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

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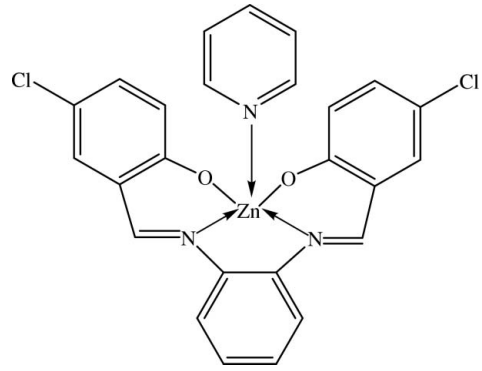
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.111; data-to-parameter ratio = 26.4.

There are two unique molecules of the title mononuclear zinc(II) complex, $[Zn(C_{20}H_{12}Cl_2N_2O_2)(C_5H_5N)]$, in the asymmetric unit. The Zn^{II} ion is five-coordinate in a distorted square-pyramidal geometry, with the basal plane defined by the two N and two O atoms of the Schiff base ligand and the apical position occupied by the N atom of the pyridine. The N and O atoms of the Schiff base ligand are mutually *cis*. The molecules are linked by weak C—H···Cl interactions into chains along the *b* axis. Other molecules are arranged diagonally between adjacent chains and bridge the chains through weak C—H···O interactions. The crystal structure is further stabilized by weak intra- and intermolecular C—H···O hydrogen bonds and C—H···π interactions.

Related literature

For a background to Schiff base coordination complexes, see: Pal *et al.* (2005); Collinson & Fenton (1996); Tarafder, Chew *et al.* (2002); Tarafder, Jin *et al.* (2002). For related literature on values of bond lengths, see: Allen *et al.* (1987). For related structures, see for example: Humphrey *et al.* (1999); Eltayeb *et al.* (2007).



Experimental

Crystal data

$[Zn(C_{20}H_{12}Cl_2N_2O_2)(C_5H_5N)]$
M_r = 527.71
Triclinic, $P\overline{1}$
a = 7.9840 (4) Å
b = 12.6632 (6) Å
c = 22.3163 (11) Å
α = 91.574 (3)°
β = 94.154 (3)°
γ = 103.791 (3)°
V = 2183.11 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 100.0 (1) K
0.60 × 0.20 × 0.12 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.489, T_{max} = 0.855
55655 measured reflections
15712 independent reflections
12030 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
S = 1.07
15712 reflections
595 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9B—H9BA···O1A^{i}	0.93	2.35	3.261 (2)	167
C21B—H21B···N1B	0.93	2.59	3.198 (3)	123
C22A—H22A···O1A^{ii}	0.93	2.42	3.199 (3)	141
C25A—H25A···O2A	0.93	2.60	3.175 (3)	121
C5B—H5BA···$Cg3^{i}$	0.93	3.06	3.463 (3)	108
C21A—H21A···$Cg1$	0.93	2.97	3.397 (3)	109
C21B—H21B···$Cg2$	0.93	2.80	3.301 (2)	115

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x-1, y, z$. $Cg1$, $Cg2$ and $Cg3$ are the centroids of rings Zn1A/O1A/C1A/C6A/C7A/N1A, Zn1B/O1B/C1B/C6B/C7B/N1B and C1A–C6A, respectively.

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: SJ2317).

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.

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

Collinson, S. R. & Fenton, D. E. (1996). *Coord. Chem. Rev.* **148**, 19–40.

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

Humphrey, E. R., Mann, K. L. V., Reeves, Z. R., Behrendt, A., Jeffery, J. C., Maher, J. P., McCleverty, J. A. & Ward, M. D. (1999). *New J. Chem.* **23**, 417–423.

Pal, S., Barik, A. K., Gupta, S., Hazra, A., Kar, S. K., Peng, S.-M., Lee, G.-H., Butcher, R. J., El Fallah, M. S. & Ribas, J. (2005). *Inorg. Chem.* **44**, 3880–3889.

Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

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

Tarafder, M. T. H., Chew, K.-B., Crouse, K. A., Ali, A. M., Yamin, B. M. & Fun, H.-K. (2002). *Polyhedron*, **21**, 2683–2690.

Tarafder, M. T. H., Jin, K. T., Crouse, K. A., Ali, A. M., Yamin, B. M. & Fun, H.-K. (2002). *Polyhedron*, **21**, 2547–2554.

supplementary materials

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

N. E. Eltayeb, S. G. Teoh, S. Chantrapromma, H.-K. Fun and K. Ibrahim

Comment

Schiff base ligands have played an important role in the development of coordination chemistry as they readily form stable complexes with most transition metal ions (Pal *et al.*, 2005). It is also well known that zinc complexes with Schiff-bases are important in biological systems and coordination chemistry (Collinson & Fenton, 1996; Tarafder, Chew *et al.*, 2002; Tarafder, Jin *et al.*, 2002). Recently, we reported the crystal structure of aqua{2,2'-[1,2-phenylenebis(nitrilomethylidyne)]bis(4-methoxyphenolato)- κ^4O,*O*',*N*,*N*'}zinc(II), (II), derived from a related Schiff base ligand (Eltayeb *et al.*, 2007). As an extension of our investigations of the structure of Schiff base zinc(II) complexes, the title mononuclear zinc(II) complex, (I) is reported here.

Complex (I) is a mononuclear zinc(II) compound (Fig. 1). There are two unique molecules in the asymmetric unit. Each Zn^{II} ion is in a distorted square pyramidal geometry and five-coordinated by two N and two O atoms of a Schiff-base ligand forming the basal plane, and by the N atom of pyridine at the axial position. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and comparable to the values in another closely related zinc(II) complex, (II) (Eltayeb *et al.*, 2007). The bond angles around the central metal zinc(II) show some deviation from ideal square pyramidal geometry. The dihedral angles between the pyridine (C21–C25/N3) and C1–C6 or C15–C20 rings are 89.75 (11)° and 74.44 (10)°, respectively in molecule A [88.32 (10)Å and 75.71 (10)° in molecule B].

In the crystal structure of (I) as shown Fig. 2, adjacent molecules are linked through weak C—H···Cl interactions into chains running along the *b* axis. Between the adjacent chains, there are molecules which are arranged diagonally and are bridging these chains through weak C—H···O interactions. The crystal is stabilized by weak C—H···O intra- and intermolecular interactions (Table 1). C—H···π were also observed; Cg_1, Cg_2 and Cg_3 are the centroids of Zn1A–O1A–C1A–C6A–C7A–N1A, Zn1B–O1B–C1B–C6B–C7B–N1B and C1A–C6A, respectively (Table 1).

Experimental

The title compound (I) was synthesized by adding 5-chloro-2-hydroxybenzaldehyde (0.624 g, 4 mmol) to a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in 95% ethanol (20 ml). The mixture was refluxed with stirring for half an hour. Zinc chloride (0.272 g, 2 mmol) in ethanol (10 ml) was then added, followed by triethylamine (0.5 ml, 3.6 mmol). The mixture was stirred at room temperature for 2 h. A yellow precipitate was obtained, washed with about 5 ml e thanol, dried, and then washed by a copious amount of diethyl ether. This precipitate was then dissolved in 20 ml of pyridine. Yellow single crystals of (I) suitable for *x*-ray structure determination formed after several days of slow evaporation of the pyridine at room temperature.

Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å. The U_{iso} values were constrained to be $1.2U_{eq}$ of the carrier atoms. The highest residual peak is located 1.17 Å from Cl1B and the deepest hole is located 0.73 Å from Zn1A.

Figures

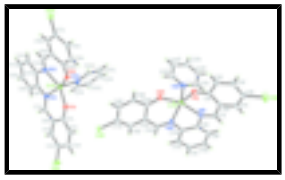

Fig. 1. The asymmetric unit of (I), showing 60% probability displacement ellipsoids and the atomic numbering.

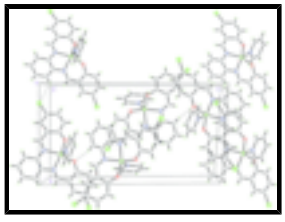

Fig. 2. The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[Zn(C_{20}H_{12}Cl_2N_2O_2)(C_5H_5N)]$	$Z = 4$
$M_r = 527.71$	$F_{000} = 1072$
Triclinic, $P\overline{1}$	$D_x = 1.606$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.9840$ (4) Å	Cell parameters from 15712 reflections
$b = 12.6632$ (6) Å	$\theta = 0.9$–32.5°
$c = 22.3163$ (11) Å	$\mu = 1.40$ mm^{-1}
$\alpha = 91.574$ (3)°	$T = 100.0$ (1) K
$\beta = 94.154$ (3)°	Needle, yellow
$\gamma = 103.791$ (3)°	0.60 × 0.20 × 0.12 mm
$V = 2183.11$ (19) Å^3	

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	15712 independent reflections
Radiation source: fine-focus sealed tube	12030 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.060$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 32.5^\circ$
$T = 100.0(1)$ K	$\theta_{min} = 0.9^\circ$

ω scans	$h = -11 \rightarrow 12$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -19 \rightarrow 19$
$T_{min} = 0.489$, $T_{max} = 0.855$	$l = -33 \rightarrow 33$
55655 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
$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.111$	$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 1.047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
15712 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
595 parameters	$\Delta\rho_{min} = -0.67$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The low-temparture 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}
Zn1A	0.07617 (3)	0.304165 (17)	0.886205 (10)	0.01428 (5)
Cl1A	−0.08004 (10)	−0.22912 (5)	0.72552 (3)	0.03907 (15)
Cl2A	0.60377 (7)	0.80907 (4)	1.03804 (2)	0.02316 (10)
O1A	0.13688 (18)	0.22551 (11)	0.81699 (6)	0.0176 (3)
O2A	0.24672 (18)	0.44173 (11)	0.87359 (6)	0.0183 (3)
N1A	−0.0384 (2)	0.15259 (13)	0.92090 (7)	0.0168 (3)
N2A	0.0915 (2)	0.34531 (13)	0.97772 (7)	0.0150 (3)
N3A	−0.1483 (2)	0.34607 (14)	0.85123 (7)	0.0179 (3)
C1A	0.0853 (2)	0.12367 (15)	0.79939 (9)	0.0165 (3)
C2A	0.1296 (3)	0.09106 (17)	0.74236 (9)	0.0209 (4)
H2AB	0.1953	0.1431	0.7194	0.025*
C3A	0.0783 (3)	−0.01512 (18)	0.72002 (10)	0.0249 (4)

H3AB	0.1075	−0.0337	0.6822	0.030*
C4A	−0.0174 (3)	−0.09444 (17)	0.75420 (10)	0.0250 (4)
C5A	−0.0601 (3)	−0.06862 (16)	0.81019 (10)	0.0222 (4)
H5AB	−0.1221	−0.1230	0.8327	0.027*
C6A	−0.0108 (2)	0.03992 (15)	0.83404 (9)	0.0178 (3)
C7A	−0.0575 (2)	0.05834 (15)	0.89393 (9)	0.0179 (3)
H7AB	−0.1052	−0.0026	0.9149	0.021*
C8A	−0.0853 (2)	0.16341 (15)	0.98018 (9)	0.0166 (3)
C9A	−0.2003 (3)	0.08306 (16)	1.00863 (10)	0.0215 (4)
H9AB	−0.2516	0.0170	0.9881	0.026*
C10A	−0.2384 (3)	0.10095 (18)	1.06700 (10)	0.0237 (4)
H10A	−0.3146	0.0468	1.0856	0.028*
C11A	−0.1638 (3)	0.19910 (18)	1.09781 (9)	0.0220 (4)
H11A	−0.1872	0.2100	1.1374	0.026*
C12A	−0.0538 (3)	0.28133 (16)	1.06969 (9)	0.0194 (4)
H12A	−0.0067	0.3479	1.0902	0.023*
C13A	−0.0133 (2)	0.26499 (15)	1.01086 (9)	0.0158 (3)
C14A	0.1872 (2)	0.43397 (15)	1.00396 (9)	0.0161 (3)
H14A	0.1856	0.4417	1.0455	0.019*
C15A	0.2958 (2)	0.52160 (15)	0.97474 (8)	0.0153 (3)
C16A	0.3845 (2)	0.61156 (15)	1.01271 (9)	0.0175 (3)
H16A	0.3680	0.6115	1.0535	0.021*
C17A	0.4945 (2)	0.69887 (15)	0.99026 (9)	0.0181 (3)
C18A	0.5231 (3)	0.69989 (16)	0.92920 (9)	0.0195 (4)
H18A	0.5982	0.7592	0.9142	0.023*
C19A	0.4393 (3)	0.61260 (16)	0.89141 (9)	0.0189 (4)
H19A	0.4602	0.6140	0.8509	0.023*
C20A	0.3216 (2)	0.52012 (15)	0.91204 (9)	0.0157 (3)
C21A	−0.3028 (3)	0.2735 (2)	0.84529 (10)	0.0243 (4)
H21A	−0.3103	0.2043	0.8595	0.029*
C22A	−0.4504 (3)	0.2972 (2)	0.81903 (11)	0.0336 (6)
H22A	−0.5547	0.2447	0.8152	0.040*
C23A	−0.4407 (3)	0.4002 (3)	0.79847 (11)	0.0393 (7)
H23A	−0.5387	0.4183	0.7809	0.047*
C24A	−0.2821 (4)	0.4764 (2)	0.80436 (11)	0.0353 (6)
H24A	−0.2720	0.5462	0.7908	0.042*
C25A	−0.1397 (3)	0.44592 (19)	0.83093 (9)	0.0237 (4)
H25A	−0.0336	0.4967	0.8349	0.028*
Zn1B	0.24994 (3)	0.750502 (17)	0.446624 (10)	0.01377 (5)
Cl1B	0.53214 (8)	1.14642 (5)	0.21623 (3)	0.03329 (13)
Cl2B	0.45724 (7)	0.33521 (4)	0.64416 (2)	0.02195 (10)
O1B	0.40173 (18)	0.89342 (11)	0.43171 (6)	0.0168 (3)
O2B	0.37564 (19)	0.72741 (11)	0.52269 (6)	0.0189 (3)
N1B	0.1634 (2)	0.73368 (12)	0.35419 (7)	0.0142 (3)
N2B	0.1587 (2)	0.58051 (13)	0.43293 (7)	0.0142 (3)
N3B	0.0454 (2)	0.80835 (13)	0.47794 (7)	0.0160 (3)
C1B	0.4220 (2)	0.94502 (15)	0.38263 (9)	0.0152 (3)
C2B	0.5361 (3)	1.05123 (16)	0.38571 (9)	0.0192 (4)
H2BA	0.5904	1.0804	0.4228	0.023*

