

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# Tetraqua(2,6-dioxo-1,2,3,6-tetrahydro-pyrimidine-4-carboxylato- $\kappa^2N^3,O$ )-cobalt(II) 2.5-hydrate

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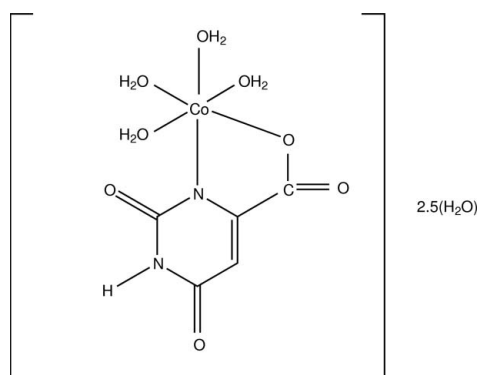
Received 25 October 2007; accepted 29 October 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.007$  Å; H-atom completeness 67%;  $R$  factor = 0.062;  $wR$  factor = 0.199; data-to-parameter ratio = 12.7.

The  $Co^{II}$  ion in the title compound,  $[Co(C_5H_2N_2O_4)(H_2O)_4] \cdot 2.5H_2O$ , is chelated by the orotate dianion through carboxylate O and pyrimidine N atoms, and its octahedral geometry is completed by four water molecules. An intermolecular  $N-H \cdots O$  hydrogen bond forms an orotate-orotate dimer. An extensive three-dimensional hydrogen-bonded network of  $O-H \cdots O$  and  $N-H \cdots O$  bonds and weak  $\pi-\pi$  interaction [ $3.754(2)$  Å] stabilize the crystal structure. One of the solvent water molecules is located on a twofold rotation axis.

## Related literature

For related literature, see: Bernstein *et al.* (1995); Icbudak *et al.* (2003); Lalioti *et al.* (1998); Panzeter & Ringer (1993); Wysokinski *et al.* (2002).



## Experimental

### Crystal data

 $[Co(C_5H_2N_2O_4)(H_2O)_4] \cdot 2.5H_2O$  $M_r = 330.12$ Orthorhombic,  $Pbcn$  $a = 20.8700(19)$  Å $b = 17.1153(16)$  Å $c = 7.3375(7)$  Å $V = 2620.9(4)$  Å<sup>3</sup> $Z = 8$ Mo  $K\alpha$  radiation  
 $\mu = 1.36$  mm<sup>-1</sup> $T = 293(2)$  K  
 $0.16 \times 0.11 \times 0.05$  mm

### Data collection

Bruker SMART CCD area-detector  
diffractometer

Absorption correction: multi-scan

(SADABS; Bruker, 2001)

 $T_{min} = 0.82$ ,  $T_{max} = 0.94$ 17563 measured reflections  
2321 independent reflections  
1971 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.038$ 

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.063$  $wR(F^2) = 0.199$  $S = 1.12$ 

2321 reflections

183 parameters

10 restraints

H atoms treated by a mixture of  
independent and constrained  
refinement $\Delta\rho_{max} = 1.39$  e Å<sup>-3</sup> $\Delta\rho_{min} = -0.71$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Co1—O5	2.075 (4)	Co1—O2W	2.112 (4)
Co1—O3W	2.078 (4)	Co1—O4W	2.123 (4)
Co1—O1W	2.086 (4)		
O5—Co1—O3W	96.2 (2)	O3W—Co1—O2W	92.1 (2)
O5—Co1—O1W	91.51 (19)	O1W—Co1—O2W	89.7 (2)
O3W—Co1—O1W	88.13 (17)	N1—Co1—O2W	93.31 (16)
O5—Co1—N1	78.39 (15)	O5—Co1—O4W	89.33 (15)
O1W—Co1—N1	90.59 (17)	O3W—Co1—O4W	88.23 (16)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H2N $\cdots$ O8 <sup>i</sup>	0.85 (4)	1.98 (4)	2.818 (5)	168 (5)
O1W—H2W $\cdots$ O5 <sup>ii</sup>	0.89 (6)	1.82 (9)	2.694 (5)	166 (10)
O1W—H1W $\cdots$ O7 <sup>iii</sup>	0.89 (8)	1.84 (4)	2.683 (5)	157 (9)
O3W—H5W $\cdots$ O6 <sup>ii</sup>	0.89 (9)	1.87 (10)	2.732 (6)	164 (11)
O3W—H6W $\cdots$ O5W	0.89 (7)	2.03 (9)	2.721 (11)	134 (10)
O4W—H7W $\cdots$ O7 <sup>iv</sup>	0.89 (7)	1.94 (4)	2.720 (5)	146 (6)
O4W—H8W $\cdots$ O6W	0.89 (5)	2.14 (5)	2.862 (11)	138 (7)
O2W—H3W $\cdots$ O8	0.88 (4)	1.82 (3)	2.666 (5)	157 (7)
O2W—H4W $\cdots$ O7W	0.89 (5)	2.24 (5)	3.014 (19)	146 (7)
O2W—H4W $\cdots$ O4W	0.89 (5)	2.43 (7)	2.994 (6)	122 (6)

