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# Dibromido[(*S*)-2-(pyrrolidin-2-yl)-1*H*-benzimidazole]zinc(II)

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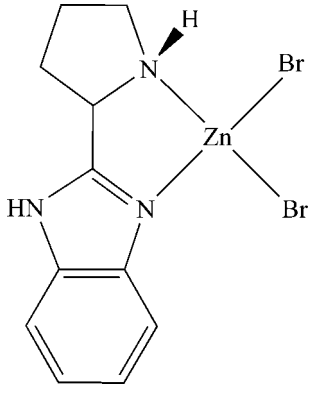
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.047; $wR$ factor = 0.115; data-to-parameter ratio = 20.6.

The title compound, $[ZnBr_2(C_{11}H_{13}N_3)]$, was synthesized by hydrothermal reaction of $ZnBr_2$ and (*S*)-2-(pyrrolidin-2-yl)-1*H*-benzimidazole. The $Zn^{II}$ atom has a distorted tetrahedral geometry and is coordinated by two N atoms from the chelating organic ligand and two terminal $Br^-$ anions. In the crystal structure, molecules are linked into a chain along the [101] direction by N—H···Br and C—H···Br hydrogen bonds.

## Related literature

For physical properties such as fluorescence and dielectric behaviors of metal-organic coordination compounds, see: Aminabhavi *et al.* (1986); Ye *et al.* (2008); Fu *et al.* (2007).




## Experimental

### Crystal data

$[ZnBr_2(C_{11}H_{13}N_3)]$
$M_r$ = 412.43
Monoclinic, $P2_1/n$
$a$ = 8.953 (3) Å
$b$ = 11.668 (2) Å
$c$ = 13.318 (2) Å
$\beta$ = 91.443 (3)°
$V$ = 1390.9 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 7.49 mm$^{-1}$
$T$ = 298 (2) K
0.30 × 0.25 × 0.15 mm

### Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.459, $T_{max}$ = 0.982
(expected range = 0.152–0.325)
13896 measured reflections
3179 independent reflections
2426 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.065

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.114
$S$ = 0.99
3179 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.00 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Br1—Zn1 | 2.3642 (8) | Zn1—N1 | 2.075 (4) |
| Zn1—N2 | 2.011 (3) | Zn1—Br2 | 2.3319 (7) |
| N2—Zn1—N1 | 82.35 (14) | N2—Zn1—Br1 | 118.99 (11) |
| N2—Zn1—Br2 | 112.70 (10) | N1—Zn1—Br1 | 110.08 (11) |
| N1—Zn1—Br2 | 117.89 (10) | Br2—Zn1—Br1 | 112.03 (3) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3*C*···Br1$^{i}$ | 0.86 | 2.74 | 3.516 (4) | 150 |
| C4—H4*A*···Br1$^{ii}$ | 0.98 | 2.86 | 3.637 (5) | 137 |
| C1—H1*A*···*Cg*1$^{iii}$ | 0.97 | 2.78 | 3.673 (6) | 153 |

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x, -y+2, -z+1$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$. *Cg*1 is the centroid of the C6–C11 ring.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2621).

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# supporting information

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## Dibromido[(*S*)-2-(pyrrolidin-2-yl)-1*H*-benzimidazole]zinc(II)

**Wei Dai and Da-Wei Fu**

### S1. Comment

Metal-organic coordination compounds provide a class of complexes displaying interesting chemical and physical properties such as fluorescence and dielectric behaviors (Aminabhavi *et al.*, 1986; Ye *et al.*, 2008; Fu *et al.*, 2007). There has been very strong interest in employing crystal-engineering strategies to generate desirable materials by the hydro-thermal reaction. Here we report the synthesis and crystal structure of the title compound.

The $Zn^{II}$ atom has a distorted tetrahedral geometry (Table 1) and is coordinated by two N atoms from the chelating *S*-2-(pyrrolidin-2-yl)-1*H*-benzimidazole ligand and two terminal $Br^-$ anions (Fig. 1).

In the crystal structure, N—H···Br and C—H···Br hydrogen bonds (Table 2) link the molecules into a chain along [1 0 1] (Fig.2).

