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Tetraaquabis(1*H*-benzimidazole-5,6-dicarboxylato- κ N³)cobalt(II) dimethylformamide disolvate dihydrate

 Hao Wang,^a Wen-Dong Song,^{b*} Shi-Jie Li,^a Dong-Liang Miao^a and Jin Liu^a

^aCollege of Food Science and Technology, Guang Dong Ocean University, Zhanjiang 524088, People's Republic of China, and ^bCollege of Science, Guang Dong Ocean University, Zhanjiang 524088, People's Republic of China
Correspondence e-mail: songwd60@163.com

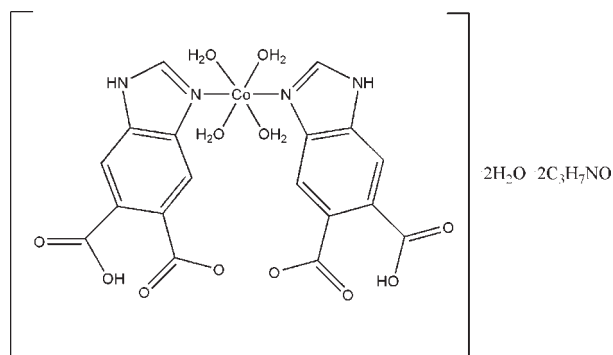
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.038; wR factor = 0.127; data-to-parameter ratio = 12.6.

In the mononuclear title compound, $[\text{Co}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_4] \cdot 2\text{C}_3\text{H}_7\text{NO} \cdot 2\text{H}_2\text{O}$, the Co^{II} atom, which lies on a center of inversion, is coordinated by four water molecules and two N atoms from two two symmetry-related 1*H*-benzimidazole-5,6-dicarboxylate ligands in a distorted octahedral geometry. The packing is governed by intermolecular O—H...O and N—H...O hydrogen-bonding interactions.

Related literature

For 1*H*-benzimidazole-5,6-dicarboxylate complexes, see: Song *et al.* (2009*a,b,c*).



Experimental

Crystal data

 $[\text{Co}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_4] \cdot 2\text{C}_3\text{H}_7\text{NO} \cdot 2\text{H}_2\text{O}$
 $M_r = 723.52$
Triclinic, $P\bar{1}$
 $a = 8.5612$ (17) Å
 $b = 9.1475$ (18) Å
 $c = 11.642$ (2) Å
 $\alpha = 100.82$ (3)°

 $\beta = 102.98$ (3)°
 $\gamma = 114.11$ (3)°
 $V = 769.9$ (3) Å³
 $Z = 1$

 Mo $K\alpha$ radiation
 $\mu = 0.64$ mm⁻¹
 $T = 293$ K
 $0.30 \times 0.24 \times 0.21$ mm

Data collection

 Rigaku/MSM Mercury CCD diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
 $T_{\text{min}} = 0.831$, $T_{\text{max}} = 0.877$

 6161 measured reflections
2751 independent reflections
2594 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.127$
 $S = 0.96$
2751 reflections
219 parameters
10 restraints

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.58$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.44$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ... <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> — <i>H</i> ... <i>A</i>
O2—H2...O5 ⁱ	0.839 (10)	1.750 (11)	2.588 (3)	177 (5)
O3W—H6W...O1 ⁱⁱ	0.84	1.98	2.800 (3)	165
O3W—H5W...O3 ⁱⁱⁱ	0.84	1.85	2.686 (3)	179
O2W—H3W...O3 ^{iv}	0.84	1.80	2.636 (3)	174
O2W—H4W...O3W	0.84	2.06	2.811 (3)	148
O1W—H1W...O4 ^{iv}	0.84	1.79	2.624 (3)	170
O1W—H2W...O3W ^v	0.84	1.94	2.749 (3)	161
N1—H1...O5 ⁱⁱ	0.86	1.98	2.782 (3)	154
N1—H1...O5 ⁱⁱ	0.86	1.98	2.782 (3)	154

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSM, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2669).

