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Bis(2,2′-bipyridyl-κ^2N,N')(carbonato-κ^2O,O')cobalt(III) bromide trihydrate

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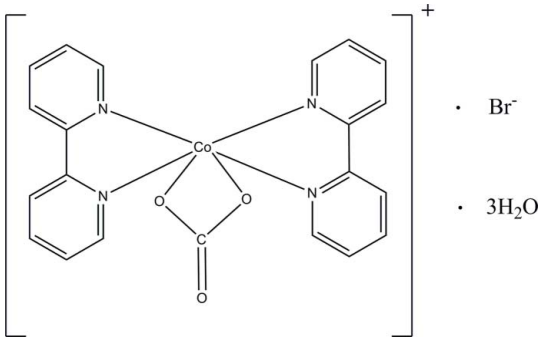
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.084; data-to-parameter ratio = 13.7.

The title complex, $[Co(CO_3)(C_{10}H_8N_2)_2]Br\cdot 3H_2O$, is isostructural with the chloride analogue. The six-coordinated octahedral $[Co(2,2'\text{-bipy})_2CO_3]^+$ cation (2,2′-bipy is 2,2′-bipyridyl), bromide ion and water molecules are linked together *via* O—H···Br and O—H···O hydrogen bonds, generating a one-dimensional chain.

Related literature

For related literature, see: Das *et al.* (1993); Thirumurugan & Natarajan (2004).



Experimental

Crystal data

$[Co(CO_3)(C_{10}H_8N_2)_2]Br\cdot 3H_2O$
M_r = 565.27
Triclinic, $P\overline{1}$
a = 9.1281 (1) Å
b = 9.6652 (2) Å
c = 13.0732 (2) Å
α = 92.054 (1)°
β = 102.315 (1)°
γ = 91.448 (1)°
V = 1125.48 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.58 mm^{-1}
T = 296 (2) K
0.18 × 0.12 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.654, T_{max} = 0.801
14734 measured reflections
4411 independent reflections
4000 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.084
S = 1.08
4411 reflections
323 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4B···O5^{i}	0.841 (10)	1.997 (11)	2.832 (3)	172 (3)
O4—H4A···O5^{ii}	0.839 (10)	2.016 (12)	2.847 (3)	171 (4)
O5—H5A···O3^{iii}	0.835 (10)	1.907 (12)	2.735 (3)	171 (3)
O5—H5B···Br1	0.837 (10)	2.422 (13)	3.247 (2)	169 (3)
O6—H6B···Br1	0.840 (10)	2.514 (12)	3.345 (2)	170 (3)
O6—H6A···Br1^{iv}	0.841 (10)	2.541 (12)	3.378 (3)	173 (3)

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

Data collection: *SMART* (Bruker, 2001); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2506).

References

Bruker (2001). *SMART*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Das, K., Sinha, U. C., Chaterjee, C. & Mishnev, A. (1993). *Z. Kristallogr.* **205**, 316–318.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Thirumurugan, A. & Natarajan, S. (2004). *Dalton Trans.* pp. 2923–2928.

supporting information

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Bis(2,2′-bipyridyl-κ^2N,N')(carbonato-κ^2O,O')cobalt(III) bromide trihydrate

Peng-Tao Ma, Yu-Xia Wang, Guo-Qian Zhang and Ming-Xue Li

S1. Comment

Recently, the design and assembly of metal coordination polymers continues attracting chemist's interests and constitutes an important area of research (Thirumurugan & Natarajan, 2004). During the past decades, lots of such compounds have been reported, which present predictable one-, two, three-dimensional frameworks by covalent bonds or hydrogen bonds interactions. Herein, we report the title compound (I).

The title complex (I), $[Co(2,2'\text{-bipy})_2CO_3]Br\cdot 3H_2O$, contains a $[Co(2,2'\text{-bipy})_2CO_3]^+$ complex cation, a bromine ion, and three water molecules (Fig.1), which is isostructural with its chloride analogue (Das *et al.*, 1993). In the molecular structure, Co atom resides in a distorted octahedral environment, which is defined by four nitrogen atoms from two 2,2-bipyridyl ligands, two oxygen dornors from the carbonate anion. In addition, the $[Co(2,2'\text{-bipy})_2CO_3]^+$ cation, bromine ion, and water molecules in the complex are linked together *via* O—H···Br and O—H···O hydrogen bonds generating a one-dimensional chain (Fig.2, Table 1).

