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Reinvestigation of bis(2,2'-bipyridine)-(nitrate- κ^2O,O')cobalt(III) hydroxide nitrate tetrahydrateA. Wojciechowska^a and M. Daszkiewicz^{b*}

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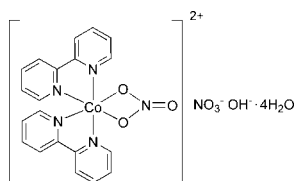
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.043; wR factor = 0.123; data-to-parameter ratio = 14.5.

Single crystals of the title compound, $[\text{Co}(\text{NO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)_2](\text{OH})(\text{NO}_3)\cdot 4\text{H}_2\text{O}$, were obtained from a Co^{2+} -2,2'-bipyridine- CrO_4^{2-} mixture as the second crystalline product. The present single-crystal study confirms a previous refinement [Reimann, Zocchi, Mighell & Santoro (1971). *Acta Cryst. B* **27**, 2211–2218], and also includes all H-atom positions, which were identified from a difference map. The structure displays an $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bonding network between the non-coordinated nitrate group, the hydroxide anion and the water molecules, forming a framework around the distorted octahedral Co complex. A twofold rotation axis passes through Co and the nitrate ligand.

Related literature

For an earlier structure refinement of the title compound, see: Reimann *et al.* (1971). For the crystal structure of $[\text{Co}(\text{bpy})_3](\text{CrO}_4)_{0.5}\text{NO}_3\cdot 7\text{H}_2\text{O}$, see: Wojciechowska *et al.* (2003). For geometrical studies of the coordination mode of the nitrate anion, see: Kleywegt *et al.* (1985); Dowling *et al.* (1996).



Experimental

Crystal data

$[\text{Co}(\text{NO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)_2](\text{OH})(\text{NO}_3)\cdot 4\text{H}_2\text{O}$
 $M_r = 584.39$
 Monoclinic, $C2/c$
 $a = 10.949$ (2) Å
 $b = 16.047$ (3) Å
 $c = 14.456$ (3) Å
 $\beta = 101.92$ (3)°

$V = 2485.1$ (9) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.76$ mm⁻¹
 $T = 298$ (2) K
 $0.38 \times 0.25 \times 0.21$ mm

Data collection

KUMA KM-4 CCD area-detector diffractometer
 Absorption correction: numerical (*CrysAlis RED*; Oxford Diffraction, 2007)
 $T_{\min} = 0.847$, $T_{\max} = 0.930$
 13043 measured reflections
 2529 independent reflections
 2212 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.123$
 $S = 1.06$
 2529 reflections
 175 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.34$ e Å⁻³
 $\Delta\rho_{\min} = -0.54$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—O12	1.8924 (17)	Co1—N1	1.9374 (19)
Co1—N2	1.926 (2)	Co1—N11	2.297 (4)
O12 ⁱ —Co1—O12	69.80 (12)	N2—Co1—N1	83.22 (8)
O12—Co1—N2	88.36 (7)	N2—Co1—N1 ⁱ	96.30 (8)
O12 ⁱ —Co1—N2	92.21 (7)	N2 ⁱ —Co1—N2	179.30 (10)
O12—Co1—N1 ⁱ	167.72 (8)	N1 ⁱ —Co1—N1	93.25 (11)
O12—Co1—N1	98.59 (8)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1—H11 \cdots O22 ⁱ	0.92	2.14	3.027 (6)	162.4
O1—H11 \cdots O21	0.92	2.40	3.165 (4)	139.9
O1—H12 \cdots O2	0.92	1.81	2.689 (5)	158.4
O2—H21 \cdots O11 ⁱⁱ	0.91	1.94	2.718 (4)	142.9
O2—H22 \cdots O3	0.92	1.97	2.748 (4)	141.5
O3—H31 \cdots O22 ⁱⁱⁱ	1.02	2.08	3.004 (6)	149.9
O3—H31 \cdots O22 ^{iv}	1.02	2.08	3.004 (6)	149.9

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *pubCIF* (Westrip, 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: E22106).

