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# Dibromidobis(quinoxaline-$\kappa N$)zinc(II)

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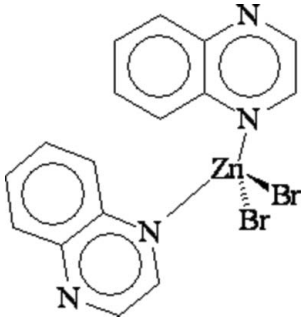
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.013 Å; $R$ factor = 0.055; $wR$ factor = 0.129; data-to-parameter ratio = 13.4.

In the title complex, $[ZnBr_2(C_8H_6N_2)_2]$, the quinoxaline ligands are monocoordinated to the $Zn^{II}$ atom and, with the bromide ions, form a distorted tetrahedral geometry. The combination of $\pi$-stacking interactions between inversion-related quinoxaline ligands and the bridging Zn creates layers parallel to the $bc$ plane [distances range from 3.250 (1) to 3.51 (1) Å].

## Related literature

For related literature, see: Landee *et al.* (2003); Lindroos & Lumme (1990); Lumme *et al.* (1988); Luo *et al.* (2004); Markowitz *et al.* (2006); Turnbull *et al.* (2005).




## Experimental

*Crystal data*

$[ZnBr_2(C_8H_6N_2)_2]$
$M_r$ = 485.49
Triclinic, $P\overline{1}$
$a$ = 8.2527 (11) Å
$b$ = 8.6670 (9) Å
$c$ = 12.4651 (17) Å
$\alpha$ = 80.067 (13)°
$\beta$ = 86.260 (12)°
$\gamma$ = 73.940 (10)°
$V$ = 843.80 (18) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 6.19 mm$^{-1}$
$T$ = 295 (2) K
0.2 × 0.15 × 0.12 mm

*Data collection*

Bruker $P4$ diffractometer
Absorption correction: $\psi$ scan (*SHELXTL*; Siemens, 1990)
$T_{min}$ = 0.363, $T_{max}$ = 0.476
3382 measured reflections
2781 independent reflections
1703 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.082
3 standard reflections
every 97 reflections
intensity decay: 2.1%

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.129
$S$ = 1.01
2781 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.53 e Å$^{-3}$

Data collection: *XSCANS* (Siemens, 1992); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXTL-Plus*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2172).

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# supplementary materials

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# Dibromidobis(quinoxaline-$\kappa N$)zinc(II)

**B. M. E. Markowitz, M. M. Turnbull and F. F. Awwadi**

## Comment

We are interested in the study of low-dimensional coordination polymers and their magnetic properties. Our previous work on two copper(II) complexes of quinoxaline (quinox) showed that Cu(quinox)$X_2$ complexes ($X$ = Cl, Br) form structural and magnetic ladders. The rungs of the ladder are formed by bridging halide ions and the rails formed by bridging quinoxaline molecules (Lindroos and Lumme, 1990; Landee *et al.*, 2003). A diamagnetic analogue of these materials would be useful for related experiments and we previously prepared the chloride analogue of (I) (Markowitz *et al.*, 2006). It resulted in a tetrahedral complex which was not a suitable analogue so the bromo complex was prepared and is reported here. Reaction of $ZnBr_2$ with quinoxaline gave Zn(quinox)$Br_2$, even in the presence of excess $ZnBr_2$.

The $Zn^{II}$ complex (I, Fig. 1) is a distorted tetrahedron with a mean angle at Zn of 120.6 (2)° (Turnbull *et al.*, 2005). The Br1—Zn—Br2 and N1—Zn1—N11 angles are both expanded and correspond with the chloride complex, unlike the pyridine and quinoline analogues (Markowitz *et al.* 2006 and references therein). The two quinoxaline ligands are nearly planar. The mean deviation from planarity for the N1 containing quinoxaline is 0.013 (12) Å and the angle between the normals to the two component rings is 1.0 (1)°; the comparable values for the N11 ring are 0.019 (17) Å and 1.4 (1)°; both are identical with the chloride complex, within experimental error. The bond lengths and angles within the quinoxaline rings are the same within experimental error and agree with those values seen in chloride analogue and similar mono-coordinated complexes such as $[Cu(quinox)_2(H_2O)_3](ClO_4)_2$ (Lumme *et al.*, 1988) and $[Cu(quinox)_2(C_2N_3)_2]$ (Luo *et al.*, 2004).

