Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaquabis(4,4′-bipyridine)cobalt(II) pyridine-2,6-dicarboxylate tetrahydrate

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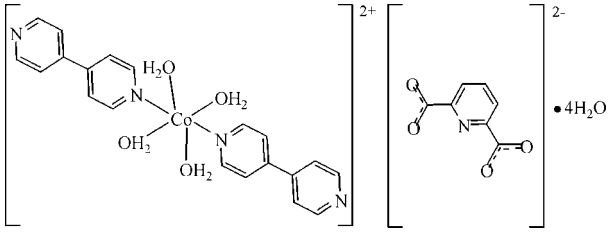
Received 18 September 2007; accepted 19 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.043; wR factor = 0.129; data-to-parameter ratio = 6.9.

In the title compound, $[Co(C_{10}H_8N_2)_2(H_2O)_4](C_7H_3NO_4)\cdot 4H_2O$, the Co^{II} ion adopts a slightly distorted *trans*-CoN_2O_4 octahedral coordination, arising from two monodentate 4,4′-bipyridine molecules and four water molecules. The constituent species interact by way of an extensive network of O—H···O and O—H···N hydrogen bonds. The crystal studied was an inversion twin.

Related literature

For general background, see: Howell *et al.* (2001).



Experimental

Crystal data

$[Co(C_{10}H_8N_2)_2(H_2O)_4]\cdot(C_7H_3NO_4)\cdot 4H_2O$
M_r = 680.53
Monoclinic, *Cc*
a = 18.1827 (5) Å
b = 6.8537 (10) Å
c = 25.1485 (5) Å
β = 99.398 (10)°
V = 3091.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 293 (2) K
0.42 × 0.28 × 0.22 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.779, T_{max} = 0.875
5091 measured reflections
3167 independent reflections
2936 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.129
S = 1.00
3167 reflections
456 parameters
26 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}
Absolute structure: Flack (1983), with 1416 Friedel pairs
Flack parameter: 0.65 (4)

Table 1
Selected bond lengths (Å).

Co1—O4	2.151 (4)	Co1—O1	2.200 (4)
Co1—O2	2.160 (4)	Co1—N1	2.279 (5)
Co1—O3	2.199 (4)	Co1—N3	2.271 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1W···O10^{i}	0.82 (6)	1.93 (6)	2.728 (6)	162 (7)
O1—H2W···O5^{ii}	0.82 (3)	1.96 (2)	2.769 (6)	169 (8)
O2—H3W···O8^{iii}	0.80 (6)	2.05 (6)	2.843 (8)	173 (8)
O2—H4W···N2^{iv}	0.81 (3)	2.06 (4)	2.755 (6)	145 (7)
O3—H5W···O7	0.82 (6)	1.95 (6)	2.772 (6)	176 (10)
O3—H6W···O8^{v}	0.816 (11)	2.01 (3)	2.789 (7)	161 (6)
O4—H7W···O5	0.82 (6)	2.06 (3)	2.826 (7)	155 (7)
O4—H8W···N4^{v}	0.82 (5)	2.00 (3)	2.769 (6)	155 (7)
O5—H9W···O9^{i}	0.81 (4)	2.00 (3)	2.777 (7)	161 (7)
O5—H10W···O7^{vi}	0.82 (7)	2.01 (6)	2.822 (8)	176 (7)
O6—H11W···O12^{vii}	0.82 (4)	2.16 (4)	2.825 (6)	137 (6)
O7—H14W···O11	0.82 (3)	1.82 (4)	2.631 (7)	174 (8)
O8—H15W···O10	0.82 (6)	1.96 (7)	2.746 (8)	162 (7)
O8—H16W···O6^{viii}	0.82 (4)	1.94 (4)	2.747 (9)	172 (8)
O6—H12W···O11	0.82 (3)	2.30 (5)	2.933 (7)	135 (7)

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

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2544).

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supplementary materials

Acta Cryst. (2007). E**63**, m2601 [**doi:10.1107/S1600536807046107**]

Tetraaquabis(4,4'-bipyridine)cobalt(II) pyridine-2,6-dicarboxylate tetrahydrate

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Comment

As part of our studies of coordination polymer networks (Howell *et al.*, 2001), the molecular title compound, (I), arose.