S2. Experimental

Solid $CoSO_4\cdot 7H_2O$ (0.5 mmol, 0.141 g), KBr(1.0 mmol, 0.119 g) and 2,2′-bipy (1 mmol, 0.156 g) was dissolved in 20 ml of the mixed solvent of ethanol and water in a ratio of 1:4(*v*/*v*). Under continuous stirring, 5 ml (1 mol/*L*) solution of Na_2CO_3 was added dropwise until a purple solution resulted. The solution was filtered and left at room temperature. After slow evaporation over a period of a week, block red crystals of (I) were obtained.

S3. Refinement

The H atoms of the water molecules were located in a difference synthesis and refined with distance restraints O—H = 0.85 (1)Å and H···H = 1.34 (2) Å. The remaining H atoms were positioned geometrically with C—H = 0.93 Å, and were refined as riding with U_{iso}(H)=1.2U_{eq}(C).

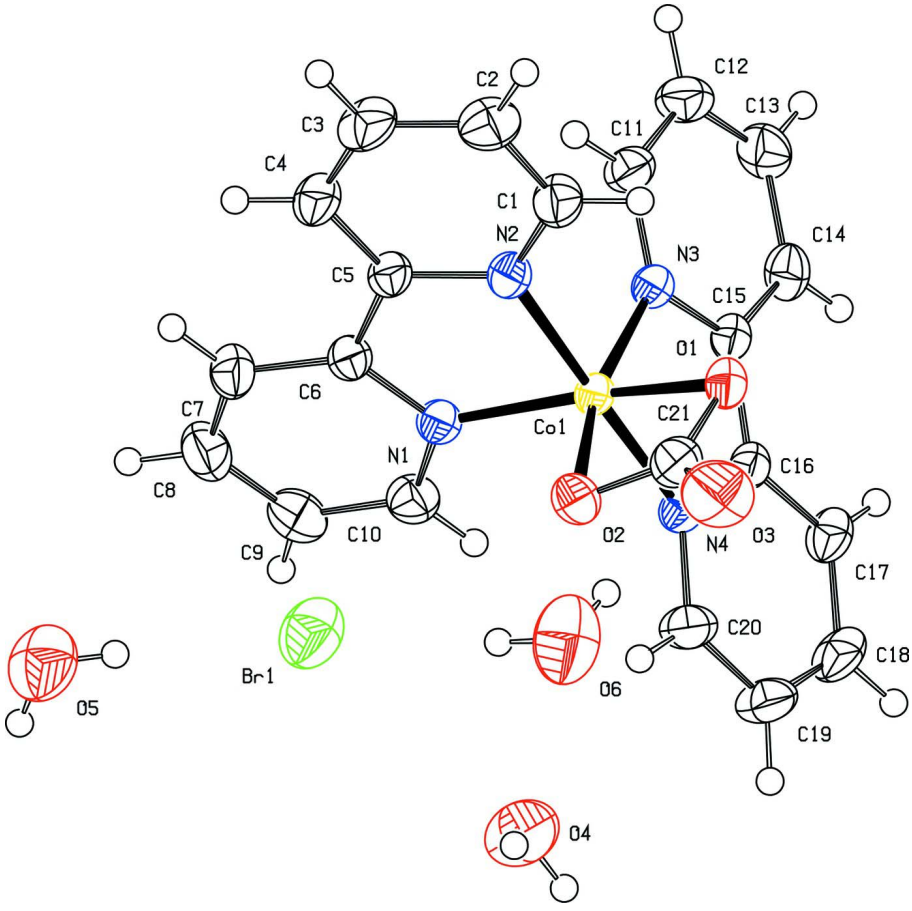

Figure 1

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

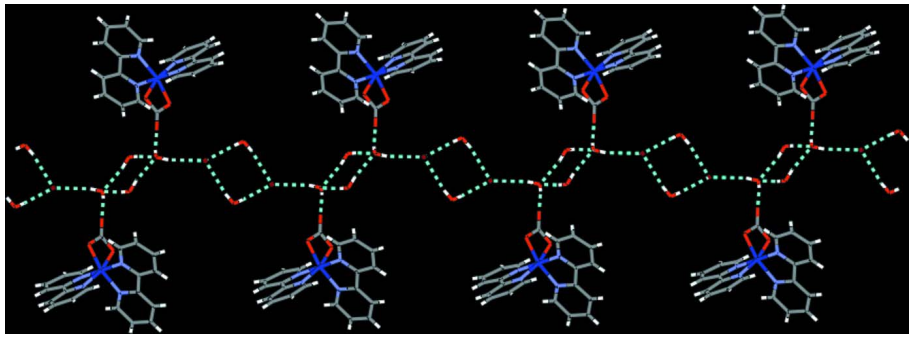

Figure 2

One-dimensional structure of (I) linked by hydrogen bonds.

