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Dibromido(6,6′-dimethyl-2,2′-bipyridine-κ^2N,N')cobalt(II)

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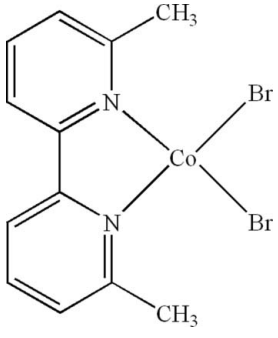
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.045; wR factor = 0.089; data-to-parameter ratio = 18.0.

In the title compound, $[CoBr_2(C_{12}H_{12}N_2)]$, the Co^{II} atom is four-coordinated in a distorted tetrahedral geometry by two N atoms from a 6,6′-dimethyl-2,2′-bipyridine ligand and by two terminal Br atoms. Intermolecular C—H···Br hydrogen bonds and π–π stacking between the pyridine rings in the bc plane [centroid–centroid distance = 3.725 (3) Å] are present in the crystal structure.

Related literature

For related structures, see: Akbarzadeh Torbati *et al.* (2010); Alizadeh *et al.* (2011, 2009); Itoh *et al.* (2005); Kou *et al.* (2008); Onggo *et al.* (2005); Shirvan & Haydari Dezfuli (2012).



Experimental

Crystal data

$[CoBr_2(C_{12}H_{12}N_2)]$
M_r = 402.97
Monoclinic, $P2_1/c$
a = 7.6550 (6) Å
b = 10.2577 (9) Å
c = 18.0030 (16) Å
β = 95.779 (7)°
V = 1406.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.88 mm^{-1}
T = 298 K
0.30 × 0.24 × 0.18 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.149, T_{max} = 0.302
7259 measured reflections
2766 independent reflections
1753 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.089
S = 0.95
2766 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N1	2.044 (4)	Co1—Br1	2.3594 (10)
Co1—N2	2.037 (4)	Co1—Br2	2.3588 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···Br1^{i}	0.93	2.92	3.696 (5)	142
C12—H12C···Br1^{ii}	0.96	2.89	3.847 (6)	172

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU5630).

References

Akbarzadeh Torbati, N., Rezvani, A. R., Safari, N., Saravani, H. & Amani, V. (2010). *Acta Cryst.* E**66**, m1284.
Alizadeh, R., Kalateh, K., Khoshtarkib, Z., Ahmadi, R. & Amani, V. (2009). *Acta Cryst.* E**65**, m1439–m1440.
Alizadeh, R., Seifi, S. & Amani, V. (2011). *Acta Cryst.* E**67**, m305.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Itoh, S., Kishikawa, N., Suzuki, T. & Takagi, H. D. (2005). *Dalton Trans.* pp. 1066–1078.
Kou, H. Z., Hishiya, S. & Sato, O. (2008). *Inorg. Chim. Acta*, **361**, 2396–2406.
Onggo, D., Scudder, M. L., Craig, D. C. & Goodwin, H. A. (2005). *J. Mol. Struct.* **738**, 129–136.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shirvan, S. A. & Haydari Dezfuli, S. (2012). *Acta Cryst.* E**68**, m1143.

supporting information

Acta Cryst. (2012). E**68**, m1363 [doi:10.1107/S1600536812041980]

Dibromido(6,6′-dimethyl-2,2′-bipyridine-κ^2N,N')cobalt(II)

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S1. Comment

6,6′-Dimethyl-2,2′-bipyridine (6,6′-dmbipy), is a good bidentate ligand, and numerous complexes with 6,6′-dmbipy have been prepared, such as that of zinc (Alizadeh *et al.*, 2009), copper (Itoh *et al.*, 2005), cadmium (Shirvan & Haydari Dezfuli, 2012), cobalt (Akbarzadeh Torbati *et al.*, 2010), nickel (Kou *et al.*, 2008), ruthenium (Onggo *et al.*, 2005) and mercury (Alizadeh *et al.*, 2011). We report herein the synthesis and crystal structure of the title compound.

In the title compound, (Fig. 1), the Co^{II} atom is four-coordinated in a distorted tetrahedral geometry by two N atoms from a 6,6′-dimethyl-2,2′-bipyridine and two terminal Br atoms. The Co—Br and Co—N bond lengths and angles are collected in Table 1.

