Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis(4-bromobenzoato-κO)-bis(nicotinamide-κN^1)cobalt(II)

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Received 8 June 2007; accepted 9 June 2007

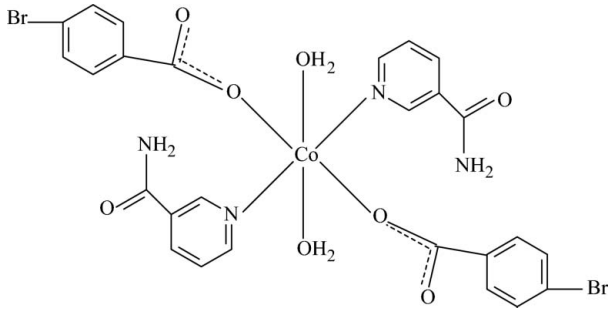
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.042; wR factor = 0.110; data-to-parameter ratio = 14.3.

The title complex, $[Co(C_7H_4BrO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, is monomeric and centrosymmetric, and contains two water molecules, two 4-bromobenzoate (BB) anions and two nicotinamide (NA) ligands, all acting as monodentate ligands. The four nearest O atoms in the equatorial plane around the Co atom form a slightly distorted square-planar arrangement, while the distorted octahedral coordination is completed by the two NA N atoms in the axial positions. Intermolecular O—H···O and N—H···O hydrogen bonds link the molecules into two-dimensional sheets.

Related literature

For general background, see: Antolini *et al.* (1982); Nadzhafov *et al.* (1981); Shnulin *et al.* (1981); Antsyshkina *et al.* (1980); Amiraslanov *et al.* (1979); Adiwidjaja *et al.* (1978); Mikelashvili (1982). For related structures, see: Hökelek & Necefoğlu (1997, 1998, 1999*a*,*b*,*c*, 2007*a*,*b*,*c*); Çaylak, Hökelek & Necefoğlu (2007); Çaylak, Hökelek *et al.* (2007).

For related literature, see: Necefoğlu *et al.* (2002).



Experimental

Crystal data

$[Co(C_7H_4BrO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$
M_r = 739.22
Triclinic, $P\overline{1}$
a = 7.6202 (1) Å
b = 9.9593 (3) Å
c = 10.1125 (2) Å
α = 77.92 (1)°
β = 85.65 (1)°
γ = 71.65 (2)°
V = 712.25 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 3.46 mm^{-1}
T = 294 (2) K
0.30 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.446, T_{max} = 0.595
3067 measured reflections
2895 independent reflections
1968 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.110
S = 1.02
2895 reflections
203 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.069 (3)	O1—C1	1.256 (5)
Co—O4	2.132 (3)	O2—C1	1.254 (5)
Co—N1	2.148 (3)		
O1^i—Co—O4	92.63 (11)	O1—Co—N1	90.30 (12)
O1—Co—O4	87.37 (11)	O4—Co—N1	87.23 (11)
O1^i—Co—N1	89.70 (12)	O4^i—Co—N1	92.77 (11)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H41···O2	0.95 (4)	1.70 (5)	2.635 (4)	166 (5)
O4—H42···O3^{ii}	0.91 (4)	2.03 (4)	2.893 (4)	156 (4)
N2—H21···O2^{iii}	0.87 (4)	2.10 (4)	2.884 (6)	151 (3)
N2—H22···O3^{iv}	0.87 (4)	2.11 (5)	2.935 (6)	160 (4)

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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).

The authors acknowledge the purchase of the CAD-4 diffractometer under grant No. DPT/TBAG1 of the Scientific and Technical Research Council of Turkey.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2273).

