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Key indicators

Single-crystal X-ray study
 T = 100 K
 Mean $\sigma(C-C)$ = 0.003 Å
 R factor = 0.036
 wR factor = 0.093
 Data-to-parameter ratio = 32.1

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

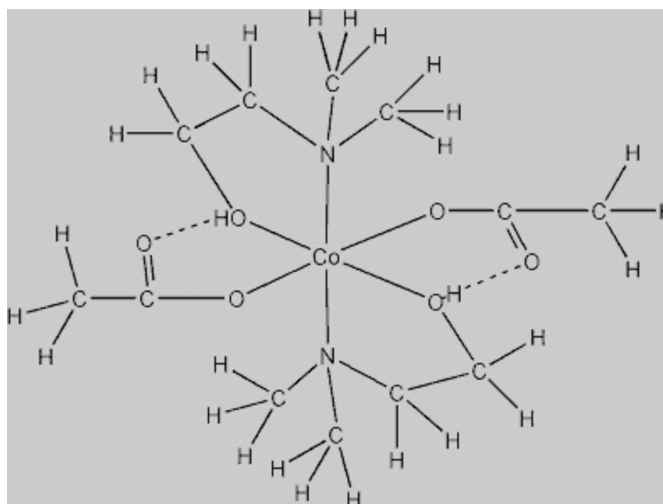
Bis(acetato-O)bis[2-(dimethylamino)ethanol- κ^2N,O]cobalt(II)

The title complex, $[Co(C_2H_3O_2)_2(C_4H_{11}NO)_2]$, was obtained in 70% yield by adding a stoichiometric amount of dmaeH [2-(dimethylamino)ethanol] to $Co(C_2H_3O_2)_2 \cdot 4H_2O$ in toluene followed by slow evaporation of the solvent. Two acetate and two dmaeH ligands are coordinated to the Co^{II} center in a slightly distorted octahedral fashion.

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Comment

The solid-state structure for octahedral complexes of the type $M(OAc)_2(dmaeH)_2$ [OAc is acetate ($OCOCH_3$) and dmaeH is *N,N*-dimethylaminoethanol ($(CH_3)_2NCH_2CH_2OH$)] have recently been reported for the Ni^{II} complex (Williams *et al.*, 2001). Such complexes are potential precursors for chemical vapor deposition to form ceramic oxides, for example CoO, which is used in ceramic material applications. The melting point of the title compound, $[Co(OAc)_2(dmaeH)_2]$, (I), (368 K) is lower than that of the parent reagent $Co(OAc)_2 \cdot 4H_2O$, making it a promising candidate as a precursor for thin films of CoO by aerosol-assisted chemical vapor deposition.



(I)

The structure determination of (I) shows it to be isotopic with its Ni counterpart (Williams *et al.*, 2001). The crystal under investigation was found to be non-merohedrally twinned with a refined twin fraction value of 0.1421 (5) (see *Experimental* section for details).

The molecular structure of (I) is shown in Fig. 1. Selected bond lengths and angles are given in Table 1. The mononuclear complex contains two monodentate acetate groups in

a *cis*-configuration and two bidentate/chelating dmaeH groups. The cobalt ion is in a distorted octahedral environment consisting of two O atoms (O3, O5) of the acetate groups, and two O atoms (O1, O2) from the OH groups of the dmaeH ligands, with the remaining two sites occupied by the N atoms (N1, N2) of the dmaeH ligands in *trans* fashion.

Two intramolecular hydrogen bonds link the hydroxy function of each dmaeH group with the non-coordinated O atoms of the acetate groups; the hydrogen bonding parameters are shown in Table 2. All bond lengths and angles are in the expected range and are in agreement with those found for similar complexes such as [Co(acac)₂(H₂O)]₂ (Cotton & Elder, 1966), [Co(acac)₂(teeda)] (Colborn *et al.*, 1988), [*cis*-NiCl₂(HOCH(Me)CH₂NMe₂)₂] (Hubert-Pfalzgraf *et al.*, 1997) or [Co(CH₃CO₂)₂(H₂O)₄] (van Niekerk & Schoening, 1953). The 'bite' angle of the dmaeH ligand, O–Co–N, is significantly less than 90° at 81.67 (5)°, but is closely comparable to that of its nickel counterpart [Ni(CH₃CO₂)₂(dmaeH)₂] (78.60 (5)°), and the Co–O(acetate) bond lengths are slightly shorter than the corresponding Ni ones (Williams *et al.*, 2001).

Experimental

[Co(CH₃CO₂)₂·4(H₂O)] (10 g, 40 mmol) was dehydrated by heating to 413 K for 1 h. THF (30 ml) was then added as a solvent. dmaeH (8.3 ml, 80.32 mmol) was introduced *via* a syringe and the mixture was stirred for 2 h. The resulting solution was filtered through a canula to remove the traces of unreacted cobalt(II) acetate. The mixture was then allowed to stand at room temperature overnight. Compound (I) was obtained as dark-pink crystals. Yield 9.71 g, 70% (based on [Co(CH₃CO₂)₂·4(H₂O)]). Similar to its Ni counterpart (Williams *et al.*, 2001) the Co complex is slightly air-sensitive.

