Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chlorobis(1,10-phenanthroline-κ^2N,N')zinc(II) nitrate monohydrate

Chun-Hui Yu* and Rong-Chang Zhang

Department of Chemistry, Beihua University, Jilin City 132013, People's Republic of China

Correspondence e-mail: jlschy@126.com

Received 4 July 2006
Accepted 4 July 2006

In the title compound, $[ZnCl(C_{12}H_8N_2)_2]NO_3\cdot H_2O$, the Zn^{II} atom is coordinated by four N atoms from two different 1,10-phenanthroline ligands and by one Cl^- ion in a distorted trigonal–bipyramidal coordination. In the crystal structure, the constituent molecules interact by way of π–π interactions between the 1,10-phenanthroline ligands and by O—H···O and O—H···Cl hydrogen bonds.

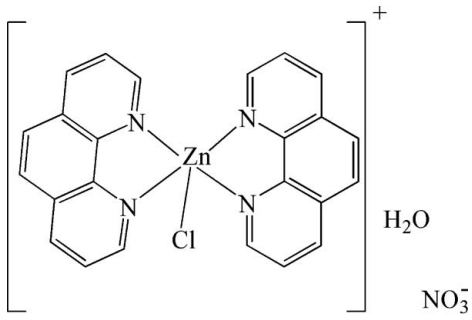
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.108
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

1,10-Phenanthroline (phen) and its derivatives have been used widely in the construction of supramolecular architectures by way of metal-organic coordination, hydrogen-bonding and π–π stacking interactions (Chen *et al.*, 2002; Zhang & Yu, 2006). As an extension of these studies, we now report the crystal structure of the title compound, (I).



(I)

Selected bond lengths and angles for (I) are given in Table 1. In (I), the Zn^{II} atom is coordinated by four N atoms from two different phen ligands and by one Cl^- ion in a distorted trigonal–bipyramidal coordination, with two N atoms in the axial positions (Fig. 1). The cationic charge of the main molecule is balanced by that of a non-coordinated nitrate ion.

The molecules of (I) are held together in the crystal structure through π–π interactions between phen ligands, generating a one-dimensional structure (Fig. 2). The distance between two adjacent phen planes is 3.47 Å. Hydrogen bonds involving the water molecule, the Cl^- ion and the nitrate ion complete the structure of (I) (Table 2).

Experimental

A solution of phen (1 mmol) in 20 ml water was added to a solution of $ZnCl_2\cdot 2H_2O$ (0.5 mmol) in 10 ml water, and the mixture was stirred at room temperature for 5 h. After removing any undissolved materials by filtration, a solution containing NH_4NO_3 (0.5 mmol) in 8 ml water was added to the filtrate. The whole was stirred for 3 h. Colorless

crystals of (I) were obtained after allowing the solution to stand at room temperature for several days (27% yield based on Zn).

Crystal data

$[ZnCl(C_{12}H_8N_2)_2]NO_3\cdot H_2O$
$M_r = 541.25$
Triclinic, $P\overline{1}$
$a = 9.6613\ (19)$ Å
$b = 11.102\ (2)$ Å
$c = 12.000\ (2)$ Å
$\alpha = 67.66\ (3)^\circ$
$\beta = 71.00\ (3)^\circ$
$\gamma = 71.65\ (3)^\circ$
$V = 1098.5\ (5)$ Å^3
$Z = 2$
$D_x = 1.636$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.28$ mm^{-1}
$T = 292\ (2)$ K
Block, colorless
0.33 × 0.31 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.641$, $T_{max} = 0.731$
10950 measured reflections
4983 independent reflections
4317 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.7^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.108$
$S = 1.06$
4983 reflections
322 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.5194P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.121 (2)	Zn1—N4	1.9834 (19)
Zn1—N2	1.9809 (19)	Zn1—Cl1	2.2723 (11)
Zn1—N3	2.084 (2)		
N2—Zn1—N4	175.76 (8)	N3—Zn1—N1	105.10 (8)
N2—Zn1—N3	96.08 (8)	N2—Zn1—Cl1	91.28 (6)
N4—Zn1—N3	81.31 (8)	N4—Zn1—Cl1	92.93 (6)
N2—Zn1—N1	81.24 (8)	N3—Zn1—Cl1	135.61 (6)
N4—Zn1—N1	96.17 (8)	N1—Zn1—Cl1	119.28 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—HW11···Cl1	0.91 (2)	2.30 (2)	3.200 (3)	169 (4)
O1W—HW12···O1^{i}	0.92 (4)	2.02 (2)	2.876 (6)	153 (4)
O1W—HW12···O2^{i}	0.92 (4)	2.45 (4)	3.236 (6)	143 (4)

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

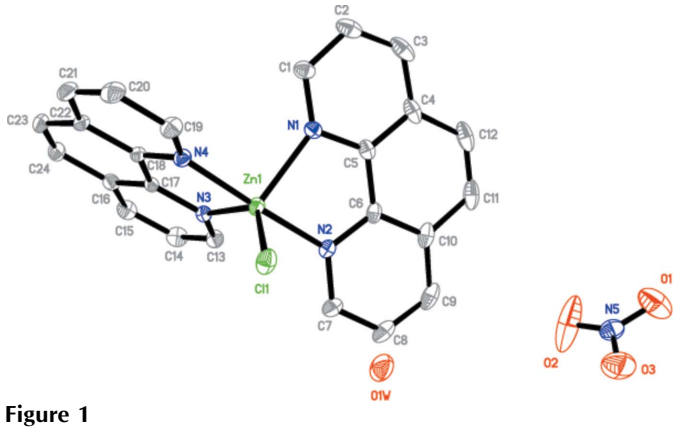


Figure 1
View of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted.

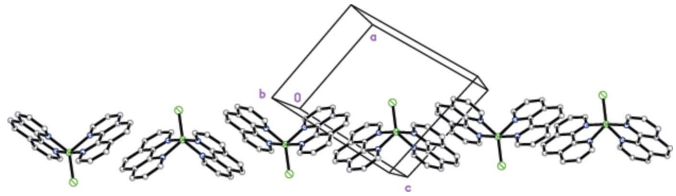


Figure 2
The π–π interactions between phen ligands in (I). H atoms have been omitted.

All H atoms on C atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the water molecule were located in a difference map and refined freely.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The authors thank Beihua University for supporting this work.

References

Chen, X. M. & Liu, D. F. (2002). *Chem. Eur. J.* **8**, 4811–4817.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, R.-C. & Yu, C.-H. (2006). *Acta Cryst.* E**62**, m807–m809.