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Dichlorido[1-(1-naphthylmethyl)-3-(2-pyridyl)-1*H*-pyrazole-κ^2N^2,N^3]zinc(II)

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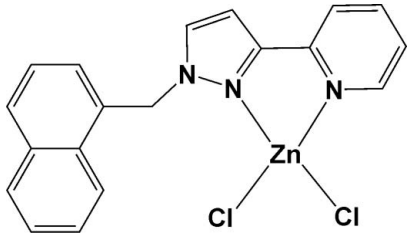
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.093; data-to-parameter ratio = 16.3.

In the title compound, $[ZnCl_2(C_{19}H_{15}N_3)]$, the Zn^{II} atom is four-coordinated by two N atoms from the 1-(1-naphthylmethyl)-3-(2-pyridyl)-1*H*-pyrazole (*L*) ligand and two terminal Cl atoms in a distorted tetrahedral coordination environment. In the crystal structure, inversion-related Zn^{II} mononuclear units are linked to form dimers through π–π stacking interactions between the pyridine and pyrazole rings, the centroid–centroid distance being 3.5166 (19) Å. The dimers are interlinked to form a chain along the *a* axis by C—H$\cdots\pi$ interactions involving both benzene rings of the *L* ligand.

Related literature

For synthesis, see: Zhang *et al.* (2005). For related literature, see: Bell *et al.* (2003); Paul *et al.* (2004); Steel (2005); Ward *et al.* (2001).



Experimental

Crystal data

$[ZnCl_2(C_{19}H_{15}N_3)]$
M_r = 421.61
Monoclinic, $P2_1/n$
a = 12.069 (2) Å
b = 10.9474 (18) Å
c = 13.609 (2) Å
β = 92.662 (3)°
V = 1796.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.67 mm^{-1}
T = 293 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.731, T_{max} = 0.776
10232 measured reflections
3673 independent reflections
2533 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.093
S = 1.02
3673 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.070 (2)	Zn1—Cl1	2.1924 (10)
Zn1—N3	2.074 (2)	Zn1—Cl2	2.2016 (9)
N2—Zn1—N3	79.77 (9)	N2—Zn1—Cl2	113.51 (7)
N2—Zn1—Cl1	115.27 (7)	N3—Zn1—Cl2	113.93 (7)
N3—Zn1—Cl1	114.91 (7)	Cl1—Zn1—Cl2	114.83 (4)

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

*Cg*1 and *Cg*2 are the centroids of the C2–C6/C11 and C6–C11 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C12—H12$\cdots$*Cg*1^{i}	0.93	2.55	3.400 (4)	152
C13—H13$\cdots$*Cg*2^{i}	0.93	2.87	3.536 (3)	129

Symmetry code: (i) $-x+1, -y, -z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: CI2416).

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supplementary materials

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Dichlorido[1-(1-naphthylmethyl)-3-(2-pyridyl)-1*H*-pyrazole-κ^2N^2,N^3]zinc(II)

C.-S. Liu, L.-F. Yan and J.-J. Wang

Comment

In recent years, much attention has been focused on the synthetic approach and the structural control of metal-organic coordination architectures with ligands based on pyrazolyl-pyridine chelating units (Steel *et al.*, 2005; Ward *et al.*, 2001). Many novel functional complexes with 3-(2-pyridyl)pyrazole and/or 3-(2-pyridyl)pyrazole ligands have been reported (Bell *et al.*, 2003; Paul *et al.*, 2004; Ward *et al.*, 2001). Recently, we have reported the preparation of a non-planar flexible ligand, 1-[3-(2-pyridyl)pyrazol-1-ylmethyl]naphthalene (*L*) (Zhang *et al.*, 2005). Now we report here the crystal structure of a zinc(II) complex of this ligand, [Zn(*L*)Cl_2], the title compound.

In the title compound, the Zn^{II} center is four-coordinated by two N donors from one *L* ligand and two Cl^- anions (Table 1). The coordination geometry around the Zn^{II} center can be described as a distorted tetrahedron (Fig. 1).

In the crystal structure, the Zn^{II} mononuclear units at (*x*, *y*, *z*) and (−*x*, −*y*, −*z*) are interconnected to form a dimer through π-π stacking interactions between the adjacent pyridine and pyrazole rings of the *L* ligand, with their centroids separated by 3.5166 (19) Å. The dimers are linked to form a chain along the *a* axis by C—H···π interactions (Table 2) involving the C2—C6/C11 (centroid *Cg*1) and C6—C11 (centroid *Cg*2) benzene rings of the *L* ligand (Fig. 2).

