metal-organic compounds

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Dichloridobis[2-(1-hydrazinylideneethyl)pyrazine- κN^1]zinc

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.078; data-to-parameter ratio = 18.5.

In the structure of the title complex, $[ZnCl_2(C_6H_8N_4)_2]$, the Zn^{II} atom has a distorted octahedral geometry. Two *cis* Cl⁻ ions and four N atoms belonging to two different 2-(1-hydrazinylideneethyl)pyrazine ligands coordinate the Zn^{II} atom, forming two five-membered Zn-N-C-C-N rings. The dihedral angle between the planes of these metallocycles is 88.13 (4)°. The organic ligands are essentially planar (r.m.s. deviations from planarity = 0.072 and 0.040 Å). Intermolecular $N-H\cdots N$ and $N-H\cdots CI$ interactions join the molecules into a three-dimensional framework.

Related literature

For the biochemical applications of complexes based on ligands containing pyrazine, see: Ha *et al.* (1999); Blackstock *et al.* (2000); Adams *et al.* (2002); Lee *et al.* (2012). For the preparation of the ligand, see: Stadler *et al.* (2010).



Experimental

Crystal data [ZnCl₂(C₆H₈N₄)₂]

 $M_r = 408.60$

Monoclinic, $P2_1/n$	
a = 8.4289 (8) Å	
b = 15.1128 (14) Å	
c = 13.4196 (13) Å	
$\beta = 104.077 \ (1)^{\circ}$	
V = 1658.1 (3) Å ³	

Data collection

Bruker APEXII CCD	11576 measured reflections
diffractometer	4132 independent reflections
Absorption correction: multi-scan	3456 reflections with $I > 2\sigma(I)$
(SADABS; Bruker, 2008)	$R_{\rm int} = 0.026$
$T_{\min} = 0.713, \ T_{\max} = 0.773$	

Z = 4

Mo $K\alpha$ radiation

 $0.20 \times 0.18 \times 0.15~\mathrm{mm}$

 $\mu = 1.81 \text{ mm}^{-1}$

T = 296 K

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$	H atoms treated by a mixture of
$vR(F^2) = 0.078$	independent and constrained
S = 1.03	refinement
132 reflections	$\Delta \rho_{\rm max} = 0.42 \ {\rm e} \ {\rm \AA}^{-3}$
223 parameters	$\Delta \rho_{\rm min} = -0.21 \text{ e } \text{\AA}^{-3}$
restraints	

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

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
N8−H2 <i>N</i> 8···Cl1	0.86 (2)	2.73 (2)	3.400 (2)	137 (2)
$N8 - H2N8 \cdot \cdot \cdot N1^{i}$	0.86 (2)	2.60 (2)	3.165 (3)	124 (2)
$N4 - H2N4 \cdot \cdot \cdot Cl2$	0.83 (2)	2.60 (2)	3.250 (2)	137 (2)
$N4 - H1N4 \cdot \cdot \cdot Cl1^{ii}$	0.81 (2)	2.66 (2)	3.4429 (19)	165 (2)

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2404).

References

Adams, T. B., Doull, J. & Feron, V. J. (2002). Food Chem. Toxicol. 40, 429–451.
Blackstock, A. W., Acostamadiedo, J. & Lesser, G. (2000). Clin. Lung Cancer, 2, 62–66.

Bruker (2008). SADABS, SAINT-Plus and APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.

Ha, T. G., Jang, J. J. & Kim, S. G. (1999). Chem. Biol. Interact. 121, 209-222.

Lee, S. E., Chung, H. & Kim, Y. S. (2012). Food Chem. 131, 1248–1254.

Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

Stadler, A. M., Puntoriero, F., Nastasi, F., Campagna, S. & Lehn, J. M. (2010). *Chem. Eur. J.* 16, 5645–5660.



supplementary materials

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Dichloridobis[2-(1-hydrazinylideneethyl)pyrazine- κN^1]zinc

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Comment

Pyrazine and its derivatives have received considerable attention and interest in the field of biochemistry. Such research has been focused on drugs (Ha *et al.*, 1999; Blackstock *et al.*, 2000), flavor ingredients (Adams *et al.*, 2002), and enzymatic modification (Lee *et al.*, 2012). In this paper, a new Zn^{II} complex, dicholorido-bis[2-(1-hydrazonethyl) pyrazine]zinc(II), is described.

