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Bis(2,4,6-triamino-1,3,5-triazin-1-ium) hexaaquacobalt(II) bis[bis(pyridine-2,6-dicarboxylato)cobaltate(II)] tetrahydrate

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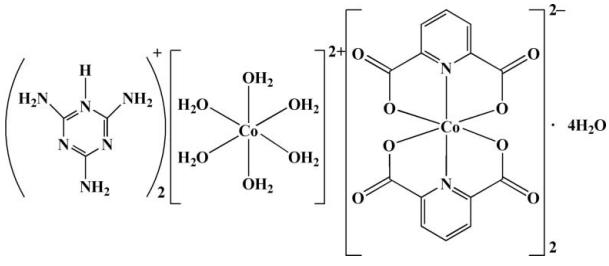
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.027; wR factor = 0.071; data-to-parameter ratio = 14.8.

The title compound, $(C_3H_7N_6)_2[Co(H_2O)_6][Co(C_7H_3NO_4)_2]_2\cdot 4H_2O$, or (tataH)$_2$[Co(H$_2$O)$_6$][Co(pydc)$_2$]$_2\cdot$4H$_2$O (where tata is 2,4,6-triamino-1,3,5-triazine and pydc is pyridine-2,6-dicarboxylic acid), was obtained by reaction of $Co(NO_3)_2\cdot 6H_2O$ with the proton-transfer compound (tataH)$_2$(pydc) in aqueous solution. The [Co(pydc)$_2$]$^{2-}$ anion is a six-coordinate Co^{II} complex with a distorted octahedral coordination geometry. The structure also contains hexaaquacobalt(II) cations (site symmetry $\overline{1}$), (tataH)$^+$ cations and uncoordinated water molecules. The two(pydc)$^{2-}$ ligands in each [Co(pydc)$_2$]$^{2-}$ anion are almost perpendicular to each other [dihedral angle between their mean planes = 82.3 (1)°]. There is extensive O—H···O, N—H···N, O—H···N and C—H···O hydrogen bonding in the structure, as well as π–π stacking between (pydc)$^{2-}$ ligands with an interplanar distance of 3.484 (15) Å.

Related literature

For related literature, see: Aghabozorg, Attar Gharamaleki *et al.* (2007); Aghabozorg, Daneshvar *et al.* (2007); Sheshmani *et al.* (2006).



Experimental

Crystal data

$(C_3H_7N_6)_2[Co(H_2O)_6]$-$[Co(C_7H_3NO_4)_2]_2\cdot 4H_2O$
M_r = 1271.66
Triclinic, $P\overline{1}$
a = 8.4003 (6) Å
b = 11.3014 (7) Å
c = 13.8794 (10) Å
α = 95.901 (6)°
β = 106.017 (5)°
γ = 107.133 (5)°
V = 1185.73 (14) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 120 (2) K
0.50 × 0.50 × 0.45 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 2004)
T_{min} = 0.570, T_{max} = 0.595
14236 measured reflections
6289 independent reflections
6111 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.071
S = 1.06
6289 reflections
426 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O13^{i}	0.83 (2)	1.97 (2)	2.7982 (18)	178 (3)
N3—H3C···O3	0.84 (2)	2.21 (2)	3.0041 (17)	159 (2)
N5—H5B···O3^{ii}	0.83 (2)	2.35 (2)	2.9713 (16)	133 (2)
N5—H5C···N4^{ii}	0.82 (2)	2.16 (2)	2.9765 (17)	178 (3)
N7—H7A···O10^{ii}	0.82 (2)	2.22 (2)	3.0291 (16)	169 (2)
N7—H7B···O7^{i}	0.80 (2)	2.26 (2)	3.0560 (17)	172 (2)
N8—H8···O8^{i}	0.85 (2)	1.89 (2)	2.7404 (17)	174 (2)
O9—H9A···N6^{ii}	0.79 (3)	1.94 (3)	2.7298 (16)	179 (4)
O9—H9B···O2^{iii}	0.87 (3)	1.89 (3)	2.7263 (16)	162 (3)
O10—H10B···O12	0.81 (2)	1.88 (3)	2.6759 (17)	167 (3)
O10—H10C···O4^{iv}	0.81 (2)	1.97 (2)	2.7675 (15)	171 (3)
O11—H11B···O5	0.80 (3)	1.97 (2)	2.7313 (14)	157 (2)
O11—H11C···O2^{v}	0.83 (2)	1.90 (2)	2.7101 (16)	165 (2)
O12—H12B···O4^{vi}	0.79 (3)	2.06 (3)	2.8389 (17)	174 (2)
O12—H12C···O6	0.84 (3)	1.98 (3)	2.8196 (16)	171 (2)
O13—H13A···O1^{vii}	0.77 (3)	2.01 (3)	2.7642 (16)	171 (3)
O13—H13B···O8	0.82 (3)	1.87 (3)	2.6642 (14)	163 (2)
C4—H4···O13^{viii}	0.93	2.43	3.164 (2)	136
C10—H10A···O6^{ix}	0.93	2.45	3.344 (2)	162

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2263).

