

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li <i>et al.</i> (2008)	Author	10.1107/S1600536807056309	RISTET
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoerbium(III)zinc(II)	Chen <i>et al.</i> (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato- $\kappa^2 O^1, O^6$)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoholmium(III)zinc(II)	Xiao, Sui <i>et al.</i> (2008)	Author	10.1107/S1600536808013743	BIZTUA
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu <i>et al.</i> (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid-4,4'-bipyridine (2I)	Wang <i>et al.</i> (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- $1\kappa^4 O^1, O^1, O^6, O^6:2\kappa^4 O^1, N, N', O^1$ } (ethanol- $1\kappa O$)- μ -nitrate- $1:2\kappa^2 O:O'$ -dinitrato- $1\kappa^2 O, O'$ -samarium(III)zinc(II)	Huang <i>et al.</i> (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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trans-Bis(ethylenediamine- κ^2N,N')-bis(nitrato- κO)zinc(II)

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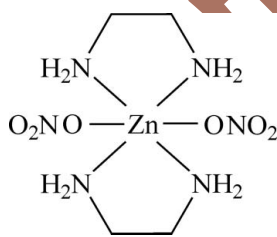
Received 14 August 2007; accepted 29 August 2007

 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.007$ Å; R factor = 0.048; wR factor = 0.148; data-to-parameter ratio = 14.1.

In the title compound, $[Zn(NO_3)_2(C_2H_8N_2)_2]$, the Zn^{II} atom lies on a centre of inversion and is coordinated by four N atoms belonging to two ethylenediamine molecules and two O atoms belonging to two nitrate anions arranged in a *trans* manner. The Zn^{II} ion displays a distorted octahedral coordination geometry. Adjacent complexes are connected by $N-H \cdots O$ hydrogen bonds formed between the H atoms of the amino groups and the uncoordinated O atoms of the nitrate anions.

Related literature

For the structure of the analogous Cu^{II} compound, see: Komiyama & Lingafelter (1964); Fronczek *et al.* (1995); Manriquez *et al.* (1996).



Experimental

Crystal data

 $[Zn(NO_3)_2(C_2H_8N_2)_2]$
 $M_r = 309.62$

 Monoclinic, $P2_1/c$
 $a = 8.2127$ (7) Å

 $b = 9.9673$ (8) Å

 $c = 7.9733$ (7) Å

 $\beta = 111.171$ (1) $^\circ$
 $V = 608.63$ (9) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 2.05$ mm⁻¹
 $T = 293$ (2) K

 $0.24 \times 0.17 \times 0.09$ mm

Data collection

Bruker APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 1997)

 $T_{\min} = 0.668$, $T_{\max} = 0.823$

 3715 measured reflections
 1116 independent reflections

 811 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.148$
 $S = 1.07$

1116 reflections

79 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.71$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.84$ e Å⁻³
Table 1

 Selected geometric parameters (Å, $^\circ$).

O2—Zn1	2.568 (3)	Zn1—N1	2.002 (4)
Zn1—N2	1.989 (4)		
N2 ⁱ —Zn1—N2	180.0	N2 ⁱ —Zn1—O2	92.14 (15)
N2 ⁱ —Zn1—N1	95.11 (16)	N2—Zn1—O2	87.86 (15)
N2—Zn1—N1	84.89 (16)	N1—Zn1—O2	91.40 (15)
N1—Zn1—N1 ⁱ	180.00(14)	N1 ⁱ —Zn1—O2	88.60 (15)

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

Table 2

 Hydrogen-bond geometry (Å, $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H3B ⁱⁱ ···O3 ⁱⁱⁱ	0.90	2.29	3.023 (6)	138
N1—H3A ⁱⁱ ···O3	0.90	2.22	3.015 (6)	147
N2—H4A ⁱⁱⁱ ···O1 ⁱⁱⁱ	0.90	2.13	3.025 (5)	176
N2—H4A ⁱⁱⁱ ···O2 ⁱⁱⁱ	0.90	2.58	3.235 (5)	130
N2—H4B ^{iv} ···O1 ^{iv}	0.90	2.16	3.027 (6)	161

 Symmetry codes: (ii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (iv) $x, y, z - 1$.