C3B	0.5683 (3)	1.11150 (16)	0.33587 (10)	0.0214 (4)
H3BA	0.6427	1.1805	0.3395	0.026*
C4B	0.4892 (3)	1.06911 (17)	0.27962 (10)	0.0222 (4)
C5B	0.3774 (3)	0.96788 (16)	0.27388 (9)	0.0198 (4)
H5BA	0.3252	0.9407	0.2362	0.024*
C6B	0.3405 (2)	0.90455 (15)	0.32454 (9)	0.0163 (3)
C7B	0.2218 (2)	0.79992 (15)	0.31328 (9)	0.0154 (3)
H7BA	0.1841	0.7781	0.2735	0.019*
C8B	0.0507 (2)	0.63124 (14)	0.33783 (8)	0.0135 (3)
C9B	−0.0596 (2)	0.60894 (15)	0.28505 (8)	0.0155 (3)
H9BA	−0.0655	0.6642	0.2590	0.019*
C10B	−0.1604 (2)	0.50445 (16)	0.27149 (9)	0.0181 (3)
H10B	−0.2319	0.4896	0.2360	0.022*
C11B	−0.1547 (3)	0.42217 (16)	0.31074 (9)	0.0187 (4)
H11B	−0.2211	0.3520	0.3011	0.022*
C12B	−0.0506 (2)	0.44382 (15)	0.36435 (9)	0.0169 (3)
H12B	−0.0498	0.3885	0.3908	0.020*
C13B	0.0531 (2)	0.54836 (15)	0.37879 (8)	0.0142 (3)
C14B	0.1999 (2)	0.50880 (15)	0.46748 (8)	0.0153 (3)
H14B	0.1559	0.4361	0.4552	0.018*
C15B	0.3069 (2)	0.53088 (15)	0.52288 (8)	0.0146 (3)
C16B	0.3296 (2)	0.43856 (15)	0.55369 (9)	0.0162 (3)
H16B	0.2727	0.3693	0.5383	0.019*
C17B	0.4345 (2)	0.45012 (16)	0.60595 (8)	0.0164 (3)
C18B	0.5276 (2)	0.55356 (17)	0.62836 (9)	0.0181 (3)
H18B	0.6021	0.5607	0.6631	0.022*
C19B	0.5087 (2)	0.64438 (16)	0.59897 (9)	0.0179 (3)
H19B	0.5729	0.7124	0.6140	0.021*
C20B	0.3942 (2)	0.63808 (15)	0.54630 (8)	0.0152 (3)
C21B	−0.0590 (3)	0.84549 (17)	0.43842 (9)	0.0201 (4)
H21B	−0.0387	0.8437	0.3979	0.024*
C22B	−0.1952 (3)	0.88633 (18)	0.45506 (11)	0.0257 (4)
H22B	−0.2652	0.9107	0.4261	0.031*
C23B	−0.2268 (3)	0.8907 (2)	0.51480 (11)	0.0291 (5)
H23B	−0.3181	0.9176	0.5270	0.035*
C24B	−0.1182 (3)	0.8536 (2)	0.55642 (10)	0.0278 (5)
H24B	−0.1354	0.8555	0.5972	0.033*
C25B	0.0159 (3)	0.81361 (17)	0.53625 (9)	0.0209 (4)
H25C	0.0885	0.7894	0.5643	0.025*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1A	0.01486 (10)	0.01347 (10)	0.01347 (10)	0.00164 (7)	0.00036 (7)	−0.00008 (7)
Cl1A	0.0577 (4)	0.0196 (3)	0.0383 (3)	0.0077 (2)	0.0031 (3)	−0.0118 (2)
Cl2A	0.0251 (2)	0.0156 (2)	0.0251 (2)	−0.00055 (16)	−0.00211 (18)	−0.00449 (17)
O1A	0.0198 (6)	0.0153 (6)	0.0171 (6)	0.0026 (5)	0.0025 (5)	−0.0008 (5)
O2A	0.0201 (6)	0.0174 (6)	0.0141 (6)	−0.0018 (5)	0.0009 (5)	−0.0014 (5)

