Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diacetato(ethylenediamine)zinc(II)

Young-Inn Kim,[a] You-Soon Lee,[b] Hoe-Joo Seo[c] and Sung Kwon Kang[b]*

[a]Department of Chemistry Education, Pusan National University, Pusan 609-735, Republic of Korea, [b]Department of Chemistry, Chungnam National University, Daejeon 305-764, Republic of Korea, and [c]Department of Chemistry, Pusan National University, Pusan 609-735, Republic of Korea
Correspondence e-mail: skkang@cnu.ac.kr

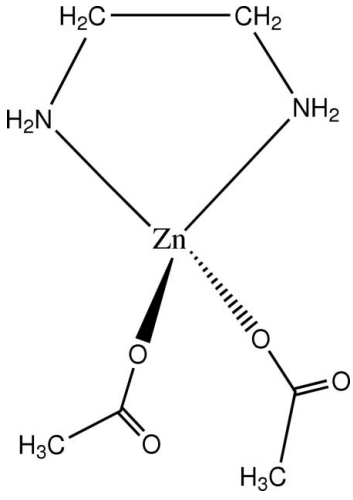
Received 17 July 2007; accepted 25 July 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.067; data-to-parameter ratio = 20.0.

In the title compound, $[Zn(C_2H_3O_2)_2(C_2H_8N_2)]$, the Zn^{II} atom is coordinated by two N atoms of one bidentate ethylenediamine ligand and two O atoms of two acetate anions in a distorted tetrahedral geometry. The compound displays [4+2] coordination, the '4' representing the distorted tetrahedral coordination, while the '2' refers to the two much longer Zn···O(uncoordinated) distances of 2.594 (2) Å. The asymmetry of the acetate coordination is reflected in the different C—O distances of 1.229 (2) and 1.280 (2) Å. The Zn atom lies on a crystallographic twofold rotation axis. The dihedral angles between the N/Zn/N′ plane and the two O/Zn/O′ planes are 85.54 (7) and 29.96 (7)°, where the prime denotes the atom related by operation of the twofold axis. N—H···O hydrogen bonding links the molecules into a three-dimensional network.

Related literature

For general background see: Amendola *et al.* (2006); Yang *et al.* (2000); Xu *et al.* (2006); Evans *et al.* (2006).



Experimental

Crystal data

$[Zn(C_2H_3O_2)_2(C_2H_8N_2)]$
M_r = 243.56
Orthorhombic, *Pbcn*
a = 12.1335 (4) Å
b = 7.7866 (2) Å
c = 10.4078 (3) Å
V = 983.32 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.48 mm^{-1}
T = 295 (2) K
0.12 × 0.12 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.745, T_{max} = 0.758
5391 measured reflections
1221 independent reflections
867 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 0.99
1221 reflections
61 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.0784 (16)	O3—C4	1.280 (2)
Zn1—O3	1.9887 (13)	C4—O5	1.229 (2)
N1—C2	1.477 (3)		
N1—Zn1—N1^{i}	85.01 (9)	N1^{i}—Zn1—O3	110.71 (6)
N1—Zn1—O3	104.95 (6)		

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O3^{ii}	0.90	2.22	3.078 (2)	160
N1—H1A···O5^{iii}	0.90	2.25	3.050 (2)	148

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by a grant from the Ministry of Commerce, Industry and Energy, and the Korea Industrial Technology Foundation. X-ray data were collected at the Center for Research Facilities at Chungnam National University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BM3031).

