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Key indicators

Single-crystal X-ray study
 T = 292 K
 Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
 R factor = 0.053
 wR factor = 0.151
 Data-to-parameter ratio = 17.9

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

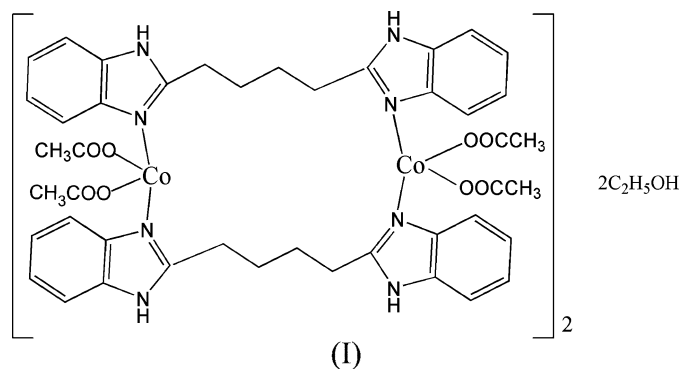
Bis[μ -2,2'-(butane-1,4-diyl)di-1*H*-benzimidazole- $\kappa^2\text{N}^3:\text{N}^{3'}$]bis[diacetatocobalt(II)] ethanol disolvate

Received 5 June 2006
 Accepted 14 July 2006

In the title compound, $[\text{Co}_2(\text{CH}_3\text{COO})_4(\text{C}_{18}\text{H}_{18}\text{N}_4)_2] \cdot 2\text{C}_2\text{H}_5\text{OH}$, the asymmetric unit consists of half each of two independent complex molecules, which are located about centres of inversion, and two molecules of ethanol. Each Co^{II} atom is four-coordinated by two N atoms from two 2,2'-(butane-1,4-diyl)-1*H*-benzimidazole ligands and two O atoms from two acetate ions in a slightly distorted tetrahedral coordination environment. In the crystal packing, the molecules are linked by a complex three-dimensional network of $\text{N}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen-bond interactions.

Comment

The field of coordination compounds formed through the appropriate selection of metal ions and multifunctional ligands has been developing rapidly and attracting increasing attention, due to their potential applications (Fujita *et al.*, 1994). To date, much of the work has focused on coordination compounds with rigid ligands (Carlucci *et al.*, 1994), while the study of flexible ligands is relatively rare (Ma *et al.*, 2003). The 2,2'-(butane-1,4-diyl)dibenzimidazole ligand (*L*), a derivative of benzimidazole, has received considerably less attention in the chemistry of coordination compounds (Yang *et al.*, 2005). Here, the crystal structure of the title compound, (I), based on the ligand *L*, is reported.



The asymmetric unit of (I) contains half each of two independent complex molecules having C_i symmetry. Each Co^{II} centre is four-coordinated by two N atoms from two *L* ligands and two O atoms from two acetate ions, giving a slightly distorted tetrahedral coordination (Fig. 1). Each Co^{II} atom is bridged by two *L* ligands, resulting in two unique cyclic units with $\text{Co}^{\text{II}} \cdots \text{Co}^{\text{II}}$ separations of 7.608 (2) and 6.990 (2) Å. The Co–N distances (Table 1) are shorter than those found in other related Co^{II} complexes [2.132 (4) and 2.159 (4) Å; Ma *et al.*, 2000].

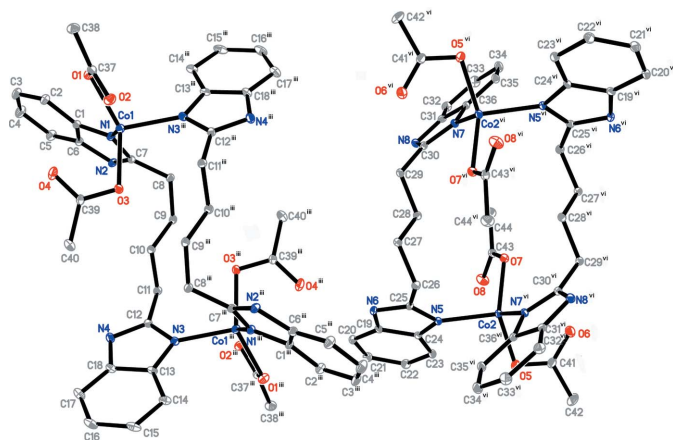


Figure 1

The two independent molecules of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 15% probability level. Ethanol molecules and H atoms have been omitted for clarity. [Symmetry codes: (iii) $2 - x, 2 - y, 1 - z$; (vi) $1 - x, 2 - y, -z$.]

