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Bis[(2-aminophenyl)methanol- κ^2N,O]-bis(nitrato- κO)zinc(II)

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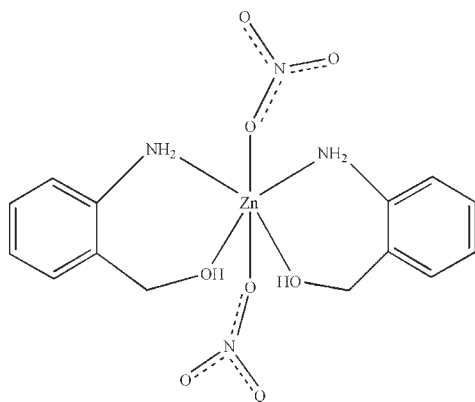
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.007$ Å; R factor = 0.088; wR factor = 0.154; data-to-parameter ratio = 22.3.

In the title compound, $[Zn(NO_3)_2(C_7H_9NO)_2]$, the Zn^{II} atom, lying on a twofold rotation axis, is six-coordinated in a distorted octahedral geometry by two N atoms and two O atoms from two (2-aminophenyl)methanol ligands and two O atoms from two monodentate nitrate anions. Intermolecular $N-H\cdots O$, $O-H\cdots O$ and $C-H\cdots O$ hydrogen bonds stabilize the crystal structure.

Related literature

For related structures, see: Bandoli *et al.* (2002); Lewiński *et al.* (1998).



Experimental

Crystal data

$[Zn(NO_3)_2(C_7H_9NO)_2]$
 $M_r = 435.71$
Orthorhombic, $Pbcn$
 $a = 23.386$ (5) Å

$b = 10.193$ (2) Å
 $c = 7.3442$ (15) Å
 $V = 1750.7$ (6) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 1.46$ mm⁻¹

$T = 298$ K
 $0.35 \times 0.03 \times 0.02$ mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{min} = 0.857$, $T_{max} = 0.980$

14935 measured reflections
3005 independent reflections
2063 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.140$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.088$
 $wR(F^2) = 0.154$
 $S = 1.26$
3005 reflections
135 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.67$ e Å⁻³
 $\Delta\rho_{min} = -0.76$ e Å⁻³

Table 1

Selected bond lengths (Å).

Zn1—O1	2.142 (3)	Zn1—N1	2.108 (4)
Zn1—O2	2.190 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1C\cdots O3^i$	0.79 (6)	2.24 (6)	2.987 (5)	157 (6)
$N1-H1D\cdots O4^{ii}$	0.86 (7)	2.24 (7)	3.096 (5)	169 (7)
$O1-H1E\cdots O2^{iii}$	0.72 (7)	2.03 (7)	2.710 (4)	159 (7)
$C1-H1B\cdots O4^{ii}$	0.97	2.56	3.441 (6)	150

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2332).

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supplementary materials

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Bis[(2-aminophenyl)methanol- κ^2N,O]bis(nitrato- κO)zinc(II)

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Comment

(2-Aminophenyl)methanol is a bidentate ligand. There is only two complexes with this ligand reported, such as those of Re (Bandoli *et al.*, 2002) and Al (Lewiński *et al.* 1998). We report herein the synthesis and structure of the title compound.

The asymmetric unit of the title compound (Fig. 1) contains half molecule. The Zn^{II} atom, lying on a twofold rotation axis, is six-coordinated in a distorted octahedral geometry by two N atoms and two O atoms from two (2-aminophenyl)methanol ligands and two O atoms from two nitrate anions (Table 1). Intermolecular N—H \cdots O, O—H \cdots O and C—H \cdots O hydrogen bonds stabilize the crystal structure (Fig. 2, Table 2).

Experimental

A solution of (2-aminophenyl)methanol (0.25 g, 2.00 mmol) in methanol (10 ml) was added to a solution of Zn(NO₃)₂·4H₂O (0.26 g, 1.00 mmol) in methanol (10 ml) and the resulting colorless solution was stirred for 20 min at 313 K. This solution was left to evaporate slowly at room temperature. After one week, colorless needle crystals of the title compound were isolated (yield: 0.32 g, 73.4%).

Refinement

C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic) and 0.97 (CH₂) Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of the amino and hydroxy groups were located in a difference Fourier map and refined isotropically.

Figures

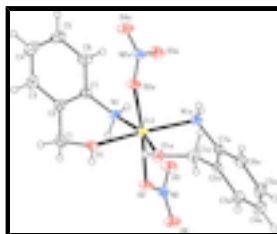


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (a) 1 - x, y, 1/2 - z.]

