Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aquachloridobis(1,10-phenanthroline-κ^2N,N')zinc(II) chloride *N*,*N*-dimethylformamide solvate

Li-Li Kong,[a] Shan Gao,[a] Li-Hua Huo[a] and Seik Weng Ng[b]*

[a]School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

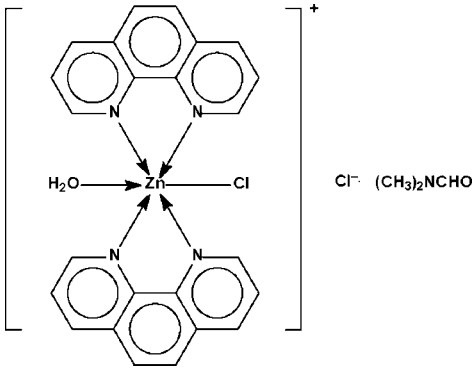
Received 7 January 2008; accepted 21 January 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.033; wR factor = 0.103; data-to-parameter ratio = 15.4.

The Zn atom in the title salt, $[ZnCl(C_{12}H_8N_2)_2(H_2O)]Cl\cdot C_3H_7NO$, is chelated by two phenanthroline molecules and is bonded to one chloride ion and one water molecule, resulting in a ZnN_4ClO octahedral coordination environment with the Cl and O atoms in a *cis* conformation. The cations and anions are linked by O—H···Cl hydrogen bonds across a center of inversion, forming a hydrogen-bonded dimeric association. The dimethylformamide solvent molecule is disordered over two orientations in a 0.56 (1):0.44 (1) ratio.

Related literature

The title compound is isostructural with the cobalt and nickel analogs: see Liu, Gao, Huo & Ng (2004); Liu, Liu & Zhong (2004).



Experimental

Crystal data

$[ZnCl(C_{12}H_8N_2)_2(H_2O)]Cl\cdot C_3H_7NO$
M_r = 587.79
Triclinic, $P\overline{1}$
a = 9.6743 (3) Å
b = 11.6096 (5) Å
c = 12.7486 (5) Å
α = 67.004 (1)°
β = 85.995 (1)°
γ = 80.025 (1)°
V = 1298.14 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.19 mm^{-1}
T = 295 (2) K
0.30 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.660, T_{max} = 0.815
12819 measured reflections
5884 independent reflections
4602 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.103
S = 1.11
5884 reflections
383 parameters
61 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.190 (2)	Zn1—N4	2.275 (2)
Zn1—N2	2.198 (2)	Zn1—O1*w*	2.090 (2)
Zn1—N3	2.157 (2)	Zn1—Cl1	2.3520 (6)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···Cl2	0.85 (3)	2.29 (3)	3.112 (2)	163 (3)
O1*w*—H1*w*2···Cl2^{i}	0.84 (3)	2.24 (3)	3.079 (2)	172 (3)

Symmetry code: (i) $-x+1, -y+2, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); method used to solve structure: atomic coordinates taken from the iostructural Co compound (Liu *et al.*, 2004); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

We thank the Heilongjiang Province Natural Science Foundation (No. B200501), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (No. 1054 G036), Heilongjiang University and the University of Malaya for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2689).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Liu, J.-W., Gao, S., Huo, L.-H. & Ng, S. W. (2004). *Acta Cryst.* E**60**, m501–m503.
Liu, H., Liu, L.-P. & Zhong, B.-H. (2004). *Anal. Sci.* **20**, x63–x64.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2008). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2008). E**64**, m423 [**doi:10.1107/S1600536808002237**]

Aquachloridobis(1,10-phenanthroline-κ^2N,N')zinc(II) chloride *N*,*N*-dimethylformamide solvate

L.-L. Kong, S. Gao, L.-H. Huo and S. W. Ng

Comment

The title compound, (I), is isostructural with its cobalt (Liu, Gao, Huo & Ng, 2004) and nickel analogs (Liu, Liu & Zhong, 2004).

The Zn atom in (I) is chelated by two phenanthroline molecules and bonded to one chloride ion and one water molecule, resulting in a ZnN_4ClO octahedral coordination environment with the Cl and O atoms in a *cis* conformation (Table 1, Fig. 1). The cations and anions are linked by O–H···Cl hydrogen bonds across a center of inversion forming a hydrogen-bonded dimeric association. Details of the hydrogen bonds are given in Table 2.