The crystal of the title compound, $[ZnCl_2(C_6H_8N_4)_2]$, consists of two Cl⁻ ions, two N atoms from two different pyrazines (N2, N6) and other two imine N atoms (N3, N7), forming a distorted octahedron (Fig. 1). The equatorial plane of the octahedron is occupied by Cl1, N2, N6 and Cl2, the four atoms are almost coplanar, with the dihedral angle of 13.28 (1)°. Atoms N3, N7 are in the axial positions of the octahedron. The distances between N3, N7 and Zn^{II} (2.158 (1) Å, 2.164 (1) Å) are shorter than those of N2, N6 of the equatorial plane with Zn^{II} (2.244 (1) Å, 2.258 (2) Å).

As shown in the packing diagram (Fig. 2), a three-dimensional framework is formed by intermolecular N—H···N and N —H···Cl interactions.

Experimental

2-(1-hydrazinylideneethyl)pyrazine (Stadler *et al.*, 2010) (0.1 mmol, 0.0136 g) was dissolved in 20 ml absolute ethanol, then ZnCl₂.2H₂O (0.2 mmol, 0.0268 g) was added, and after 0.5 h of stirring at 333 K, the mixture was filtered and held at room temperature to allow slow evaporation of solvent. Shiny pale yellow crystals suitable for X-ray diffraction were collected after one week (Yield = 64%).

Refinement

H atoms of the pyrazine ring were placed in calculated positions, with C—H = 0.93 Å, and refined using ariding modea, with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of the methyl group were located in difference Fourier maps and included as part of a rigid rotor, with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C \text{ methyl})$. H atoms of the NH₂ groups were refined subject to a variable distance restraint that refined to N—H = 0.83 (2) Å and with $U_{iso}(H) = 1.5U_{eq}(N)$.

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).



Figure 1

The crystal structure of the title complex. Ellipsoids are drawn at the 50% probability level. Hydrogen atoms are depicted as small spheres of arbitrary radius.



Figure 2

The packing diagram of the title complex, viewed along the *a* axis. Intermolecular interactions are shown as dashed lines.

Dichloridobis[2-(1-hydrazinylideneethyl)pyrazine- κN^1]zinc

Crystal data	
$[ZnCl_{2}(C_{6}H_{8}N_{4})_{2}]$ $M_{r} = 408.60$ Monoclinic, $P2_{1}/n$ Hall symbol: -P 2yn a = 8.4289 (8) Å b = 15.1128 (14) Å c = 13.4196 (13) Å $\beta = 104.077$ (1)° V = 1658.1 (3) Å ³ Z = 4	F(000) = 832 $D_x = 1.637 \text{ Mg m}^{-3}$ Mo Ka radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 4411 reflections $\theta = 2.7-28.2^{\circ}$ $\mu = 1.81 \text{ mm}^{-1}$ T = 296 K Block, colourless $0.20 \times 0.18 \times 0.15 \text{ mm}$
Data collection	
Bruker APEXII CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator φ and ω scans	Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2008) $T_{min} = 0.713$, $T_{max} = 0.773$ 11576 measured reflections 4132 independent reflections 3456 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.026$	
$\theta_{\rm max} = 28.3^{\circ}, \theta_{\rm min} = 2.1^{\circ}$	
$h = -10 \rightarrow 11$	

Refinement	
Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.029$	Hydrogen site location: inferred from
$wR(F^2) = 0.078$	neighbouring sites
<i>S</i> = 1.03	H atoms treated by a mixture of independent
4132 reflections	and constrained refinement
223 parameters	$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.3057P]$
4 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: structure-invariant	$(\Delta/\sigma)_{\rm max} = 0.009$
direct methods	$\Delta \rho_{\rm max} = 0.42 \text{ e } \text{\AA}^{-3}$
	$\Delta \rho_{\rm min} = -0.21 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

 $k = -18 \rightarrow 20$ $l = -9 \rightarrow 17$

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.

