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2-Amino-5-bromopyridin-1-ium (2-amino-5-bromopyridine-κN^1)trichloridozincate

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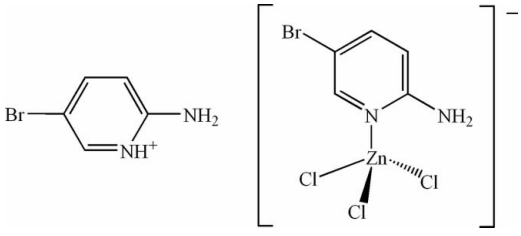
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.086; data-to-parameter ratio = 15.2.

The structure of the title salt, $(C_5H_6BrN_2)[ZnCl_3(C_5H_5BrN_2)]$, consists of discrete 2-amino-5-bromopyridin-1-ium cations and distorted tetrahedral (2-amino-5-bromopyridine)trichloridozincate anions. In the crystal, the complex anions and cations are linked *via* N—H···Cl hydrogen bonds into layers parallel to (101). Short Br···Cl contacts of 3.4239 (11) and 3.4503 (12) Å are observed, as well as π–π stacking interactions between the pyridine and pyridinium rings, with alternating centroid-to-centroid distances of 3.653 (2) and 3.845 (2) Å.

Related literature

For background to the chemistry of substituted pyridines, see: Janiak *et al.* (1999); Hubrich *et al.* (2010); Wei *et al.* (2012). For the biological activities and electrochemical properties of pyridine derivatives, see: Jo *et al.* (2004); Xiao *et al.* (2012).



Experimental

Crystal data

$(C_5H_6BrN_2)[ZnCl_3(C_5H_5BrN_2)]$
M_r = 518.77
Monoclinic, $P2_1/n$
a = 9.4238 (4) Å
b = 13.6544 (6) Å
c = 13.5679 (6) Å
β = 104.349 (1)°
V = 1691.40 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.64 mm^{-1}
T = 293 K
0.26 × 0.16 × 0.08 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.286, T_{max} = 0.576
18043 measured reflections
2979 independent reflections
2491 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.086
S = 1.02
2979 reflections
196 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl1	0.87 (2)	2.50 (3)	3.315 (4)	156 (4)
N2—H2B···Cl2^{i}	0.87 (2)	2.43 (2)	3.288 (4)	169 (5)
N3—H3A···Cl1^{ii}	0.87 (2)	2.75 (4)	3.309 (4)	124 (3)
N3—H3A···Cl1^{iii}	0.87 (2)	2.74 (4)	3.297 (4)	123 (4)
N4—H4A···Cl3^{iii}	0.88 (2)	2.49 (3)	3.328 (4)	159 (4)
N4—H4B···Cl2^{iv}	0.87 (2)	2.46 (3)	3.295 (4)	160 (4)

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-1, y, z$; (iii) $-x+1, -y, -z+1$; (iv) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2739).

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2-Amino-5-bromopyridin-1-ium (2-amino-5-bromopyridine-κN^1)trichloridozincate

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S1. Comment

In recent years, pyridine and its derivatives were found to be suitable ligands for transition metal coordination compounds involving Fe^{II}, Ni^{II} (Janiak *et al.*, 1999); Cu^{II}, Co^{II} (Hubrich *et al.*, 2010) and Zn^{II} (Wei *et al.*, 2012). Several pyridine derivatives play important roles in biological activities (Jo *et al.*, 2004) or have interesting electrochemical properties (Xiao *et al.*, 2012).

In the present work, 2-amino-5-bromopyridine was reacted with $ZnCl_2$ in acidic solution, forming the pyridinium cation, $[C_5H_6BrN_2]^+$, accompanied by the complex anion, $[ZnCl_3(C_5H_5BrN_2]^-$ (Fig. 1). In the anion, the Zn^{II} atom is in a distorted tetrahedral coordination geometry, bonded to the N atom of the pyridine ring of neutral 2-amino-5-bromopyridine and to three Cl atoms. The amino group is not involved in metal coordination. The Zn1—N1 bond length is 2.052 (3) Å, and the three Zn—Cl bond lengths are Zn1—Cl1 = 2.2494 (11) Å; Zn1—Cl2 = 2.2691 (11) Å; Zn1—Cl3 = 2.2499 (11) Å. The angles around the Zn^{II} atom range from 104.99 (9) to 114.22 (4)°, indicating a slight deviation from the the ideal tetrahedral angles.