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supplementary materials

Acta Cryst. (2008). E**64**, m187-m188 [**doi:10.1107/S1600536807066032**]

Bis(2,4,6-triamino-1,3,5-triazin-1-ium) hexaaquacobalt(II) bis[bis(pyridine-2,6-dicarboxylato)cobaltate(II)] tetrahydrate

H. Aghabozorg, J. Attar Gharamaleki, S. Daneshvar, M. Ghadermazi and H. R. Khavasi

Comment

Recently, we have reported the reactions between $Co(NO_3)_2{\cdot}6H_2O$ and two proton-transfer compounds: $(GH)_2(pydc)$ (where G is guanidine) and $(pipzH_2)(pydc)$ (where pipz is piperazine) in a 1:2 molar ratio. These reactions lead to the formation of the complexes $(GH)_2[Co(H_2O)_6][Co(pydc)_2]_2$ (Sheshmani *et al.*, 2006) and $(pipzH_2)[Co(H_2O)_6][Co(pydc)_2]_2{\cdot}8H_2O$ (Aghabozorg, Attar Gharamaleki *et al.*, 2007), respectively.

Here, we report the synthesis and X-ray crystal structure of the title compound (Fig. 1). The compound contains $[Co(pydc)_2]^{2-}$ anions, $[Co(H_2O)_6]^{2+}$ cations (site symmetry $\bar{1}$), and $(tataH)^+$ cations. In the $[Co(pydc)_2]^{2-}$ anions, the Co^{II} atom is hexacoordinated by two N atoms (N1 and N2) and four O atoms (O1, O3, O5 and O7) from the carboxylate groups of two $(pydc)^{2-}$ groups that act as tridentate ligands. The coordination geometry is distorted octahedral, with atoms N1 and N2 occupying axial positions and the O atoms forming the equatorial plane. The N1—Co2—N2 angle deviates *ca* 7.7° from linearity. The mean Co—N and Co—O bond lengths for Co1 are 2.0214 (11) and 2.1658 (10) Å, respectively, consistent with similar complexes in the literature. The dihedral angle between the mean planes of the two $(pydc)^{2-}$ groups is 82.3 (1)°.

There is extensive O—H···O, N—H···O, N—H···N and C—H···O hydrogen bonding in the structure, as well as π–π stacking between $(pydc)^{2-}$ ligands with an interplanar distance of 3.484 (15) Å (symmetry operator: $-x, -y + 1, -z + 1$). Atom O8 of the C14═O8 carboxyl group lies above the N2/C9–C13 ring with an O···centroid distance of 3.240 (1) Å (symmetry operator: $x, -y + 1, -z$).

Experimental

The proton-transfer compound, $(tataH)_2(pydc)$, was prepared by the reaction of pyridine-2,6-dicarboxylic acid ($pydcH_2$) with 2,4,6-triamino-1,3,5-triazine (tata). The reaction between $Co(NO_3)_2{\cdot}6H_2O$ (115 mg, 0.5 mmol) in water (20 ml) and $(tataH)_2(pydc)$ (420 mg, 1.0 mmol) in water (20 ml), in a 1:2 molar ratio gave a violet crystalline compound after slow evaporation of the solvent at room temperature.

Refinement

The N-bound and O-bound H atoms were located in difference Fourier maps and their positions were freely refined. Other H atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

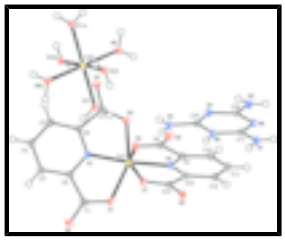

Fig. 1. The molecular structure with displacement ellipsoids drawn at the 50% probability level for non-H atoms. Water molecules are omitted. The suffix a denotes atoms generated by the symmetry operator −*x*, −*y*, −*z* + 1.

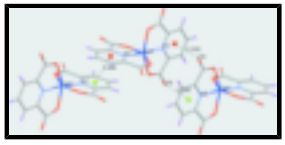

Fig. 2. π···π Stacking interaction between two aromatic rings of $(pydc)^{2-}$ units, with inter-planar distance of 3.484 (15) Å [−*x*, −*y* + 1, −*z* + 1]; C—O···π stacking interactions between CO groups of carboxylate fragments with aromatic rings of $(pydc)^{2-}$ with distances of 3.240 (1) Å for C14–O8···*Cg*1 (*x*, −*y* + 1, −*z*) [*Cg*1 is the centroid for N2/C9–C13 ring].

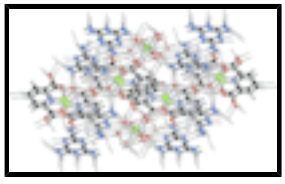

Fig. 3. Unit cell packing. Hydrogen bonds are shown as dashed lines.

