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{4,4′-Dibromo-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,O',N,N'}(pyridine-κN)zinc(II)

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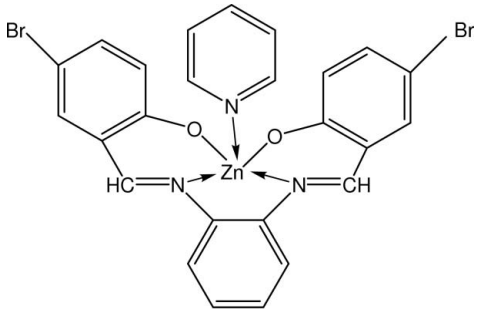
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.068; data-to-parameter ratio = 13.2.

In the title compound, $[Zn(C_{20}H_{12}Br_2N_2O_2)(C_5H_5N)]$, the Zn^{II} atom is in a distorted square-pyramidal environment in both independent molecules. The crystal structure is stabilized by C—H···O and C—H···π interactions, together with short Br···N contacts.

Related literature

For related structures, see Eltayeb, Teoh, Ng *et al.* (2007); Eltayeb, Teoh, Chantrapromma *et al.* (2007).

For related literature, see: Allen *et al.* (1987); Bernstein *et al.* (1995).



Experimental

Crystal data

$[Zn(C_{20}H_{12}Br_2N_2O_2)(C_5H_5N)]$
M_r = 616.61
Triclinic, $P\overline{1}$
a = 8.0236 (2) Å
b = 12.7930 (3) Å
c = 22.4773 (7) Å
α = 91.989 (2)°
β = 94.233 (2)°
γ = 103.566 (2)°
V = 2233.49 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.71 mm^{-1}
T = 100.0 (1) K
0.48 × 0.32 × 0.31 mm

Data collection

Bruker SMART APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.213, T_{max} = 0.319
(expected range = 0.155–0.232)
36723 measured reflections
7830 independent reflections
6908 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.068
S = 1.06
7830 reflections
595 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1*A*—O1*A*	1.966 (2)	Zn1*B*—O2*B*	1.973 (2)
Zn1*A*—O2*A*	1.979 (2)	Zn1*B*—O1*B*	1.976 (2)
Zn1*A*—N2*A*	2.082 (2)	Zn1*B*—N3*B*	2.096 (2)
Zn1*A*—N3*A*	2.092 (2)	Zn1*B*—N2*B*	2.101 (2)
Zn1*A*—N1*A*	2.114 (2)	Zn1*B*—N1*B*	2.117 (2)
O1*A*—Zn1*A*—O2*A*	94.05 (8)	O2*B*—Zn1*B*—O1*B*	96.53 (8)
O1*A*—Zn1*A*—N2*A*	151.54 (8)	O2*B*—Zn1*B*—N3*B*	101.28 (9)
O2*A*—Zn1*A*—N2*A*	90.27 (9)	O1*B*—Zn1*B*—N3*B*	97.35 (8)
O1*A*—Zn1*A*—N3*A*	102.03 (8)	O2*B*—Zn1*B*—N2*B*	89.32 (8)
O2*A*—Zn1*A*—N3*A*	99.03 (9)	O1*B*—Zn1*B*—N2*B*	153.76 (8)
N2*A*—Zn1*A*—N3*A*	105.04 (9)	N3*B*—Zn1*B*—N2*B*	106.58 (9)
O1*A*—Zn1*A*—N1*A*	89.02 (9)	O2*B*—Zn1*B*—N1*B*	159.18 (8)
O2*A*—Zn1*A*—N1*A*	160.97 (9)	O1*B*—Zn1*B*—N1*B*	88.92 (8)
N2*A*—Zn1*A*—N1*A*	78.44 (9)	N3*B*—Zn1*B*—N1*B*	97.91 (9)
N3*A*—Zn1*A*—N1*A*	98.68 (9)	N2*B*—Zn1*B*—N1*B*	77.45 (9)

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

*Cg*1 and *Cg*2 are the centroids of the N3*A*/C8*A*–C12*A* and N3*B*/C8*B*–C12*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9*A*—H9*AA*···O1*A*^{i}	0.93	2.44	3.233 (4)	143
C8*B*—H8*BA*···N1*B*	0.93	2.61	3.216 (4)	123
C12*A*—H12*A*···O2*A*	0.93	2.60	3.178 (4)	121
C24*B*—H24*B*···O1*A*^{ii}	0.93	2.36	3.267 (3)	166
C17*A*—H17*A*···*Cg*1^{iii}	0.93	2.89	3.820 (3)	174
C17*B*—H17*B*···*Cg*2^{ii}	0.93	2.96	3.882 (3)	173

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2268).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.

Eltayeb, N. E., Teoh, S. G., Chantrapromma, S., Fun, H.-K. & Ibrahim, K. (2007). *Acta Cryst.* E**63**, m1633–m1634.

Eltayeb, N. E., Teoh, S. G., Ng, S.-L., Fun, H.-K. & Ibrahim, K. (2007). *Acta Cryst.* E**63**, m1284–m1285.

Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

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{4,4'-Dibromo-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,O',N,N'}(pyridine-κN)zinc(II)

N. E. Eltayeb, S. G. Teoh, J. B.-J. Teh, H.-K. Fun and K. Ibrahim

Comment

Recently, we reported the crystal structure of {2,2'-[1,2-phenylenebis(nitrilomethylylidyne)]diphenolato}pyridinezinc (Eltayeb, Teoh, Ng *et al.*, 2007) and aqua{4,4'-dimethoxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato}zinc (Eltayeb, Teoh, Chantrapromma *et al.*, 2007). The structure of the zinc derivative of 2,2'-{1,2-phenylenebis[nitrilomethylidene]}bis(4-bromophenol) is described here.

There are two independent molecules. The Zn atom is five-coordinate, with the two O atoms and two N atoms forming the basal plane, and with the N atom of the pyridine ring in the apical position, to give a square-pyramidal geometry (Fig. 1 and Table 1). In molecule A, the Zn^{II} ion is displaced from the basal plane (N1A/N2A/O2A/O1A) by −0.3918 (3) Å. The pyridine ring of N3A/C8A—C12A is attached axially to Zn1A with O1A—Zn1A—N3A—C8A torsion angle of 78.5 (2)°. In molecule B, the Zn^{II} ion is displaced from the basal plane (N1B/N2B/O2B/O1B) by −0.3765 (3) Å. The pyridine ring of N3B/C8B—C12B is attached axially to Zn1B with O1B—Zn1B—N3B—C8B torsion angle of 73.6 (2)°. The bond lengths and angles in (I) have normal values (Allen *et al.*, 1987), comparable with those found in the two related structures (Eltayeb, Teoh, Ng *et al.*, 2007; Eltayeb, Teoh, Chantrapromma *et al.*,2007).