The Co^{ii} atom is (I) is coordinated by two monodentate 4,4'-bipyridine molecules in the axial sites and four associated water molecules in the equatorial plane with the r.m.s. deviation for the fitted atoms (Co1, O1, O2, O3, O4) being 0.012 Å (Fig. 1, Table 1). The dihedral angle between the N1 and N2 rings is 6.2 (3)°; that between the N3 and N4 rings is 6.9 (3)°.

A network of O—H···O and O—H···N hydrogen bonds (Table 2, Fig. 2) helps to establish the packing for (I).

Experimental

A mixture of cobalt dichloride (0.5 mmol), benzene-1,3-dicarboxylic acid (0.5 mmol), sodium hydroxide (1 mmol), 4,4'-bipyridine (0.5 mmol), H_2O (8 ml) and ethanol (8 ml) in a 25-ml Teflon-lined stainless steel autoclave was heated at 453 K for one week, and then cooled to room temperature. Red blocks of (I) were obtained with a yield of 8%. Anal. Calc. for $C_{27}H_{35}CoN_5O_{12}$: C 47.61, H 5.14, N 10.29%; Found: C 47.56, H 5.18, N 10.22%.

Refinement

The H atoms of the water molecule were located from difference density maps and were refined with distance restraints of H···H = 1.38 (2) Å and O—H = 0.82 (2) Å. All other H atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}$ of the respective carrier atom.

Figures

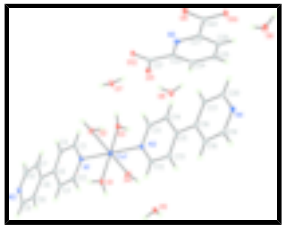

Fig. 1. The molecular structure of (I), drawn with 30% probability displacement ellipsoids for the non-hydrogen atoms.

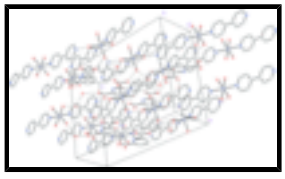

Fig. 2. The packing in (I) with the O···O and O···N contacts for the hydrogen bonds indicated by dashed lines.

Tetraaquabis(4,4'-bipyridine)cobalt(II) pyridine-2,6-dicarboxylate tetrahydrate

Crystal data

$[Co(C_{10}H_8N_2)_2(H_2O)_4](C_7H_3NO_4)\cdot 4H_2O$	$F_{000} = 1420$
$M_r = 680.53$	$D_x = 1.462$ Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 3167 reflections
a = 18.1827 (5) Å	θ = 1.6–25.0º
b = 6.8537 (10) Å	μ = 0.63 mm^{-1}
c = 25.1485 (5) Å	*T* = 293 (2) K
β = 99.398 (10)º	Block, red
V = 3091.9 (5) Å^3	0.42 × 0.28 × 0.22 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	3167 independent reflections
Radiation source: fine-focus sealed tube	2936 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
T = 293(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.6$º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −19→21
$T_{min} = 0.779$, $T_{max} = 0.875$	*k* = −8→4
5091 measured reflections	*l* = −29→12