Both intra- and inter-molecular N—H···Cl hydrogen-bonding interactions are observed (Fig. 2). The only intramolecular hydrogen bond is in the complex anion, namely between the N2 atom of the amino group and the Cl1 atom [N2—H2A···Cl1, N2···Cl1 = 3.315 (4) Å]. The N2 donor is also connected to the $Cl2^{i}$ atom (i: -*x* + 3/2, *y* + 1/2, -*z* + 1/2) of an adjacent anionic complex as an inter-molecular interaction [N2—H2B···$Cl2^{i}$, N2···$Cl2^{i}$ = 3.288 (4) Å]. Other inter-molecular hydrogen bonds are found between the *N*-amino group of the cation and Cl atoms of different anionic complexes [N4—H4A···$Cl3^{iii}$, N4···$Cl3^{iii}$ = 3.328 (4) Å; iii: -*x* + 1, -*y*, -*z* + 1; N4—H4B···$Cl2^{iv}$, N4···$Cl2^{iv}$ = 3.295 (4) Å; iv: *x* - 1/2, -*y* + 1/2, *z* + 1/2]. In addition, inter-molecular hydrogen bonding of the type N—H···Cl is also found among the protonated N atom of the cation and other two Cl atoms of two nearby anionic complexes [N3—H3A···$Cl1^{ii}$, N3···$Cl1^{ii}$ = 3.309 (4) Å; ii: *x* - 1, *y*, *z*; N3—H3A···$Cl1^{iii}$, N3···$Cl1^{iii}$ = 3.297 (4) Å]. All these inter-molecular hydrogen-bonding interactions generate a layer-like arrangement parallel to (101).

A short halogen···halogen contact of the type Br···Cl is found between the Br1 atom of the 2-amino-5-bromopyridine ligand of the complex anion and the Cl2 atom of an adjacent complex anion [Br1···Cl2 = 3.4239 (11) Å]. Furthermore, the Br2 atom of the neighbouring 2-amino-5-bromopyridinium cation also has a short contact to this Cl2 atom with a Br2···Cl2 distance of 3.4503 (12) Å as depicted in Fig. 3.

The crystal packing is futher stabilized by π–π stacking interactions between the pyridine ring (*Cg*1) of the anionic complex and the pyridinium ring (*Cg*2) with alternating centroid···centroid distances of *Cg*2···*Cg*1 = 3.653 (2) Å and *Cg*1···*Cg*2 = 3.845 (2) Å (Fig. 4). These interactions generate π–π stacking chains parallel to [$10\bar{1}$]. All in all, the stability of the crystal packing is governed by various interactions, including N—H···Cl hydrogen bonds, Br···Cl short contacts

and π–π stacking, respectively.

S2. Experimental

The title compound was synthesized by dissolving zinc chloride (480 mg, 3 mmol) in methanol (10 ml) which was added to a methanolic solution of 2-amino-5-bromopyridine (519 mg, 3 mmol). The reaction mixture was stirred in the presence of a few drops of concentrated hydrochloric acid. The final pH of the solution was adjusted to 3. After stirring for 5 h, the resulting solution was filtered off and the filtrate was left for slow evaporation of the solvent at ambient temperature. After several days, brown crystals suitable for X-ray diffraction analysis were collected by filtration, washed several times with methanol and dried in a desiccator over silica gel.

The analytical data of the zinc(II) complex are given as follows. $[C_5H_6BrN_2]^+.[ZnCl_3(C_5H_5BrN_2)]^-$. Yield 0.42 g, 27%. m.p. 461–463 K. Anal. Calcd. for $[C_5H_6BrN_2]^+.[ZnCl_3(C_5H_5BrN_2)]^-$: C 23.15, H 2.14, N 10.80%. Found: C 23.31, H 2.09, N 10.64%.

S3. Refinement

All carbon H-atoms of were placed in calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C). The H atoms of all N atoms were located in a difference map and were restrained to N—H = 0.88 (2) Å with U_{iso}(H) = 1.2U_{eq}(N).