Intramolecular C8B—H8BA···N1B and C12A—H12A···O2A interactions generate S(5) ring motifs (Fig. 1 and Table 2) (Bernstein *et al.*, 1995). The crystal structure (Fig. 2) is stabilized by C—H···O and C—H···π interactions, the latter involving N3A/C8A—C12A (centroid *Cg*1) and N3B/C8B—C12B (centroid *Cg*2) rings (Table 2). The relatively short distance [3.392 (2) Å] between the Br2B and $N1B^{i}$ [symmetry code: (i) $1-x,1-y,1-z$] atoms indicate the presence of intermolecular Br···N interactions, which contribute to the further stabilization of the crystal packing.

Experimental

To a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol (20 ml) was added 5-bromosalicylaldehyde (0.804 g, 4 mmol). The mixture was refluxed with stirring for half an hour. Zinc chloride (0.272 g, 2 mmol) in 10 ml e thanol was then added, followed by triethylamine (0.5 ml, 3.6 mmol). The mixture was stirred at room temperature for two h. The yellow precipitate that was obtained was washed by about 5 ml e thanol, dried, and then washed with diethyl ether. This precipitate was dissolved in 15 ml of pyridine, following which orange crystals were formed after two weeks.

Refinement

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å and the $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

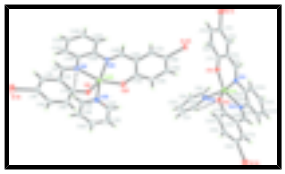


Fig. 1. **Figure 1**. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Intramolecular hydrogen bonds are shown as dashed lines.

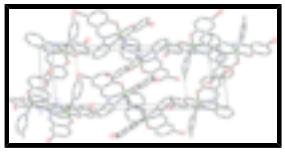


Fig. 2. **Figure 2**. The crystal packing of (I), viewed down the *b* axis. H atoms not involved in intermolecular hydrogen bonding have been omitted.

{4,4'-Dibromo-2,2'-[1,2-phenylenebis(nitrilomethylidene)]diphenolato-\ κ^4*O*,*O*',*N*,*N*'}(pyridine-*κN*)zinc(II)

Crystal data

$[Zn(C_{20}H_{12}Br_2N_2O_2)(C_5H_5N)]$	$Z = 4$
$M_r = 616.61$	$F_{000} = 1216$
Triclinic, $P\overline{1}$	$D_x = 1.834$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.0236$ (2) Å	Cell parameters from 7987 reflections
$b = 12.7930$ (3) Å	$\theta = 0.9$–25.0º
$c = 22.4773$ (7) Å	$\mu = 4.71$ mm^{-1}
$\alpha = 91.989$ (2)º	$T = 100.0$ (1) K
$\beta = 94.233$ (2)º	Block, yellow
$\gamma = 103.566$ (2)º	0.48 × 0.32 × 0.31 mm
$V = 2233.49$ (10) Å^3	

Data collection

Bruker SMART APEX II CCD diffractometer	7830 independent reflections
Radiation source: fine-focus sealed tube	6908 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 25.0$º
$T = 100.0(1)$ K	$\theta_{min} = 0.9$º
ω scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -15 \rightarrow 15$
$T_{min} = 0.213$, $T_{max} = 0.319$	$l = -26 \rightarrow 26$
36723 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 2.2079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.002$
7830 reflections	$\Delta\rho_{max} = 0.70$ e Å^{-3}
595 parameters	$\Delta\rho_{min} = -0.62$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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}
Br1A	−0.07547 (5)	−0.23450 (2)	0.726142 (16)	0.03649 (9)
Br2A	0.60641 (4)	0.81989 (2)	1.039570 (13)	0.02463 (8)
Zn1A	0.07733 (4)	0.30831 (2)	0.885341 (14)	0.01721 (8)
O1A	0.1376 (2)	0.22931 (15)	0.81676 (9)	0.0202 (4)
O2A	0.2470 (2)	0.44360 (15)	0.87258 (9)	0.0213 (4)
N1A	−0.0375 (3)	0.15936 (18)	0.91996 (11)	0.0193 (5)
N2A	0.0960 (3)	0.34958 (18)	0.97641 (10)	0.0176 (5)
C1A	−0.0541 (3)	0.0659 (2)	0.89351 (13)	0.0202 (6)
H1AA	−0.1003	0.0060	0.9145	0.024*
C2A	−0.0075 (4)	0.0465 (2)	0.83453 (13)	0.0204 (6)
C3A	−0.0542 (4)	−0.0613 (2)	0.81136 (14)	0.0229 (6)
H3AA	−0.1146	−0.1146	0.8340	0.027*
C4A	−0.0119 (4)	−0.0883 (2)	0.75623 (14)	0.0258 (7)
C5A	0.0815 (4)	−0.0104 (2)	0.72177 (14)	0.0260 (7)
H5AA	0.1104	−0.0297	0.6843	0.031*
C6A	0.1305 (4)	0.0944 (2)	0.74322 (14)	0.0236 (6)
H6AA	0.1946	0.1453	0.7201	0.028*
C7A	0.0868 (3)	0.1283 (2)	0.79977 (13)	0.0190 (6)
N3A	−0.1462 (3)	0.34966 (19)	0.85053 (10)	0.0198 (5)
C8A	−0.2992 (4)	0.2786 (3)	0.84481 (13)	0.0249 (6)
H8AA	−0.3060	0.2099	0.8581	0.030*