Experimental

The ligand 1-[3-(2-pyridyl)pyrazol-1-ylmethyl]naphthalene (*L*) was synthesized according to the method reported in the literature (Zhang *et al.*, 2005). A solution of $ZnCl_2$ (0.1 mmol) in methanol (15 ml) was added to *L* (0.1 mmol). A yellow solid formed was filtered off and the resulting solution was kept at room temperature. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent after several days (yield: 30%). Analysis calculated for ($C_{19}H_{15}ZnCl_2N_3$): C 54.12, H 3.59, N 9.97%; found: C 54.26, H 3.44, N 10.11%.

Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 (aromatic) or 0.97 Å (methylene) and U_{iso}(H) = 1.2U_{eq}(C).

Figures

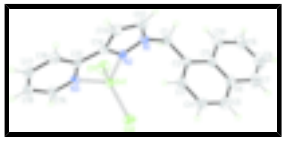


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

Dichlorido[1-(1-naphthylmethyl)-3-(2-pyridyl)-1*H*-pyrazole- κ^2N^2,N^3]zinc(II)

Crystal data

$[ZnCl_2(C_{19}H_{15}N_3)]$	F_{000} = 856
M_r = 421.61	D_x = 1.559 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3039 reflections
a = 12.069 (2) Å	θ = 2.3–25.2º
b = 10.9474 (18) Å	μ = 1.67 mm^{-1}
c = 13.609 (2) Å	T = 293 (2) K
β = 92.662 (3)º	Block, yellow
V = 1796.1 (5) Å^3	0.24 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3673 independent reflections
Radiation source: fine-focus sealed tube	2533 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 293(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	h = −15→14
T_{min} = 0.731, T_{max} = 0.776	k = −9→13
10232 measured reflections	l = −17→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.093	$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.4714P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
3673 reflections	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.11994 (3)	0.26266 (3)	0.11428 (2)	0.03872 (13)
Cl1	0.05436 (8)	0.22829 (10)	0.25927 (7)	0.0695 (3)
Cl2	0.20707 (8)	0.43809 (7)	0.10055 (6)	0.0578 (2)
N1	0.29477 (18)	0.0502 (2)	0.06734 (18)	0.0383 (6)
N2	0.20198 (18)	0.1170 (2)	0.05350 (17)	0.0337 (5)
N3	0.01157 (18)	0.2225 (2)	−0.00402 (17)	0.0374 (6)
C1	0.3734 (2)	0.0719 (3)	0.1492 (2)	0.0430 (7)
H1A	0.4103	−0.0042	0.1669	0.052*
H1B	0.3335	0.0990	0.2055	0.052*
C2	0.4602 (2)	0.1669 (3)	0.1263 (2)	0.0353 (6)
C3	0.4487 (3)	0.2406 (3)	0.0461 (2)	0.0460 (8)
H3	0.3860	0.2327	0.0042	0.055*
C4	0.5288 (3)	0.3285 (3)	0.0250 (3)	0.0554 (9)
H4	0.5186	0.3782	−0.0301	0.066*
C5	0.6204 (3)	0.3410 (3)	0.0844 (3)	0.0557 (9)
H5	0.6729	0.3999	0.0703	0.067*
C6	0.6377 (2)	0.2655 (3)	0.1679 (2)	0.0461 (8)
C7	0.7348 (3)	0.2733 (4)	0.2298 (3)	0.0634 (11)
H7	0.7889	0.3306	0.2160	0.076*
C8	0.7505 (3)	0.1995 (4)	0.3082 (3)	0.0733 (13)
H8	0.8158	0.2047	0.3470	0.088*
C9	0.6694 (3)	0.1152 (4)	0.3315 (2)	0.0648 (11)
H9	0.6803	0.0666	0.3872	0.078*
C10	0.5742 (3)	0.1026 (3)	0.2744 (2)	0.0511 (8)
H10	0.5215	0.0450	0.2907	0.061*
C11	0.5558 (2)	0.1775 (3)	0.1901 (2)	0.0383 (7)
C12	0.3038 (3)	−0.0296 (3)	−0.0065 (2)	0.0491 (8)
H12	0.3614	−0.0850	−0.0132	0.059*
C13	0.2143 (3)	−0.0156 (3)	−0.0703 (2)	0.0475 (8)
H13	0.1984	−0.0585	−0.1282	0.057*
C14	0.1521 (2)	0.0764 (3)	−0.0301 (2)	0.0348 (7)
C15	0.0460 (2)	0.1310 (3)	−0.0620 (2)	0.0359 (7)
C16	−0.0163 (3)	0.0922 (3)	−0.1437 (2)	0.0472 (8)