Bis(2,4,6-triamino-1,3,5-triazin-1-ium) hexaaquacobalt(II) bis[bis(pyridine-2,6-dicarboxylato)cobaltate(II)] tetrahydrate

Crystal data

$(C_3H_7N_6)_2[Co(H_2O)_6][Co(C_7H_3NO_4)_2]_2{\cdot}4H_2O$	$Z = 1$
$M_r = 1271.66$	$F_{000} = 651$
Triclinic, $P\overline{1}$	$D_x = 1.781$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.4003$ (6) Å	Cell parameters from 2500 reflections
$b = 11.3014$ (7) Å	$\theta = 1.9$–29.2°
$c = 13.8794$ (10) Å	$\mu = 1.15$ mm^{-1}
$\alpha = 95.901$ (6)°	$T = 120$ (2) K
$\beta = 106.017$ (5)°	Block, violet
$\gamma = 107.133$ (5)°	0.50 × 0.50 × 0.45 mm
$V = 1185.73$ (14) Å^3	

Data collection

Stoe IPDSII diffractometer	6289 independent reflections
Radiation source: fine-focus sealed tube	6111 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.021$
$T = 120(2)$ K	$\theta_{max} = 29.2^\circ$
φ scans	$\theta_{min} = 1.9^\circ$
Absorption correction: numerical (X-SHAPE; Stoe & Cie, 2004)	$h = -11 \rightarrow 11$

T_{min} = 0.570, T_{max} = 0.595
14236 measured reflections

k = −15→15
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.071
S = 1.06
6289 reflections
426 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 1.0178P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.019
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}
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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.09807 (17)	0.59767 (12)	0.39201 (10)	0.0120 (2)
C2	0.19794 (16)	0.52881 (12)	0.46046 (9)	0.0100 (2)
C3	0.26752 (17)	0.56041 (12)	0.56675 (10)	0.0120 (2)
H3A	0.2520	0.6273	0.6035	0.014*
C4	0.36138 (17)	0.48851 (12)	0.61643 (10)	0.0123 (2)
H4	0.4087	0.5068	0.6874	0.015*
C5	0.38413 (17)	0.38926 (12)	0.55950 (10)	0.0110 (2)
H5A	0.4481	0.3416	0.5917	0.013*
C6	0.30917 (16)	0.36313 (11)	0.45369 (9)	0.0092 (2)
C7	0.32416 (16)	0.26121 (11)	0.37973 (10)	0.0099 (2)
C8	−0.23329 (17)	0.17773 (12)	0.16471 (10)	0.0110 (2)
C9	−0.17660 (16)	0.21879 (12)	0.07477 (10)	0.0102 (2)
C10	−0.26571 (17)	0.16132 (12)	−0.02722 (10)	0.0118 (2)
H10A	−0.3694	0.0926	−0.0460	0.014*
C11	−0.19517 (17)	0.20971 (12)	−0.10097 (10)	0.0125 (2)

