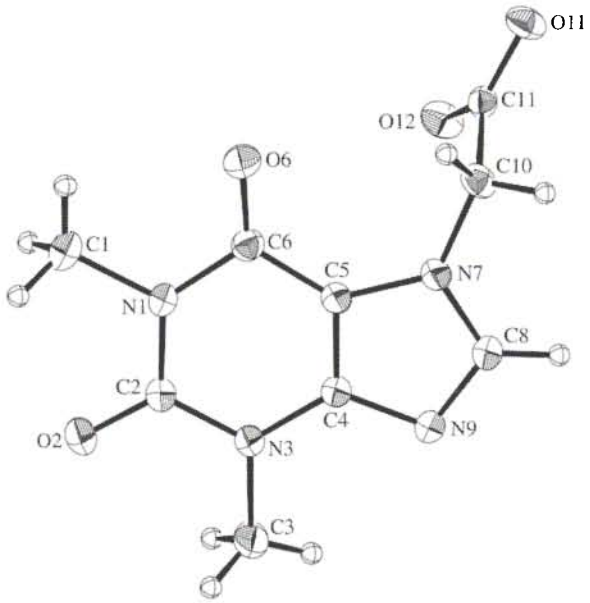
Crystal structure of hexaaquocobalt(II) theophylline-7-acetate tetrahydrate, $[Co(OH_2)_6][C_9H_9N_4O_4]_2 \cdot 4H_2O$

E. Horn[I], A. F. Botello[II], J. M. Salas[II] and E. R. T. Tiekink*,[III]

[I] Rikkyo University, Department of Chemistry, Tokyo 171-8501 and University of Tsukuba, Department of Chemistry, Ibaraki 305, Japan
[II] Universidad de Granada, Departamento de Quimica Inorganica, 18071 Granada, Spain
[III] The University of Adelaide, Department of Chemistry, Australia 5005

Received January 15, 2000, CCDC-No. 1267/382



Abstract

$C_{18}H_{38}CoN_8O_{18}$, triclinic, $P\bar{1}$ (No. 2), a = 8.141(2) Å, b = 9.117(1) Å, c = 11.893(1) Å, α = 105.4(3)°, β = 95.25(1)°, γ = 115.08(1)°, V = 749.5 Å^3, Z = 1, $R_{gt}(F)$ = 0.036, $wR_{ref}(F)$ = 0.039, T = 293 K.

Source of material

The compound was prepared as in the literature [1].

Discussion

The structure of the title compound is isomorphous with the nickel analogue [1]. The unit cell comprises centrosymmetric octahedral $[Co(OH_2)_6]^{2+}$ cations {d(Co—O) = 2.074(4) Å – 2.096(2) Å}, two non- coordinated theophylline-7-acetate anions (Fig.) and four water molecules of crystallisation. The mean deviation of the non-hydrogen atoms comprising the anion (excluding the CO_2 atoms) is 0.019 Å. The carboxylate group occupies a position normal to this plane as seen in the C(5)–N(7)–C(10)–C(11) torsion angle of –79.3(2)°. Extensive hydrogen bonding is present in the structure as detailed in [1].

Table 1. Data collection and handling.

Crystal:	pale pink, prismatic, size 0.20 × 0.20 × 0.40 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	6.65 cm^{-1}
Diffractometer, scan mode:	AFC7R, ω/2θ
$2\theta_{max}$:	60°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4630, 4375
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\ \sigma(I_{obs})$, 3756
$N(param)_{refined}$:	205
Programs:	teXsan [2], DIRDIF92 [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1a)	2*i*	–0.0996	0.0186	0.6434	0.028
H(1b)	2*i*	–0.1430	0.1759	0.7025	0.028
H(1c)	2*i*	0.0089	0.1897	0.6496	0.028
H(1w1)	2*i*	0.3682	0.2295	0.0894	0.028
H(1w2)	2*i*	0.3309	0.0982	0.1319	0.028
H(2w1)	2*i*	–0.0332	0.1127	0.2204	0.028
H(2w2)	2*i*	–0.1631	–0.0646	0.1704	0.028
H(3a)	2*i*	–0.4071	0.3998	0.4437	0.028
H(3b)	2*i*	–0.4002	0.3213	0.3012	0.028
H(3c)	2*i*	–0.2334	0.4378	0.3956	0.028
H(3w1)	2*i*	0.0039	–0.3051	–0.0390	0.028
H(3w2)	2*i*	–0.0701	–0.2694	0.0604	0.028
H(4w1)	2*i*	0.1756	0.2653	0.4336	0.028
H(4w2)	2*i*	0.1355	0.3935	0.3955	0.028
H(5w1)	2*i*	–0.0033	–0.5090	–0.2345	0.028
H(5w2)	2*i*	0.1477	–0.4683	–0.1417	0.028
H(8)	2*i*	–0.6647	–0.2377	0.0712	0.028
H(10a)	2*i*	–0.6597	–0.4825	0.1275	0.028
H(10b)	2*i*	–0.5896	–0.4680	0.2568	0.028