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supplementary materials

Acta Cryst. (2007). E**63**, m1873-m1874 [**doi:10.1107/S1600536807028358**]

Diaquabis(4-bromobenzoato-κO)bis(nicotinamide-κN^1)cobalt(II)

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Comment

Transition metal complexes with biochemical molecules show interesting physical and/or chemical properties, in which they may find applications in biological systems (Antolini *et al.*, 1982). The structure-function-coordination relationships of the arylcarboxylate ion in Co^{II} complexes of benzoic acid derivatives change depending on the nature and position of the substituted groups in the phenyl ring, the nature of the additional ligand molecule or solvent, and the medium of synthesis (Nadzhafov *et al.*, 1981; Shnulin *et al.*, 1981; Antsyshkina *et al.*, 1980; Amiraslanov *et al.*, 1979; Adiwidjaja *et al.*, 1978). To the best of our knowledge, only a few structures of Co^{II} complexes with nicotinic and/or benzoic acid derivatives as ligands have been reported to date (Amiraslanov *et al.*, 1979; Nadzhafov *et al.*, 1981; Mikelashvili, 1982; Hökelek & Necefoğlu, 1997; 1998; 1999*a*,b,c; 2007*a*; Çaylak, Hökelek & Necefoğlu, 2007; Çaylak, Hökelek *et al.*, 2007).

The structure determination of the title compound, (I), a cobalt complex with two bromobenzoate (BB), two nicotinamide (NA) ligands and two water molecules, was undertaken in order to determine the properties of the BB and NA ligands and also to compare the results obtained with those reported previously.

The title monomeric complex, (I), with the Co atom on a centre of symmetry contains two BB and two NA ligands and two water molecules denoted by primed and unprimed labels, respectively, in Fig. 1. A l l ligands are monodentate. The four symmetry-related carboxylate and water O atoms (O1, O4, and the symmetry related atoms, O1', O4') in the equatorial plane around the Co atom form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the NA ligands (N1, and the symmetry related atom, N1') in the axial positions (Table 1 and Fig. 1), as in the similar compounds (Hökelek & Necefoğlu, 1997; 1998; 1999*a*,b,c; 2007*a*; Çaylak, Hökelek & Necefoğlu, 2007; Çaylak, Hökelek *et al.*, 2007).

The near equality of the C1—O1 [1.256 (5) Å] and C1—O2 [1.254 (5) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds, as in bis(4-hydroxybenzoato-κ*O*)bis(nicotinamide-κ*N*)zinc(II) (Necefoğlu *et al.*, 2002), diaquabis[4-(dimethylamino)benzoato-κ*O*]-(nicotinamide-κN^1)cobalt(II) dihydrate (Hökelek & Necefoğlu, 2007*a*), tetraaquabis[4-(dimethylamino)benzoato-κ*O*]manganese(II) dihydrate (Hökelek & Necefoğlu, 2007*b*), diaquabis[4-(dimethylamino)benzoato-κ*O*]-(nicotinamide-κN^1)manganese(II) dihydrate (Hökelek & Necefoğlu, 2007*c*), diaquabis(4-fluorobenzoato-κ*O*)bis(nicotinamide-κN^1)cobalt(II) (Çaylak, Hökelek & Necefoğlu, 2007) and diaquabis(4-chlorobenzoato-κ*O*)bis(nicotinamide-κ*N*)cobalt(II) (Çaylak, Hökelek *et al.*, 2007). This may influenced by the intra- and intermolecular O—H···O and N—H···O hydrogen bonds involving the carboxylate O atoms (Table 2). The Co atom is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by −0.465 (1) Å. The dihedral angle between the planar carboxyl group and the benzene ring A (C2—C7) is 23.2 (3)°, while that between rings A and B (N1/C8—C12) is A/B = 88.82 (11)°.

As can be seen from the packing diagram (Fig. 2), intermolecular O—H···O and N—H···O hydrogen bonds (Table 2), firstly link the amide groups of NA molecules to form centrosymmetric hydrogen bonded dimers, they further link the molecules into two-dimensional sheets lying parallel to the *ab* plane.

Experimental

The title compound, (I), was prepared by the reaction of $CoSO_4$ (1.55 g, 10 mmol) and NA (2.44 g, 20 mmol) in H_2O (100 ml) with sodium 4-bromobenzoate (4.46 g, 20 mmol) in H_2O (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for several days, giving pink single crystals.

