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Tetraaquabis(4,6-dioxidopyrimidin-1-ium-κ^3N)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.082
Data-to-parameter ratio = 8.4

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

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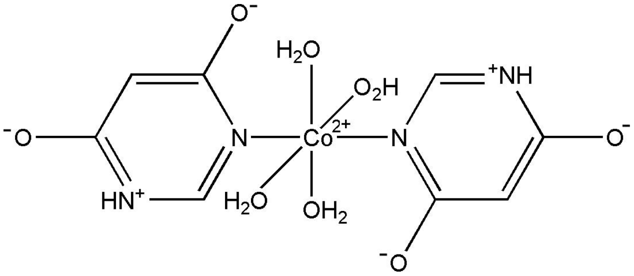
In the title complex, $[Co(C_4H_3N_2O_2)_2(H_2O)_4]$, the central Co^{II} ion is located at an inversion centre and is coordinated by two N atoms from 4,6-dihydroxypyrimidine ligands and four O atoms from water molecules in an approximately octahedral geometry. This discrete structure is further extended into a three-dimensional supramolecular structure *via* weak hydrogen bonds.

Comment

The study of cobalt coordination complexes is especially interesting as these compounds exhibit special magnetic properties, due to strong orbital contributions to the magnetic moments (Liu *et al.*, 2003; Pali *et al.*, 2003). In our work on the preparation of cobalt complexes, the title mononuclear compound, (I), was obtained, and its synthesis and structure are reported here.



(I)

The crystallographic analysis reveals that (I) consists of a centrosymmetric mononuclear $[Co(C_4H_3N_2O_2)_2(H_2O)_4]$ complex, in which each Co^{II} ion is in an N_2O_4 six-coordinated environment. Two deprotonated 4,6-dihydroxypyrimidine ligands use one of their N atoms to coordinate to the metal centre and the other to bind an H atom, while four water molecules occupy the equatorial sites to complete a slightly distorted octahedral geometry, as shown in Fig. 1.

The crystal structure of (I) involves eight different hydrogen bonds (Table 2), which connect the discrete molecules into a three-dimensional supramolecular structure, as shown in Fig. 2 (Lavalette *et al.*, 2003).

Experimental

An aqueous solution (5 ml) of 4,6-dihydroxypyrimidine (0.045 g, 0.4 mmol) was added to a solution of $CoCl_2{\cdot}6H_2O$ (0.048 g, 0.2 mmol) in water (3 ml). The solution was stirred for 10 min and its pH was adjusted to 7.0 with NaOH solution (0.5 M). The reaction mixture was allowed to stand at room temperature for several days, and red crystals of the title compound were obtained in 78% yield (based on

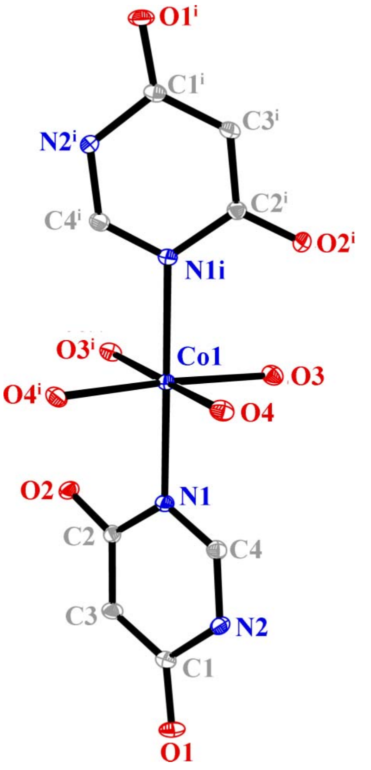


Figure 1
The structure of the title complex. H atoms have been omitted. Displacement ellipsoids are plotted at the 50% probability level. [Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$

Co). Analysis, calculated (%): C 27.18, O 36.24, N 15.86, H 3.96; found (%): C 27.14, O 36.21, N 15.84, H 3.94.