C9A	−0.4477 (4)	0.3031 (3)	0.81993 (15)	0.0336 (8)
H9AA	−0.5520	0.2518	0.8163	0.040*
C10A	−0.4367 (5)	0.4056 (3)	0.80067 (15)	0.0374 (8)
H10A	−0.5343	0.4246	0.7840	0.045*
C11A	−0.2805 (5)	0.4794 (3)	0.80621 (15)	0.0346 (8)
H11A	−0.2709	0.5488	0.7934	0.042*
C12A	−0.1382 (4)	0.4486 (2)	0.83108 (13)	0.0254 (6)
H12A	−0.0325	0.4984	0.8345	0.030*
C13A	0.3222 (3)	0.5223 (2)	0.91086 (13)	0.0192 (6)
C14A	0.4374 (4)	0.6135 (2)	0.89022 (13)	0.0219 (6)
H14A	0.4575	0.6143	0.8500	0.026*
C15A	0.5198 (4)	0.7000 (2)	0.92751 (14)	0.0224 (6)
H15A	0.5939	0.7586	0.9126	0.027*
C16A	0.4917 (4)	0.6997 (2)	0.98794 (13)	0.0201 (6)
C17A	0.3854 (4)	0.6139 (2)	1.01044 (13)	0.0204 (6)
H17A	0.3701	0.6145	1.0511	0.024*
C18A	0.2982 (4)	0.5240 (2)	0.97296 (13)	0.0187 (6)
C19A	0.1925 (3)	0.4375 (2)	1.00225 (13)	0.0189 (6)
H19A	0.1935	0.4454	1.0436	0.023*
C20A	−0.0057 (3)	0.2711 (2)	1.00963 (13)	0.0197 (6)
C21A	−0.0413 (4)	0.2875 (2)	1.06881 (13)	0.0219 (6)
H21A	0.0078	0.3531	1.0894	0.026*
C22A	−0.1484 (4)	0.2073 (2)	1.09675 (14)	0.0244 (6)
H22A	−0.1692	0.2186	1.1363	0.029*
C23A	−0.2255 (4)	0.1100 (2)	1.06643 (14)	0.0248 (6)
H23A	−0.2994	0.0568	1.0854	0.030*
C24A	−0.1926 (4)	0.0921 (2)	1.00808 (14)	0.0226 (6)
H24A	−0.2453	0.0268	0.9877	0.027*
C25A	−0.0808 (4)	0.1710 (2)	0.97943 (13)	0.0199 (6)
Br1B	0.53308 (4)	1.14490 (3)	0.211994 (15)	0.03487 (9)
Br2B	0.45592 (4)	0.33200 (2)	0.645408 (13)	0.02358 (8)
Zn1B	0.24696 (4)	0.75184 (2)	0.446619 (14)	0.01731 (8)
O1B	0.3972 (2)	0.89302 (15)	0.43195 (9)	0.0201 (4)
O2B	0.3728 (3)	0.72934 (15)	0.52202 (9)	0.0233 (4)
N1B	0.1589 (3)	0.73430 (18)	0.35485 (10)	0.0177 (5)
N2B	0.1568 (3)	0.58417 (18)	0.43259 (10)	0.0170 (5)
C1B	0.2168 (3)	0.7995 (2)	0.31420 (13)	0.0189 (6)
H1BA	0.1782	0.7780	0.2746	0.023*
C2B	0.3358 (4)	0.9026 (2)	0.32548 (13)	0.0208 (6)
C3B	0.3734 (4)	0.9643 (2)	0.27532 (14)	0.0231 (6)
H3BA	0.3212	0.9373	0.2378	0.028*
C4B	0.4852 (4)	1.0630 (2)	0.28103 (14)	0.0247 (6)
C5B	0.5651 (4)	1.1055 (2)	0.33632 (14)	0.0252 (7)
H5BA	0.6399	1.1734	0.3397	0.030*
C6B	0.5338 (4)	1.0474 (2)	0.38584 (14)	0.0228 (6)
H6BA	0.5893	1.0766	0.4225	0.027*
C7B	0.4187 (3)	0.9434 (2)	0.38308 (13)	0.0193 (6)
N3B	0.0443 (3)	0.80924 (18)	0.47850 (11)	0.0201 (5)
C8B	−0.0598 (4)	0.8468 (2)	0.44046 (14)	0.0248 (6)

H8BA	−0.0402	0.8455	0.4002	0.030*
C9B	−0.1952 (4)	0.8876 (3)	0.45728 (16)	0.0320 (7)
H9BA	−0.2648	0.9130	0.4291	0.038*
C10B	−0.2245 (4)	0.8898 (3)	0.51684 (16)	0.0351 (8)
H10B	−0.3150	0.9162	0.5297	0.042*
C11B	−0.1174 (4)	0.8521 (3)	0.55712 (16)	0.0342 (8)
H11B	−0.1343	0.8531	0.5976	0.041*
C12B	0.0156 (4)	0.8128 (2)	0.53650 (14)	0.0255 (6)
H12B	0.0878	0.7879	0.5639	0.031*
C13B	0.3927 (3)	0.6409 (2)	0.54518 (13)	0.0185 (6)
C14B	0.5050 (4)	0.6473 (2)	0.59747 (13)	0.0219 (6)
H14B	0.5679	0.7147	0.6127	0.026*
C15B	0.5248 (4)	0.5578 (2)	0.62670 (13)	0.0217 (6)
H15B	0.5987	0.5652	0.6613	0.026*
C16B	0.4331 (4)	0.4556 (2)	0.60417 (13)	0.0205 (6)
C17B	0.3296 (3)	0.4439 (2)	0.55211 (13)	0.0197 (6)
H17B	0.2740	0.3753	0.5365	0.024*
C18B	0.3060 (3)	0.5350 (2)	0.52170 (13)	0.0183 (6)
C19B	0.1991 (3)	0.5127 (2)	0.46679 (13)	0.0184 (6)
H19B	0.1558	0.4407	0.4544	0.022*
C20B	0.0504 (3)	0.5518 (2)	0.37908 (12)	0.0179 (6)
C21B	−0.0534 (4)	0.4481 (2)	0.36509 (13)	0.0193 (6)
H21B	−0.0529	0.3941	0.3917	0.023*
C22B	−0.1560 (4)	0.4257 (2)	0.31207 (13)	0.0211 (6)
H22B	−0.2226	0.3564	0.3026	0.025*
C23B	−0.1601 (4)	0.5065 (2)	0.27283 (13)	0.0209 (6)
H23B	−0.2306	0.4911	0.2374	0.025*
C24B	−0.0604 (4)	0.6096 (2)	0.28590 (13)	0.0207 (6)
H24B	−0.0657	0.6637	0.2597	0.025*
C25B	0.0479 (3)	0.6323 (2)	0.33832 (13)	0.0176 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1A	0.0529 (2)	0.02217 (16)	0.0329 (2)	0.00699 (14)	0.00489 (15)	−0.00938 (13)
Br2A	0.02792 (15)	0.01889 (14)	0.02338 (17)	−0.00025 (11)	−0.00122 (12)	−0.00287 (11)
Zn1A	0.02032 (16)	0.01708 (16)	0.01329 (17)	0.00260 (12)	0.00171 (12)	−0.00011 (12)
O1A	0.0240 (10)	0.0184 (10)	0.0180 (11)	0.0039 (8)	0.0038 (8)	0.0005 (8)
O2A	0.0251 (10)	0.0206 (10)	0.0157 (11)	0.0004 (8)	0.0028 (8)	−0.0003 (8)
N1A	0.0219 (12)	0.0182 (12)	0.0174 (13)	0.0037 (9)	0.0015 (9)	0.0008 (10)
N2A	0.0208 (12)	0.0175 (11)	0.0146 (12)	0.0042 (9)	0.0032 (9)	0.0022 (9)
C1A	0.0201 (14)	0.0194 (14)	0.0194 (15)	0.0021 (11)	−0.0007 (11)	0.0017 (12)
C2A	0.0198 (14)	0.0213 (14)	0.0203 (16)	0.0063 (11)	−0.0006 (11)	−0.0010 (12)
C3A	0.0231 (15)	0.0199 (14)	0.0246 (17)	0.0040 (11)	−0.0004 (12)	0.0002 (12)
C4A	0.0300 (16)	0.0201 (14)	0.0270 (17)	0.0077 (12)	−0.0014 (13)	−0.0053 (13)
C5A	0.0274 (15)	0.0318 (16)	0.0206 (16)	0.0121 (13)	0.0015 (12)	−0.0067 (13)
C6A	0.0230 (15)	0.0271 (15)	0.0218 (16)	0.0070 (12)	0.0057 (12)	0.0008 (13)
C7A	0.0183 (13)	0.0213 (14)	0.0176 (15)	0.0064 (11)	−0.0014 (11)	−0.0012 (11)