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.104P)^2 + 1.0603P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.129$	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max} = 0.40$ e Å^{-3}
3167 reflections	$\Delta\rho_{min} = -0.58$ e Å^{-3}
456 parameters	Extinction correction: none
26 restraints	Absolute structure: Flack (1983), with how many Friedel pairs?
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.65 (4)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.67783 (8)	0.76266 (9)	0.87717 (6)	0.0355 (2)
C1	0.6043 (3)	0.8586 (8)	0.9833 (2)	0.0364 (12)
H1	0.5597	0.8604	0.9591	0.044*
C2	0.7306 (3)	0.8503 (9)	0.9992 (2)	0.0437 (14)
H2	0.7757	0.8458	0.9864	0.052*
C3	0.7327 (3)	0.8594 (8)	1.0542 (2)	0.0395 (13)
H3	0.7782	0.8620	1.0773	0.047*
C4	0.6013 (3)	0.8673 (9)	1.0380 (2)	0.0389 (13)
H4	0.5556	0.8749	1.0499	0.047*
C5	0.6670 (3)	0.8644 (6)	1.0746 (2)	0.0265 (10)
C6	0.6670 (3)	0.8625 (7)	1.1340 (2)	0.0277 (11)
C7	0.6017 (3)	0.8496 (9)	1.1560 (2)	0.0444 (14)
H7	0.5557	0.8446	1.1335	0.053*
C8	0.7334 (3)	0.8700 (10)	1.1714 (2)	0.0467 (14)
H8	0.7790	0.8794	1.1594	0.056*
C9	0.7313 (4)	0.8637 (9)	1.2261 (2)	0.0461 (14)
H9	0.7763	0.8682	1.2498	0.055*
C10	0.6052 (4)	0.8443 (10)	1.2112 (3)	0.0553 (17)
H10	0.5605	0.8351	1.2245	0.066*
C11	0.6226 (3)	0.6744 (10)	0.7540 (2)	0.0452 (14)
H11	0.5770	0.6870	0.7658	0.054*
C12	0.7481 (4)	0.6476 (10)	0.7726 (2)	0.0481 (15)
H12	0.7920	0.6429	0.7974	0.058*
C13	0.7532 (3)	0.6281 (10)	0.7186 (2)	0.0459 (14)
H13	0.7994	0.6063	0.7083	0.055*
C14	0.6228 (3)	0.6587 (9)	0.6993 (2)	0.0430 (14)
H14	0.5777	0.6599	0.6757	0.052*
C15	0.6886 (3)	0.6411 (6)	0.6791 (2)	0.0261 (10)
C16	0.6920 (3)	0.6373 (6)	0.62062 (19)	0.0272 (11)
C17	0.6269 (3)	0.6348 (8)	0.5828 (2)	0.0359 (12)
H17	0.5804	0.6339	0.5937	0.043*
C18	0.7592 (3)	0.6372 (8)	0.6013 (2)	0.0388 (12)
H18	0.8043	0.6375	0.6249	0.047*

