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Dibromido{2-[1-(cyclopropylimino)-ethyl]pyridine}zinc(II)

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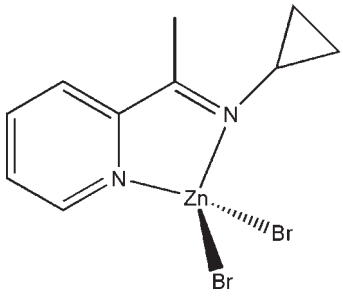
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.019 Å; R factor = 0.063; wR factor = 0.165; data-to-parameter ratio = 17.6.

In the title compound, $[ZnBr_2(C_{10}H_{12}N_2)]$, the Zn^{2+} ion is coordinated by the N,N'-bidentate Schiff base ligand and two bromode ions in a distorted tetrahedral arrangement. The dihedral angle between the pyridine and the cyclopropyl rings is 95.4 (8)°.

Related literature

For background to Schiff bases as chelating ligands, see: Hamaker *et al.* (2010); Wang *et al.* (2010); Mirkhani *et al.* (2010); Liu & Yang (2009). For similar zinc complexes, see: Zakrzewski & Lingafelter (1970); Gourbatsis *et al.* (1999); Merino *et al.* (2001); Majumder *et al.* (2006).



Experimental

Crystal data

$[ZnBr_2(C_{10}H_{12}N_2)]$
M_r = 385.41
Monoclinic, $P2_1$
a = 7.029 (3) Å
b = 14.090 (3) Å
c = 7.037 (2) Å
β = 111.820 (3)°
V = 647.0 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.04 mm^{-1}
T = 298 K
0.23 × 0.23 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.259, T_{max} = 0.283
4060 measured reflections
2408 independent reflections
1708 reflections with $I > 2\sigma(I)$
R_{int} = 0.104

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.165
S = 0.95
2408 reflections
137 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −1.09 e Å^{-3}
Absolute structure: Flack (1983), 957 Friedel pairs
Flack parameter: −0.05 (3)

Table 1
Selected bond lengths (Å).

Zn1—N1	2.041 (9)	Zn1—Br1	2.3488 (18)
Zn1—N2	2.073 (10)	Zn1—Br2	2.3616 (19)

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: *SHELXTL* (Sheldrick, 2008); 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: HB5526).

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supporting information

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Dibromido{2-[1-(cyclopropylimino)ethyl]pyridine}zinc(II)

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S1. Comment

Schiff bases have often been used as chelating ligands in coordination chemistry (Hamaker *et al.*, 2010; Wang *et al.*, 2010; Mirkhani *et al.*, 2010; Liu & Yang, 2009). We report here the crystal structure of the title new zinc complex with the chelating Schiff base ligand cyclopropyl-(1-pyridin-2-ylethylidene)amine.

The Zn atom in the complex is four-coordinated by one pyridine N and one imine N atoms of the Schiff base ligand, and by two bromide atoms, forming a tetrahedral geometry (Fig. 1). The dihedral angle between the pyridine and the cyclopropyl rings is 95.4 (8)°. The bond lengths (Table 1) related to the Zn atom are comparable to those observed in similar zinc complexes (Zakrzewski & Lingafelter, 1970; Gourbatsis *et al.*, 1999; Merino *et al.*, 2001; Majumder *et al.*, 2006).

S2. Experimental

2-Acetylpyridine (0.1 mmol, 12.1 mg) and cyclopropylamine (0.1 mmol, 5.7 mg) were mixed and stirred in methanol (10 ml) for 30 min. Then a methanol solution (5 ml) of zinc bromide (0.1 mmol, 22.5 mg) was added to the mixture. The final mixture was stirred for another 30 min to give a colourless solution. Colourless blocks of (I) were obtained by slow evaporation of the solution at room temperature.

S3. Refinement

H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined using a riding model, with with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). A rotating group model was used for the methyl group.