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
Zn1	0.79801 (2)	0.074400 (13)	0.764996 (15)	0.03098 (8)	
Cl1	0.74457 (6)	0.17192 (3)	0.89354 (4)	0.04074 (12)	
Cl2	0.61902 (6)	-0.03984 (4)	0.78802 (4)	0.04526 (13)	
N1	1.2922 (2)	0.25410 (13)	0.75292 (16)	0.0535 (5)	
N2	1.00732 (17)	0.16076 (10)	0.75046 (11)	0.0322 (3)	
N3	1.01610 (18)	0.01092 (10)	0.85368 (11)	0.0331 (3)	
N4	1.0037 (3)	-0.06823 (12)	0.89868 (16)	0.0478 (5)	
H1N4	1.076 (3)	-0.0850 (16)	0.9461 (18)	0.057*	
H2N4	0.909 (3)	-0.0860 (17)	0.892 (2)	0.057*	
N5	0.8091 (3)	-0.09261 (13)	0.44379 (15)	0.0533 (5)	
N6	0.82991 (18)	-0.00119 (10)	0.62587 (11)	0.0327 (3)	
N7	0.65102 (18)	0.14165 (10)	0.63190 (12)	0.0330 (3)	
N8	0.5788 (2)	0.22084 (12)	0.64252 (16)	0.0473 (4)	
H1N8	0.493 (3)	0.2340 (17)	0.5969 (17)	0.057*	
H2N8	0.568 (3)	0.2228 (17)	0.7042 (15)	0.057*	
C1	1.1478 (3)	0.28105 (15)	0.69904 (19)	0.0508 (5)	
H1	1.1414	0.3328	0.6607	0.061*	
C2	1.0057 (2)	0.23502 (12)	0.69773 (16)	0.0405 (4)	
H2	0.9065	0.2567	0.6589	0.049*	
C3	1.1533 (2)	0.13197 (12)	0.80650 (14)	0.0329 (4)	
C4	1.2941 (2)	0.18004 (14)	0.80619 (18)	0.0459 (5)	
H4	1.3939	0.1593	0.8451	0.055*	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

C5	1.1551 (2)	0.05001 (13)	0.86525 (14)	0.0333 (4)
C6	1.3119 (2)	0.01689 (16)	0.93253 (16)	0.0478 (5)
H6A	1.2922	-0.0376	0.9643	0.072*
H6B	1.3546	0.0600	0.9847	0.072*
H6C	1.3894	0.0070	0.8919	0.072*
C7	0.9003 (3)	-0.12098 (14)	0.53299 (17)	0.0476 (5)
H7	0.9594	-0.1731	0.5344	0.057*
C8	0.9103 (3)	-0.07594 (12)	0.62350 (17)	0.0405 (4)
H8	0.9752	-0.0986	0.6843	0.049*
С9	0.7363 (2)	0.02954 (12)	0.53650 (14)	0.0321 (4)
C10	0.7270 (3)	-0.01761 (14)	0.44637 (15)	0.0433 (5)
H10	0.6608	0.0040	0.3854	0.052*
C11	0.6464 (2)	0.11247 (12)	0.54143 (14)	0.0332 (4)
C12	0.5611 (3)	0.15970 (16)	0.44551 (17)	0.0542 (6)
H12A	0.4486	0.1689	0.4459	0.081*
H12B	0.5671	0.1247	0.3868	0.081*
H12C	0.6128	0.2159	0.4422	0.081*