Refinement

H atoms of water molecule and NH_2 group were located in a difference Fourier map and refined isotropically [O—H = 0.91 (2) and 0.95 (5) Å and U_{iso}(H) = 0.055 (15) and 0.072 (17) Å^2; N—H = 0.87 (2) and 0.87 (4) Å and U_{iso}(H) = 0.046 (14) and 0.076 (18) Å^2]. The remaining H atoms were positioned geometrically with C—H = 0.93 Å, for aromatic H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

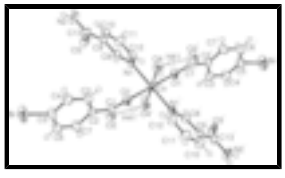

Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. Primed atoms are generated by the symmetry operator (−*x*, −*y*, −*z*).

Fig. 2. A partial packing diagram of the title compound, showing hydrogen bonds (dashed lines) linking the complexes into two-dimensional sheets in the *ab* planes. H atoms not involved in hydrogen bonding are omitted.

Diaquabis(4-bromobenzoato-κ*O*)bis(nicotinamide-κ*N*^{1})cobalt(II)

Crystal data

$[Co(C_7H_4BrO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$	$Z = 1$
$M_r = 739.22$	$F_{000} = 369$
Triclinic, $P\overline{1}$	$D_x = 1.723$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.6202$ (1) Å	Cell parameters from 25 reflections
$b = 9.9593$ (3) Å	$\theta = 3.6$–22.2º
$c = 10.1125$ (2) Å	$\mu = 3.46$ mm^{-1}
$\alpha = 77.92$ (1)º	$T = 294$ (2) K
$\beta = 85.65$ (1)º	Prism, pink

$\gamma = 71.65\ (2)^{\circ}$	0.30 × 0.20 × 0.15 mm
$V = 712.25\ (9)\ Å^3$	

Data collection

Enraf–Nonius TurboCAD-4 diffractometer	$R_{int} = 0.022$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.3^{\circ}$
Monochromator: graphite	$\theta_{min} = 3.0^{\circ}$
$T = 294(2)$ K	$h = -9 \rightarrow 9$
non–profiled ω scans	$k = -12 \rightarrow 12$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = -12 \rightarrow 0$
$T_{min} = 0.446$, $T_{max} = 0.595$	3 standard reflections
3067 measured reflections	every 120 min
2895 independent reflections	intensity decay: 1%
1968 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.47P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
2895 reflections	$\Delta\rho_{max} = 0.93$ e Å^{-3}
203 parameters	$\Delta\rho_{min} = -0.58$ e Å^{-3}
8 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co	0.0000	0.0000	0.5000	0.0266 (2)
Br	0.51245 (9)	0.28767 (7)	1.09652 (7)	0.0754 (3)
O1	0.1170 (4)	0.0145 (3)	0.6725 (3)	0.0351 (7)
O2	−0.1297 (4)	0.1515 (4)	0.7667 (3)	0.0456 (8)
O3	0.4344 (4)	0.3394 (3)	0.4903 (4)	0.0480 (8)
O4	0.2740 (4)	−0.0730 (3)	0.4218 (3)	0.0366 (7)
H41	0.241 (7)	−0.107 (5)	0.349 (4)	0.072 (17)*
H42	0.357 (5)	−0.150 (4)	0.473 (4)	0.055 (15)*
N1	−0.0003 (4)	0.2151 (3)	0.4081 (3)	0.0306 (7)
N2	0.3329 (6)	0.5588 (4)	0.3608 (5)	0.0491 (10)
H21	0.261 (5)	0.628 (4)	0.304 (4)	0.046 (14)*
H22	0.423 (5)	0.579 (5)	0.391 (5)	0.076 (18)*
C1	0.0411 (5)	0.0925 (4)	0.7565 (4)	0.0298 (9)
C2	0.1624 (5)	0.1255 (4)	0.8464 (4)	0.0283 (8)
C3	0.3438 (6)	0.1150 (4)	0.8117 (4)	0.0348 (9)
H3	0.3959	0.0759	0.7367	0.042*
C4	0.4502 (6)	0.1617 (5)	0.8863 (4)	0.0408 (10)
H4	0.5719	0.1558	0.8613	0.049*
C5	0.3718 (6)	0.2168 (5)	0.9980 (4)	0.0390 (10)
C6	0.1944 (7)	0.2219 (6)	1.0394 (5)	0.0497 (12)
H6	0.1456	0.2548	1.1180	0.060*
C7	0.0898 (6)	0.1773 (5)	0.9623 (4)	0.0425 (11)
H7	−0.0313	0.1821	0.9885	0.051*
C8	0.1419 (5)	0.2577 (4)	0.4292 (4)	0.0308 (9)
H8	0.2383	0.1926	0.4825	0.037*
C9	0.1538 (5)	0.3957 (4)	0.3753 (4)	0.0308 (9)
C10	0.0106 (6)	0.4892 (4)	0.2960 (5)	0.0416 (11)
H10	0.0128	0.5821	0.2578	0.050*
C11	−0.1365 (6)	0.4450 (5)	0.2729 (5)	0.0451 (11)
H11	−0.2337	0.5071	0.2185	0.054*
C12	−0.1373 (5)	0.3087 (4)	0.3312 (4)	0.0352 (9)
H12	−0.2378	0.2799	0.3165	0.042*
C13	0.3196 (6)	0.4291 (5)	0.4132 (5)	0.0376 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0225 (4)	0.0273 (4)	0.0340 (4)	−0.0106 (3)	−0.0033 (3)	−0.0088 (3)
Br	0.0728 (4)	0.0981 (5)	0.0812 (5)	−0.0396 (4)	−0.0130 (3)	−0.0487 (4)
O1	0.0310 (15)	0.0391 (16)	0.0392 (16)	−0.0102 (13)	−0.0060 (12)	−0.0151 (13)
O2	0.0283 (16)	0.062 (2)	0.0497 (19)	−0.0106 (14)	−0.0019 (14)	−0.0227 (16)
O3	0.0409 (17)	0.0350 (17)	0.072 (2)	−0.0151 (14)	−0.0194 (16)	−0.0062 (16)
O4	0.0265 (15)	0.0399 (17)	0.0454 (18)	−0.0111 (13)	−0.0009 (13)	−0.0107 (14)
N1	0.0282 (17)	0.0294 (18)	0.0370 (19)	−0.0124 (14)	−0.0038 (14)	−0.0060 (15)