### S2. Experimental

The homochiral ligand *S*-2-(pyrrolidin-2-yl)-1*H*-benzimidazole was synthesized by reaction of *S*-pyrrolidine-2-carboxylic acid and benzene-1,2-diamine according to the procedure described in the literature (Aminabhavi *et al.*, 1986). A mixture of *S*-2-(pyrrolidin-2-yl)-1*H*-benzimidazole (18.7 mg, 0.1 mmol), $ZnBr_2$ (33.9 mg, 0.1 mmol) and water (1 ml) sealed in a glass tube was maintained at 343 K. Crystals suitable for X-ray ananlysis were obtained after 3 d.

### S3. Refinement

All H atoms attached to C and N atoms were fixed geometrically and treated as riding with C-H = 0.93 Å (aromatic), 0.97 Å (methylene) or 0.98 Å (methine) and N-H = 0.91 Å with $U_{iso}$(H) = 1.2$U_{eq}$(C,N).

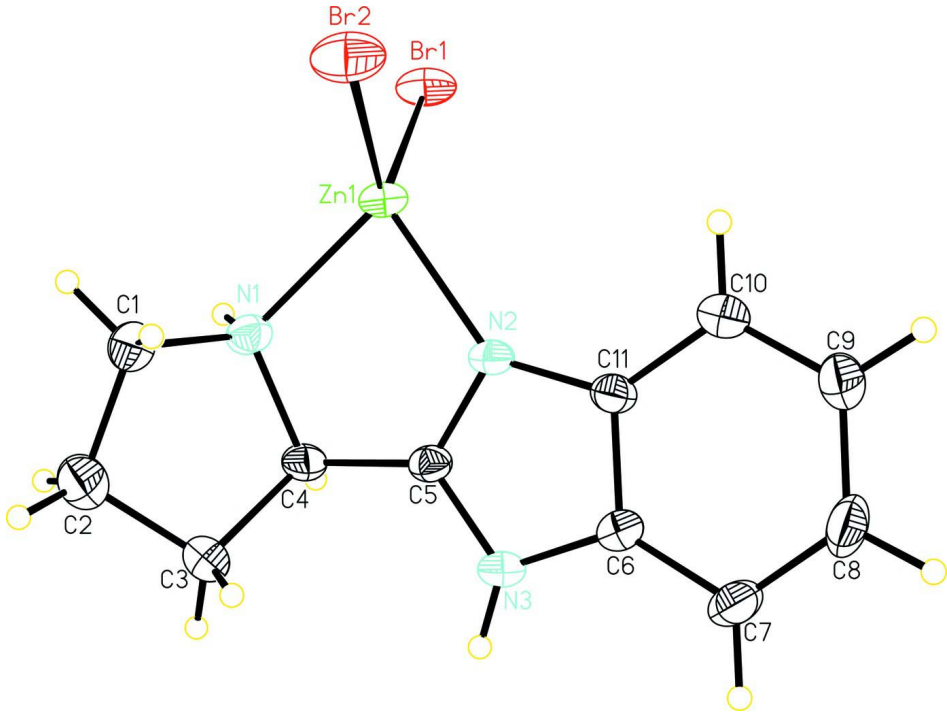


**Figure 1**

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

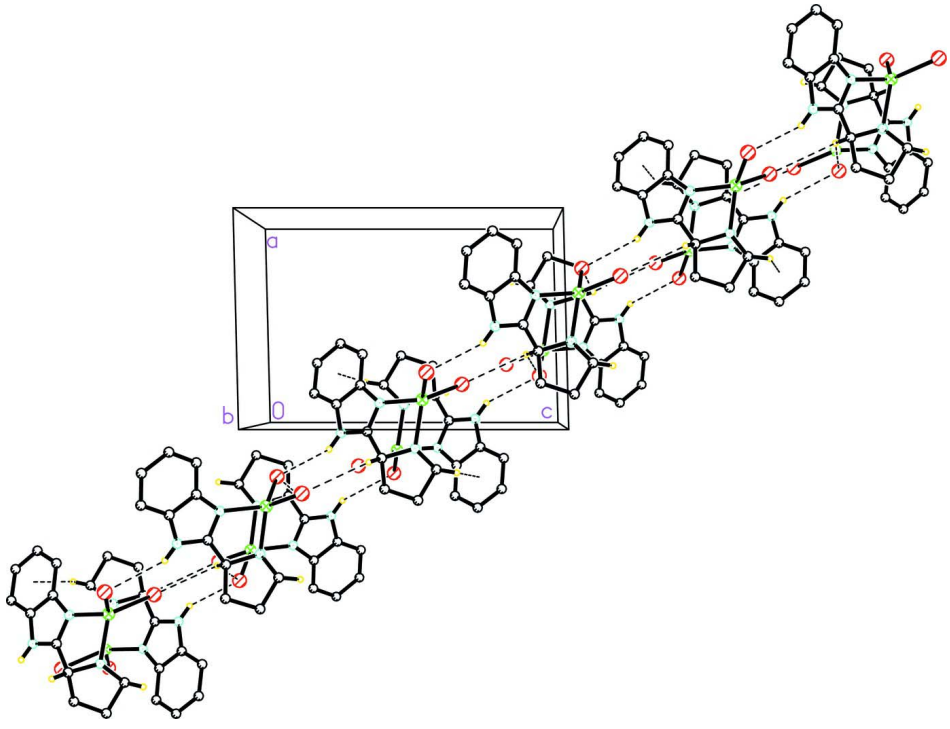


**Figure 2**

The crystal packing of the title compound, viewed along the *b* axis. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

**Dibromido[(*S*)-2-(pyrrolidin-2-yl)-1*H*-benzimidazole]zinc(II)**

*Crystal data*

$[ZnBr_2(C_{11}H_{13}N_3)]$
$M_r = 412.43$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.953$ (3) Å
$b = 11.668$ (2) Å
$c = 13.318$ (2) Å
$\beta = 91.443$ (3)°
$V = 1390.9$ (6) Å$^3$
$Z = 4$
$F(000) = 800$
$D_x = 1.970$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3615 reflections
$\theta = 2.7$–$27.5°$
$\mu = 7.49$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.30 × 0.25 × 0.15 mm

*Data collection*

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.459$, $T_{max} = 0.982$
13896 measured reflections
3179 independent reflections
2426 reflections with $I > 2\sigma(I)$
$R_{int} = 0.065$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.7°$
$h = -11 \rightarrow 11$
$k = -15 \rightarrow 15$
$l = -17 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.114$
$S = 0.99$
3179 reflections
154 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
$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.67$ e Å$^{-3}$
$\Delta\rho_{min} = -1.00$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.25768 (6) | 0.93780 (4) | 0.57154 (4) | 0.04999 (18) |
| Zn1 | 0.13105 (6) | 0.76113 (4) | 0.55176 (4) | 0.03634 (16) |
| Br2 | 0.20151 (7) | 0.62945 (5) | 0.67586 (4) | 0.0600 (2) |
| C6 | 0.1068 (5) | 0.5895 (4) | 0.2708 (3) | 0.0378 (10) |