Experimental

Zinc diacetate dihydrate (1 mmol) and 1,10-phenanthroline (2 mmol) were dissolved in a DMF-water mixture. Several drops of hydrochloric acid were added, and the mixture set aside for the growth of crystals.. The mixture was filtered and colorless blocks of (I) were isolated after several days.

Refinement

The carbon-bound H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) 1.2–1.5U_{eq}(C).

The water H-atoms were located in a difference map, and were refined with a distance restraint of O–H = 0.85±0.01 Å; their U_{iso} values were refined.

The DMF solvate molecule is disordered but the disorder components share a nitrogen atom. The C–O distance was restrained to 1.25±0.01 Å, the *N*–$C_{carbonyl}$ distance to 1.35±0.01 Å and the *N*–C_{methyl} distance to 1.45±0.01 Å. The molecule was restrained to be nearly flat. The occupations of the disorder components refined to 0.56 (1):0.44 (1).

Figures

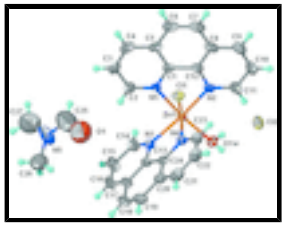


Fig. 1. View of the molecular structure of (I); displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. Only one disorder component of the DMF molecule is shown.

Aquachloridobis(1,10-phenanthroline-κ^2*N*,*N*^{1})zinc(II) chloride *N*,*N*-dimethylformamide solvate

Crystal data

$[ZnCl(C_{12}H_8N_2)_2(H_2O)]Cl·C_3H_7NO$	$Z = 2$
$M_r = 587.79$	$F(000) = 604$
Triclinic, $P\overline{1}$	$D_x = 1.504$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.6743$ (3) Å	Cell parameters from 10359 reflections
$b = 11.6096$ (5) Å	$\theta = 3.1–27.5°$
$c = 12.7486$ (5) Å	$\mu = 1.19$ mm^{-1}
$\alpha = 67.004$ (1)°	$T = 295$ K
$\beta = 85.995$ (1)°	Block, colorless
$\gamma = 80.025$ (1)°	0.30 × 0.24 × 0.18 mm
$V = 1298.14$ (9) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	5884 independent reflections
Radiation source: fine-focus sealed tube	4602 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.022$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
ω scans	$h = -12\rightarrow12$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$k = -15\rightarrow15$
$T_{min} = 0.660$, $T_{max} = 0.815$	$l = -15\rightarrow16$
12819 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.033$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.103$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.11$	$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
5884 reflections	$(\Delta/\sigma)_{max} = 0.001$
383 parameters	$\Delta\rho_{max} = 0.43$ e Å^{-3}
61 restraints	$\Delta\rho_{min} = -0.36$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.69100 (2)	0.67147 (2)	0.71925 (2)	0.02999 (10)	
Cl1	0.57695 (6)	0.68729 (6)	0.88327 (5)	0.04014 (15)	
Cl2	0.39933 (7)	1.05103 (6)	0.64297 (5)	0.04871 (17)	
O1W	0.53618 (17)	0.80418 (17)	0.61027 (14)	0.0387 (4)	
H1W1	0.498 (3)	0.861 (2)	0.634 (2)	0.059 (9)*	
H1W2	0.553 (3)	0.837 (3)	0.5398 (10)	0.055 (8)*	
N1	0.88448 (17)	0.55649 (18)	0.80695 (15)	0.0324 (4)	
N2	0.83314 (19)	0.80984 (18)	0.68954 (16)	0.0352 (4)	
N3	0.61286 (18)	0.50502 (17)	0.72752 (15)	0.0316 (4)	
N4	0.78178 (18)	0.63714 (18)	0.56257 (15)	0.0317 (4)	
N5	0.7617 (3)	0.0237 (3)	0.9642 (3)	0.0874 (10)	
C1	0.9880 (2)	0.6243 (2)	0.80178 (18)	0.0324 (5)	
C2	0.9080 (2)	0.4331 (2)	0.8658 (2)	0.0402 (5)	
H2	0.8381	0.3861	0.8686	0.048*	
C3	1.0332 (3)	0.3698 (3)	0.9242 (2)	0.0464 (6)	
H3	1.0454	0.2826	0.9651	0.056*	
C4	1.1368 (3)	0.4364 (3)	0.9207 (2)	0.0481 (6)	
H4	1.2201	0.3953	0.9601	0.058*	
C5	1.1177 (2)	0.5674 (3)	0.8576 (2)	0.0400 (6)	
C6	1.2211 (2)	0.6458 (3)	0.8478 (2)	0.0509 (7)	
H6	1.3063	0.6092	0.8855	0.061*	
C7	1.1979 (3)	0.7700 (3)	0.7860 (3)	0.0532 (7)	
H7	1.2687	0.8175	0.7786	0.064*	
C8	1.0664 (2)	0.8316 (3)	0.7308 (2)	0.0439 (6)	
C9	1.0341 (3)	0.9631 (3)	0.6682 (2)	0.0530 (7)	
H9	1.1007	1.0150	0.6596	0.064*	
C10	0.9053 (3)	1.0136 (3)	0.6203 (3)	0.0553 (7)	
H10	0.8825	1.1005	0.5799	0.066*	
C11	0.8071 (3)	0.9338 (2)	0.6322 (2)	0.0456 (6)	
H11	0.7196	0.9696	0.5984	0.055*	
C12	0.9604 (2)	0.7587 (2)	0.73849 (18)	0.0339 (5)	
C13	0.6459 (2)	0.4679 (2)	0.63922 (19)	0.0324 (5)	
C14	0.5353 (2)	0.4368 (2)	0.8115 (2)	0.0421 (6)	
H14	0.5150	0.4599	0.8737	0.050*	
C15	0.4828 (3)	0.3327 (3)	0.8111 (3)	0.0546 (7)	
H15	0.4287	0.2878	0.8716	0.065*	
C16	0.5120 (3)	0.2975 (3)	0.7202 (3)	0.0527 (7)	
H16	0.4758	0.2295	0.7175	0.063*	
C17	0.5967 (2)	0.3644 (2)	0.6314 (2)	0.0415 (6)	
C18	0.6358 (3)	0.3313 (3)	0.5352 (2)	0.0525 (7)	
H18	0.6026	0.2636	0.5291	0.063*	
C19	0.7204 (3)	0.3973 (3)	0.4532 (2)	0.0541 (7)	
H19	0.7447	0.3740	0.3916	0.065*	
C20	0.7732 (2)	0.5017 (3)	0.4589 (2)	0.0417 (5)	
C21	0.8641 (3)	0.5729 (3)	0.3765 (2)	0.0530 (7)	