References

- Brandenburg, K. (2005). *DIAMOND*. Release 3.0e. Crystal Impact GbR, Bonn, Germany.
 Dowling, C., Murphy, V. J. & Parkin, G. (1996). *Inorg. Chem.* **35**, 2415–2420.
 Kleywegt, G. J., Wiesmeijer, W. G. R., Van Driel, G. J., Driessen, W. L., Reedijk, J. & Noordik, J. H. (1985). *J. Chem. Soc. Dalton Trans.* pp. 2177–2184.
 Oxford Diffraction (2007). *CrysAlis RED* and *CrysAlis CCD*. Versions 1.171.31.8. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.

metal-organic compounds

Reimann, C. W., Zocchi, M., Mighell, A. D. & Santoro, A. (1971). *Acta Cryst.* **B27**, 2211–2218.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Westrip (2007). *publCIF*. in preparation.
Wojciechowska, A., Staszak, Z., Bronowska, W., Pietraszko, A. & Cieslak-Golonka, M. (2003). *J. Mol. Struct.* **654**, 197–204.

supplementary materials

Acta Cryst. (2007). E63, m2975-m2976 [doi:10.1107/S160053680705605X]

Reinvestigation of bis(2,2'-bipyridine)(nitrate- κ^2O,O')cobalt(III) hydroxide nitrate tetrahydrate

A. Wojciechowska and M. Daszkiewicz

Comment

Bis(2,2'-bipyridine)(nitrate- O,O')cobalt(III) hydroxide nitrate tetrahydrate (I) was unintentionally obtained from a $[\text{Co}^{2+}-2,2'\text{-bipyridine}-\text{CrO}_4^{2-}]$ mixture as the second product. The first product was identified as $[\text{Co}(\text{bpy})_3](\text{CrO}_4)_{0.5}\cdot\text{NO}_3\cdot 7\text{H}_2\text{O}$ (Wojciechowska *et al.*, 2003). The present single-crystal study confirms the previous refinement (Reimann *et al.*, 1971), but with all hydrogen atoms, which were visible in the difference maps, included in the refinement (Fig. 1). Two organic ligands and one nitrate ion form a distorted octahedral coordination sphere around the Co(III) ion. The differences between the Co—O_{nitrate} bond lengths, and the Co—O—N and Co—N—O_{terminal} angles are 0 Å, 0° and 180° respectively, which correlate exactly with the bidentate mode of the nitrate group (Kleywegt *et al.*, 1985; Dowling *et al.*, 1996). The nitrate groups, hydroxide ions and water molecules form a rich hydrogen bonding network, which surrounds the $[\text{Co}(\text{bpy})_2(\text{NO}_3-O,O')^+]$ cation and links to it *via* an O_{water}—H \cdots O_{nitrate} hydrogen bond (Fig. 2).

Experimental

15 cm³ of a 0.50 M methanolic solution of 2,2'-bipyridine was added to 20 cm³ of an aqueous solution of K₂CrO₄ (0.25 M). After 15 min of mixing, 10 cm³ of an 0.25 M aqueous solution of cobalt nitrate was added dropwise. This mixture of $[\text{Co}^{2+}-2,2'\text{-bipyridine}-\text{CrO}_4^{2-}]$ reagents in a 1:3:2 molar ratio was slowly evaporated at room temperature. After 14 days orange crystals of $[\text{Co}(\text{bpy})_3](\text{CrO}_4)_{0.5}\cdot\text{NO}_3\cdot 7\text{H}_2\text{O}$ were obtained. The crystals were filtered off and the filtrate was left to stand. After 30 days pink prismatic crystals of the title compound were isolated.

Refinement

All the hydrogen atoms were visible on difference maps and were refined with isotropic displacement parameters correlated with the anisotropic displacement parameters of the atoms to which they were bonded [C—H 0.93 (2) Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. The positions of hydrogen atoms in the hydroxide ion and water molecules were determined from difference maps and were not refined [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$].

Figures

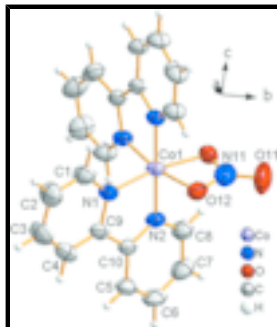


Fig. 1. A view of $[\text{Co}(\text{bpy})_2(\text{NO}_3\text{-}O,O')^+]$ cation, showing the atom numbering scheme of the asymmetric unit. Displacement ellipsoids are shown at the 50% probability level.

