Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[*N*,*N*-bis(2-hydroxyethyl)glycinato]-cobalt(II)

Jiong-Peng Zhao and Fu-Chen Liu*

School of Chemistry and Chemical Engineering, Tianjin University of Technology, Tianjin 300191, People's Republic of China
Correspondence e-mail: fuchenliutj@yahoo.com

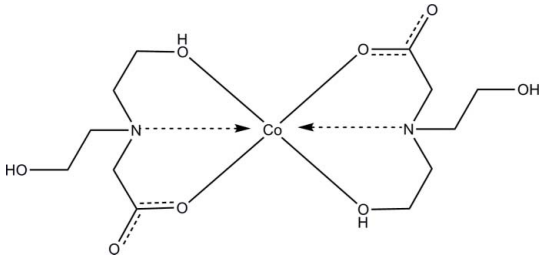
Received 19 May 2010; accepted 19 June 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.057; wR factor = 0.159; data-to-parameter ratio = 17.2.

The asymmetric unit of the title compound, $[Co(C_6H_{12}NO_4)_2]$, contains one half-molecule with the Co^{II} ion situated on an inversion center. Intermolecular O—H···O hydrogen bonds generate a three-dimensional hydrogen-bonding network, which consolidates the crystal packing.

Related literature

For related structures, see: Ammar *et al.* (2001); Chuklanova *et al.* (1981); Thakuria & Das (2007).



Experimental

Crystal data

$[Co(C_6H_{12}NO_4)_2]$
M_r = 383.26
Monoclinic, $P2_1/c$
a = 9.932 (2) Å
b = 11.388 (2) Å
c = 7.4477 (15) Å
β = 110.12 (3)°
V = 791.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 293 K
0.20 × 0.18 × 0.18 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.736, T_{max} = 1.000
8129 measured reflections
1819 independent reflections
1357 reflections with $I > 2\sigma(I)$
R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.159
S = 1.00
1819 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H12···O3^{i}	0.85	1.79	2.632 (4)	171
O1—H11···O3^{ii}	0.85	1.89	2.744 (4)	178

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

Data collection: *SCXmini Benchtop Crystallography System Software* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

The authors acknowledge financial support from Tianjin Municipal Education Commission (grant No. 20060503).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2723).

References

Ammar, M. K., Amor, F. B., Driss, A. & Jouini, T. (2001). *Z. Kristallogr. New Cryst. Struct.* **216**, 631–633.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Chuklanova, E. B., Polynova, T. N., Porai-Koshits, M. A. & Babeshkina, G. K. (1981). *Koord. Khim.* **7**, 944–951.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Americas Corporation, The Woodlands, Texas, USA.
Rigaku (2006). *SCXmini Benchtop Crystallography System Software*. Rigaku Americas Corporation, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Thakuria, H. & Das, G. (2007). *Polyhedron*, **26**, 149–153.

supplementary materials

Acta Cryst. (2010). E**66**, m848 [**doi:10.1107/S1600536810023810**]

Bis[*N*,*N*-bis(2-hydroxyethyl)glycinato]cobalt(II)

J.-P. Zhao and F.-C. Liu

Comment

As a contribution to a structural study of ML_2 complexes, where *L* = N,N-bis(2-hydroxyethyl)glycinato ligand, and M = Cu (Ammar *et al.*, 2001; Thakuria & Das, 2007) and Ni (Chuklanova *et al.*, 1981), herewith we report the crystal structure of the title compound CoL_2 (I).

In (I) (Fig. 1), the Co(II) ions are located on the inversion centers and are coordinated by two *L* ligands forming an octahedral enviromental geometry with four oxygen and two nitrogen atoms. The bond lengths are: Co1—N1 = 2.172 (3) Å, Co1—O2 = 2.088 (3) Å and Co1—O4 = 2.046 (2) Å. Though ML_2 complexes (M = Co, Ni, Cu) have similar structures, there are some differences. The Co and Ni centers are in a regular octahedron coordinated geometry, while the Cu center has an elongated octahedral coordination with two hydroxy atoms in axial positions.

Intermolecular O—H···O hydrogen bonds (Table 1) generate three-dimensional hydrogen-bonding network, which consolidate the crystal packing (Fig. 2).

Experimental

A mixture of Co(II) nitrate (1.0mmol), Dy(III)nitrate (0.5mmol) and N,N-bis(2-hydroxyethyl)glycine, (1 mmol), in 10 ml solvent wITH DMF:MeOH = 1:1 was sealed in a Teflon-lined stainless-steel Parr bomb that was heated at 413 K for 48 h. Red crystals of the title complex were collected after the bomb was allowed to cool to room temperature.Yield 20% based on metal salt.