N2	0.053 (3)	0.035 (2)	0.067 (3)	−0.026 (2)	−0.015 (2)	−0.003 (2)
C1	0.031 (2)	0.029 (2)	0.031 (2)	−0.0111 (17)	−0.0032 (17)	−0.0030 (17)
C2	0.0273 (19)	0.028 (2)	0.029 (2)	−0.0059 (16)	−0.0043 (16)	−0.0065 (17)
C3	0.033 (2)	0.040 (2)	0.034 (2)	−0.0122 (18)	0.0012 (17)	−0.0122 (19)
C4	0.033 (2)	0.051 (3)	0.042 (3)	−0.015 (2)	−0.0011 (19)	−0.014 (2)
C5	0.038 (2)	0.043 (3)	0.041 (2)	−0.014 (2)	−0.0072 (19)	−0.014 (2)
C6	0.051 (3)	0.067 (3)	0.039 (3)	−0.017 (2)	0.003 (2)	−0.030 (2)
C7	0.034 (2)	0.058 (3)	0.040 (3)	−0.018 (2)	0.007 (2)	−0.018 (2)
C8	0.029 (2)	0.030 (2)	0.036 (2)	−0.0104 (17)	−0.0064 (17)	−0.0069 (17)
C9	0.034 (2)	0.025 (2)	0.035 (2)	−0.0113 (17)	0.0002 (17)	−0.0086 (17)
C10	0.045 (2)	0.025 (2)	0.053 (3)	−0.0119 (19)	−0.005 (2)	−0.001 (2)
C11	0.042 (3)	0.035 (2)	0.055 (3)	−0.010 (2)	−0.012 (2)	0.000 (2)
C12	0.026 (2)	0.038 (2)	0.042 (2)	−0.0100 (18)	−0.0054 (18)	−0.0073 (19)
C13	0.041 (2)	0.033 (2)	0.047 (3)	−0.020 (2)	0.003 (2)	−0.015 (2)

Geometric parameters (Å, °)