In the crystal structure, intermolecular C—H···Br hydrogen bonds (Table 2) and π-π contacts (Fig. 2) between the pyridine rings, *Cg*2—*Cg*3^{i} [symmetry cods: (i) -*x*, 1 - y, -*z*, where *Cg*2 and *Cg*3 are centroids of the rings (N1/C2–C6) and (N2/C7–C11), respectively] may stabilize the structure, with centroid–centroid distance of 3.725 (3) Å.

S2. Experimental

For the preparation of the title compound, a solution of 6,6′-dimethyl-2,2′-bipyridine (0.25 g, 1.33 mmol) in methanol (10 ml) was added to a solution of $CoBr_2$ (0.29 g, 1.33 mmol) in acetonitrile (15 ml) and the resulting blue solution was stirred for 15 min at 313 K. This solution was left to evaporate slowly at room temperature. After one week, blue block crystals of the title compound were isolated (yield 0.41 g, 76.5%).

S3. Refinement

H atoms were positioned geometrically with C—H = 0.93 and 0.96 Å and constrained to ride on their parent atoms, U_{iso}(H) = 1.2U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for aromatic H atoms.

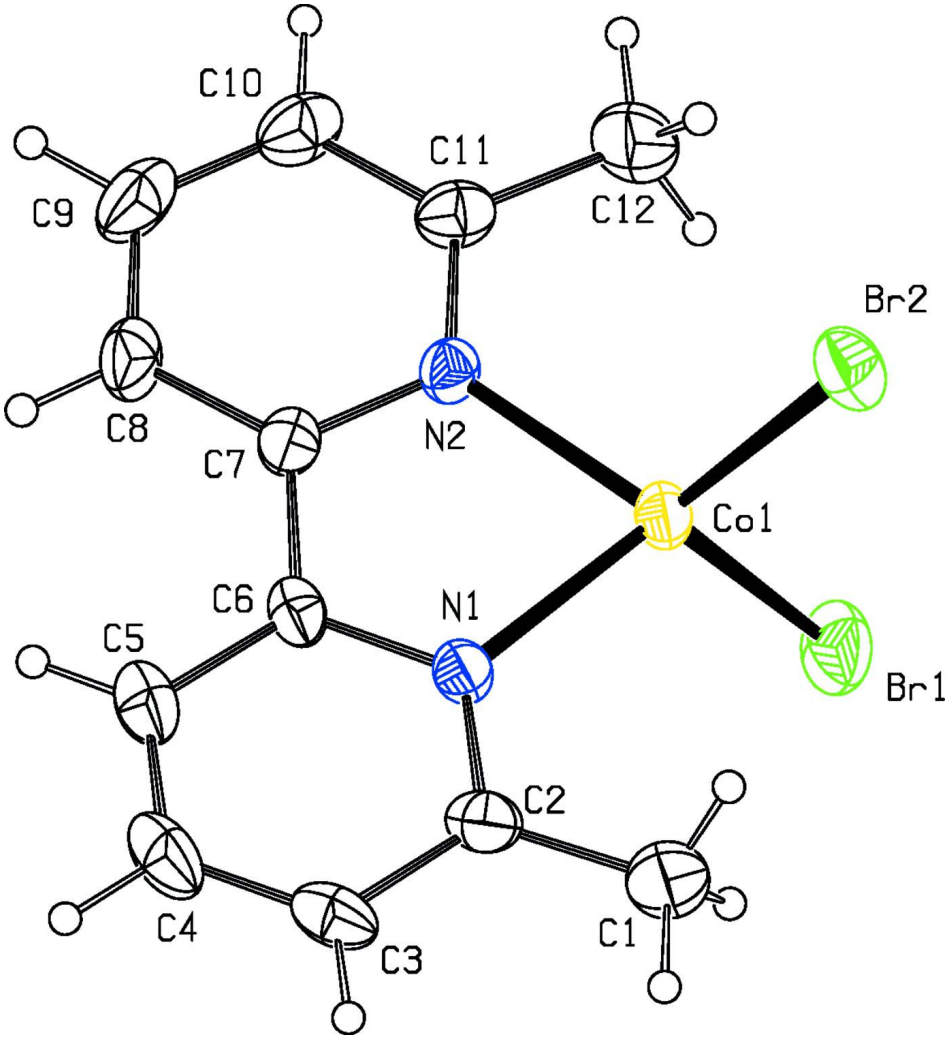

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

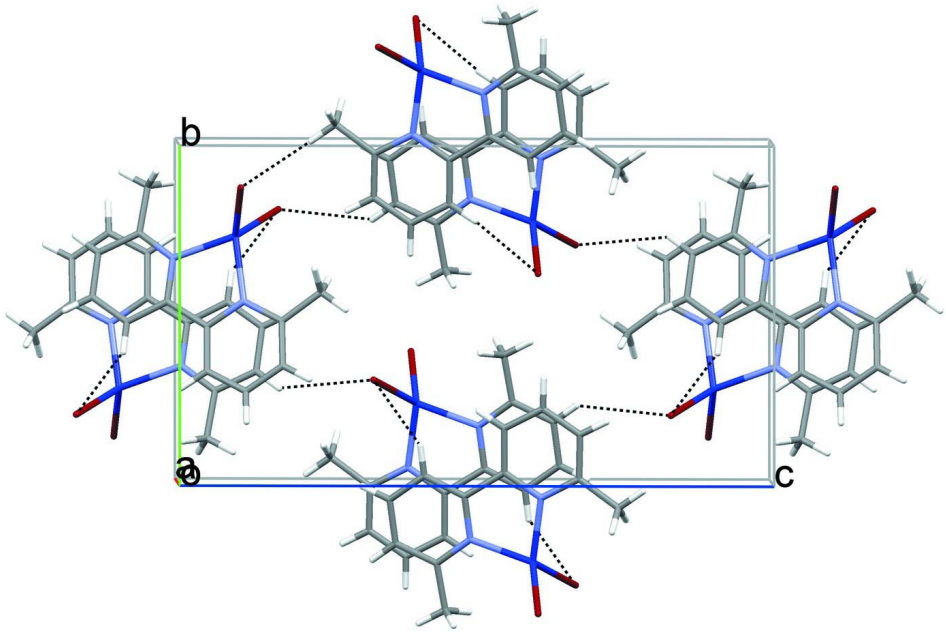

Figure 2

Unit-cell packing diagram for title molecule. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[CoBr_2(C_{12}H_{12}N_2)]$
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$a = 7.6550$ (6) Å
$b = 10.2577$ (9) Å
$c = 18.0030$ (16) Å
$\beta = 95.779$ (7)°
$V = 1406.5$ (2) Å^3
$Z = 4$
$F(000) = 780$
$D_x = 1.903$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7259 reflections
$\theta = 2.3$–$26.0°$
$\mu = 6.88$ mm^{-1}
$T = 298$ K
Block, blue
0.30 × 0.24 × 0.18 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.149$, $T_{max} = 0.302$
7259 measured reflections
2766 independent reflections
1753 reflections with $I > 2\sigma(I)$
