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Synthesis and crystal structure of *catena*-poly[[dibromidozinc(II)]-μ-2,3-dimethylpyrazine-$\kappa^2N^1:N^4$]

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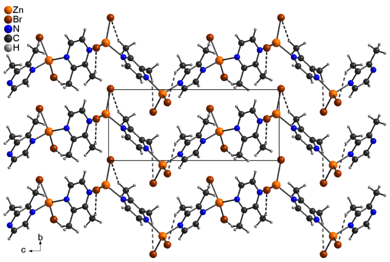
The title compound, $[ZnBr_2(C_6H_8N_2)_2]_n$, was prepared by the reaction of zinc bromide with 2,3-dimethylpyrazine in acetonitrile and is isotypic to the corresponding compound with zinc chloride reported recently [Näther & Bhosekar (2025). *Acta Cryst.* E**4**, 813–820]. The asymmetric unit consists of one zinc cation, two crystallographically independent bromide anions and one 2,3-dimethylpyrazine ligand, all of which are located in general positions. In the crystal, the Zn cations are tetrahedrally coordinated by two bromide anions and two 2,3-dimethylpyrazine ligands and are linked by bridging 2,3-dimethylpyrazine ligands into corrugated chains that proceed along the *c*-axis direction. Measurements using powder X-ray diffraction show that a pure crystalline phase was obtained.

1. Chemical context

We have been interested in the synthesis and structures of transition-metal halide and pseudo halide compounds with N-donor coligands for a very long time because they show a versatile coordination and structural behavior. This is especially the case for compounds based on Cu^I, in which the metal cations forms mono or dinuclear complexes or they are linked by the halide or pseudo halide anions into one-dimensional or two-dimensional networks (Näther *et al.*, 2001, 2002; Kromp & Sheldrick, 1999; Peng *et al.*, 2010; Li *et al.*, 2005). In most cases, for a given copper(I) halide or pseudo halide and a given coligand, compounds of different stoichiometry are observed, which include coligand-rich and coligand-deficient compounds. In this context we have found that the coligand-rich compounds can be transformed into the corresponding coligand-deficient compounds by heating (Näther & Jess, 2002, 2004).

In contrast to copper(I), compounds with twofold positively charged cations such as, for example, Zn^{II} or Cd^{II}, show a limited number of MX_2 networks (M = Zn, Cd). In these structures a tetrahedral and also an octahedral coordination can be observed. The former coordination dominates for Zn^{II}, whereas the latter is frequently found for Cd^{II} (Neumann *et al.*, 2018*a*,*b*). For Zn^{II} mainly discrete complexes are observed, whereas for Cd^{II} examples are known in which the metal cations are linked into chains (Neumann *et al.*, 2018*a*,*b*). The MX_2 complexes or chains can additionally be connected if bridging coligands like pyrazine are used, and several such compounds are reported in the literature (Bailey & Pennington, 1997; Pickardt & Staub, 1997; Bhosekar *et al.*, 2006; Bourne *et al.*, 2001; Song *et al.*, 2004). Based on these observations, we prepared new $ZnCl_2$ compounds with 2,3-



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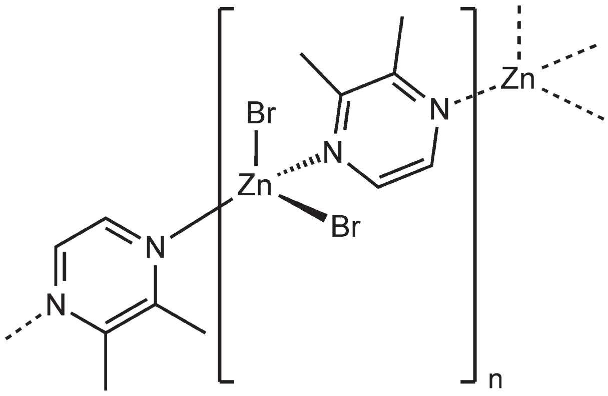
dimethylpyrazine as ligand with the composition $ZnCl_2$(2,3-dimethylpyrazine) and $ZnCl_2$(2,3-dimethylpyrazine)$_2$ (Näther & Bhosekar, 2025). In both compounds the Zn cations are tetrahedrally coordinated, leading to the formation of discrete complexes in the 2,3-dimethylpyrazine-rich compound, whereas in the 2,3-dimethylpyrazine-deficient compounds the Zn cations are linked into chains. Very recently a corresponding compound with the composition $ZnBr_2$(2,3-dimethylpyrazine)$_2$ was reported that is isotypic to $ZnCl_2$(2,3-dimethylpyrazine)$_2$ and which was investigated for its photophysical properties (Yang *et al.*, 2025). Based on these results, we assumed that a further compound with $ZnBr_2$ with the composition $ZnBr_2$(2,3-dimethylpyrazine) could be prepared that might be isotypic to its $ZnCl_2$ analog. Therefore, zinc bromide was reacted with equivalent amounts of 2,3-dimethylpyrazine and the crystals obtained were characterized by X-ray single crystal and powder diffraction.