H11A	−0.2524	0.1736	−0.1700	0.015*
C12	−0.03839 (17)	0.31260 (12)	−0.07062 (10)	0.0118 (2)
H12A	0.0096	0.3464	−0.1188	0.014*
C13	0.04411 (16)	0.36325 (11)	0.03343 (9)	0.0096 (2)
C14	0.21779 (16)	0.47113 (12)	0.08186 (10)	0.0102 (2)
C15	0.34004 (16)	0.22483 (12)	0.01662 (10)	0.0102 (2)
C16	0.12106 (17)	0.07415 (12)	−0.11206 (10)	0.0112 (2)
C17	0.33515 (17)	0.21334 (12)	−0.15514 (10)	0.0111 (2)
N1	0.21838 (14)	0.43202 (10)	0.40734 (8)	0.00895 (19)
N2	−0.02564 (14)	0.31650 (10)	0.10290 (8)	0.00952 (19)
N3	0.41635 (16)	0.28384 (11)	0.11324 (9)	0.0126 (2)
H3B	0.504 (3)	0.349 (2)	0.1304 (17)	0.027 (5)*
H3C	0.370 (3)	0.258 (2)	0.1568 (17)	0.021 (5)*
N4	0.19481 (15)	0.12353 (10)	−0.01054 (8)	0.0114 (2)
N5	−0.02803 (16)	−0.02294 (11)	−0.14102 (9)	0.0145 (2)
H5B	−0.079 (3)	−0.057 (2)	−0.2023 (19)	0.029 (6)*
H5C	−0.073 (3)	−0.049 (2)	−0.0984 (18)	0.025 (5)*
N6	0.18535 (15)	0.11571 (11)	−0.18643 (8)	0.0118 (2)
N7	0.41327 (17)	0.25597 (11)	−0.22155 (9)	0.0142 (2)
H7A	0.369 (3)	0.218 (2)	−0.2810 (17)	0.022 (5)*
H7B	0.497 (3)	0.320 (2)	−0.2040 (17)	0.022 (5)*
N8	0.41245 (15)	0.27160 (11)	−0.05467 (8)	0.0113 (2)
H8	0.504 (3)	0.337 (2)	−0.0403 (19)	0.034 (6)*
O1	0.04288 (13)	0.54960 (9)	0.29686 (7)	0.01419 (18)
O2	0.07887 (16)	0.69381 (10)	0.43161 (8)	0.0199 (2)
O3	0.26322 (13)	0.26350 (9)	0.28504 (7)	0.01189 (17)
O4	0.39502 (13)	0.18586 (9)	0.41537 (8)	0.01399 (18)
O5	−0.12884 (13)	0.24112 (9)	0.25325 (7)	0.01391 (18)
O6	−0.37131 (13)	0.08811 (10)	0.14719 (8)	0.01572 (19)
O7	0.27238 (12)	0.50218 (9)	0.17825 (7)	0.01198 (17)
O8	0.29441 (13)	0.52186 (9)	0.02292 (7)	0.01449 (18)
O9	0.04230 (14)	−0.08822 (10)	0.37722 (8)	0.01480 (19)
H9A	−0.024 (4)	−0.097 (3)	0.322 (2)	0.043 (7)*
H9B	0.053 (3)	−0.162 (3)	0.381 (2)	0.043 (7)*
O10	−0.27658 (13)	−0.08879 (9)	0.43229 (8)	0.01282 (18)
H10B	−0.331 (3)	−0.047 (2)	0.404 (2)	0.035 (6)*
H10C	−0.321 (3)	−0.116 (2)	0.4736 (19)	0.032 (6)*
O11	−0.02330 (13)	0.15266 (9)	0.42733 (8)	0.01306 (18)
H11B	−0.071 (3)	0.158 (2)	0.370 (2)	0.033 (6)*
H11C	−0.044 (3)	0.207 (2)	0.4624 (18)	0.028 (6)*
O12	−0.47942 (15)	0.01920 (11)	0.31460 (9)	0.0196 (2)
H12B	−0.512 (3)	0.069 (2)	0.340 (2)	0.036 (6)*
H12C	−0.443 (3)	0.048 (2)	0.268 (2)	0.033 (6)*
O13	0.29453 (14)	0.49240 (11)	−0.16999 (8)	0.0180 (2)
H13A	0.205 (4)	0.480 (2)	−0.210 (2)	0.039 (7)*
H13B	0.277 (3)	0.488 (2)	−0.115 (2)	0.037 (6)*
Co1	0.10510 (2)	0.385862 (16)	0.253625 (12)	0.00886 (5)
Co2	0.0000	0.0000	0.5000	0.01165 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0127 (5)	0.0121 (5)	0.0124 (6)	0.0050 (4)	0.0048 (4)	0.0029 (4)
C2	0.0104 (5)	0.0095 (5)	0.0101 (5)	0.0027 (4)	0.0042 (4)	0.0016 (4)
C3	0.0132 (5)	0.0119 (5)	0.0100 (5)	0.0032 (4)	0.0047 (4)	−0.0005 (4)
C4	0.0133 (5)	0.0131 (5)	0.0086 (5)	0.0016 (4)	0.0039 (4)	0.0011 (4)
C5	0.0112 (5)	0.0108 (5)	0.0101 (5)	0.0022 (4)	0.0032 (4)	0.0037 (4)
C6	0.0094 (5)	0.0083 (5)	0.0096 (5)	0.0019 (4)	0.0039 (4)	0.0018 (4)
C7	0.0100 (5)	0.0087 (5)	0.0111 (5)	0.0019 (4)	0.0049 (4)	0.0017 (4)
C8	0.0118 (5)	0.0109 (5)	0.0111 (5)	0.0045 (4)	0.0037 (4)	0.0034 (4)
C9	0.0107 (5)	0.0094 (5)	0.0108 (5)	0.0036 (4)	0.0034 (4)	0.0023 (4)
C10	0.0110 (5)	0.0107 (5)	0.0120 (6)	0.0029 (4)	0.0019 (4)	0.0015 (4)
C11	0.0137 (6)	0.0137 (6)	0.0082 (5)	0.0046 (5)	0.0012 (4)	0.0001 (4)
C12	0.0133 (6)	0.0131 (6)	0.0089 (5)	0.0044 (5)	0.0035 (4)	0.0022 (4)
C13	0.0104 (5)	0.0092 (5)	0.0092 (5)	0.0034 (4)	0.0029 (4)	0.0018 (4)
C14	0.0108 (5)	0.0087 (5)	0.0108 (5)	0.0032 (4)	0.0036 (4)	0.0015 (4)
C15	0.0116 (5)	0.0102 (5)	0.0104 (5)	0.0055 (4)	0.0040 (4)	0.0024 (4)
C16	0.0129 (5)	0.0092 (5)	0.0118 (6)	0.0045 (4)	0.0036 (4)	0.0020 (4)
C17	0.0132 (5)	0.0107 (5)	0.0103 (5)	0.0054 (4)	0.0039 (4)	0.0018 (4)
N1	0.0094 (4)	0.0086 (4)	0.0083 (4)	0.0019 (4)	0.0032 (4)	0.0015 (4)
N2	0.0105 (5)	0.0094 (4)	0.0084 (4)	0.0034 (4)	0.0026 (4)	0.0017 (4)
N3	0.0137 (5)	0.0129 (5)	0.0095 (5)	0.0021 (4)	0.0039 (4)	0.0012 (4)
N4	0.0123 (5)	0.0107 (5)	0.0098 (5)	0.0024 (4)	0.0032 (4)	0.0015 (4)
N5	0.0147 (5)	0.0131 (5)	0.0115 (5)	−0.0002 (4)	0.0039 (4)	0.0000 (4)
N6	0.0131 (5)	0.0113 (5)	0.0094 (5)	0.0025 (4)	0.0032 (4)	0.0014 (4)
N7	0.0169 (5)	0.0126 (5)	0.0103 (5)	0.0003 (4)	0.0059 (4)	0.0005 (4)
N8	0.0115 (5)	0.0113 (5)	0.0092 (5)	0.0013 (4)	0.0038 (4)	0.0008 (4)
O1	0.0176 (5)	0.0155 (4)	0.0107 (4)	0.0089 (4)	0.0033 (4)	0.0020 (3)
O2	0.0300 (6)	0.0169 (5)	0.0167 (5)	0.0149 (4)	0.0067 (4)	0.0016 (4)
O3	0.0142 (4)	0.0128 (4)	0.0088 (4)	0.0053 (3)	0.0035 (3)	0.0011 (3)
O4	0.0184 (5)	0.0137 (4)	0.0146 (4)	0.0089 (4)	0.0078 (4)	0.0057 (3)
O5	0.0141 (4)	0.0150 (4)	0.0096 (4)	0.0009 (4)	0.0034 (3)	0.0028 (3)
O6	0.0131 (4)	0.0149 (4)	0.0155 (4)	−0.0006 (4)	0.0049 (4)	0.0029 (4)
O7	0.0126 (4)	0.0122 (4)	0.0092 (4)	0.0018 (3)	0.0033 (3)	0.0015 (3)
O8	0.0157 (4)	0.0147 (4)	0.0110 (4)	0.0005 (4)	0.0061 (4)	0.0026 (3)
O9	0.0201 (5)	0.0161 (5)	0.0092 (4)	0.0093 (4)	0.0034 (4)	0.0011 (4)
O10	0.0156 (4)	0.0126 (4)	0.0115 (4)	0.0053 (4)	0.0050 (4)	0.0044 (3)
O11	0.0183 (5)	0.0114 (4)	0.0108 (4)	0.0066 (4)	0.0045 (4)	0.0036 (3)
O12	0.0271 (6)	0.0227 (5)	0.0190 (5)	0.0157 (5)	0.0131 (4)	0.0095 (4)
O13	0.0139 (5)	0.0264 (5)	0.0110 (4)	0.0030 (4)	0.0041 (4)	0.0031 (4)
Co1	0.01010 (9)	0.00890 (8)	0.00667 (8)	0.00262 (6)	0.00218 (6)	0.00084 (6)
Co2	0.01542 (12)	0.01014 (11)	0.00968 (11)	0.00476 (9)	0.00401 (9)	0.00194 (8)