C19	0.7576 (4)	0.6368 (8)	0.5461 (2)	0.0429 (13)
H19	0.8031	0.6383	0.5337	0.051*
C20	0.6327 (3)	0.6335 (8)	0.5279 (2)	0.0379 (12)
H20	0.5889	0.6318	0.5029	0.045*
C21	0.4269 (3)	0.8255 (8)	0.6808 (2)	0.0369 (12)
C22	0.4210 (3)	0.9008 (7)	0.4797 (2)	0.0329 (10)
C23	0.4286 (6)	0.7341 (6)	0.6267 (4)	0.0317 (8)
C24	0.4309 (3)	0.5329 (7)	0.6202 (2)	0.0372 (11)
H24	0.4319	0.4520	0.6500	0.045*
C25	0.4317 (3)	0.4511 (7)	0.5695 (2)	0.0381 (11)
H25	0.4338	0.3163	0.5658	0.046*
C26	0.4295 (3)	0.5684 (7)	0.5248 (2)	0.0371 (11)
H26	0.4301	0.5125	0.4911	0.044*
C27	0.4265 (4)	0.7722 (7)	0.5299 (3)	0.0321 (14)
N1	0.6684 (2)	0.8477 (6)	0.96340 (16)	0.0301 (10)
N2	0.6678 (3)	0.8514 (6)	1.24685 (19)	0.0403 (11)
N3	0.6852 (2)	0.6725 (6)	0.79132 (17)	0.0325 (10)
N4	0.6963 (3)	0.6345 (6)	0.50961 (18)	0.0367 (11)
N5	0.4265 (3)	0.8515 (7)	0.5801 (2)	0.0432 (11)
O1	0.7932 (2)	0.8702 (5)	0.88665 (16)	0.0386 (9)
O2	0.6401 (3)	1.0475 (5)	0.84774 (15)	0.0448 (10)
O3	0.5623 (2)	0.6581 (6)	0.86976 (17)	0.0434 (9)
O4	0.7151 (2)	0.4793 (6)	0.90703 (17)	0.0445 (9)
O5	0.8406 (4)	0.2547 (5)	0.8925 (2)	0.0455 (14)
O6	0.4356 (3)	0.3084 (8)	0.7615 (2)	0.0700 (13)
O7	0.4362 (3)	0.8505 (6)	0.81861 (18)	0.0525 (11)
O8	0.5140 (4)	0.7287 (7)	0.3640 (3)	0.0559 (16)
O9	0.4161 (2)	1.0788 (5)	0.48651 (15)	0.0432 (9)
O10	0.4189 (2)	0.8175 (6)	0.43492 (16)	0.0446 (9)
O11	0.4273 (3)	0.7097 (7)	0.72046 (19)	0.0511 (13)
O12	0.4261 (2)	1.0060 (6)	0.68432 (16)	0.0459 (9)
H1W	0.825 (3)	0.793 (7)	0.901 (3)	0.069*
H2W	0.804 (4)	0.986 (3)	0.892 (3)	0.069*
H3W	0.607 (3)	1.117 (9)	0.854 (2)	0.069*
H4W	0.645 (4)	1.026 (10)	0.8169 (10)	0.069*
H5W	0.526 (3)	0.715 (8)	0.853 (3)	0.069*
H6W	0.559 (4)	0.5395 (18)	0.870 (3)	0.069*
H7W	0.745 (3)	0.416 (8)	0.893 (3)	0.069*
H8W	0.702 (4)	0.419 (8)	0.932 (2)	0.069*
H9W	0.859 (4)	0.280 (10)	0.9234 (10)	0.069*
H10W	0.867 (4)	0.278 (11)	0.870 (2)	0.069*
H11W	0.415 (4)	0.262 (8)	0.7327 (16)	0.069*
H13W	0.458 (4)	0.956 (5)	0.823 (2)	0.069*
H14W	0.431 (5)	0.813 (9)	0.7873 (10)	0.069*
H15W	0.492 (4)	0.739 (10)	0.3897 (19)	0.069*
H16W	0.487 (3)	0.724 (11)	0.3347 (14)	0.069*
H12W	0.425 (4)	0.422 (4)	0.767 (3)	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0370 (3)	0.0440 (3)	0.0255 (3)	0.0009 (3)	0.0054 (2)	0.0012 (3)
C1	0.028 (3)	0.057 (3)	0.023 (3)	0.008 (2)	0.001 (2)	−0.005 (2)
C2	0.032 (3)	0.070 (4)	0.030 (3)	−0.007 (3)	0.007 (2)	−0.007 (3)
C3	0.027 (3)	0.068 (3)	0.022 (3)	−0.007 (3)	0.001 (2)	−0.006 (2)
C4	0.030 (3)	0.066 (3)	0.020 (3)	0.003 (3)	0.003 (2)	−0.003 (2)
C5	0.034 (3)	0.027 (2)	0.019 (2)	0.0008 (19)	0.004 (2)	−0.0007 (18)