Complex (I) packs in the lattice such that π-stacking is observed between inversion related quinoxaline rings, generating layers parallel to the *bc*-plane. The ring overlap occurs between both the nitrogen-containing rings and the non-nitrogen containing rings. The interplanar distance between the stacked N1-rings is 3.30 (1)Å and the displacement angle (defined as the angle between the mean plane of the ring and the line connecting the ring centroids) is 19.1 (1)° while the values for the carbocyclic rings containing C6 are 3.41 (1)Å and 13.9 (1)°, respectively. For the stacked N11 rings the distance is 3.25 (2)Å with a displacement angle of 19.3 (1)° while the carbocyclic C16 rings are separated by 3.51 (1) Å and 6.0 (1)°. Both show that the carbocyclic rings are slightly further apart, but show greater overlap compared to the heterocyclic rings.

## Experimental

A solution of quinoxaline (1.4 g, 10 mmol) in absolute ethanol (10 ml) was added to a solution of $ZnBr_2$ (2.3 g, 10 mmol) in absolute ethanol (10 ml) yielding a pale-orange solution. The flask was wrapped in aluminium foil and allowed to evaporate under a slow flow of argon. After 12 h, light-brown crystals of (I) were collected, washed with cold ethanol and allowed to air dry yielding 1.62 g (67%). IR (KBr, $cm^{-1}$): 1504 s, 1466*m*, 1383w, 1360 s, 1215*m*, 1147*m*, 1131*m*, 1046 s, 965 s,876*m*, 772 s, 766 s.

## Figures

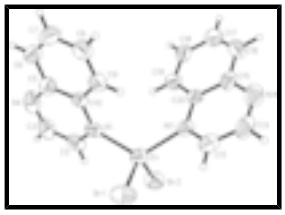


Fig. 1. Molecular structure of (I), showing atom labelling scheme and 50% atom displacement ellipsoids.

## Dibromidobis(quinoxaline-κ*N*)zinc(II)

*Crystal data*

| | |
|---|---|
| $[ZnBr_2(C_8H_6N_2)_2]$ | $Z = 2$ |
| $M_r = 485.49$ | $F_{000} = 472$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.911$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 8.2527$ (11) Å | Cell parameters from 31 reflections |
| $b = 8.6670$ (9) Å | $\theta = 3.3$–$15.6^\circ$ |
| $c = 12.4651$ (17) Å | $\mu = 6.19$ mm$^{-1}$ |
| $\alpha = 80.067$ (13)° | $T = 295$ (2) K |
| $\beta = 86.260$ (12)° | Parallelpiped, colourless |
| $\gamma = 73.940$ (10)° | 0.2 × 0.15 × 0.12 mm |
| $V = 843.80$ (18) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker P4<br>diffractometer | $R_{int} = 0.082$ |
| Radiation source: fine-focus sealed tube | $\theta_{max} = 24.6^\circ$ |
| Monochromator: graphite | $\theta_{min} = 2.5^\circ$ |
| $T = 295$(2) K | $h = -9 \rightarrow 1$ |
| ω scans | $k = -10 \rightarrow 9$ |
| Absorption correction: ψ scan<br>(SHELXTL; Siemens, 1990) | $l = -14 \rightarrow 14$ |
| $T_{min} = 0.363$, $T_{max} = 0.476$ | 3 standard reflections |
| 3382 measured reflections | every 97 reflections |
| 2781 independent reflections | intensity decay: 2.1% |
| 1703 reflections with $I > 2\sigma(I)$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.055$ | H-atom parameters constrained |