H21	0.8931	0.5519	0.3142	0.064*	
C22	0.9091 (3)	0.6714 (3)	0.3882 (2)	0.0501 (7)	
H22	0.9683	0.7188	0.3341	0.060*	
C23	0.8649 (2)	0.7005 (2)	0.4829 (2)	0.0412 (5)	
H23	0.8960	0.7686	0.4899	0.049*	
C24	0.7357 (2)	0.5379 (2)	0.55131 (18)	0.0322 (5)	
O1	0.8615 (13)	0.1721 (13)	0.8303 (11)	0.145 (5)	0.560 (9)
C25	0.8320 (9)	0.1203 (9)	0.9327 (10)	0.153 (5)	0.560 (9)
H25	0.8587	0.1486	0.9860	0.184*	0.560 (9)
C26	0.7138 (10)	−0.0335 (9)	0.8953 (7)	0.105 (3)	0.560 (9)
H26A	0.7384	0.0105	0.8171	0.157*	0.560 (9)
H26B	0.6137	−0.0287	0.9020	0.157*	0.560 (9)
H26C	0.7571	−0.1207	0.9204	0.157*	0.560 (9)
C27	0.7266 (10)	−0.0410 (11)	1.0865 (6)	0.137 (4)	0.560 (9)
H27A	0.8004	−0.0406	1.1329	0.206*	0.560 (9)
H27B	0.7166	−0.1269	1.1017	0.206*	0.560 (9)
H27C	0.6401	0.0027	1.1039	0.206*	0.560 (9)
O1'	0.9009 (13)	0.1667 (11)	0.8546 (11)	0.115 (4)	0.440 (9)
C25'	0.8264 (10)	0.0799 (9)	0.8675 (9)	0.100 (4)	0.440 (9)
H25'	0.8180	0.0563	0.8067	0.120*	0.440 (9)
C26'	0.7784 (13)	0.0665 (13)	1.0524 (9)	0.135 (5)	0.440 (9)
H26D	0.8736	0.0797	1.0528	0.202*	0.440 (9)
H26E	0.7569	0.0040	1.1246	0.202*	0.440 (9)
H26F	0.7161	0.1447	1.0393	0.202*	0.440 (9)
C27'	0.6808 (12)	−0.0719 (10)	0.9728 (17)	0.168 (7)	0.440 (9)
H27D	0.7428	−0.1478	0.9772	0.253*	0.440 (9)
H27E	0.6220	−0.0425	0.9069	0.253*	0.440 (9)
H27F	0.6234	−0.0895	1.0401	0.253*	0.440 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02905 (14)	0.03305 (16)	0.03096 (15)	−0.00828 (10)	0.00059 (10)	−0.01436 (11)
Cl1	0.0364 (3)	0.0549 (4)	0.0340 (3)	−0.0079 (3)	0.0019 (2)	−0.0225 (3)
Cl2	0.0604 (4)	0.0398 (3)	0.0463 (4)	−0.0088 (3)	0.0078 (3)	−0.0180 (3)
O1W	0.0421 (9)	0.0380 (10)	0.0353 (9)	−0.0009 (7)	−0.0029 (7)	−0.0151 (8)
N1	0.0296 (8)	0.0378 (10)	0.0310 (9)	−0.0059 (8)	0.0007 (7)	−0.0146 (8)
N2	0.0348 (9)	0.0380 (11)	0.0381 (10)	−0.0104 (8)	0.0016 (8)	−0.0187 (9)
N3	0.0311 (9)	0.0338 (10)	0.0328 (10)	−0.0085 (8)	0.0026 (7)	−0.0149 (8)
N4	0.0330 (9)	0.0334 (10)	0.0288 (9)	−0.0045 (8)	0.0006 (7)	−0.0126 (8)
N5	0.106 (2)	0.069 (2)	0.099 (2)	−0.0437 (19)	0.034 (2)	−0.0382 (18)
C1	0.0259 (9)	0.0473 (13)	0.0299 (11)	−0.0061 (9)	0.0024 (8)	−0.0216 (10)
C2	0.0375 (11)	0.0439 (14)	0.0372 (13)	−0.0055 (10)	0.0016 (10)	−0.0140 (11)
C3	0.0460 (13)	0.0473 (15)	0.0370 (13)	0.0054 (11)	−0.0050 (10)	−0.0111 (11)
C4	0.0369 (12)	0.0707 (19)	0.0369 (13)	0.0060 (12)	−0.0041 (10)	−0.0263 (13)
C5	0.0291 (10)	0.0619 (17)	0.0347 (12)	−0.0006 (11)	−0.0019 (9)	−0.0272 (12)
C6	0.0282 (11)	0.081 (2)	0.0568 (17)	−0.0059 (12)	−0.0015 (11)	−0.0421 (16)
C7	0.0324 (12)	0.080 (2)	0.0638 (18)	−0.0224 (13)	0.0055 (12)	−0.0414 (17)