H16	0.0084	0.0291	−0.1829	0.057*
C17	−0.1174 (3)	0.1499 (3)	−0.1659 (2)	0.0541 (9)
H17	−0.1614	0.1253	−0.2203	0.065*
C18	−0.1514 (3)	0.2421 (3)	−0.1078 (3)	0.0553 (9)
H18	−0.2187	0.2811	−0.1219	0.066*
C19	−0.0850 (2)	0.2770 (3)	−0.0280 (3)	0.0485 (8)
H19	−0.1082	0.3411	0.0109	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0406 (2)	0.0404 (2)	0.0348 (2)	0.00353 (16)	−0.00087 (14)	−0.00799 (16)
Cl1	0.0731 (6)	0.0930 (8)	0.0437 (5)	−0.0062 (5)	0.0168 (4)	−0.0042 (5)
Cl2	0.0793 (6)	0.0408 (5)	0.0524 (5)	−0.0079 (4)	−0.0084 (4)	−0.0040 (4)
N1	0.0338 (13)	0.0375 (14)	0.0440 (15)	0.0029 (11)	0.0055 (11)	−0.0011 (11)
N2	0.0326 (12)	0.0311 (13)	0.0375 (13)	−0.0001 (10)	0.0042 (10)	−0.0028 (10)
N3	0.0336 (13)	0.0432 (15)	0.0353 (13)	−0.0015 (11)	−0.0005 (10)	0.0008 (11)
C1	0.0388 (17)	0.0491 (19)	0.0409 (17)	0.0051 (14)	0.0003 (14)	0.0091 (14)
C2	0.0321 (15)	0.0385 (17)	0.0356 (16)	0.0067 (13)	0.0036 (12)	−0.0018 (13)
C3	0.0401 (17)	0.051 (2)	0.0463 (18)	0.0010 (15)	−0.0032 (14)	0.0073 (15)
C4	0.064 (2)	0.049 (2)	0.053 (2)	−0.0014 (18)	0.0043 (18)	0.0124 (16)
C5	0.057 (2)	0.048 (2)	0.063 (2)	−0.0116 (17)	0.0121 (18)	−0.0066 (17)
C6	0.0394 (17)	0.051 (2)	0.0480 (18)	0.0022 (15)	0.0041 (14)	−0.0226 (16)
C7	0.046 (2)	0.082 (3)	0.062 (2)	−0.0041 (19)	0.0001 (18)	−0.035 (2)
C8	0.052 (2)	0.108 (3)	0.058 (3)	0.020 (2)	−0.0153 (19)	−0.042 (2)
C9	0.067 (2)	0.087 (3)	0.0384 (19)	0.031 (2)	−0.0111 (18)	−0.0100 (18)
C10	0.054 (2)	0.061 (2)	0.0379 (18)	0.0166 (17)	−0.0013 (15)	−0.0043 (15)
C11	0.0362 (16)	0.0444 (18)	0.0345 (16)	0.0085 (14)	0.0038 (13)	−0.0113 (13)
C12	0.051 (2)	0.0397 (19)	0.057 (2)	0.0072 (15)	0.0144 (17)	−0.0105 (16)
C13	0.061 (2)	0.0406 (18)	0.0415 (18)	−0.0003 (16)	0.0081 (16)	−0.0126 (14)
C14	0.0411 (16)	0.0339 (16)	0.0297 (14)	−0.0093 (13)	0.0052 (13)	−0.0033 (12)
C15	0.0399 (16)	0.0370 (17)	0.0306 (15)	−0.0126 (13)	0.0009 (13)	0.0030 (12)
C16	0.060 (2)	0.0465 (19)	0.0340 (16)	−0.0136 (16)	−0.0032 (15)	0.0026 (14)
C17	0.055 (2)	0.063 (2)	0.0422 (19)	−0.0263 (18)	−0.0177 (16)	0.0178 (18)
C18	0.0400 (18)	0.071 (3)	0.054 (2)	−0.0074 (17)	−0.0097 (15)	0.018 (2)
C19	0.0384 (17)	0.052 (2)	0.055 (2)	0.0029 (15)	−0.0005 (15)	0.0057 (15)

Geometric parameters (Å, °)

Zn1—N2	2.070 (2)	C6—C11	1.422 (4)
Zn1—N3	2.074 (2)	C7—C8	1.345 (6)
Zn1—Cl1	2.1924 (10)	C7—H7	0.93
Zn1—Cl2	2.2016 (9)	C8—C9	1.392 (5)
N1—C12	1.340 (4)	C8—H8	0.93
N1—N2	1.344 (3)	C9—C10	1.363 (4)
N1—C1	1.450 (3)	C9—H9	0.93
N2—C14	1.338 (3)	C10—C11	1.420 (4)
N3—C19	1.337 (4)	C10—H10	0.93
N3—C15	1.352 (4)	C12—C13	1.363 (4)

