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Diaquabis(2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylato-κ^2O,O')-cobalt(II)

Hui-Hui Xing,[a] Zi-Lu Chen[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Chemical Engineering, Guangxi Normal University, Gulin 541004, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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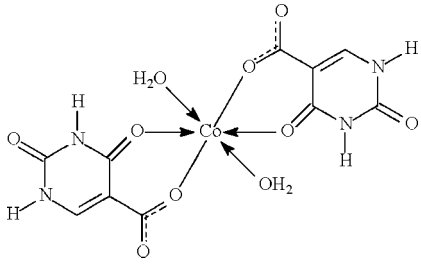
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.086; data-to-parameter ratio = 11.9.

The Co atom of the title compound, $[Co(C_5H_3N_2O_4)_2(H_2O)_2]$, lies on a center of inversion and is chelated by the 2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate anion through its 5-carboxylate and 4-oxo donor atoms. The other two sites of the octahedron around the metal atom are occupied by water molecules. The water molecules and amino groups serve as donors to other acceptor sites, giving rise to a three-dimensional hydrogen-bonded network.

Related literature

For the crystal structure of 2,4-dioxo-1,2,3,4-tetrahydropyridimine-5-carboxylic acid as the monohydrate, see Law *et al.* (2004). For the crystal structures of other water-coordinated metal derivatives, see Maistralis *et al.* (1991) (Mn), Baran *et al.* (1996) (Fe), Sun & Jin (2004) (Fe and Co) and Luo *et al.* (2002) (Cu).



Experimental

Crystal data

$[Co(C_5H_3N_2O_4)_2(H_2O)_2]$
M_r = 405.15
Monoclinic, $P2_1/n$
a = 5.0608 (6) Å
b = 15.087 (2) Å
c = 9.290 (1) Å
β = 99.389 (1)°
V = 699.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.30 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.743, T_{max} = 0.881
4291 measured reflections
1605 independent reflections
1308 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.086
S = 1.05
1605 reflections
135 parameters
5 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	2.037 (1)	Co1—O1*W*	2.135 (2)
Co1—O3	2.058 (1)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*w*—H11···O1^{i}	0.85 (1)	1.98 (1)	2.823 (2)	175 (3)
O1*w*—H12···O4^{ii}	0.85 (1)	2.14 (1)	2.959 (2)	165 (3)
N1—H1···O2^{iii}	0.85 (1)	1.81 (1)	2.667 (2)	177 (3)
N2—H2···O4^{iv}	0.85 (1)	1.98 (1)	2.822 (2)	171 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2460).

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supplementary materials

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Diaquabis(2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylato-κ^2O,O')cobalt(II)

H.-H. Xing, Z.-L. Chen and S. W. Ng

Comment

2,4-Dihydroxypyridimine-5-carboxylic acid crystallizes as a monohydrate; the 2,4-dihydroxypyrimidinyl portion of the molecule exists a 2,4-dioxo-1,2,3,4-tetrahydropyrimidinyl entity having secondary nitrogen atoms and exocyclic carbon–oxygen double bonds (Law *et al.*, 2004). The features are retained in the diaquamanganese(II) (Maistralis *et al.*, 1991), dihydrated diaquairon(II) (Baran *et al.*, 1996), triaquacobalt(II), triaquanickel(II) (Sun & Jin, 2004) and diaquacopper(II) (Luo *et al.*, 2002) derivatives; the anion chelates to the metal atoms through the 5-carboxylato and 4-oxo oxygen atoms. The diaquamanganese (Maistralis *et al.*, 1991), diaquacopper (Luo *et al.*, 2002) and the present diaquacobalt(II) compounds are isostructural; two carboxylate monoanions chelate in this manner across a center of inversion. Hydrogen bonds link adjacent octahedral molecules into a three-dimensional network.

Experimental

Cobalt(II) acetate hexahydrate (0.062 g, 0.25 mmol) and 2,4-dihydroxypyrimidine-5-carboxylic acid (0.087 g, 0.5 mmol) were placed in a 23-ml, Telefon-lined, stainless-steel Parr bomb together with water (6 ml) and THF (4 ml). The bomb was heated to 383 K for 144 h; it was then cooled over 48 h. Pink crystals were isolated in 70% yield.

Refinement

All hydrogen atoms were located in a difference Fourier map, and were refined with distance restraints of C—H 0.95 (1) Å, N—H = O—H = 0.85 (1) Å. Their temperature factors were freely refined.

Figures

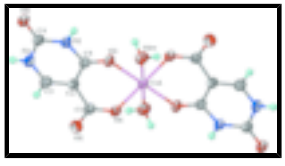

Fig. 1. Thermal ellipsoid plot of $Co(C_5H_3N_2O_4)_2(H_2O)_2$. The molecule lies about a center-of-inversion, and the unlabeled atoms are related to the labeled ones by $1-x$, $1-y$, $1-z$.