N1A	0.0170 (7)	0.0156 (7)	0.0165 (7)	0.0018 (5)	0.0007 (6)	0.0003 (6)
N2A	0.0157 (7)	0.0138 (7)	0.0150 (7)	0.0024 (5)	0.0010 (5)	0.0014 (5)
N3A	0.0174 (7)	0.0215 (8)	0.0156 (7)	0.0064 (6)	0.0015 (6)	−0.0031 (6)
C1A	0.0147 (8)	0.0179 (8)	0.0171 (8)	0.0061 (6)	−0.0029 (6)	−0.0017 (7)
C2A	0.0211 (9)	0.0235 (9)	0.0189 (9)	0.0071 (7)	0.0021 (7)	−0.0024 (7)
C3A	0.0272 (10)	0.0257 (10)	0.0234 (10)	0.0110 (8)	−0.0007 (8)	−0.0077 (8)
C4A	0.0297 (10)	0.0164 (9)	0.0293 (11)	0.0085 (7)	−0.0022 (8)	−0.0074 (8)
C5A	0.0259 (10)	0.0152 (8)	0.0247 (10)	0.0047 (7)	−0.0017 (8)	−0.0025 (7)
C6A	0.0183 (8)	0.0147 (8)	0.0201 (9)	0.0043 (6)	−0.0017 (7)	−0.0002 (7)
C7A	0.0190 (8)	0.0142 (8)	0.0191 (9)	0.0025 (6)	−0.0014 (7)	0.0014 (7)
C8A	0.0176 (8)	0.0158 (8)	0.0161 (8)	0.0036 (6)	0.0002 (6)	0.0022 (6)
C9A	0.0237 (9)	0.0162 (8)	0.0233 (10)	0.0014 (7)	0.0039 (7)	0.0031 (7)
C10A	0.0249 (10)	0.0218 (9)	0.0244 (10)	0.0029 (7)	0.0087 (8)	0.0063 (8)
C11A	0.0243 (9)	0.0251 (10)	0.0177 (9)	0.0061 (7)	0.0071 (7)	0.0051 (7)
C12A	0.0206 (9)	0.0191 (9)	0.0183 (9)	0.0043 (7)	0.0032 (7)	0.0007 (7)
C13A	0.0141 (7)	0.0167 (8)	0.0164 (8)	0.0033 (6)	0.0013 (6)	0.0038 (6)
C14A	0.0179 (8)	0.0163 (8)	0.0141 (8)	0.0044 (6)	0.0008 (6)	0.0002 (6)
C15A	0.0157 (8)	0.0136 (8)	0.0166 (8)	0.0035 (6)	0.0014 (6)	0.0000 (6)
C16A	0.0192 (8)	0.0164 (8)	0.0168 (8)	0.0047 (6)	0.0002 (7)	0.0001 (7)
C17A	0.0182 (8)	0.0142 (8)	0.0207 (9)	0.0027 (6)	−0.0019 (7)	−0.0033 (7)
C18A	0.0172 (8)	0.0162 (8)	0.0237 (10)	0.0010 (6)	0.0014 (7)	0.0014 (7)
C19A	0.0197 (8)	0.0172 (8)	0.0186 (9)	0.0014 (7)	0.0030 (7)	0.0015 (7)
C20A	0.0151 (8)	0.0154 (8)	0.0167 (8)	0.0033 (6)	0.0018 (6)	0.0013 (6)
C21A	0.0176 (9)	0.0337 (11)	0.0204 (10)	0.0041 (8)	0.0023 (7)	−0.0041 (8)
C22A	0.0175 (9)	0.0593 (17)	0.0241 (11)	0.0113 (10)	−0.0012 (8)	−0.0093 (11)
C23A	0.0324 (12)	0.071 (2)	0.0242 (11)	0.0350 (13)	−0.0038 (9)	−0.0073 (12)
C24A	0.0454 (14)	0.0474 (15)	0.0237 (11)	0.0317 (12)	0.0031 (10)	0.0035 (10)
C25A	0.0282 (10)	0.0273 (10)	0.0191 (9)	0.0134 (8)	0.0017 (8)	0.0007 (8)
Zn1B	0.01546 (10)	0.01179 (10)	0.01394 (10)	0.00336 (7)	0.00016 (7)	0.00078 (7)
Cl1B	0.0322 (3)	0.0312 (3)	0.0329 (3)	−0.0022 (2)	0.0057 (2)	0.0176 (2)
Cl2B	0.0260 (2)	0.0213 (2)	0.0208 (2)	0.01013 (17)	−0.00032 (17)	0.00674 (17)
O1B	0.0184 (6)	0.0147 (6)	0.0163 (6)	0.0023 (5)	0.0009 (5)	0.0009 (5)
O2B	0.0241 (7)	0.0144 (6)	0.0171 (6)	0.0045 (5)	−0.0044 (5)	0.0004 (5)
N1B	0.0142 (7)	0.0117 (6)	0.0170 (7)	0.0038 (5)	0.0012 (5)	0.0014 (5)
N2B	0.0155 (7)	0.0135 (7)	0.0133 (7)	0.0031 (5)	0.0011 (5)	0.0004 (5)
N3B	0.0160 (7)	0.0133 (7)	0.0188 (7)	0.0029 (5)	0.0031 (6)	0.0008 (6)
C1B	0.0150 (8)	0.0135 (8)	0.0181 (8)	0.0045 (6)	0.0030 (6)	0.0009 (6)
C2B	0.0185 (8)	0.0152 (8)	0.0229 (9)	0.0019 (6)	0.0029 (7)	−0.0008 (7)
C3B	0.0190 (9)	0.0140 (8)	0.0309 (11)	0.0015 (6)	0.0069 (8)	0.0034 (7)
C4B	0.0220 (9)	0.0200 (9)	0.0253 (10)	0.0044 (7)	0.0062 (7)	0.0105 (8)
C5B	0.0186 (8)	0.0187 (9)	0.0218 (9)	0.0034 (7)	0.0028 (7)	0.0041 (7)
C6B	0.0153 (8)	0.0152 (8)	0.0186 (9)	0.0035 (6)	0.0029 (6)	0.0021 (7)
C7B	0.0154 (8)	0.0158 (8)	0.0157 (8)	0.0046 (6)	0.0016 (6)	0.0015 (6)
C8B	0.0138 (7)	0.0125 (7)	0.0139 (8)	0.0025 (6)	0.0024 (6)	−0.0007 (6)
C9B	0.0171 (8)	0.0163 (8)	0.0136 (8)	0.0047 (6)	0.0018 (6)	0.0022 (6)
C10B	0.0180 (8)	0.0201 (9)	0.0157 (8)	0.0044 (7)	−0.0009 (6)	−0.0005 (7)
C11B	0.0189 (8)	0.0158 (8)	0.0197 (9)	0.0013 (6)	0.0012 (7)	−0.0018 (7)
C12B	0.0190 (8)	0.0140 (8)	0.0172 (8)	0.0026 (6)	0.0015 (6)	0.0026 (6)
C13B	0.0150 (7)	0.0150 (8)	0.0126 (8)	0.0032 (6)	0.0017 (6)	0.0015 (6)

C14B	0.0173 (8)	0.0128 (7)	0.0153 (8)	0.0028 (6)	0.0017 (6)	−0.0004 (6)
C15B	0.0146 (7)	0.0152 (8)	0.0145 (8)	0.0041 (6)	0.0019 (6)	0.0021 (6)
C16B	0.0161 (8)	0.0164 (8)	0.0169 (8)	0.0050 (6)	0.0032 (6)	0.0026 (6)
C17B	0.0172 (8)	0.0188 (8)	0.0153 (8)	0.0078 (6)	0.0026 (6)	0.0045 (7)
C18B	0.0177 (8)	0.0235 (9)	0.0142 (8)	0.0076 (7)	−0.0008 (6)	0.0017 (7)
C19B	0.0168 (8)	0.0187 (8)	0.0174 (9)	0.0034 (6)	0.0001 (6)	−0.0012 (7)
C20B	0.0158 (8)	0.0156 (8)	0.0143 (8)	0.0040 (6)	0.0020 (6)	0.0009 (6)
C21B	0.0206 (9)	0.0209 (9)	0.0201 (9)	0.0079 (7)	0.0015 (7)	0.0013 (7)
C22B	0.0197 (9)	0.0245 (10)	0.0341 (12)	0.0088 (8)	0.0008 (8)	−0.0030 (9)
C23B	0.0181 (9)	0.0313 (11)	0.0367 (12)	0.0037 (8)	0.0072 (8)	−0.0120 (9)
C24B	0.0257 (10)	0.0316 (11)	0.0232 (10)	0.0003 (8)	0.0076 (8)	−0.0067 (9)
C25B	0.0211 (9)	0.0195 (9)	0.0192 (9)	−0.0013 (7)	0.0030 (7)	−0.0003 (7)

Geometric parameters (Å, °)