Geometric parameters (Å, °)

C1—O2	1.2401 (16)	C16—N4	1.3541 (16)
C1—O1	1.2729 (16)	C16—N6	1.3548 (16)

C1—C2	1.5195 (17)	C17—N7	1.3232 (17)
C2—N1	1.3358 (16)	C17—N6	1.3310 (17)
C2—C3	1.3922 (17)	C17—N8	1.3636 (16)
C3—C4	1.3965 (18)	N1—Co1	2.0218 (11)
C3—H3A	0.930	N2—Co1	2.0211 (11)
C4—C5	1.3952 (18)	N3—H3B	0.83 (2)
C4—H4	0.930	N3—H3C	0.84 (2)
C5—C6	1.3898 (17)	N5—H5B	0.83 (2)
C5—H5A	0.930	N5—H5C	0.82 (2)
C6—N1	1.3356 (16)	N7—H7A	0.82 (2)
C6—C7	1.5199 (17)	N7—H7B	0.81 (2)
C7—O4	1.2438 (16)	N8—H8	0.86 (3)
C7—O3	1.2781 (15)	O1—Co1	2.1383 (10)
C8—O6	1.2373 (16)	O3—Co1	2.1802 (10)
C8—O5	1.2833 (16)	O5—Co1	2.1532 (10)
C8—C9	1.5223 (17)	O7—Co1	2.1916 (9)
C9—N2	1.3391 (16)	O9—Co2	2.0538 (10)
C9—C10	1.3877 (17)	O9—H9A	0.79 (3)
C10—C11	1.3989 (18)	O9—H9B	0.87 (3)
C10—H10A	0.930	O10—Co2	2.1250 (10)
C11—C12	1.3982 (18)	O10—H10B	0.81 (3)
C11—H11A	0.930	O10—H10C	0.81 (3)
C12—C13	1.3920 (17)	O11—Co2	2.1166 (10)
C12—H12A	0.930	O11—H11B	0.81 (3)
C13—N2	1.3364 (16)	O11—H11C	0.83 (3)
C13—C14	1.5196 (17)	O12—H12B	0.79 (3)
C14—O8	1.2576 (15)	O12—H12C	0.85 (3)
C14—O7	1.2624 (15)	O13—H13A	0.77 (3)
C15—N3	1.3205 (17)	O13—H13B	0.83 (3)
C15—N4	1.3324 (16)	Co2—O9^{i}	2.0538 (10)
C15—N8	1.3706 (16)	Co2—O11^{i}	2.1166 (10)
C16—N5	1.3251 (17)	Co2—O10^{i}	2.1250 (10)
O2—C1—O1	126.05 (12)	C15—N3—H3C	118.9 (14)
O2—C1—C2	118.92 (12)	H3B—N3—H3C	120 (2)
O1—C1—C2	115.03 (11)	C15—N4—C16	115.97 (11)
N1—C2—C3	121.29 (12)	C16—N5—H5B	121.4 (16)
N1—C2—C1	112.54 (11)	C16—N5—H5C	120.0 (16)
C3—C2—C1	126.15 (11)	H5B—N5—H5C	119 (2)
C2—C3—C4	117.93 (12)	C17—N6—C16	115.98 (11)
C2—C3—H3A	121.0	C17—N7—H7A	117.6 (15)
C4—C3—H3A	121.0	C17—N7—H7B	120.4 (15)
C5—C4—C3	119.94 (12)	H7A—N7—H7B	122 (2)
C5—C4—H4	120.0	C17—N8—C15	119.54 (11)
C3—C4—H4	120.0	C17—N8—H8	116.7 (16)
C6—C5—C4	118.55 (12)	C15—N8—H8	123.8 (16)
C6—C5—H5A	120.7	C1—O1—Co1	116.52 (8)
C4—C5—H5A	120.7	C7—O3—Co1	114.43 (8)
N1—C6—C5	120.80 (11)	C8—O5—Co1	115.52 (8)