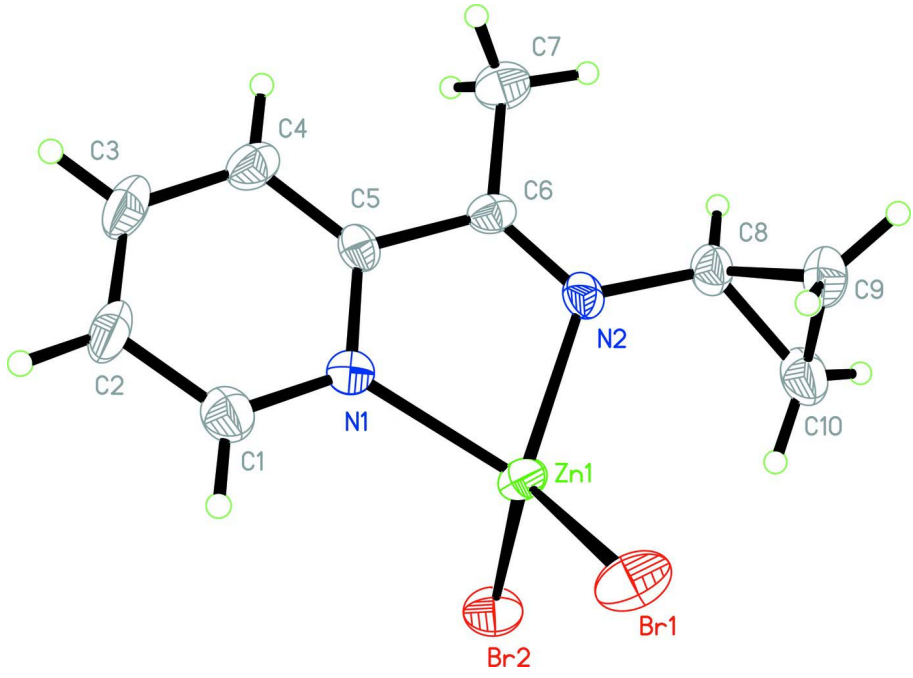

Figure 1

The molecular structure of the title complex, showing 30% probability displacement ellipsoids.

Dibromido{2-[1-(cyclopropylimino)ethyl]pyridine}zinc(II)

Crystal data

$[ZnBr_2(C_{10}H_{12}N_2)]$
$M_r = 385.41$
Monoclinic, $P2_1$
$a = 7.029$ (3) Å
$b = 14.090$ (3) Å
$c = 7.037$ (2) Å
$\beta = 111.820$ (3)°
$V = 647.0$ (4) Å^3
$Z = 2$
$F(000) = 372$
$D_x = 1.978$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1405 reflections
$\theta = 2.8$–25.0°
$\mu = 8.04$ mm^{-1}
$T = 298$ K
Block, colourless
0.23 × 0.23 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.259$, $T_{max} = 0.283$
4060 measured reflections
2408 independent reflections
1708 reflections with $I > 2\sigma(I)$
$R_{int} = 0.104$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.9°$
$h = -8 \rightarrow 8$
$k = -18 \rightarrow 17$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.165$
$S = 0.95$
2408 reflections
137 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.96$ e Å^{-3}
$\Delta\rho_{min} = -1.09$ e Å^{-3}
Absolute structure: Flack (1983), 957 Friedel pairs
Absolute structure parameter: −0.05 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Zn1	0.01583 (18)	0.10050 (8)	0.5412 (2)	0.0380 (3)
Br1	−0.0650 (2)	−0.05302 (9)	0.6175 (2)	0.0601 (4)
Br2	0.0576 (2)	0.12235 (9)	0.2262 (2)	0.0559 (4)
N1	−0.1663 (14)	0.2047 (7)	0.5832 (15)	0.040 (2)
N2	0.2313 (14)	0.1748 (7)	0.7783 (14)	0.036 (2)
C1	−0.3710 (18)	0.2147 (10)	0.491 (2)	0.050 (3)
H1	−0.4447	0.1674	0.4022	0.060*
C2	−0.477 (2)	0.2918 (10)	0.524 (2)	0.053 (3)
H2	−0.6184	0.2965	0.4582	0.064*
C3	−0.369 (2)	0.3597 (10)	0.652 (2)	0.057 (4)
H3	−0.4351	0.4134	0.6742	0.069*
C4	−0.158 (2)	0.3503 (9)	0.753 (2)	0.047 (3)
H4	−0.0833	0.3966	0.8450	0.056*
C5	−0.0622 (16)	0.2727 (8)	0.7166 (16)	0.034 (2)
C6	0.1628 (17)	0.2531 (8)	0.8195 (16)	0.036 (2)
C7	0.288 (2)	0.3276 (9)	0.968 (2)	0.058 (4)
H7A	0.2300	0.3390	1.0702	0.087*
H7B	0.2870	0.3854	0.8960	0.087*
H7C	0.4265	0.3057	1.0337	0.087*
C8	0.4414 (17)	0.1441 (9)	0.8788 (19)	0.044 (3)
H8	0.5438	0.1939	0.9385	0.053*
C9	0.471 (2)	0.0526 (10)	0.995 (2)	0.051 (3)
H9A	0.3501	0.0188	0.9917	0.061*
H9B	0.5889	0.0474	1.1220	0.061*
C10	0.511 (2)	0.0589 (11)	0.799 (2)	0.058 (4)
H10A	0.6518	0.0572	0.8084	0.070*
H10B	0.4131	0.0285	0.6781	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0393 (6)	0.0335 (7)	0.0441 (7)	−0.0027 (6)	0.0189 (5)	−0.0084 (6)
Br1	0.0749 (9)	0.0420 (7)	0.0784 (10)	−0.0192 (7)	0.0460 (8)	−0.0117 (7)
Br2	0.0672 (8)	0.0607 (9)	0.0464 (7)	−0.0071 (6)	0.0287 (7)	−0.0038 (6)
N1	0.039 (5)	0.039 (6)	0.039 (5)	0.000 (4)	0.010 (4)	−0.005 (4)
N2	0.040 (5)	0.037 (5)	0.029 (5)	0.004 (4)	0.011 (4)	0.009 (4)
C1	0.043 (7)	0.061 (8)	0.045 (7)	0.001 (6)	0.016 (6)	0.001 (6)
C2	0.056 (8)	0.056 (8)	0.056 (8)	0.029 (7)	0.030 (7)	0.009 (7)
C3	0.069 (9)	0.045 (8)	0.066 (9)	0.028 (7)	0.035 (8)	0.013 (7)
C4	0.066 (8)	0.034 (6)	0.045 (7)	0.006 (6)	0.026 (7)	0.001 (5)
C5	0.035 (6)	0.038 (6)	0.028 (5)	0.003 (5)	0.009 (5)	0.009 (5)
C6	0.051 (7)	0.031 (6)	0.030 (6)	−0.002 (5)	0.020 (5)	0.001 (4)
C7	0.065 (9)	0.041 (8)	0.061 (9)	−0.007 (6)	0.016 (8)	−0.014 (6)
C8	0.032 (6)	0.043 (7)	0.052 (7)	0.002 (5)	0.009 (5)	0.001 (6)
C9	0.052 (8)	0.047 (7)	0.054 (7)	0.012 (6)	0.019 (7)	0.015 (6)
C10	0.046 (7)	0.079 (10)	0.047 (7)	0.018 (7)	0.015 (6)	0.007 (7)