Zn1A—O1A	1.9665 (14)	Zn1B—O2B	1.9734 (14)
Zn1A—O2A	1.9798 (13)	Zn1B—O1B	1.9750 (13)
Zn1A—N2A	2.0815 (16)	Zn1B—N3B	2.0971 (17)
Zn1A—N3A	2.0919 (17)	Zn1B—N2B	2.1076 (16)
Zn1A—N1A	2.1138 (16)	Zn1B—N1B	2.1160 (16)
Cl1A—C4A	1.748 (2)	Cl1B—C4B	1.750 (2)
Cl2A—C17A	1.7459 (19)	Cl2B—C17B	1.7462 (19)
O1A—C1A	1.297 (2)	O1B—C1B	1.291 (2)
O2A—C20A	1.294 (2)	O2B—C20B	1.296 (2)
N1A—C7A	1.293 (3)	N1B—C7B	1.293 (2)
N1A—C8A	1.412 (3)	N1B—C8B	1.413 (2)
N2A—C14A	1.295 (2)	N2B—C14B	1.293 (2)
N2A—C13A	1.416 (2)	N2B—C13B	1.414 (2)
N3A—C25A	1.343 (3)	N3B—C21B	1.341 (3)
N3A—C21A	1.347 (3)	N3B—C25B	1.342 (3)
C1A—C2A	1.422 (3)	C1B—C2B	1.430 (3)
C1A—C6A	1.433 (3)	C1B—C6B	1.431 (3)
C2A—C3A	1.377 (3)	C2B—C3B	1.371 (3)
C2A—H2AB	0.9300	C2B—H2BA	0.9300
C3A—C4A	1.391 (3)	C3B—C4B	1.396 (3)
C3A—H3AB	0.9300	C3B—H3BA	0.9300
C4A—C5A	1.370 (3)	C4B—C5B	1.373 (3)
C5A—C6A	1.414 (3)	C5B—C6B	1.412 (3)
C5A—H5AB	0.9300	C5B—H5BA	0.9300
C6A—C7A	1.441 (3)	C6B—C7B	1.437 (3)
C7A—H7AB	0.9300	C7B—H7BA	0.9300
C8A—C9A	1.399 (3)	C8B—C9B	1.398 (3)
C8A—C13A	1.413 (3)	C8B—C13B	1.413 (3)
C9A—C10A	1.384 (3)	C9B—C10B	1.387 (3)
C9A—H9AB	0.9300	C9B—H9BA	0.9300
C10A—C11A	1.383 (3)	C10B—C11B	1.386 (3)
C10A—H10A	0.9300	C10B—H10B	0.9300
C11A—C12A	1.389 (3)	C11B—C12B	1.388 (3)
C11A—H11A	0.9300	C11B—H11B	0.9300

C12A—C13A	1.396 (3)	C12B—C13B	1.399 (3)
C12A—H12A	0.9300	C12B—H12B	0.9300
C14A—C15A	1.439 (3)	C14B—C15B	1.432 (3)
C14A—H14A	0.9300	C14B—H14B	0.9300
C15A—C16A	1.412 (3)	C15B—C16B	1.414 (3)
C15A—C20A	1.429 (3)	C15B—C20B	1.435 (3)
C16A—C17A	1.370 (3)	C16B—C17B	1.369 (3)
C16A—H16A	0.9300	C16B—H16B	0.9300
C17A—C18A	1.398 (3)	C17B—C18B	1.402 (3)
C18A—C19A	1.377 (3)	C18B—C19B	1.373 (3)
C18A—H18A	0.9300	C18B—H18B	0.9300
C19A—C20A	1.426 (3)	C19B—C20B	1.424 (3)
C19A—H19A	0.9300	C19B—H19B	0.9300
C21A—C22A	1.378 (3)	C21B—C22B	1.380 (3)
C21A—H21A	0.9300	C21B—H21B	0.9300
C22A—C23A	1.381 (4)	C22B—C23B	1.377 (3)
C22A—H22A	0.9300	C22B—H22B	0.9300
C23A—C24A	1.392 (4)	C23B—C24B	1.391 (4)
C23A—H23A	0.9300	C23B—H23B	0.9300
C24A—C25A	1.385 (3)	C24B—C25B	1.386 (3)
C24A—H24A	0.9300	C24B—H24B	0.9300
C25A—H25A	0.9300	C25B—H25C	0.9300
O1A—Zn1A—O2A	94.27 (6)	O2B—Zn1B—O1B	96.46 (6)
O1A—Zn1A—N2A	152.35 (6)	O2B—Zn1B—N3B	101.63 (6)
O2A—Zn1A—N2A	90.19 (6)	O1B—Zn1B—N3B	97.23 (6)
O1A—Zn1A—N3A	101.93 (6)	O2B—Zn1B—N2B	89.26 (6)
O2A—Zn1A—N3A	98.92 (7)	O1B—Zn1B—N2B	153.84 (6)
N2A—Zn1A—N3A	104.30 (6)	N3B—Zn1B—N2B	106.60 (6)
O1A—Zn1A—N1A	88.80 (6)	O2B—Zn1B—N1B	159.13 (6)
O2A—Zn1A—N1A	160.78 (6)	O1B—Zn1B—N1B	88.79 (6)
N2A—Zn1A—N1A	78.67 (6)	N3B—Zn1B—N1B	97.70 (6)
N3A—Zn1A—N1A	98.99 (7)	N2B—Zn1B—N1B	77.66 (6)
C1A—O1A—Zn1A	130.17 (13)	C1B—O1B—Zn1B	130.18 (12)
C20A—O2A—Zn1A	129.38 (12)	C20B—O2B—Zn1B	130.32 (12)
C7A—N1A—C8A	121.75 (17)	C7B—N1B—C8B	120.31 (16)
C7A—N1A—Zn1A	125.75 (14)	C7B—N1B—Zn1B	126.05 (13)
C8A—N1A—Zn1A	112.40 (12)	C8B—N1B—Zn1B	112.91 (11)
C14A—N2A—C13A	121.22 (16)	C14B—N2B—C13B	120.78 (16)
C14A—N2A—Zn1A	125.28 (13)	C14B—N2B—Zn1B	125.35 (13)
C13A—N2A—Zn1A	113.50 (12)	C13B—N2B—Zn1B	113.74 (12)
C25A—N3A—C21A	117.93 (19)	C21B—N3B—C25B	117.53 (18)
C25A—N3A—Zn1A	120.16 (14)	C21B—N3B—Zn1B	119.04 (13)
C21A—N3A—Zn1A	121.81 (15)	C25B—N3B—Zn1B	123.39 (14)
O1A—C1A—C2A	118.42 (18)	O1B—C1B—C2B	118.05 (17)
O1A—C1A—C6A	124.65 (18)	O1B—C1B—C6B	125.45 (16)
C2A—C1A—C6A	116.91 (18)	C2B—C1B—C6B	116.50 (17)
C3A—C2A—C1A	122.1 (2)	C3B—C2B—C1B	122.30 (19)
C3A—C2A—H2AB	118.9	C3B—C2B—H2BA	118.8
C1A—C2A—H2AB	118.9	C1B—C2B—H2BA	118.8