$R_{int} = 0.068$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.3°$
$h = -8 \rightarrow 9$
$k = -12 \rightarrow 11$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.089$
$S = 0.95$
2766 reflections
154 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} = 0.005$
H-atom parameters constrained	$\Delta\rho_{max} = 0.51$ e Å^{-3}
	$\Delta\rho_{min} = -0.56$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3959 (11)	0.8727 (6)	−0.0503 (3)	0.074 (2)
H1A	0.4872	0.8803	−0.0098	0.089*
H1B	0.2921	0.9159	−0.0372	0.089*
H1C	0.4338	0.9122	−0.0942	0.089*
C2	0.3572 (8)	0.7343 (6)	−0.0648 (3)	0.0494 (14)
C3	0.3757 (8)	0.6766 (7)	−0.1338 (3)	0.0566 (16)
H3	0.4156	0.7252	−0.1723	0.068*
C4	0.3342 (9)	0.5468 (7)	−0.1441 (3)	0.0651 (18)
H4	0.3435	0.5077	−0.1901	0.078*
C5	0.2791 (8)	0.4753 (6)	−0.0865 (3)	0.0550 (15)
H5	0.2506	0.3876	−0.0930	0.066*
C6	0.2665 (7)	0.5352 (5)	−0.0188 (3)	0.0397 (12)
C7	0.2137 (7)	0.4644 (5)	0.0477 (3)	0.0421 (12)
C8	0.1766 (8)	0.3330 (5)	0.0476 (3)	0.0570 (16)
H8	0.1821	0.2838	0.0045	0.068*
C9	0.1312 (9)	0.2751 (6)	0.1121 (4)	0.0687 (19)
H9	0.1056	0.1865	0.1131	0.082*
C10	0.1245 (8)	0.3503 (6)	0.1744 (4)	0.0592 (16)
H10	0.0960	0.3120	0.2185	0.071*
C11	0.1592 (8)	0.4813 (6)	0.1731 (3)	0.0504 (14)
C12	0.1535 (10)	0.5666 (7)	0.2391 (3)	0.077 (2)
H12A	0.0704	0.6355	0.2275	0.092*
H12B	0.2677	0.6033	0.2525	0.092*
H12C	0.1187	0.5164	0.2801	0.092*
N1	0.3039 (6)	0.6627 (4)	−0.0087 (2)	0.0385 (10)
N2	0.2047 (6)	0.5381 (4)	0.1095 (2)	0.0387 (10)
Co1	0.26905 (10)	0.72871 (7)	0.09589 (3)	0.0414 (2)
Br1	0.03425 (10)	0.87570 (7)	0.10302 (4)	0.0703 (2)
Br2	0.52149 (9)	0.80174 (6)	0.17019 (3)	0.0598 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.109 (6)	0.062 (4)	0.054 (3)	−0.021 (4)	0.019 (4)	0.010 (3)
C2	0.053 (4)	0.056 (3)	0.039 (3)	0.008 (3)	0.002 (3)	0.006 (2)