Diaquabis(2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylato- κ^2O,O')cobalt(II)

Crystal data

$[Co(C_5H_3N_2O_4)_2(H_2O)_2]$	$F_{000} = 410$
$M_r = 405.15$	$D_x = 1.923$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1901 reflections

a = 5.0608 (6) Å	θ = 2.6–27.5º
b = 15.087 (2) Å	μ = 1.30 mm^{-1}
c = 9.290 (1) Å	T = 295 (2) K
β = 99.389 (1)º	Block, pink
V = 699.8 (2) Å^3	0.20 × 0.20 × 0.10 mm
Z = 2	

Data collection

Bruker APEXII area-detector diffractometer	1605 independent reflections
Radiation source: fine-focus sealed tube	1308 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −6→6
T_{min} = 0.743, T_{max} = 0.881	k = −19→17
4291 measured reflections	l = −9→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.030	All H-atom parameters refined
$wR(F^2)$ = 0.086	$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.1507P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
1605 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
135 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
5 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.02430 (14)
O1	0.2334 (3)	0.4047 (1)	0.4163 (2)	0.0289 (3)
O2	0.0616 (3)	0.2948 (1)	0.2730 (2)	0.0292 (3)
O3	0.6389 (3)	0.5050 (1)	0.3040 (2)	0.0267 (3)
O4	0.8892 (3)	0.4044 (1)	−0.1094 (2)	0.0314 (4)
O1W	0.7933 (3)	0.4003 (1)	0.5678 (2)	0.0322 (4)
N1	0.5619 (4)	0.3281 (1)	−0.0207 (2)	0.0264 (4)
N2	0.7483 (3)	0.4527 (1)	0.0975 (2)	0.0223 (4)
C1	0.2244 (4)	0.3567 (1)	0.3041 (2)	0.0218 (4)
C2	0.4114 (4)	0.3746 (1)	0.1976 (2)	0.0219 (4)

C3	0.4047 (4)	0.3190 (1)	0.0823 (2)	0.0257 (4)
C4	0.7430 (4)	0.3953 (1)	−0.0169 (2)	0.0240 (4)
C5	0.5999 (4)	0.4468 (1)	0.2087 (2)	0.0215 (4)
H11	0.930 (4)	0.403 (2)	0.527 (3)	0.07 (1)*
H12	0.842 (5)	0.394 (2)	0.659 (1)	0.05 (1)*
H1	0.557 (5)	0.288 (1)	−0.085 (2)	0.04 (1)*
H2	0.848 (5)	0.498 (1)	0.107 (3)	0.04 (1)*
H3	0.289 (4)	0.270 (1)	0.064 (2)	0.03 (1)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0236 (2)	0.0294 (2)	0.0220 (2)	−0.0043 (2)	0.0099 (2)	−0.0052 (2)
O1	0.0257 (7)	0.0373 (8)	0.0264 (8)	−0.0079 (6)	0.0118 (6)	−0.0074 (6)
O2	0.0324 (8)	0.0296 (8)	0.0266 (8)	−0.0086 (6)	0.0071 (6)	0.0023 (6)
O3	0.0303 (8)	0.0298 (8)	0.0223 (8)	−0.0066 (6)	0.0114 (6)	−0.0064 (6)
O4	0.0318 (8)	0.0403 (9)	0.0249 (8)	−0.0068 (6)	0.0130 (6)	−0.0051 (6)
O1W	0.0298 (9)	0.0377 (9)	0.0309 (9)	0.0008 (7)	0.0104 (7)	0.0001 (7)
N1	0.0294 (9)	0.0270 (9)	0.0245 (9)	−0.0028 (7)	0.0091 (7)	−0.0066 (7)
N2	0.0230 (9)	0.0247 (9)	0.0204 (8)	−0.0033 (7)	0.0075 (7)	−0.0015 (7)
C1	0.021 (1)	0.024 (1)	0.021 (1)	0.002 (1)	0.005 (1)	0.003 (1)
C2	0.022 (1)	0.023 (1)	0.022 (1)	0.000 (1)	0.006 (1)	0.000 (1)
C3	0.025 (1)	0.024 (1)	0.029 (1)	−0.002 (1)	0.008 (1)	−0.001 (1)
C4	0.022 (1)	0.028 (1)	0.022 (1)	0.001 (1)	0.006 (1)	0.000 (1)
C5	0.021 (1)	0.024 (1)	0.020 (1)	0.002 (1)	0.006 (1)	0.003 (1)

Geometric parameters (Å, °)