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL/PC (Sheldrick, 1990) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

The authors thank Dr J. S. Yadav, Director, IICT, Hyderabad, for his kind encouragement.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2564).

## References

- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (2001). *SAINTE* (Version 6.28a) and *SMART* (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
- Icbudak, H., Olmez, H., Yesilel, O. Z., Arslan, F., Naumov, P., Jovanovski, G., Ibrahim, A. R., Usman, A., Fun, H.-K., Chantrapromma, S. & Ng, S. W. (2003). *J. Mol. Struct.* **789**, 147–155.
- Lalioti, N., Raptopoulou, C. P., Terzis, C. P., Panagiotopoulos, A., Perlepes, S. P. & Manessi-Zoupa, E. (1998). *J. Chem. Soc. Dalton Trans.* pp. 1327–1333.
- Panzeter, P. L. & Ringer, D. P. (1993). *Biochem. J.* **293**, 775–779.
- Sheldrick, G. M. (1990). *SHELXTL/PC*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Wysokinski, R., Ociepa, B. M., Glowiak, T. & Michalska, D. (2002). *J. Mol. Struct.* **606**, 241–251.

**supplementary materials**

*Acta Cryst.* (2007). E63, m2887-m2888 [ doi:10.1107/S1600536807054050 ]

## Tetraaqua(2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylato- $\kappa^2N^3,O$ )cobalt(II) 2.5-hydrate

**B. Sridhar and K. Ravikumar**

### Comment

Orotic acid (vitamin B13, H<sub>3</sub>Or) plays a significant role in biosynthesis of pyrimidine nucleosides (Panzeter & Ringer, 1993) and also found in cell and body fluids of many living organisms (Lalioti *et al.*, 1998). Orotic acid is a good organic building block in coordination chemistry and has a multidentate nature. The most potential coordination sites (pH range of 5–9) are the carboxylate oxygen and the adjacent nitrogen atom for the formation of a stable five-membered chelate ring. The crystal structures of nickel(II) orotate pentahydrate (Wysokinski *et al.*, 2002) and the analogous pentahydrate salt of cobalt (Icbudak *et al.*, 2003) were recently reported. In the present study, we are reporting the crystal structure of tetraaqua(orotato)cobalt(II) 2.5 hydrate (I).

The molecular structure of (I) is shown in Fig. 1 and selected geometrical parameters are given in Table 1. Compound (I) comprises of one Co<sup>II</sup> ion, one orotate ligand, four coordinated water molecule and 2.5 uncoordinated solvent water molecules. The central Co<sup>II</sup> ion has a distorted octahedral coordination geometry, comprised of atoms N1 and O4 from a doubly deprotonated bidentate orotate ligand and four water (O1W, O2W, O3W and O4W) molecules.

The orotate ligand is essentially planar. The dihedral angle between the pyrimidine ring and the carboxylate group is 0.8 (4)°. The atom N and carboxylate O atom of the orotate ring form a five-membered chelate ring with the Co<sup>II</sup> ion. The dihedral angle between the five-membered ring and the six-membered pyrimidine ring is 4.3 (1)°. The Co—N distance is 2.104 (4) Å and Co—O distances lie in the range 2.075 (3)–2.123 (4) Å (Table 1).

The structure is stabilized by N—H···O and O—H···O hydrogen bonding. The intramolecular O—H···O hydrogen bond forms an S(6) motif (Bernstein *et al.*, 1995). The intermolecular N—H···O hydrogen bonding leads to the formation of centrosymmetric dimer of R<sub>2</sub><sup>2</sup>(8)-type motif. The four water molecules link the carboxylate (O5 & O6) groups and carbonyl (O7 & O8) atoms through intra and intermolecular hydrogen bond interactions (Table. 2). Hydrogen-bonding interactions between the coordinated and uncoordinated water molecules and between the water molecules and the ligand result in a three-dimensional network structure (Fig. 2).