Crystal data

[Co(C ₂ H ₃ O ₂) ₂ (C ₄ H ₁₁ NO) ₂]	$V = 851.4 (3) \text{ \AA}^3$
$M_r = 355.29$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.386 \text{ Mg m}^{-3}$
$a = 8.3661 (15) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.5562 (16) \text{ \AA}$	$\mu = 1.03 \text{ mm}^{-1}$
$c = 12.837 (2) \text{ \AA}$	$T = 100 (2) \text{ K}$
$\alpha = 95.555 (5)^\circ$	Block, pink
$\beta = 96.244 (4)^\circ$	$0.50 \times 0.40 \times 0.40 \text{ mm}$
$\gamma = 109.664 (4)^\circ$	

Data collection

Bruker SMART APEX CCD diffractometer	6513 measured reflections
ω scans	6513 independent reflections
Absorption correction: multi-scan (TWINABS in SAINT-Plus; Bruker, 2003)	6105 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.465$, $T_{\max} = 0.661$	$\theta_{\max} = 28.3^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.7996P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.093$	$(\Delta/\sigma)_{\max} = 0.002$
$S = 1.15$	$\Delta\rho_{\max} = 0.91 \text{ e \AA}^{-3}$
6513 reflections	$\Delta\rho_{\min} = -0.78 \text{ e \AA}^{-3}$
203 parameters	
H atoms treated by a mixture of independent and constrained refinement	

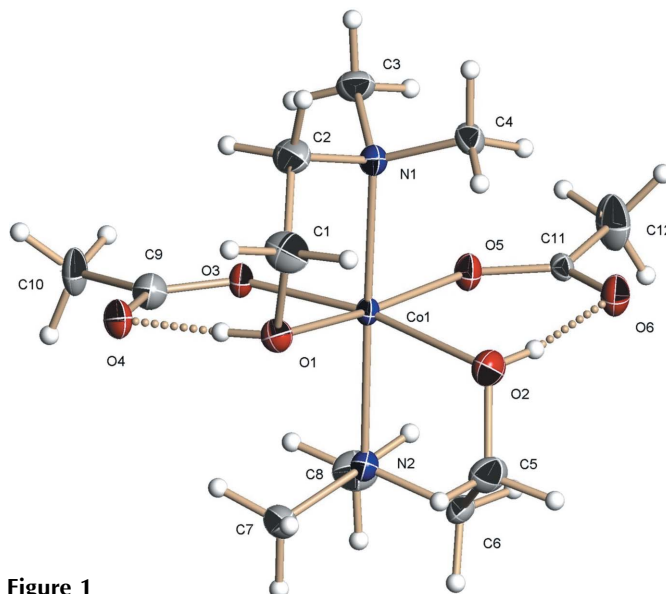


Figure 1
View of the title complex, showing the atom labeling scheme. Ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as broken lines.

Table 1

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

Co1–O3	2.0537 (13)	Co1–O2	2.1566 (13)
Co1–O5	2.0605 (13)	Co1–N2	2.1886 (15)
Co1–O1	2.1531 (13)	Co1–N1	2.1920 (15)
O3–Co1–O5	96.74 (5)	O1–Co1–N2	95.70 (5)
O3–Co1–O1	89.09 (5)	O2–Co1–N2	81.51 (5)
O5–Co1–O1	170.45 (5)	O3–Co1–N1	92.22 (6)
O3–Co1–O2	170.16 (5)	O5–Co1–N1	90.53 (5)
O5–Co1–O2	89.58 (5)	O1–Co1–N1	81.67 (5)
O1–Co1–O2	85.69 (5)	O2–Co1–N1	95.27 (5)
O3–Co1–N2	90.73 (6)	N2–Co1–N1	176.01 (5)
O5–Co1–N2	91.79 (5)		

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 \cdots O4	0.822 (16)	1.748 (17)	2.556 (2)	167 (3)
O2–H2 \cdots O6	0.808 (16)	1.776 (17)	2.5703 (19)	167 (3)

The crystal under investigation was found to be non-merohedrally twinned, so equivalent reflections cannot be merged before refinement. The two components were integrated using *SAINTE*, and were corrected for absorption using *TWINABS* (Bruker, 2003). The twin law was identified to be approximately $\bar{1} 0 0, 0 \bar{1} 0, 0.4903 0.4558 1$, and the refined twin fraction was 0.1421 (5). The hydroxyl H atoms were located in a difference density Fourier map and their O–H distances were restrained to be 0.80 (2) \AA . All other H atoms were placed in calculated positions. For all H atoms, U_{iso} was set to 1.5 (methyl, hydroxyl) or 1.2 times (all others) that $U_{\text{eq}}(\text{C}, \text{O})$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE-Plus* (Bruker, 2003); data reduction: *SAINTE-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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