References

Amendola, V., Fabbrizzi, L., Foti, F., Licchelli, M., Mangano, C., Pallavicini, P., Poggi, A., Sacchi, D. & Taglietti, A. (2006). *Coord. Chem. Rev.* **250**, 273–299.
Bruker (2002). *SADABS* (Version 2.03), *SAINT* (Version 6.02) and *SMART* (Version 5.62). Bruker AXS Inc., Madison, Wisconsin, USA.
Evans, R. C., Douglas, P. & Winscom, C. J. (2006). *Coord. Chem. Rev.* **250**, 2093–2126.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

 doi:10.1107/S1600536807036616 © 2007 International Union of Crystallography

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (2002). *SADABS*. University of Göttingen, Germany.
Xu, Y., Chen, B., Gong, Y., Yuan, D., Jiang, F. & Hong, M. (2006). *J. Mol. Struct.* **789**, 220–224.
Yang, W., Schmider, H., Wu, Q., Zhang, Y.-S. & Wang, S. (2000). *Inorg. Chem.* **39**, 2397–2404.

supplementary materials

Acta Cryst. (2007). E**63**, m2239-m2240 [**doi:10.1107/S1600536807036616**]

Diacetato(ethylenediamine)zinc(II)

Y.-I. Kim, Y.-S. Lee, H.-J. Seo and S. K. Kang

Comment

Luminescent coordination compounds have been investigated extensively due to their various potential applications in material sciences (Amendola *et al.* 2006). Many Zn(II) complexes are known to exhibit an intense fluorescence at room temperature (Yang, *et al.* 2000; Xu, *et al.* 2006), and they are proposed as candidates for the fluorescent based organic light-emitting diods (OLED) devices (Evans, *et al.* 2006). The title compound displays distorted tetrahedral coordination, with two N atoms from ethylenediamine and two O atoms from two acetate ligands. The title compound displays [4 + 2] coordination: the "4" represnets the distorted tetrahedral coordination, while the "2" means the two much longer Zn1—O5 distances of 2.594 (2) Å. The asymmetry of the acetate coordination is reflected in the different C—O distances of 1.229 (2) and 1.280 (2) Å. The Zn1 lies on a crystallographic twofold axis. The dihedral angle between N1—Zn1—N1' and O3—Zn1—O3' planes is 85.54 (7) °, where the prime denotes the symetry operation about the twofold axis. While the dihedral angle between N1—Zn1—N1' and O5—Zn1—O5' planes is 29.96 (7) °. N—H···O hydrogen bonding links molecules into a three-dimensional network. The title compound exhibits an intense blue emission at 444 nm in $CHCl_3$ upon 368 nm excitation.

Experimental

A solution of zinc acetate (2.195 g, 10.0 mmol) and ethylenediamine (0.601 g, 10.0 mmol) in absolute ethanol (50 ml) was stirred for 8 hrs at room temperature under a nitrogen atmosphere. The resulting colorless solution was allowed to stand at room temperature for two weeks to produce colorless crystals (yield 65.0%) suitable for X-ray diffraction.

Refinement

Apart from those of sp^2-bound methyl groups, which were located in ΔF syntheses, H atoms were positioned geometrically. Thereafter they were constrained to ride on their carrier atoms, with N—H = 0.90 Å and U_{iso}(H) = 1.2U_{iso}(N) for NH_2, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{iso}(C) for CH_2, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{iso}(C) for CH_3 groups.

Figures

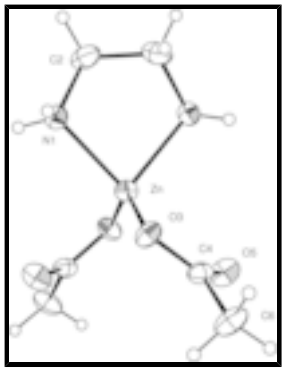


Fig. 1. Molecular structure of (I), showing the atom-numbering scheme and 30% probability ellipsoids.

Diacetato(ethylenediamine)zinc(II)

Crystal data

$[Zn(C_2H_3O_2)_2(C_2H_8N_2)]$	F_{000} = 504
M_r = 243.56	D_x = 1.645 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 1923 reflections
a = 12.1335 (4) Å	θ = 3.1–26.9º
b = 7.7866 (2) Å	μ = 2.48 mm^{-1}
c = 10.4078 (3) Å	*T* = 295 (2) K
V = 983.32 (5) Å^3	Block, colourless
Z = 4	0.12 × 0.12 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer	R_{int} = 0.028
φ and ω scans	θ_{max} = 28.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	θ_{min} = 3.1º
T_{min} = 0.745, T_{max} = 0.758	*h* = −16→11
5391 measured reflections	*k* = −7→10
1221 independent reflections	*l* = −9→13
867 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.026	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.067	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
S = 0.99	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
1221 reflections	Extinction correction: none
61 parameters	