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supplementary materials

Acta Cryst. (2009). E65, m1423 [doi:10.1107/S1600536809043177]

Tetraaquabis(1*H*-benzimidazole-5,6-dicarboxylato- κ N³)cobalt(II) dimethylformamide disolvate dihydrate

H. Wang, W.-D. Song, S.-J. Li, D.-L. Miao and J. Liu

Comment

From the structural point of view, 1*H*-benzimidazole-5,6-dicarboxylic acid possesses two nitrogen atoms of imidazole ring and four oxygen atoms of carboxylate groups, and might be used as versatile linker in constructing coordination polymers with abundant hydrogen bonds. And based on this idea a series of coordination polymers formed by this ligand have been reported by us: Pentaqua(1*H*-benzimidazole-5,6-dicarboxylato- κ N³)cobalt(II)pentahydrate (Song *et al.*, 2009b), Pentaqua(1*H*-benzimidazole-5,6-dicarboxylato- κ N³)nickel(II)pentahydrate (Song *et al.*, 2009c), *catena*-Poly[[diaqua(1,10-phenanthroline- κ^2 N,N') nickel(II)]- μ -1*H*-benzimidazole-5,6-dicarboxylato- κ^2 N³:O⁶] (Song *et al.*, 2009a). In the present paper, we synthesized a novel coordination complex [Co(C₉H₄N₂O₄)₂(H₂O)₄].2H₂O.2C₃H₇NO.

As shown in Figure 1, the Co^{II} atom exhibits an octahedral coordination sphere, defined by two N atoms from two different 1*H*-benzimidazole-5,6-dicarboxylate ligands, and four water molecules. The equatorial plane is defined by O1_w, O2_w, O1_wⁱ and O2_wⁱ atoms, while N1 and N1ⁱ occupy the axial position (symmetry codes: $i = -x, 1 - y, 1 - z$). The solvent (water and dimethylformamide) molecules are also present in the asymmetric unit. Inter/intramolecular O—H \cdots O and N—H \cdots O hydrogen bonds form a three-dimensional supramolecular network making the structure more stable (Fig 2). The hydrogen bonds are in the normal range (Table 1).

Experimental

A C₃H₇NO solution (20 mL) containing Co(NO₃)₂ (0.1 mmol) and 1*H*-benzimidazole-5,6-dicarboxylic acid (0.2 mmol) was stirred for a few minutes in air, and left to stand at room temperature for about a few weeks, then the red crystals were obtained.

Refinement

Carbon and nitrogen bound H atoms were placed at calculated positions and were treated as riding on the parent C or N atoms with C—H = 0.93 Å, N—H = 0.86 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$. The water H-atoms were located in a difference map, and were refined with a distance restraint of O—H = 0.84 Å; their U_{iso} values were refined.

Figures

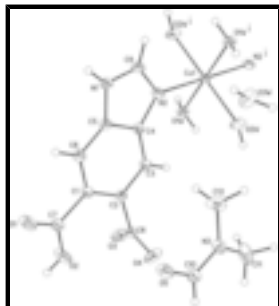


Fig. 1. The structure of the title compound, showing the atomic numbering scheme with 30% probability displacement ellipsoids. [Symmetry codes: (i) $-x, 1 - y, 1 - z$.]

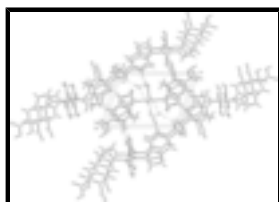


Fig. 2. A view of the three-dimensional network constructed by O—H...O and N—H...O hydrogen bonding interactions.

Tetraaquabis(1*H*-benzimidazole-5,6-dicarboxylato- κN^3)cobalt(II) dimethylformamide disolvate dihydrate

Crystal data

$[\text{Co}(\text{C}_9\text{H}_5\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_4] \cdot 2\text{C}_3\text{H}_7\text{NO} \cdot 2\text{H}_2\text{O}$

$M_r = 723.52$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.5612\ (17)\ \text{\AA}$

$b = 9.1475\ (18)\ \text{\AA}$

$c = 11.642\ (2)\ \text{\AA}$

$\alpha = 100.82\ (3)^\circ$

$\beta = 102.98\ (3)^\circ$

$\gamma = 114.11\ (3)^\circ$

$V = 769.9\ (3)\ \text{\AA}^3$

$Z = 1$

$F_{000} = 377$

$D_x = 1.561\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3420 reflections

