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#### Key indicators

Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.029  
 $wR$  factor = 0.084  
Data-to-parameter ratio = 19.2

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

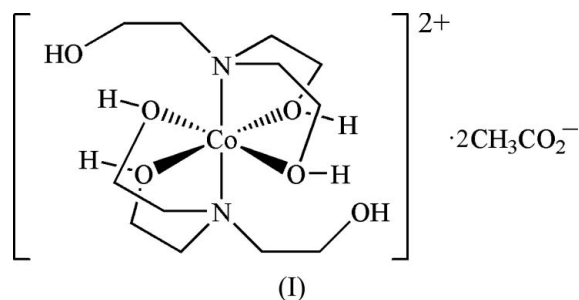
## Bis(2,2',2''-nitrilotriethanol)cobalt(II) bis(acetate)

The title compound,  $[\text{Co}(\text{C}_6\text{H}_{15}\text{NO}_3)_2](\text{CH}_3\text{CO}_2)_2$ , contains two triethanolamine ligands bound to a  $\text{Co}^{2+}$  metal centre, which lies on a crystallographic inversion site such that the asymmetric unit contains half of the cation and one acetate anion. The triethanolamine ligands coordinate *via* each axial N and two of the three O atoms, while the third arm of the ligand is pendant with the hydroxyl group pointing away from the metal centre. The acetate anions are hydrogen bonded to the coordinated hydroxyl groups and also to the free arm, forming a two-dimensional sheet-like motif.

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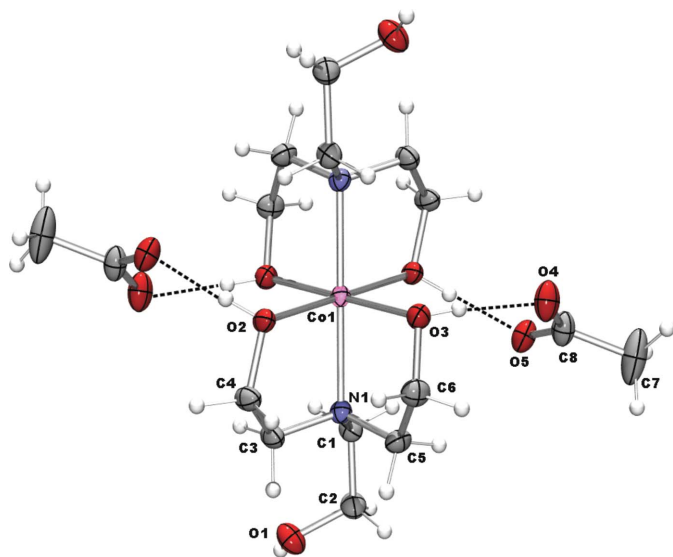
#### Comment

The synthesis of mesoporous siliceous materials involves the hydrolysis of an organosilicon source in the presence of a structure-directing template. In the synthesis of mesoporous silica, denoted TUD-1 (Jansen *et al.*, 2001), the structure-directing template is triethanolamine. Within our group there has been much effort dedicated to the incorporation of metals into the silica framework of such materials (Shan *et al.*, 2001; Hamdy *et al.*, 2005). One approach that has been targeted is the complexation of the metal precursors with the structure-directing template prior to hydrolysis of the silicon source (Hamdy *et al.*, 2006).



The title compound, (I), was isolated upon heating a solution of triethanolamine, cobalt(II) acetate tetrahydrate and 2-propanol at 353 K. Removal of the solvent resulted in an orange oil, which deposited crystals of (I) upon standing. There have been numerous reports of triethanolamine as either a tridentate ligand (for Cu, Ni and Co) (Krabbes *et al.*, 1999, 2000; Gao *et al.*, 2004) or a tetradentate ligand for Mn (Andruh *et al.*, 1993). The previously reported cobalt complex possesses an identical ligand arrangement as observed in this example with a single benzene-1,4-dioxyacetate dianion counter-ion (Gao *et al.*, 2004).

The complex cation of (I) has a distorted octahedral geometry in which the coordinated atoms of one ligand are


**Figure 1**

The structure of (I), with displacement ellipsoids drawn at the 50% probability level. Hydrogen bonds are indicated by dashed lines. [Symmetry operation used to generate equivalent atoms:  $-x, -y, -z$ .]

*trans* to the corresponding atoms of the other ligand (Fig. 1 and Table 1).