N3A	0.0233 (12)	0.0244 (12)	0.0119 (12)	0.0065 (10)	0.0024 (9)	−0.0028 (10)
C8A	0.0248 (15)	0.0328 (16)	0.0162 (16)	0.0051 (13)	0.0032 (12)	−0.0027 (13)
C9A	0.0249 (16)	0.053 (2)	0.0216 (17)	0.0085 (15)	0.0017 (13)	−0.0084 (15)
C10A	0.0373 (19)	0.064 (2)	0.0207 (18)	0.0319 (18)	0.0013 (14)	−0.0004 (16)
C11A	0.045 (2)	0.0405 (19)	0.0250 (18)	0.0238 (16)	0.0042 (15)	0.0028 (15)
C12A	0.0319 (16)	0.0278 (16)	0.0186 (16)	0.0104 (13)	0.0066 (12)	−0.0013 (12)
C13A	0.0181 (13)	0.0206 (14)	0.0200 (15)	0.0070 (11)	0.0006 (11)	−0.0003 (12)
C14A	0.0252 (15)	0.0238 (15)	0.0169 (15)	0.0064 (12)	0.0019 (11)	0.0005 (12)
C15A	0.0228 (14)	0.0177 (14)	0.0258 (17)	0.0022 (11)	0.0028 (12)	0.0040 (12)
C16A	0.0208 (14)	0.0165 (13)	0.0210 (16)	0.0023 (11)	−0.0022 (11)	−0.0028 (11)
C17A	0.0245 (14)	0.0206 (14)	0.0162 (15)	0.0062 (12)	0.0011 (11)	−0.0011 (11)
C18A	0.0218 (14)	0.0172 (13)	0.0181 (15)	0.0068 (11)	0.0007 (11)	0.0007 (11)
C19A	0.0211 (14)	0.0210 (14)	0.0153 (15)	0.0062 (11)	0.0025 (11)	0.0003 (11)
C20A	0.0190 (13)	0.0220 (14)	0.0182 (15)	0.0049 (11)	0.0021 (11)	0.0031 (12)
C21A	0.0258 (15)	0.0219 (14)	0.0174 (16)	0.0045 (12)	0.0034 (12)	−0.0016 (12)
C22A	0.0286 (15)	0.0289 (16)	0.0163 (15)	0.0073 (13)	0.0044 (12)	0.0032 (12)
C23A	0.0278 (15)	0.0235 (15)	0.0241 (17)	0.0049 (12)	0.0094 (12)	0.0073 (13)
C24A	0.0262 (15)	0.0186 (14)	0.0224 (16)	0.0035 (12)	0.0032 (12)	0.0017 (12)
C25A	0.0243 (14)	0.0206 (14)	0.0155 (15)	0.0071 (11)	0.0010 (11)	0.0011 (11)
Br1B	0.03360 (17)	0.03722 (18)	0.03095 (19)	−0.00047 (14)	0.00568 (13)	0.01775 (14)
Br2B	0.02856 (15)	0.02544 (15)	0.01949 (16)	0.01116 (12)	0.00222 (11)	0.00614 (12)
Zn1B	0.02121 (16)	0.01680 (15)	0.01404 (17)	0.00474 (12)	0.00144 (12)	0.00084 (12)
O1B	0.0243 (10)	0.0202 (10)	0.0150 (11)	0.0031 (8)	0.0033 (8)	0.0015 (8)
O2B	0.0294 (11)	0.0205 (10)	0.0187 (11)	0.0052 (8)	−0.0036 (8)	0.0015 (8)
N1B	0.0195 (11)	0.0181 (11)	0.0168 (13)	0.0069 (9)	0.0028 (9)	0.0008 (10)
N2B	0.0191 (11)	0.0190 (11)	0.0133 (12)	0.0046 (9)	0.0025 (9)	0.0014 (9)
C1B	0.0216 (14)	0.0228 (14)	0.0140 (14)	0.0088 (11)	0.0006 (11)	0.0002 (12)
C2B	0.0195 (14)	0.0208 (14)	0.0241 (16)	0.0079 (11)	0.0037 (11)	0.0026 (12)
C3B	0.0243 (15)	0.0273 (15)	0.0183 (16)	0.0068 (12)	0.0030 (12)	0.0042 (12)
C4B	0.0251 (15)	0.0246 (15)	0.0265 (17)	0.0066 (12)	0.0094 (12)	0.0122 (13)
C5B	0.0252 (15)	0.0189 (14)	0.0318 (18)	0.0045 (12)	0.0070 (13)	0.0025 (13)
C6B	0.0239 (15)	0.0217 (14)	0.0225 (16)	0.0049 (12)	0.0027 (12)	−0.0017 (12)
C7B	0.0181 (13)	0.0213 (14)	0.0208 (16)	0.0083 (11)	0.0046 (11)	0.0011 (12)
N3B	0.0227 (12)	0.0174 (11)	0.0200 (14)	0.0038 (9)	0.0030 (10)	−0.0003 (10)
C8B	0.0261 (15)	0.0272 (15)	0.0230 (17)	0.0102 (12)	0.0030 (12)	−0.0016 (13)
C9B	0.0271 (16)	0.0330 (17)	0.037 (2)	0.0107 (14)	−0.0018 (14)	−0.0052 (15)
C10B	0.0239 (16)	0.0386 (18)	0.042 (2)	0.0060 (14)	0.0077 (14)	−0.0124 (16)
C11B	0.0331 (18)	0.0391 (18)	0.0264 (19)	−0.0011 (14)	0.0135 (14)	−0.0080 (15)
C12B	0.0295 (16)	0.0246 (15)	0.0201 (17)	0.0016 (12)	0.0036 (12)	−0.0007 (12)
C13B	0.0199 (14)	0.0214 (14)	0.0152 (15)	0.0058 (11)	0.0047 (11)	0.0006 (11)
C14B	0.0214 (14)	0.0240 (15)	0.0191 (16)	0.0036 (12)	0.0020 (11)	−0.0018 (12)
C15B	0.0229 (14)	0.0278 (15)	0.0153 (15)	0.0080 (12)	0.0014 (11)	0.0002 (12)
C16B	0.0208 (14)	0.0253 (15)	0.0181 (15)	0.0093 (12)	0.0060 (11)	0.0055 (12)
C17B	0.0205 (14)	0.0209 (14)	0.0193 (15)	0.0064 (11)	0.0060 (11)	0.0013 (11)
C18B	0.0199 (13)	0.0212 (14)	0.0153 (15)	0.0074 (11)	0.0043 (11)	0.0016 (11)
C19B	0.0200 (13)	0.0174 (13)	0.0175 (15)	0.0028 (11)	0.0046 (11)	0.0009 (11)
C20B	0.0197 (13)	0.0214 (14)	0.0136 (14)	0.0069 (11)	0.0039 (11)	−0.0013 (11)
C21B	0.0231 (14)	0.0192 (14)	0.0162 (15)	0.0057 (11)	0.0036 (11)	0.0011 (11)
C22B	0.0213 (14)	0.0202 (14)	0.0209 (16)	0.0036 (11)	0.0028 (11)	−0.0018 (12)

C23B	0.0205 (14)	0.0271 (15)	0.0148 (15)	0.0062 (12)	0.0003 (11)	−0.0029 (12)
C24B	0.0229 (14)	0.0251 (15)	0.0160 (15)	0.0088 (12)	0.0033 (11)	0.0032 (12)
C25B	0.0182 (13)	0.0185 (13)	0.0174 (15)	0.0056 (11)	0.0069 (11)	0.0005 (11)