Bis(2,2′-bipyridyl-κ^2N,N')(carbonato-κ^2O,O')cobalt(III) bromide trihydrate

Crystal data

$[Co(CO_3)(C_{10}H_8N_2)_2]Br\cdot 3H_2O$
$M_r = 565.27$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.1281$ (1) Å
$b = 9.6652$ (2) Å

c = 13.0732 (2) Å
α = 92.054 (1)°
β = 102.315 (1)°
γ = 91.448 (1)°
V = 1125.48 (3) Å^3
Z = 2
F(000) = 572
D_x = 1.668 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9295 reflections
θ = 2.6–26.7°
μ = 2.58 mm^{-1}
T = 296 K
Block, red
0.18 × 0.12 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.654, T_{max} = 0.801

14734 measured reflections
4411 independent reflections
4000 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 26.0°, θ_{min} = 2.1°
h = −10→11
k = −11→11
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.084
S = 1.08
4411 reflections
323 parameters
9 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.4188P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0160 (12)

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}
Co1	0.26787 (3)	0.01455 (3)	0.244258 (18)	0.02444 (10)
Br1	0.68362 (3)	0.61581 (3)	0.14986 (2)	0.06088 (12)
C1	0.3267 (2)	−0.2651 (2)	0.31331 (18)	0.0361 (5)

H1	0.2315	−0.2896	0.2742	0.043*
C2	0.4099 (3)	−0.3639 (2)	0.37077 (19)	0.0421 (5)
H2	0.3717	−0.4542	0.3702	0.051*
C3	0.5510 (3)	−0.3268 (2)	0.42920 (18)	0.0422 (5)
H3	0.6083	−0.3917	0.4694	0.051*
C4	0.6063 (2)	−0.1933 (2)	0.42761 (17)	0.0369 (5)
H4	0.7016	−0.1672	0.4660	0.044*
C5	0.5184 (2)	−0.0982 (2)	0.36814 (14)	0.0278 (4)
C6	0.5627 (2)	0.0465 (2)	0.35739 (14)	0.0278 (4)
C7	0.7009 (2)	0.1073 (2)	0.40451 (17)	0.0366 (5)
H7	0.7727	0.0569	0.4478	0.044*
C8	0.7303 (3)	0.2439 (3)	0.38614 (19)	0.0436 (5)
H8	0.8224	0.2865	0.4169	0.052*
C9	0.6221 (3)	0.3167 (2)	0.3219 (2)	0.0430 (5)
H9	0.6406	0.4087	0.3086	0.052*
C10	0.4857 (2)	0.2511 (2)	0.27730 (17)	0.0354 (5)
H10	0.4126	0.3004	0.2342	0.042*
C11	0.3835 (2)	−0.1361 (2)	0.07871 (17)	0.0331 (4)
H11	0.4386	−0.1880	0.1312	0.040*
C12	0.3882 (3)	−0.1675 (2)	−0.02410 (18)	0.0390 (5)
H12	0.4445	−0.2404	−0.0409	0.047*
C13	0.3086 (3)	−0.0894 (3)	−0.10162 (17)	0.0399 (5)
H13	0.3101	−0.1097	−0.1715	0.048*
C14	0.2262 (2)	0.0193 (2)	−0.07523 (15)	0.0341 (5)
H14	0.1740	0.0744	−0.1266	0.041*
C15	0.2232 (2)	0.0443 (2)	0.02917 (15)	0.0263 (4)
C16	0.1368 (2)	0.1543 (2)	0.06733 (15)	0.0265 (4)
C17	0.0429 (2)	0.2405 (2)	0.00477 (17)	0.0338 (4)
H17	0.0303	0.2332	−0.0677	0.041*
C18	−0.0327 (2)	0.3386 (2)	0.0514 (2)	0.0413 (5)
H18	−0.0990	0.3964	0.0106	0.050*
C19	−0.0085 (3)	0.3493 (2)	0.1585 (2)	0.0447 (6)
H19	−0.0560	0.4167	0.1910	0.054*
C20	0.0864 (3)	0.2598 (2)	0.21795 (18)	0.0395 (5)
H20	0.1021	0.2673	0.2906	0.047*
O3	−0.0230 (2)	−0.0747 (2)	0.37222 (16)	0.0604 (5)
C21	0.0755 (2)	−0.0408 (2)	0.32724 (17)	0.0368 (5)
N1	0.45605 (18)	0.11867 (17)	0.29456 (13)	0.0282 (3)
N2	0.37927 (18)	−0.13463 (17)	0.31232 (12)	0.0281 (3)
N3	0.30138 (17)	−0.03247 (17)	0.10536 (12)	0.0265 (3)
N4	0.15670 (18)	0.16221 (17)	0.17294 (13)	0.0292 (4)
O1	0.08496 (15)	−0.08699 (15)	0.23240 (11)	0.0321 (3)
O2	0.18851 (16)	0.04514 (16)	0.36505 (11)	0.0341 (3)
O4	0.1357 (3)	0.4381 (3)	0.43419 (18)	0.0666 (6)
O5	0.9249 (3)	0.6454 (3)	0.37190 (19)	0.0676 (6)
O6	0.3364 (3)	0.4743 (3)	0.1049 (2)	0.0754 (7)
H4A	0.109 (4)	0.409 (3)	0.4873 (19)	0.084 (12)*
H4B	0.075 (3)	0.498 (3)	0.410 (2)	0.061 (9)*