2. Structural commentary

The new compound $ZnBr_2$(2,3-dimethylpyrazine) is isotypic to the corresponding chloride compound $ZnCl_2$(2,3-dimethylpyrazine) reported recently (Näther & Bhosekar, 2025). The asymmetric unit of the title compound consists of one Zn cation, two crystallographically independent bromide anions and one crystallographically independent 2,3-dimethylpyrazine ligand in general positions (Fig. 1). The Zn cations are fourfold coordinated by two N atoms of the 2,3-dimethylpyrazine coligands and two bromide anions in a distorted tetrahedral geometry. The N—Zn—Br angles deviate only slightly from the ideal tetrahedral values, whereas the Br—Zn—Br angles are larger and the N—Zn—N angles are smaller (Table 1), presumably because of steric repulsion between the halide anions. The metal cations are linked into chains along the crystallographic *c*-axis direction by bridging 2,3-dimethylpyrazine ligands (Fig. 2). These chains are corrugated because of the tetrahedral coordination (Fig. 2).

Table 1
Selected geometric parameters (Å, °).

Zn1—N2^{i}	2.085 (6)	Zn1—Br1	2.3380 (12)
Zn1—N1	2.118 (7)	Zn1—Br2	2.3501 (12)
N2^{i}—Zn1—N1	103.1 (3)	N2^{i}—Zn1—Br2	115.18 (19)
N2^{i}—Zn1—Br1	109.2 (2)	N1—Zn1—Br2	108.13 (19)
N1—Zn1—Br1	105.25 (19)	Br1—Zn1—Br2	114.87 (5)

Symmetry code: (i) $-x+y+1, -x+1, z-\frac{1}{3}$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Br1^{ii}	0.94	2.95	3.604 (8)	128
C3—H3···Br2^{iii}	0.94	2.99	3.687 (8)	132
C4—H4···Br2	0.94	2.95	3.605 (8)	128
C5—H5*C*···Br1	0.97	2.95	3.824 (10)	151
C6—H6*A*···Br1^{iv}	0.97	2.99	3.710 (10)	132
C6—H6*C*···Br2^{ii}	0.97	2.95	3.820 (10)	150

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

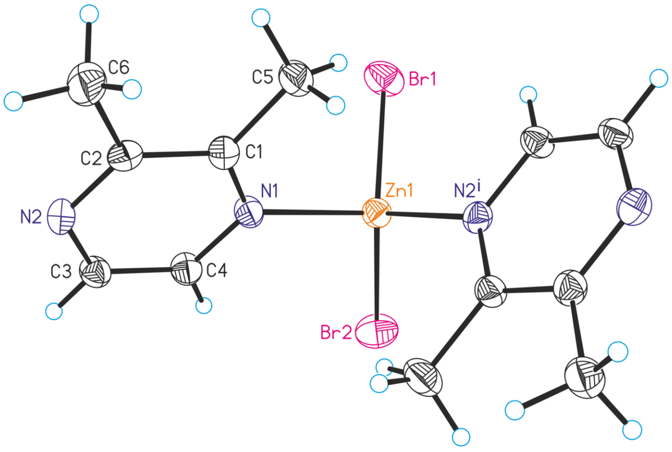


Figure 1
Crystal structure of the title compound with atom labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry code for the generation of equivalent atoms: (i) $-x+y+1, -x+1, z-\frac{1}{3}$.