C1—C2	1.518 (4)	C12—H12	0.93
C1—H1A	0.97	C13—C14	1.384 (4)
C1—H1B	0.97	C13—H13	0.93
C2—C3	1.359 (4)	C14—C15	1.461 (4)
C2—C11	1.417 (4)	C15—C16	1.380 (4)
C3—C4	1.404 (4)	C16—C17	1.395 (4)
C3—H3	0.93	C16—H16	0.93
C4—C5	1.345 (4)	C17—C18	1.358 (5)
C4—H4	0.93	C17—H17	0.93
C5—C6	1.413 (5)	C18—C19	1.374 (5)
C5—H5	0.93	C18—H18	0.93
C6—C7	1.414 (5)	C19—H19	0.93
N2—Zn1—N3	79.77 (9)	C6—C7—H7	119.4
N2—Zn1—Cl1	115.27 (7)	C7—C8—C9	120.3 (3)
N3—Zn1—Cl1	114.91 (7)	C7—C8—H8	119.9
N2—Zn1—Cl2	113.51 (7)	C9—C8—H8	119.9
N3—Zn1—Cl2	113.93 (7)	C10—C9—C8	121.3 (4)
Cl1—Zn1—Cl2	114.83 (4)	C10—C9—H9	119.3
C12—N1—N2	110.3 (2)	C8—C9—H9	119.3
C12—N1—C1	127.6 (3)	C9—C10—C11	119.9 (3)
N2—N1—C1	122.0 (2)	C9—C10—H10	120.1
C14—N2—N1	106.1 (2)	C11—C10—H10	120.1
C14—N2—Zn1	113.01 (18)	C2—C11—C10	122.7 (3)
N1—N2—Zn1	140.77 (18)	C2—C11—C6	118.7 (3)
C19—N3—C15	118.5 (3)	C10—C11—C6	118.6 (3)
C19—N3—Zn1	127.3 (2)	N1—C12—C13	108.3 (3)
C15—N3—Zn1	114.23 (18)	N1—C12—H12	125.9
N1—C1—C2	112.8 (2)	C13—C12—H12	125.9
N1—C1—H1A	109.0	C12—C13—C14	105.0 (3)
C2—C1—H1A	109.0	C12—C13—H13	127.5
N1—C1—H1B	109.0	C14—C13—H13	127.5
C2—C1—H1B	109.0	N2—C14—C13	110.3 (3)
H1A—C1—H1B	107.8	N2—C14—C15	118.1 (2)
C3—C2—C11	119.5 (3)	C13—C14—C15	131.6 (3)
C3—C2—C1	121.8 (3)	N3—C15—C16	121.8 (3)
C11—C2—C1	118.7 (2)	N3—C15—C14	114.7 (2)
C2—C3—C4	121.7 (3)	C16—C15—C14	123.4 (3)
C2—C3—H3	119.1	C15—C16—C17	118.3 (3)
C4—C3—H3	119.1	C15—C16—H16	120.9
C5—C4—C3	120.1 (3)	C17—C16—H16	120.9
C5—C4—H4	119.9	C18—C17—C16	119.7 (3)
C3—C4—H4	119.9	C18—C17—H17	120.2
C4—C5—C6	120.7 (3)	C16—C17—H17	120.2
C4—C5—H5	119.7	C17—C18—C19	119.1 (3)
C6—C5—H5	119.7	C17—C18—H18	120.4
C5—C6—C7	122.1 (3)	C19—C18—H18	120.4
C5—C6—C11	119.3 (3)	N3—C19—C18	122.6 (3)
C7—C6—C11	118.6 (3)	N3—C19—H19	118.7
C8—C7—C6	121.2 (4)	C18—C19—H19	118.7

