addenda and errata

Acta Crystallographica Section E Structure Reports Online

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Retraction of articles

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This article reports the retraction of 11 articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), 11 additional articles are retracted by the authors or by the journal as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
[N,N'-Bis(2-hydroxynaphthylmethylene)-1,2-ethanediaminato]zinc(II)	Chen et al. (2005)	10.1107/S1600536805026796	YAWZOM
Diazidobis(2,2'-biimidazole)copper(II)	Liu et al. (2007)	10.1107/S1600536807047873	SILZIX
Dichlorido(1,10-phenanthroline)copper(II)	Liu (2007)	10.1107/S1600536807056735	MISSAJ
Diazidobis(2,2'-biimidazole)cobalt(II)	Li et al. (2008)	10.1107/S1600536807062873	MIRYAO
Diazidobis(2,2'-biimidazole)manganese(II)	Zhang et al. (2008)	10.1107/S1600536808017984	MODBUD
Diazidobis(2,2'-biimidazole)iron(II)	Hao et al. (2008a)	10.1107/S1600536808018539	MODFOB
Bis(pentane-2,4-dionato)bis[2-(4-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl 3-oxide]nickel(II)	Hao <i>et al.</i> (2008 <i>b</i>)	10.1107/S1600536808018552	MODFUH
Bis(pentane-2,4-dionato-κ ² O,O')bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline- 1-oxyl 3-oxide-κN ²]manganese(II)	Liu, Zhang <i>et al.</i> (2008)	10.1107/S1600536808022952	MODLUN
Bis[2,4-pentanedionato(1-)]bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline- 1-oxyl 3-oxide]manganese(II)	Liu, He et al. (2008)	10.1107/S1600536808038440	MODLUN01
Di-µ-chlorido-bis[chlorido(1,10-phenanthroline-ĸ ² N,N')zinc(II)] Tris(ethylenediamine)manganese(II) sulfate	Yang <i>et al.</i> (2009) Lu (2009)	10.1107/S1600536809014482 10.1107/S1600536809034874	JOLBOC YUCZEC

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Chen, G., Zhao, B., Sun, M. & Qi, W. (2005). Acta Cryst. E61, m1869-m1870.

Hao, L., Mu, C. & Kong, B. (2008a). Acta Cryst. E64, m956.

Hao, L., Mu, C. & Kong, B. (2008b). Acta Cryst. E64, m957.

Harrison, W. T. A., Simpson, J. & Weil, M. (2010). Acta Cryst. E66, e1-e2.

Li, S., Wang, S.-B., Zhang, F.-L. & Tang, K. (2008). Acta Cryst. E64, m76.

Liu, Y.-Q. (2007). Acta Cryst. E63, m2991.

Liu, Y., Dou, J., Li, D. & Zhang, X. (2007). Acta Cryst. E63, m2661.

Liu, Y., He, Q., Zhang, X., Xue, Z. & Lv, C. (2008). Acta Cryst. E64, m1604.

Liu, Y., Zhang, X., Xue, Z., He, Q. & Zhang, Y. (2008). *Acta Cryst.* E**64**, m1077. Lu, J. (2009). *Acta Cryst.* E**65**, m1187.

Yang, X.-M., Leng, Q.-B., Chen, Y., He, Y.-G. & Luo, S.-W. (2009). Acta Cryst. E65, m567.

Zhang, X., Wei, P. & Li, B. (2008). Acta Cryst. E64, m934.

 $0.19 \times 0.16 \times 0.12 \text{ mm}$

7229 measured reflections

4218 independent reflections

3453 reflections with $I > 2\sigma(I)$

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Di-*u*-chlorido-bis[chlorido(1,10-phenanthroline- $\kappa^2 N, N'$ zinc(II)]

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.009 Å; R factor = 0.033; wR factor = 0.073; data-to-parameter ratio = 13.7.