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

The authors are grateful to the Natural Science Foundation of Jiangxi Province (grant Nos. 0520036 and 0620029) for support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2235).

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supplementary materials

Article retracted

Acta Cryst. (2007). E63, m2462 [doi:10.1107/S1600536807042390]

***trans*-Bis(ethylenediamine- κ^2N,N')bis(nitrato- κO)zinc(II)**

Y.-Q. Liu, X.-R. Zeng and W.-T. Chen

Comment

The title compound (Fig. 1) is a mononuclear Zn^{II} complex. The Zn^{II} atom lies on a centre of inversion and is coordinated to four N atoms belonging to two ethylenediamine molecules and two O atoms belonging to two nitrate anions arranged in a *trans* manner. In the crystal, adjacent molecules are connected by N—H \cdots O hydrogen bonds involving the H atoms of the amino groups and the non-bonded O atoms of the nitrate ions (Fig. 2).

Experimental

Ethylenediamine (0.120 g, 0.002 mol) and $Zn(NO_3)_2$ (0.189 g, 0.001 mol) were added to 25 ml methanol. The mixture was heated for 5 h under reflux with stirring and the resulting solution was filtered. Single crystals suitable for X-ray diffraction were formed after a week by slow evaporation of the filtrate.

Refinement

H atoms were placed at calculated positions and refined as riding on their parent C or N atoms, with C—H = 0.97 Å or N—H = 0.90 Å, and with $U_{iso}(H) = 1.2U_{eq}(C/N)$.

Figures

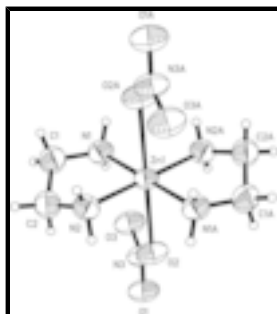


Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at 50% probability for non-H atoms.

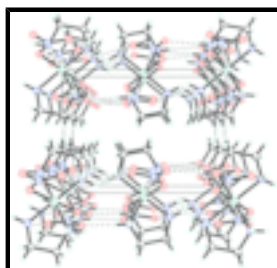


Fig. 2. Unit-cell contents viewed along the *c* axis. H bonds are shown as dashed lines.

trans-Bis(ethylenediamine- κ^2N,N')bis(nitrato- κO) zinc(II)

Crystal data

$[Zn(NO_3)_2(C_2H_8N_2)_2]$

$M_r = 309.62$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.2127$ (7) Å

$b = 9.9673$ (8) Å

$c = 7.9733$ (7) Å

$\beta = 111.171$ (1)°

$V = 608.63$ (9) Å³

$Z = 2$

$F_{000} = 320$

$D_x = 1.689$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2202 reflections

$\theta = 2.7$ – 27.8°

$\mu = 2.05$ mm⁻¹

$T = 293$ (2) K

Block, colourless

$0.24 \times 0.17 \times 0.09$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 1997)

$T_{\min} = 0.668$, $T_{\max} = 0.823$

3715 measured reflections

1116 independent reflections

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

$R_{\text{int}} = 0.026$

$\theta_{\max} = 25.5^\circ$

$\theta_{\min} = 2.7^\circ$

$h = -9 \rightarrow 9$

$k = -12 \rightarrow 11$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.148$

$S = 1.07$

1116 reflections

79 parameters

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0901P)^2 + 0.4042P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.71$ e Å⁻³