Co—O1^{i}	2.069 (3)	C2—C7	1.386 (6)
Co—O1	2.069 (3)	C3—H3	0.9300
Co—O4	2.132 (3)	C4—C3	1.386 (6)
Co—O4^{i}	2.132 (3)	C4—H4	0.9300
Co—N1	2.148 (3)	C5—C4	1.373 (6)
Co—N1^{i}	2.148 (3)	C5—C6	1.373 (6)
Br—C5	1.889 (4)	C6—H6	0.9300
O1—C1	1.256 (5)	C7—C6	1.379 (6)
O2—C1	1.254 (5)	C7—H7	0.9300
O3—C13	1.221 (5)	C8—N1	1.329 (5)
O4—H41	0.95 (5)	C8—C9	1.397 (5)
O4—H42	0.91 (2)	C8—H8	0.9300
N2—C13	1.323 (5)	C11—C12	1.364 (6)
N2—H21	0.87 (4)	C11—C10	1.378 (6)
N2—H22	0.87 (2)	C11—H11	0.9300
C1—C2	1.495 (5)	C12—N1	1.330 (5)
C2—C3	1.377 (6)	C12—H12	0.9300
O1^{i}—Co—O1	180.0	C2—C3—H3	119.4
O1^{i}—Co—O4	92.63 (11)	C4—C3—H3	119.4
O1—Co—O4	87.37 (11)	C5—C4—C3	118.5 (4)
O1^{i}—Co—O4^{i}	87.37 (11)	C5—C4—H4	120.7
O1—Co—O4^{i}	92.63 (11)	C3—C4—H4	120.7
O4—Co—O4^{i}	180.0	C4—C5—C6	121.6 (4)
O1^{i}—Co—N1	89.70 (12)	C4—C5—Br	118.9 (3)
O1—Co—N1	90.30 (12)	C6—C5—Br	119.5 (3)
O4—Co—N1	87.23 (11)	C5—C6—C7	118.8 (4)
O4^{i}—Co—N1	92.77 (11)	C5—C6—H6	120.6
O1^{i}—Co—N1^{i}	90.30 (12)	C7—C6—H6	120.6
O1—Co—N1^{i}	89.70 (12)	C6—C7—C2	121.0 (4)

O4—Co—N1^{i}	92.77 (11)	C6—C7—H7	119.5
O4^{i}—Co—N1^{i}	87.23 (11)	C2—C7—H7	119.5
N1—Co—N1^{i}	180.0	N1—C8—C9	123.2 (4)
C1—O1—Co	126.9 (2)	N1—C8—H8	118.4
Co—O4—H42	118 (3)	C9—C8—H8	118.4
Co—O4—H41	96 (3)	C10—C9—C8	117.2 (4)
H42—O4—H41	106 (3)	C10—C9—C13	126.1 (4)
C8—N1—C12	118.0 (3)	C8—C9—C13	116.7 (4)
C8—N1—Co	118.8 (3)	C9—C10—C11	119.8 (4)
C12—N1—Co	123.1 (3)	C9—C10—H10	120.1
C13—N2—H21	129 (3)	C11—C10—H10	120.1
C13—N2—H22	115 (3)	C12—C11—C10	118.9 (4)
H21—N2—H22	115 (4)	C12—C11—H11	120.5
O2—C1—O1	125.1 (4)	C10—C11—H11	120.5
O2—C1—C2	116.7 (3)	N1—C12—C11	122.8 (4)
O1—C1—C2	118.1 (3)	N1—C12—H12	118.6
C3—C2—C7	118.6 (4)	C11—C12—H12	118.6
C3—C2—C1	121.1 (4)	O3—C13—N2	122.6 (4)
C7—C2—C1	120.1 (3)	O3—C13—C9	120.5 (4)
C2—C3—C4	121.2 (4)	N2—C13—C9	116.9 (4)
O4—Co—O1—C1	156.5 (3)	C1—C2—C7—C6	−173.5 (4)
O4^{i}—Co—O1—C1	−23.5 (3)	C5—C4—C3—C2	1.1 (7)
N1—Co—O1—C1	69.3 (3)	Br—C5—C4—C3	−177.6 (3)
N1^{i}—Co—O1—C1	−110.7 (3)	C6—C5—C4—C3	2.3 (7)
O1^{i}—Co—N1—C8	−141.9 (3)	C4—C5—C6—C7	−3.4 (7)
O1—Co—N1—C8	38.1 (3)	Br—C5—C6—C7	176.4 (4)
O4—Co—N1—C8	−49.3 (3)	C2—C7—C6—C5	1.2 (7)
O4^{i}—Co—N1—C8	130.7 (3)	N1—C8—C9—C10	−0.6 (6)
O1^{i}—Co—N1—C12	38.5 (3)	N1—C8—C9—C13	177.6 (4)
O1—Co—N1—C12	−141.5 (3)	C9—C8—N1—C12	0.3 (6)
O4—Co—N1—C12	131.1 (3)	C9—C8—N1—Co	−179.3 (3)
O4^{i}—Co—N1—C12	−48.9 (3)	C8—C9—C10—C11	0.1 (7)
Co—O1—C1—O2	16.3 (6)	C13—C9—C10—C11	−177.9 (4)
Co—O1—C1—C2	−159.9 (3)	C10—C9—C13—O3	176.2 (4)
O2—C1—C2—C3	−154.9 (4)	C8—C9—C13—O3	−1.8 (6)
O1—C1—C2—C3	21.6 (6)	C10—C9—C13—N2	−2.9 (7)
O2—C1—C2—C7	20.5 (6)	C8—C9—C13—N2	179.0 (4)
O1—C1—C2—C7	−163.0 (4)	C10—C11—C12—N1	−1.1 (7)
C7—C2—C3—C4	−3.2 (6)	C12—C11—C10—C9	0.7 (7)
C1—C2—C3—C4	172.3 (4)	C11—C12—N1—C8	0.5 (6)
C3—C2—C7—C6	2.0 (7)	C11—C12—N1—Co	−179.9 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H41···O2	0.95 (4)	1.70 (5)	2.635 (4)	166 (5)