In the crystal structure of the title complex, [Zn₂Cl₄- $(C_{12}H_8N_2)_2$], each of the two five-coordinated Zn^{II} atoms displays a strongly distorted trigonal-bipyramidal geometry defined by two N atoms from the chelate ligand and by one terminal and two bridging chloride anions. The crystal structure is stabilized by C-H···Cl interactions. There is intermolecular π - π stacking between adjacent phenanthroline ligands, with a centroid-centroid distance of 3.151 (3) Å.

Related literature

For the use of metal complexes of phenanthroline and its derivatives with π - π stacking to study the hydrolysis of biologically important phosphate diesters with poor leaving groups, see: Wall et al. (1999). For the structures of a series of metal complexes, see: Wu et al. (2003); Pan & Xu (2004); Li et al. (2005). For bond-length data, see: Allen et al. (1987).



Experimental

Crystal data

$[Zn_2Cl_4(C_{12}H_8N_2)_2]$
$M_r = 632.95$
Monoclinic, Cc
a = 9.8537 (12) Å
b = 17.873 (2) Å

c = 13.3798 (12) Å $\beta = 106.502 \ (3)^{\circ}$ V = 2259.3 (4) Å³ Z = 4Mo Ka radiation

$\mu = 2.62 \text{ mm}^{-1}$ T = 293 K

Data collection

Bruker APEXII area-detector diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2000) $T_{\rm min}=0.636,\;T_{\rm max}=0.744$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$ $wR(F^2) = 0.073$ S = 1.004218 reflections 307 parameters

2 restraints

H-atom parameters constrained $\Delta \rho_{\text{max}} = 0.47 \text{ e} \text{ Å}^{-3}$ $\Delta \rho_{\rm min} = -0.43 \text{ e } \text{\AA}^{-3}$

 $R_{\rm int} = 0.033$

Absolute structure: Flack (1983), 1983 Friedel pairs Flack parameter: 0.079 (12)

Table 1

Selected geometric parameters (

Zn1-Cl1	2.2629 (16)	Zn2-Cl2	2.8525 (15)
Zn1-Cl2	2.2596 (15)	Zn2-Cl3	2.2839 (14)
Zn1-Cl3	2.7049 (14)	Zn2-Cl4	2.2545 (14)
Zn1-N1	2.041 (4)	Zn2-N3	2.031 (4)
Zn1-N2	2.046 (4)	Zn2-N4	2.032 (4)

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

$D-\mathrm{H}\cdot\cdot A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
C1-H1···Cl1	0.93	2.68	3.229 (7)	118
$C6-H6\cdots Cl2^{i}$	0.93	2.77	3.525 (6)	139
$C10-H10\cdots Cl2$	0.93	2.68	3.235 (6)	119
C13−H13···Cl3	0.93	2.62	3.200 (6)	121
C17-H17···Cl3 ⁱⁱ	0.93	2.67	3.500 (7)	149
C18−H18···Cl4 ⁱⁱ	0.93	2.82	3.742 (7)	173
$C22-H22\cdots Cl4$	0.93	2.68	3.238 (6)	119

Symmetry codes: (i) $x - \frac{1}{2}, y + \frac{1}{2}, z$; (ii) $x + \frac{1}{2}, y - \frac{1}{2}, z$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

We thank the Youth Program of Jiangxi University of Finance and Economics for financial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2764).

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Wu, Z.-Y., Xue, Y.-H. & Xu, D.-J. (2003). Acta Cryst. E59, m809-m811.

supporting information

Acta Cryst. (2009). E65, m567 [doi:10.1107/S1600536809014482]

Di- μ -chlorido-bis[chlorido(1,10-phenanthroline- $\kappa^2 N, N'$)zinc(II)]

Xiao-Mao Yang, Qing-Bo Leng, Yi Chen, You-Gang He and Shi-Wu Luo

S1. Comment

Simple metal complexes of phenanthroline and its derivatives with π - π stacking have attracted great interest because they can be used to study the hydrolysis of biologically important phosphate diesters with poor leaving groups (Wall *et al.*, 1999). A series of metal complexes incorporating different aromatic ligands such as phenanthroline(phen), benzimidazole and quinoline have been prepared and their crystal structures provide useful information about π - π stacking (Wu *et al.*, 2003; Pan & Xu, 2004; Li *et al.*, 2005). We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). In the crystal structure of the title complex, each of the two five-coordinated Zn^{II} atoms displays a strongly distorted trigonalbipyramidal geometry, defined by two N atom from the organic ligand, and by one terminal and two bridging chloride anions (Table 1).