C8	0.0368 (12)	0.0597 (17)	0.0487 (14)	−0.0210 (12)	0.0099 (11)	−0.0315 (13)
C9	0.0509 (15)	0.0574 (18)	0.0607 (17)	−0.0311 (14)	0.0095 (13)	−0.0259 (14)
C10	0.0678 (18)	0.0410 (15)	0.0591 (17)	−0.0207 (14)	0.0046 (14)	−0.0170 (13)
C11	0.0455 (13)	0.0433 (14)	0.0507 (15)	−0.0128 (11)	0.0008 (11)	−0.0186 (12)
C12	0.0300 (10)	0.0463 (14)	0.0334 (11)	−0.0120 (10)	0.0046 (9)	−0.0221 (10)
C13	0.0298 (10)	0.0337 (12)	0.0373 (12)	−0.0033 (9)	−0.0034 (9)	−0.0178 (10)
C14	0.0396 (12)	0.0439 (14)	0.0473 (14)	−0.0132 (11)	0.0116 (11)	−0.0217 (12)
C15	0.0525 (15)	0.0464 (16)	0.0701 (19)	−0.0239 (13)	0.0183 (14)	−0.0245 (14)
C16	0.0493 (14)	0.0397 (14)	0.078 (2)	−0.0167 (12)	0.0029 (14)	−0.0287 (14)
C17	0.0383 (12)	0.0397 (13)	0.0556 (15)	−0.0055 (10)	−0.0061 (11)	−0.0272 (12)
C18	0.0564 (15)	0.0518 (17)	0.0673 (19)	−0.0064 (13)	−0.0096 (14)	−0.0413 (15)
C19	0.0628 (16)	0.0637 (19)	0.0514 (16)	0.0021 (14)	−0.0078 (13)	−0.0426 (15)
C20	0.0448 (12)	0.0485 (15)	0.0347 (12)	0.0034 (11)	−0.0042 (10)	−0.0229 (11)
C21	0.0577 (15)	0.0673 (19)	0.0321 (13)	0.0035 (14)	0.0048 (11)	−0.0235 (13)
C22	0.0520 (15)	0.0549 (17)	0.0351 (13)	−0.0078 (13)	0.0126 (11)	−0.0108 (12)
C23	0.0424 (12)	0.0421 (14)	0.0358 (13)	−0.0077 (11)	0.0062 (10)	−0.0119 (11)
C24	0.0324 (10)	0.0346 (12)	0.0303 (11)	0.0019 (9)	−0.0046 (9)	−0.0156 (9)
O1	0.171 (8)	0.152 (8)	0.109 (6)	−0.028 (6)	0.017 (5)	−0.050 (5)
C25	0.202 (9)	0.147 (8)	0.135 (8)	−0.061 (7)	0.015 (7)	−0.069 (7)
C26	0.142 (7)	0.100 (6)	0.083 (5)	−0.003 (5)	−0.017 (5)	−0.049 (5)
C27	0.172 (8)	0.157 (8)	0.094 (6)	−0.049 (6)	0.027 (6)	−0.054 (6)
O1'	0.147 (7)	0.097 (6)	0.107 (7)	−0.089 (5)	0.063 (6)	−0.030 (4)
C25'	0.139 (8)	0.088 (6)	0.095 (7)	−0.033 (6)	0.029 (6)	−0.058 (5)
C26'	0.144 (8)	0.169 (10)	0.094 (7)	−0.052 (7)	0.020 (6)	−0.046 (7)
C27'	0.149 (9)	0.152 (10)	0.203 (12)	−0.045 (8)	0.008 (8)	−0.059 (8)