C6	0.031 (3)	0.029 (2)	0.025 (3)	0.002 (2)	0.009 (2)	−0.0010 (18)
C7	0.031 (3)	0.071 (4)	0.031 (3)	−0.005 (3)	0.006 (2)	−0.005 (3)
C8	0.034 (3)	0.073 (4)	0.034 (3)	0.002 (3)	0.008 (3)	0.000 (3)
C9	0.044 (3)	0.070 (3)	0.025 (3)	0.003 (3)	0.006 (3)	0.002 (3)
C10	0.054 (4)	0.083 (4)	0.034 (3)	−0.008 (3)	0.021 (3)	−0.007 (3)
C11	0.028 (3)	0.084 (4)	0.025 (3)	−0.005 (3)	0.010 (2)	−0.007 (3)
C12	0.038 (3)	0.076 (4)	0.028 (3)	0.014 (3)	0.000 (3)	−0.004 (3)
C13	0.029 (3)	0.079 (4)	0.032 (3)	0.008 (3)	0.010 (2)	−0.010 (3)
C14	0.023 (3)	0.077 (4)	0.027 (3)	−0.001 (3)	−0.002 (2)	−0.006 (3)
C15	0.028 (3)	0.028 (2)	0.022 (3)	0.0014 (19)	0.005 (2)	0.0001 (18)
C16	0.032 (3)	0.025 (2)	0.023 (3)	0.0024 (19)	0.002 (2)	−0.0028 (18)
C17	0.033 (3)	0.057 (3)	0.018 (3)	0.000 (2)	0.005 (2)	−0.003 (2)
C18	0.035 (3)	0.055 (3)	0.028 (3)	0.003 (2)	0.009 (2)	−0.003 (2)
C19	0.043 (3)	0.055 (3)	0.033 (3)	0.001 (3)	0.015 (3)	0.000 (2)
C20	0.037 (3)	0.047 (3)	0.026 (3)	−0.004 (2)	−0.006 (2)	−0.003 (2)
C21	0.028 (3)	0.045 (3)	0.036 (3)	0.006 (2)	0.003 (2)	−0.002 (2)
C22	0.027 (2)	0.041 (2)	0.031 (2)	−0.003 (2)	0.0067 (19)	−0.005 (2)
C23	0.0186 (16)	0.042 (2)	0.033 (2)	0.002 (2)	−0.0011 (14)	0.002 (2)
C24	0.032 (2)	0.041 (2)	0.036 (3)	0.002 (2)	0.000 (2)	0.002 (2)
C25	0.037 (3)	0.029 (2)	0.046 (3)	0.004 (2)	0.001 (2)	−0.002 (2)
C26	0.035 (3)	0.041 (3)	0.034 (3)	−0.001 (2)	0.001 (2)	−0.011 (2)
C27	0.024 (3)	0.036 (3)	0.037 (3)	0.000 (2)	0.005 (2)	−0.007 (2)
N1	0.031 (2)	0.037 (2)	0.021 (2)	−0.0023 (18)	0.0028 (19)	−0.0010 (17)
N2	0.053 (3)	0.042 (2)	0.026 (2)	−0.005 (2)	0.010 (2)	−0.004 (2)
N3	0.034 (2)	0.040 (2)	0.024 (2)	0.0030 (19)	0.0038 (19)	−0.0017 (18)
N4	0.049 (3)	0.041 (2)	0.021 (2)	0.003 (2)	0.009 (2)	−0.0004 (18)
N5	0.033 (2)	0.050 (3)	0.046 (3)	0.003 (2)	0.005 (2)	−0.002 (2)
O1	0.035 (2)	0.0408 (17)	0.039 (2)	−0.0036 (16)	0.0040 (17)	0.0008 (16)
O2	0.066 (3)	0.044 (2)	0.0266 (19)	0.0210 (19)	0.0154 (18)	0.0088 (17)
O3	0.034 (2)	0.050 (2)	0.045 (2)	−0.0060 (18)	0.0060 (18)	−0.0033 (19)
O4	0.057 (3)	0.045 (2)	0.036 (2)	0.0186 (18)	0.0198 (18)	0.0104 (17)
O5	0.047 (3)	0.051 (3)	0.040 (3)	−0.0054 (17)	0.008 (3)	−0.0061 (17)
O6	0.087 (4)	0.077 (3)	0.045 (3)	−0.010 (3)	0.009 (2)	−0.014 (2)
O7	0.066 (3)	0.049 (2)	0.043 (3)	−0.008 (2)	0.012 (2)	−0.0047 (19)
O8	0.056 (4)	0.063 (3)	0.055 (4)	−0.009 (2)	0.028 (3)	−0.015 (2)
O9	0.055 (2)	0.0404 (19)	0.0336 (19)	0.0007 (17)	0.0046 (17)	−0.0005 (16)
O10	0.049 (2)	0.055 (2)	0.031 (2)	−0.005 (2)	0.0108 (18)	−0.0114 (18)
O11	0.067 (4)	0.061 (2)	0.025 (2)	0.005 (3)	0.006 (2)	0.003 (2)