N1—C6—C7	113.45 (11)	C14—O7—Co1	114.48 (8)
C5—C6—C7	125.72 (11)	Co2—O9—H9A	119 (2)
O4—C7—O3	126.28 (12)	Co2—O9—H9B	116.3 (18)
O4—C7—C6	118.49 (11)	H9A—O9—H9B	105 (3)
O3—C7—C6	115.22 (11)	Co2—O10—H10B	117.2 (18)
O6—C8—O5	126.18 (12)	Co2—O10—H10C	111.2 (17)
O6—C8—C9	118.67 (11)	H10B—O10—H10C	107 (2)
O5—C8—C9	115.14 (11)	Co2—O11—H11B	134.2 (18)
N2—C9—C10	121.47 (12)	Co2—O11—H11C	113.0 (16)
N2—C9—C8	113.40 (11)	H11B—O11—H11C	102 (2)
C10—C9—C8	125.11 (11)	H12B—O12—H12C	108 (2)
C9—C10—C11	118.14 (12)	H13A—O13—H13B	107 (3)
C9—C10—H10A	120.9	N2—Co1—N1	172.24 (4)
C11—C10—H10A	120.9	N2—Co1—O1	107.89 (4)
C12—C11—C10	119.79 (12)	N1—Co1—O1	76.33 (4)
C12—C11—H11A	120.1	N2—Co1—O5	76.99 (4)
C10—C11—H11A	120.1	N1—Co1—O5	96.02 (4)
C13—C12—C11	118.36 (12)	O1—Co1—O5	99.47 (4)
C13—C12—H12A	120.8	N2—Co1—O3	100.34 (4)
C11—C12—H12A	120.8	N1—Co1—O3	76.35 (4)
N2—C13—C12	121.12 (11)	O1—Co1—O3	151.15 (4)
N2—C13—C14	112.50 (11)	O5—Co1—O3	92.44 (4)
C12—C13—C14	126.37 (11)	N2—Co1—O7	76.19 (4)
O8—C14—O7	125.66 (12)	N1—Co1—O7	110.86 (4)
O8—C14—C13	117.54 (11)	O1—Co1—O7	87.05 (4)
O7—C14—C13	116.80 (11)	O5—Co1—O7	153.11 (4)
N3—C15—N4	120.51 (12)	O3—Co1—O7	94.11 (4)
N3—C15—N8	118.32 (12)	O9—Co2—O9^{i}	180.000 (1)
N4—C15—N8	121.16 (11)	O9—Co2—O11^{i}	88.64 (4)
N5—C16—N4	116.86 (12)	O9^{i}—Co2—O11^{i}	91.36 (4)
N5—C16—N6	117.28 (12)	O9—Co2—O11	91.36 (4)
N4—C16—N6	125.86 (12)	O9^{i}—Co2—O11	88.64 (4)
N7—C17—N6	120.34 (12)	O11^{i}—Co2—O11	180.0
N7—C17—N8	118.30 (12)	O9—Co2—O10^{i}	89.04 (4)
N6—C17—N8	121.36 (12)	O9^{i}—Co2—O10^{i}	90.96 (4)
C6—N1—C2	121.47 (11)	O11^{i}—Co2—O10^{i}	87.97 (4)
C6—N1—Co1	119.06 (8)	O11—Co2—O10^{i}	92.03 (4)
C2—N1—Co1	119.45 (9)	O9—Co2—O10	90.96 (4)
C13—N2—C9	121.11 (11)	O9^{i}—Co2—O10	89.04 (4)
C13—N2—Co1	119.93 (9)	O11^{i}—Co2—O10	92.03 (4)
C9—N2—Co1	118.84 (9)	O11—Co2—O10	87.97 (4)
C15—N3—H3B	121.1 (16)	O10^{i}—Co2—O10	180.00 (6)
O2—C1—C2—N1	−175.99 (12)	N5—C16—N6—C17	179.97 (12)
O1—C1—C2—N1	3.28 (16)	N4—C16—N6—C17	0.49 (19)
O2—C1—C2—C3	2.4 (2)	N7—C17—N8—C15	−176.18 (12)
O1—C1—C2—C3	−178.33 (12)	N6—C17—N8—C15	3.55 (19)