H6A	0.331 (3)	0.445 (4)	0.0429 (13)	0.074 (12)*
H5A	0.939 (3)	0.7312 (12)	0.379 (2)	0.055 (9)*
H6B	0.423 (2)	0.510 (4)	0.125 (2)	0.082 (12)*
H5B	0.856 (3)	0.630 (3)	0.3190 (19)	0.086 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02552 (15)	0.02518 (16)	0.02032 (14)	0.00563 (10)	−0.00088 (10)	0.00176 (10)
Br1	0.05214 (18)	0.0591 (2)	0.0695 (2)	0.00644 (13)	0.00614 (14)	0.01561 (15)
C1	0.0349 (11)	0.0304 (11)	0.0403 (12)	0.0004 (8)	0.0015 (9)	0.0057 (9)
C2	0.0496 (13)	0.0294 (11)	0.0486 (13)	0.0054 (9)	0.0114 (11)	0.0107 (10)
C3	0.0474 (13)	0.0386 (13)	0.0398 (12)	0.0159 (10)	0.0036 (10)	0.0143 (10)
C4	0.0358 (11)	0.0412 (13)	0.0302 (10)	0.0108 (9)	−0.0025 (8)	0.0049 (9)
C5	0.0287 (9)	0.0325 (11)	0.0212 (9)	0.0064 (8)	0.0022 (7)	0.0016 (8)
C6	0.0295 (9)	0.0318 (11)	0.0210 (9)	0.0051 (8)	0.0027 (7)	0.0001 (8)
C7	0.0312 (10)	0.0439 (13)	0.0311 (10)	0.0020 (9)	−0.0008 (8)	−0.0013 (9)
C8	0.0387 (12)	0.0451 (14)	0.0438 (13)	−0.0090 (10)	0.0043 (10)	−0.0082 (10)
C9	0.0501 (13)	0.0308 (12)	0.0478 (13)	−0.0054 (10)	0.0111 (11)	−0.0022 (10)
C10	0.0403 (11)	0.0289 (11)	0.0361 (11)	0.0032 (9)	0.0054 (9)	0.0035 (9)
C11	0.0323 (10)	0.0320 (11)	0.0349 (11)	0.0084 (8)	0.0064 (8)	0.0028 (8)
C12	0.0407 (12)	0.0376 (12)	0.0410 (12)	0.0079 (9)	0.0142 (10)	−0.0039 (10)
C13	0.0415 (12)	0.0504 (14)	0.0286 (10)	0.0009 (10)	0.0109 (9)	−0.0057 (9)
C14	0.0323 (10)	0.0435 (12)	0.0245 (10)	0.0009 (9)	0.0010 (8)	0.0048 (9)
C15	0.0230 (9)	0.0283 (10)	0.0261 (9)	0.0007 (7)	0.0017 (7)	0.0027 (8)
C16	0.0235 (9)	0.0263 (10)	0.0279 (9)	0.0004 (7)	0.0009 (7)	0.0034 (8)
C17	0.0303 (10)	0.0341 (11)	0.0351 (11)	0.0037 (8)	0.0008 (8)	0.0110 (9)
C18	0.0345 (11)	0.0324 (12)	0.0550 (14)	0.0109 (9)	0.0016 (10)	0.0155 (10)
C19	0.0439 (12)	0.0327 (12)	0.0583 (15)	0.0143 (10)	0.0116 (11)	0.0008 (11)
C20	0.0456 (12)	0.0354 (12)	0.0377 (11)	0.0143 (10)	0.0082 (9)	−0.0017 (9)
O3	0.0540 (11)	0.0702 (13)	0.0655 (12)	−0.0069 (9)	0.0345 (10)	−0.0080 (10)
C21	0.0353 (11)	0.0412 (12)	0.0339 (11)	0.0074 (9)	0.0065 (9)	0.0011 (9)
N1	0.0304 (8)	0.0269 (9)	0.0257 (8)	0.0042 (7)	0.0023 (6)	0.0010 (6)
N2	0.0292 (8)	0.0282 (9)	0.0251 (8)	0.0036 (6)	0.0012 (6)	0.0031 (6)
N3	0.0264 (8)	0.0259 (8)	0.0256 (8)	0.0043 (6)	0.0015 (6)	0.0015 (6)
N4	0.0295 (8)	0.0291 (9)	0.0274 (8)	0.0063 (7)	0.0019 (6)	0.0005 (7)
O1	0.0260 (7)	0.0374 (8)	0.0298 (7)	0.0018 (6)	−0.0003 (5)	−0.0014 (6)
O2	0.0387 (8)	0.0394 (8)	0.0229 (7)	0.0030 (6)	0.0040 (6)	−0.0022 (6)
O4	0.0692 (14)	0.0753 (16)	0.0579 (13)	0.0224 (12)	0.0159 (11)	0.0070 (11)
O5	0.0678 (14)	0.0646 (15)	0.0665 (14)	0.0084 (11)	0.0022 (11)	0.0222 (11)
O6	0.0618 (14)	0.0878 (18)	0.0730 (17)	−0.0079 (12)	0.0045 (11)	0.0232 (14)