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5	0.61106 (4)	0.75	0.03233 (13)
N1	0.39968 (13)	0.4143 (2)	0.68272 (16)	0.0361 (4)
H1A	0.3286	0.4352	0.7017	0.043*
H1B	0.4064	0.4028	0.597	0.043*
C2	0.43883 (19)	0.2582 (3)	0.7493 (2)	0.0531 (7)
H2A	0.412	0.1568	0.7051	0.064*
H2B	0.4109	0.2562	0.8366	0.064*
O3	0.56408 (11)	0.71701 (18)	0.59300 (13)	0.0405 (4)
C4	0.63853 (17)	0.8189 (3)	0.6350 (2)	0.0364 (5)
O5	0.66115 (15)	0.8299 (2)	0.74983 (13)	0.0513 (4)
C6	0.6980 (2)	0.9260 (3)	0.5362 (2)	0.0526 (6)
H6A	0.7507	0.9984	0.5783	0.079*
H6B	0.6453	0.9962	0.4912	0.079*
H6C	0.7348	0.8523	0.4763	0.079*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0364 (2)	0.0318 (2)	0.02885 (18)	0	0.00367 (14)	0
N1	0.0369 (10)	0.0397 (11)	0.0316 (9)	−0.0031 (8)	−0.0019 (8)	0.0034 (7)
C2	0.0726 (17)	0.0370 (13)	0.0495 (13)	−0.0147 (12)	−0.0162 (14)	0.0061 (11)
O3	0.0420 (9)	0.0408 (9)	0.0386 (8)	−0.0132 (7)	0.0047 (7)	0.0014 (6)
C4	0.0424 (13)	0.0280 (11)	0.0386 (11)	0.0004 (10)	0.0077 (10)	−0.0027 (9)
O5	0.0634 (11)	0.0538 (10)	0.0367 (8)	−0.0129 (9)	0.0037 (7)	−0.0030 (8)
C6	0.0665 (16)	0.0486 (14)	0.0427 (12)	−0.0260 (13)	0.0051 (12)	0.0027 (11)

Geometric parameters (Å, °)

Zn1—N1	2.0784 (16)	C2—H2B	0.97
Zn1—O3	1.9887 (13)	O3—C4	1.280 (2)
N1—C2	1.477 (3)	C4—O5	1.229 (2)
N1—H1A	0.90	C4—C6	1.508 (3)
N1—H1B	0.90	C6—H6A	0.96
C2—C2^{i}	1.485 (5)	C6—H6B	0.96
C2—H2A	0.97	C6—H6C	0.96
N1—Zn1—N1^{i}	85.01 (9)	C2^{i}—C2—H2B	109.9
N1—Zn1—O3	104.95 (6)	H2A—C2—H2B	108.3
N1^{i}—Zn1—O3	110.71 (6)	C4—O3—Zn1	104.61 (12)
C2—N1—Zn1	105.09 (12)	O5—C4—O3	122.23 (19)
C2—N1—H1A	110.7	O5—C4—C6	121.2 (2)
Zn1—N1—H1A	110.7	O3—C4—C6	116.56 (18)
C2—N1—H1B	110.7	C4—C6—H6A	109.5
Zn1—N1—H1B	110.7	C4—C6—H6B	109.5
H1A—N1—H1B	108.8	H6A—C6—H6B	109.5

N1—C2—C2^{i}	109.05 (16)	C4—C6—H6C	109.5
N1—C2—H2A	109.9	H6A—C6—H6C	109.5
C2^{i}—C2—H2A	109.9	H6B—C6—H6C	109.5
N1—C2—H2B	109.9		

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1B···O3^{ii}	0.90	2.22	3.078 (2)	160
N1—H1A···O5^{iii}	0.90	2.25	3.050 (2)	148

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1/2, *y*−1/2, −*z*+3/2.

Fig. 1