Atomic displacement parameters $(Å^2)$

	U^{11}	<i>U</i> ²²	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02815 (12)	0.03323 (12)	0.02997 (12)	-0.00097 (8)	0.00402 (8)	0.00062 (8)
Cl1	0.0421 (2)	0.0393 (3)	0.0413 (3)	0.00117 (19)	0.01106 (19)	-0.00545 (19)
Cl2	0.0444 (3)	0.0473 (3)	0.0443 (3)	-0.0159 (2)	0.0113 (2)	-0.0026 (2)
N1	0.0427 (10)	0.0487 (11)	0.0738 (14)	-0.0098 (8)	0.0232 (10)	-0.0013 (9)
N2	0.0295 (7)	0.0318 (7)	0.0353 (8)	-0.0001 (6)	0.0078 (6)	-0.0032 (6)
N3	0.0339 (8)	0.0326 (8)	0.0309 (8)	0.0006 (6)	0.0044 (6)	0.0015 (6)
N4	0.0466 (11)	0.0423 (10)	0.0485 (11)	-0.0012 (8)	-0.0003 (9)	0.0142 (8)
N5	0.0660 (13)	0.0522 (11)	0.0441 (11)	0.0055 (9)	0.0181 (9)	-0.0093 (8)
N6	0.0328 (8)	0.0319 (8)	0.0326 (8)	0.0006 (6)	0.0064 (6)	0.0008 (6)
N7	0.0286 (7)	0.0313 (7)	0.0390 (9)	0.0020 (6)	0.0081 (6)	0.0001 (6)
N8	0.0458 (10)	0.0413 (10)	0.0545 (11)	0.0136 (8)	0.0115 (9)	0.0010 (8)
C1	0.0531 (13)	0.0376 (11)	0.0671 (15)	-0.0016 (9)	0.0250 (11)	0.0061 (10)
C2	0.0400 (10)	0.0351 (10)	0.0466 (11)	0.0033 (8)	0.0110 (8)	0.0030 (8)
C3	0.0275 (8)	0.0381 (10)	0.0334 (9)	-0.0009 (7)	0.0084 (7)	-0.0060 (7)
C4	0.0317 (10)	0.0515 (12)	0.0557 (13)	-0.0047 (9)	0.0130 (9)	-0.0018 (10)
C5	0.0290 (9)	0.0412 (10)	0.0284 (9)	0.0034 (7)	0.0047 (7)	-0.0043 (7)
C6	0.0331 (10)	0.0616 (14)	0.0448 (12)	0.0089 (9)	0.0018 (9)	0.0065 (10)
C7	0.0530 (13)	0.0399 (11)	0.0527 (13)	0.0083 (9)	0.0185 (10)	-0.0033 (9)
C8	0.0412 (11)	0.0369 (10)	0.0432 (11)	0.0056 (8)	0.0098 (9)	0.0018 (8)
C9	0.0300 (8)	0.0349 (9)	0.0319 (9)	-0.0030 (7)	0.0083 (7)	0.0019 (7)
C10	0.0498 (12)	0.0462 (11)	0.0330 (10)	0.0011 (9)	0.0079 (9)	-0.0016 (8)
C11	0.0293 (9)	0.0340 (9)	0.0343 (9)	-0.0004 (7)	0.0042 (7)	0.0054 (7)
C12	0.0656 (15)	0.0501 (13)	0.0408 (12)	0.0119 (11)	0.0011 (10)	0.0117 (9)

Geometric parameters (Å, °)

Zn1—N3	2.1568 (15)	N8—H2N8	0.857 (18)
Zn1—N7	2.1637 (15)	C1—C2	1.382 (3)
Zn1—N2	2.2408 (15)	C1—H1	0.9300

Zn1—N6	2,2600 (15)	С2—Н2	0.9300
Zn1-Cl2	2,3620 (5)	C3—C4	1 392 (3)
Zn1—Cl1	2.3934 (5)	C3—C5	1.466 (3)
N1-C1	1.320 (3)	C4—H4	0.9300
N1—C4	1.326 (3)	C5—C6	1.493 (3)
N2—C2	1.325 (2)	C6—H6A	0.9600
N2—C3	1.349 (2)	C6—H6B	0.9600
N3-C5	1 288 (2)	C6—H6C	0.9600
N3—N4	1 355 (2)	C7—C8	1377(3)