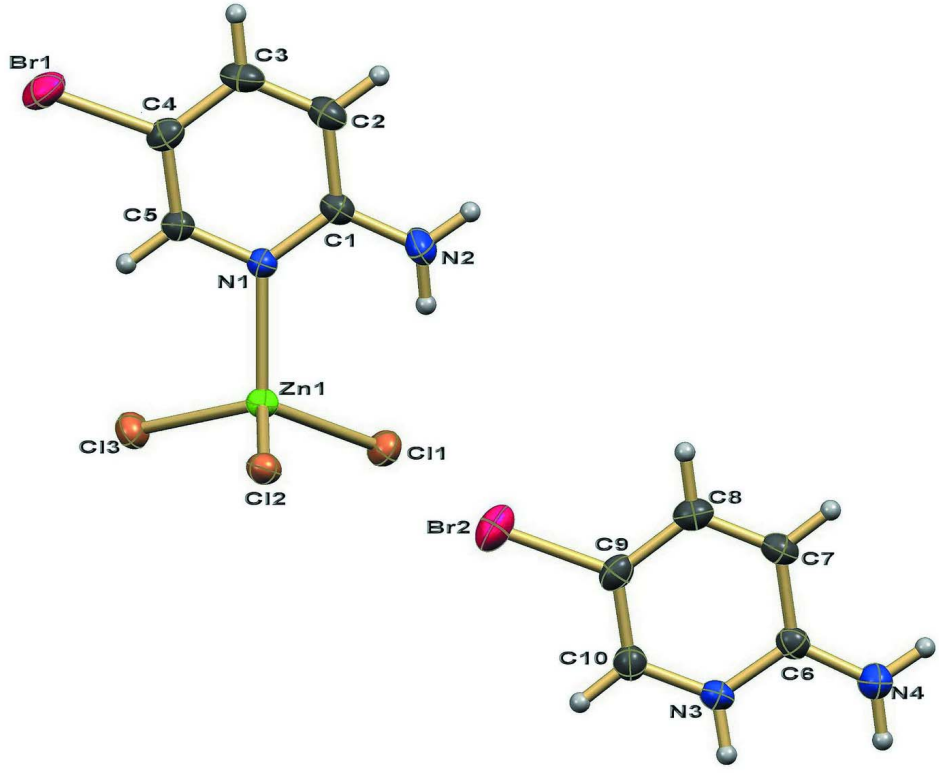

Figure 1

The molecular entities of cation and anion in the structure of $[C_5H_6BrN_2]^+.[ZnCl_3(C_5H_5BrN_2)]^-$, drawn with anisotropic displacement ellipsoids at the 30% probability level.