A  $\pi$ - $\pi$  interaction is observed between the symmetry-related pyrimidine rings (N1/C1/C2/C3/C4/N2/C5). The six-membered ring at (x,y,z) and (x, 1 - y, z + 1/2) are parallel with an interplanar spacing of 3.267 Å; the ring centroid separation is 3.755 (3) Å.

### Experimental

A solution of CoCl<sub>2</sub>·6H<sub>2</sub>O (1.2 g, 1 mmol) in water (25 ml) was added to a solution of orotic acid (0.9 g, 1 mmol) in water (25 ml). The solution refluxed and stirred in a temperature-controlled bath. The mixture was then left for crystallization.

## Refinement

The H atom attached to the N atom was located in a difference Fourier map and refined isotropically. H atoms of coordinated water molecules were located in a difference Fourier map and refined isotropically with  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$ . The N2—H2N and coordinated water H atoms were restrained to values of 0.85 (1) and 0.89 (1) Å, respectively. The H atom attached to the C atom was positioned geometrically and treated as riding on its parent C atom with C—H distance = 0.93 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The O atoms of the uncoordinated water (O5W, O6W & O7W) molecules show high displacement parameters, but attempts to refine them as disordered were unsuccessful. Hence, the O atoms were refined isotropically. The H atoms of O5W, O6W and O7W could not be located from electron density maps. These H atoms were not included in the calculations (although they are included in the empirical formula). A maximum (positive) residual density was observed 0.88 Å from atom O5W.

## Figures

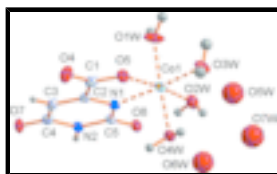


Fig. 1. A view of the (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

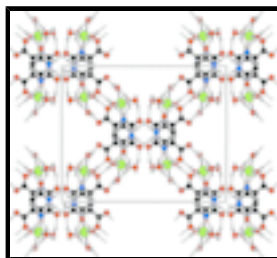


Fig. 2. A packing diagram for (I), viewed down the *c* axis. H atom attached to the C atom and three uncoordinated water molecules have been omitted for clarity.

## Tetraaqua(2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylato- $\kappa^2\text{N}^3,\text{O}$ )cobalt(II) 2.5-hydrate

### Crystal data

$[\text{Co}(\text{C}_5\text{H}_2\text{N}_2\text{O}_4)(\text{H}_2\text{O})_4] \cdot 2.5\text{H}_2\text{O}$

$M_r = 330.12$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 20.8700$  (19) Å

$b = 17.1153$  (16) Å

$c = 7.3375$  (7) Å

$V = 2620.9$  (4) Å<sup>3</sup>

$Z = 8$

$F_{000} = 1360$

$D_x = 1.673$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 7524 reflections

$\theta = 2.4$ – $24.3^\circ$

$\mu = 1.36$  mm<sup>-1</sup>

$T = 293$  (2) K

Block, brown

$0.16 \times 0.11 \times 0.05$  mm

*Data collection*

Bruker SMART CCD area-detector diffractometer	2321 independent reflections
Radiation source: fine-focus sealed tube	1971 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.038$
$T = 294(2)$ K	$\theta_{\text{max}} = 25.0^\circ$
$\omega$ scans	$\theta_{\text{min}} = 1.5^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -24 \rightarrow 24$
$T_{\text{min}} = 0.82$ , $T_{\text{max}} = 0.94$	$k = -20 \rightarrow 19$
17563 measured reflections	$l = -8 \rightarrow 8$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.063$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.199$	$w = 1/[\sigma^2(F_o^2) + (0.1193P)^2 + 6.0462P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
2321 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
183 parameters	$\Delta\rho_{\text{max}} = 1.39 \text{ e } \text{\AA}^{-3}$
10 restraints	$\Delta\rho_{\text{min}} = -0.70 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7263 (2)	0.3856 (3)	0.3371 (7)	0.0385 (12)
C2	0.6732 (2)	0.4366 (3)	0.2594 (7)	0.0309 (10)
C3	0.6769 (2)	0.5154 (3)	0.2676 (7)	0.0338 (11)
H3	0.7118	0.5399	0.3216	0.041*
C4	0.6257 (2)	0.5599 (3)	0.1911 (6)	0.0312 (11)
C5	0.5743 (2)	0.4364 (3)	0.1159 (6)	0.0286 (10)
Co1	0.63880 (3)	0.27419 (4)	0.18230 (9)	0.0331 (3)
N1	0.62351 (19)	0.3957 (2)	0.1868 (5)	0.0299 (9)