Refinement

C-bound H atoms were included in calculated positions and treated as riding on their parent atoms, with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C). Hydroxy H atoms were located on difference Fourier maps, but placed in idealized positions (O—H = 0.85Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(O).

Figures

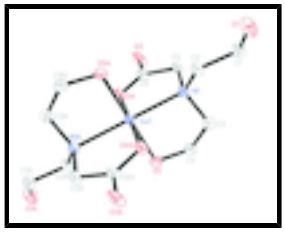


Fig. 1. The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level. H atom have been omitted for clarity. Symmetry code: (A) -x+1, -y-1, -z+1.

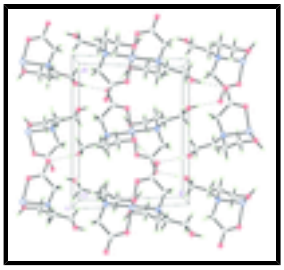


Fig. 2. A portion of the crystal packing viewed down the *c* axis. Dashed lines denote O—H···O hydrogen bonds.

Bis[*N*,*N*-bis(2-hydroxyethyl)glycinato]cobalt(II)

Crystal data

$[Co(C_6H_{12}NO_4)_2]$	$F(000) = 402$
$M_r = 383.26$	$D_x = 1.609$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.932$ (2) Å	Cell parameters from 7077 reflections
$b = 11.388$ (2) Å	$\theta = 3.4$–$27.6°$
$c = 7.4477$ (15) Å	$\mu = 1.13$ mm^{-1}
$\beta = 110.12$ (3)°	$T = 293$ K
$V = 791.0$ (3) Å^3	Block, red
$Z = 2$	0.2 × 0.18 × 0.18 mm

Data collection

Rigaku SCXmini diffractometer	1819 independent reflections
Radiation source: fine-focus sealed tube	1357 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.072$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -12 \rightarrow 12$
$T_{min} = 0.736$, $T_{max} = 1.000$	$k = -14 \rightarrow 14$
8129 measured reflections	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.057$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.159$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
1819 reflections	$(\Delta/\sigma)_{max} < 0.001$
106 parameters	$\Delta\rho_{max} = 0.48$ e Å^{-3}

0 restraints $\Delta\rho_{min} = -0.36$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.0244 (3)
O1	0.0043 (3)	0.3365 (3)	0.0259 (4)	0.0552 (9)
H11	−0.0846	0.3211	−0.0073	0.066*
O2	0.5173 (3)	0.4447 (3)	0.7743 (4)	0.0347 (7)
H12	0.5746	0.3883	0.8218	0.042*
O3	0.2823 (3)	0.7874 (2)	0.5700 (4)	0.0449 (8)
O4	0.4555 (3)	0.6656 (2)	0.5703 (4)	0.0333 (6)
N1	0.2727 (3)	0.4762 (2)	0.4479 (5)	0.0270 (7)
C1	0.0483 (4)	0.3862 (4)	0.2103 (6)	0.0431 (10)
H1A	0.0377	0.3299	0.3022	0.052*
H1B	−0.0090	0.4550	0.2118	0.052*
C2	0.2040 (4)	0.4198 (3)	0.2589 (5)	0.0329 (9)
H2A	0.2579	0.3496	0.2538	0.040*
H2B	0.2115	0.4730	0.1610	0.040*
C3	0.2708 (4)	0.3967 (4)	0.6042 (6)	0.0363 (9)
H3A	0.2918	0.3173	0.5750	0.044*
H3B	0.1758	0.3970	0.6137	0.044*
C4	0.3792 (4)	0.4339 (4)	0.7929 (6)	0.0401 (10)
H4A	0.3510	0.5086	0.8317	0.048*
H4B	0.3830	0.3762	0.8902	0.048*
C5	0.2141 (4)	0.5937 (3)	0.4614 (6)	0.0309 (8)
H5A	0.1554	0.5882	0.5416	0.037*
H5B	0.1521	0.6172	0.3347	0.037*
C6	0.3256 (4)	0.6887 (3)	0.5411 (5)	0.0310 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0203 (4)	0.0227 (4)	0.0279 (4)	0.0026 (3)	0.0055 (3)	−0.0003 (3)
O1	0.0397 (18)	0.066 (2)	0.053 (2)	−0.0136 (15)	0.0076 (15)	−0.0177 (16)
O2	0.0302 (14)	0.0401 (16)	0.0306 (15)	0.0078 (13)	0.0065 (11)	0.0075 (12)