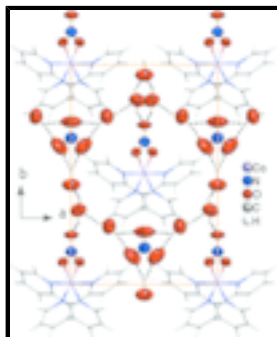


Fig. 2. The hydrogen bonding network of (I) viewed along the c axis. Hydrogen bonds are indicated by dashed lines.

bis(2,2'-bipyridine)(nitrato- κ^2O,O')cobalt(III) hydroxide nitrate tetrahydrate

Crystal data

$[\text{Co}(\text{NO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)_2](\text{OH})(\text{NO}_3)\cdot 4\text{H}_2\text{O}$

$M_r = 584.39$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 10.949\ (2)\ \text{\AA}$

$b = 16.047\ (3)\ \text{\AA}$

$c = 14.456\ (3)\ \text{\AA}$

$\beta = 101.92\ (3)^\circ$

$V = 2485.1\ (9)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1208$

$D_x = 1.562\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2212 reflections

$\theta = 2.9\text{--}26.4^\circ$

$\mu = 0.76\ \text{mm}^{-1}$

$T = 298\ (2)\ \text{K}$

Prism, pink

$0.38 \times 0.25 \times 0.21\ \text{mm}$

Data collection

KUMA KM-4 with CCD area detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 1024×1024 with blocks 2×2 , $33.133\ \text{pixel/mm pixels mm}^{-1}$

$T = 298\ (2)\ \text{K}$

2529 independent reflections

2212 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\text{max}} = 26.4^\circ$

$\theta_{\text{min}} = 2.9^\circ$

ω -scan $h = -13 \rightarrow 13$
 Absorption correction: numerical
 (CrysAlis RED; Oxford Diffraction, 2007) $k = -19 \rightarrow 20$
 $T_{\min} = 0.847$, $T_{\max} = 0.930$ $l = -18 \rightarrow 16$
 13043 measured reflections

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.0763P)^2 + 1.6632P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
2529 reflections	$(\Delta/\sigma)_{\max} < 0.001$
175 parameters	$\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > \sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.50622 (2)	0.2500	0.03378 (17)
N11	0.5000	0.6494 (2)	0.2500	0.0744 (11)
O11	0.5000	0.72623 (19)	0.2500	0.1021 (13)
O12	0.55680 (17)	0.60295 (11)	0.19693 (12)	0.0486 (4)
N21	0.5000	0.1667 (3)	0.2500	0.0739 (10)
O21	0.5000	0.2402 (3)	0.2500	0.177 (3)
O22	0.5834 (4)	0.1293 (3)	0.3002 (3)	0.1659 (18)
N1	0.56282 (17)	0.42330 (12)	0.17425 (12)	0.0374 (4)
N2	0.35747 (19)	0.50549 (11)	0.14648 (13)	0.0361 (4)
C1	0.6699 (2)	0.38072 (17)	0.19718 (18)	0.0497 (6)
H1	0.7232	0.3913	0.2549	0.060*
C2	0.7033 (3)	0.3220 (2)	0.1382 (2)	0.0639 (8)
H2	0.7784	0.2934	0.1557	0.077*