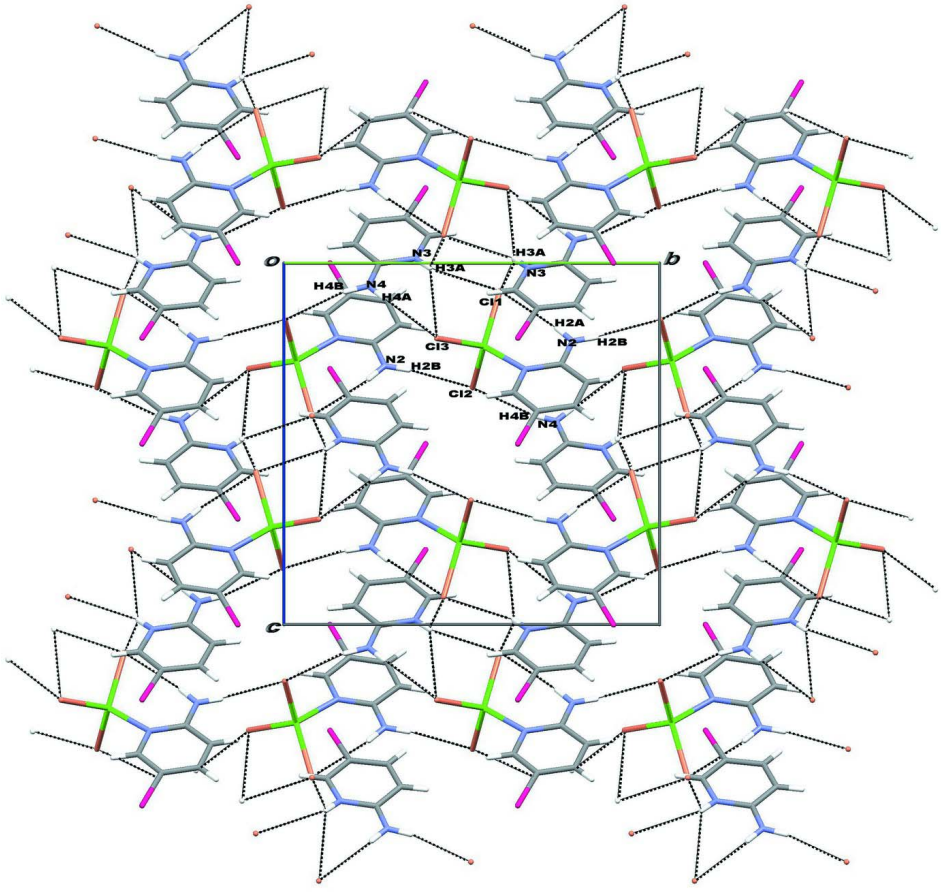

Figure 2

The inter- and intra-molecular hydrogen bonding interactions in $[C_5H_6BrN_2]^+.[ZnCl_3(C_5H_5BrN_2)]^-$, as viewed down the *a* axis.

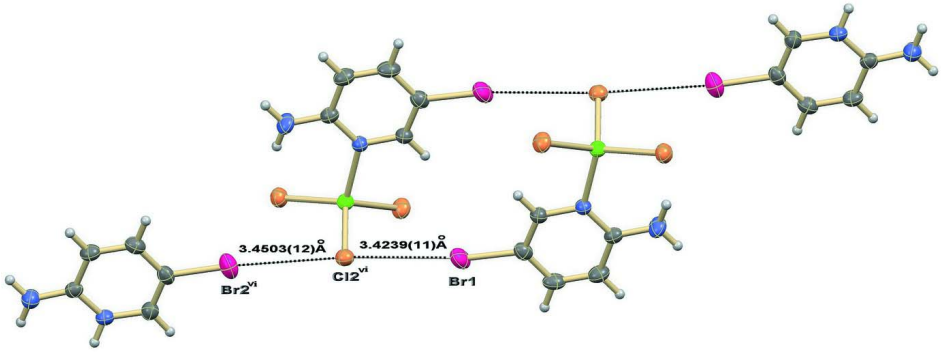

Figure 3

The Br···Cl short contacts in $[C_5H_6BrN_2]^+.[ZnCl_3(C_5H_5BrN_2)]^-$, as viewed down the *a* axis [symmetry code: (vi) -*x* + 2, -*y*, -*z*].