$\theta = 3.3\text{--}27.4^\circ$

$\mu = 0.64\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, red

$0.30 \times 0.24 \times 0.21\ \text{mm}$

Data collection

Rigaku/MSM Mercury CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293\ \text{K}$

ω scans

Absorption correction: multi-scan
(*REQAB*; Jacobson, 1998)

$T_{\min} = 0.831, T_{\max} = 0.877$

6161 measured reflections

2751 independent reflections

2594 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\text{max}} = 25.2^\circ$

$\theta_{\text{min}} = 3.3^\circ$

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 1.194P]$
$S = 0.96$	where $P = (F_o^2 + 2F_c^2)/3$
2751 reflections	$(\Delta/\sigma)_{\max} < 0.001$
219 parameters	$\Delta\rho_{\max} = 0.58 \text{ e } \text{\AA}^{-3}$
10 restraints	$\Delta\rho_{\min} = -0.44 \text{ e } \text{\AA}^{-3}$
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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1417 (4)	0.8422 (3)	0.1200 (2)	0.0279 (6)
C2	0.2484 (3)	0.8904 (3)	0.2467 (2)	0.0247 (5)
C3	0.1906 (3)	0.7887 (3)	0.3191 (2)	0.0269 (5)
H3	0.2595	0.8201	0.4020	0.032*
C4	0.0277 (3)	0.6389 (3)	0.2654 (2)	0.0248 (5)
C5	-0.0742 (3)	0.5940 (3)	0.1405 (2)	0.0272 (6)
C6	-0.0194 (4)	0.6932 (4)	0.0667 (2)	0.0309 (6)
H6	-0.0888	0.6606	-0.0163	0.037*
C7	0.1921 (4)	0.9449 (4)	0.0363 (3)	0.0324 (6)
C8	0.4297 (3)	1.0478 (3)	0.3103 (2)	0.0263 (5)
C9	-0.2117 (4)	0.4034 (3)	0.2225 (3)	0.0310 (6)
H9	-0.2984	0.3064	0.2299	0.037*
C10	0.6732 (4)	0.7964 (4)	0.1713 (3)	0.0344 (6)
H10	0.7801	0.8972	0.1955	0.041*
N3	0.6382 (3)	0.7242 (3)	0.2550 (2)	0.0340 (5)
Co1	0.0000	0.5000	0.5000	0.02238 (18)