| | |
|---|---|
| $wR(F^2) = 0.129$ | $w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.6175P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.01$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2781 reflections | $\Delta\rho_{max} = 0.68$ e Å$^{-3}$ |
| 208 parameters | $\Delta\rho_{min} = -0.53$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn | 0.34064 (11) | 0.66777 (11) | 0.75037 (8) | 0.0414 (3) |
| Br1 | 0.48802 (12) | 0.39624 (11) | 0.73519 (9) | 0.0618 (3) |
| Br2 | 0.48360 (11) | 0.86374 (11) | 0.76689 (8) | 0.0560 (3) |
| N1 | 0.2157 (8) | 0.7537 (7) | 0.6045 (5) | 0.0396 (16) |
| C2 | 0.2853 (11) | 0.8412 (10) | 0.5272 (7) | 0.048 (2) |
| H2A | 0.3835 | 0.8650 | 0.5427 | 0.058* |
| C3 | 0.2186 (13) | 0.8992 (11) | 0.4236 (8) | 0.057 (2) |
| H3A | 0.2736 | 0.9606 | 0.3733 | 0.068* |
| N4 | 0.0816 (11) | 0.8707 (9) | 0.3944 (6) | 0.058 (2) |
| C5 | 0.0051 (11) | 0.7813 (10) | 0.4701 (8) | 0.049 (2) |
| C6 | −0.1435 (11) | 0.7466 (12) | 0.4439 (8) | 0.057 (3) |
| H6A | −0.1895 | 0.7856 | 0.3751 | 0.069* |
| C7 | −0.2190 (12) | 0.6551 (12) | 0.5204 (9) | 0.060 (3) |
| H7A | −0.3178 | 0.6336 | 0.5035 | 0.072* |
| C8 | −0.1515 (11) | 0.5936 (11) | 0.6230 (8) | 0.056 (2) |
| H8A | −0.2055 | 0.5305 | 0.6728 | 0.067* |
| C9 | −0.0086 (10) | 0.6229 (10) | 0.6527 (7) | 0.047 (2) |
| H9A | 0.0359 | 0.5801 | 0.7215 | 0.057* |
| C10 | 0.0702 (9) | 0.7198 (9) | 0.5763 (7) | 0.038 (2) |
| N11 | 0.2023 (8) | 0.6495 (8) | 0.8954 (5) | 0.0393 (16) |
| C12 | 0.2657 (11) | 0.5273 (11) | 0.9726 (8) | 0.051 (2) |
| H12A | 0.3641 | 0.4501 | 0.9577 | 0.061* |
| C13 | 0.1906 (13) | 0.5087 (12) | 1.0769 (8) | 0.060 (3) |
| H13A | 0.2438 | 0.4226 | 1.1294 | 0.071* |
| N14 | 0.0498 (11) | 0.6075 (10) | 1.1023 (6) | 0.059 (2) |