Geometric parameters (Å, °)

Zn1—N1	2.190 (2)	C10—C11	1.399 (3)
Zn1—N2	2.198 (2)	C10—H10	0.9300
Zn1—N3	2.157 (2)	C11—H11	0.9300
Zn1—N4	2.275 (2)	C13—C17	1.407 (3)
Zn1—O1w	2.090 (2)	C13—C24	1.438 (3)
Zn1—Cl1	2.3520 (6)	C14—C15	1.391 (4)
O1W—H1W1	0.85 (3)	C14—H14	0.9300
O1W—H1W2	0.84 (3)	C15—C16	1.369 (4)
N1—C2	1.319 (3)	C15—H15	0.9300
N1—C1	1.360 (3)	C16—C17	1.400 (4)
N2—C11	1.322 (3)	C16—H16	0.9300
N2—C12	1.350 (3)	C17—C18	1.431 (4)
N3—C14	1.329 (3)	C18—C19	1.349 (4)
N3—C13	1.355 (3)	C18—H18	0.9300
N4—C23	1.314 (3)	C19—C20	1.423 (4)
N4—C24	1.365 (3)	C19—H19	0.9300
N5—C25'	1.320 (10)	C20—C24	1.404 (3)
N5—C25	1.325 (11)	C20—C21	1.416 (4)
N5—C26'	1.424 (8)	C21—C22	1.354 (4)
N5—C26	1.431 (7)	C21—H21	0.9300
N5—C27'	1.432 (9)	C22—C23	1.397 (4)