supplementary materials

N1	-0.2262 (3)	0.4426 (3)	0.1168 (2)	0.0315 (5)
H1	-0.3137	0.3846	0.0473	0.038*
N2	-0.0630 (3)	0.5150 (3)	0.3148 (2)	0.0282 (5)
C12	0.4674 (5)	0.5710 (5)	0.2251 (4)	0.0552 (9)
H3A	0.3742	0.6008	0.2330	0.083*
H3B	0.4829	0.5094	0.2812	0.083*
H3C	0.4330	0.5021	0.1414	0.083*
C11	0.7568 (6)	0.8059 (5)	0.3848 (3)	0.0547 (9)
H4A	0.8640	0.9036	0.3911	0.082*
H4B	0.7907	0.7283	0.4145	0.082*
H4C	0.6937	0.8393	0.4340	0.082*
O1	0.1079 (3)	0.8972 (3)	-0.0726 (2)	0.0582 (7)
O2	0.3337 (4)	1.0933 (3)	0.0904 (2)	0.0635 (8)
O3	0.4308 (3)	1.1767 (3)	0.3708 (2)	0.0458 (6)
O4	0.5660 (3)	1.0359 (3)	0.3035 (3)	0.0524 (6)
O5	0.5725 (3)	0.7391 (3)	0.06005 (19)	0.0457 (6)
O1W	0.0884 (2)	0.7574 (2)	0.57397 (17)	0.0300 (4)
H2W	0.0296	0.7784	0.6176	0.045*
H1W	0.2007	0.8133	0.6126	0.045*
O2W	0.2619 (3)	0.5455 (2)	0.50191 (19)	0.0360 (5)
H4W	0.2576	0.4881	0.4347	0.054*
H3W	0.3630	0.6321	0.5381	0.054*
O3W	0.1590 (3)	0.2539 (3)	0.3083 (2)	0.0498 (6)
H5W	0.2452	0.2312	0.3275	0.075*
H6W	0.0905	0.2004	0.2343	0.075*
H2	0.367 (6)	1.146 (5)	0.041 (3)	0.075*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0271 (13)	0.0262 (13)	0.0258 (13)	0.0076 (11)	0.0094 (10)	0.0090 (10)
C2	0.0231 (12)	0.0223 (12)	0.0259 (13)	0.0076 (10)	0.0088 (10)	0.0076 (10)
C3	0.0258 (13)	0.0260 (13)	0.0217 (12)	0.0073 (11)	0.0052 (10)	0.0071 (10)
C4	0.0247 (12)	0.0238 (12)	0.0245 (12)	0.0089 (10)	0.0098 (10)	0.0089 (10)
C5	0.0248 (13)	0.0230 (13)	0.0260 (13)	0.0052 (11)	0.0080 (10)	0.0062 (10)
C6	0.0303 (14)	0.0302 (14)	0.0224 (13)	0.0067 (12)	0.0060 (11)	0.0082 (11)
C7	0.0322 (14)	0.0304 (14)	0.0262 (14)	0.0071 (12)	0.0081 (11)	0.0111 (11)
C8	0.0232 (13)	0.0248 (13)	0.0257 (13)	0.0066 (11)	0.0064 (10)	0.0101 (11)
C9	0.0277 (14)	0.0244 (13)	0.0306 (14)	0.0026 (11)	0.0088 (11)	0.0103 (11)
C10	0.0334 (15)	0.0294 (14)	0.0290 (14)	0.0074 (12)	0.0047 (12)	0.0088 (11)
N3	0.0404 (13)	0.0350 (13)	0.0270 (12)	0.0174 (11)	0.0105 (10)	0.0122 (10)
Co1	0.0203 (3)	0.0186 (3)	0.0219 (3)	0.0040 (2)	0.00591 (19)	0.00645 (19)
N1	0.0243 (11)	0.0260 (12)	0.0229 (11)	-0.0027 (9)	0.0002 (9)	0.0055 (9)
N2	0.0271 (11)	0.0238 (11)	0.0262 (11)	0.0046 (9)	0.0083 (9)	0.0097 (9)
C12	0.052 (2)	0.057 (2)	0.060 (2)	0.0169 (18)	0.0275 (18)	0.0332 (18)
C11	0.085 (3)	0.055 (2)	0.0270 (16)	0.041 (2)	0.0084 (16)	0.0138 (15)
O1	0.0560 (15)	0.0498 (14)	0.0286 (11)	-0.0072 (11)	-0.0002 (10)	0.0191 (10)
O2	0.0580 (15)	0.0463 (14)	0.0325 (12)	-0.0183 (12)	-0.0036 (11)	0.0210 (11)

O3	0.0293 (11)	0.0302 (11)	0.0569 (14)	0.0051 (9)	0.0109 (10)	-0.0062 (10)
O4	0.0218 (10)	0.0340 (12)	0.0823 (18)	0.0077 (9)	0.0093 (11)	-0.0002 (11)
O5	0.0399 (12)	0.0433 (12)	0.0270 (11)	-0.0014 (10)	0.0014 (9)	0.0144 (9)
O1W	0.0238 (9)	0.0245 (9)	0.0318 (10)	0.0058 (8)	0.0057 (8)	0.0051 (8)
O2W	0.0250 (10)	0.0296 (10)	0.0399 (11)	0.0049 (8)	0.0114 (8)	0.0004 (8)
O3W	0.0428 (13)	0.0590 (15)	0.0395 (12)	0.0271 (12)	0.0088 (10)	-0.0033 (11)

Geometric parameters (Å, °)