| | | | | |
|---|---|---|---|---|
| C15 | −0.0207 (11) | 0.7367 (10) | 1.0254 (7) | 0.046 (2) |
| C16 | −0.1749 (11) | 0.8485 (12) | 1.0501 (8) | 0.054 (2) |
| H16A | −0.2280 | 0.8339 | 1.1178 | 0.065* |
| C17 | −0.2415 (12) | 0.9746 (12) | 0.9740 (8) | 0.057 (2) |
| H17A | −0.3427 | 1.0474 | 0.9899 | 0.068* |
| C18 | −0.1666 (11) | 1.0026 (11) | 0.8715 (7) | 0.051 (2) |
| H18A | −0.2165 | 1.0938 | 0.8216 | 0.062* |
| C19 | −0.0202 (10) | 0.8964 (10) | 0.8445 (7) | 0.044 (2) |
| H19A | 0.0291 | 0.9138 | 0.7759 | 0.052* |
| C20 | 0.0556 (9) | 0.7603 (9) | 0.9212 (6) | 0.0368 (19) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn | 0.0367 (6) | 0.0398 (6) | 0.0459 (7) | −0.0105 (4) | −0.0020 (5) | −0.0017 (5) |
| Br1 | 0.0525 (6) | 0.0409 (5) | 0.0840 (8) | −0.0006 (4) | −0.0017 (5) | −0.0081 (5) |
| Br2 | 0.0524 (6) | 0.0567 (6) | 0.0657 (7) | −0.0249 (5) | 0.0031 (5) | −0.0132 (5) |
| N1 | 0.031 (4) | 0.035 (4) | 0.046 (4) | −0.003 (3) | 0.003 (3) | 0.001 (3) |
| C2 | 0.044 (5) | 0.045 (5) | 0.051 (6) | −0.011 (4) | 0.013 (4) | −0.001 (5) |
| C3 | 0.072 (7) | 0.054 (6) | 0.042 (6) | −0.021 (5) | 0.014 (5) | 0.001 (5) |
| N4 | 0.084 (6) | 0.043 (4) | 0.040 (5) | −0.010 (4) | −0.001 (4) | −0.001 (4) |
| C5 | 0.052 (5) | 0.040 (5) | 0.050 (6) | 0.000 (4) | −0.006 (5) | −0.014 (5) |
| C6 | 0.047 (6) | 0.066 (6) | 0.055 (7) | 0.000 (5) | −0.013 (5) | −0.020 (5) |
| C7 | 0.043 (5) | 0.061 (6) | 0.080 (8) | −0.008 (5) | −0.010 (5) | −0.030 (6) |
| C8 | 0.052 (6) | 0.067 (6) | 0.053 (7) | −0.021 (5) | 0.006 (5) | −0.017 (5) |
| C9 | 0.047 (5) | 0.051 (5) | 0.046 (6) | −0.014 (4) | 0.002 (4) | −0.011 (4) |
| C10 | 0.032 (5) | 0.034 (4) | 0.044 (6) | 0.000 (4) | 0.001 (4) | −0.010 (4) |
| N11 | 0.036 (4) | 0.041 (4) | 0.040 (4) | −0.014 (3) | −0.007 (3) | 0.006 (3) |
| C12 | 0.044 (5) | 0.050 (5) | 0.057 (7) | −0.013 (4) | −0.011 (5) | −0.002 (5) |
| C13 | 0.068 (7) | 0.060 (6) | 0.050 (7) | −0.027 (6) | −0.018 (5) | 0.017 (5) |
| N14 | 0.068 (6) | 0.066 (5) | 0.047 (5) | −0.031 (5) | −0.004 (4) | 0.002 (4) |
| C15 | 0.051 (5) | 0.051 (5) | 0.040 (5) | −0.023 (5) | −0.011 (4) | −0.001 (4) |
| C16 | 0.054 (6) | 0.069 (6) | 0.044 (6) | −0.023 (5) | 0.009 (5) | −0.012 (5) |
| C17 | 0.049 (5) | 0.065 (6) | 0.060 (7) | −0.009 (5) | −0.002 (5) | −0.031 (6) |
| C18 | 0.054 (6) | 0.055 (6) | 0.043 (6) | −0.004 (5) | −0.010 (5) | −0.016 (5) |
| C19 | 0.041 (5) | 0.045 (5) | 0.044 (5) | −0.015 (4) | 0.001 (4) | 0.002 (4) |
| C20 | 0.030 (4) | 0.046 (5) | 0.035 (5) | −0.018 (4) | −0.003 (4) | 0.002 (4) |

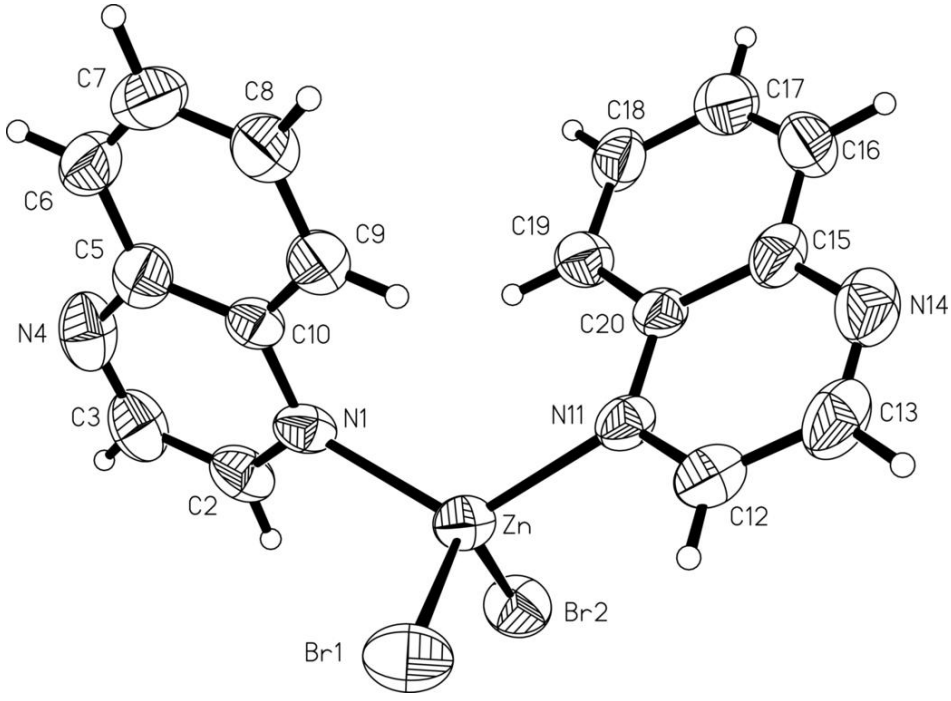
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Zn—N1 | 2.068 (7) | C9—C10 | 1.406 (11) |
| Zn—N11 | 2.080 (6) | C9—H9A | 0.9300 |
| Zn—Br2 | 2.3623 (12) | N11—C12 | 1.315 (10) |
| Zn—Br1 | 2.3650 (13) | N11—C20 | 1.380 (10) |
| N1—C2 | 1.323 (10) | C12—C13 | 1.406 (13) |
| N1—C10 | 1.392 (9) | C12—H12A | 0.9300 |
| C2—C3 | 1.391 (13) | C13—N14 | 1.296 (12) |
| C2—H2A | 0.9300 | C13—H13A | 0.9300 |
| C3—N4 | 1.308 (11) | N14—C15 | 1.361 (11) |