O12	0.054 (2)	0.048 (2)	0.035 (2)	0.0018 (18)	0.0044 (17)	−0.0097 (17)

Geometric parameters (Å, °)

Co1—O4	2.151 (4)	C17—C20	1.402 (8)
Co1—O2	2.160 (4)	C17—H17	0.9300
Co1—O3	2.199 (4)	C18—C19	1.384 (8)
Co1—O1	2.200 (4)	C18—H18	0.9300
Co1—N1	2.279 (5)	C19—N4	1.323 (8)
Co1—N3	2.271 (5)	C19—H19	0.9300
C1—N1	1.344 (7)	C20—N4	1.311 (8)
C1—C4	1.388 (8)	C20—H20	0.9300
C1—H1	0.9300	C21—O12	1.241 (7)
C2—N1	1.326 (7)	C21—O11	1.274 (8)
C2—C3	1.377 (8)	C21—C23	1.503 (11)
C2—H2	0.9300	C22—O9	1.237 (6)
C3—C5	1.377 (7)	C22—O10	1.258 (6)
C3—H3	0.9300	C22—C27	1.529 (8)
C4—C5	1.384 (7)	C23—C24	1.390 (7)
C4—H4	0.9300	C23—N5	1.416 (10)
C5—C6	1.493 (6)	C24—C25	1.397 (8)
C6—C7	1.392 (8)	C24—H24	0.9300
C6—C8	1.407 (8)	C25—C26	1.377 (8)
C7—C10	1.380 (9)	C25—H25	0.9300
C7—H7	0.9300	C26—C27	1.405 (7)
C8—C9	1.381 (8)	C26—H26	0.9300
C8—H8	0.9300	C27—N5	1.375 (8)
C9—N2	1.346 (8)	O1—H1W	0.82 (6)
C9—H9	0.9300	O1—H2W	0.82 (3)
C10—N2	1.329 (9)	O2—H3W	0.80 (6)
C10—H10	0.9300	O2—H4W	0.81 (3)
C11—N3	1.351 (7)	O3—H5W	0.82 (6)
C11—C14	1.379 (8)	O3—H6W	0.816 (11)
C11—H11	0.9300	O4—H7W	0.82 (6)
C12—N3	1.317 (8)	O4—H8W	0.82 (5)
C12—C13	1.383 (8)	O5—H9W	0.81 (4)
C12—H12	0.9300	O5—H10W	0.82 (7)
C13—C15	1.413 (8)	O6—H11W	0.82 (4)
C13—H13	0.9300	O6—H12W	0.82 (3)
C14—C15	1.380 (8)	O7—H13W	0.82 (5)
C14—H14	0.9300	O7—H14W	0.82 (3)
C15—C16	1.482 (7)	O8—H15W	0.82 (6)
C16—C18	1.387 (8)	O8—H16W	0.82 (4)
C16—C17	1.393 (7)		
O4—Co1—O2	179.6 (2)	C18—C16—C15	122.0 (5)
O4—Co1—O3	88.71 (17)	C17—C16—C15	120.7 (4)
O2—Co1—O3	91.11 (18)	C16—C17—C20	118.7 (5)
O4—Co1—O1	91.40 (17)	C16—C17—H17	120.6
O2—Co1—O1	88.77 (17)	C20—C17—H17	120.6