## supplementary materials

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N2	0.57606 (18)	0.5165 (2)	0.1237 (5)	0.0292 (9)
H2N	0.5431 (16)	0.542 (3)	0.090 (7)	0.039 (15)*
O5	0.71873 (17)	0.3129 (2)	0.3242 (5)	0.0435 (9)
O6	0.77339 (19)	0.4172 (2)	0.4090 (7)	0.0578 (12)
O7	0.62424 (19)	0.6324 (2)	0.1820 (5)	0.0397 (9)
O8	0.52739 (15)	0.40450 (19)	0.0404 (5)	0.0360 (8)
O1W	0.6869 (2)	0.2836 (3)	-0.0659 (6)	0.0688 (15)
H1W	0.674 (5)	0.306 (5)	-0.169 (7)	0.108*
H2W	0.715 (4)	0.252 (5)	-0.120 (13)	0.108*
O2W	0.5526 (2)	0.2518 (2)	0.0408 (6)	0.0525 (10)
H3W	0.534 (3)	0.298 (2)	0.030 (10)	0.073*
H4W	0.548 (4)	0.221 (4)	0.137 (6)	0.073*
O3W	0.6630 (3)	0.1565 (3)	0.1854 (6)	0.0619 (13)
H5W	0.686 (5)	0.142 (7)	0.089 (10)	0.144*
H6W	0.680 (5)	0.144 (7)	0.293 (8)	0.144*
O4W	0.5907 (2)	0.2568 (2)	0.4340 (5)	0.0452 (9)
H7W	0.589 (4)	0.3028 (18)	0.491 (8)	0.082*
H8W	0.608 (4)	0.216 (2)	0.491 (8)	0.082*
O5W	0.6640 (5)	0.0575 (6)	0.4756 (14)	0.148 (3)*
O6W	0.5927 (4)	0.1499 (6)	0.7340 (14)	0.141 (3)*
O7W	0.5000	0.1145 (14)	0.2500	0.251 (9)*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.029 (2)	0.045 (3)	0.042 (3)	0.004 (2)	-0.005 (2)	0.010 (2)
C2	0.024 (2)	0.039 (3)	0.030 (2)	0.0022 (19)	-0.0005 (19)	0.005 (2)
C3	0.027 (2)	0.040 (3)	0.035 (2)	-0.003 (2)	-0.007 (2)	0.005 (2)
C4	0.032 (2)	0.035 (3)	0.027 (2)	0.003 (2)	-0.0020 (19)	0.0046 (19)
C5	0.025 (2)	0.031 (2)	0.029 (2)	0.0065 (18)	0.0007 (19)	-0.0014 (19)
Co1	0.0328 (5)	0.0306 (5)	0.0359 (5)	0.0094 (2)	0.0009 (3)	-0.0006 (3)
N1	0.0249 (19)	0.029 (2)	0.035 (2)	0.0053 (16)	-0.0030 (16)	0.0001 (16)
N2	0.027 (2)	0.027 (2)	0.034 (2)	0.0063 (15)	-0.0047 (17)	0.0012 (17)
O5	0.0367 (19)	0.038 (2)	0.056 (2)	0.0099 (16)	-0.0112 (16)	0.0036 (16)
O6	0.039 (2)	0.050 (2)	0.085 (3)	-0.0030 (18)	-0.027 (2)	0.015 (2)
O7	0.050 (2)	0.0253 (19)	0.044 (2)	-0.0024 (15)	-0.0124 (16)	0.0031 (15)
O8	0.0307 (17)	0.0303 (17)	0.047 (2)	0.0050 (13)	-0.0119 (15)	-0.0028 (15)
O1W	0.072 (3)	0.087 (3)	0.047 (3)	0.053 (3)	0.023 (2)	0.021 (2)
O2W	0.049 (2)	0.044 (2)	0.065 (3)	0.0031 (19)	-0.011 (2)	-0.008 (2)
O3W	0.096 (4)	0.039 (2)	0.051 (3)	0.028 (2)	0.020 (2)	0.0046 (19)
O4W	0.054 (2)	0.0392 (19)	0.042 (2)	-0.0014 (18)	0.0065 (18)	-0.0056 (17)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C1—O6	1.240 (6)	Co1—O1W	2.086 (4)
C1—O5	1.258 (7)	Co1—N1	2.104 (4)
C1—C2	1.521 (7)	Co1—O2W	2.112 (4)
C2—C3	1.352 (7)	Co1—O4W	2.123 (4)
C2—N1	1.360 (6)	N2—H2N	0.85 (4)