C3	0.057 (4)	0.082 (5)	0.032 (3)	0.006 (3)	0.009 (3)	0.003 (3)
C4	0.067 (5)	0.085 (5)	0.043 (3)	0.013 (4)	0.007 (3)	−0.025 (3)
C5	0.056 (4)	0.058 (4)	0.051 (3)	0.002 (3)	0.005 (3)	−0.019 (3)
C6	0.034 (3)	0.043 (3)	0.040 (3)	0.003 (2)	−0.001 (2)	−0.011 (2)
C7	0.035 (3)	0.037 (3)	0.051 (3)	0.002 (2)	−0.007 (2)	−0.003 (2)
C8	0.056 (4)	0.041 (3)	0.070 (4)	−0.008 (3)	−0.012 (3)	−0.012 (3)
C9	0.066 (5)	0.038 (3)	0.099 (5)	−0.010 (3)	−0.010 (4)	0.012 (3)
C10	0.054 (4)	0.051 (4)	0.072 (4)	−0.013 (3)	0.001 (3)	0.018 (3)
C11	0.046 (4)	0.053 (4)	0.052 (3)	−0.005 (3)	0.006 (3)	0.011 (3)
C12	0.112 (6)	0.076 (5)	0.047 (3)	−0.018 (4)	0.027 (4)	0.006 (3)
N1	0.042 (3)	0.039 (2)	0.035 (2)	−0.002 (2)	0.0043 (19)	−0.0038 (17)
N2	0.038 (3)	0.034 (2)	0.043 (2)	−0.005 (2)	0.0007 (19)	−0.0013 (18)
Co1	0.0525 (5)	0.0357 (4)	0.0369 (3)	−0.0046 (3)	0.0083 (3)	−0.0058 (3)
Br1	0.0725 (5)	0.0601 (4)	0.0781 (4)	0.0177 (4)	0.0062 (3)	−0.0207 (3)
Br2	0.0619 (4)	0.0660 (4)	0.0508 (3)	−0.0135 (3)	0.0023 (3)	−0.0131 (3)

Geometric parameters (Å, º)

C1—C2	1.468 (8)	C8—C9	1.379 (8)
C1—H1A	0.9600	C8—H8	0.9300
C1—H1B	0.9600	C9—C10	1.367 (9)
C1—H1C	0.9600	C9—H9	0.9300
C2—N1	1.345 (6)	C10—C11	1.370 (8)
C2—C3	1.396 (7)	C10—H10	0.9300
C3—C4	1.377 (9)	C11—N2	1.360 (6)
C3—H3	0.9300	C11—C12	1.481 (8)
C4—C5	1.371 (9)	C12—H12A	0.9600
C4—H4	0.9300	C12—H12B	0.9600
C5—C6	1.378 (7)	C12—H12C	0.9600
C5—H5	0.9300	Co1—N1	2.044 (4)
C6—N1	1.347 (6)	Co1—N2	2.037 (4)
C6—C7	1.490 (7)	Co1—Br1	2.3594 (10)
C7—N2	1.354 (6)	Co1—Br2	2.3588 (10)
C7—C8	1.377 (7)		
C2—C1—H1A	109.5	C10—C9—C8	118.8 (6)
C2—C1—H1B	109.5	C10—C9—H9	120.6
H1A—C1—H1B	109.5	C8—C9—H9	120.6
C2—C1—H1C	109.5	C9—C10—C11	121.0 (6)
H1A—C1—H1C	109.5	C9—C10—H10	119.5
H1B—C1—H1C	109.5	C11—C10—H10	119.5
N1—C2—C3	120.1 (5)	N2—C11—C10	120.1 (5)
N1—C2—C1	117.7 (5)	N2—C11—C12	116.9 (5)