| | | | |
|---|---|---|---|
| C3—H3A | 0.9300 | C15—C20 | 1.414 (11) |
| N4—C5 | 1.353 (11) | C15—C16 | 1.422 (12) |
| C5—C6 | 1.412 (12) | C16—C17 | 1.333 (13) |
| C5—C10 | 1.421 (12) | C16—H16A | 0.9300 |
| C6—C7 | 1.364 (13) | C17—C18 | 1.395 (12) |
| C6—H6A | 0.9300 | C17—H17A | 0.9300 |
| C7—C8 | 1.386 (13) | C18—C19 | 1.363 (11) |
| C7—H7A | 0.9300 | C18—H18A | 0.9300 |
| C8—C9 | 1.360 (11) | C19—C20 | 1.406 (11) |
| C8—H8A | 0.9300 | C19—H19A | 0.9300 |
| N1—Zn—N11 | 119.5 (2) | N1—C10—C9 | 119.6 (7) |
| N1—Zn—Br2 | 104.56 (18) | N1—C10—C5 | 119.4 (7) |
| N11—Zn—Br2 | 103.95 (18) | C9—C10—C5 | 121.0 (8) |
| N1—Zn—Br1 | 103.70 (18) | C12—N11—C20 | 116.5 (7) |
| N11—Zn—Br1 | 104.58 (18) | C12—N11—Zn | 117.3 (6) |
| Br2—Zn—Br1 | 121.69 (5) | C20—N11—Zn | 125.9 (5) |
| C2—N1—C10 | 116.0 (7) | N11—C12—C13 | 122.7 (9) |
| C2—N1—Zn | 117.5 (6) | N11—C12—H12A | 118.7 |
| C10—N1—Zn | 126.4 (5) | C13—C12—H12A | 118.7 |
| N1—C2—C3 | 123.2 (9) | N14—C13—C12 | 122.2 (9) |
| N1—C2—H2A | 118.4 | N14—C13—H13A | 118.9 |
| C3—C2—H2A | 118.4 | C12—C13—H13A | 118.9 |
| N4—C3—C2 | 122.6 (8) | C13—N14—C15 | 117.5 (8) |
| N4—C3—H3A | 118.7 | N14—C15—C20 | 121.1 (8) |
| C2—C3—H3A | 118.7 | N14—C15—C16 | 119.3 (9) |
| C3—N4—C5 | 116.9 (8) | C20—C15—C16 | 119.6 (8) |
| N4—C5—C6 | 119.8 (9) | C17—C16—C15 | 118.4 (8) |
| N4—C5—C10 | 122.0 (8) | C17—C16—H16A | 120.8 |
| C6—C5—C10 | 118.3 (8) | C15—C16—H16A | 120.8 |
| C7—C6—C5 | 119.4 (9) | C16—C17—C18 | 123.1 (9) |
| C7—C6—H6A | 120.3 | C16—C17—H17A | 118.4 |
| C5—C6—H6A | 120.3 | C18—C17—H17A | 118.4 |
| C6—C7—C8 | 121.4 (9) | C19—C18—C17 | 120.0 (9) |
| C6—C7—H7A | 119.3 | C19—C18—H18A | 120.0 |
| C8—C7—H7A | 119.3 | C17—C18—H18A | 120.0 |
| C9—C8—C7 | 121.8 (9) | C18—C19—C20 | 119.6 (8) |
| C9—C8—H8A | 119.1 | C18—C19—H19A | 120.2 |
| C7—C8—H8A | 119.1 | C20—C19—H19A | 120.2 |
| C8—C9—C10 | 118.2 (9) | N11—C20—C19 | 120.7 (7) |
| C8—C9—H9A | 120.9 | N11—C20—C15 | 119.9 (7) |
| C10—C9—H9A | 120.9 | C19—C20—C15 | 119.4 (8) |
| N11—Zn—N1—C2 | 145.7 (6) | N1—Zn—N11—C12 | 145.1 (6) |
| Br2—Zn—N1—C2 | 30.0 (6) | Br2—Zn—N11—C12 | −98.9 (6) |
| Br1—Zn—N1—C2 | −98.5 (6) | Br1—Zn—N11—C12 | 29.7 (6) |
| N11—Zn—N1—C10 | −38.9 (7) | N1—Zn—N11—C20 | −39.9 (7) |
| Br2—Zn—N1—C10 | −154.6 (5) | Br2—Zn—N11—C20 | 76.2 (6) |
| Br1—Zn—N1—C10 | 76.9 (6) | Br1—Zn—N11—C20 | −155.2 (6) |
| C10—N1—C2—C3 | 0.8 (11) | C20—N11—C12—C13 | −0.4 (11) |

