Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{2-[2-(diethylamino)ethyliminomethyl]-4-nitrophenolato}dimethanolzinc(II) dinitrate

Xiao-Yang Qiu

Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China

Correspondence e-mail: xiaoyang_qiu@126.com

Received 17 April 2006
Accepted 19 April 2006

Key indicators

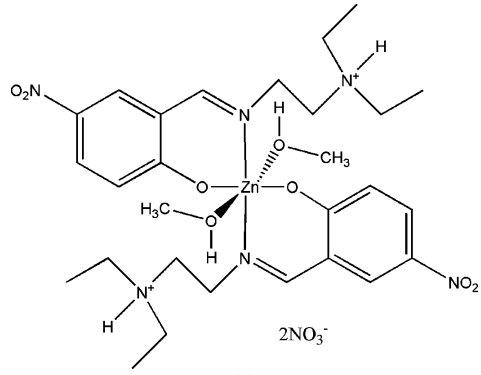
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
Disorder in solvent or counterion
R factor = 0.057
wR factor = 0.171
Data-to-parameter ratio = 14.9

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

The title compound, $[Zn(C_{13}H_{19}N_3O_3)_2(CH_4O)_2](NO_3)_2$, is isostructural with the nickel complex reported previously [Chen (2006). *Acta Cryst.* E**62**, m204–m206]. The Zn atom lies on an inversion centre and is coordinated octahedrally by N and O atoms of two Schiff base ligands and two MeOH molecules in a *trans* orientation. In the crystal structure, molecules are linked through O—H···N, O—H···O, N—H···N and N—H···O intermolecular hydrogen bonds, forming chains running along the *b* axis.

Comment

The crystal structure of the nickel(II) complex derived from the Schiff base ligand 2-[2-(diethylamino)ethyliminomethyl]-4-nitrophenol was reported previously (Chen, 2006). An isostructural zinc(II) complex with the same ligand is reported here.



(I)

The title mononuclear zinc(II) compound, (I), consists of a $[Zn(C_{13}H_{19}N_3O_3)_2(CH_3OH)_2]^{2+}$ cation and two disordered nitrate anions. The Zn atom lies on an inversion centre and is six-coordinated by N and O atoms from two Schiff base ligands and two MeOH molecules in a *trans* orientation, forming an octahedral geometry (Fig. 1 and Table 1). All the bond lengths around the metal centre are slightly longer than the corresponding values observed in the nickel(II) complex cited above.

In the crystal structure, molecules are linked through O—H···N, O—H···O, N—H···N and N—H···O intermolecular hydrogen bonds, forming chains running along the *b* axis (Table 2 and Fig. 2).

Experimental

5-Nitrosalicylaldehyde (1.0 mmol, 167.5 mg), *N*,*N*-diethylethane-1,2-diamine (1.0 mmol, 116.2 mg) and $Zn(NO_3)_2{\cdot}6H_2O$ (0.5 mmol,

148.7 mg) were dissolved in MeOH (50 ml). The mixture was stirred for 20 min at room temperature and then allowed to evaporate slowly in air for about a week to give colourless block-like crystals.

Crystal data

$[Zn(C_{13}H_{19}N_3O_3)_2(CH_4O)_2](NO_3)_2$
M_r = 784.10
Triclinic, $P\overline{1}$
a = 8.305 (1) Å
b = 11.083 (2) Å
c = 11.126 (2) Å
α = 69.584 (1)°
β = 71.080 (1)°
γ = 84.204 (1)°
V = 907.8 (3) Å^3
Z = 1
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 298 (2) K
Block, colourless
0.30 × 0.25 × 0.22 mm