O3—Co1—O1	178.5 (2)	C19—C18—C16	118.4 (5)
O4—Co1—N1	88.11 (16)	C19—C18—H18	120.8
O2—Co1—N1	91.48 (15)	C16—C18—H18	120.8
O3—Co1—N1	86.82 (17)	N4—C19—C18	125.0 (6)
O1—Co1—N1	91.71 (16)	N4—C19—H19	117.6
O4—Co1—N3	91.27 (16)	C18—C19—H19	117.5
O2—Co1—N3	89.13 (16)	N4—C20—C17	123.9 (5)
O3—Co1—N3	91.97 (17)	N4—C20—H20	118.0
O1—Co1—N3	89.49 (17)	C17—C20—H20	118.0
N1—Co1—N3	178.66 (19)	O12—C21—O11	124.3 (6)
N1—C1—C4	123.2 (5)	O12—C21—C23	118.8 (5)
N1—C1—H1	118.4	O11—C21—C23	116.8 (5)
C4—C1—H1	118.4	O9—C22—O10	125.3 (5)
N1—C2—C3	124.4 (6)	O9—C22—C27	116.9 (4)
N1—C2—H2	117.8	O10—C22—C27	117.7 (4)
C3—C2—H2	117.8	C24—C23—N5	117.7 (8)
C2—C3—C5	119.4 (5)	C24—C23—C21	121.6 (7)
C2—C3—H3	120.3	N5—C23—C21	120.7 (4)
C5—C3—H3	120.3	C23—C24—C25	120.6 (7)
C5—C4—C1	119.4 (5)	C23—C24—H24	119.7
C5—C4—H4	120.3	C25—C24—H24	119.7
C1—C4—H4	120.3	C26—C25—C24	120.6 (5)
C3—C5—C4	117.3 (5)	C26—C25—H25	119.7
C3—C5—C6	121.0 (5)	C24—C25—H25	119.7
C4—C5—C6	121.7 (5)	C25—C26—C27	120.1 (5)
C7—C6—C8	115.5 (5)	C25—C26—H26	119.9
C7—C6—C5	122.5 (5)	C27—C26—H26	119.9
C8—C6—C5	121.9 (5)	N5—C27—C26	118.9 (6)
C10—C7—C6	120.0 (6)	N5—C27—C22	121.4 (4)
C10—C7—H7	120.0	C26—C27—C22	119.7 (5)
C6—C7—H7	120.0	C2—N1—C1	116.2 (5)
C9—C8—C6	120.3 (6)	C2—N1—Co1	117.5 (4)
C9—C8—H8	119.9	C1—N1—Co1	124.9 (3)
C6—C8—H8	119.8	C10—N2—C9	115.8 (5)
N2—C9—C8	123.6 (6)	C12—N3—C11	115.8 (5)
N2—C9—H9	118.2	C12—N3—Co1	124.3 (4)
C8—C9—H9	118.2	C11—N3—Co1	119.0 (4)
N2—C10—C7	124.8 (6)	C20—N4—C19	116.6 (5)
N2—C10—H10	117.6	C27—N5—C23	122.1 (5)
C7—C10—H10	117.6	Co1—O1—H1W	115 (5)
N3—C11—C14	123.6 (5)	Co1—O1—H2W	123 (5)
N3—C11—H11	118.2	H1W—O1—H2W	115 (3)
C14—C11—H11	118.2	Co1—O2—H3W	132 (5)
N3—C12—C13	124.4 (5)	Co1—O2—H4W	95 (5)
N3—C12—H12	117.8	H3W—O2—H4W	120 (3)
C13—C12—H12	117.8	Co1—O3—H5W	125 (5)
C12—C13—C15	120.2 (5)	Co1—O3—H6W	114 (5)
C12—C13—H13	119.9	H5W—O3—H6W	114 (3)
C15—C13—H13	119.9	Co1—O4—H7W	122 (4)

C11—C14—C15	121.2 (5)	Co1—O4—H8W	127 (4)
C11—C14—H14	119.4	H7W—O4—H8W	111 (7)
C15—C14—H14	119.4	H9W—O5—H10W	115 (7)
C14—C15—C13	114.7 (5)	H11W—O6—H12W	116 (7)
C14—C15—C16	123.1 (4)	H13W—O7—H14W	112 (3)
C13—C15—C16	122.2 (5)	H15W—O8—H16W	115 (3)
C18—C16—C17	117.4 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1W···O10^{i}	0.82 (6)	1.93 (6)	2.728 (6)	162 (7)
O1—H2W···O5^{ii}	0.82 (3)	1.96 (2)	2.769 (6)	169 (8)
O2—H3W···O8^{iii}	0.80 (6)	2.05 (6)	2.843 (8)	173 (8)
O2—H4W···N2^{iv}	0.81 (3)	2.06 (4)	2.755 (6)	145 (7)
O3—H5W···O7	0.82 (6)	1.95 (6)	2.772 (6)	176 (10)
O3—H6W···O8^{v}	0.816 (11)	2.01 (3)	2.789 (7)	161 (6)
O4—H7W···O5	0.82 (6)	2.06 (3)	2.826 (7)	155 (7)
O4—H8W···N4^{v}	0.82 (5)	2.00 (3)	2.769 (6)	155 (7)
O5—H9W···O9^{i}	0.81 (4)	2.00 (3)	2.777 (7)	161 (7)
O5—H10W···O7^{vi}	0.82 (7)	2.01 (6)	2.822 (8)	176 (7)
O6—H11W···O12^{vii}	0.82 (4)	2.16 (4)	2.825 (6)	137 (6)
O7—H14W···O11	0.82 (3)	1.82 (4)	2.631 (7)	174 (8)
O8—H15W···O10	0.82 (6)	1.96 (7)	2.746 (8)	162 (7)
O8—H16W···O6^{viii}	0.82 (4)	1.94 (4)	2.747 (9)	172 (8)
O6—H12W···O11	0.82 (3)	2.30 (5)	2.933 (7)	135 (7)