The crystal structure is stabilized by C—H···Cl interactions (Table 1). There is intermolecular π - π stacking between adjacent phenanthrolines, with a centroid-centroid distance of 3.151 (3) Å (symmetry code: -1/2 + x, 1/2 + y, z). These π - π stacking interactions lead to a supramolecular network structure (Fig. 2).

S2. Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Zinc(II) chloride (136.3 mg, 1 mmol), phen (396 mg, 2 mmol) and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colourless solution was decanted from small colourless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.



Figure 1

The molecular structure of the title complex, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.



Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Di- μ -chlorido-bis[chlorido(1,10-phenanthroline- $\kappa^2 N, N'$)zinc(II)]

Crystal data

 $[Zn_2Cl_4(C_{12}H_8N_2)_2]$ $M_r = 632.95$ Monoclinic, *Cc* Hall symbol: C -2yc a = 9.8537 (12) Å b = 17.873 (2) Å c = 13.3798 (12) Å $\beta = 106.502$ (3)° V = 2259.3 (4) Å³ Z = 4 F(000) = 1264 $D_x = 1.861 \text{ Mg m}^{-3}$ Mo K\alpha radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 3822 reflections $\theta = 2.3-27.3^{\circ}$ $\mu = 2.62 \text{ mm}^{-1}$ T = 293 KPlane, colourless $0.19 \times 0.16 \times 0.12 \text{ mm}$ Data collection

Bruker APEXII area-detector diffractometer	7229 measured reflections 4218 independent reflections
Radiation source: fine-focus sealed tube	3453 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.033$
φ and ω scans	$\theta_{\text{max}} = 26.0^{\circ}, \ \theta_{\text{min}} = 2.3^{\circ}$
Absorption correction: multi-scan	$h = -12 \rightarrow 11$
(SADABS; Bruker, 2000))	$k = -22 \rightarrow 21$
$T_{\min} = 0.636, T_{\max} = 0.744$	$l = -16 \rightarrow 16$
Refinement	
Refinement on F^2	Hydrogen site location: inferred from
Least-squares matrix: full	neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.073$	$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.16P]$
S = 1.00	where $P = (F_o^2 + 2F_c^2)/3$
4218 reflections	$(\Delta/\sigma)_{\rm max} < 0.001$
307 parameters	$\Delta \rho_{\rm max} = 0.47 \text{ e} \text{ Å}^{-3}$
2 restraints	$\Delta \rho_{\rm min} = -0.43 \text{ e} \text{ Å}^{-3}$
Primary atom site location: structure-invariant	Absolute structure: Flack (1983), 1983 Freidel
direct methods	pairs
Secondary atom site location: difference Fourier	Absolute structure parameter: 0.079 (12)
map	
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	V	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
Zn1	0.69851 (5)	0.33467 (3)	0.27140 (4)	0.03385 (16)	
Zn2	0.99585 (6)	0.30433 (3)	0.49316 (5)	0.03673 (16)	
C13	0.76987 (13)	0.34082 (7)	0.48194 (10)	0.0360 (3)	
Cl2	0.91611 (14)	0.29488 (8)	0.27124 (10)	0.0366 (4)	
Cl1	0.60068 (15)	0.21961 (8)	0.23650 (12)	0.0457 (4)	
Cl4	1.08005 (15)	0.42235 (7)	0.50920 (12)	0.0478 (4)	
N1	0.5066 (4)	0.3839(2)	0.2553 (3)	0.0315 (10)	
N2	0.7513 (4)	0.4444 (2)	0.2596 (3)	0.0321 (10)	
C11	0.6385 (5)	0.4924 (3)	0.2474 (3)	0.0277 (11)	
C12	0.5088 (5)	0.4583 (3)	0.2469 (4)	0.0303 (12)	
C1	0.3845 (6)	0.3509 (4)	0.2559 (4)	0.0489 (16)	
H1	0.3828	0.2993	0.2635	0.059*	
C2	0.2584 (6)	0.3918 (4)	0.2455 (5)	0.0515 (16)	
H2	0.1752	0.3675	0.2461	0.062*	
C8	0.7830 (7)	0.5967 (3)	0.2373 (4)	0.0468 (16)	