C3—C4	1.427 (7)	O1W—H1W	0.89 (6)
C3—H3	0.9300	O1W—H2W	0.89 (8)
C4—O7	1.243 (6)	O2W—H3W	0.88 (4)
C4—N2	1.367 (6)	O2W—H4W	0.89 (5)
C5—O8	1.249 (6)	O3W—H5W	0.89 (9)
C5—N1	1.347 (6)	O3W—H6W	0.89 (7)
C5—N2	1.374 (6)	O4W—H7W	0.89 (4)
Co1—O5	2.075 (4)	O4W—H8W	0.89 (5)
Co1—O3W	2.078 (4)		
O6—C1—O5	124.2 (5)	O5—Co1—O4W	89.33 (15)
O6—C1—C2	119.1 (5)	O3W—Co1—O4W	88.23 (16)
O5—C1—C2	116.6 (4)	O1W—Co1—O4W	176.33 (17)
C3—C2—N1	125.0 (4)	N1—Co1—O4W	93.08 (15)
C3—C2—C1	121.0 (4)	O2W—Co1—O4W	89.99 (17)
N1—C2—C1	114.0 (4)	C5—N1—C2	117.8 (4)
C2—C3—C4	118.3 (4)	C5—N1—Co1	128.4 (3)
C2—C3—H3	120.9	C2—N1—Co1	113.6 (3)
C4—C3—H3	120.9	C4—N2—C5	125.3 (4)
O7—C4—N2	120.2 (4)	C4—N2—H2N	116 (4)
O7—C4—C3	125.0 (5)	C5—N2—H2N	118 (4)
N2—C4—C3	114.8 (4)	C1—O5—Co1	117.0 (3)
O8—C5—N1	122.9 (4)	Co1—O1W—H1W	130 (7)
O8—C5—N2	118.4 (4)	Co1—O1W—H2W	131 (7)
N1—C5—N2	118.7 (4)	H1W—O1W—H2W	94 (8)
O5—Co1—O3W	96.2 (2)	Co1—O2W—H3W	105 (5)
O5—Co1—O1W	91.51 (19)	Co1—O2W—H4W	79 (5)
O3W—Co1—O1W	88.13 (17)	H3W—O2W—H4W	123 (7)
O5—Co1—N1	78.39 (15)	Co1—O3W—H5W	113 (8)
O3W—Co1—N1	174.4 (2)	Co1—O3W—H6W	109 (8)
O1W—Co1—N1	90.59 (17)	H5W—O3W—H6W	115 (10)
O5—Co1—O2W	171.62 (15)	Co1—O4W—H7W	108 (5)
O3W—Co1—O2W	92.1 (2)	Co1—O4W—H8W	109 (5)
O1W—Co1—O2W	89.7 (2)	H7W—O4W—H8W	119 (5)
N1—Co1—O2W	93.31 (16)		
O6—C1—C2—C3	0.1 (8)	O1W—Co1—N1—C5	88.8 (4)
O5—C1—C2—C3	179.7 (5)	O2W—Co1—N1—C5	-0.9 (4)
O6—C1—C2—N1	-179.0 (5)	O4W—Co1—N1—C5	-91.1 (4)
O5—C1—C2—N1	0.6 (7)	O5—Co1—N1—C2	5.7 (3)
N1—C2—C3—C4	-1.5 (8)	O1W—Co1—N1—C2	-85.7 (4)
C1—C2—C3—C4	179.6 (4)	O2W—Co1—N1—C2	-175.4 (3)
C2—C3—C4—O7	-176.6 (5)	O4W—Co1—N1—C2	94.4 (3)
C2—C3—C4—N2	2.9 (7)	O7—C4—N2—C5	175.7 (4)
O8—C5—N1—C2	177.5 (4)	C3—C4—N2—C5	-3.9 (7)
N2—C5—N1—C2	-1.3 (6)	O8—C5—N2—C4	-175.7 (4)
O8—C5—N1—Co1	3.2 (7)	N1—C5—N2—C4	3.2 (7)
N2—C5—N1—Co1	-175.6 (3)	O6—C1—O5—Co1	-175.9 (4)
C3—C2—N1—C5	0.6 (7)	C2—C1—O5—Co1	4.5 (6)
C1—C2—N1—C5	179.6 (4)	O3W—Co1—O5—C1	172.9 (4)