| | | | | |
|---|---|---|---|---|
| N2 | 0.1146 (4) | 0.6901 (3) | 0.4143 (2) | 0.0344 (8) |
| N1 | −0.0955 (4) | 0.7895 (3) | 0.5261 (3) | 0.0378 (8) |
| H10B | −0.1140 | 0.8650 | 0.5377 | 0.045* |
| N3 | −0.0296 (4) | 0.6401 (3) | 0.2863 (3) | 0.0391 (9) |
| H3C | −0.1073 | 0.6357 | 0.2471 | 0.047* |
| C8 | 0.3041 (6) | 0.4841 (5) | 0.2047 (4) | 0.0554 (14) |
| H8A | 0.3427 | 0.4362 | 0.1559 | 0.066* |
| C5 | −0.0198 (5) | 0.6977 (4) | 0.3735 (3) | 0.0315 (9) |
| C11 | 0.1978 (5) | 0.6223 (4) | 0.3510 (3) | 0.0354 (9) |
| C7 | 0.1572 (6) | 0.5177 (4) | 0.1952 (3) | 0.0489 (12) |
| H7A | 0.0955 | 0.4941 | 0.1419 | 0.059* |
| C3 | −0.2915 (5) | 0.6980 (5) | 0.4237 (4) | 0.0550 (13) |
| H3A | −0.3632 | 0.7284 | 0.3748 | 0.066* |
| H3B | −0.2771 | 0.6170 | 0.4107 | 0.066* |
| C10 | 0.3458 (6) | 0.5868 (5) | 0.3582 (4) | 0.0508 (12) |
| H10A | 0.4074 | 0.6090 | 0.4120 | 0.061* |
| C9 | 0.3976 (6) | 0.5188 (5) | 0.2844 (4) | 0.0555 (14) |
| H9A | 0.4967 | 0.4949 | 0.2869 | 0.067* |
| C1 | −0.1969 (6) | 0.7209 (5) | 0.5893 (3) | 0.0512 (13) |
| H1A | −0.2104 | 0.7573 | 0.6539 | 0.061* |
| H1B | −0.1578 | 0.6442 | 0.6002 | 0.061* |
| C4 | −0.1416 (5) | 0.7637 (4) | 0.4201 (3) | 0.0361 (10) |
| H4A | −0.1568 | 0.8357 | 0.3834 | 0.043* |
| C2 | −0.3426 (6) | 0.7174 (6) | 0.5290 (4) | 0.0631 (15) |
| H2A | −0.4059 | 0.6553 | 0.5510 | 0.076* |
| H2B | −0.3965 | 0.7892 | 0.5344 | 0.076* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0629 (3) | 0.0386 (3) | 0.0474 (3) | −0.0098 (2) | −0.0209 (2) | 0.0027 (2) |
| Zn1 | 0.0395 (3) | 0.0392 (3) | 0.0299 (3) | −0.0022 (2) | −0.0093 (2) | −0.0028 (2) |
| Br2 | 0.0757 (4) | 0.0521 (3) | 0.0509 (3) | −0.0016 (3) | −0.0220 (3) | 0.0139 (2) |
| C6 | 0.040 (2) | 0.042 (2) | 0.032 (2) | −0.001 (2) | −0.0023 (19) | −0.0055 (18) |
| N2 | 0.0326 (18) | 0.041 (2) | 0.0290 (17) | −0.0002 (16) | −0.0077 (15) | −0.0026 (15) |
| N1 | 0.041 (2) | 0.0366 (19) | 0.0357 (19) | −0.0010 (17) | −0.0034 (16) | −0.0067 (16) |
| N3 | 0.035 (2) | 0.050 (2) | 0.0319 (18) | −0.0031 (17) | −0.0084 (16) | −0.0051 (16) |
| C8 | 0.057 (3) | 0.063 (3) | 0.046 (3) | 0.018 (3) | 0.014 (3) | −0.013 (3) |
| C5 | 0.034 (2) | 0.035 (2) | 0.0255 (19) | −0.0055 (18) | −0.0032 (17) | 0.0030 (17) |
| C11 | 0.031 (2) | 0.041 (2) | 0.033 (2) | −0.0023 (19) | −0.0051 (18) | −0.0002 (18) |
| C7 | 0.058 (3) | 0.054 (3) | 0.035 (2) | 0.001 (3) | −0.004 (2) | −0.012 (2) |
| C3 | 0.035 (3) | 0.077 (4) | 0.053 (3) | −0.008 (3) | 0.002 (2) | −0.015 (3) |