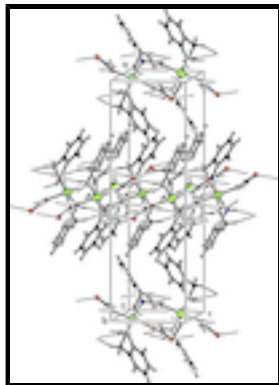


Fig. 2. Crystal packing diagram for the title compound. Dashed lines denote hydrogen bonds.

Bis[(2-aminophenyl)methanol- κ^2 N,O]bis(nitrato- κ O)zinc(II)

Crystal data

[Zn(NO₃)₂(C₇H₉NO)₂]

$M_r = 435.71$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 23.386$ (5) Å

$b = 10.193$ (2) Å

$c = 7.3442$ (15) Å

$V = 1750.7$ (6) Å³

$Z = 4$

$F(000) = 896$

$D_x = 1.653$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1421 reflections

$\theta = 2.2$ – 32.0°

$\mu = 1.46$ mm⁻¹

$T = 298$ K

Needle, colorless

$0.35 \times 0.03 \times 0.02$ mm

Data collection

Bruker APEX CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.857$, $T_{\max} = 0.980$

14935 measured reflections

3005 independent reflections

2063 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.140$

$\theta_{\max} = 32.0^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -34 \rightarrow 34$

$k = -15 \rightarrow 13$

$l = -9 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.088$

$wR(F^2) = 0.154$

$S = 1.26$

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 3.223P]$

3005 reflections

135 parameters

0 restraints

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.004$$

$$\Delta\rho_{\max} = 0.67 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.76 \text{ e } \text{\AA}^{-3}$$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3876 (2)	0.4320 (4)	0.3878 (6)	0.0324 (9)
H1A	0.3663	0.5136	0.3834	0.039*
H1B	0.3910	0.4056	0.5142	0.039*
C2	0.35648 (17)	0.3286 (4)	0.2831 (5)	0.0270 (8)
C3	0.3046 (2)	0.3574 (5)	0.1974 (7)	0.0408 (11)
H3	0.2892	0.4413	0.2074	0.049*
C4	0.2756 (2)	0.2623 (7)	0.0976 (8)	0.0519 (15)
H4	0.2411	0.2826	0.0417	0.062*
C5	0.2980 (2)	0.1394 (7)	0.0818 (8)	0.0499 (14)
H5	0.2790	0.0768	0.0124	0.060*
C6	0.3488 (2)	0.1067 (5)	0.1679 (6)	0.0381 (10)
H6	0.3633	0.0220	0.1589	0.046*
C7	0.37800 (17)	0.2015 (4)	0.2681 (5)	0.0279 (7)
N1	0.43276 (16)	0.1728 (4)	0.3456 (5)	0.0262 (7)
H1C	0.439 (2)	0.097 (6)	0.339 (8)	0.040 (15)*
H1D	0.433 (3)	0.192 (7)	0.460 (9)	0.06 (2)*
N2	0.44748 (15)	0.2148 (4)	-0.1135 (4)	0.0286 (7)
O1	0.44352 (14)	0.4515 (3)	0.3116 (5)	0.0305 (7)
H1E	0.457 (3)	0.510 (7)	0.344 (9)	0.054 (19)*
O2	0.46612 (15)	0.3154 (3)	-0.0261 (4)	0.0316 (7)
O3	0.46254 (17)	0.1044 (3)	-0.0629 (5)	0.0427 (8)
O4	0.41587 (17)	0.2329 (4)	-0.2447 (5)	0.0484 (9)
Zn1	0.5000	0.29214 (6)	0.2500	0.02484 (16)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.038 (2)	0.030 (2)	0.029 (2)	0.0063 (18)	0.0021 (18)	-0.0027 (16)
C2	0.0273 (17)	0.0312 (19)	0.022 (2)	-0.0029 (15)	0.0007 (13)	0.0042 (13)
C3	0.031 (2)	0.047 (3)	0.045 (3)	0.003 (2)	0.0000 (18)	0.009 (2)
C4	0.030 (2)	0.074 (4)	0.052 (3)	-0.005 (2)	-0.012 (2)	0.006 (3)
C5	0.039 (3)	0.065 (4)	0.046 (3)	-0.021 (3)	-0.007 (2)	-0.005 (3)
C6	0.044 (3)	0.037 (2)	0.033 (2)	-0.010 (2)	-0.004 (2)	-0.001 (2)
C7	0.0324 (16)	0.0315 (17)	0.0199 (17)	-0.0051 (16)	-0.0010 (15)	0.0002 (17)
N1	0.0344 (18)	0.0186 (15)	0.0257 (17)	-0.0002 (14)	-0.0053 (14)	0.0003 (12)
N2	0.0364 (17)	0.0277 (16)	0.0218 (14)	-0.0003 (16)	-0.0019 (13)	-0.0022 (14)
O1	0.0335 (15)	0.0188 (13)	0.0391 (16)	-0.0032 (12)	-0.0028 (13)	-0.0081 (12)
O2	0.0494 (18)	0.0201 (14)	0.0253 (14)	-0.0007 (13)	-0.0107 (13)	0.0000 (11)
O3	0.061 (2)	0.0234 (15)	0.0440 (19)	0.0019 (15)	-0.0116 (17)	-0.0025 (14)
O4	0.062 (2)	0.053 (2)	0.0302 (15)	-0.0018 (17)	-0.0188 (18)	-0.0012 (19)