supplementary materials

C3	0.6250 (3)	0.30562 (19)	0.0530 (2)	0.0629 (7)
H3	0.6459	0.2652	0.0128	0.075*
C4	0.5152 (2)	0.34973 (17)	0.02769 (18)	0.0508 (6)
H4	0.4615	0.3400	-0.0301	0.061*
C5	0.2822 (2)	0.45824 (17)	-0.01124 (16)	0.0495 (6)
H5	0.2927	0.4256	-0.0622	0.059*
C6	0.1773 (3)	0.50778 (17)	-0.0174 (2)	0.0571 (7)
H6	0.1169	0.5093	-0.0730	0.068*
C7	0.1630 (2)	0.55457 (18)	0.0591 (2)	0.0572 (7)
H7	0.0924	0.5874	0.0562	0.069*
C8	0.2546 (2)	0.55237 (16)	0.14060 (18)	0.0486 (6)
H8	0.2448	0.5840	0.1925	0.058*
C9	0.4859 (2)	0.40857 (14)	0.08920 (14)	0.0380 (5)
C10	0.3712 (2)	0.45814 (14)	0.07220 (14)	0.0382 (5)
O1	0.2572 (3)	0.2652 (2)	0.0904 (3)	0.1321 (12)
H11	0.3083	0.2320	0.1342	0.198*
H12	0.1874	0.2802	0.1126	0.198*
O2	0.0487 (4)	0.33863 (18)	0.1216 (2)	0.1137 (10)
H21	0.0504	0.2873	0.1485	0.171*
H22	0.0588	0.3895	0.1520	0.171*
O3	0.0000	0.4538 (3)	0.2500	0.1300 (18)
H31	0.0000	0.5172	0.2500	0.195*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0356 (3)	0.0405 (3)	0.0229 (2)	0.000	0.00068 (16)	0.000
N11	0.080 (3)	0.055 (2)	0.075 (2)	0.000	-0.014 (2)	0.000
O11	0.129 (3)	0.0345 (16)	0.133 (3)	0.000	0.004 (3)	0.000
O12	0.0555 (10)	0.0477 (9)	0.0398 (9)	-0.0063 (8)	0.0033 (7)	0.0071 (7)
N21	0.086 (3)	0.063 (2)	0.075 (3)	0.000	0.022 (2)	0.000
O21	0.257 (9)	0.067 (3)	0.218 (7)	0.000	0.078 (7)	0.000
O22	0.161 (4)	0.161 (4)	0.147 (4)	0.060 (3)	-0.033 (3)	0.016 (3)
N1	0.0374 (9)	0.0447 (10)	0.0286 (8)	-0.0001 (7)	0.0031 (7)	-0.0012 (7)
N2	0.0364 (10)	0.0425 (10)	0.0274 (9)	0.0009 (7)	0.0020 (8)	0.0033 (7)
C1	0.0428 (13)	0.0601 (15)	0.0439 (13)	0.0087 (11)	0.0033 (10)	-0.0034 (11)
C2	0.0544 (16)	0.0712 (19)	0.0656 (18)	0.0173 (14)	0.0112 (13)	-0.0103 (14)
C3	0.0657 (18)	0.0674 (18)	0.0578 (16)	0.0080 (14)	0.0179 (14)	-0.0198 (14)
C4	0.0560 (15)	0.0588 (15)	0.0371 (11)	-0.0078 (11)	0.0089 (10)	-0.0112 (11)
C5	0.0537 (15)	0.0549 (15)	0.0333 (12)	-0.0088 (11)	-0.0064 (10)	0.0003 (10)
C6	0.0502 (16)	0.0656 (17)	0.0439 (15)	-0.0060 (12)	-0.0168 (12)	0.0080 (11)
C7	0.0414 (13)	0.0614 (16)	0.0617 (16)	0.0056 (11)	-0.0054 (12)	0.0104 (13)
C8	0.0435 (13)	0.0547 (14)	0.0452 (13)	0.0056 (11)	0.0035 (10)	0.0020 (11)
C9	0.0422 (12)	0.0436 (12)	0.0272 (10)	-0.0063 (9)	0.0051 (9)	0.0002 (8)
C10	0.0438 (12)	0.0398 (12)	0.0278 (10)	-0.0068 (9)	0.0003 (9)	0.0033 (8)
O1	0.101 (2)	0.135 (3)	0.147 (3)	0.003 (2)	-0.004 (2)	0.015 (2)
O2	0.139 (3)	0.094 (2)	0.105 (2)	0.0196 (19)	0.017 (2)	0.0046 (16)
O3	0.191 (5)	0.076 (3)	0.106 (3)	0.000	-0.008 (3)	0.000

Geometric parameters (Å, °)