N5—C27	1.487 (7)	C22—H22	0.9300
C1—C5	1.410 (3)	C23—H23	0.9300
C1—C12	1.435 (3)	O1—C25	1.242 (9)
C2—C3	1.397 (3)	C25—H25	0.9300
C2—H2	0.9300	C26—H26A	0.9600
C3—C4	1.357 (4)	C26—H26B	0.9600
C3—H3	0.9300	C26—H26C	0.9600
C4—C5	1.401 (4)	C27—H27A	0.9600
C4—H4	0.9300	C27—H27B	0.9600
C5—C6	1.433 (4)	C27—H27C	0.9600
C6—C7	1.332 (4)	O1'—C25'	1.291 (19)
C6—H6	0.9300	C25'—H25'	0.9300
C7—C8	1.428 (4)	C26'—H26D	0.9600
C7—H7	0.9300	C26'—H26E	0.9600
C8—C9	1.408 (4)	C26'—H26F	0.9600
C8—C12	1.414 (3)	C27'—H27D	0.9600
C9—C10	1.357 (4)	C27'—H27E	0.9600
C9—H9	0.9300	C27'—H27F	0.9600
O1W—Zn1—N3	96.59 (7)	N2—C11—C10	122.9 (2)
O1W—Zn1—N1	167.57 (6)	N2—C11—H11	118.5
N3—Zn1—N1	91.38 (7)	C10—C11—H11	118.5
O1W—Zn1—N2	93.77 (7)	N2—C12—C8	123.0 (2)
N3—Zn1—N2	160.59 (7)	N2—C12—C1	118.07 (19)
N1—Zn1—N2	75.98 (7)	C8—C12—C1	118.9 (2)
O1W—Zn1—N4	86.13 (7)	N3—C13—C17	122.6 (2)
N3—Zn1—N4	75.15 (6)	N3—C13—C24	117.74 (19)
N1—Zn1—N4	86.72 (6)	C17—C13—C24	119.6 (2)
N2—Zn1—N4	89.27 (7)	N3—C14—C15	123.4 (2)
O1W—Zn1—Cl1	93.08 (5)	N3—C14—H14	118.3
N3—Zn1—Cl1	97.30 (5)	C15—C14—H14	118.3
N1—Zn1—Cl1	95.36 (5)	C16—C15—C14	119.0 (2)
N2—Zn1—Cl1	98.48 (5)	C16—C15—H15	120.5
N4—Zn1—Cl1	172.25 (5)	C14—C15—H15	120.5
Zn1—O1W—H1W1	114 (2)	C15—C16—C17	119.6 (2)
Zn1—O1W—H1W2	120 (2)	C15—C16—H16	120.2
H1W1—O1W—H1W2	110 (3)	C17—C16—H16	120.2
C2—N1—C1	118.2 (2)	C16—C17—C13	117.6 (2)
C2—N1—Zn1	127.51 (15)	C16—C17—C18	123.1 (2)
C1—N1—Zn1	114.19 (15)	C13—C17—C18	119.3 (2)
C11—N2—C12	118.1 (2)	C19—C18—C17	120.6 (2)
C11—N2—Zn1	127.78 (16)	C19—C18—H18	119.7
C12—N2—Zn1	114.09 (15)	C17—C18—H18	119.7
C14—N3—C13	117.80 (19)	C18—C19—C20	121.6 (2)
C14—N3—Zn1	125.44 (16)	C18—C19—H19	119.2
C13—N3—Zn1	116.76 (14)	C20—C19—H19	119.2
C23—N4—C24	117.9 (2)	C24—C20—C21	116.6 (2)
C23—N4—Zn1	129.65 (17)	C24—C20—C19	119.4 (2)
C24—N4—Zn1	112.42 (13)	C21—C20—C19	124.0 (2)
C25'—N5—C26'	115.4 (8)	C22—C21—C20	120.2 (2)