supplementary materials

Zn1 0.0289 (3) 0.0202 (2) 0.0254 (3) 0.000 -0.0063 (3) 0.000

Geometric parameters (Å, °)

C1—O1	1.436 (6)	C6—C7	1.394 (6)
C1—C2	1.494 (6)	C6—H6	0.9300
C1—H1A	0.9700	C7—N1	1.432 (5)
C1—H1B	0.9700	N1—H1C	0.79 (6)
C2—C7	1.394 (6)	N1—H1D	0.86 (7)
C2—C3	1.399 (6)	N2—O4	1.228 (5)
C3—C4	1.391 (8)	N2—O3	1.236 (5)
C3—H3	0.9300	N2—O2	1.286 (5)
C4—C5	1.363 (9)	Zn1—O1	2.142 (3)
C4—H4	0.9300	O1—H1E	0.72 (7)
C5—C6	1.386 (7)	Zn1—O2	2.190 (3)
C5—H5	0.9300	Zn1—N1	2.108 (4)
O1—C1—C2	109.9 (3)	Zn1—N1—H1C	114 (4)
O1—C1—H1A	109.7	C7—N1—H1D	111 (4)
C2—C1—H1A	109.7	Zn1—N1—H1D	100 (4)
O1—C1—H1B	109.7	H1C—N1—H1D	106 (6)
C2—C1—H1B	109.7	O4—N2—O3	123.0 (4)
H1A—C1—H1B	108.2	O4—N2—O2	118.4 (4)
C7—C2—C3	118.2 (4)	O3—N2—O2	118.6 (3)
C7—C2—C1	121.3 (4)	C1—O1—Zn1	122.6 (3)
C3—C2—C1	120.4 (4)	C1—O1—H1E	113 (5)
C4—C3—C2	120.8 (5)	Zn1—O1—H1E	115 (5)
C4—C3—H3	119.6	N2—O2—Zn1	119.9 (2)
C2—C3—H3	119.6	N1—Zn1—N1 ⁱ	109.5 (2)
C5—C4—C3	120.0 (5)	N1—Zn1—O1	84.67 (14)
C5—C4—H4	120.0	N1 ⁱ —Zn1—O1	165.41 (13)
C3—C4—H4	120.0	N1—Zn1—O1 ⁱ	165.41 (13)
C4—C5—C6	120.7 (5)	N1 ⁱ —Zn1—O1 ⁱ	84.67 (14)
C4—C5—H5	119.6	O1—Zn1—O1 ⁱ	81.37 (18)
C6—C5—H5	119.6	N1—Zn1—O2 ⁱ	91.37 (13)
C5—C6—C7	119.6 (5)	N1 ⁱ —Zn1—O2 ⁱ	95.81 (13)
C5—C6—H6	120.2	O1—Zn1—O2 ⁱ	86.87 (12)
C7—C6—H6	120.2	O1 ⁱ —Zn1—O2 ⁱ	83.69 (12)
C6—C7—C2	120.6 (4)	N1—Zn1—O2	95.81 (13)
C6—C7—N1	120.4 (4)	N1 ⁱ —Zn1—O2	91.37 (13)
C2—C7—N1	118.8 (4)	O1—Zn1—O2	83.69 (12)
C7—N1—Zn1	114.6 (3)	O1 ⁱ —Zn1—O2	86.88 (12)
C7—N1—H1C	110 (4)	O2 ⁱ —Zn1—O2	167.55 (15)
O1—C1—C2—C7	59.5 (5)	O3—N2—O2—Zn1	-19.1 (5)
O1—C1—C2—C3	-120.7 (4)	C7—N1—Zn1—N1 ⁱ	-126.8 (3)
C7—C2—C3—C4	-1.0 (7)	C7—N1—Zn1—O1	49.8 (3)
C1—C2—C3—C4	179.1 (5)	C7—N1—Zn1—O1 ⁱ	66.7 (6)