Geometric parameters (Å, °)

Br1A—C4A	1.905 (3)	Br1B—C4B	1.914 (3)
Br2A—C16A	1.901 (3)	Br2B—C16B	1.899 (3)
Zn1A—O1A	1.9656 (19)	Zn1B—O2B	1.973 (2)
Zn1A—O2A	1.979 (2)	Zn1B—O1B	1.9757 (19)
Zn1A—N2A	2.082 (2)	Zn1B—N3B	2.096 (2)
Zn1A—N3A	2.092 (2)	Zn1B—N2B	2.101 (2)
Zn1A—N1A	2.114 (2)	Zn1B—N1B	2.117 (2)
O1A—C7A	1.296 (3)	O1B—C7B	1.295 (4)
O2A—C13A	1.302 (3)	O2B—C13B	1.299 (3)
N1A—C1A	1.290 (4)	N1B—C1B	1.297 (4)
N1A—C25A	1.417 (4)	N1B—C25B	1.417 (4)
N2A—C19A	1.297 (4)	N2B—C19B	1.303 (4)
N2A—C20A	1.410 (4)	N2B—C20B	1.413 (4)
C1A—C2A	1.433 (4)	C1B—C2B	1.437 (4)
C1A—H1AA	0.9300	C1B—H1BA	0.9300
C2A—C3A	1.412 (4)	C2B—C3B	1.409 (4)
C2A—C7A	1.432 (4)	C2B—C7B	1.433 (4)
C3A—C4A	1.363 (4)	C3B—C4B	1.363 (4)
C3A—H3AA	0.9300	C3B—H3BA	0.9300
C4A—C5A	1.395 (5)	C4B—C5B	1.387 (5)
C5A—C6A	1.364 (4)	C5B—C6B	1.366 (4)
C5A—H5AA	0.9300	C5B—H5BA	0.9300
C6A—C7A	1.423 (4)	C6B—C7B	1.427 (4)
C6A—H6AA	0.9300	C6B—H6BA	0.9300
N3A—C8A	1.339 (4)	N3B—C8B	1.331 (4)
N3A—C12A	1.343 (4)	N3B—C12B	1.341 (4)
C8A—C9A	1.386 (4)	C8B—C9B	1.382 (4)
C8A—H8AA	0.9300	C8B—H8BA	0.9300
C9A—C10A	1.380 (5)	C9B—C10B	1.377 (5)
C9A—H9AA	0.9300	C9B—H9BA	0.9300
C10A—C11A	1.376 (5)	C10B—C11B	1.379 (5)
C10A—H10A	0.9300	C10B—H10B	0.9300
C11A—C12A	1.379 (5)	C11B—C12B	1.383 (5)
C11A—H11A	0.9300	C11B—H11B	0.9300
C12A—H12A	0.9300	C12B—H12B	0.9300
C13A—C18A	1.423 (4)	C13B—C14B	1.415 (4)
C13A—C14A	1.423 (4)	C13B—C18B	1.433 (4)
C14A—C15A	1.370 (4)	C14B—C15B	1.375 (4)
C14A—H14A	0.9300	C14B—H14B	0.9300
C15A—C16A	1.393 (4)	C15B—C16B	1.397 (4)
C15A—H15A	0.9300	C15B—H15B	0.9300
C16A—C17A	1.360 (4)	C16B—C17B	1.367 (4)
C17A—C18A	1.411 (4)	C17B—C18B	1.415 (4)

C17A—H17A	0.9300	C17B—H17B	0.9300
C18A—C19A	1.438 (4)	C18B—C19B	1.430 (4)
C19A—H19A	0.9300	C19B—H19B	0.9300
C20A—C21A	1.400 (4)	C20B—C21B	1.403 (4)
C20A—C25A	1.407 (4)	C20B—C25B	1.404 (4)
C21A—C22A	1.377 (4)	C21B—C22B	1.379 (4)
C21A—H21A	0.9300	C21B—H21B	0.9300
C22A—C23A	1.383 (4)	C22B—C23B	1.386 (4)
C22A—H22A	0.9300	C22B—H22B	0.9300
C23A—C24A	1.379 (4)	C23B—C24B	1.382 (4)
C23A—H23A	0.9300	C23B—H23B	0.9300
C24A—C25A	1.394 (4)	C24B—C25B	1.391 (4)
C24A—H24A	0.9300	C24B—H24B	0.9300
O1A—Zn1A—O2A	94.05 (8)	O2B—Zn1B—O1B	96.53 (8)
O1A—Zn1A—N2A	151.54 (8)	O2B—Zn1B—N3B	101.28 (9)
O2A—Zn1A—N2A	90.27 (9)	O1B—Zn1B—N3B	97.35 (8)
O1A—Zn1A—N3A	102.03 (8)	O2B—Zn1B—N2B	89.32 (8)
O2A—Zn1A—N3A	99.03 (9)	O1B—Zn1B—N2B	153.76 (8)
N2A—Zn1A—N3A	105.04 (9)	N3B—Zn1B—N2B	106.58 (9)
O1A—Zn1A—N1A	89.02 (9)	O2B—Zn1B—N1B	159.18 (8)
O2A—Zn1A—N1A	160.97 (9)	O1B—Zn1B—N1B	88.92 (8)
N2A—Zn1A—N1A	78.44 (9)	N3B—Zn1B—N1B	97.91 (9)
N3A—Zn1A—N1A	98.68 (9)	N2B—Zn1B—N1B	77.45 (9)
C7A—O1A—Zn1A	129.87 (18)	C7B—O1B—Zn1B	130.36 (18)
C13A—O2A—Zn1A	129.37 (19)	C13B—O2B—Zn1B	130.36 (18)
C1A—N1A—C25A	121.8 (2)	C1B—N1B—C25B	120.2 (2)
C1A—N1A—Zn1A	125.4 (2)	C1B—N1B—Zn1B	125.86 (19)
C25A—N1A—Zn1A	112.53 (17)	C25B—N1B—Zn1B	113.05 (18)
C19A—N2A—C20A	121.2 (2)	C19B—N2B—C20B	120.5 (2)
C19A—N2A—Zn1A	125.0 (2)	C19B—N2B—Zn1B	125.38 (19)
C20A—N2A—Zn1A	113.81 (18)	C20B—N2B—Zn1B	113.97 (17)
N1A—C1A—C2A	125.6 (3)	N1B—C1B—C2B	125.1 (3)
N1A—C1A—H1AA	117.2	N1B—C1B—H1BA	117.4
C2A—C1A—H1AA	117.2	C2B—C1B—H1BA	117.4
C3A—C2A—C7A	119.4 (3)	C3B—C2B—C7B	119.5 (3)
C3A—C2A—C1A	116.5 (3)	C3B—C2B—C1B	116.1 (3)
C7A—C2A—C1A	124.1 (3)	C7B—C2B—C1B	124.3 (3)
C4A—C3A—C2A	120.9 (3)	C4B—C3B—C2B	120.9 (3)
C4A—C3A—H3AA	119.6	C4B—C3B—H3BA	119.6
C2A—C3A—H3AA	119.6	C2B—C3B—H3BA	119.6
C3A—C4A—C5A	120.8 (3)	C3B—C4B—C5B	120.9 (3)
C3A—C4A—Br1A	120.1 (2)	C3B—C4B—Br1B	119.8 (2)
C5A—C4A—Br1A	119.2 (2)	C5B—C4B—Br1B	119.3 (2)
C6A—C5A—C4A	119.8 (3)	C6B—C5B—C4B	119.9 (3)
C6A—C5A—H5AA	120.1	C6B—C5B—H5BA	120.0
C4A—C5A—H5AA	120.1	C4B—C5B—H5BA	120.0
C5A—C6A—C7A	122.2 (3)	C5B—C6B—C7B	122.1 (3)
C5A—C6A—H6AA	118.9	C5B—C6B—H6BA	118.9
C7A—C6A—H6AA	118.9	C7B—C6B—H6BA	118.9