| C10 | 0.039 (3) | 0.067 (3) | 0.046 (3) | 0.002 (3) | −0.008 (2) | −0.010 (2) |
| C9 | 0.041 (3) | 0.076 (4) | 0.050 (3) | 0.014 (3) | 0.004 (2) | −0.006 (3) |
| C1 | 0.048 (3) | 0.068 (3) | 0.038 (3) | −0.009 (3) | 0.004 (2) | 0.004 (2) |
| C4 | 0.033 (2) | 0.044 (3) | 0.031 (2) | 0.0022 (19) | −0.0080 (18) | 0.0031 (18) |
| C2 | 0.046 (3) | 0.087 (4) | 0.057 (3) | −0.002 (3) | 0.002 (3) | 0.004 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—Zn1 | 2.3642 (8) | C5—C4 | 1.484 (6) |
| Zn1—N2 | 2.011 (3) | C11—C10 | 1.390 (6) |
| Zn1—N1 | 2.075 (4) | C7—H7A | 0.93 |
| Zn1—Br2 | 2.3319 (7) | C3—C2 | 1.504 (7) |
| C6—N3 | 1.377 (6) | C3—C4 | 1.547 (6) |
| C6—C11 | 1.382 (6) | C3—H3A | 0.97 |
| C6—C7 | 1.393 (6) | C3—H3B | 0.97 |
| N2—C5 | 1.311 (5) | C10—C9 | 1.354 (7) |
| N2—C11 | 1.387 (5) | C10—H10A | 0.93 |
| N1—C1 | 1.488 (6) | C9—H9A | 0.93 |
| N1—C4 | 1.492 (5) | C1—C2 | 1.515 (7) |
| N1—H10B | 0.91 | C1—H1A | 0.97 |
| N3—C5 | 1.343 (5) | C1—H1B | 0.97 |
| N3—H3C | 0.86 | C4—H4A | 0.98 |
| C8—C7 | 1.376 (7) | C2—H2A | 0.97 |
| C8—C9 | 1.395 (7) | C2—H2B | 0.97 |
| C8—H8A | 0.93 | | |
| | | | |
| N2—Zn1—N1 | 82.35 (14) | C6—C7—H7A | 122.2 |
| N2—Zn1—Br2 | 112.70 (10) | C2—C3—C4 | 103.8 (4) |
| N1—Zn1—Br2 | 117.89 (10) | C2—C3—H3A | 111.0 |
| N2—Zn1—Br1 | 118.99 (11) | C4—C3—H3A | 111.0 |
| N1—Zn1—Br1 | 110.08 (11) | C2—C3—H3B | 111.0 |
| Br2—Zn1—Br1 | 112.03 (3) | C4—C3—H3B | 111.0 |
| N3—C6—C11 | 105.8 (4) | H3A—C3—H3B | 109.0 |
| N3—C6—C7 | 132.1 (4) | C9—C10—C11 | 118.0 (5) |
| C11—C6—C7 | 122.0 (4) | C9—C10—H10A | 121.0 |
| C5—N2—C11 | 106.7 (3) | C11—C10—H10A | 121.0 |
| C5—N2—Zn1 | 113.3 (3) | C10—C9—C8 | 120.8 (5) |
| C11—N2—Zn1 | 139.5 (3) | C10—C9—H9A | 119.6 |
| C1—N1—C4 | 105.6 (3) | C8—C9—H9A | 119.6 |
| C1—N1—Zn1 | 115.4 (3) | N1—C1—C2 | 104.1 (4) |
| C4—N1—Zn1 | 111.7 (3) | N1—C1—H1A | 110.9 |
| C1—N1—H10B | 108.0 | C2—C1—H1A | 110.9 |
| C4—N1—H10B | 108.0 | N1—C1—H1B | 110.9 |
| Zn1—N1—H10B | 108.0 | C2—C1—H1B | 110.9 |
| C5—N3—C6 | 107.8 (3) | H1A—C1—H1B | 109.0 |
| C5—N3—H3C | 126.1 | C5—C4—N1 | 108.1 (3) |
| C6—N3—H3C | 126.1 | C5—C4—C3 | 113.8 (4) |
| C7—C8—C9 | 122.8 (5) | N1—C4—C3 | 106.9 (3) |
| C7—C8—H8A | 118.6 | C5—C4—H4A | 109.3 |
| C9—C8—H8A | 118.6 | N1—C4—H4A | 109.3 |
| N2—C5—N3 | 111.4 (4) | C3—C4—H4A | 109.3 |
| N2—C5—C4 | 122.6 (4) | C3—C2—C1 | 102.7 (4) |
| N3—C5—C4 | 126.0 (4) | C3—C2—H2A | 111.2 |
| C6—C11—N2 | 108.2 (4) | C1—C2—H2A | 111.2 |