C3—C2—C1	122.1 (5)	C10—C11—C12	122.9 (5)
C4—C3—C2	119.2 (5)	C11—C12—H12A	109.5
C4—C3—H3	120.4	C11—C12—H12B	109.5
C2—C3—H3	120.4	H12A—C12—H12B	109.5
C5—C4—C3	120.0 (5)	C11—C12—H12C	109.5
C5—C4—H4	120.0	H12A—C12—H12C	109.5
C3—C4—H4	120.0	H12B—C12—H12C	109.5
C4—C5—C6	119.0 (6)	C2—N1—C6	120.4 (4)
C4—C5—H5	120.5	C2—N1—Co1	126.0 (3)
C6—C5—H5	120.5	C6—N1—Co1	113.5 (3)
N1—C6—C5	121.3 (5)	C7—N2—C11	119.4 (4)
N1—C6—C7	115.9 (4)	C7—N2—Co1	113.8 (3)
C5—C6—C7	122.8 (5)	C11—N2—Co1	126.8 (3)
N2—C7—C8	121.3 (5)	N2—Co1—N1	81.30 (15)
N2—C7—C6	115.4 (4)	N2—Co1—Br2	115.50 (12)
C8—C7—C6	123.3 (5)	N1—Co1—Br2	116.88 (13)
C7—C8—C9	119.4 (6)	N2—Co1—Br1	114.33 (13)
C7—C8—H8	120.3	N1—Co1—Br1	115.65 (12)
C9—C8—H8	120.3	Br2—Co1—Br1	110.57 (4)

N1—C2—C3—C4	1.8 (9)	C5—C6—N1—Co1	178.5 (4)
C1—C2—C3—C4	−178.9 (6)	C7—C6—N1—Co1	−2.2 (6)
C2—C3—C4—C5	−1.4 (10)	C8—C7—N2—C11	0.4 (8)
C3—C4—C5—C6	−0.1 (10)	C6—C7—N2—C11	−179.4 (5)
C4—C5—C6—N1	1.3 (9)	C8—C7—N2—Co1	179.1 (5)
C4—C5—C6—C7	−177.9 (5)	C6—C7—N2—Co1	−0.6 (6)
N1—C6—C7—N2	1.9 (7)	C10—C11—N2—C7	0.6 (8)
C5—C6—C7—N2	−178.8 (5)	C12—C11—N2—C7	179.4 (5)
N1—C6—C7—C8	−177.9 (5)	C10—C11—N2—Co1	−177.9 (4)
C5—C6—C7—C8	1.4 (9)	C12—C11—N2—Co1	0.8 (8)
N2—C7—C8—C9	−0.7 (9)	C7—N2—Co1—N1	−0.4 (4)
C6—C7—C8—C9	179.0 (5)	C11—N2—Co1—N1	178.2 (5)
C7—C8—C9—C10	0.0 (10)	C7—N2—Co1—Br2	−116.1 (3)
C8—C9—C10—C11	1.1 (10)	C11—N2—Co1—Br2	62.5 (5)
C9—C10—C11—N2	−1.4 (10)	C7—N2—Co1—Br1	113.9 (3)
C9—C10—C11—C12	180.0 (6)	C11—N2—Co1—Br1	−67.5 (5)
C3—C2—N1—C6	−0.6 (8)	C2—N1—Co1—N2	−179.1 (5)
C1—C2—N1—C6	−180.0 (6)	C6—N1—Co1—N2	1.5 (4)
C3—C2—N1—Co1	180.0 (4)	C2—N1—Co1—Br2	−64.8 (5)
C1—C2—N1—Co1	0.6 (8)	C6—N1—Co1—Br2	115.7 (3)
C5—C6—N1—C2	−0.9 (8)	C2—N1—Co1—Br1	68.0 (5)
C7—C6—N1—C2	178.3 (5)	C6—N1—Co1—Br1	−111.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···Br1^{i}	0.93	2.92	3.696 (5)	142

C12—H12*C*···Br1^{ii}	0.96	2.89	3.847 (6)	172

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*, *y*−1/2, −*z*+1/2.