$\Delta\rho_{\min} = -0.84$ e Å⁻³

Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	1.0000	0.5000	0.5000	0.0411 (3)
N3	0.8252 (6)	0.5573 (4)	0.8297 (6)	0.0547 (11)
O1	0.7756 (5)	0.6261 (4)	0.9285 (5)	0.0637 (10)
O2	0.9006 (5)	0.6110 (3)	0.7375 (5)	0.0600 (10)
O3	0.7984 (5)	0.4342 (4)	0.8202 (6)	0.0675 (11)
C2	0.6379 (8)	0.5160 (5)	0.3000 (9)	0.0620 (15)
H2A	0.5473	0.5332	0.1840	0.074*
H2B	0.5968	0.5474	0.3929	0.074*
N1	0.8360 (5)	0.3461 (4)	0.4743 (6)	0.0544 (11)
H3B	0.8856	0.2696	0.4563	0.065*
H3A	0.8125	0.3370	0.5755	0.065*
N2	0.7978 (5)	0.5876 (4)	0.3128 (6)	0.0515 (11)
H4A	0.7904	0.6739	0.3423	0.062*
H4B	0.8120	0.5853	0.2061	0.062*
C1	0.6745 (7)	0.3712 (5)	0.3217 (8)	0.0649 (15)
H1A	0.5784	0.3256	0.3408	0.078*
H1B	0.6851	0.3356	0.2128	0.078*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.090 (3)	0.044 (2)	0.062 (2)	-0.0035 (18)	0.045 (2)	-0.0026 (16)
O3	0.095 (3)	0.039 (2)	0.075 (3)	-0.0047 (19)	0.039 (2)	0.0023 (19)
Zn1	0.0495 (5)	0.0314 (5)	0.0439 (5)	0.0007 (3)	0.0187 (3)	0.0030 (3)
N3	0.082 (3)	0.037 (2)	0.056 (3)	-0.001 (2)	0.039 (2)	0.000 (2)
O1	0.093 (3)	0.052 (2)	0.060 (2)	0.0047 (19)	0.044 (2)	-0.0022 (17)
C2	0.058 (3)	0.052 (3)	0.069 (4)	-0.001 (2)	0.014 (3)	0.002 (2)
N1	0.057 (2)	0.037 (2)	0.069 (3)	-0.0039 (18)	0.021 (2)	-0.0027 (19)
N2	0.054 (2)	0.044 (2)	0.054 (3)	0.0043 (18)	0.0172 (19)	0.0036 (18)
C1	0.061 (3)	0.049 (3)	0.076 (4)	-0.004 (2)	0.014 (3)	-0.003 (3)

Geometric parameters (Å, °)

O2—N3	1.241 (5)	C2—H2A	0.970
O2—Zn1	2.568 (3)	C2—H2B	0.970
O3—N3	1.243 (6)	N1—C1	1.462 (6)
Zn1—N2 ⁱ	1.989 (4)	N1—H3B	0.900
Zn1—N2	1.989 (4)	N1—H3A	0.900
Zn1—N1	2.002 (4)	N2—H4A	0.900
Zn1—N1 ⁱ	2.002 (4)	N2—H4B	0.900
N3—O1	1.221 (5)	C1—H1A	0.970
C2—N2	1.466 (7)	C1—H1B	0.970
C2—C1	1.472 (7)		
N3—O2—Zn1	127.6 (3)	H2A—C2—H2B	108.3
N2 ⁱ —Zn1—N2	180.0	C1—N1—Zn1	109.2 (3)
N2 ⁱ —Zn1—N1	95.11 (16)	C1—N1—H3B	109.8
N2—Zn1—N1	84.89 (16)	Zn1—N1—H3B	109.8
N2 ⁱ —Zn1—N1 ⁱ	84.89 (16)	C1—N1—H3A	109.8
N2—Zn1—N1 ⁱ	95.11 (16)	Zn1—N1—H3A	109.8
N1—Zn1—N1 ⁱ	180.00 (14)	H3B—N1—H3A	108.3
N2 ⁱ —Zn1—O2	92.14 (15)	C2—N2—Zn1	108.9 (3)
N2—Zn1—O2	87.86 (15)	C2—N2—H4A	109.9
N1—Zn1—O2	91.40 (15)	Zn1—N2—H4A	109.9
N1 ⁱ —Zn1—O2	88.60 (15)	C2—N2—H4B	109.9
O1—N3—O2	119.6 (4)	Zn1—N2—H4B	109.9
O1—N3—O3	120.0 (4)	H4A—N2—H4B	108.3
O2—N3—O3	120.3 (4)	N1—C1—C2	110.6 (4)
N2—C2—C1	109.2 (5)	N1—C1—H1A	109.5
N2—C2—H2A	109.8	C2—C1—H1A	109.5
C1—C2—H2A	109.8	N1—C1—H1B	109.5
N2—C2—H2B	109.8	C2—C1—H1B	109.5
C1—C2—H2B	109.8	H1A—C1—H1B	108.1