H8	0.7944	0.6476	0.2278	0.056*
C7	0.6504 (6)	0.5691 (3)	0.2363 (4)	0.0367 (13)
C10	0.8756 (6)	0.4746 (3)	0.2632 (4)	0.0366 (12)
H10	0.9538	0.4433	0.2739	0.044*
C3	0.2615 (6)	0.4669 (4)	0.2345 (4)	0.0495 (15)
Н3	0.1788	0.4943	0.2266	0.059*
C4	0.3884 (6)	0.5051 (3)	0.2347 (4)	0.0401 (14)
C6	0.5230 (6)	0.6132 (3)	0.2241 (4)	0.0447 (14)
H6	0.5271	0.6646	0.2145	0.054*
C5	0.4016 (7)	0.5830 (3)	0.2260 (4)	0.0497 (16)
Н5	0.3238	0.6136	0.2215	0.060*
N4	0.9434 (4)	0.1943 (2)	0.4907 (3)	0.0284 (9)
N3	1.1864 (4)	0.2591 (2)	0.4971 (3)	0.0357 (10)
C13	0.8177 (6)	0.1637 (3)	0.4836 (4)	0.0408 (13)
H13	0.7405	0.1948	0.4789	0.049*
C23	1.1830 (5)	0.1816 (3)	0.4989 (4)	0.0342 (13)
C22	1.3047 (6)	0.2925 (3)	0.4985 (4)	0.0403 (15)
H22	1.3085	0.3445	0.4992	0.048*
C24	1.0533 (6)	0.1489 (3)	0.4961 (4)	0.0309 (12)
C16	1.0413 (7)	0.0691 (3)	0.4961 (4)	0.0429 (15)
C17	1.1629 (7)	0.0258 (4)	0.5004 (4)	0.0515 (17)
H17	1.1565	-0.0261	0.5016	0.062*
C15	0.9031 (7)	0.0404 (3)	0.4884 (4)	0.0477 (15)
H15	0.8885	-0.0110	0.4873	0.057*
C18	1.2876 (7)	0.0575 (4)	0.5027 (4)	0.0545 (18)
H18	1.3657	0.0274	0.5057	0.065*
C14	0.7984 (7)	0.0854 (3)	0.4831 (4)	0.0428 (15)
H14	0.7094	0.0660	0.4788	0.051*
C19	1.3008 (6)	0.1378 (3)	0.5006 (4)	0.0450 (15)
C20	1.4266 (7)	0.1761 (4)	0.5006 (5)	0.063 (2)
H20	1.5086	0.1500	0.5016	0.075*
C21	1.4242 (7)	0.2522 (5)	0.4989 (5)	0.0599 (19)
H21	1.5059	0.2779	0.4980	0.072*
C9	0.8946 (7)	0.5507 (3)	0.2517 (5)	0.0473 (16)
H9	0.9834	0.5695	0.2540	0.057*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0277 (3)	0.0256 (3)	0.0473 (3)	0.0018 (3)	0.0090 (2)	0.0012 (3)
Zn2	0.0278 (3)	0.0222 (3)	0.0593 (4)	0.0017 (3)	0.0111 (3)	-0.0001 (3)
C13	0.0305 (8)	0.0301 (7)	0.0480 (8)	0.0072 (5)	0.0121 (6)	-0.0017 (6)
Cl2	0.0308 (8)	0.0313 (8)	0.0493 (8)	0.0074 (6)	0.0141 (6)	-0.0001 (6)
Cl1	0.0413 (9)	0.0267 (8)	0.0675 (10)	-0.0035 (7)	0.0127 (7)	-0.0038 (7)
Cl4	0.0398 (8)	0.0239 (7)	0.0723 (10)	-0.0047 (6)	0.0037 (7)	0.0008 (6)
N1	0.025 (3)	0.033 (3)	0.036 (2)	0.0032 (19)	0.0084 (18)	-0.0008 (18)
N2	0.029 (2)	0.027 (2)	0.042 (2)	0.009 (2)	0.0108 (18)	0.0046 (18)
C11	0.030 (3)	0.022 (3)	0.030 (2)	0.002 (2)	0.006 (2)	0.0006 (19)