O1A—C7A—C6A	118.4 (3)	O1B—C7B—C6B	118.4 (3)
O1A—C7A—C2A	124.7 (3)	O1B—C7B—C2B	125.0 (3)
C6A—C7A—C2A	116.9 (3)	C6B—C7B—C2B	116.6 (3)
C8A—N3A—C12A	117.9 (3)	C8B—N3B—C12B	117.4 (3)
C8A—N3A—Zn1A	121.9 (2)	C8B—N3B—Zn1B	119.6 (2)
C12A—N3A—Zn1A	120.1 (2)	C12B—N3B—Zn1B	123.0 (2)
N3A—C8A—C9A	122.9 (3)	N3B—C8B—C9B	123.8 (3)
N3A—C8A—H8AA	118.5	N3B—C8B—H8BA	118.1
C9A—C8A—H8AA	118.5	C9B—C8B—H8BA	118.1
C10A—C9A—C8A	118.1 (3)	C10B—C9B—C8B	118.3 (3)
C10A—C9A—H9AA	120.9	C10B—C9B—H9BA	120.9
C8A—C9A—H9AA	120.9	C8B—C9B—H9BA	120.9
C11A—C10A—C9A	119.6 (3)	C9B—C10B—C11B	118.9 (3)
C11A—C10A—H10A	120.2	C9B—C10B—H10B	120.6
C9A—C10A—H10A	120.2	C11B—C10B—H10B	120.6
C10A—C11A—C12A	118.7 (3)	C10B—C11B—C12B	119.1 (3)
C10A—C11A—H11A	120.6	C10B—C11B—H11B	120.4
C12A—C11A—H11A	120.6	C12B—C11B—H11B	120.4
N3A—C12A—C11A	122.6 (3)	N3B—C12B—C11B	122.5 (3)
N3A—C12A—H12A	118.7	N3B—C12B—H12B	118.7
C11A—C12A—H12A	118.7	C11B—C12B—H12B	118.7
O2A—C13A—C18A	124.5 (3)	O2B—C13B—C14B	119.2 (2)
O2A—C13A—C14A	118.8 (3)	O2B—C13B—C18B	124.3 (2)
C18A—C13A—C14A	116.7 (3)	C14B—C13B—C18B	116.5 (3)
C15A—C14A—C13A	122.3 (3)	C15B—C14B—C13B	122.6 (3)
C15A—C14A—H14A	118.8	C15B—C14B—H14B	118.7
C13A—C14A—H14A	118.8	C13B—C14B—H14B	118.7
C14A—C15A—C16A	119.5 (3)	C14B—C15B—C16B	119.6 (3)
C14A—C15A—H15A	120.3	C14B—C15B—H15B	120.2
C16A—C15A—H15A	120.3	C16B—C15B—H15B	120.2
C17A—C16A—C15A	120.8 (3)	C17B—C16B—C15B	120.5 (3)
C17A—C16A—Br2A	119.8 (2)	C17B—C16B—Br2B	119.7 (2)
C15A—C16A—Br2A	119.4 (2)	C15B—C16B—Br2B	119.8 (2)
C16A—C17A—C18A	120.8 (3)	C16B—C17B—C18B	120.7 (3)
C16A—C17A—H17A	119.6	C16B—C17B—H17B	119.6
C18A—C17A—H17A	119.6	C18B—C17B—H17B	119.6
C17A—C18A—C13A	119.8 (3)	C17B—C18B—C19B	115.7 (2)
C17A—C18A—C19A	115.6 (3)	C17B—C18B—C13B	119.9 (3)
C13A—C18A—C19A	124.6 (3)	C19B—C18B—C13B	124.3 (3)
N2A—C19A—C18A	126.1 (3)	N2B—C19B—C18B	125.9 (3)
N2A—C19A—H19A	117.0	N2B—C19B—H19B	117.1
C18A—C19A—H19A	117.0	C18B—C19B—H19B	117.1
C21A—C20A—C25A	118.7 (3)	C21B—C20B—C25B	119.0 (3)
C21A—C20A—N2A	124.7 (3)	C21B—C20B—N2B	125.0 (3)
C25A—C20A—N2A	116.5 (3)	C25B—C20B—N2B	115.9 (2)
C22A—C21A—C20A	120.5 (3)	C22B—C21B—C20B	120.4 (3)
C22A—C21A—H21A	119.7	C22B—C21B—H21B	119.8
C20A—C21A—H21A	119.7	C20B—C21B—H21B	119.8
C21A—C22A—C23A	120.6 (3)	C21B—C22B—C23B	120.1 (3)