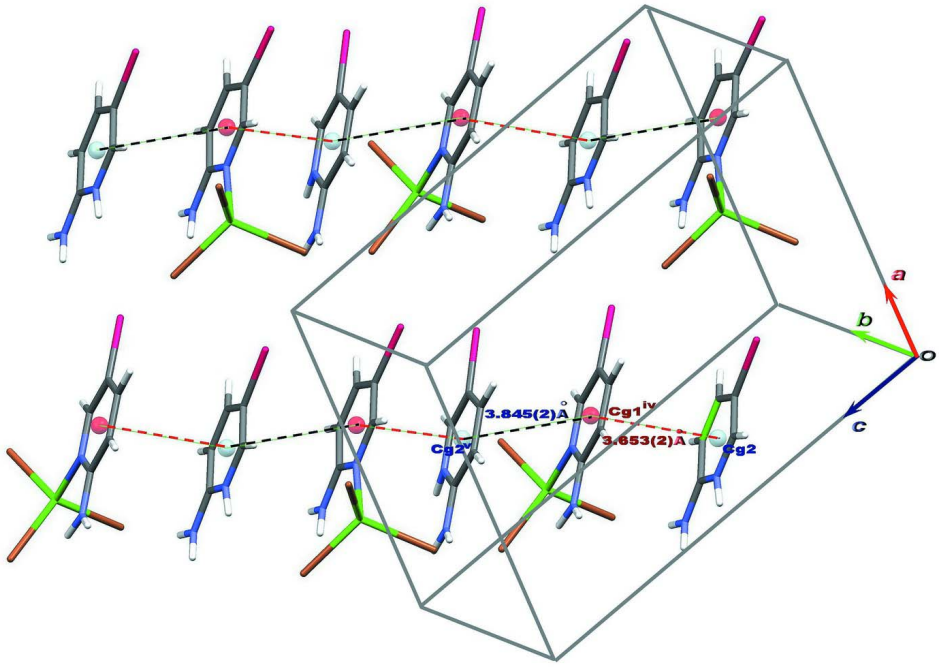

Figure 4

The one-dimensional inter-molecular π–π stacking in $[C_5H_6BrN_2]^+.[ZnCl_3(C_5H_5BrN_2)]^-$ [symmetry codes: (iv) x - 1/2, -y + 1/2, z + 1/2; (v) x + 1/2, -y + 1/2, z + 1/2).

2-Amino-5-bromopyridin-1-ium (2-amino-5-bromopyridine-κN^1)trichloridozincate

Crystal data

$(C_5H_6BrN_2)[ZnCl_3(C_5H_5BrN_2)]$
M_r = 518.77
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 9.4238 (4) Å
b = 13.6544 (6) Å
c = 13.5679 (6) Å
β = 104.349 (1)°
V = 1691.40 (13) Å^3
Z = 4
$F(000)$ = 1000
D_x = 2.037 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4332 reflections
θ = 2.2–24.1°
μ = 6.64 mm^{-1}
T = 293 K
Block, brown
0.26 × 0.16 × 0.08 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
0.3° ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.286, T_{max} = 0.576
18043 measured reflections
2979 independent reflections
2491 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −11→11
k = −16→16
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.086$
$S = 1.02$
2979 reflections
196 parameters
5 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 2.1357P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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}
Zn1	0.84827 (5)	0.03227 (3)	0.27004 (3)	0.04549 (14)
N1	0.9443 (3)	0.1421 (2)	0.2061 (2)	0.0424 (7)
N2	0.8519 (5)	0.2686 (3)	0.2841 (3)	0.0656 (10)
H2A	0.816 (5)	0.226 (3)	0.320 (3)	0.079*
H2B	0.843 (5)	0.3311 (17)	0.295 (4)	0.079*
N3	0.1587 (4)	0.1505 (2)	0.4873 (3)	0.0519 (8)
H3A	0.104 (4)	0.112 (3)	0.513 (3)	0.062*
N4	0.0611 (5)	0.2750 (3)	0.5635 (3)	0.0642 (10)
H4A	0.019 (5)	0.234 (3)	0.597 (3)	0.077*
H4B	0.056 (5)	0.3368 (17)	0.579 (4)	0.077*
Cl1	0.81449 (12)	0.07487 (8)	0.42275 (8)	0.0559 (3)
Cl2	0.63220 (11)	0.00231 (7)	0.15590 (7)	0.0509 (2)
Cl3	1.00795 (13)	−0.09311 (7)	0.29181 (8)	0.0589 (3)
C1	0.9311 (4)	0.2387 (3)	0.2208 (3)	0.0461 (9)
C2	1.0012 (5)	0.3065 (3)	0.1699 (3)	0.0588 (11)
H2	0.9933	0.3733	0.1810	0.071*
C3	1.0794 (5)	0.2747 (3)	0.1055 (3)	0.0614 (12)
H3	1.1252	0.3191	0.0716	0.074*
C4	1.0908 (4)	0.1746 (3)	0.0904 (3)	0.0521 (10)
C5	1.0238 (4)	0.1116 (3)	0.1420 (3)	0.0461 (9)
H5	1.0333	0.0446	0.1326	0.055*
C6	0.1411 (4)	0.2466 (3)	0.5014 (3)	0.0469 (9)
C7	0.2104 (5)	0.3113 (3)	0.4476 (3)	0.0538 (10)
H7	0.2005	0.3786	0.4547	0.065*