C12	0.029 (3)	0.029 (3)	0.032 (3)	0.009 (2)	0.006 (2)	-0.003 (2)
C1	0.047 (4)	0.043 (4)	0.058 (4)	0.000 (3)	0.016 (3)	0.007 (3)
C2	0.026 (3)	0.066 (5)	0.065 (4)	0.004 (3)	0.016 (3)	0.004 (3)
C8	0.067 (5)	0.020 (3)	0.049 (3)	-0.008 (3)	0.010 (3)	-0.002 (2)
C7	0.048 (3)	0.022 (3)	0.038 (3)	0.012 (2)	0.008 (2)	0.001 (2)
C10	0.029 (3)	0.027 (3)	0.052 (3)	0.002 (2)	0.009 (2)	0.003 (2)
C3	0.033 (3)	0.060 (4)	0.056 (4)	0.016 (3)	0.013 (3)	0.002 (3)
C4	0.031 (3)	0.049 (4)	0.039 (3)	0.014 (3)	0.008 (2)	-0.002 (3)
C6	0.062 (4)	0.028 (3)	0.042 (3)	0.016 (3)	0.011 (3)	0.005 (2)
C5	0.045 (4)	0.047 (4)	0.056 (4)	0.027 (3)	0.011 (3)	-0.002 (3)
N4	0.025 (2)	0.021 (2)	0.040 (2)	-0.0010 (18)	0.0112 (17)	0.0033 (17)
N3	0.030 (3)	0.034 (3)	0.042 (2)	0.007 (2)	0.0083 (19)	0.0000 (19)
C13	0.031 (3)	0.034 (3)	0.054 (3)	-0.004 (3)	0.007 (2)	0.009 (3)
C23	0.034 (3)	0.039 (4)	0.029 (3)	0.010 (2)	0.007 (2)	0.001 (2)
C22	0.021 (3)	0.049 (4)	0.052 (4)	-0.009 (3)	0.011 (2)	0.000 (3)
C24	0.038 (3)	0.022 (3)	0.033 (3)	0.010 (2)	0.010(2)	0.001 (2)
C16	0.071 (4)	0.025 (3)	0.032 (3)	0.012 (3)	0.013 (3)	0.002 (2)
C17	0.081 (5)	0.037 (3)	0.036 (3)	0.027 (4)	0.016 (3)	-0.001 (2)
C15	0.073 (5)	0.021 (3)	0.049 (3)	-0.008 (3)	0.016 (3)	-0.004 (2)
C18	0.066 (5)	0.047 (4)	0.050 (4)	0.032 (4)	0.015 (3)	0.004 (3)
C14	0.047 (4)	0.021 (3)	0.059 (4)	-0.008 (3)	0.012 (3)	0.002 (2)
C19	0.045 (4)	0.054 (4)	0.034 (3)	0.025 (3)	0.009 (2)	0.005 (3)
C20	0.031 (3)	0.098 (6)	0.059 (4)	0.019 (4)	0.012 (3)	-0.010 (4)
C21	0.022 (3)	0.085 (6)	0.074 (5)	0.000 (4)	0.015 (3)	0.001 (4)
C9	0.042 (4)	0.031 (3)	0.070 (4)	-0.007 (3)	0.017 (3)	0.007 (3)