C25—N5—C26	128.7 (7)	C22—C21—H21	119.9
C25'—N5—C27'	119.3 (10)	C20—C21—H21	119.9
C26'—N5—C27'	125.4 (9)	C21—C22—C23	118.9 (2)
C25—N5—C27	119.5 (8)	C21—C22—H22	120.6
C26—N5—C27	111.8 (6)	C23—C22—H22	120.6
N1—C1—C5	122.3 (2)	N4—C23—C22	123.6 (2)
N1—C1—C12	117.64 (19)	N4—C23—H23	118.2
C5—C1—C12	120.0 (2)	C22—C23—H23	118.2
N1—C2—C3	122.9 (2)	N4—C24—C20	122.8 (2)
N1—C2—H2	118.6	N4—C24—C13	117.76 (19)
C3—C2—H2	118.6	C20—C24—C13	119.4 (2)
C4—C3—C2	119.5 (3)	O1—C25—N5	118.4 (13)
C4—C3—H3	120.2	O1—C25—H25	120.8
C2—C3—H3	120.2	N5—C25—H25	120.8
C3—C4—C5	119.6 (2)	N5—C26—H26A	109.5
C3—C4—H4	120.2	N5—C26—H26B	109.5
C5—C4—H4	120.2	N5—C26—H26C	109.5
C4—C5—C1	117.3 (2)	N5—C27—H27A	109.5
C4—C5—C6	123.9 (2)	N5—C27—H27B	109.5
C1—C5—C6	118.8 (2)	N5—C27—H27C	109.5
C7—C6—C5	121.4 (2)	O1'—C25'—N5	122.1 (11)
C7—C6—H6	119.3	O1'—C25'—H25'	118.9
C5—C6—H6	119.3	N5—C25'—H25'	118.9
C6—C7—C8	121.4 (2)	N5—C26'—H26D	109.5
C6—C7—H7	119.3	N5—C26'—H26E	109.5
C8—C7—H7	119.3	H26D—C26'—H26E	109.5
C9—C8—C12	116.8 (2)	N5—C26'—H26F	109.5
C9—C8—C7	123.9 (2)	H26D—C26'—H26F	109.5
C12—C8—C7	119.4 (3)	H26E—C26'—H26F	109.5
C10—C9—C8	119.7 (2)	N5—C27'—H27D	109.5
C10—C9—H9	120.1	N5—C27'—H27E	109.5
C8—C9—H9	120.1	H27D—C27'—H27E	109.5
C9—C10—C11	119.4 (3)	N5—C27'—H27F	109.5
C9—C10—H10	120.3	H27D—C27'—H27F	109.5
C11—C10—H10	120.3	H27E—C27'—H27F	109.5
O1W—Zn1—N1—C2	−146.2 (3)	C7—C8—C9—C10	−178.8 (3)
N3—Zn1—N1—C2	−16.20 (19)	C8—C9—C10—C11	−1.1 (4)
N2—Zn1—N1—C2	178.7 (2)	C12—N2—C11—C10	0.0 (4)
N4—Zn1—N1—C2	−91.24 (19)	Zn1—N2—C11—C10	178.9 (2)
Cl1—Zn1—N1—C2	81.27 (19)	C9—C10—C11—N2	0.6 (4)
O1W—Zn1—N1—C1	36.5 (4)	C11—N2—C12—C8	−0.2 (3)
N3—Zn1—N1—C1	166.52 (14)	Zn1—N2—C12—C8	−179.21 (17)
N2—Zn1—N1—C1	1.41 (14)	C11—N2—C12—C1	179.3 (2)
N4—Zn1—N1—C1	91.48 (14)	Zn1—N2—C12—C1	0.3 (2)
Cl1—Zn1—N1—C1	−96.01 (14)	C9—C8—C12—N2	−0.2 (3)
O1W—Zn1—N2—C11	7.4 (2)	C7—C8—C12—N2	179.5 (2)
N3—Zn1—N2—C11	129.6 (2)	C9—C8—C12—C1	−179.8 (2)
N1—Zn1—N2—C11	−179.8 (2)	C7—C8—C12—C1	0.0 (3)
N4—Zn1—N2—C11	93.4 (2)	N1—C1—C12—N2	1.0 (3)