O3	0.0249 (15)	0.0323 (15)	0.068 (2)	0.0053 (12)	0.0029 (14)	−0.0206 (14)
O4	0.0227 (13)	0.0269 (13)	0.0468 (17)	0.0006 (11)	0.0076 (12)	−0.0064 (11)
N1	0.0241 (16)	0.0217 (15)	0.0329 (17)	−0.0002 (12)	0.0067 (13)	−0.0023 (11)
C1	0.037 (2)	0.047 (2)	0.039 (2)	−0.013 (2)	0.0060 (18)	−0.0058 (19)
C2	0.0244 (19)	0.037 (2)	0.036 (2)	−0.0001 (16)	0.0081 (16)	−0.0030 (17)
C3	0.034 (2)	0.035 (2)	0.041 (2)	−0.0042 (18)	0.0142 (18)	0.0034 (17)
C4	0.034 (2)	0.050 (3)	0.036 (2)	0.003 (2)	0.0119 (18)	0.0074 (19)
C5	0.0216 (18)	0.034 (2)	0.035 (2)	0.0020 (16)	0.0072 (15)	−0.0028 (16)
C6	0.0258 (19)	0.032 (2)	0.031 (2)	0.0047 (16)	0.0048 (15)	−0.0049 (15)

Geometric parameters (Å, °)

Co1—O4	2.046 (2)	N1—C2	1.483 (5)
Co1—O4^{i}	2.046 (2)	C1—C2	1.512 (5)
Co1—O2	2.088 (3)	C1—H1A	0.9700
Co1—O2^{i}	2.088 (3)	C1—H1B	0.9700
Co1—N1^{i}	2.172 (3)	C2—H2A	0.9700
Co1—N1	2.172 (3)	C2—H2B	0.9700
O1—C1	1.409 (5)	C3—C4	1.507 (5)
O1—H11	0.8499	C3—H3A	0.9700
O2—C4	1.430 (5)	C3—H3B	0.9700
O2—H12	0.8500	C4—H4A	0.9700
O3—C6	1.249 (4)	C4—H4B	0.9700
O4—C6	1.260 (4)	C5—C6	1.515 (5)
N1—C5	1.476 (4)	C5—H5A	0.9700
N1—C3	1.480 (5)	C5—H5B	0.9700
O4—Co1—O4^{i}	180.0	C2—C1—H1B	110.4
O4—Co1—O2	88.86 (11)	H1A—C1—H1B	108.6
O4^{i}—Co1—O2	91.14 (11)	N1—C2—C1	115.8 (3)
O4—Co1—O2^{i}	91.14 (11)	N1—C2—H2A	108.3
O4^{i}—Co1—O2^{i}	88.86 (11)	C1—C2—H2A	108.3
O2—Co1—O2^{i}	180.0	N1—C2—H2B	108.3
O4—Co1—N1^{i}	98.17 (10)	C1—C2—H2B	108.3
O4^{i}—Co1—N1^{i}	81.83 (10)	H2A—C2—H2B	107.4
O2—Co1—N1^{i}	97.61 (11)	N1—C3—C4	111.3 (3)
O2^{i}—Co1—N1^{i}	82.39 (11)	N1—C3—H3A	109.4
O4—Co1—N1	81.83 (10)	C4—C3—H3A	109.4
O4^{i}—Co1—N1	98.17 (10)	N1—C3—H3B	109.4
O2—Co1—N1	82.39 (11)	C4—C3—H3B	109.4
O2^{i}—Co1—N1	97.61 (11)	H3A—C3—H3B	108.0
N1^{i}—Co1—N1	180.0	O2—C4—C3	109.6 (3)
C1—O1—H11	108.0	O2—C4—H4A	109.8
C4—O2—Co1	111.2 (2)	C3—C4—H4A	109.8
C4—O2—H12	115.0	O2—C4—H4B	109.8
Co1—O2—H12	116.9	C3—C4—H4B	109.8
C6—O4—Co1	116.5 (2)	H4A—C4—H4B	108.2