N1—C2—C3—C4	0.67 (19)	N3—C15—N8—C17	−179.25 (12)
C1—C2—C3—C4	−177.60 (12)	N4—C15—N8—C17	−0.25 (19)
C2—C3—C4—C5	0.53 (19)	O2—C1—O1—Co1	178.25 (11)
C3—C4—C5—C6	−1.09 (18)	C2—C1—O1—Co1	−0.95 (14)
C4—C5—C6—N1	0.48 (18)	O4—C7—O3—Co1	168.69 (10)
C4—C5—C6—C7	178.42 (11)	C6—C7—O3—Co1	−12.44 (13)
N1—C6—C7—O4	−174.80 (11)	O6—C8—O5—Co1	177.49 (11)
C5—C6—C7—O4	7.12 (19)	C9—C8—O5—Co1	−1.93 (14)
N1—C6—C7—O3	6.23 (15)	O8—C14—O7—Co1	−177.89 (10)
C5—C6—C7—O3	−171.84 (12)	C13—C14—O7—Co1	2.28 (14)
O6—C8—C9—N2	179.96 (12)	C13—N2—Co1—O1	84.95 (10)
O5—C8—C9—N2	−0.58 (16)	C9—N2—Co1—O1	−99.00 (10)
O6—C8—C9—C10	−1.74 (19)	C13—N2—Co1—O5	−179.15 (10)
O5—C8—C9—C10	177.73 (12)	C9—N2—Co1—O5	−3.10 (9)
N2—C9—C10—C11	−1.12 (19)	C13—N2—Co1—O3	−89.02 (10)
C8—C9—C10—C11	−179.30 (12)	C9—N2—Co1—O3	87.03 (10)
C9—C10—C11—C12	0.45 (19)	C13—N2—Co1—O7	2.71 (9)
C10—C11—C12—C13	0.63 (19)	C9—N2—Co1—O7	178.76 (10)
C11—C12—C13—N2	−1.12 (19)	C6—N1—Co1—O1	−178.41 (10)
C11—C12—C13—C14	177.53 (12)	C2—N1—Co1—O1	2.95 (9)
N2—C13—C14—O8	−179.98 (11)	C6—N1—Co1—O5	83.28 (9)
C12—C13—C14—O8	1.28 (19)	C2—N1—Co1—O5	−95.36 (9)
N2—C13—C14—O7	−0.13 (16)	C6—N1—Co1—O3	−7.78 (9)
C12—C13—C14—O7	−178.88 (12)	C2—N1—Co1—O3	173.58 (10)
C5—C6—N1—C2	0.73 (18)	C6—N1—Co1—O7	−97.00 (9)
C7—C6—N1—C2	−177.45 (11)	C2—N1—Co1—O7	84.36 (10)
C5—C6—N1—Co1	−177.89 (9)	C1—O1—Co1—N2	172.32 (9)
C7—C6—N1—Co1	3.94 (14)	C1—O1—Co1—N1	−0.91 (9)
C3—C2—N1—C6	−1.32 (18)	C1—O1—Co1—O5	93.04 (10)
C1—C2—N1—C6	177.17 (11)	C1—O1—Co1—O3	−20.05 (14)
C3—C2—N1—Co1	177.29 (9)	C1—O1—Co1—O7	−113.22 (10)
C1—C2—N1—Co1	−4.23 (14)	C8—O5—Co1—N2	2.70 (9)
C12—C13—N2—C9	0.48 (19)	C8—O5—Co1—N1	−173.89 (9)
C14—C13—N2—C9	−178.34 (11)	C8—O5—Co1—O1	109.02 (9)
C12—C13—N2—Co1	176.44 (9)	C8—O5—Co1—O3	−97.36 (9)
C14—C13—N2—Co1	−2.38 (14)	C8—O5—Co1—O7	6.70 (15)
C10—C9—N2—C13	0.67 (19)	C7—O3—Co1—N2	−161.61 (9)
C8—C9—N2—C13	179.04 (11)	C7—O3—Co1—N1	11.20 (9)
C10—C9—N2—Co1	−175.33 (9)	C7—O3—Co1—O1	30.34 (13)
C8—C9—N2—Co1	3.04 (14)	C7—O3—Co1—O5	−84.40 (9)
N3—C15—N4—C16	176.38 (12)	C7—O3—Co1—O7	121.69 (9)
N8—C15—N4—C16	−2.61 (18)	C14—O7—Co1—N2	−2.67 (9)
N5—C16—N4—C15	−176.90 (12)	C14—O7—Co1—N1	173.94 (9)
N6—C16—N4—C15	2.58 (19)	C14—O7—Co1—O1	−111.90 (9)
N7—C17—N6—C16	176.15 (12)	C14—O7—Co1—O5	−6.68 (14)
N8—C17—N6—C16	−3.57 (18)	C14—O7—Co1—O3	96.99 (9)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···O13^{ii}	0.83 (2)	1.97 (2)	2.7982 (18)	178 (3)
N3—H3C···O3	0.84 (2)	2.21 (2)	3.0041 (17)	159 (2)
N5—H5B···O3^{iii}	0.83 (2)	2.35 (2)	2.9713 (16)	133 (2)
N5—H5C···N4^{iii}	0.82 (2)	2.16 (2)	2.9765 (17)	178 (3)
N7—H7A···O10^{iii}	0.82 (2)	2.22 (2)	3.0291 (16)	169 (2)
N7—H7B···O7^{ii}	0.80 (2)	2.26 (2)	3.0560 (17)	172 (2)
N8—H8···O8^{ii}	0.85 (2)	1.89 (2)	2.7404 (17)	174 (2)
O9—H9A···N6^{iii}	0.79 (3)	1.94 (3)	2.7298 (16)	179 (4)
O9—H9B···O2^{iv}	0.87 (3)	1.89 (3)	2.7263 (16)	162 (3)
O10—H10B···O12	0.81 (2)	1.88 (3)	2.6759 (17)	167 (3)
O10—H10C···O4^{i}	0.81 (2)	1.97 (2)	2.7675 (15)	171 (3)
O11—H11B···O5	0.80 (3)	1.97 (2)	2.7313 (14)	157 (2)
O11—H11C···O2^{v}	0.83 (2)	1.90 (2)	2.7101 (16)	165 (2)
O12—H12B···O4^{vi}	0.79 (3)	2.06 (3)	2.8389 (17)	174 (2)
O12—H12C···O6	0.84 (3)	1.98 (3)	2.8196 (16)	171 (2)
O13—H13A···O1^{vii}	0.77 (3)	2.01 (3)	2.7642 (16)	171 (3)
O13—H13B···O8	0.82 (3)	1.87 (3)	2.6642 (14)	163 (2)
C4—H4···O13^{viii}	0.93	2.43	3.164 (2)	136
C10—H10A···O6^{ix}	0.93	2.45	3.344 (2)	162