3. Supramolecular features

In the crystal, intrachain C—H···Br hydrogen bonding with C—H···Br angles of 151 and 150° is observed (Fig. 2 and Table 2). These chains are linked by interchain C—H···Br contacts that show much smaller angles and thus should represent only very weak interactions (Fig. 3 and Table 2).

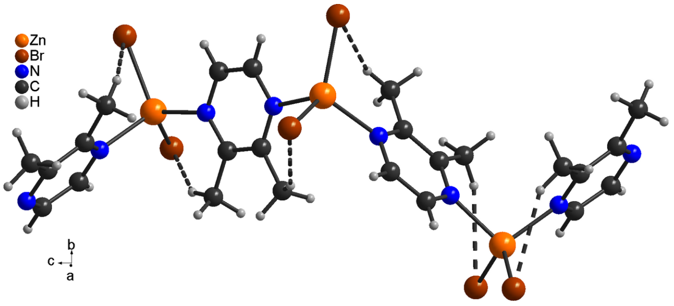


Figure 2
Fragment of the extended structure of the title compound with a view of part of a chain and intrachain C···H—Br hydrogen bonding shown as dashed lines.

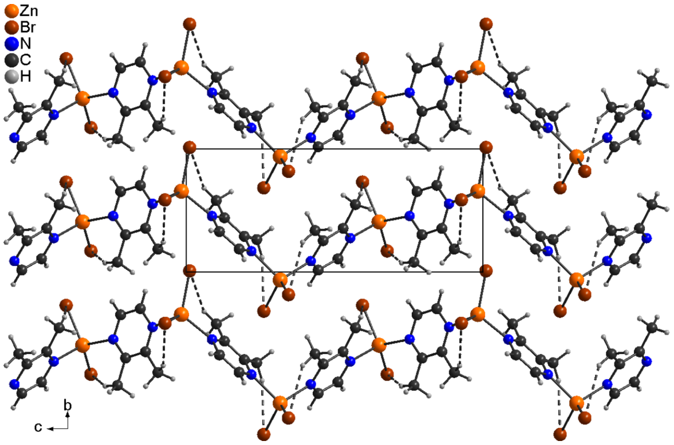


Figure 3
Crystal structure of the title compound with a view along the crystallographic *a*-axis direction and intrachain C$\cdots$H—Br hydrogen bonding shown as dashed lines.

4. Database survey

As mentioned above, the title compound is isotypic to the corresponding 2,3-dimethylpyrazine compound with $ZnCl_2$ already reported in the literature (Näther & Bhosekar, 2025). There are two additional compounds with the composition $ZnCl_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025) and $ZnBr_2$(2,3-dimethylpyrazine) (Yang *et al.*, 2025) that are isotypic and that are built up of discrete complexes with a tetrahedral Zn coordination. Further compounds with twofold positively charged transition-metal halides and 2,3-dimethylpyrazine as ligand are not reported in the CCDC database (CSD Version 5.43, January 2025; Groom *et al.*, 2016) using CONQUEST (Bruno *et al.*, 2002). However, some compounds are known with the unsubstituted ligand pyrazine. These include CdX_2(pyrazine) [X = Cl, Refcode TISSUJ ((Pickardt & Staub, 1997)]), X = Br, RINSIQ and RINSOW (Bailey & Pennington, 1997); X = I, RINSIQ01 and RINSOW01 (Pickardt & Staub, 1997)] in which the metal cations are octahedrally coordinated and are linked by pairs of halide anions into chains that are further connected into layers by the pyrazine ligands.