N4—H1N4	0.806 (19)	C7—H7	0.9300
N4—H2N4	0.827(19)	C8—H8	0.9300
N5-C7	1 326 (3)	C9—C10	1 389 (3)
N5-C10	1.323(3)	C9C11	1.505(3) 1 474(3)
N6-C8	1.322(2)	C10—H10	0.9300
N6-C9	1.322(2) 1.348(2)	C11-C12	1494(3)
N7-C11	1.346(2) 1.283(2)	C12—H12A	0.9600
N7 N8	1.265 (2)	C12 H12R	0.9600
N8_H1N8	1.300(2) 0.850(19)	C12—H12D	0.9600
110-111100	0.050 (19)	012—11120	0.9000
N3 7n1 N7	154 76 (6)	N2 C2 H2	110.2
$N_3 = Zn_1 = N_2$	73.96 (6)	$12 - C_2 - H_2$	119.2
N7 Tn1 N2	73.90 (0) 87.67 (5)	$N_2 C_3 C_4$	119.2
$N_{1} = N_{1} = N_{2}$	87.07 (5) 88.53 (6)	$N_2 = C_3 = C_4$	117.46 (16)
N7 Tn1 N6	73 43 (6)	12-03-03	117.40(10) 122.03(17)
$N_2 = Zn_1 = N_0$	73.43 (0) 88.17 (5)	C_{4}	123.03(17) 122.06(10)
$N_2 = Z_{III} = N_0$ $N_3 = Z_{III} = C_{III}^2$	95.08(4)	N1 = C4 = C3 N1 = C4 = H4	122.90 (19)
N7 Tr1 C12	35.08(4)	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	118.5
$N_{-}Z_{11} - C_{12}$	101.20(4) 168 11 (4)	C_{3} C_{4} C_{14} C_{5} C_{2}	110.3 115.62(15)
$N_2 = Z_{III} = C_{IZ}$	100.11(4) 86.04(4)	$N_{3} = C_{5} = C_{5}$	113.03(13) 124.36(18)
$N_{2} = 2n_{1} = C_{12}$	80.94(4)	C_{3}^{2} C_{5}^{2} C_{6}^{6}	124.30(18) 120.01(17)
N7 Tr1 C11	99.23 (4) 07.78 (4)	C_{5}	120.01 (17)
$N_{$	97.78 (4) 80.67 (4)	C_{5} C_{6} H_{6} H_{6}	109.5
$N_2 = Z_{III} = C_{II}$	(4)		109.5
$\frac{1}{10} - 2 \prod - C \prod$	1/1.02(4)	HOA - CO - HOB	109.5
C1 = N1 = C4	90.70(2)		109.5
C1 - N1 - C4	110.34(18) 117.42(16)	HoA = Co = HoC	109.5
$C_2 = N_2 = C_3$	117.43(10) 120.22(12)	HOB - CO - HOC	109.3
$C_2 = N_2 = Z_{\rm m} I$	129.32 (13)	N5	122.3 (2)
$C_5 = N_2 = N_4$	113.23(12)	N3-C7-H7	118.9
C5 N2 Tr1	121.17(10)	$C_8 - C_7 - H_7$	118.9
C3—N3—ZIII	119.41(12)		121.45 (19)
N4 - N5 - Zn1	119.40 (13)	NO-CS-HS	119.5
N2 N4 U2N4	120.3(19)	$C/-C\delta$ -H8	119.5
IN3-IN4-H2IN4	114.0 (18)	$N_{0} = C_{0} = C_{10}$	119.07 (18)
H1N4 $N4$ $H2N4$	120(3)		110.07(10)
$C_1 - N_2 - C_1 U$	110.23(18) 117.76(17)	10 - 0 - 0	123.03(17)
$C_{0} = 1 \times C_{0} = 1$	11/./0(1/) 128.07(12)	$N_{2} = C_{10} = C_{20}$	122.01 (19)
$C_0 = N_0 = Z_{n-1}$	120.07 (13) 112.55 (12)	$\frac{1}{10} - \frac{1}{10} = \frac{1}{10}$	110./
$C_{2} = 100 - 2\Pi I$	113.33(12) 110.22(10)	$\begin{array}{c} \mathbf{U} = $	116./
	119.22 (10)	IN/	113.91 (13)