Data collection

Buker SMART APEX 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.806, T_{max} = 0.852
7642 measured reflections
3881 independent reflections
3423 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.171
S = 1.04
3881 reflections
260 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.12P)^2 + 0.2978P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.021 (2)	Zn1—O4	2.217 (3)
Zn1—N1	2.107 (2)		
O1^i—Zn1—O1	180	O1—Zn1—O4	91.34 (13)
O1—Zn1—N1^i	91.27 (10)	N1^i—Zn1—O4	89.47 (11)
O1—Zn1—N1	88.73 (10)	N1—Zn1—O4	90.53 (11)
N1^i—Zn1—N1	180	O4—Zn1—O4^i	180
O1^i—Zn1—O4	88.66 (13)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···N3^{ii}	0.84 (3)	2.58 (3)	3.417 (4)	177 (4)
O4—H4A···O2^{ii}	0.84 (3)	2.34 (2)	3.112 (4)	153 (4)
O4—H4A···O3^{ii}	0.84 (3)	2.22 (3)	2.978 (4)	150 (4)
N2—H2···N4	0.89 (3)	2.63 (3)	3.509 (4)	170 (4)
N2—H2···O6	0.89 (3)	2.59 (3)	3.348 (7)	142 (4)
N2—H2···O7′	0.89 (3)	2.43 (2)	3.284 (12)	159 (4)
N2—H2···O6′	0.89 (3)	1.93 (3)	2.736 (9)	148 (4)
N2—H2···O7	0.89 (3)	1.93 (2)	2.798 (6)	163 (5)

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

Atoms H2 and H4*A* were located in a difference Fourier map and refined isotropically, with the O—H2 and N—H4*A* distances restrained to 0.84 (1) and 0.90 (1) Å, respectively, and U_{iso}(H) = 0.08 Å. All other H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). The O atoms of the nitrate anions were disordered over two distinct sites with occupancies of 0.605 (3) and 0.395 (3). The N—O and O···O distances in both disordered components were restrained to be equal. An unassigned maximum residual density was observed 1.14 Å from C10.

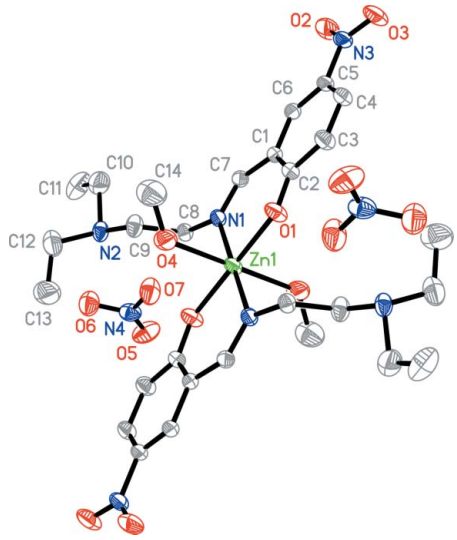


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. Only the major components of the disordered nitrate anions are shown, and H atoms have been omitted. Labelled atoms are related to unlabelled atoms by the symmetry operation $(2-x, 2-y, -z)$.

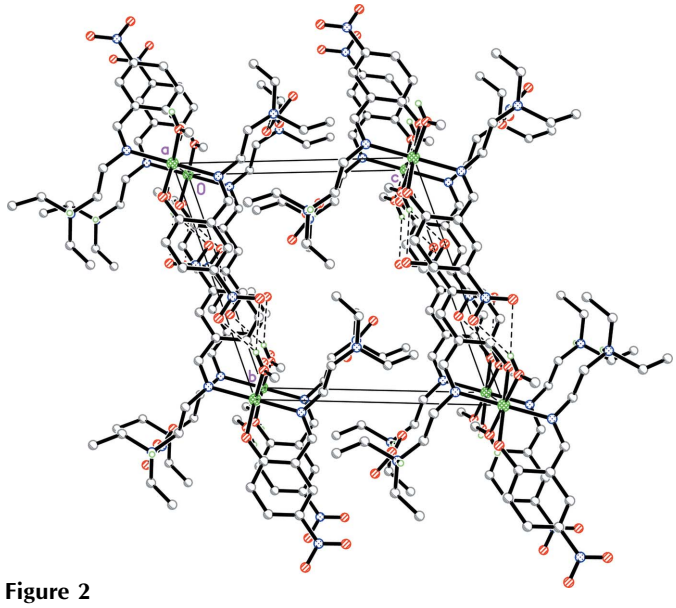


Figure 2
The molecular packing of (I). Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The author acknowledges Fuyang Normal College for financial support.

References

Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Y. (2006). *Acta Cryst.* E**62**, m204–m206.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS, Inc., Madison, Wisconsin, USA.