Symmetry codes: (i) *x*+1/2, −*y*+3/2, *z*+1/2; (ii) *x*, *y*+1, *z*; (iii) *x*, −*y*+2, *z*+1/2; (iv) *x*, −*y*+2, *z*−1/2; (v) *x*, −*y*+1, *z*+1/2; (vi) *x*+1/2, *y*−1/2, *z*; (vii) *x*, *y*−1, *z*; (viii) *x*, −*y*+1, *z*−1/2.

Fig. 1

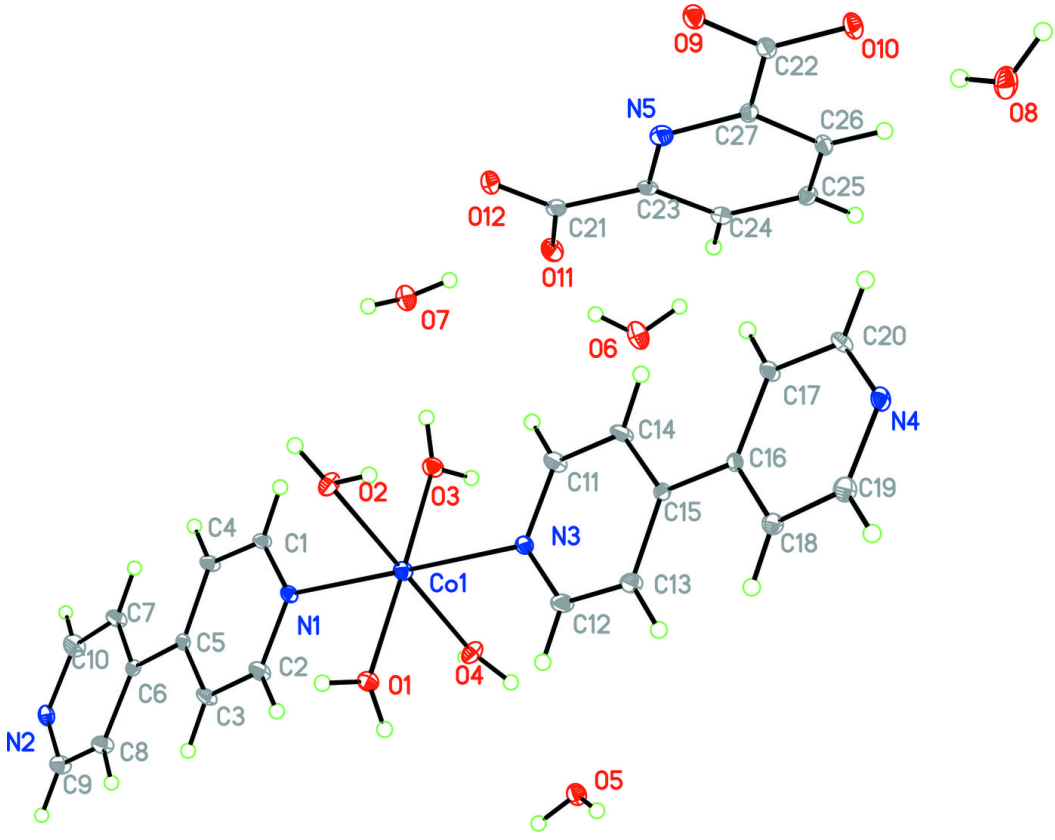
O9
O10
C22
O8
N5
C27
C26
C25
O12
C23
C21
C24
O11
O7
O6
C20
C17
N4
C14
C16
C11
C19
O2
O3
C15
C4
C1
N3
C18
Co1
C13
C7
N1
C12
C5
C10
C2
O1
O4
C6
C3
N2
C8
C9
O5

Fig. 2