O4—H42···O3^{ii}	0.91 (4)	2.03 (4)	2.893 (4)	156 (4)
N2—H21···O2^{iii}	0.87 (4)	2.10 (4)	2.884 (6)	151 (3)
N2—H22···O3^{iv}	0.87 (4)	2.11 (5)	2.935 (6)	160 (4)

Symmetry codes: (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1.

Fig. 1

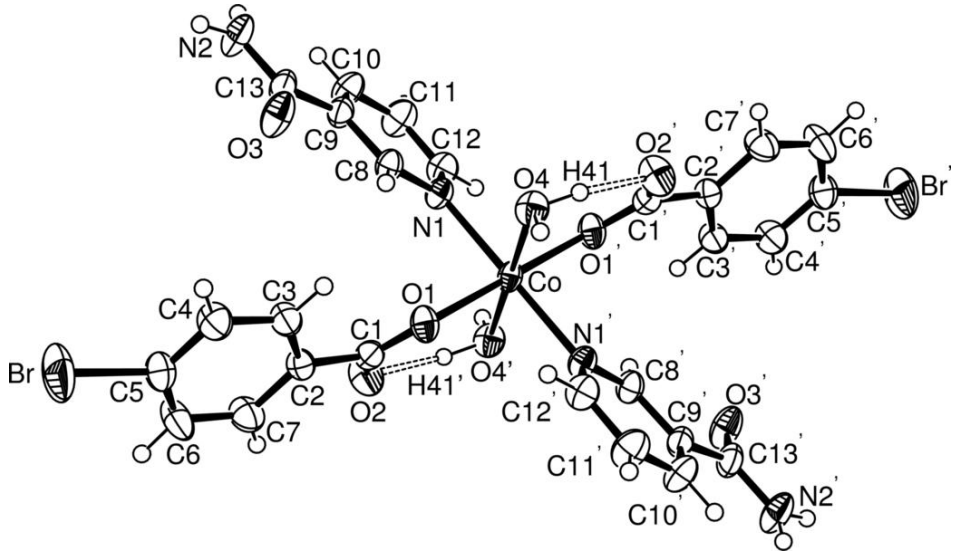
N2
C10
C13
C11
O3
C9
C12
C8
N1
O4
H41
O2'
C7'
C6'
C2'
Br'
C5'
C1'
O1'
C3'
C4'
Co
O1
C4
C3
C1
N1'
Br
C5
C2
O2
H41'
O4'
C8'
C12'
C9'
O3'
C7
C6
C11'
C13'
C10'
N2'

Fig. 2