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Cobalt diacetate tetrahydrate

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Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.001 Å
R factor = 0.018
wR factor = 0.047
Data-to-parameter ratio = 27.0

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

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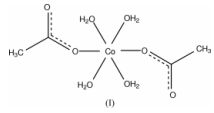
The crystal structure of tetra-aqua-bis(acetato-*O*)cobalt(II), $Co(C_2H_3O_2)_2(H_2O)_4$, has been determined at 153 K, providing a precise description of the geometric parameters and details of the hydrogen-bonding system operating in the crystal.

Comment

A number of divalent metal acetates crystallize from aqueous solution as tetrahydrates. The crystal structures of the isomorphous magnesium (Irish *et al.*, 1991; Trunov & Endeladze, 1986) and nickel (Treushnikov *et al.*, 1980; Cramer *et al.*, 1975; Downie *et al.*, 1971; van Niekerk & Schoening, 1953) derivatives have been established in detail, while earlier it was shown that the cobalt(II) analogue was also isomorphous (van Niekerk & Schoening, 1953). The structure of the latter has not otherwise been determined, a deficiency which we rectify here.



(I)

Like its magnesium and nickel counterparts, cobalt(II) acetate tetrahydrate crystallizes in monoclinic space group $P2_1/c$, $Z = 2$, so that one half of the formula unit comprises the asymmetric unit of the structure. All component moieties are coordinated to the metal, the unidentate *O*-acetate anions lying obligate *trans* about it, by virtue of the $[Co(H_2O)_4(O\text{-}CO\text{-}CH_3)_2]$ molecule being centrosymmetric, the cobalt lying on a crystallographic inversion centre. As in the magnesium and nickel analogues, the metal–oxygen distances span a range of less than 0.05 Å (Table 1), the distances to the two water molecules straddling that to the acetate [M—O 2.0761 (8), 2.1091 (8), 2.0577 (9) Å, M = Mg (Irish *et al.*, 1991); M—O 2.072 (1), 2.092 (1), 2.048 (1) Å, M = Ni (derivative of the electron-density-distribution study, Treushnikov *et al.*, 1980)]. The water molecule H atoms are all involved in hydrogen bonding, one of these bonds being intramolecular, tethering the uncoordinated oxygen of the acetate. Geometries within the acetate are unexceptional; Co—O may be compared with corresponding distances in $[Co(H_2O)_4(OOC\text{-}(CH_2)_2\text{-}COO)]_n$ [Co-OH_2 2.079 (2)–2.138 (2), Co—$O_{(carboxylate)}$ 2.089 (2) and 2.096 (2); Zheng & Lin, 2000)] and $[Co(H_2O)_4(OOC\text{-}(CH_2)_4\text{-}COO)]_n$ [Co—OH_2 2.085 (3), 2.106 (3), Co—$O_{(carboxylate)}$ 2.090 (4) Å; Suresh *et al.*, 1999]. The unique set of hydrogen bonds is tabulated in Table 2 and the hydrogen-bonding

system involving one molecule of cobalt diacetate tetrahydrate are shown in Fig. 1.

Experimental

Pink crystals of tetra-aqua-bis(acetato-*O*)cobalt(II) were obtained as a by-product during the synthesis of complexes of the 3*d* metals with organic ligands from aqueous solution (Shvelashvili *et al.*, 2001).

Crystal data

$[Co(C_2H_3O_2)_2(H_2O)_4]$	D_x = 1.767 Mg m^{-3}
M_r = 249.08	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6622 reflections
a = 4.7744 (3) Å	θ = 3.0–37.5°
b = 11.8425 (8) Å	μ = 1.85 mm^{-1}
c = 8.2904 (6) Å	T = 153 (2) K
β = 93.142 (2)°	Cuboid, pink
V = 468.04 (5) Å^3	0.48 × 0.42 × 0.38 mm
Z = 2	

Data collection

Bruker AXS SMART CCD diffractometer	2429 independent reflections
	2241 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.018
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	θ_{max} = 37.5°
	$h = -8 \rightarrow 7$
T_{min} = 0.430, T_{max} = 0.499	$k = 0 \rightarrow 20$
9443 measured reflections	$l = 0 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 0.1094P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.018	
$wR(F^2)$ = 0.047	
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
2429 reflections	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
90 parameters	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
All H-atom parameters refined	Extinction correction: *SHELXTL*
	Extinction coefficient: 0.041 (2)