	Geometric	parameters	(Å.	<i>o</i>)
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Geometric parameters (Å, °)		•	
Zn1—Cl1	2.2629 (16)	C4—C5	1.406 (8)
Zn1—Cl2	2.2596 (15)	C6—C5	1.318 (8)
Zn1—Cl3	2.7049 (14)	С6—Н6	0.9300
Zn1—N1	2.041 (4)	С5—Н5	0.9300
Zn1—N2	2.046 (4)	N4—C13	1.332 (6)
Zn2—Cl2	2.8525 (15)	N4—C24	1.338 (6)
Zn2—Cl3	2.2839 (14)	N3—C22	1.305 (7)
Zn2—Cl4	2.2545 (14)	N3—C23	1.387 (7)
Zn2—N3	2.031 (4)	C13—C14	1.412 (7)
Zn2—N4	2.032 (4)	C13—H13	0.9300
N1—C12	1.335 (6)	C23—C19	1.395 (7)
N1—C1	1.341 (7)	C23—C24	1.397 (7)
N2—C10	1.328 (6)	C22—C21	1.380 (9)
N2—C11	1.376 (6)	C22—H22	0.9300
C11—C7	1.388 (7)	C24—C16	1.431 (7)
C11—C12	1.414 (7)	C16—C17	1.413 (7)
C12—C4	1.423 (7)	C16—C15	1.431 (8)
C1—C2	1.413 (8)	C17—C18	1.345 (8)
C1—H1	0.9300	C17—H17	0.9300
C2—C3	1.353 (8)	C15—C14	1.294 (9)