More compounds are reported with Zn^{II} cations and pyrazine. In contrast to the title compound with 2,3-dimethylpyrazine as coligand, these compounds show an octahedral coordination. This is the case in, *e.g.*, $ZnCl_2(pyrazine)_2$ (Refcode REMPAB; Bhosekar *et al.*, 2006) in which the Zn cations are linked into layers by the pyrazine ligands. In the pyrazine-deficient compound $ZnCl_2$(pyrazine) (Refcode TISTAQ; Pickardt & Staub, 1997), the Zn cations are linked into chains by pairs of bridging chloride anions that are further connected into layers by the pyrazine ligands. With $ZnBr_2$, two compounds are known of which the pyrazine-rich compound $ZnBr_2(pyrazine)_2$ crystallizes in two modifications with layered networks of the same topology. One of them is isotypic to the corresponding chloride compound [Refcodes EBOLAI (Bourne *et al.*, 2001) and EBOLAI01 (Bhosekar *et al.*, 2006)]. They also include $ZnBr_2$(pyrazine), which crystallizes differently from the chloride compound (Refcode EBOKUB; Bourne *et al.*, 2001). Finally, ZnI_2(pyrazine) is reported that shows a structure similar to that of the bromide compound [Refcodes ISOPOV (Song *et al.*, 2004) and ISOPOV01 (Bhosekar *et al.*, 2006)].

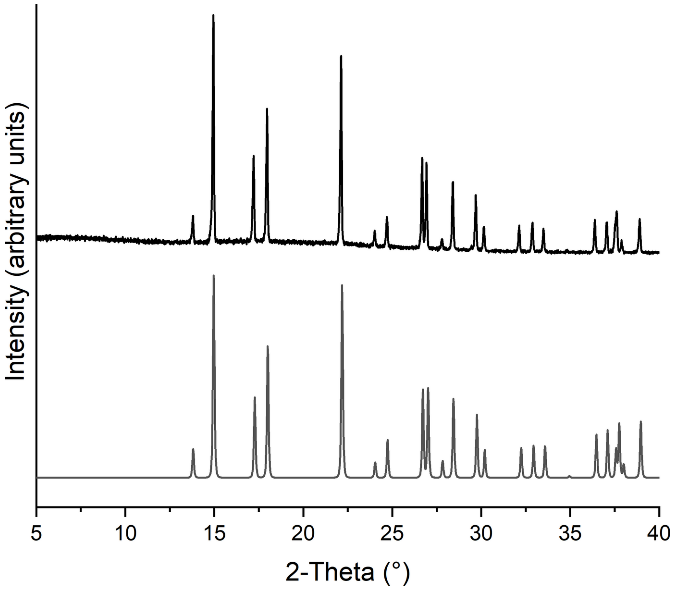


Figure 4
Experimental (top) and calculated (bottom) X-ray powder pattern of the title compound.

5. Synthesis and crystallization

Zinc bromide and 2,3-dimethylpyrazine were purchased from Sigma-Aldrich.

Synthesis

0.5 mmol (112.6 mg) of zinc bromide were reacted with 0.5 mmol (54.1 mg) of 2,3-dimethylpyrazine in 1 mL of acetonitrile. The reaction mixture was stirred for 3 d and the precipitate was filtered off and dried. Single crystals were obtained using the same ratio of reactants without stirring.

The title compound was additionally investigated by X-ray powder diffraction, which shows that a pure sample has been obtained (Fig. 4).

Experimental details

The PXRD measurements were performed with Cu $K\alpha_1$ radiation (λ = 1.540598 Å) using a Stoe Transmission Powder Diffraction System (STADI P) that is equipped with a MYTHEN 1K detector and a Johansson-type Ge(111) monochromator.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and were refined isotropically with U_{iso}(H) = 1.2 U_{eq}(C) (1.5 for methyl H atoms).

Acknowledgements

Financial support by the State of Schleswig-Holstein is gratefully acknowledged.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[ZnBr_2(C_6H_8N_2)_2]$
M_r	333.33
Crystal system, space group	Trigonal, $P3_1$
Temperature (K)	220
a, c (Å)	7.3972 (3), 15.3874 (8)
V (Å^3)	729.17 (7)
Z	3
Radiation type	Mo $K\alpha$
μ (mm^{-1})	10.69
Crystal size (mm)	0.11 × 0.07 × 0.06
Data collection	
Diffractometer	Stoe *IPDS1*
Absorption correction	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)
$T_{\min}$, $T_{\max}$	0.067, 0.156
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7080, 2343, 2231
$R_{\rm int}$	0.076
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.660
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.102, 1.06
No. of reflections	2343
No. of parameters	103
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.71, −0.73
Absolute structure	Flack x determined using 1049 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.01 (2)

Computer programs: *X-AREA* (Stoe, 2008), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 1999) and *XP* in *SHELXTL-PC* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