Co1—O12 ⁱ	1.8924 (17)	C2—H2	0.9300
Co1—O12	1.8924 (17)	C3—C4	1.378 (4)
Co1—N2 ⁱ	1.926 (2)	C3—H3	0.9300
Co1—N2	1.926 (2)	C4—C9	1.379 (3)
Co1—N1 ⁱ	1.9374 (19)	C4—H4	0.9300
Co1—N1	1.9374 (19)	C5—C6	1.384 (4)
Co1—N11	2.297 (4)	C5—C10	1.385 (3)
N11—O11	1.233 (4)	C5—H5	0.9300
N11—O12	1.314 (3)	C6—C7	1.372 (4)
N11—O12 ⁱ	1.314 (3)	C6—H6	0.9300
N21—O21	1.180 (6)	C7—C8	1.380 (4)
N21—O22 ⁱ	1.202 (4)	C7—H7	0.9300
N21—O22	1.202 (4)	C8—H8	0.9300
N1—C1	1.338 (3)	C9—C10	1.464 (3)
N1—C9	1.360 (3)	O1—H11	0.9218
N2—C8	1.342 (3)	O1—H12	0.9194
N2—C10	1.349 (3)	O2—H21	0.9100
C1—C2	1.371 (4)	O2—H22	0.9225
C1—H1	0.9300	O3—H31	1.0180
C2—C3	1.372 (4)		
O12 ⁱ —Co1—O12	69.80 (12)	C8—N2—Co1	125.47 (17)
O12 ⁱ —Co1—N2 ⁱ	88.36 (7)	C10—N2—Co1	114.60 (15)
O12—Co1—N2 ⁱ	92.21 (8)	N1—C1—C2	122.0 (2)
O12—Co1—N2	88.36 (7)	N1—C1—H1	119.0
O12 ⁱ —Co1—N2	92.21 (7)	C2—C1—H1	119.0
O12—Co1—N1 ⁱ	167.72 (8)	C1—C2—C3	119.5 (3)
O12—Co1—N1	98.59 (8)	C1—C2—H2	120.3
N2—Co1—N1	83.22 (8)	C3—C2—H2	120.3
N2—Co1—N1 ⁱ	96.30 (8)	C2—C3—C4	119.3 (2)
N2 ⁱ —Co1—N2	179.30 (10)	C2—C3—H3	120.4
O12 ⁱ —Co1—N1 ⁱ	98.59 (8)	C4—C3—H3	120.4
N2 ⁱ —Co1—N1 ⁱ	83.22 (8)	C3—C4—C9	119.1 (2)
O12 ⁱ —Co1—N1	167.72 (8)	C3—C4—H4	120.4
N2 ⁱ —Co1—N1	96.30 (8)	C9—C4—H4	120.4
N1 ⁱ —Co1—N1	93.25 (11)	C6—C5—C10	118.8 (2)
O12 ⁱ —Co1—N11	34.90 (6)	C6—C5—H5	120.6
O12—Co1—N11	34.90 (6)	C10—C5—H5	120.6
N2 ⁱ —Co1—N11	90.35 (5)	C7—C6—C5	119.6 (2)
N2—Co1—N11	90.35 (5)	C7—C6—H6	120.2
N1 ⁱ —Co1—N11	133.38 (6)	C5—C6—H6	120.2
N1—Co1—N11	133.38 (6)	C6—C7—C8	119.3 (3)
O11—N11—O12	124.54 (15)	C6—C7—H7	120.3