С2—Н2	0.9300	C15—H15	0.9300
C8—C9	1.342 (8)	C18—C19	1.443 (9)
C8—C7	1.393 (8)	C18—H18	0.9300
C8—H8	0.9300	C14—H14	0.9300
C7—C6	1.452 (7)	C19—C20	1.416 (9)
C10—C9	1.386 (8)	C20—C21	1.359 (10)
C10—H10	0.9300	C20—H20	0.9300
C3-C4	1 424 (8)	C21—H21	0.9300
C3—H3	0.9300	C9H9	0.9300
05-115	0.9500	0	0.7500
Cl1—Zn1—Cl2	93.58 (6)	С5—С6—Н6	118.8
Cl1—Zn1—Cl3	102.79 (5)	С7—С6—Н6	118.8
Cl2—Zn1—Cl3	92.74 (5)	C6—C5—C4	120.8 (5)
N1—Zn1—Cl1	92.42 (13)	С6—С5—Н5	119.6
N2—Zn1—Cl1	163.25 (11)	С4—С5—Н5	119.6
N1—Zn1—Cl2	170.64 (13)	C13—N4—C24	118.5 (5)
N2—Zn1—Cl2	92.27 (12)	C13—N4—Zn2	128.7 (4)
N1—Zn1—Cl3	92.93 (11)	C24—N4—Zn2	112.8 (3)
N2—Zn1—Cl3	92.59 (11)	C22—N3—C23	118.8 (5)
N1— $Zn1$ — $N2$	80.04 (17)	C22 - N3 - 7n2	129.3 (4)
C_13 — Z_n2 — C_14	93.71 (6)	$C_{23} = N_{3} = Z_{n2}$	111.8(3)
N_3 — Z_n^2 — C_1^3	172.83 (13)	N4-C13-C14	121.8 (5)
N4— $Zn2$ — $Cl3$	92.09(12)	N4-C13-H13	119.1
$N_3 = 7n^2 = Cl^4$	93 28 (14)	C14_C13_H13	119.1
N4 $Zn2$ $Cl4$	172 95 (12)	$N_{2} = (22) = (19)$	122 5 (5)
$N_3 = 7n^2 = N_4$	81.04 (16)	$N_{3} = C_{23} = C_{24}$	122.3(3)
$7n^2 - C^{13} - 7n^1$	90 98 (<i>A</i>)	C_{19} C_{23} C_{24}	110.4(4) 1211(5)
C12 N1 C1	118 3 (5)	$N_{3} C_{23} C_{24}$	121.1(5) 121.3(6)
C12 - N1 - C1	112.6 (2)	$N_3 = C_{22} = C_{21}$	121.3 (0)
C_{12} N_{1} Z_{n1}	128 0 (4)	$N_{3} = C_{22} = H_{22}$	119.4
$C_1 = N_1 = Z_{11}$	128.0(4)	N4 C24 C22	119.4
$C_{10} = N_2 = C_{11}$	117.2(4) 120.8(4)	N4 - C24 - C25	117.9(4)
C_{10} N_2 Z_{n1}	129.0(4)	N4 - C24 - C10	122.0(3)
$N_2 = C_{11} = C_7$	113.1(3)	$C_{23} = C_{24} = C_{16}$	119.4(3)
N2_C11_C12	122.0(5)	C17 - C16 - C15	125.8 (5)
N2-CII-CI2	115.5 (4)	C1/-C16-C24	118.5 (6)
	122.0(5)	C13 - C10 - C24	115.7 (5)
NI-CI2-CII	11/./ (4)	C18 - C17 - C16	121.9 (6)
NI-CI2-C4	124.2 (5)	C18—C17—H17	119.1
C11—C12—C4	118.0 (5)	C16—C17—H17	119.1
NI—CI—C2	122.5 (6)	C14—C15—C16	120.6 (5)
N1—C1—H1	118.8	С14—С15—Н15	119.7
C2—C1—H1	118.8	C16—C15—H15	119.7
C3—C2—C1	118.5 (6)	C17—C18—C19	120.4 (6)
C3—C2—H2	120.7	C17—C18—H18	119.8
C1—C2—H2	120.7	C19—C18—H18	119.8
C9—C8—C7	120.8 (5)	C15—C14—C13	120.8 (6)
С9—С8—Н8	119.6	C15—C14—H14	119.6
С7—С8—Н8	119.6	C13—C14—H14	119.6

C11—C7—C8	117.2 (5)	C23—C19—C20	117.0 (6)
C11—C7—C6	116.8 (5)	C23—C19—C18	118.6 (6)
C8—C7—C6	126.0 (5)	C20-C19-C18	124.4 (6)
N2—C10—C9	123.2 (5)	C21—C20—C19	118.2 (6)
N2—C10—H10	118.4	C21—C20—H20	120.9
С9—С10—Н10	118.4	C19—C20—H20	120.9
C2—C3—C4	121.5 (5)	C20—C21—C22	122.2 (7)
С2—С3—Н3	119.3	C20—C21—H21	118.9
С4—С3—Н3	119.3	C22—C21—H21	118.9
C5—C4—C12	119.9 (5)	C8—C9—C10	119.1 (6)
C5—C4—C3	125.2 (5)	С8—С9—Н9	120.5
C12—C4—C3	114.9 (5)	С10—С9—Н9	120.5
C5—C6—C7	122.4 (5)		

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	D···A	D—H··· A
C1—H1···Cl1	0.93	2.68	3.229 (7)	118
C6—H6···Cl2 ⁱ	0.93	2.77	3.525 (6)	139
C10—H10…Cl2	0.93	2.68	3.235 (6)	119
C13—H13…Cl3	0.93	2.62	3.200 (6)	121
C17—H17···Cl3 ⁱⁱ	0.93	2.67	3.500 (7)	149
C18—H18····Cl4 ⁱⁱ	0.93	2.82	3.742 (7)	173
C22—H22…Cl4	0.93	2.68	3.238 (6)	119
	¢			