C21A—C22A—H22A	119.7	C21B—C22B—H22B	120.0
C23A—C22A—H22A	119.7	C23B—C22B—H22B	120.0
C24A—C23A—C22A	119.9 (3)	C24B—C23B—C22B	120.7 (3)
C24A—C23A—H23A	120.0	C24B—C23B—H23B	119.7
C22A—C23A—H23A	120.0	C22B—C23B—H23B	119.7
C23A—C24A—C25A	120.5 (3)	C23B—C24B—C25B	119.8 (3)
C23A—C24A—H24A	119.8	C23B—C24B—H24B	120.1
C25A—C24A—H24A	119.8	C25B—C24B—H24B	120.1
C24A—C25A—C20A	119.7 (3)	C24B—C25B—C20B	120.1 (3)
C24A—C25A—N1A	124.5 (3)	C24B—C25B—N1B	124.1 (3)
C20A—C25A—N1A	115.8 (3)	C20B—C25B—N1B	115.8 (2)
O2A—Zn1A—O1A—C7A	173.0 (2)	O2B—Zn1B—O1B—C7B	159.8 (2)
N2A—Zn1A—O1A—C7A	75.0 (3)	N3B—Zn1B—O1B—C7B	−97.9 (2)
N3A—Zn1A—O1A—C7A	−86.8 (2)	N2B—Zn1B—O1B—C7B	57.9 (3)
N1A—Zn1A—O1A—C7A	11.8 (2)	N1B—Zn1B—O1B—C7B	−0.1 (2)
O1A—Zn1A—O2A—C13A	−154.9 (2)	O1B—Zn1B—O2B—C13B	−149.2 (2)
N2A—Zn1A—O2A—C13A	−3.0 (2)	N3B—Zn1B—O2B—C13B	112.0 (2)
N3A—Zn1A—O2A—C13A	102.3 (2)	N2B—Zn1B—O2B—C13B	5.2 (2)
N1A—Zn1A—O2A—C13A	−56.1 (4)	N1B—Zn1B—O2B—C13B	−44.9 (4)
O1A—Zn1A—N1A—C1A	−4.4 (2)	O2B—Zn1B—N1B—C1B	−100.5 (3)
O2A—Zn1A—N1A—C1A	−104.1 (3)	O1B—Zn1B—N1B—C1B	5.2 (2)
N2A—Zn1A—N1A—C1A	−158.7 (2)	N3B—Zn1B—N1B—C1B	102.5 (2)
N3A—Zn1A—N1A—C1A	97.6 (2)	N2B—Zn1B—N1B—C1B	−152.2 (2)
O1A—Zn1A—N1A—C25A	169.47 (18)	O2B—Zn1B—N1B—C25B	68.9 (3)
O2A—Zn1A—N1A—C25A	69.9 (3)	O1B—Zn1B—N1B—C25B	174.53 (17)
N2A—Zn1A—N1A—C25A	15.18 (18)	N3B—Zn1B—N1B—C25B	−88.20 (18)
N3A—Zn1A—N1A—C25A	−88.51 (19)	N2B—Zn1B—N1B—C25B	17.12 (17)
O1A—Zn1A—N2A—C19A	99.7 (3)	O2B—Zn1B—N2B—C19B	−3.4 (2)
O2A—Zn1A—N2A—C19A	0.7 (2)	O1B—Zn1B—N2B—C19B	100.1 (3)
N3A—Zn1A—N2A—C19A	−98.7 (2)	N3B—Zn1B—N2B—C19B	−104.9 (2)
N1A—Zn1A—N2A—C19A	165.3 (2)	N1B—Zn1B—N2B—C19B	160.4 (2)
O1A—Zn1A—N2A—C20A	−79.2 (3)	O2B—Zn1B—N2B—C20B	−179.50 (19)
O2A—Zn1A—N2A—C20A	−178.21 (18)	O1B—Zn1B—N2B—C20B	−76.0 (3)
N3A—Zn1A—N2A—C20A	82.37 (19)	N3B—Zn1B—N2B—C20B	78.93 (19)
N1A—Zn1A—N2A—C20A	−13.64 (18)	N1B—Zn1B—N2B—C20B	−15.71 (18)
C25A—N1A—C1A—C2A	−177.5 (3)	C25B—N1B—C1B—C2B	−177.0 (2)
Zn1A—N1A—C1A—C2A	−4.1 (4)	Zn1B—N1B—C1B—C2B	−8.4 (4)
N1A—C1A—C2A—C3A	−173.0 (3)	N1B—C1B—C2B—C3B	−175.8 (3)
N1A—C1A—C2A—C7A	9.2 (4)	N1B—C1B—C2B—C7B	5.7 (4)
C7A—C2A—C3A—C4A	−0.5 (4)	C7B—C2B—C3B—C4B	−1.2 (4)
C1A—C2A—C3A—C4A	−178.4 (3)	C1B—C2B—C3B—C4B	−179.7 (3)
C2A—C3A—C4A—C5A	1.2 (4)	C2B—C3B—C4B—C5B	0.0 (4)
C2A—C3A—C4A—Br1A	179.7 (2)	C2B—C3B—C4B—Br1B	−179.9 (2)
C3A—C4A—C5A—C6A	−0.4 (4)	C3B—C4B—C5B—C6B	0.9 (4)
Br1A—C4A—C5A—C6A	−178.9 (2)	Br1B—C4B—C5B—C6B	−179.2 (2)
C4A—C5A—C6A—C7A	−1.2 (4)	C4B—C5B—C6B—C7B	−0.7 (4)
Zn1A—O1A—C7A—C6A	170.82 (19)	Zn1B—O1B—C7B—C6B	178.19 (18)
Zn1A—O1A—C7A—C2A	−10.8 (4)	Zn1B—O1B—C7B—C2B	−2.1 (4)
C5A—C6A—C7A—O1A	−179.7 (3)	C5B—C6B—C7B—O1B	179.3 (3)