C11—N7—Zn1	119.93 (12)	N7-C11-C12	123.24 (18)
N8—N7—Zn1	120.38 (13)	C9—C11—C12	120.81 (18)
N7—N8—H1N8	117.0 (17)	C11—C12—H12A	109.5
N7—N8—H2N8	106.8 (17)	C11—C12—H12B	109.5
H1N8 - N8 - H2N8	114(2)	H12A - C12 - H12B	109.5
N1 C1 C2	117(2)	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	109.5
N1 = C1 = U2	122.2 (2)	H_{12} H_{12} H_{12}	109.5
$C_2 C_1 H_1$	118.9	H12R - C12 - H12C	109.5
$C_2 = C_1 = H_1$	110.9	H12B-C12-H12C	109.5
N2-C2-C1	121.33 (19)		
N3—Zn1—N2—C2	178.63 (17)	C4—N1—C1—C2	0.0 (3)
N7— $Zn1$ — $N2$ — $C2$	16.15 (17)	C3 - N2 - C2 - C1	0.6 (3)
N6-Zn1-N2-C2	89.63 (17)	Zn1-N2-C2-C1	178.73 (15)
C12— $Zn1$ — $N2$ — $C2$	155 39 (16)	N1-C1-C2-N2	-0.3(3)
C11 - Zn1 - N2 - C2	-81.65 (16)	$C_{2} = N_{2} = C_{3} = C_{4}$	-0.5(3)
N_{3} T_{n1} N_{2} C_{3}	-3.15(12)	7n1 - N2 - C3 - C4	-17893(14)
N7 Tn1 N2 C3	-165.63.(13)	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	170.72(14)
$N_{-2} = N_{2} = C_{3}$	-92.15(13)	7n1 N2 C3 C5	179.72(10)
10 - 211 - 112 - C3	-264(3)	$\sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{i=1}^{n} \sum_{i$	1.3(2)
C12 - Z111 - N2 - C3	-20.4(3)	C1— $N1$ — $C4$ — $C3$	0.1(3)
$V_1 = Z_1 = N_2 = C_3$	90.57 (12) 50.1 (2)	$N_2 - C_3 - C_4 - N_1$	0.1(3)
N = 2n1 = N3 = C5	50.1(2)	C_{3} C_{4} N_{1} C_{5} C_{2}	179.9 (2)
N_2 — Zn_1 — N_3 — C_5	5.20 (13)	N4 - N3 - C5 - C3	1/5./3(1/)
N6—Zn1—N3—C5	93.72 (14)	Zn1—N3—C5—C3	-6.2 (2)
Cl2—Zn1—N3—C5	-179.49 (13)	N4—N3—C5—C6	-4.0 (3)
Cl1—Zn1—N3—C5	-81.77 (14)	Zn1—N3—C5—C6	174.13 (15)
N7—Zn1—N3—N4	-131.82 (16)	N2—C3—C5—N3	3.1 (3)
N2—Zn1—N3—N4	-176.68 (16)	C4—C3—C5—N3	-176.72 (18)
N6—Zn1—N3—N4	-88.16 (15)	N2—C3—C5—C6	-177.23 (17)
Cl2—Zn1—N3—N4	-1.36 (15)	C4—C3—C5—C6	3.0 (3)
Cl1—Zn1—N3—N4	96.35 (15)	C10—N5—C7—C8	0.0 (3)
N3—Zn1—N6—C8	23.01 (17)	C9—N6—C8—C7	0.4 (3)
N7—Zn1—N6—C8	-174.88 (17)	Zn1—N6—C8—C7	170.70 (15)
N2—Zn1—N6—C8	97.01 (17)	N5-C7-C8-N6	-0.5 (3)
Cl2—Zn1—N6—C8	-72.15 (16)	C8—N6—C9—C10	0.3 (3)
N3—Zn1—N6—C9	-166.32 (13)	Zn1—N6—C9—C10	-171.45 (14)
N7—Zn1—N6—C9	-4.21 (12)	C8—N6—C9—C11	179.32 (17)
N2—Zn1—N6—C9	-92.33 (13)	Zn1—N6—C9—C11	7.6 (2)
C12—Zn1—N6—C9	98.51 (12)	C7—N5—C10—C9	0.7 (3)
N3—Zn1—N7—C11	46.0 (2)	N6—C9—C10—N5	-0.8(3)
N2— $Zn1$ — $N7$ — $C11$	88.76 (14)	$C_{11} - C_{9} - C_{10} - N_{5}$	-179.8(2)
N6-Zn1-N7-C11	-0.03(14)	N8—N7—C11—C9	17615(16)
C12 - 7n1 - N7 - C11	-83.36(14)	7n1 - N7 - C11 - C9	40(2)
C12 = Zn1 = N7 = C11	178 11 (14)	N8_N7_C11_C12	-1.8(3)
$N_{3}_{7n1}N_{7}N_{8}$	-126.06 (16)	7n1 N7 C11 C12	$-174\ 00\ (16)$
$N_2 = 2n_1 = N_7 = N_0$	-82.32(14)	$N_{11} - N_{11} - C_{11} - C_{12}$	-70(2)
$\frac{1}{2} - \frac{1}{2} - \frac{1}{1} - \frac{1}{1} - \frac{1}{10} = \frac{1}{10}$	-172 11 (15)	$\frac{1}{10} - \frac{1}{10} $	1.9 (4) 171 15 (19)
$\frac{110}{211} \frac{11}{11} \frac{11}{10} \frac{110}{100}$	1/2.11(13) 104.55(14)	$N_{10} = 0.000000000000000000000000000000000$	171.13(10) 170.15(10)
$C_{12} - C_{111} - I_{N} / - I_{NO}$	6 02 (14)	110 - 07 - 011 - 012	-10.2(2)
-11 - 2111 - 107 - 100	0.02(14)	UIU-U7-UII-UI2	10.0 (3)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H···A
N8—H2 <i>N</i> 8…C11	0.86 (2)	2.73 (2)	3.400 (2)	137 (2)
N8—H2N8····N1 ⁱ	0.86 (2)	2.60 (2)	3.165 (3)	124 (2)
N4—H2 <i>N</i> 4····Cl2	0.83 (2)	2.60 (2)	3.250 (2)	137 (2)
N4—H1 <i>N</i> 4····Cl1 ⁱⁱ	0.81 (2)	2.66 (2)	3.4429 (19)	165 (2)

Hydrogen-bond geometry (Å, °)

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