C2A—C3A—C4A	119.7 (2)	C2B—C3B—C4B	119.90 (18)
C2A—C3A—H3AB	120.1	C2B—C3B—H3BA	120.0
C4A—C3A—H3AB	120.1	C4B—C3B—H3BA	120.0
C5A—C4A—C3A	120.89 (19)	C5B—C4B—C3B	120.48 (19)
C5A—C4A—Cl1A	119.88 (18)	C5B—C4B—Cl1B	119.99 (17)
C3A—C4A—Cl1A	119.21 (17)	C3B—C4B—Cl1B	119.53 (15)
C4A—C5A—C6A	120.6 (2)	C4B—C5B—C6B	120.79 (19)
C4A—C5A—H5AB	119.7	C4B—C5B—H5BA	119.6
C6A—C5A—H5AB	119.7	C6B—C5B—H5BA	119.6
C5A—C6A—C1A	119.68 (19)	C5B—C6B—C1B	120.01 (17)
C5A—C6A—C7A	116.47 (18)	C5B—C6B—C7B	116.05 (17)
C1A—C6A—C7A	123.82 (17)	C1B—C6B—C7B	123.94 (17)
N1A—C7A—C6A	125.36 (18)	N1B—C7B—C6B	125.12 (18)
N1A—C7A—H7AB	117.3	N1B—C7B—H7BA	117.4
C6A—C7A—H7AB	117.3	C6B—C7B—H7BA	117.4
C9A—C8A—N1A	124.64 (17)	C9B—C8B—N1B	124.22 (16)
C9A—C8A—C13A	119.23 (18)	C9B—C8B—C13B	119.84 (16)
N1A—C8A—C13A	116.09 (16)	N1B—C8B—C13B	115.94 (16)
C10A—C9A—C8A	120.60 (19)	C10B—C9B—C8B	120.11 (17)
C10A—C9A—H9AB	119.7	C10B—C9B—H9BA	119.9
C8A—C9A—H9AB	119.7	C8B—C9B—H9BA	119.9
C11A—C10A—C9A	120.23 (19)	C11B—C10B—C9B	120.19 (18)
C11A—C10A—H10A	119.9	C11B—C10B—H10B	119.9
C9A—C10A—H10A	119.9	C9B—C10B—H10B	119.9
C10A—C11A—C12A	120.09 (19)	C10B—C11B—C12B	120.42 (17)
C10A—C11A—H11A	120.0	C10B—C11B—H11B	119.8
C12A—C11A—H11A	120.0	C12B—C11B—H11B	119.8
C11A—C12A—C13A	120.62 (19)	C11B—C12B—C13B	120.42 (17)
C11A—C12A—H12A	119.7	C11B—C12B—H12B	119.8
C13A—C12A—H12A	119.7	C13B—C12B—H12B	119.8
C12A—C13A—C8A	119.17 (17)	C12B—C13B—C8B	118.95 (16)
C12A—C13A—N2A	124.60 (17)	C12B—C13B—N2B	125.21 (16)
C8A—C13A—N2A	116.19 (17)	C8B—C13B—N2B	115.80 (15)
N2A—C14A—C15A	125.94 (18)	N2B—C14B—C15B	126.11 (17)
N2A—C14A—H14A	117.0	N2B—C14B—H14B	116.9
C15A—C14A—H14A	117.0	C15B—C14B—H14B	116.9
C16A—C15A—C20A	120.06 (17)	C16B—C15B—C14B	115.75 (16)
C16A—C15A—C14A	115.59 (17)	C16B—C15B—C20B	120.06 (17)
C20A—C15A—C14A	124.31 (17)	C14B—C15B—C20B	124.14 (17)
C17A—C16A—C15A	120.92 (18)	C17B—C16B—C15B	120.67 (18)
C17A—C16A—H16A	119.5	C17B—C16B—H16B	119.7
C15A—C16A—H16A	119.5	C15B—C16B—H16B	119.7
C16A—C17A—C18A	120.47 (18)	C16B—C17B—C18B	120.48 (17)
C16A—C17A—Cl2A	120.21 (16)	C16B—C17B—Cl2B	119.96 (15)
C18A—C17A—Cl2A	119.31 (15)	C18B—C17B—Cl2B	119.54 (15)
C19A—C18A—C17A	119.63 (18)	C19B—C18B—C17B	119.85 (17)
C19A—C18A—H18A	120.2	C19B—C18B—H18B	120.1
C17A—C18A—H18A	120.2	C17B—C18B—H18B	120.1
C18A—C19A—C20A	122.41 (18)	C18B—C19B—C20B	122.29 (18)

C18A—C19A—H19A	118.8	C18B—C19B—H19B	118.9
C20A—C19A—H19A	118.8	C20B—C19B—H19B	118.9
O2A—C20A—C19A	118.70 (17)	O2B—C20B—C19B	119.03 (17)
O2A—C20A—C15A	124.80 (16)	O2B—C20B—C15B	124.47 (17)
C19A—C20A—C15A	116.50 (17)	C19B—C20B—C15B	116.49 (17)
N3A—C21A—C22A	122.9 (2)	N3B—C21B—C22B	123.0 (2)
N3A—C21A—H21A	118.6	N3B—C21B—H21B	118.5
C22A—C21A—H21A	118.6	C22B—C21B—H21B	118.5
C21A—C22A—C23A	118.9 (2)	C23B—C22B—C21B	119.5 (2)
C21A—C22A—H22A	120.6	C23B—C22B—H22B	120.3
C23A—C22A—H22A	120.6	C21B—C22B—H22B	120.3
C22A—C23A—C24A	119.1 (2)	C22B—C23B—C24B	118.2 (2)
C22A—C23A—H23A	120.5	C22B—C23B—H23B	120.9
C24A—C23A—H23A	120.5	C24B—C23B—H23B	120.9
C25A—C24A—C23A	118.5 (3)	C25B—C24B—C23B	119.0 (2)
C25A—C24A—H24A	120.7	C25B—C24B—H24B	120.5
C23A—C24A—H24A	120.7	C23B—C24B—H24B	120.5
N3A—C25A—C24A	122.7 (2)	N3B—C25B—C24B	122.8 (2)
N3A—C25A—H25A	118.6	N3B—C25B—H25C	118.6
C24A—C25A—H25A	118.6	C24B—C25B—H25C	118.6
O2A—Zn1A—O1A—C1A	173.52 (16)	O2B—Zn1B—O1B—C1B	160.82 (16)
N2A—Zn1A—O1A—C1A	74.9 (2)	N3B—Zn1B—O1B—C1B	−96.53 (17)
N3A—Zn1A—O1A—C1A	−86.41 (17)	N2B—Zn1B—O1B—C1B	59.2 (2)
N1A—Zn1A—O1A—C1A	12.52 (17)	N1B—Zn1B—O1B—C1B	1.08 (17)
O1A—Zn1A—O2A—C20A	−154.74 (17)	O1B—Zn1B—O2B—C20B	−149.62 (17)
N2A—Zn1A—O2A—C20A	−2.06 (17)	N3B—Zn1B—O2B—C20B	111.60 (17)
N3A—Zn1A—O2A—C20A	102.45 (17)	N2B—Zn1B—O2B—C20B	4.79 (17)
N1A—Zn1A—O2A—C20A	−56.1 (3)	N1B—Zn1B—O2B—C20B	−45.9 (3)
O1A—Zn1A—N1A—C7A	−5.56 (17)	O2B—Zn1B—N1B—C7B	−100.1 (2)
O2A—Zn1A—N1A—C7A	−105.1 (2)	O1B—Zn1B—N1B—C7B	4.98 (16)
N2A—Zn1A—N1A—C7A	−160.76 (18)	N3B—Zn1B—N1B—C7B	102.11 (16)
N3A—Zn1A—N1A—C7A	96.33 (17)	N2B—Zn1B—N1B—C7B	−152.48 (17)
O1A—Zn1A—N1A—C8A	170.79 (13)	O2B—Zn1B—N1B—C8B	70.0 (2)
O2A—Zn1A—N1A—C8A	71.2 (2)	O1B—Zn1B—N1B—C8B	175.10 (13)
N2A—Zn1A—N1A—C8A	15.59 (13)	N3B—Zn1B—N1B—C8B	−87.77 (13)
N3A—Zn1A—N1A—C8A	−87.32 (13)	N2B—Zn1B—N1B—C8B	17.63 (12)
O1A—Zn1A—N2A—C14A	100.08 (19)	O2B—Zn1B—N2B—C14B	−3.12 (16)
O2A—Zn1A—N2A—C14A	0.49 (17)	O1B—Zn1B—N2B—C14B	100.12 (19)
N3A—Zn1A—N2A—C14A	−98.77 (17)	N3B—Zn1B—N2B—C14B	−105.04 (16)
N1A—Zn1A—N2A—C14A	164.72 (17)	N1B—Zn1B—N2B—C14B	160.49 (17)
O1A—Zn1A—N2A—C13A	−79.03 (18)	O2B—Zn1B—N2B—C13B	−179.06 (13)
O2A—Zn1A—N2A—C13A	−178.63 (13)	O1B—Zn1B—N2B—C13B	−75.83 (19)
N3A—Zn1A—N2A—C13A	82.11 (14)	N3B—Zn1B—N2B—C13B	79.01 (13)
N1A—Zn1A—N2A—C13A	−14.40 (13)	N1B—Zn1B—N2B—C13B	−15.45 (12)
O1A—Zn1A—N3A—C25A	−98.16 (15)	O2B—Zn1B—N3B—C21B	172.35 (14)
O2A—Zn1A—N3A—C25A	−1.84 (16)	O1B—Zn1B—N3B—C21B	74.19 (15)
N2A—Zn1A—N3A—C25A	90.65 (16)	N2B—Zn1B—N3B—C21B	−94.92 (15)
N1A—Zn1A—N3A—C25A	171.16 (15)	N1B—Zn1B—N3B—C21B	−15.56 (15)
O1A—Zn1A—N3A—C21A	78.24 (16)	O2B—Zn1B—N3B—C25B	−5.46 (16)