Cl1—Zn1—N2—C11	−86.3 (2)	C5—C1—C12—N2	−177.85 (19)
O1W—Zn1—N2—C12	−173.77 (15)	N1—C1—C12—C8	−179.48 (19)
N3—Zn1—N2—C12	−51.5 (3)	C5—C1—C12—C8	1.7 (3)
N1—Zn1—N2—C12	−0.90 (15)	C14—N3—C13—C17	2.6 (3)
N4—Zn1—N2—C12	−87.70 (15)	Zn1—N3—C13—C17	−177.17 (17)
Cl1—Zn1—N2—C12	92.54 (15)	C14—N3—C13—C24	−176.9 (2)
O1W—Zn1—N3—C14	−99.15 (19)	Zn1—N3—C13—C24	3.3 (3)
N1—Zn1—N3—C14	90.41 (19)	C13—N3—C14—C15	−2.3 (4)
N2—Zn1—N3—C14	139.0 (2)	Zn1—N3—C14—C15	177.5 (2)
N4—Zn1—N3—C14	176.6 (2)	N3—C14—C15—C16	0.2 (4)
Cl1—Zn1—N3—C14	−5.17 (19)	C14—C15—C16—C17	1.7 (4)
O1W—Zn1—N3—C13	80.64 (16)	C15—C16—C17—C13	−1.3 (4)
N1—Zn1—N3—C13	−89.80 (16)	C15—C16—C17—C18	178.0 (3)
N2—Zn1—N3—C13	−41.2 (3)	N3—C13—C17—C16	−0.9 (4)
N4—Zn1—N3—C13	−3.56 (15)	C24—C13—C17—C16	178.7 (2)
Cl1—Zn1—N3—C13	174.62 (15)	N3—C13—C17—C18	179.8 (2)
O1W—Zn1—N4—C23	82.8 (2)	C24—C13—C17—C18	−0.6 (3)
N3—Zn1—N4—C23	−179.3 (2)	C16—C17—C18—C19	−178.5 (3)
N1—Zn1—N4—C23	−87.0 (2)	C13—C17—C18—C19	0.8 (4)
N2—Zn1—N4—C23	−11.0 (2)	C17—C18—C19—C20	−0.2 (4)
O1W—Zn1—N4—C24	−94.44 (15)	C18—C19—C20—C24	−0.6 (4)
N3—Zn1—N4—C24	3.43 (14)	C18—C19—C20—C21	178.9 (3)
N1—Zn1—N4—C24	95.73 (15)	C24—C20—C21—C22	−0.8 (4)
N2—Zn1—N4—C24	171.73 (15)	C19—C20—C21—C22	179.7 (3)
C2—N1—C1—C5	−0.5 (3)	C20—C21—C22—C23	0.4 (4)
Zn1—N1—C1—C5	177.05 (16)	C24—N4—C23—C22	−0.4 (4)
C2—N1—C1—C12	−179.31 (19)	Zn1—N4—C23—C22	−177.58 (18)
Zn1—N1—C1—C12	−1.8 (2)	C21—C22—C23—N4	0.3 (4)
C1—N1—C2—C3	1.0 (3)	C23—N4—C24—C20	0.0 (3)
Zn1—N1—C2—C3	−176.18 (17)	Zn1—N4—C24—C20	177.58 (17)
N1—C2—C3—C4	−0.4 (4)	C23—N4—C24—C13	179.4 (2)
C2—C3—C4—C5	−0.8 (4)	Zn1—N4—C24—C13	−3.0 (2)
C3—C4—C5—C1	1.2 (3)	C21—C20—C24—N4	0.7 (3)
C3—C4—C5—C6	−179.4 (2)	C19—C20—C24—N4	−179.8 (2)
N1—C1—C5—C4	−0.6 (3)	C21—C20—C24—C13	−178.7 (2)
C12—C1—C5—C4	178.2 (2)	C19—C20—C24—C13	0.8 (3)
N1—C1—C5—C6	−180.0 (2)	N3—C13—C24—N4	0.0 (3)
C12—C1—C5—C6	−1.2 (3)	C17—C13—C24—N4	−179.6 (2)
C4—C5—C6—C7	179.6 (2)	N3—C13—C24—C20	179.4 (2)
C1—C5—C6—C7	−1.1 (4)	C17—C13—C24—C20	−0.1 (3)
C5—C6—C7—C8	2.9 (4)	C26—N5—C25—O1	0.8 (4)
C6—C7—C8—C9	177.4 (3)	C27—N5—C25—O1	179.3 (3)
C6—C7—C8—C12	−2.3 (4)	C26'—N5—C25'—O1'	0.8 (3)
C12—C8—C9—C10	0.9 (4)	C27'—N5—C25'—O1'	−179.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···Cl2	0.85 (3)	2.29 (3)	3.112 (2)	163 (3)

O1w—H1w2···Cl2^{i}	0.84 (3)	2.24 (3)	3.079 (2)	172 (3)

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

Fig. 1