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supporting information

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Synthesis and crystal structure of *catena*-poly[[dibromidozinc(II)]-*μ*-2,3-dimethylpyrazine-κ^2N^1:N^4]

Christian Näther and Gaurav Bhosekar

Computing details

catena-Poly[[dibromidozinc(II)]-*μ*-2,3-dimethylpyrazine-κ^2N^1:N^4]

Crystal data

$[ZnBr_2(C_6H_8N_2)_2]$
$M_r = 333.33$
Trigonal, $P3_1$
$a = 7.3972$ (3) Å
$c = 15.3874$ (8) Å
$V = 729.17$ (7) Å^3
$Z = 3$
$F(000) = 474$

$D_x = 2.277$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7962 reflections
$\theta = 10.4$–27.1°
$\mu = 10.69$ mm^{-1}
$T = 220$ K
Block, light yellow
0.11 × 0.07 × 0.06 mm

Data collection

Stoe IPDS-1
diffractometer
Phi scans
Absorption correction: numerical
(X-Red and X-Shape; Stoe, 2008)
$T_{min} = 0.067$, $T_{max} = 0.156$
7080 measured reflections

2343 independent reflections
2231 reflections with $I > 2\sigma(I)$
$R_{int} = 0.076$
$\theta_{max} = 28.0°$, $\theta_{min} = 3.2°$
$h = -9\rightarrow9$
$k = -9\rightarrow9$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.102$
$S = 1.06$
2343 reflections
103 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 0.5878P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.043 (4)
Absolute structure: Flack x determined using 1049 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.01 (2)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Zn1	1.06358 (14)	0.65633 (14)	0.01689 (5)	0.0206 (3)
Br1	1.31606 (14)	0.58557 (16)	0.07229 (6)	0.0339 (3)
Br2	1.18263 (16)	1.01071 (14)	−0.01098 (6)	0.0364 (3)
N1	0.8300 (11)	0.5540 (10)	0.1140 (4)	0.0214 (13)
C1	0.7097 (13)	0.3550 (13)	0.1380 (5)	0.0218 (14)
C2	0.5591 (13)	0.3036 (12)	0.2051 (5)	0.0209 (14)
N2	0.5454 (10)	0.4553 (11)	0.2470 (4)	0.0203 (12)
C3	0.6710 (12)	0.6539 (12)	0.2219 (5)	0.0217 (14)
H3	0.662006	0.761430	0.250495	0.026*
C4	0.8122 (13)	0.7038 (12)	0.1554 (5)	0.0222 (15)
H4	0.896891	0.844010	0.138842	0.027*
C5	0.7352 (15)	0.1869 (14)	0.0961 (6)	0.0286 (17)
H5A	0.644589	0.133729	0.045754	0.043*
H5B	0.698387	0.074531	0.137308	0.043*
H5C	0.879174	0.243448	0.078088	0.043*
C6	0.4191 (16)	0.0817 (14)	0.2324 (7)	0.0322 (19)
H6A	0.502059	0.028064	0.258741	0.048*
H6B	0.346705	−0.002001	0.181996	0.048*
H6C	0.317974	0.075293	0.274258	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0210 (4)	0.0201 (4)	0.0207 (4)	0.0102 (3)	−0.0004 (3)	−0.0012 (3)
Br1	0.0299 (4)	0.0399 (5)	0.0389 (5)	0.0228 (4)	−0.0114 (4)	−0.0094 (4)
Br2	0.0393 (5)	0.0218 (4)	0.0445 (6)	0.0126 (4)	0.0007 (4)	0.0070 (4)
N1	0.022 (3)	0.025 (3)	0.020 (3)	0.014 (3)	0.001 (2)	−0.001 (3)
C1	0.023 (4)	0.023 (3)	0.020 (3)	0.012 (3)	0.002 (3)	0.000 (3)
C2	0.023 (3)	0.018 (3)	0.022 (3)	0.010 (3)	−0.002 (3)	0.002 (3)
N2	0.020 (3)	0.022 (3)	0.017 (3)	0.009 (3)	0.003 (2)	0.000 (2)
C3	0.022 (3)	0.018 (3)	0.025 (3)	0.010 (3)	0.003 (3)	0.001 (3)
C4	0.024 (3)	0.016 (3)	0.025 (4)	0.008 (3)	0.003 (3)	0.000 (3)
C5	0.037 (4)	0.024 (4)	0.028 (4)	0.018 (3)	0.008 (4)	0.002 (3)
C6	0.037 (5)	0.022 (4)	0.033 (4)	0.011 (3)	0.011 (4)	0.005 (3)