C2—C3—C4—C5	-0.3 (8)	C7—N1—Zn1—O2 ⁱ	136.5 (3)
C3—C4—C5—C6	1.6 (9)	C7—N1—Zn1—O2	-33.3 (3)
C4—C5—C6—C7	-1.6 (8)	C1—O1—Zn1—N1	0.8 (3)
C5—C6—C7—C2	0.3 (7)	C1—O1—Zn1—N1 ⁱ	168.0 (5)
C5—C6—C7—N1	-174.9 (4)	C1—O1—Zn1—O1 ⁱ	-175.0 (4)
C3—C2—C7—C6	1.0 (6)	C1—O1—Zn1—O2 ⁱ	-90.9 (3)
C1—C2—C7—C6	-179.2 (4)	C1—O1—Zn1—O2	97.3 (3)
C3—C2—C7—N1	176.2 (4)	N2—O2—Zn1—N1	-46.2 (3)
C1—C2—C7—N1	-3.9 (6)	N2—O2—Zn1—N1 ⁱ	63.6 (3)
C6—C7—N1—Zn1	118.9 (4)	N2—O2—Zn1—O1	-130.2 (3)
C2—C7—N1—Zn1	-56.4 (4)	N2—O2—Zn1—O1 ⁱ	148.2 (3)
C2—C1—O1—Zn1	-48.3 (4)	N2—O2—Zn1—O2 ⁱ	-171.1 (3)
O4—N2—O2—Zn1	161.5 (3)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1C \cdots O3 ⁱⁱ	0.79 (6)	2.24 (6)	2.987 (5)	157 (6)
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O1—H1E \cdots O2 ^{iv}	0.72 (7)	2.03 (7)	2.710 (4)	159 (7)
C1—H1B \cdots O4 ⁱⁱⁱ	0.97	2.56	3.441 (6)	150

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Fig. 1

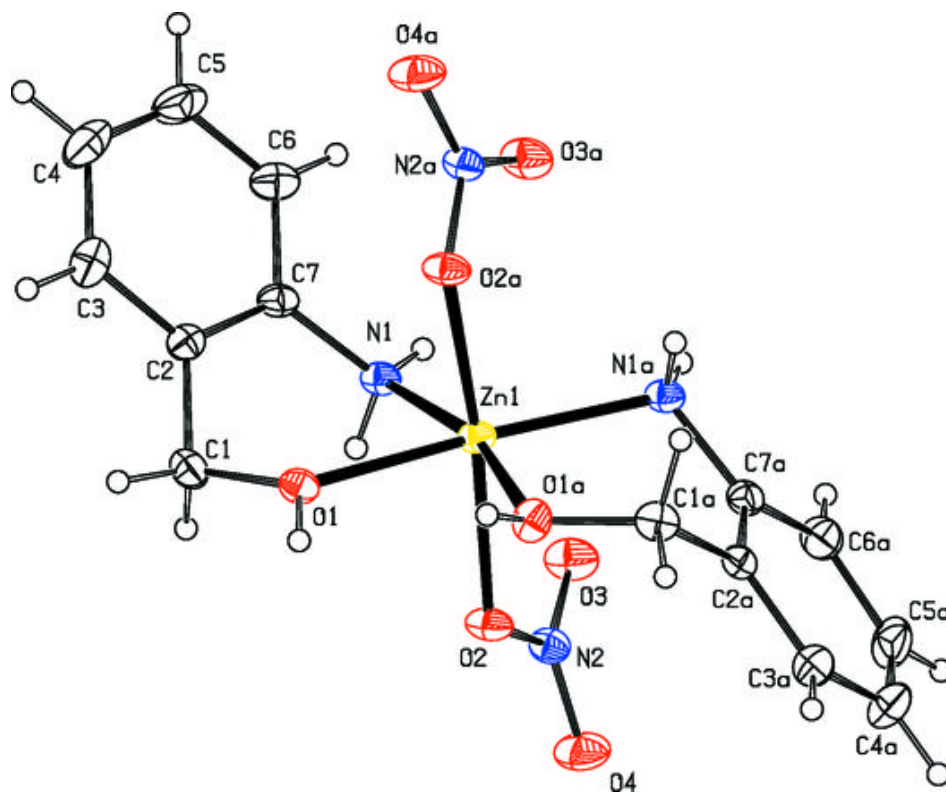


Fig. 2