supplementary materials

O11—N11—O12 ⁱ	124.54 (15)	C8—C7—H7	120.3
O12—N11—O12 ⁱ	110.9 (3)	N2—C8—C7	121.4 (2)
O11—N11—Co1	180.0	N2—C8—H8	119.3
O12—N11—Co1	55.46 (15)	C7—C8—H8	119.3
O12 ⁱ —N11—Co1	55.46 (15)	N1—C9—C4	121.3 (2)
N11—O12—Co1	89.64 (17)	N1—C9—C10	114.01 (19)
O21—N21—O22 ⁱ	119.9 (3)	C4—C9—C10	124.7 (2)
O21—N21—O22	119.9 (3)	N2—C10—C5	121.2 (2)
O22 ⁱ —N21—O22	120.2 (6)	N2—C10—C9	113.90 (18)
C1—N1—C9	118.8 (2)	C5—C10—C9	124.9 (2)
C1—N1—Co1	127.28 (16)	H11—O1—H12	110.0
C9—N1—Co1	113.87 (15)	H21—O2—H22	127.5
C8—N2—C10	119.7 (2)		
O12 ⁱ —Co1—N11—O12	180.0	N11—Co1—N2—C8	-46.18 (19)
N2 ⁱ —Co1—N11—O12	93.37 (11)	O12 ⁱ —Co1—N2—C10	162.94 (16)
N2—Co1—N11—O12	-86.63 (11)	O12—Co1—N2—C10	93.23 (16)
N1 ⁱ —Co1—N11—O12	174.35 (11)	N1 ⁱ —Co1—N2—C10	-98.16 (16)
N1—Co1—N11—O12	-5.65 (11)	N1—Co1—N2—C10	-5.62 (15)
O12—Co1—N11—O12 ⁱ	180.000 (1)	N11—Co1—N2—C10	128.08 (15)
N2 ⁱ —Co1—N11—O12 ⁱ	-86.63 (11)	C9—N1—C1—C2	-1.0 (4)
N2—Co1—N11—O12 ⁱ	93.37 (11)	Co1—N1—C1—C2	178.6 (2)
N1 ⁱ —Co1—N11—O12 ⁱ	-5.65 (11)	N1—C1—C2—C3	-0.3 (5)
N1—Co1—N11—O12 ⁱ	174.35 (11)	C1—C2—C3—C4	1.1 (5)
O11—N11—O12—Co1	180.0	C2—C3—C4—C9	-0.8 (4)
O12 ⁱ —N11—O12—Co1	0.0	C10—C5—C6—C7	-0.8 (4)
O12 ⁱ —Co1—O12—N11	0.0	C5—C6—C7—C8	1.0 (4)
N2 ⁱ —Co1—O12—N11	-87.44 (9)	C10—N2—C8—C7	-1.3 (4)
N2—Co1—O12—N11	92.96 (9)	Co1—N2—C8—C7	172.68 (19)
N1 ⁱ —Co1—O12—N11	-19.6 (4)	C6—C7—C8—N2	0.1 (4)
N1—Co1—O12—N11	175.85 (8)	C1—N1—C9—C4	1.3 (3)
O12 ⁱ —Co1—N1—C1	114.8 (3)	Co1—N1—C9—C4	-178.29 (18)
O12—Co1—N1—C1	96.2 (2)	C1—N1—C9—C10	179.5 (2)
N2 ⁱ —Co1—N1—C1	2.9 (2)	Co1—N1—C9—C10	-0.1 (2)
N2—Co1—N1—C1	-176.5 (2)	C3—C4—C9—N1	-0.5 (4)
N1 ⁱ —Co1—N1—C1	-80.6 (2)	C3—C4—C9—C10	-178.4 (2)
N11—Co1—N1—C1	99.4 (2)	C8—N2—C10—C5	1.4 (3)
O12 ⁱ —Co1—N1—C9	-65.6 (4)	Co1—N2—C10—C5	-173.18 (17)
O12—Co1—N1—C9	-84.26 (16)	C8—N2—C10—C9	-178.4 (2)
N2 ⁱ —Co1—N1—C9	-177.47 (15)	Co1—N2—C10—C9	7.0 (2)
N2—Co1—N1—C9	3.04 (15)	C6—C5—C10—N2	-0.4 (4)
N1 ⁱ —Co1—N1—C9	99.00 (16)	C6—C5—C10—C9	179.5 (2)
N11—Co1—N1—C9	-81.00 (16)	N1—C9—C10—N2	-4.4 (3)
O12 ⁱ —Co1—N2—C8	-11.3 (2)	C4—C9—C10—N2	173.6 (2)
O12—Co1—N2—C8	-81.0 (2)	N1—C9—C10—C5	175.7 (2)

N1 ⁱ —Co1—N2—C8	87.6 (2)	C4—C9—C10—C5	-6.2 (4)
N1—Co1—N2—C8	-179.9 (2)		

