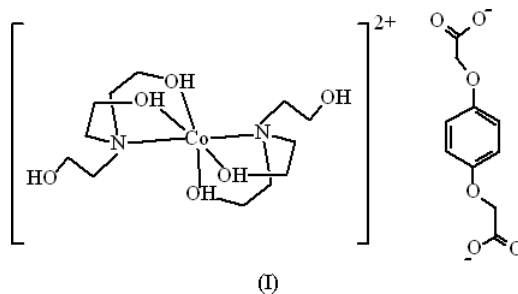


Shan Gao,<sup>a\*</sup> Ji-Wei Liu,<sup>a</sup> Li-Hua  
Huo<sup>a</sup> and Seik Weng Ng<sup>b</sup><sup>a</sup>College of Chemistry and Chemical  
Technology, Heilongjiang University, Harbin  
150080, People's Republic of China, and<sup>b</sup>Department of Chemistry, University of  
Malaya, Kuala Lumpur 50603, MalaysiaCorrespondence e-mail:  
shangao67@yahoo.com

## Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
Disorder in main residue  
R factor = 0.056  
wR factor = 0.165  
Data-to-parameter ratio = 16.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(triethanolamine)cobalt(II)  
benzene-1,4-dioxydiacetateThe title complex,  $[\text{Co}(\text{C}_6\text{H}_{15}\text{NO}_3)_2](\text{C}_{10}\text{H}_8\text{O}_6)$ , comprises a  $\text{Co}^{\text{II}}$  cation, coordinated centrosymmetrically in an octahedral  $\text{N}_2\text{O}_4$  mode by two tridentate triethanolamine ligands, and a centrosymmetric benzene-1,4-dioxyacetate dianion. The ions are linked by hydrogen bonds into a supramolecular network.

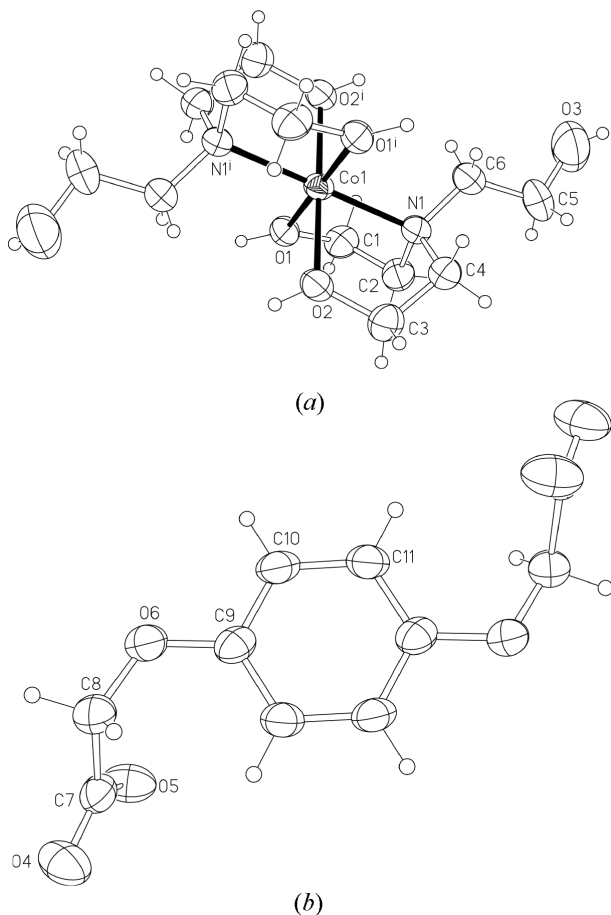
## Comment

Among transition metal complexes containing triethanolamine and organic acid ligands, triethanolamine functions either as a tridentate ligand, *e.g.* in Cu and Ni salts (Krabbes *et al.*, 1999, 2000), or as a tetradentate ligand, *e.g.* in an Mn salt (Andruh *et al.*, 1993). Recently, we reported the structure of the complex  $[\text{Cu}(\text{triethanolamine})(\text{imidazole})(\text{H}_2\text{O})](\text{ClO}_4)(\text{C}_{10}\text{H}_8\text{O}_6)_{0.5}$ , which incorporates benzene-1,4-dioxyacetate as a counterion (Gao *et al.*, 2004). Here, our study is extended to the title  $\text{Co}^{\text{II}}$  complex,  $[\text{Co}(\text{C}_6\text{H}_{15}\text{NO}_3)_2](\text{C}_{10}\text{H}_8\text{O}_6)$ , (I), obtained from the assembly reaction of cobalt diacetate trihydrate, benzene-1,4-dioxyacetic acid and triethanolamine.As shown in Figs. 1 and 2, the crystal structure of (I) reveals that the asymmetric unit comprises half of a mononuclear  $\text{Co}^{\text{II}}$  complex cation,  $[\text{Co}(\text{C}_6\text{H}_{15}\text{NO}_3)_2]^{2+}$ , and half of a benzene-1,4-dioxyacetate dianion. Both the cation and anion lie on inversion sites.The triethanolamine ligand is bonded in a tridentate chelating mode. This contrasts with the situation in the related  $\text{Cu}^{\text{II}}$  complex (Gao *et al.*, 2004), where the triethanolamine is coordinated in a tetradentate fashion. The  $\text{Co}^{\text{II}}$  cation is coordinated by four hydroxyl O atoms and two N atoms, so as to define a distorted octahedral configuration (Table 1). In the anion of (I), the acetate groups and the benzene ring are not coplanar, as seen in the  $\text{C}9-\text{O}6-\text{C}8-\text{C}7$  torsion angle of  $98.8(4)^\circ$ .The uncoordinated hydroxy O atom forms an intermolecular hydrogen bond with a carboxyl O atom, resulting in the formation of a one-dimensional chain, with an  $\text{O}\cdots\text{O}$  distance of  $2.743(5) \text{ \AA}$  and an  $\text{O}-\text{H}\cdots\text{O}$  angle of  $148^\circ$ . Another description of the crystal structure of (I) is that in