C1—C6	1.381 (4)	N3—C12	1.462 (4)
C1—C2	1.424 (4)	N3—C11	1.463 (4)
C1—C7	1.489 (4)	Co1—O1W	2.086 (2)
C2—C3	1.387 (4)	Co1—O1W ⁱ	2.086 (2)
C2—C8	1.513 (4)	Co1—O2W ⁱ	2.1007 (19)
C3—C4	1.393 (4)	Co1—O2W	2.1007 (19)
C3—H3	0.9300	Co1—N2	2.146 (2)
C4—N2	1.395 (3)	Co1—N2 ⁱ	2.146 (2)
C4—C5	1.398 (4)	N1—H1	0.8600
C5—C6	1.382 (4)	C12—H3A	0.9600
C5—N1	1.382 (3)	C12—H3B	0.9600
C6—H6	0.9300	C12—H3C	0.9600
C7—O1	1.201 (4)	C11—H4A	0.9600
C7—O2	1.304 (4)	C11—H4B	0.9600
C8—O4	1.234 (3)	C11—H4C	0.9600
C8—O3	1.250 (3)	O2—H2	0.839 (10)
C9—N2	1.315 (4)	O1W—H2W	0.8400
C9—N1	1.338 (4)	O1W—H1W	0.8400
C9—H9	0.9300	O2W—H4W	0.8399
C10—O5	1.253 (3)	O2W—H3W	0.8399
C10—N3	1.299 (4)	O3W—H5W	0.8400
C10—H10	0.9300	O3W—H6W	0.8399
C6—C1—C2	120.8 (2)	O1W ⁱ —Co1—O2W	88.64 (8)
C6—C1—C7	115.4 (2)	O2W ⁱ —Co1—O2W	180.0
C2—C1—C7	123.8 (2)	O1W—Co1—N2	90.82 (9)
C3—C2—C1	120.3 (2)	O1W ⁱ —Co1—N2	89.18 (9)
C3—C2—C8	115.8 (2)	O2W ⁱ —Co1—N2	90.29 (9)
C1—C2—C8	123.9 (2)	O2W—Co1—N2	89.71 (9)
C2—C3—C4	118.9 (2)	O1W—Co1—N2 ⁱ	89.18 (9)
C2—C3—H3	120.6	O1W ⁱ —Co1—N2 ⁱ	90.82 (9)
C4—C3—H3	120.6	O2W ⁱ —Co1—N2 ⁱ	89.71 (9)
C3—C4—N2	131.3 (2)	O2W—Co1—N2 ⁱ	90.29 (9)
C3—C4—C5	119.7 (2)	N2—Co1—N2 ⁱ	179.999 (1)
N2—C4—C5	108.9 (2)	C9—N1—C5	107.1 (2)
C6—C5—N1	132.1 (2)	C9—N1—H1	126.5
C6—C5—C4	122.4 (2)	C5—N1—H1	126.5
N1—C5—C4	105.5 (2)	C9—N2—C4	104.9 (2)

supplementary materials

C1—C6—C5	117.9 (2)	C9—N2—Co1	124.00 (18)
C1—C6—H6	121.0	C4—N2—Co1	130.98 (18)
C5—C6—H6	121.0	N3—C12—H3A	109.5
O1—C7—O2	121.9 (3)	N3—C12—H3B	109.5
O1—C7—C1	123.1 (3)	H3A—C12—H3B	109.5
O2—C7—C1	115.0 (2)	N3—C12—H3C	109.5
O4—C8—O3	125.2 (3)	H3A—C12—H3C	109.5
O4—C8—C2	117.0 (2)	H3B—C12—H3C	109.5
O3—C8—C2	117.7 (2)	N3—C11—H4A	109.5
N2—C9—N1	113.6 (2)	N3—C11—H4B	109.5
N2—C9—H9	123.2	H4A—C11—H4B	109.5
N1—C9—H9	123.2	N3—C11—H4C	109.5
O5—C10—N3	124.3 (3)	H4A—C11—H4C	109.5
O5—C10—H10	117.8	H4B—C11—H4C	109.5
N3—C10—H10	117.8	C7—O2—H2	114 (3)
C10—N3—C12	120.6 (3)	Co1—O1W—H2W	113.1
C10—N3—C11	120.7 (3)	Co1—O1W—H1W	113.3
C12—N3—C11	118.2 (3)	H2W—O1W—H1W	110.9
O1W—Co1—O1W ⁱ	180.0	Co1—O2W—H4W	110.8
O1W—Co1—O2W ⁱ	88.64 (8)	Co1—O2W—H3W	130.9
O1W ⁱ —Co1—O2W ⁱ	91.36 (8)	H4W—O2W—H3W	112.2
O1W—Co1—O2W	91.36 (8)	H5W—O3W—H6W	112.2