Geometric parameters (Å, º)

Zn1—N2$^{\rm i}$	2.085 (6)	N2—C3	1.344 (10)
Zn1—N1	2.118 (7)	C3—C4	1.374 (11)

Zn1—Br1	2.3380 (12)	C3—H3	0.9400
Zn1—Br2	2.3501 (12)	C4—H4	0.9400
N1—C1	1.336 (10)	C5—H5A	0.9700
N1—C4	1.340 (10)	C5—H5B	0.9700
C1—C2	1.424 (12)	C5—H5C	0.9700
C1—C5	1.494 (11)	C6—H6A	0.9700
C2—N2	1.341 (11)	C6—H6B	0.9700
C2—C6	1.498 (11)	C6—H6C	0.9700

N2^{i}—Zn1—N1	103.1 (3)	N2—C3—C4	121.6 (7)
N2^{i}—Zn1—Br1	109.2 (2)	N2—C3—H3	119.2
N1—Zn1—Br1	105.25 (19)	C4—C3—H3	119.2
N2^{i}—Zn1—Br2	115.18 (19)	N1—C4—C3	120.5 (7)
N1—Zn1—Br2	108.13 (19)	N1—C4—H4	119.8
Br1—Zn1—Br2	114.87 (5)	C3—C4—H4	119.8
C1—N1—C4	119.5 (7)	C1—C5—H5A	109.5
C1—N1—Zn1	124.3 (5)	C1—C5—H5B	109.5
C4—N1—Zn1	116.1 (5)	H5A—C5—H5B	109.5
N1—C1—C2	119.7 (7)	C1—C5—H5C	109.5
N1—C1—C5	120.4 (7)	H5A—C5—H5C	109.5
C2—C1—C5	119.9 (7)	H5B—C5—H5C	109.5
N2—C2—C1	120.1 (7)	C2—C6—H6A	109.5
N2—C2—C6	118.8 (7)	C2—C6—H6B	109.5
C1—C2—C6	121.1 (7)	H6A—C6—H6B	109.5
C2—N2—C3	118.5 (7)	C2—C6—H6C	109.5
C2—N2—Zn1^{ii}	124.8 (5)	H6A—C6—H6C	109.5
C3—N2—Zn1^{ii}	116.7 (5)	H6B—C6—H6C	109.5

C4—N1—C1—C2	2.2 (11)	C6—C2—N2—C3	−179.8 (8)
Zn1—N1—C1—C2	179.1 (6)	C1—C2—N2—Zn1^{ii}	−177.0 (6)
C4—N1—C1—C5	−176.6 (8)	C6—C2—N2—Zn1^{ii}	0.8 (11)
Zn1—N1—C1—C5	0.3 (11)	C2—N2—C3—C4	−0.5 (12)
N1—C1—C2—N2	−3.3 (12)	Zn1^{ii}—N2—C3—C4	179.0 (6)
C5—C1—C2—N2	175.4 (8)	C1—N1—C4—C3	−0.2 (12)
N1—C1—C2—C6	178.9 (8)	Zn1—N1—C4—C3	−177.4 (6)
C5—C1—C2—C6	−2.3 (12)	N2—C3—C4—N1	−0.7 (13)
C1—C2—N2—C3	2.4 (12)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Br1^{ii}	0.94	2.95	3.604 (8)	128
C3—H3···Br2^{iii}	0.94	2.99	3.687 (8)	132
C4—H4···Br2	0.94	2.95	3.605 (8)	128
C5—H5*C*···Br1	0.97	2.95	3.824 (10)	151

C6—H6*A*···Br1$^{\mathrm{iv}}$	0.97	2.99	3.710 (10)	132
C6—H6*C*···Br2$^{\mathrm{ii}}$	0.97	2.95	3.820 (10)	150

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