O2A—Zn1A—N3A—C21A	174.57 (15)	O1B—Zn1B—N3B—C25B	−103.61 (15)
N2A—Zn1A—N3A—C21A	−92.94 (16)	N2B—Zn1B—N3B—C25B	87.28 (15)
N1A—Zn1A—N3A—C21A	−12.43 (16)	N1B—Zn1B—N3B—C25B	166.64 (15)
Zn1A—O1A—C1A—C2A	170.62 (14)	Zn1B—O1B—C1B—C2B	176.85 (13)
Zn1A—O1A—C1A—C6A	−10.9 (3)	Zn1B—O1B—C1B—C6B	−3.7 (3)
O1A—C1A—C2A—C3A	−179.22 (19)	O1B—C1B—C2B—C3B	178.84 (19)
C6A—C1A—C2A—C3A	2.2 (3)	C6B—C1B—C2B—C3B	−0.7 (3)
C1A—C2A—C3A—C4A	−1.1 (3)	C1B—C2B—C3B—C4B	−0.4 (3)
C2A—C3A—C4A—C5A	−0.7 (3)	C2B—C3B—C4B—C5B	0.9 (3)
C2A—C3A—C4A—Cl1A	−179.45 (17)	C2B—C3B—C4B—Cl1B	−179.64 (17)
C3A—C4A—C5A—C6A	1.3 (3)	C3B—C4B—C5B—C6B	−0.2 (3)
Cl1A—C4A—C5A—C6A	−179.88 (16)	Cl1B—C4B—C5B—C6B	−179.70 (16)
C4A—C5A—C6A—C1A	−0.2 (3)	C4B—C5B—C6B—C1B	−0.9 (3)
C4A—C5A—C6A—C7A	−178.3 (2)	C4B—C5B—C6B—C7B	−179.95 (19)
O1A—C1A—C6A—C5A	−179.97 (19)	O1B—C1B—C6B—C5B	−178.17 (19)
C2A—C1A—C6A—C5A	−1.5 (3)	C2B—C1B—C6B—C5B	1.3 (3)
O1A—C1A—C6A—C7A	−2.1 (3)	O1B—C1B—C6B—C7B	0.8 (3)
C2A—C1A—C6A—C7A	176.47 (19)	C2B—C1B—C6B—C7B	−179.71 (18)
C8A—N1A—C7A—C6A	−179.00 (18)	C8B—N1B—C7B—C6B	−178.18 (18)
Zn1A—N1A—C7A—C6A	−3.0 (3)	Zn1B—N1B—C7B—C6B	−8.7 (3)
C5A—C6A—C7A—N1A	−173.03 (19)	C5B—C6B—C7B—N1B	−175.09 (19)
C1A—C6A—C7A—N1A	9.0 (3)	C1B—C6B—C7B—N1B	5.9 (3)
C7A—N1A—C8A—C9A	−20.4 (3)	C7B—N1B—C8B—C9B	−27.0 (3)
Zn1A—N1A—C8A—C9A	163.06 (17)	Zn1B—N1B—C8B—C9B	162.22 (15)
C7A—N1A—C8A—C13A	161.92 (18)	C7B—N1B—C8B—C13B	153.22 (18)
Zn1A—N1A—C8A—C13A	−14.6 (2)	Zn1B—N1B—C8B—C13B	−17.5 (2)
N1A—C8A—C9A—C10A	180.0 (2)	N1B—C8B—C9B—C10B	177.18 (18)
C13A—C8A—C9A—C10A	−2.4 (3)	C13B—C8B—C9B—C10B	−3.1 (3)
C8A—C9A—C10A—C11A	0.4 (3)	C8B—C9B—C10B—C11B	1.2 (3)
C9A—C10A—C11A—C12A	1.8 (3)	C9B—C10B—C11B—C12B	1.1 (3)
C10A—C11A—C12A—C13A	−1.9 (3)	C10B—C11B—C12B—C13B	−1.5 (3)
C11A—C12A—C13A—C8A	−0.2 (3)	C11B—C12B—C13B—C8B	−0.3 (3)
C11A—C12A—C13A—N2A	177.24 (19)	C11B—C12B—C13B—N2B	177.46 (18)
C9A—C8A—C13A—C12A	2.3 (3)	C9B—C8B—C13B—C12B	2.6 (3)
N1A—C8A—C13A—C12A	−179.89 (18)	N1B—C8B—C13B—C12B	−177.65 (17)
C9A—C8A—C13A—N2A	−175.29 (18)	C9B—C8B—C13B—N2B	−175.37 (17)
N1A—C8A—C13A—N2A	2.5 (3)	N1B—C8B—C13B—N2B	4.4 (2)
C14A—N2A—C13A—C12A	14.5 (3)	C14B—N2B—C13B—C12B	17.1 (3)
Zn1A—N2A—C13A—C12A	−166.32 (16)	Zn1B—N2B—C13B—C12B	−166.78 (16)
C14A—N2A—C13A—C8A	−168.00 (18)	C14B—N2B—C13B—C8B	−165.12 (17)
Zn1A—N2A—C13A—C8A	11.1 (2)	Zn1B—N2B—C13B—C8B	11.0 (2)
C13A—N2A—C14A—C15A	−178.79 (18)	C13B—N2B—C14B—C15B	179.31 (17)
Zn1A—N2A—C14A—C15A	2.2 (3)	Zn1B—N2B—C14B—C15B	3.6 (3)
N2A—C14A—C15A—C16A	178.22 (19)	N2B—C14B—C15B—C16B	178.27 (18)
N2A—C14A—C15A—C20A	−4.0 (3)	N2B—C14B—C15B—C20B	−4.3 (3)
C20A—C15A—C16A—C17A	0.7 (3)	C14B—C15B—C16B—C17B	177.56 (17)
C14A—C15A—C16A—C17A	178.59 (18)	C20B—C15B—C16B—C17B	0.0 (3)
C15A—C16A—C17A—C18A	−0.9 (3)	C15B—C16B—C17B—C18B	−3.0 (3)
C15A—C16A—C17A—Cl2A	−179.71 (15)	C15B—C16B—C17B—Cl2B	178.64 (14)

