | C2A—C3A—H3AA | 120.1 |
| C2—C3—H3A | 120.0 | C3A—C4A—C5A | 119.3 (11) |
| C3—C4—C5 | 119.4 (11) | C3A—C4A—H4AA | 120.4 |
| C3—C4—H4A | 120.3 | C5A—C4A—H4AA | 120.4 |
| C5—C4—H4A | 120.3 | N1A—C5A—C4A | 122.7 (10) |
| N1—C5—C4 | 122.6 (10) | N1A—C5A—C6A | 115.1 (9) |
| N1—C5—C6 | 115.1 (9) | C4A—C5A—C6A | 122.1 (12) |
| C4—C5—C6 | 122.1 (11) | N2A—C6A—C5A | 119.5 (9) |
| N2—C6—C5 | 119.5 (9) | N2A—C6A—H6AA | 120.2 |
| N2—C6—H6A | 120.2 | C5A—C6A—H6AA | 120.2 |
| C5—C6—H6A | 120.2 | C8A—C7A—C12A | 119.9 (9) |

| | | | |
|---|---|---|---|
| C8—C7—C12 | 119.9 (8) | C8A—C7A—N2A | 123.9 (8) |
| C8—C7—N2 | 123.9 (8) | C12A—C7A—N2A | 116.0 (8) |
| C12—C7—N2 | 116.1 (8) | C9A—C8A—C7A | 121.2 (10) |
| C9—C8—C7 | 121.2 (10) | C9A—C8A—H8AA | 119.4 |
| C9—C8—H8A | 119.4 | C7A—C8A—H8AA | 119.4 |
| C7—C8—H8A | 119.4 | C8A—C9A—C10A | 117.6 (12) |
| C8—C9—C10 | 117.6 (11) | C8A—C9A—H9AA | 121.2 |
| C8—C9—H9A | 121.2 | C10A—C9A—H9AA | 121.2 |
| C10—C9—H9A | 121.2 | C11A—C10A—C9A | 122.9 (9) |
| C11—C10—C9 | 122.9 (8) | C11A—C10A—N3A | 118.6 (12) |
| C11—C10—N3 | 118.7 (12) | C9A—C10A—N3A | 118.4 (13) |
| C9—C10—N3 | 118.4 (13) | C10A—C11A—C12A | 119.5 (10) |
| C10—C11—C12 | 119.4 (9) | C10A—C11A—H11B | 120.3 |
| C10—C11—H11A | 120.3 | C12A—C11A—H11B | 120.3 |
| C12—C11—H11A | 120.3 | C11A—C12A—C7A | 118.7 (10) |
| C11—C12—C7 | 118.7 (10) | C11A—C12A—H12B | 120.6 |
| C11—C12—H12A | 120.6 | C7A—C12A—H12B | 120.6 |

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