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

Fig. 1

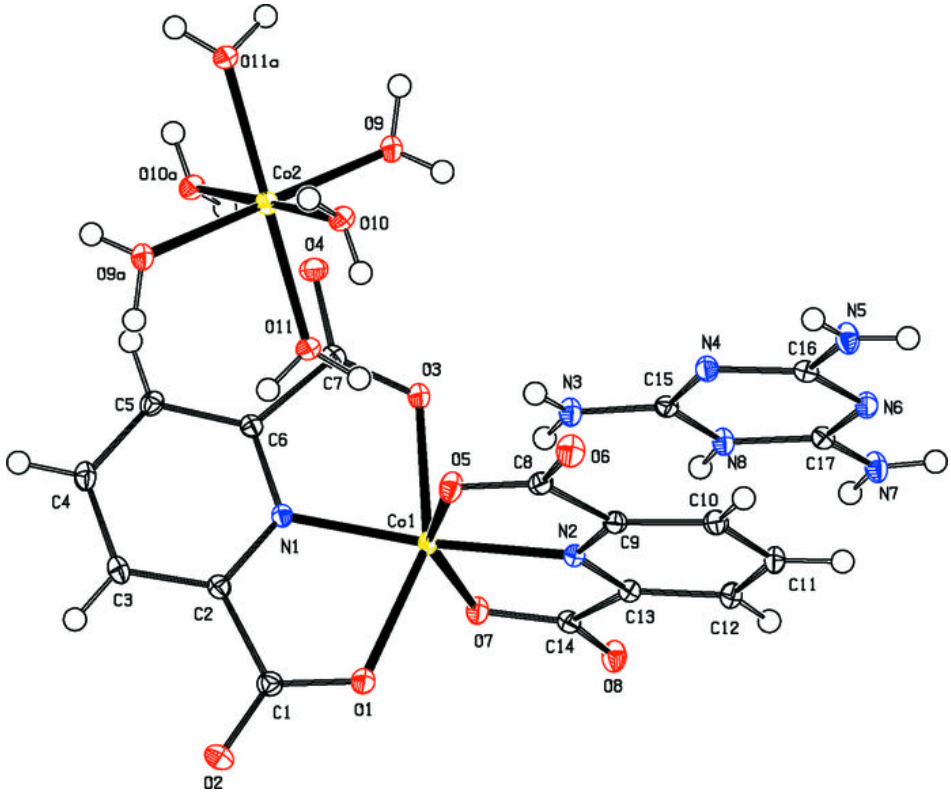
O11a
O9
O10a
Co2
O10
O4
O9a
O11
C7
O3
C5
C6
C4
N1
Co1
O5
C8
O6
N3
C15
N4
C16
N5
N6
N8
C17
N7
C10
N2
C9
C11
C3
C2
C13
C12
O7
C14
O8
C1
O1
O2

Fig. 2

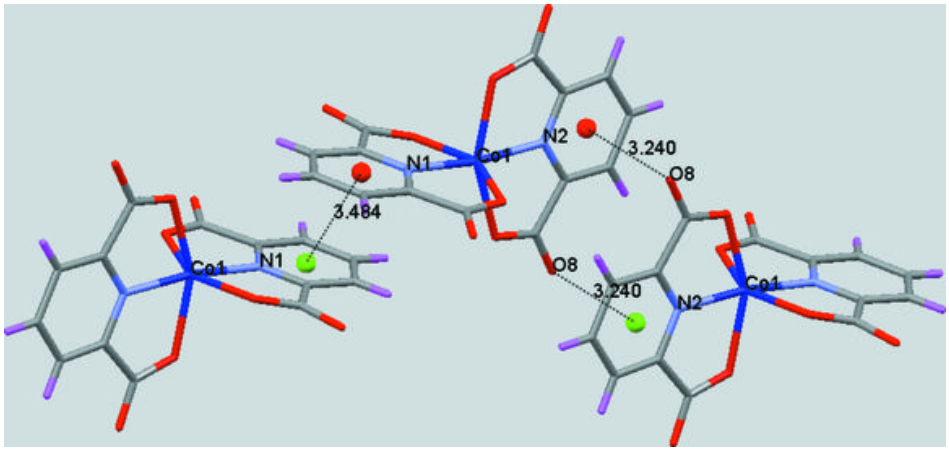

Fig. 3