Symmetry codes: (i) $-x, -y+1, -z+1$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2 \cdots O5 ⁱⁱ	0.839 (10)	1.750 (11)	2.588 (3)	177 (5)
O3W—H6W \cdots O1 ⁱⁱⁱ	0.84	1.98	2.800 (3)	165
O3W—H5W \cdots O3 ^{iv}	0.84	1.85	2.686 (3)	179
O2W—H3W \cdots O3 ^v	0.84	1.80	2.636 (3)	174
O2W—H4W \cdots O3W	0.84	2.06	2.811 (3)	148
O1W—H1W \cdots O4 ^v	0.84	1.79	2.624 (3)	170
O1W—H2W \cdots O3W ⁱ	0.84	1.94	2.749 (3)	161
N1—H1 \cdots O5 ⁱⁱⁱ	0.86	1.98	2.782 (3)	154
N1—H1 \cdots O5 ⁱⁱⁱ	0.86	1.98	2.782 (3)	154

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

Fig. 1

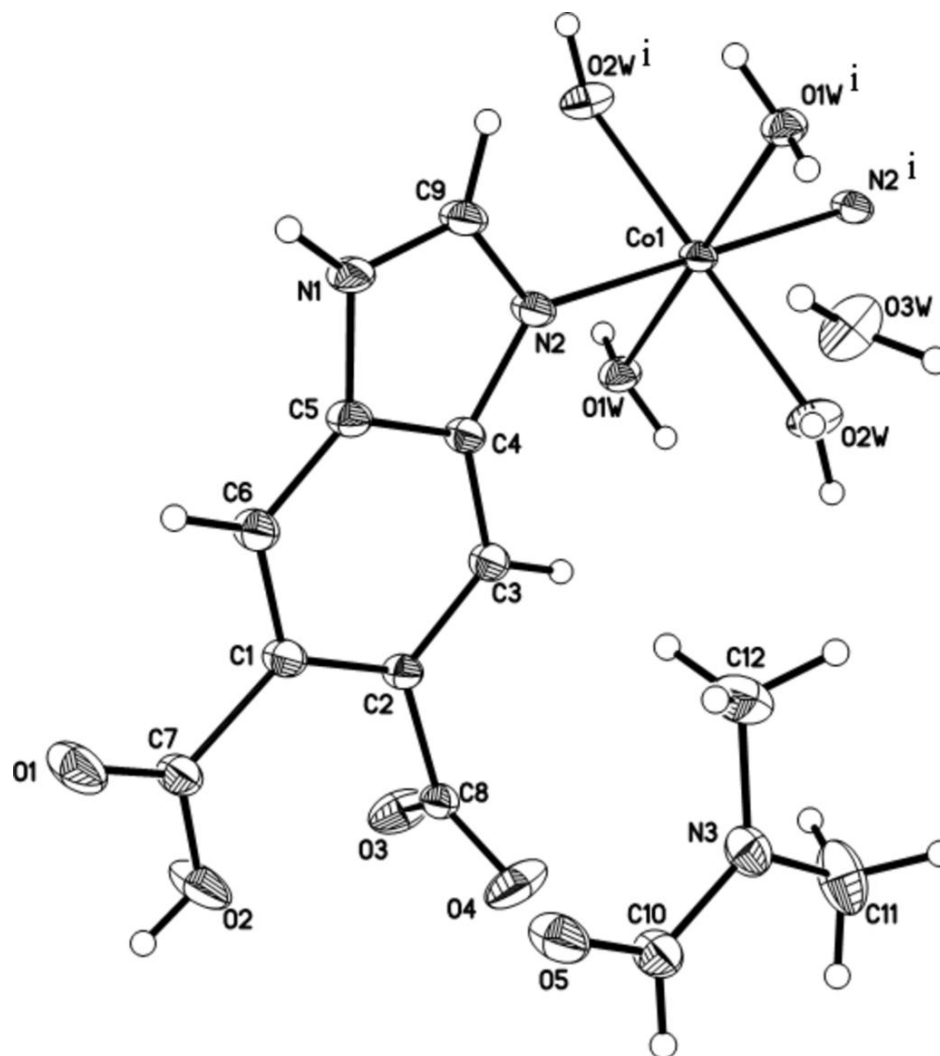


Fig. 2