C16A—C17A—C18A—C19A	0.3 (3)	C16B—C17B—C18B—C19B	2.4 (3)
Cl2A—C17A—C18A—C19A	179.07 (16)	Cl2B—C17B—C18B—C19B	−179.17 (15)
C17A—C18A—C19A—C20A	0.6 (3)	C17B—C18B—C19B—C20B	1.1 (3)
Zn1A—O2A—C20A—C19A	−179.07 (14)	Zn1B—O2B—C20B—C19B	172.92 (13)
Zn1A—O2A—C20A—C15A	1.0 (3)	Zn1B—O2B—C20B—C15B	−6.8 (3)
C18A—C19A—C20A—O2A	179.36 (19)	C18B—C19B—C20B—O2B	176.31 (18)
C18A—C19A—C20A—C15A	−0.7 (3)	C18B—C19B—C20B—C15B	−3.9 (3)
C16A—C15A—C20A—O2A	179.99 (19)	C16B—C15B—C20B—O2B	−176.93 (18)
C14A—C15A—C20A—O2A	2.3 (3)	C14B—C15B—C20B—O2B	5.7 (3)
C16A—C15A—C20A—C19A	0.1 (3)	C16B—C15B—C20B—C19B	3.3 (3)
C14A—C15A—C20A—C19A	−177.60 (18)	C14B—C15B—C20B—C19B	−174.00 (17)
C25A—N3A—C21A—C22A	0.6 (3)	C25B—N3B—C21B—C22B	−1.2 (3)
Zn1A—N3A—C21A—C22A	−175.93 (17)	Zn1B—N3B—C21B—C22B	−179.15 (16)
N3A—C21A—C22A—C23A	−0.8 (3)	N3B—C21B—C22B—C23B	0.5 (3)
C21A—C22A—C23A—C24A	0.6 (4)	C21B—C22B—C23B—C24B	0.2 (3)
C22A—C23A—C24A—C25A	−0.2 (4)	C22B—C23B—C24B—C25B	−0.3 (3)
C21A—N3A—C25A—C24A	−0.1 (3)	C21B—N3B—C25B—C24B	1.2 (3)
Zn1A—N3A—C25A—C24A	176.41 (17)	Zn1B—N3B—C25B—C24B	178.99 (15)
C23A—C24A—C25A—N3A	0.0 (4)	C23B—C24B—C25B—N3B	−0.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9B—H9BA···O1A^{i}	0.93	2.35	3.261 (2)	167
C21B—H21B···N1B	0.93	2.59	3.198 (3)	123
C22A—H22A···O1A^{ii}	0.93	2.42	3.199 (3)	141
C25A—H25A···O2A	0.93	2.60	3.175 (3)	121
C5B—H5BA···Cg3^{i}	0.93	3.06	3.463 (3)	108
C21A—H21A···Cg1	0.93	2.97	3.397 (3)	109
C21B—H21B···Cg2	0.93	2.80	3.301 (2)	115

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

Fig. 1

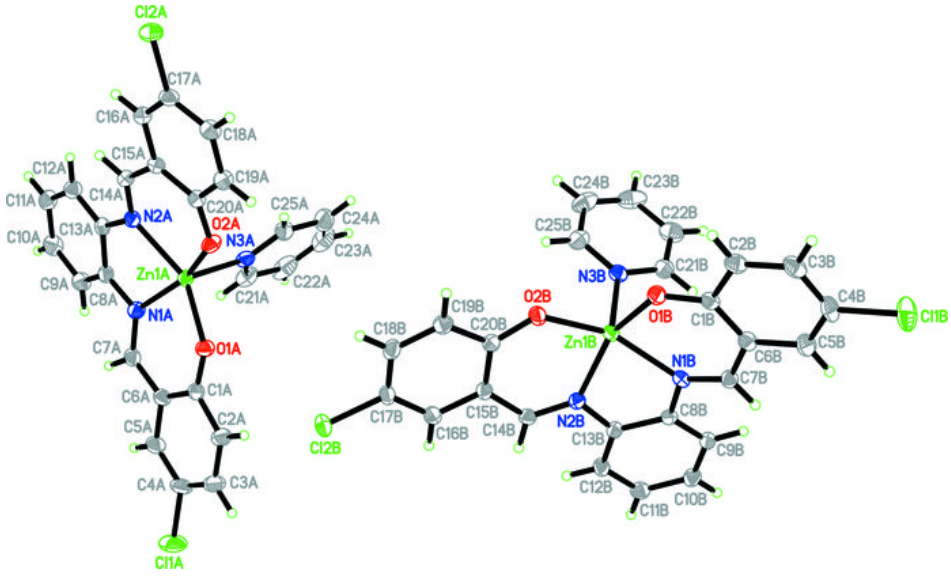
Cl2A
C17A
C16A
C18A
C15A
C19A
C12A
C11A
C14A
C20A
C25A
C24A
N2A
O2A
N3A
C10A
C13A
C23A
Zn1A
C22A
C9A
C8A
C21A
N1A
C7A
O1A
C6A
C1A
C5A
C2A
C4A
C3A
Cl1A
C24B
C23B
C22B
C25B
C2B
C3B
N3B
C21B
C4B
Cl1B
C19B
O2B
O1B
C1B
C18B
C20B
Zn1B
C6B
C5B
N1B
C7B
C17B
C15B
C8B
C16B
C14B
N2B
C13B
C9B
Cl2B
C12B
C10B
C11B

Fig. 2