Geometric parameters (Å, º)

Co1—O1	1.8896 (14)	C11—C12	1.377 (3)
Co1—O2	1.8897 (14)	C11—H11	0.9300
Co1—N2	1.9195 (16)	C12—C13	1.376 (3)
Co1—N4	1.9238 (16)	C12—H12	0.9300

Co1—N1	1.9440 (17)	C13—C14	1.383 (3)
Co1—N3	1.9447 (16)	C13—H13	0.9300
Co1—C21	2.314 (2)	C14—C15	1.384 (3)
C1—N2	1.339 (3)	C14—H14	0.9300
C1—C2	1.378 (3)	C15—N3	1.352 (2)
C1—H1	0.9300	C15—C16	1.474 (3)
C2—C3	1.381 (3)	C16—N4	1.353 (3)
C2—H2	0.9300	C16—C17	1.373 (3)
C3—C4	1.377 (3)	C17—C18	1.385 (3)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.384 (3)	C18—C19	1.370 (4)
C4—H4	0.9300	C18—H18	0.9300
C5—N2	1.353 (2)	C19—C20	1.379 (3)
C5—C6	1.467 (3)	C19—H19	0.9300
C6—N1	1.357 (2)	C20—N4	1.342 (3)
C6—C7	1.387 (3)	C20—H20	0.9300
C7—C8	1.380 (3)	O3—C21	1.219 (3)
C7—H7	0.9300	C21—O2	1.307 (3)
C8—C9	1.378 (4)	C21—O1	1.324 (3)
C8—H8	0.9300	O4—H4A	0.839 (10)
C9—C10	1.384 (3)	O4—H4B	0.841 (10)
C9—H9	0.9300	O5—H5A	0.835 (10)
C10—N1	1.339 (3)	O5—H5B	0.837 (10)
C10—H10	0.9300	O6—H6A	0.841 (10)
C11—N3	1.346 (3)	O6—H6B	0.840 (10)