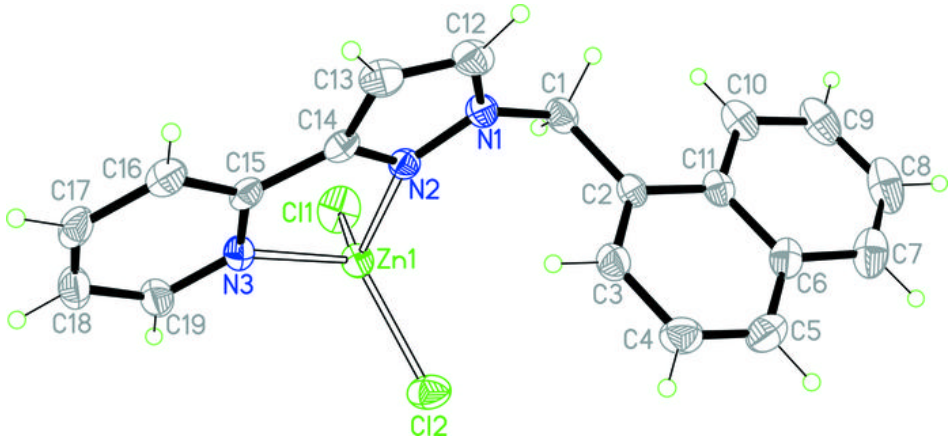
C8—C7—H7	119.4		
C12—N1—N2—C14	0.8 (3)	C3—C2—C11—C6	−0.2 (4)
C1—N1—N2—C14	177.3 (2)	C1—C2—C11—C6	179.3 (3)
C12—N1—N2—Zn1	−175.0 (2)	C9—C10—C11—C2	178.3 (3)
C1—N1—N2—Zn1	1.6 (4)	C9—C10—C11—C6	−0.6 (4)
N3—Zn1—N2—C14	3.88 (18)	C5—C6—C11—C2	1.2 (4)
Cl1—Zn1—N2—C14	116.72 (18)	C7—C6—C11—C2	−177.9 (3)
Cl2—Zn1—N2—C14	−107.90 (18)	C5—C6—C11—C10	−179.8 (3)
N3—Zn1—N2—N1	179.4 (3)	C7—C6—C11—C10	1.1 (4)
Cl1—Zn1—N2—N1	−67.7 (3)	N2—N1—C12—C13	−0.5 (3)
Cl2—Zn1—N2—N1	67.7 (3)	C1—N1—C12—C13	−176.8 (3)
N2—Zn1—N3—C19	178.1 (3)	N1—C12—C13—C14	0.0 (3)
Cl1—Zn1—N3—C19	64.9 (3)	N1—N2—C14—C13	−0.8 (3)
Cl2—Zn1—N3—C19	−70.6 (2)	Zn1—N2—C14—C13	176.28 (19)
N2—Zn1—N3—C15	−2.49 (19)	N1—N2—C14—C15	178.2 (2)
Cl1—Zn1—N3—C15	−115.73 (18)	Zn1—N2—C14—C15	−4.8 (3)
Cl2—Zn1—N3—C15	108.82 (18)	C12—C13—C14—N2	0.5 (3)
C12—N1—C1—C2	88.0 (4)	C12—C13—C14—C15	−178.3 (3)
N2—N1—C1—C2	−87.9 (3)	C19—N3—C15—C16	−0.9 (4)
N1—C1—C2—C3	13.6 (4)	Zn1—N3—C15—C16	179.7 (2)
N1—C1—C2—C11	−166.0 (2)	C19—N3—C15—C14	−179.8 (2)
C11—C2—C3—C4	−0.6 (5)	Zn1—N3—C15—C14	0.8 (3)
C1—C2—C3—C4	179.9 (3)	N2—C14—C15—N3	2.7 (4)
C2—C3—C4—C5	0.5 (5)	C13—C14—C15—N3	−178.6 (3)
C3—C4—C5—C6	0.6 (5)	N2—C14—C15—C16	−176.2 (3)
C4—C5—C6—C7	177.7 (3)	C13—C14—C15—C16	2.5 (5)
C4—C5—C6—C11	−1.4 (5)	N3—C15—C16—C17	0.0 (4)
C5—C6—C7—C8	−179.0 (3)	C14—C15—C16—C17	178.8 (3)
C11—C6—C7—C8	0.1 (5)	C15—C16—C17—C18	0.4 (4)
C6—C7—C8—C9	−1.6 (5)	C16—C17—C18—C19	0.1 (5)
C7—C8—C9—C10	2.1 (5)	C15—N3—C19—C18	1.4 (4)
C8—C9—C10—C11	−0.9 (5)	Zn1—N3—C19—C18	−179.2 (2)
C3—C2—C11—C10	−179.2 (3)	C17—C18—C19—N3	−1.0 (5)
C1—C2—C11—C10	0.4 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···Cg1^{i}	0.93	2.55	3.400 (4)	152
C13—H13···Cg2^{i}	0.93	2.87	3.536 (3)	129

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

Fig. 1


C12
C13
C1
C10
C14
N1
C9
C16
C15
N2
C11
C8
C17
C2
Cl1
Zn1
C7
N3
C3
C6
C18
C19
C4
C5
Cl2