In the crystal structure of (I), the $-NH$ group and the ethanol molecules play the roles of both acceptors and donors for hydrogen bonds, whereas the coordinated acetate anions act only as acceptors of hydrogen bonds (Table 2).

Experimental

Ligand *L* was synthesized according to the method reported by Berends & Stephan (1984). A mixture of $\text{Co}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ (1.0 mmol) and *L* (1.0 mmol) in ethanol (20 ml) was refluxed for 30 min and a purple solution was obtained. This solution was allowed to stand in air at room temperature for two weeks, yielding purple crystals of (I) (yield 29% based on Co).

Crystal data

$[\text{Co}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_{18}\text{H}_{18}\text{N}_4)_2] \cdot 2\text{C}_2\text{H}_6\text{O}$	$\gamma = 75.17 (3)^\circ$
$M_r = 1026.90$	$V = 2568.6 (11) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 12.723 (3) \text{ \AA}$	$D_x = 1.328 \text{ Mg m}^{-3}$
$b = 14.082 (3) \text{ \AA}$	Mo $K\alpha$ radiation
$c = 15.462 (3) \text{ \AA}$	$\mu = 0.71 \text{ mm}^{-1}$
$\alpha = 73.74 (3)^\circ$	$T = 292 (2) \text{ K}$
$\beta = 88.11 (3)^\circ$	Block, purple
	$0.41 \times 0.37 \times 0.31 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID diffractometer	21073 measured reflections
ω scans	10986 independent reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	6829 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.751, T_{\max} = 0.800$	$R_{\text{int}} = 0.046$
	$\theta_{\text{max}} = 27.4^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0886P)^2]$
$wR(F^2) = 0.151$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{\text{max}} = 0.001$
10986 reflections	$\Delta\rho_{\text{max}} = 1.01 \text{ e \AA}^{-3}$
613 parameters	$\Delta\rho_{\text{min}} = -0.53 \text{ e \AA}^{-3}$

Table 1

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

$\text{N1}-\text{Co1}$	2.055 (3)	$\text{O1}-\text{Co1}$	2.006 (2)
$\text{N3}-\text{Co1}^i$	2.063 (3)	$\text{O3}-\text{Co1}$	2.005 (2)
$\text{N5}-\text{Co2}$	2.045 (3)	$\text{O5}-\text{Co2}$	1.966 (3)
$\text{N7}-\text{Co2}^{ii}$	2.053 (3)	$\text{O7}-\text{Co2}$	1.969 (2)
$\text{O3}-\text{Co1}-\text{O1}$	138.91 (10)	$\text{O5}-\text{Co2}-\text{O7}$	136.66 (11)
$\text{O3}-\text{Co1}-\text{N1}$	99.63 (11)	$\text{O5}-\text{Co2}-\text{N5}$	100.24 (11)
$\text{O1}-\text{Co1}-\text{N1}$	102.51 (10)	$\text{O7}-\text{Co2}-\text{N5}$	103.01 (10)
$\text{O3}-\text{Co1}-\text{N3}^i$	100.38 (10)	$\text{O5}-\text{Co2}-\text{N7}^{ii}$	103.71 (11)
$\text{O1}-\text{Co1}-\text{N3}^i$	106.23 (11)	$\text{O7}-\text{Co2}-\text{N7}^{ii}$	100.22 (10)
$\text{N1}-\text{Co1}-\text{N3}^i$	105.72 (10)	$\text{N5}-\text{Co2}-\text{N7}^{ii}$	112.80 (10)

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

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N2}-\text{H2A} \cdots \text{O8}^{iii}$	0.86	1.87	2.707 (4)	166
$\text{N4}-\text{H4A} \cdots \text{O10}^{iv}$	0.86	1.93	2.780 (4)	170
$\text{N8}-\text{H8} \cdots \text{O9}$	0.86	1.87	2.720 (4)	167
$\text{N6}-\text{H6} \cdots \text{O4}^i$	0.86	1.87	2.719 (4)	172
$\text{O9}-\text{H9} \cdots \text{O2}^v$	0.82	2.03	2.636 (4)	130
$\text{O10}-\text{H10} \cdots \text{O6}$	0.82	1.89	2.687 (4)	165

Symmetry codes: (i) $-x + 2, -y + 2, -z + 1$; (iii) $-x + 1, -y + 2, -z + 1$; (iv) $x + 1, y, z + 1$; (v) $x - 1, y, z$.

All H atoms were positioned geometrically and refined as riding atoms, with $C-H = 0.93 \text{ \AA}$, $N-H = 0.86 \text{ \AA}$ and $O-H = 0.82 \text{ \AA}$, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N,O})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The maximum residual electron density is located 0.45 \AA from atom C47.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The author thanks Jilin University for supporting this work.

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