Geometric parameters (Å, º)

Zn1—N1	2.041 (9)	C4—H4	0.9300
Zn1—N2	2.073 (10)	C5—C6	1.500 (15)
Zn1—Br1	2.3488 (18)	C6—C7	1.514 (16)
Zn1—Br2	2.3616 (19)	C7—H7A	0.9600
N1—C1	1.348 (15)	C7—H7B	0.9600
N1—C5	1.350 (15)	C7—H7C	0.9600
N2—C6	1.279 (15)	C8—C10	1.48 (2)
N2—C8	1.446 (14)	C8—C9	1.498 (18)
C1—C2	1.383 (18)	C8—H8	0.9800
C1—H1	0.9300	C9—C10	1.506 (19)
C2—C3	1.34 (2)	C9—H9A	0.9700
C2—H2	0.9300	C9—H9B	0.9700
C3—C4	1.392 (19)	C10—H10A	0.9700
C3—H3	0.9300	C10—H10B	0.9700
C4—C5	1.358 (17)		
N1—Zn1—N2	80.2 (4)	N2—C6—C5	117.9 (10)
N1—Zn1—Br1	114.3 (3)	N2—C6—C7	125.7 (11)
N2—Zn1—Br1	116.6 (3)	C5—C6—C7	116.4 (10)
N1—Zn1—Br2	110.2 (3)	C6—C7—H7A	109.5
N2—Zn1—Br2	112.4 (3)	C6—C7—H7B	109.5
Br1—Zn1—Br2	117.36 (7)	H7A—C7—H7B	109.5
C1—N1—C5	117.7 (10)	C6—C7—H7C	109.5
C1—N1—Zn1	128.4 (8)	H7A—C7—H7C	109.5
C5—N1—Zn1	113.8 (7)	H7B—C7—H7C	109.5
C6—N2—C8	123.3 (11)	N2—C8—C10	118.4 (11)
C6—N2—Zn1	113.2 (7)	N2—C8—C9	115.8 (10)

C8—N2—Zn1	123.4 (8)	C10—C8—C9	60.7 (9)
N1—C1—C2	123.2 (13)	N2—C8—H8	116.7
N1—C1—H1	118.4	C10—C8—H8	116.7
C2—C1—H1	118.4	C9—C8—H8	116.7
C3—C2—C1	117.8 (12)	C8—C9—C10	59.1 (9)
C3—C2—H2	121.1	C8—C9—H9A	117.9
C1—C2—H2	121.1	C10—C9—H9A	117.9
C2—C3—C4	120.3 (12)	C8—C9—H9B	117.9
C2—C3—H3	119.8	C10—C9—H9B	117.9
C4—C3—H3	119.8	H9A—C9—H9B	115.0
C5—C4—C3	119.3 (12)	C8—C10—C9	60.2 (8)
C5—C4—H4	120.4	C8—C10—H10A	117.8
C3—C4—H4	120.4	C9—C10—H10A	117.8
N1—C5—C4	121.6 (10)	C8—C10—H10B	117.8
N1—C5—C6	114.0 (10)	C9—C10—H10B	117.8
C4—C5—C6	124.3 (11)	H10A—C10—H10B	114.9