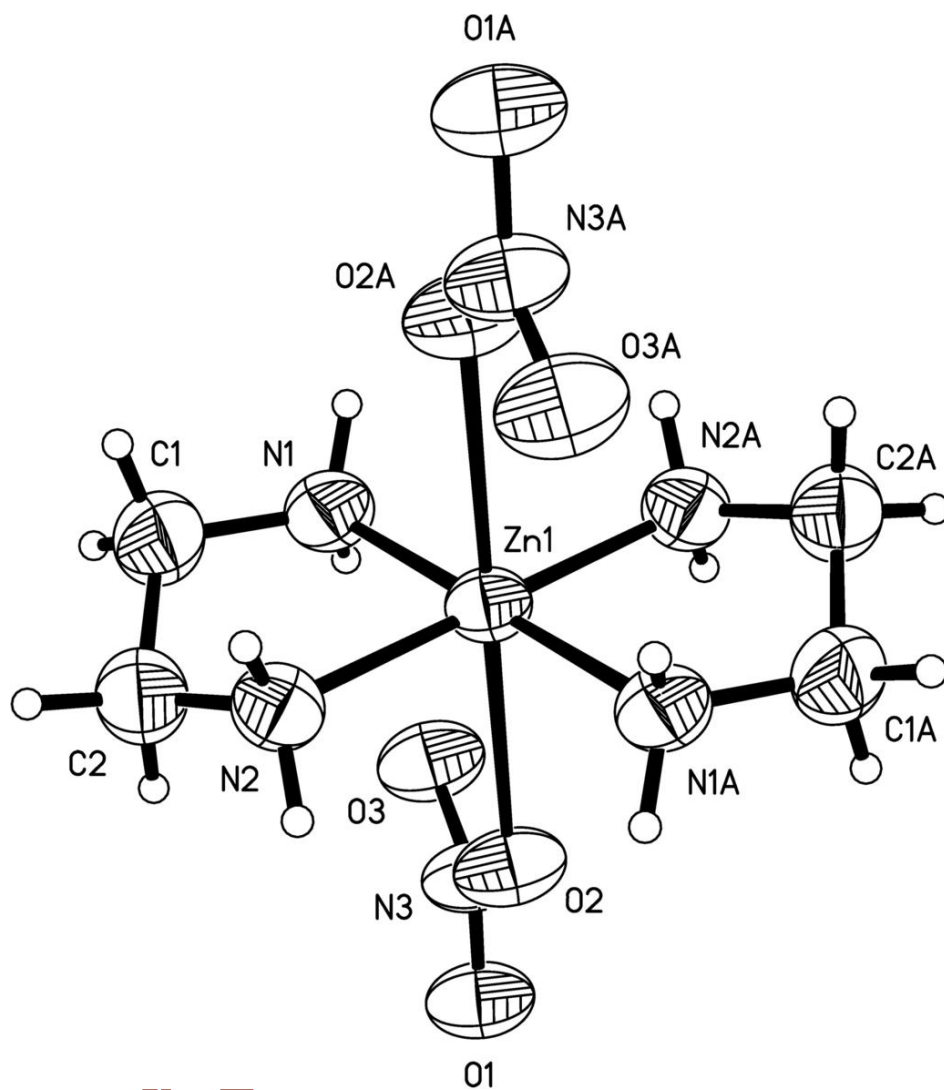
Symmetry codes: (i) $-x+2, -y+1, -z+1$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H3B...O3 ⁱⁱ	0.90	2.29	3.023 (6)	138
N1—H3A...O3	0.90	2.22	3.015 (6)	147
N2—H4A...O1 ⁱⁱⁱ	0.90	2.13	3.025 (5)	176
N2—H4A...O2 ⁱⁱⁱ	0.90	2.58	3.235 (5)	130
N2—H4B...O1 ^{iv}	0.90	2.16	3.027 (6)	161