| | | | |
|---|---|---|---|
| C6—C11—C10 | 120.8 (4) | C3—C2—H2B | 111.2 |
| N2—C11—C10 | 130.9 (4) | C1—C2—H2B | 111.2 |
| C8—C7—C6 | 115.6 (4) | H2A—C2—H2B | 109.1 |
| C8—C7—H7A | 122.2 | | |

| | | | |
|---|---|---|---|
| N1—Zn1—N2—C5 | 2.2 (3) | Zn1—N2—C11—C6 | 170.4 (3) |
| Br2—Zn1—N2—C5 | 119.3 (3) | C5—N2—C11—C10 | −179.8 (5) |
| Br1—Zn1—N2—C5 | −106.5 (3) | Zn1—N2—C11—C10 | −9.2 (8) |
| N1—Zn1—N2—C11 | −168.0 (5) | C9—C8—C7—C6 | 0.1 (8) |
| Br2—Zn1—N2—C11 | −50.9 (5) | N3—C6—C7—C8 | 179.6 (5) |
| Br1—Zn1—N2—C11 | 83.2 (5) | C11—C6—C7—C8 | −1.4 (7) |
| N2—Zn1—N1—C1 | 110.8 (3) | C6—C11—C10—C9 | −0.2 (8) |
| Br2—Zn1—N1—C1 | −0.8 (3) | N2—C11—C10—C9 | 179.3 (5) |
| Br1—Zn1—N1—C1 | −131.0 (3) | C11—C10—C9—C8 | −1.1 (8) |
| N2—Zn1—N1—C4 | −9.8 (3) | C7—C8—C9—C10 | 1.2 (9) |
| Br2—Zn1—N1—C4 | −121.4 (3) | C4—N1—C1—C2 | −32.6 (5) |
| Br1—Zn1—N1—C4 | 108.4 (3) | Zn1—N1—C1—C2 | −156.5 (3) |
| C11—C6—N3—C5 | −1.6 (5) | N2—C5—C4—N1 | −14.3 (6) |
| C7—C6—N3—C5 | 177.5 (5) | N3—C5—C4—N1 | 166.5 (4) |
| C11—N2—C5—N3 | −0.8 (5) | N2—C5—C4—C3 | −132.8 (4) |
| Zn1—N2—C5—N3 | −174.2 (3) | N3—C5—C4—C3 | 47.9 (6) |
| C11—N2—C5—C4 | 179.8 (4) | C1—N1—C4—C5 | −111.7 (4) |
| Zn1—N2—C5—C4 | 6.5 (5) | Zn1—N1—C4—C5 | 14.4 (4) |
| C6—N3—C5—N2 | 1.5 (5) | C1—N1—C4—C3 | 11.1 (5) |
| C6—N3—C5—C4 | −179.2 (4) | Zn1—N1—C4—C3 | 137.3 (3) |
| N3—C6—C11—N2 | 1.1 (5) | C2—C3—C4—C5 | 133.9 (4) |
| C7—C6—C11—N2 | −178.1 (4) | C2—C3—C4—N1 | 14.6 (5) |
| N3—C6—C11—C10 | −179.2 (4) | C4—C3—C2—C1 | −34.0 (6) |
| C7—C6—C11—C10 | 1.6 (7) | N1—C1—C2—C3 | 41.8 (6) |
| C5—N2—C11—C6 | −0.2 (5) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*C*···Br1$^{i}$ | 0.86 | 2.74 | 3.516 (4) | 150 |
| C4—H4*A*···Br1$^{ii}$ | 0.98 | 2.86 | 3.637 (5) | 137 |
| C1—H1*A*···*Cg*1$^{iii}$ | 0.97 | 2.78 | 3.673 (6) | 153 |

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