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.0929 (5)	O1—C1	1.2767 (8)
Co—O3	2.0853 (5)	O2—C1	1.2550 (8)
Co—O4	2.1144 (5)	C1—C2	1.5001 (9)
O1—Co—O3	90.54 (2)	O3—Co—O4^{i}	89.52 (2)
O1—Co—O4	89.72 (2)	C1—O1—Co	125.47 (4)
O3—Co—O4	90.48 (2)	O2—C1—O1	123.11 (6)
O1—Co—O3^{i}	89.46 (2)	O2—C1—C2	119.55 (6)
O1—Co—O4^{i}	90.28 (2)	O1—C1—C2	117.32 (6)

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···O2	0.83 (2)	1.84 (2)	2.6282 (8)	160 (2)
O3—H32···O4^{ii}	0.82 (2)	2.05 (2)	2.8041 (7)	153 (1)
O4—H41···O1^{iii}	0.82 (2)	1.93 (2)	2.7084 (7)	159 (1)
O4—H42···O2^{iv}	0.85 (2)	1.85 (2)	2.6935 (7)	174 (1)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

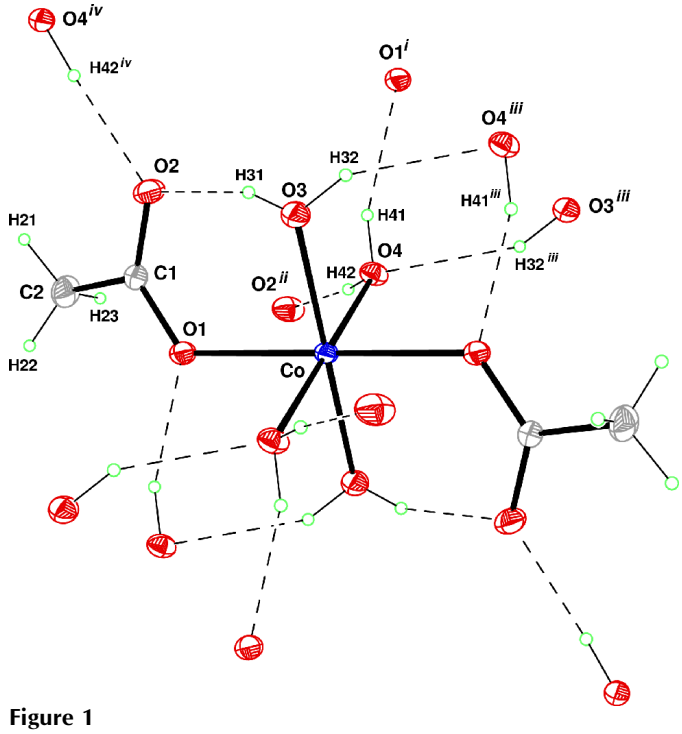


Figure 1
Details of the hydrogen-bonding of the cobalt diacetate tetrahydrate crystal structure. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level. Symmetry codes: (i) $x+1, y, z$; (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (iii) $1-x, -y, -z$; (iv) $x, \frac{1}{2}-y+\frac{1}{2}, z+\frac{1}{2}$ with their centrosymmetric complement $(-x, -y, -z)$.

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References

Bruker (1997). *SMART, SAINT, SADABS* (Version 5.0) and *SHELXTL* (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.

Cramer, R. E., van Doorne, M. & Dubois, R. (1975). *Inorg. Chem.* **14**, 2462–2466.

Downie, T. C., Harrison, W. & Raper, E. S. (1971). *Acta Cryst.* B**27**, 706–712.

Irish, D. E., Semmler, J, Taylor, N. J. & Toogood, G. E. (1991). *Acta Cryst.* C**47**, 2322–2324.

Niekerk, J. N. van & Schoening, F. R. L. (1953). *Acta Cryst.* **6**, 609–612.

Shvelashvili, A., Amirkhanashvili, K., Sakvarelidze, T. & Adeishvili, G. (2001). *Bull. Georgian Acad. Sci.* **164**, 488–491.

Suresh, E., Bhadbhade, M. M. & Venkatasubramanian, K. (1999). *Polyhedron*, **18**, 657–667.

Treushnikov, E. N., Kuskov, V. I., Aslanov, L. A. & Soboleva, L. V. (1980). *Sov. Phys. Crystallogr.* **25**, 160–170.

Trunov, V. K. & Endeladze, N. O. (1986). *J. Struct. Chem.* **27**, 812–814 (translation from Russian).

Zheng, Y.-O. & Lin, J.-L. (2000). *Z. Kristallogr. New Cryst. Struct.* **215**, 159–160.