C8	0.2913 (4)	0.2767 (3)	0.3856 (3)	0.0552 (10)
H8	0.3366	0.3199	0.3501	0.066*
C9	0.3068 (4)	0.1754 (3)	0.3750 (3)	0.0528 (10)
C10	0.2379 (5)	0.1142 (3)	0.4251 (3)	0.0536 (10)
H10	0.2447	0.0469	0.4171	0.064*
Br1	1.19546 (6)	0.12257 (4)	0.00001 (4)	0.07623 (18)
Br2	0.42174 (6)	0.12277 (5)	0.29263 (4)	0.07970 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0510 (3)	0.0391 (2)	0.0496 (3)	−0.00250 (19)	0.0187 (2)	0.00095 (19)
N1	0.0439 (17)	0.0370 (16)	0.0489 (18)	−0.0010 (13)	0.0163 (14)	0.0004 (13)
N2	0.086 (3)	0.040 (2)	0.079 (3)	0.0100 (19)	0.036 (2)	−0.0003 (19)
N3	0.056 (2)	0.0417 (19)	0.061 (2)	−0.0096 (15)	0.0204 (17)	−0.0032 (16)
N4	0.076 (3)	0.055 (2)	0.070 (2)	−0.005 (2)	0.033 (2)	−0.006 (2)
Cl1	0.0633 (6)	0.0595 (6)	0.0492 (6)	0.0011 (5)	0.0218 (5)	−0.0012 (5)
Cl2	0.0517 (6)	0.0443 (5)	0.0568 (6)	−0.0039 (4)	0.0137 (5)	0.0020 (4)
Cl3	0.0694 (7)	0.0455 (5)	0.0646 (6)	0.0112 (5)	0.0219 (5)	0.0063 (5)
C1	0.047 (2)	0.039 (2)	0.049 (2)	−0.0024 (16)	0.0062 (18)	0.0020 (17)
C2	0.072 (3)	0.042 (2)	0.060 (3)	−0.008 (2)	0.011 (2)	0.0033 (19)
C3	0.070 (3)	0.054 (3)	0.058 (3)	−0.019 (2)	0.012 (2)	0.011 (2)
C4	0.048 (2)	0.065 (3)	0.044 (2)	−0.0064 (19)	0.0119 (18)	0.0017 (19)
C5	0.047 (2)	0.043 (2)	0.049 (2)	−0.0042 (17)	0.0143 (18)	0.0007 (17)
C6	0.043 (2)	0.045 (2)	0.050 (2)	−0.0043 (17)	0.0064 (18)	−0.0033 (17)
C7	0.058 (3)	0.040 (2)	0.062 (3)	−0.0053 (18)	0.010 (2)	0.0050 (19)
C8	0.051 (2)	0.061 (3)	0.055 (2)	−0.008 (2)	0.014 (2)	0.008 (2)
C9	0.039 (2)	0.068 (3)	0.052 (2)	0.0020 (19)	0.0130 (18)	−0.001 (2)
C10	0.052 (2)	0.052 (2)	0.057 (2)	0.0014 (19)	0.015 (2)	−0.005 (2)
Br1	0.0751 (3)	0.1016 (4)	0.0625 (3)	−0.0195 (3)	0.0369 (3)	−0.0081 (3)
Br2	0.0638 (3)	0.1060 (4)	0.0769 (4)	0.0159 (3)	0.0318 (3)	0.0004 (3)

Geometric parameters (Å, º)

Zn1—N1	2.052 (3)	C2—C3	1.347 (6)
Zn1—Cl1	2.2494 (11)	C2—H2	0.9300
Zn1—Cl3	2.2499 (11)	C3—C4	1.390 (6)
Zn1—Cl2	2.2691 (11)	C3—H3	0.9300
N1—C1	1.344 (5)	C4—C5	1.359 (5)
N1—C5	1.347 (5)	C4—Br1	1.892 (4)
N2—C1	1.334 (5)	C5—H5	0.9300
N2—H2A	0.874 (19)	C6—C7	1.406 (6)
N2—H2B	0.873 (19)	C7—C8	1.354 (6)
N3—C6	1.342 (5)	C7—H7	0.9300
N3—C10	1.351 (5)	C8—C9	1.401 (6)
N3—H3A	0.868 (19)	C8—H8	0.9300
N4—C6	1.320 (6)	C9—C10	1.342 (6)
N4—H4A	0.881 (19)	C9—Br2	1.882 (4)