| | | | |
|---|---|---|---|
| Zn—N1—C2—C3 | 176.7 (7) | Zn—N11—C12—C13 | 175.1 (6) |
| N1—C2—C3—N4 | −0.4 (14) | N11—C12—C13—N14 | 2.9 (14) |
| C2—C3—N4—C5 | 0.2 (13) | C12—C13—N14—C15 | −3.1 (13) |
| C3—N4—C5—C6 | 179.8 (8) | C13—N14—C15—C20 | 1.1 (12) |
| C3—N4—C5—C10 | −0.4 (12) | C13—N14—C15—C16 | −179.7 (8) |
| N4—C5—C6—C7 | 179.5 (9) | N14—C15—C16—C17 | 179.7 (8) |
| C10—C5—C6—C7 | −0.3 (12) | C20—C15—C16—C17 | −1.1 (13) |
| C5—C6—C7—C8 | −0.9 (14) | C15—C16—C17—C18 | −0.4 (14) |
| C6—C7—C8—C9 | 0.8 (14) | C16—C17—C18—C19 | 1.5 (14) |
| C7—C8—C9—C10 | 0.6 (13) | C17—C18—C19—C20 | −1.0 (12) |
| C2—N1—C10—C9 | 177.9 (8) | C12—N11—C20—C19 | 179.0 (7) |
| Zn—N1—C10—C9 | 2.4 (10) | Zn—N11—C20—C19 | 3.9 (10) |
| C2—N1—C10—C5 | −1.0 (10) | C12—N11—C20—C15 | −1.6 (10) |
| Zn—N1—C10—C5 | −176.5 (5) | Zn—N11—C20—C15 | −176.7 (5) |
| C8—C9—C10—N1 | 179.3 (7) | C18—C19—C20—N11 | 178.9 (7) |
| C8—C9—C10—C5 | −1.9 (12) | C18—C19—C20—C15 | −0.5 (11) |
| N4—C5—C10—N1 | 0.8 (12) | N14—C15—C20—N11 | 1.3 (12) |
| C6—C5—C10—N1 | −179.4 (7) | C16—C15—C20—N11 | −177.9 (7) |
| N4—C5—C10—C9 | −178.1 (7) | N14—C15—C20—C19 | −179.3 (7) |
| C6—C5—C10—C9 | 1.8 (11) | C16—C15—C20—C19 | 1.5 (12) |

**Fig. 1**


C7
C8
C6
C5
C9
N4
C10
C3
N1
C2
Zn
Br1
Br2
C18
C17
C16
C19
C15
N14
C20
N11
C13
C12