C5—N1—C3	112.9 (3)	N1—C5—C6	114.9 (3)
C5—N1—C2	113.2 (3)	N1—C5—H5A	108.5
C3—N1—C2	110.9 (3)	C6—C5—H5A	108.5
C5—N1—Co1	106.5 (2)	N1—C5—H5B	108.5
C3—N1—Co1	103.3 (2)	C6—C5—H5B	108.5
C2—N1—Co1	109.5 (2)	H5A—C5—H5B	107.5
O1—C1—C2	106.5 (3)	O3—C6—O4	123.4 (3)
O1—C1—H1A	110.4	O3—C6—C5	117.5 (3)
C2—C1—H1A	110.4	O4—C6—C5	119.1 (3)
O1—C1—H1B	110.4		
O4—Co1—O2—C4	75.2 (3)	$O4^{i}$—Co1—N1—C2	−48.4 (2)
$O4^{i}$—Co1—O2—C4	−104.8 (3)	O2—Co1—N1—C2	−138.4 (2)
$O2^{i}$—Co1—O2—C4	−9(84)	$O2^{i}$—Co1—N1—C2	41.6 (2)
$N1^{i}$—Co1—O2—C4	173.3 (3)	$N1^{i}$—Co1—N1—C2	35 (100)
N1—Co1—O2—C4	−6.7 (3)	C5—N1—C2—C1	−67.2 (4)
$O4^{i}$—Co1—O4—C6	37 (100)	C3—N1—C2—C1	60.8 (4)
O2—Co1—O4—C6	−88.4 (3)	Co1—N1—C2—C1	174.1 (3)
$O2^{i}$—Co1—O4—C6	91.6 (3)	O1—C1—C2—N1	179.1 (3)
$N1^{i}$—Co1—O4—C6	174.1 (3)	C5—N1—C3—C4	−70.5 (4)
N1—Co1—O4—C6	−5.9 (3)	C2—N1—C3—C4	161.4 (3)
O4—Co1—N1—C5	8.9 (2)	Co1—N1—C3—C4	44.2 (3)
$O4^{i}$—Co1—N1—C5	−171.1 (2)	Co1—O2—C4—C3	32.5 (4)
O2—Co1—N1—C5	98.9 (2)	N1—C3—C4—O2	−53.5 (4)
$O2^{i}$—Co1—N1—C5	−81.1 (2)	C3—N1—C5—C6	101.7 (4)
$N1^{i}$—Co1—N1—C5	−88 (100)	C2—N1—C5—C6	−131.4 (3)
O4—Co1—N1—C3	−110.2 (2)	Co1—N1—C5—C6	−11.0 (4)
$O4^{i}$—Co1—N1—C3	69.8 (2)	Co1—O4—C6—O3	−177.0 (3)
O2—Co1—N1—C3	−20.3 (2)	Co1—O4—C6—C5	1.1 (5)
$O2^{i}$—Co1—N1—C3	159.7 (2)	N1—C5—C6—O3	−174.3 (3)
$N1^{i}$—Co1—N1—C3	153 (100)	N1—C5—C6—O4	7.4 (5)
O4—Co1—N1—C2	131.6 (2)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H12···$O3^{ii}$	0.85	1.79	2.632 (4)	171
O1—H11···$O3^{iii}$	0.85	1.89	2.744 (4)	178

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

Fig. 1

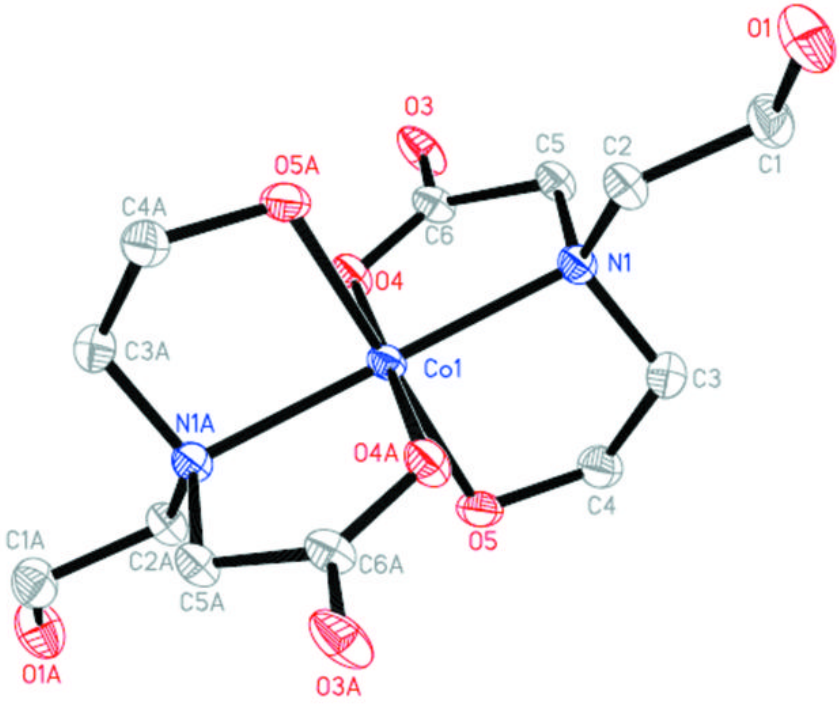

O1
O3
C5
C2
C1
O5A
C4A
C6
O4
N1
C3A
Co1
C3
N1A
O4A
C4
O5
C1A
C2A
C6A
C5A
O1A
O3A

Fig. 2