N4—H4B	0.874 (19)	C10—H10	0.9300
C1—C2	1.413 (6)		
N1—Zn1—Cl1	112.23 (9)	C2—C3—C4	119.2 (4)
N1—Zn1—Cl3	105.12 (9)	C2—C3—H3	120.4
Cl1—Zn1—Cl3	108.58 (4)	C4—C3—H3	120.4
N1—Zn1—Cl2	104.99 (9)	C5—C4—C3	118.9 (4)
Cl1—Zn1—Cl2	111.55 (4)	C5—C4—Br1	118.6 (3)
Cl3—Zn1—Cl2	114.22 (4)	C3—C4—Br1	122.5 (3)
C1—N1—C5	119.1 (3)	N1—C5—C4	122.7 (4)
C1—N1—Zn1	126.0 (3)	N1—C5—H5	118.7
C5—N1—Zn1	114.9 (2)	C4—C5—H5	118.7
C1—N2—H2A	121 (3)	N4—C6—N3	119.3 (4)
C1—N2—H2B	120 (3)	N4—C6—C7	123.9 (4)
H2A—N2—H2B	119 (5)	N3—C6—C7	116.8 (4)
C6—N3—C10	123.7 (4)	C8—C7—C6	120.6 (4)
C6—N3—H3A	116 (3)	C8—C7—H7	119.7
C10—N3—H3A	120 (3)	C6—C7—H7	119.7
C6—N4—H4A	123 (3)	C7—C8—C9	119.8 (4)
C6—N4—H4B	121 (3)	C7—C8—H8	120.1
H4A—N4—H4B	115 (5)	C9—C8—H8	120.1
N2—C1—N1	118.9 (4)	C10—C9—C8	119.2 (4)
N2—C1—C2	121.2 (4)	C10—C9—Br2	119.0 (3)
N1—C1—C2	120.0 (4)	C8—C9—Br2	121.9 (3)
C3—C2—C1	120.1 (4)	C9—C10—N3	119.9 (4)
C3—C2—H2	119.9	C9—C10—H10	120.0
C1—C2—H2	119.9	N3—C10—H10	120.0
Cl1—Zn1—N1—C1	−29.5 (3)	C1—N1—C5—C4	−0.6 (6)
Cl3—Zn1—N1—C1	−147.3 (3)	Zn1—N1—C5—C4	177.7 (3)
Cl2—Zn1—N1—C1	91.9 (3)	C3—C4—C5—N1	1.2 (6)
Cl1—Zn1—N1—C5	152.4 (2)	Br1—C4—C5—N1	−178.5 (3)
Cl3—Zn1—N1—C5	34.5 (3)	C10—N3—C6—N4	179.7 (4)
Cl2—Zn1—N1—C5	−86.3 (3)	C10—N3—C6—C7	0.0 (6)
C5—N1—C1—N2	179.8 (4)	N4—C6—C7—C8	179.7 (4)
Zn1—N1—C1—N2	1.7 (5)	N3—C6—C7—C8	−0.5 (6)
C5—N1—C1—C2	−0.5 (5)	C6—C7—C8—C9	−0.2 (6)
Zn1—N1—C1—C2	−178.6 (3)	C7—C8—C9—C10	1.5 (6)
N2—C1—C2—C3	−179.3 (4)	C7—C8—C9—Br2	−178.4 (3)
N1—C1—C2—C3	1.0 (6)	C8—C9—C10—N3	−2.0 (6)
C1—C2—C3—C4	−0.4 (7)	Br2—C9—C10—N3	177.8 (3)
C2—C3—C4—C5	−0.7 (6)	C6—N3—C10—C9	1.3 (6)
C2—C3—C4—Br1	179.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Cl1	0.87 (2)	2.50 (3)	3.315 (4)	156 (4)

N2—H2*B*···Cl2^{i}	0.87 (2)	2.43 (2)	3.288 (4)	169 (5)
N3—H3*A*···Cl1^{ii}	0.87 (2)	2.75 (4)	3.309 (4)	124 (3)
N3—H3*A*···Cl1^{iii}	0.87 (2)	2.74 (4)	3.297 (4)	123 (4)
N4—H4*A*···Cl3^{iii}	0.88 (2)	2.49 (3)	3.328 (4)	159 (4)
N4—H4*B*···Cl2^{iv}	0.87 (2)	2.46 (3)	3.295 (4)	160 (4)

Symmetry codes: (i) $-x+3/2, y+1/2, -z+1/2$; (ii) $x-1, y, z$; (iii) $-x+1, -y, -z+1$; (iv) $x-1/2, -y+1/2, z+1/2$.