Co1—O1	2.037 (1)	N1—C4	1.364 (3)
Co1—O1^{i}	2.037 (1)	N2—C4	1.367 (2)
Co1—O3	2.058 (1)	N2—C5	1.376 (2)
Co1—O3^{i}	2.058 (1)	C1—C2	1.501 (3)
Co1—O1W	2.135 (2)	C2—C3	1.357 (3)
Co1—O1W^{i}	2.135 (2)	C2—C5	1.440 (3)
O1—C1	1.265 (2)	O1W—H11	0.85 (1)
O2—C1	1.247 (2)	O1W—H12	0.85 (1)
O3—C5	1.239 (2)	N1—H1	0.85 (1)
O4—C4	1.230 (2)	N2—H2	0.85 (1)
N1—C3	1.347 (3)	C3—H3	0.94 (1)
O1^{i}—Co1—O1	180.0	O1—C1—C2	119.9 (2)
O1^{i}—Co1—O3^{i}	89.33 (5)	C3—C2—C5	117.1 (2)
O1—Co1—O3^{i}	90.67 (5)	C3—C2—C1	118.1 (2)
O1^{i}—Co1—O3	90.67 (5)	C5—C2—C1	124.8 (2)
O1—Co1—O3	89.33 (5)	N1—C3—C2	123.8 (2)
O3^{i}—Co1—O3	180.0	O4—C4—N1	122.9 (2)
O1^{i}—Co1—O1W	89.97 (7)	O4—C4—N2	122.3 (2)
O1—Co1—O1W	90.03 (7)	N1—C4—N2	114.8 (2)

O3^{i}—Co1—O1W	92.00 (6)	O3—C5—N2	116.6 (2)
O3—Co1—O1W	88.00 (6)	O3—C5—C2	127.8 (2)
O1^{i}—Co1—O1W^{i}	90.03 (7)	N2—C5—C2	115.5 (2)
O1—Co1—O1W^{i}	89.97 (7)	Co1—O1W—H11	114 (2)
O3^{i}—Co1—O1W^{i}	88.00 (6)	Co1—O1W—H12	117 (2)
O3—Co1—O1W^{i}	92.00 (6)	H11—O1W—H12	109 (3)
O1W—Co1—O1W^{i}	180.0	C3—N1—H1	118 (2)
C1—O1—Co1	130.7 (1)	C4—N1—H1	120 (2)
C5—O3—Co1	124.7 (1)	C4—N2—H2	122 (2)
C3—N1—C4	122.0 (2)	C5—N2—H2	111 (2)
C4—N2—C5	126.8 (2)	N1—C3—H3	112.0 (13)
O2—C1—O1	123.6 (2)	C2—C3—H3	124.2 (13)
O2—C1—C2	116.5 (2)		
O3^{i}—Co1—O1—C1	−164.2 (2)	C5—C2—C3—N1	−0.4 (3)
O3—Co1—O1—C1	15.8 (2)	C1—C2—C3—N1	179.9 (2)
O1W—Co1—O1—C1	−72.2 (2)	C3—N1—C4—O4	179.6 (2)
O1W^{i}—Co1—O1—C1	107.8 (2)	C3—N1—C4—N2	−1.0 (3)
O1^{i}—Co1—O3—C5	162.5 (2)	C5—N2—C4—O4	−177.8 (2)
O1—Co1—O3—C5	−17.5 (2)	C5—N2—C4—N1	2.8 (3)
O1W—Co1—O3—C5	72.5 (2)	Co1—O3—C5—N2	−168.1 (1)
O1W^{i}—Co1—O3—C5	−107.5 (2)	Co1—O3—C5—C2	13.9 (3)
Co1—O1—C1—O2	173.1 (1)	C4—N2—C5—O3	178.5 (2)
Co1—O1—C1—C2	−8.7 (3)	C4—N2—C5—C2	−3.2 (3)
O2—C1—C2—C3	−4.9 (3)	C3—C2—C5—O3	179.9 (2)
O1—C1—C2—C3	176.8 (2)	C1—C2—C5—O3	−0.4 (3)
O2—C1—C2—C5	175.4 (2)	C3—C2—C5—N2	1.8 (3)
O1—C1—C2—C5	−2.9 (3)	C1—C2—C5—N2	−178.5 (2)
C4—N1—C3—C2	−0.1 (3)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H11···O1^{ii}	0.85 (1)	1.98 (1)	2.823 (2)	175 (3)
O1W—H12···O4^{iii}	0.85 (1)	2.14 (1)	2.959 (2)	165 (3)
N1—H1···O2^{iv}	0.85 (1)	1.81 (1)	2.667 (2)	177 (3)
N2—H2···O4^{v}	0.85 (1)	1.98 (1)	2.822 (2)	171 (3)

Symmetry codes: (ii) *x*+1, *y*, *z*; (iii) *x*, *y*, *z*+1; (iv) *x*+1/2, −*y*+1/2, *z*−1/2; (v) −*x*+2, −*y*+1, −*z*.

Fig. 1