Crystal data

$[Co(C_4H_3N_2O_2)_2(H_2O)_4]$
$M_r = 353.16$
Monoclinic, $C2/c$
$a = 13.5324$ (15) Å
$b = 7.2128$ (8) Å
$c = 12.9880$ (15) Å
$\beta = 109.501$ (2)°
$V = 1195.0$ (2) Å^3
$Z = 4$
$D_x = 1.963$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1567 reflections
$\theta = 3.2$–$25.0°$
$\mu = 1.49$ mm^{-1}
$T = 293$ (2) K
Prism, red
0.30 × 0.30 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.600$, $T_{\max} = 0.809$
1915 measured reflections
1037 independent reflections
974 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 25.0°$
$h = -16 \rightarrow 9$
$k = -5 \rightarrow 8$
$l = -12 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.082$
$S = 1.17$
1037 reflections
124 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 3.5596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.43$ e Å^{-3}
$\Delta\rho_{\min} = -0.49$ e Å^{-3}

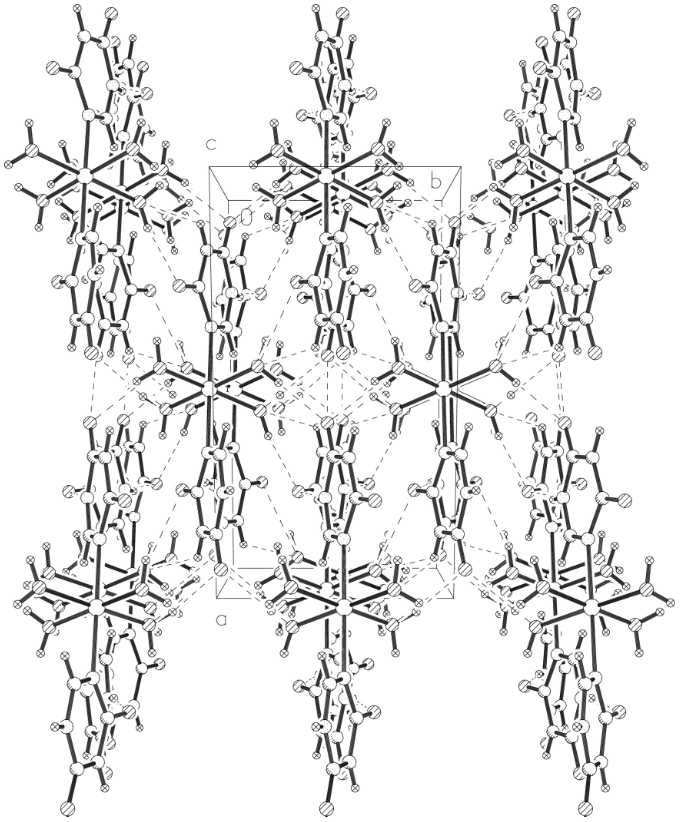


Figure 2
The three-dimensional packing of (I). Dashed lines indicate hydrogen bonds.

Table 1
Selected geometric parameters (Å, °).

Co1—O3	2.079 (2)	Co1—N1	2.192 (2)
Co1—O4	2.098 (2)		
O3^{i}—Co1—O3	93.59 (13)	O3—Co1—N1^{i}	92.42 (9)
O3^{i}—Co1—O4^{i}	89.91 (9)	O4^{i}—Co1—N1^{i}	90.33 (8)
O3—Co1—O4^{i}	175.63 (8)	O4—Co1—N1^{i}	89.30 (9)
O4^{i}—Co1—O4	86.72 (13)	N1^{i}—Co1—N1	179.48 (13)
O3^{i}—Co1—N1^{i}	87.93 (8)		

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{ii}	0.79 (4)	2.12 (4)	2.901 (3)	169 (4)
N2—H2···O3^{iii}	0.79 (4)	2.96 (4)	3.523 (3)	130 (3)
O3—H3A···O1^{iv}	0.84 (5)	1.93 (5)	2.748 (3)	166 (4)
O3—H3A···O1^{v}	0.84 (5)	2.76 (4)	3.250 (3)	119 (3)
O4—H4A···O1^{vi}	0.81 (5)	1.93 (5)	2.738 (3)	174 (5)
O4—H4A···O1^{vii}	0.81 (5)	2.75 (5)	3.134 (3)	111 (4)
O3—H3B···O2^{i}	0.84 (4)	1.88 (4)	2.652 (3)	152 (4)
O4—H4B···O2^{viii}	0.82 (4)	2.02 (4)	2.825 (3)	167 (4)

Symmetry codes: (i) $-x+1, y, -z+\frac{1}{2}$; (ii) $x, -y+2, z-\frac{1}{2}$; (iii) $-x+1, -y+2, -z$; (iv) $-x+\frac{1}{2}, -y+\frac{5}{2}, -z$; (v) $x+\frac{1}{2}, -y+\frac{5}{2}, z+\frac{1}{2}$; (vi) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (vii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (viii) $x+\frac{1}{2}, y-\frac{1}{2}, z$.

Acta Cryst. (2005). E**61**, m832–m834 Huang *et al.* • $[Co(C_4H_3N_2O_2)_2(H_2O)_4]$ **m833**

All H atoms were located in difference Fourier maps and refined freely.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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