Symmetry codes: (i) $-x+1, y, -z+1/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H11...O22 ⁱ	0.92	2.14	3.027 (6)	162.4
O1—H11...O21	0.92	2.40	3.165 (4)	139.9
O1—H12...O2	0.92	1.81	2.689 (5)	158.4
O2—H21...O11 ⁱⁱ	0.91	1.94	2.718 (4)	142.9
O2—H22...O3	0.92	1.97	2.748 (4)	141.5
O3—H31...O22 ⁱⁱⁱ	1.02	2.08	3.004 (6)	149.9
O3—H31...O22 ^{iv}	1.02	2.08	3.004 (6)	149.9

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

Fig. 1

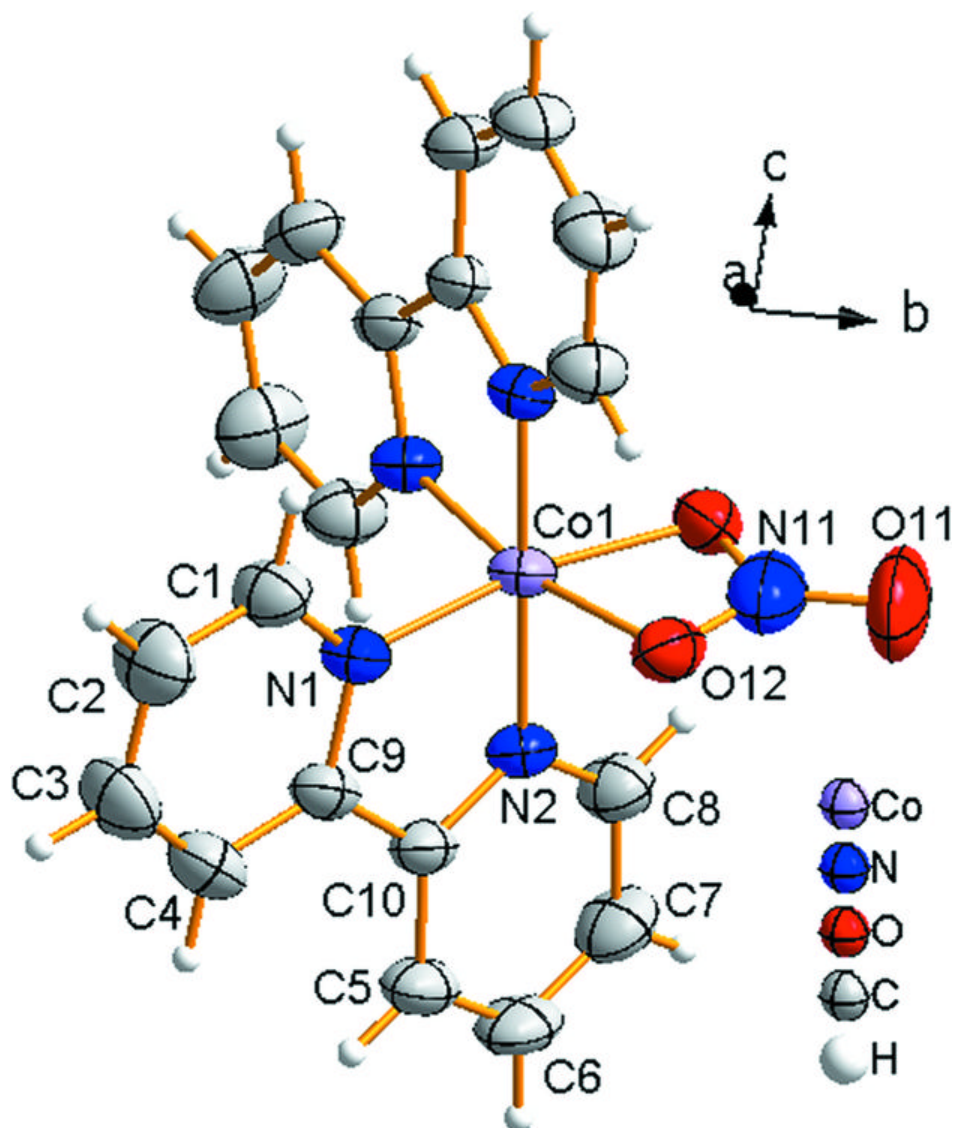


Fig. 2