* Correspondence author (e-mail: edward.tiekink@adelaide.edu.au)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co	1*a*	0	0	0	0.0242(1)	0.0194(1)	0.0256(1)	0.0087(1)	0.0037(1)	0.0073(1)
O(1w)	2*i*	0.2728(2)	0.1463(2)	0.1011(1)	0.0270(6)	0.0293(6)	0.0542(8)	0.0062(5)	–0.0041(5)	0.0192(5)
O(2w)	2*i*	–0.0998(2)	0.0350(2)	0.1550(1)	0.0482(7)	0.0289(6)	0.0327(6)	0.0120(5)	0.0147(5)	0.0088(5)
O(3w)	2*i*	0.0064(2)	–0.2194(1)	0.0196(1)	0.0416(6)	0.0269(6)	0.0417(7)	0.0181(5)	0.0148(5)	0.0149(5)
O(4w)	2*i*	0.0910(3)	0.2817(2)	0.3757(1)	0.102(1)	0.0393(8)	0.0472(9)	0.0355(9)	–0.0199(9)	–0.0020(7)
O(5w)	2*i*	0.0388(2)	–0.4577(2)	–0.1553(1)	0.066(1)	0.075(1)	0.0491(9)	0.0501(9)	0.0046(8)	–0.0042(8)
O(2)	2*i*	–0.1634(2)	0.3631(2)	0.5862(1)	0.0519(8)	0.0318(6)	0.0317(6)	0.0182(6)	–0.0044(5)	–0.0001(5)
O(6)	2*i*	–0.3049(2)	–0.2075(2)	0.4596(1)	0.0522(8)	0.0375(7)	0.0399(7)	0.0252(6)	0.0027(6)	0.0143(5)
O(11)	2*i*	–0.4057(2)	–0.5750(1)	0.1088(1)	0.0374(6)	0.0237(5)	0.0509(8)	0.0140(5)	0.0112(6)	0.0087(5)
O(12)	2*i*	–0.2445(2)	–0.2924(1)	0.1561(1)	0.0327(6)	0.0264(6)	0.0536(8)	0.0091(5)	0.0165(5)	0.0139(5)
N(1)	2*i*	–0.2333(2)	0.0793(2)	0.5211(1)	0.0333(7)	0.0329(7)	0.0252(6)	0.0168(6)	0.0008(5)	0.0074(5)
N(3)	2*i*	–0.3471(2)	0.1985(2)	0.3997(1)	0.0376(7)	0.0263(6)	0.0282(6)	0.0157(6)	–0.0006(5)	0.0047(5)
N(7)	2*i*	–0.5265(2)	–0.2353(2)	0.2239(1)	0.0302(7)	0.0276(6)	0.0319(7)	0.0146(5)	0.0002(5)	0.0020(5)
N(9)	2*i*	–0.5378(2)	–0.0030(2)	0.2025(1)	0.0412(8)	0.0352(7)	0.0307(7)	0.0215(6)	–0.0043(6)	0.0043(6)
C(1)	2*i*	–0.1150(3)	0.1099(3)	0.6343(2)	0.054(1)	0.050(1)	0.0313(9)	0.0273(9)	–0.0082(8)	0.0073(8)
C(2)	2*i*	–0.2430(2)	0.2218(2)	0.5062(1)	0.0317(8)	0.0309(8)	0.0274(7)	0.0145(6)	0.0033(6)	0.0063(6)
C(3)	2*i*	–0.3589(3)	0.3454(2)	0.3792(2)	0.069(1)	0.0304(9)	0.040(1)	0.0244(9)	–0.0065(9)	0.0064(7)
C(4)	2*i*	–0.4329(2)	0.0389(2)	0.3123(1)	0.0289(7)	0.0290(7)	0.0262(7)	0.0151(6)	0.0019(6)	0.0053(6)
C(5)	2*i*	–0.4216(2)	–0.0995(2)	0.3297(1)	0.0276(7)	0.0270(7)	0.0268(7)	0.0136(6)	0.0038(6)	0.0053(6)
C(6)	2*i*	–0.3199(2)	–0.0887(2)	0.4374(1)	0.0286(7)	0.0320(8)	0.0296(7)	0.0157(6)	0.0067(6)	0.0106(6)
C(8)	2*i*	–0.5896(3)	–0.1698(2)	0.1521(2)	0.0393(9)	0.0387(9)	0.0315(8)	0.0219(8)	–0.0049(7)	0.0014(7)
C(10)	2*i*	–0.5499(2)	–0.4095(2)	0.1907(2)	0.0272(7)	0.0234(7)	0.0403(9)	0.0081(6)	0.0066(6)	0.0040(6)
C(11)	2*i*	–0.3861(2)	–0.4256(2)	0.1479(1)	0.0270(7)	0.0240(7)	0.0249(7)	0.0100(6)	0.0027(5)	0.0076(5)

Acknowledgment. The Australian Research Council is thanked for support.

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