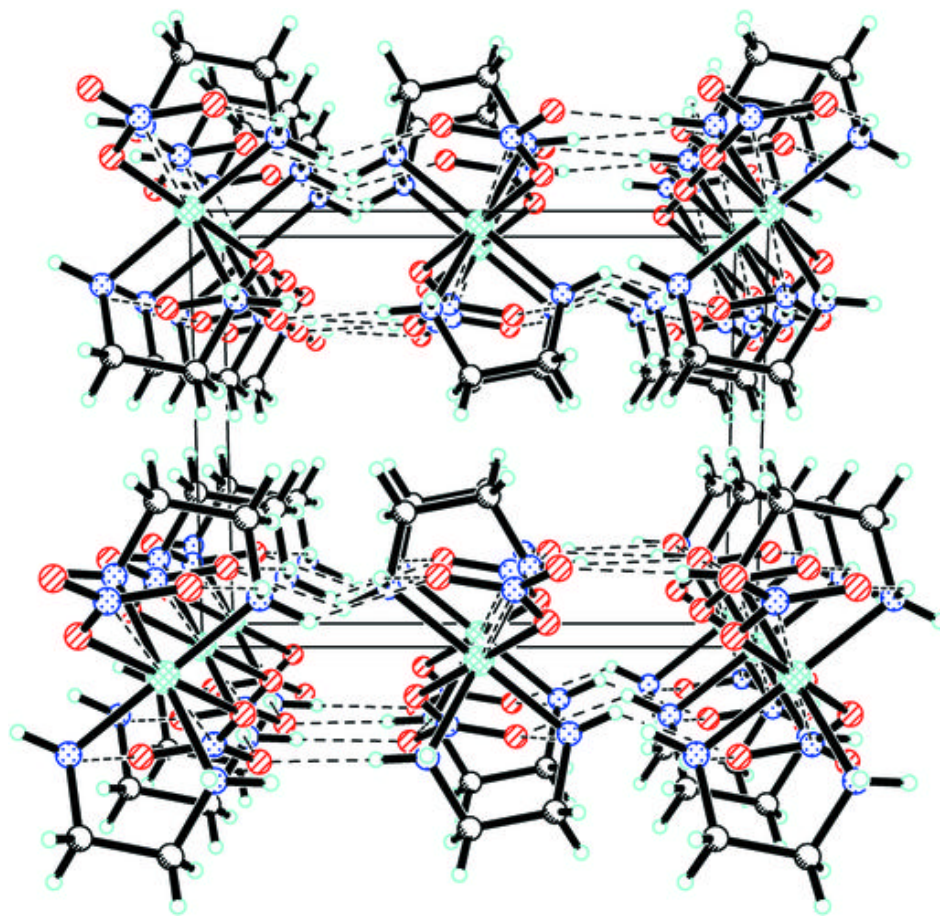
Symmetry codes: (ii) $x, -y+1/2, z-1/2$; (iii) $x, -y+3/2, z-1/2$; (iv) $x, y, z-1$.

Fig. 1



A1

Fig. 2



Article