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**Figure 1**

Displacement ellipsoid plots, at the 30% probability level, for (a) the [Co(C<sub>6</sub>H<sub>15</sub>NO<sub>3</sub>)<sub>2</sub>]<sup>2+</sup> cation in (I) and (b) the [C<sub>10</sub>H<sub>8</sub>O<sub>6</sub>]<sup>2-</sup> anion in (I). [Symmetry code: (i) 1 - x, 1 - y, 1 - z].

which layers of anions alternate with layers of cations, the layers being linked *via* hydrogen bonds to give rise to a supramolecular network (Table 2, Fig. 2).

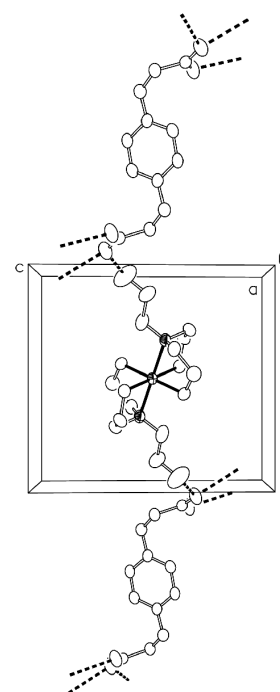
## Experimental

Benzene-1,4-dioxyacetic acid was prepared by the method described for the synthesis of benzene-1,2-dioxyacetic acid (Mirci, 1990). Cobalt diacetate trihydrate (4.76 g, 20 mmol) and benzene-1,4-dioxyacetic acid (9.04 g, 40 mmol) were dissolved in water and the pH was adjusted to 7 with triethanolamine. Pink crystals of (I) separated from the filtered solution at room temperature over several days. CHN analysis: calculated for C<sub>22</sub>H<sub>38</sub>N<sub>2</sub>O<sub>12</sub>Co: C 45.44, H 6.59, N 4.82%; found: C 45.70, H 6.66, N 4.69%.

### Crystal data

[Co(C<sub>6</sub>H<sub>15</sub>NO<sub>3</sub>)<sub>2</sub>](C<sub>10</sub>H<sub>8</sub>O<sub>6</sub>)  
*M<sub>r</sub>* = 581.47  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 11.116 (2) Å  
*b* = 10.480 (2) Å  
*c* = 11.369 (2) Å  
 $\beta$  = 94.88 (3)°  
*V* = 1319.7 (4) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 1.463 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 5364 reflections  
 $\theta$  = 3.1–27.4°  
 $\mu$  = 0.72 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, pink  
 0.38 × 0.27 × 0.18 mm


**Figure 2**

The packing of (I).

### Data collection

Rigaku R-AXIS RAPID diffractometer

$\omega$  scans

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

*T*<sub>min</sub> = 0.773, *T*<sub>max</sub> = 0.882

5772 measured reflections

3013 independent reflections

1996 reflections with *I* > 2σ(*I*)

*R*<sub>int</sub> = 0.026

$\theta$ <sub>max</sub> = 27.5°

*h* = -14 → 14

*k* = -13 → 13

*l* = -14 → 14

### Refinement

Refinement on *F*<sup>2</sup>

$R[F^2 > 2\sigma(F^2)] = 0.056$

*wR*(*F*<sup>2</sup>) = 0.165

*S* = 0.98

3013 reflections

182 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1059P)^2]$

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

( $\Delta/\sigma$ )<sub>max</sub> = 0.001

$\Delta\rho$ <sub>max</sub> = 1.05 e Å<sup>-3</sup>

$\Delta\rho$ <sub>min</sub> = -0.48 e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Co1—O1	2.068 (2)	Co1—N1	2.172 (3)
Co1—O2	2.103 (2)		
O1—Co1—O2	92.87 (9)	O2—Co1—N1	80.8 (1)
O1—Co1—N1	82.3 (1)		

**Table 2**

Hydrogen-bonding 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>
O1—H1...O4 <sup>ii</sup>	0.93	1.93	2.564 (4)	123
O2—H2...O5 <sup>ii</sup>	0.93	2.17	2.597 (3)	107
O3—H3...O4	0.82	2.01	2.743 (5)	148

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

Two of the aminoethyl groups of the triethanolamine molecule are disordered over two sites, with assumed equal occupancy. Within each group, the pairs of C—O, N—C and C—C distances were restrained to be approximately equal. Additionally, the displacement parameters of the unprimed and primed atoms were set to be equal to each other. The distance restraints gave a model in which these distances are sensible. However, the model has an intramolecular H2'1...H6B contact of 1.65 Å. Attempts at using other distance restraints led to a wider spread of bond distances. H atoms bound to C and O atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (aliphatic) and O—H = 0.82 Å (hydroxyl group), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{O})$ , using a riding model approximation.

Data collection: *RAPID AUTO* (Rigaku, 1998); cell refinement: *RAPID AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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