C5A—C6A—C7A—C2A	1.8 (4)	C5B—C6B—C7B—C2B	−0.4 (4)
C3A—C2A—C7A—O1A	−179.3 (3)	C3B—C2B—C7B—O1B	−178.4 (3)
C1A—C2A—C7A—O1A	−1.7 (4)	C1B—C2B—C7B—O1B	0.0 (4)
C3A—C2A—C7A—C6A	−0.9 (4)	C3B—C2B—C7B—C6B	1.3 (4)
C1A—C2A—C7A—C6A	176.8 (3)	C1B—C2B—C7B—C6B	179.8 (3)
O1A—Zn1A—N3A—C8A	78.5 (2)	O2B—Zn1B—N3B—C8B	171.8 (2)
O2A—Zn1A—N3A—C8A	174.6 (2)	O1B—Zn1B—N3B—C8B	73.6 (2)
N2A—Zn1A—N3A—C8A	−92.7 (2)	N2B—Zn1B—N3B—C8B	−95.6 (2)
N1A—Zn1A—N3A—C8A	−12.4 (2)	N1B—Zn1B—N3B—C8B	−16.4 (2)
O1A—Zn1A—N3A—C12A	−99.1 (2)	O2B—Zn1B—N3B—C12B	−6.5 (2)
O2A—Zn1A—N3A—C12A	−2.9 (2)	O1B—Zn1B—N3B—C12B	−104.7 (2)
N2A—Zn1A—N3A—C12A	89.8 (2)	N2B—Zn1B—N3B—C12B	86.2 (2)
N1A—Zn1A—N3A—C12A	170.1 (2)	N1B—Zn1B—N3B—C12B	165.4 (2)
C12A—N3A—C8A—C9A	0.0 (4)	C12B—N3B—C8B—C9B	−0.8 (4)
Zn1A—N3A—C8A—C9A	−177.6 (2)	Zn1B—N3B—C8B—C9B	−179.1 (2)
N3A—C8A—C9A—C10A	−0.5 (5)	N3B—C8B—C9B—C10B	0.1 (5)
C8A—C9A—C10A—C11A	0.5 (5)	C8B—C9B—C10B—C11B	0.5 (5)
C9A—C10A—C11A—C12A	0.0 (5)	C9B—C10B—C11B—C12B	−0.3 (5)
C8A—N3A—C12A—C11A	0.5 (4)	C8B—N3B—C12B—C11B	0.9 (4)
Zn1A—N3A—C12A—C11A	178.2 (2)	Zn1B—N3B—C12B—C11B	179.2 (2)
C10A—C11A—C12A—N3A	−0.5 (5)	C10B—C11B—C12B—N3B	−0.4 (5)
Zn1A—O2A—C13A—C18A	2.0 (4)	Zn1B—O2B—C13B—C14B	173.5 (2)
Zn1A—O2A—C13A—C14A	−178.32 (18)	Zn1B—O2B—C13B—C18B	−7.3 (4)
O2A—C13A—C14A—C15A	179.2 (3)	O2B—C13B—C14B—C15B	175.9 (3)
C18A—C13A—C14A—C15A	−1.1 (4)	C18B—C13B—C14B—C15B	−3.4 (4)
C13A—C14A—C15A—C16A	0.3 (4)	C13B—C14B—C15B—C16B	0.8 (4)
C14A—C15A—C16A—C17A	0.9 (4)	C14B—C15B—C16B—C17B	2.6 (4)
C14A—C15A—C16A—Br2A	179.9 (2)	C14B—C15B—C16B—Br2B	−178.5 (2)
C15A—C16A—C17A—C18A	−1.3 (4)	C15B—C16B—C17B—C18B	−3.4 (4)
Br2A—C16A—C17A—C18A	179.7 (2)	Br2B—C16B—C17B—C18B	177.8 (2)
C16A—C17A—C18A—C13A	0.4 (4)	C16B—C17B—C18B—C19B	178.2 (3)
C16A—C17A—C18A—C19A	178.7 (3)	C16B—C17B—C18B—C13B	0.7 (4)
O2A—C13A—C18A—C17A	−179.6 (2)	O2B—C13B—C18B—C17B	−176.6 (3)
C14A—C13A—C18A—C17A	0.7 (4)	C14B—C13B—C18B—C17B	2.6 (4)
O2A—C13A—C18A—C19A	2.3 (4)	O2B—C13B—C18B—C19B	6.1 (4)
C14A—C13A—C18A—C19A	−177.4 (3)	C14B—C13B—C18B—C19B	−174.7 (3)
C20A—N2A—C19A—C18A	−178.5 (3)	C20B—N2B—C19B—C18B	179.8 (3)
Zn1A—N2A—C19A—C18A	2.7 (4)	Zn1B—N2B—C19B—C18B	3.8 (4)
C17A—C18A—C19A—N2A	177.0 (3)	C17B—C18B—C19B—N2B	178.1 (3)
C13A—C18A—C19A—N2A	−4.8 (4)	C13B—C18B—C19B—N2B	−4.5 (5)
C19A—N2A—C20A—C21A	13.7 (4)	C19B—N2B—C20B—C21B	17.3 (4)
Zn1A—N2A—C20A—C21A	−167.3 (2)	Zn1B—N2B—C20B—C21B	−166.3 (2)
C19A—N2A—C20A—C25A	−168.8 (2)	C19B—N2B—C20B—C25B	−164.3 (2)
Zn1A—N2A—C20A—C25A	10.1 (3)	Zn1B—N2B—C20B—C25B	12.0 (3)
C25A—C20A—C21A—C22A	−0.3 (4)	C25B—C20B—C21B—C22B	0.0 (4)
N2A—C20A—C21A—C22A	177.1 (3)	N2B—C20B—C21B—C22B	178.4 (3)
C20A—C21A—C22A—C23A	−1.4 (4)	C20B—C21B—C22B—C23B	−1.5 (4)
C21A—C22A—C23A—C24A	1.2 (4)	C21B—C22B—C23B—C24B	0.8 (4)
C22A—C23A—C24A—C25A	0.6 (4)	C22B—C23B—C24B—C25B	1.3 (4)

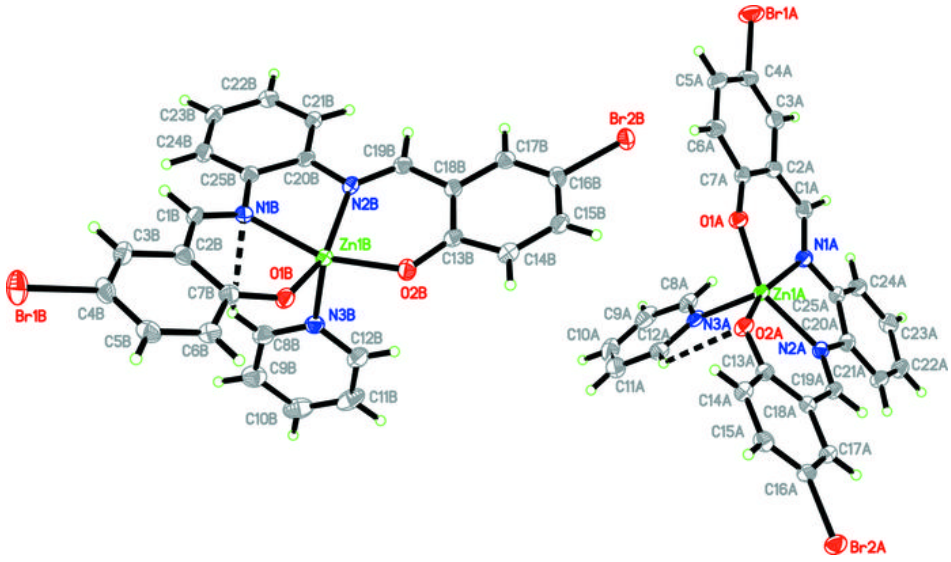
C23A—C24A—C25A—C20A	−2.2 (4)	C23B—C24B—C25B—C20B	−2.8 (4)
C23A—C24A—C25A—N1A	179.1 (3)	C23B—C24B—C25B—N1B	177.9 (2)
C21A—C20A—C25A—C24A	2.0 (4)	C21B—C20B—C25B—C24B	2.1 (4)
N2A—C20A—C25A—C24A	−175.5 (2)	N2B—C20B—C25B—C24B	−176.4 (2)
C21A—C20A—C25A—N1A	−179.2 (2)	C21B—C20B—C25B—N1B	−178.6 (2)
N2A—C20A—C25A—N1A	3.2 (4)	N2B—C20B—C25B—N1B	3.0 (3)
C1A—N1A—C25A—C24A	−21.8 (4)	C1B—N1B—C25B—C24B	−27.0 (4)
Zn1A—N1A—C25A—C24A	164.1 (2)	Zn1B—N1B—C25B—C24B	163.0 (2)
C1A—N1A—C25A—C20A	159.5 (3)	C1B—N1B—C25B—C20B	153.7 (2)
Zn1A—N1A—C25A—C20A	−14.7 (3)	Zn1B—N1B—C25B—C20B	−16.3 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9A—H9AA···O1A^{i}	0.93	2.44	3.233 (4)	143
C8B—H8BA···N1B	0.93	2.61	3.216 (4)	123
C12A—H12A···O2A	0.93	2.60	3.178 (4)	121
C24B—H24B···O1A^{ii}	0.93	2.36	3.267 (3)	166
C17A—H17A···Cg1^{iii}	0.93	2.89	3.820 (3)	174
C17B—H17B···Cg2^{ii}	0.93	2.96	3.882 (3)	173

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

Fig. 1


Br1A
C4A
C5A
C3A
C6A
C2A
C7A
C1A
O1A
N1A
C8A
Zn1A
C24A
C25A
C9A
N3A
O2A
C20A
C23A
C10A
C12A
N2A
C22A
C13A
C21A
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N3B
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C8B
C12B
C6B
C9B
C11B
C10B

Fig. 2