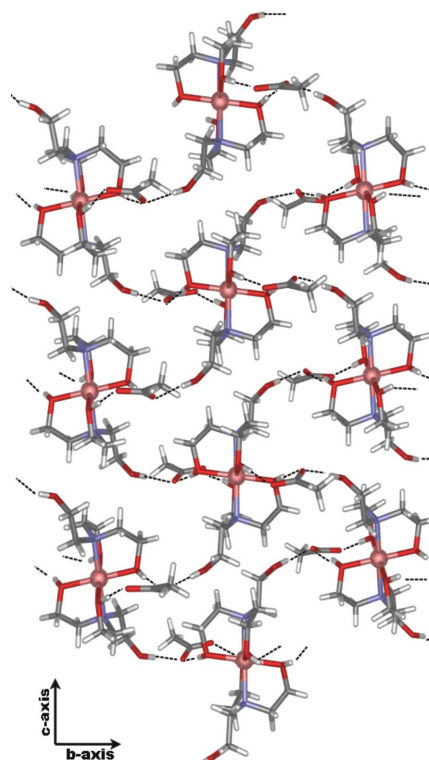
The third arm of the triethanolamine ligand is oriented away from the cobalt. The acetate anions are positioned in the voids created by the uncoordinated arm of the triethanolamine. One of the acetate O atoms is strongly hydrogen bonded to the hydroxyl group [ $H \cdots O = 1.77(2) \text{ \AA}$ ] of the coordinated arms of the triethanolamine of one dication as well as to that [ $1.89(2) \text{ \AA}$ ] of the pendant arm of another dication (Table 2), forming a two-dimensional array which propagates in the *bc* plane (Fig. 2). This is a different hydrogen-bonding network to that of  $[\text{Co}((\text{HOCH}_2\text{CH}_2)_3\text{N})_2][(\text{C}_6\text{H}_4\text{O}_2)(\text{CH}_2\text{CO}_2)_2]$ , in which all four diacetate O atoms are involved in weaker hydrogen bonding (1.93, 2.01 and 2.17  $\text{\AA}$ ; Gao *et al.*, 2004).

## Experimental

Cobalt(II) acetate tetrahydrate (0.5 g, 2.0 mmol) was added to a solution of triethanolamine (TEA) (10 ml) and 2-propanol (10 ml). The resulting suspension was heated at 353 K for 24 h to afford a deep orange solution. The solvent was removed *in vacuo* to afford an orange oil. Orange single crystals suitable for X-ray diffraction were obtained upon prolonged standing. MS (ESI<sup>+</sup>) (*m/z*, %): 356 ( $[M - H]^+$ , 27), 267 ( $[\text{Co}(\text{TEA})(\text{OAc})]^+$ , 3), 207 ( $[\text{Co}(\text{TEA}) - H]^+$ , 20). Analysis found: C 40.12, H 7.23, N 5.69%; calculated for  $\text{C}_{16}\text{H}_{36}\text{CoN}_2\text{O}_{10}$ : C 40.42, H 7.63, N 5.89%.

### Crystal data

$[\text{Co}(\text{C}_6\text{H}_{15}\text{NO}_3)_2](\text{C}_2\text{H}_3\text{O}_2)_2$	$Z = 4$
$M_r = 475.4$	$D_x = 1.440 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 14.847(2) \text{ \AA}$	$\mu = 0.84 \text{ mm}^{-1}$
$b = 9.5480(11) \text{ \AA}$	$T = 150(2) \text{ K}$
$c = 15.473(2) \text{ \AA}$	Prism, orange
$V = 2193.4(4) \text{ \AA}^3$	$0.54 \times 0.48 \times 0.19 \text{ mm}$


**Figure 2**

A schematic representation of part of the two-dimensional hydrogen-bonding network present in the title compound. Dashed lines indicate hydrogen bonds.

### Data collection

Siemens SMART 1000 CCD diffractometer	20387 measured reflections
$\omega$ scans	2710 independent reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1999)	2314 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.701, T_{\max} = 0.853$	$R_{\text{int}} = 0.021$
	$\theta_{\max} = 28.3^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 1.1747P]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.084$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.04$	$\Delta\rho_{\max} = 0.67 \text{ e \AA}^{-3}$
2710 reflections	$\Delta\rho_{\min} = -0.37 \text{ e \AA}^{-3}$
141 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Co1—O2	2.0890 (10)	Co1—N1	2.1557 (12)
Co1—O3	2.0906 (11)		
O2—Co1—O2 <sup>i</sup>	180	O3—Co1—N1	82.82 (4)
O2—Co1—O3 <sup>i</sup>	89.67 (4)	O3—Co1—N1 <sup>i</sup>	97.18 (4)
O2 <sup>i</sup> —Co1—O3 <sup>i</sup>	90.33 (4)	O2—Co1—N1	81.16 (4)
O3 <sup>i</sup> —Co1—O3	180	N1 <sup>i</sup> —Co1—N1	180
O2—Co1—N1 <sup>i</sup>	98.84 (4)		

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3–H3 $\cdots$ O4	0.83 (2)	1.77 (2)	2.5952 (16)	173.7 (19)
O2–H2 $\cdots$ O5 <sup>i</sup>	0.85 (2)	1.71 (2)	2.5584 (15)	176.9 (19)
O1–H1 $\cdots$ O4 <sup>ii</sup>	0.84 (2)	1.89 (2)	2.7240 (16)	176

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

All H atoms bound to carbon were refined using a riding model with  $C-H = 0.98-0.99$  Å and  $U_{iso}(H) = 1.2U_{eq}(C)$  or  $1.5U_{eq}(C_{methyl})$ . O-bound H atoms were located in a difference Fourier map and refined without bond length restraints, with  $U_{iso}(H) = 1.5U_{eq}(O)$ .

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT* and *XPREP* (Siemens, 1995); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997), *WinGX32* (Farrugia, 1999), *POV-RAY* 3.5 (Cason, 2002) and *WebLab ViewerPro* 3.7 (Molecular Simulations, 2000); software used to prepare material for publication: *enCIFer 1.0* (Allen *et al.*, 2004).

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