O1—Co1—O2	69.26 (6)	N3—C11—H11	119.1
O1—Co1—N2	91.31 (7)	C12—C11—H11	119.1
O2—Co1—N2	88.81 (7)	C13—C12—C11	119.1 (2)
O1—Co1—N4	88.69 (7)	C13—C12—H12	120.4
O2—Co1—N4	92.44 (7)	C11—C12—H12	120.4
N2—Co1—N4	178.66 (7)	C12—C13—C14	119.7 (2)
O1—Co1—N1	165.27 (7)	C12—C13—H13	120.2
O2—Co1—N1	96.93 (7)	C14—C13—H13	120.2
N2—Co1—N1	83.06 (7)	C13—C14—C15	118.66 (19)
N4—Co1—N1	97.25 (7)	C13—C14—H14	120.7
O1—Co1—N3	97.79 (6)	C15—C14—H14	120.7
O2—Co1—N3	166.44 (7)	N3—C15—C14	121.61 (18)
N2—Co1—N3	95.69 (7)	N3—C15—C16	114.35 (16)
N4—Co1—N3	82.99 (7)	C14—C15—C16	124.04 (18)
N1—Co1—N3	96.31 (7)	N4—C16—C17	121.78 (18)
O1—Co1—C21	34.90 (7)	N4—C16—C15	113.11 (16)
O2—Co1—C21	34.39 (7)	C17—C16—C15	125.10 (18)
N2—Co1—C21	89.09 (7)	C16—C17—C18	118.9 (2)
N4—Co1—C21	91.68 (7)	C16—C17—H17	120.6
N1—Co1—C21	131.00 (7)	C18—C17—H17	120.6
N3—Co1—C21	132.64 (7)	C19—C18—C17	119.2 (2)
N2—C1—C2	121.8 (2)	C19—C18—H18	120.4

N2—C1—H1	119.1	C17—C18—H18	120.4
C2—C1—H1	119.1	C18—C19—C20	119.7 (2)
C1—C2—C3	118.9 (2)	C18—C19—H19	120.1
C1—C2—H2	120.5	C20—C19—H19	120.1
C3—C2—H2	120.5	N4—C20—C19	121.3 (2)
C4—C3—C2	119.6 (2)	N4—C20—H20	119.4
C4—C3—H3	120.2	C19—C20—H20	119.4
C2—C3—H3	120.2	O3—C21—O2	125.6 (2)
C3—C4—C5	119.1 (2)	O3—C21—O1	124.9 (2)
C3—C4—H4	120.4	O2—C21—O1	109.44 (18)
C5—C4—H4	120.4	O3—C21—Co1	177.39 (19)
N2—C5—C4	121.01 (19)	O2—C21—Co1	54.74 (10)
N2—C5—C6	113.60 (16)	O1—C21—Co1	54.75 (10)
C4—C5—C6	125.38 (18)	C10—N1—C6	119.14 (17)
N1—C6—C7	121.44 (19)	C10—N1—Co1	126.97 (14)
N1—C6—C5	114.04 (17)	C6—N1—Co1	113.81 (14)
C7—C6—C5	124.51 (18)	C1—N2—C5	119.56 (17)
C8—C7—C6	118.9 (2)	C1—N2—Co1	125.30 (14)
C8—C7—H7	120.5	C5—N2—Co1	115.00 (14)
C6—C7—H7	120.5	C11—N3—C15	119.05 (17)
C9—C8—C7	119.6 (2)	C11—N3—Co1	127.02 (14)
C9—C8—H8	120.2	C15—N3—Co1	113.76 (12)
C7—C8—H8	120.2	C20—N4—C16	119.12 (17)
C8—C9—C10	119.1 (2)	C20—N4—Co1	125.47 (14)
C8—C9—H9	120.4	C16—N4—Co1	115.00 (13)
C10—C9—H9	120.4	C21—O1—Co1	90.36 (12)
N1—C10—C9	121.8 (2)	C21—O2—Co1	90.87 (12)
N1—C10—H10	119.1	H4A—O4—H4B	106.4 (16)
C9—C10—H10	119.1	H5A—O5—H5B	106.9 (16)
N3—C11—C12	121.83 (19)	H6A—O6—H6B	105.4 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*B*···O5^{i}	0.84 (1)	2.00 (1)	2.832 (3)	172 (3)
O4—H4*A*···O5^{ii}	0.84 (1)	2.02 (1)	2.847 (3)	171 (4)
O5—H5*A*···O3^{iii}	0.84 (1)	1.91 (1)	2.735 (3)	171 (3)
O5—H5*B*···Br1	0.84 (1)	2.42 (1)	3.247 (2)	169 (3)
O6—H6*B*···Br1	0.84 (1)	2.51 (1)	3.345 (2)	170 (3)
O6—H6*A*···Br1^{iv}	0.84 (1)	2.54 (1)	3.378 (3)	173 (3)

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