## supplementary materials

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C3—C2—N1—Co1	175.7 (4)	O1W—Co1—O5—C1	84.7 (4)
C1—C2—N1—Co1	-5.2 (5)	N1—Co1—O5—C1	-5.6 (4)
O5—Co1—N1—C5	-179.8 (4)	O4W—Co1—O5—C1	-98.9 (4)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2N $\cdots$ O8 <sup>i</sup>	0.85 (4)	1.98 (4)	2.818 (5)	168 (5)
O1W—H2W $\cdots$ O5 <sup>ii</sup>	0.89 (6)	1.82 (9)	2.694 (5)	166 (10)
O1W—H1W $\cdots$ O7 <sup>iii</sup>	0.89 (8)	1.84 (4)	2.683 (5)	157 (9)
O3W—H5W $\cdots$ O6 <sup>ii</sup>	0.89 (9)	1.87 (10)	2.732 (6)	164 (11)
O3W—H6W $\cdots$ O5W	0.89 (7)	2.03 (9)	2.721 (11)	134 (10)
O4W—H7W $\cdots$ O7 <sup>iv</sup>	0.89 (7)	1.94 (4)	2.720 (5)	146 (6)
O4W—H8W $\cdots$ O6W	0.89 (5)	2.14 (5)	2.862 (11)	138 (7)
O2W—H3W $\cdots$ O8	0.88 (4)	1.82 (3)	2.666 (5)	157 (7)
O2W—H4W $\cdots$ O7W	0.89 (5)	2.24 (5)	3.014 (19)	146 (7)
O2W—H4W $\cdots$ O4W	0.89 (5)	2.43 (7)	2.994 (6)	122 (6)

Symmetry codes: (i)  $-x+1, -y+1, -z$ ; (ii)  $-x+3/2, -y+1/2, z-1/2$ ; (iii)  $x, -y+1, z-1/2$ ; (iv)  $x, -y+1, z+1/2$ .

Fig. 1

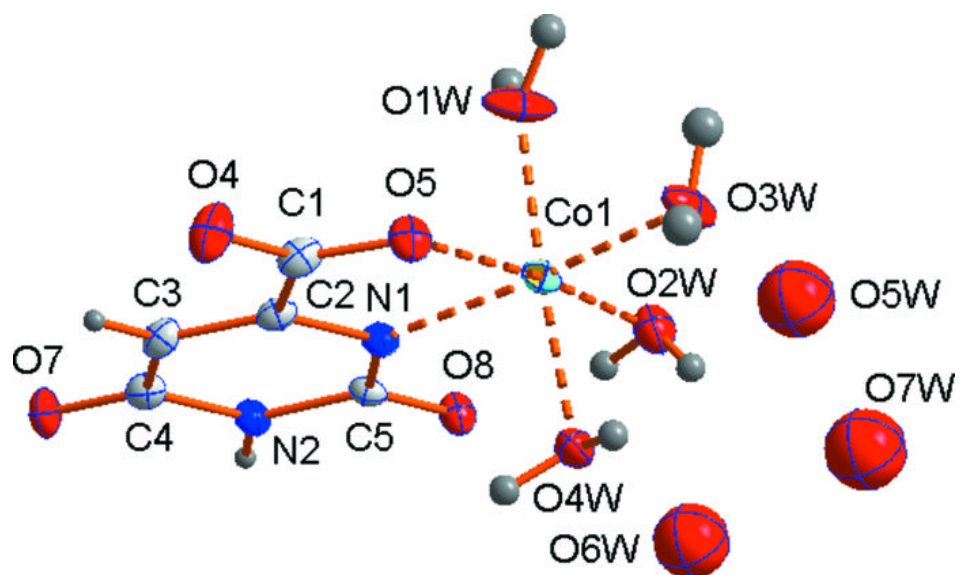


Fig. 2

