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# 4-(Dimethylamino)pyridinium tribromido{3-[bromo/hydro(0.9/0.1)]-4-(dimethylamino)pyridine-$\kappa N^1$}cobaltate(II)

**Kong Mun Lo and Seik Weng Ng***

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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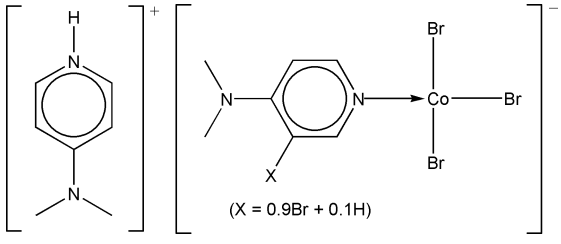
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.010 Å; disorder in main residue; $R$ factor = 0.046; $wR$ factor = 0.130; data-to-parameter ratio = 20.1.

The reaction of a cobalt(II) salt with 4-(dimethylamino)-pyridinium hydrobromide perbromide yielded the title compound, $(C_7H_{11}N_2)[CoBr_3(C_7H_{9.1}Br_{0.9}N_2)]$. In the anion, the $Co^{II}$ atom is coordinated in a distorted tetrahedral geometry by three Br atoms and the pyridine N atom of a bromine-substituted 4-(dimethylamino)pyridine molecule, whose formation probably results from an incomplete substitution (90%) catalysed by the $Co^{II}$ ion. One of the three bromine atoms bonded to the metal is disordered over two sites in a 0.9:0.1 ratio. An N—H···Br hydrogen bond connects the cation and anion.

## Related literature

For bis(4-(dimethylamino)pyridinium) tetrabromidocobaltate, see: Lo & Ng (2009). For other trihalocobaltate(II) anions having a pyridine-type donor ligand, see: Bogdanović *et al.* (2001); Crane *et al.* (2004); Divjaković *et al.* (1982); Hahn *et al.* (1997); Mueller-Westerhoff *et al.* (1996); Sumner & Steinmetz (1985).




## Experimental

### Crystal data

$(C_7H_{11}N_2)[CoBr_3(C_7H_{9.1}Br_{0.9}N_2)]$
$M_r$ = 615.02
Triclinic, $P\overline{1}$
$a$ = 8.3768 (2) Å
$b$ = 10.2622 (2) Å
$c$ = 12.4691 (3) Å
$\alpha$ = 99.028 (2)°
$\beta$ = 98.927 (1)°
$\gamma$ = 106.933 (2)°
$V$ = 989.57 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 8.74 mm$^{-1}$
$T$ = 150 K
0.40 × 0.20 × 0.10 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.128, $T_{max}$ = 0.475
(expected range = 0.112–0.417)
7974 measured reflections
4451 independent reflections
3019 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.053

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.130
$S$ = 0.97
4451 reflections
221 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.04 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Co1—Br1 | 2.4086 (11) | Co1—Br3′ | 2.376 (9) |
| Co1—Br2 | 2.3958 (10) | Co1—N1 | 2.032 (5) |
| Co1—Br3 | 2.3814 (13) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···Br1 | 0.88 | 2.74 | 3.434 (6) | 137 |

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2210).

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# supporting information

*Acta Cryst.* (2009). E**65**, m958–m959 [doi:10.1107/S1600536809027913]

## 4-(Dimethylamino)pyridinium tribromido{3-[bromo/hydro(0.9/0.1)]-4-(dimethylamino)pyridine-$\kappa N^1$}cobaltate(II)

**Kong Mun Lo and Seik Weng Ng**

### S1. Comment

The reaction of cobalt(II) nitrate and 4-(dimethylamino)pyridinium hydrobromide perbromide yields bis(4-(dimethylamino)pyridinium) tetrabromidocobaltate (Lo & Ng, 2009). A similar reaction with cobalt acetate in place of cobalt nitrate yields a new 4-(dimethylamino)pyridinium salt, $[C_7H_{11}N_2][CoBr_3(C_7H_{9.1}Br_{0.9}N_2)]$ (Scheme 1, Fig. 1). The $Co^{II}$ atom is coordinated by a bromine-substituted 4-(dimethylamino)pyridine molecule, whose formation probably results from an incomplete (90%) electrophilic substitution of 4-(dimethylamino)pyridine that is probabably catalyzed by the cobaltous ion.

### S2. Experimental

Green cobalt acetate (0.70 g, 2.8 mmol) dissolved in water (2 ml) and 4-(dimethylamino)pyridinium hydrobromide perbromide (1.00 g, 2.8 mmol) dissolved in ethanol (50 ml) were mixed and the mixture was heated for one hour. The red solution was filtered; well-formed deep-blue crystals were isolated from the solution after several days.

### S3. Refinement

H atoms were placed at calculated positions (C—H = 0.95 and 0.98, N—H = 0.88 Å) and were treated as riding on their parent atoms, with $U_{iso}$(H) = 1.2(or 1.5)$U_{eq}$(C).

One of the three Br atoms that are bonded to Co1 is disordered over two positions (Br3 and Br3′). The Br3 atom is 3.5 Å from $Br4^{i}$ atom [symmetry code: (i) = 1-x, 1-y, 2-z]. However, as the Br3′ atom is only 3.0 Å from $Br4^{i}$, the atom that is linked to the C2 atom should then be a mixture of Br and H atoms, with the provision that the occupancies of the Br3 and Br4 atoms are identical. As the occupancies refined to nearly 0.9:0.1, the occupancy factors were then fixed as 0.90 and 0.1 for Br3 and Br3′, as well as for Br4 and H2. Other ratios, e.g. 0.85:0.15 and 0.95:0.05, gave less satisfactory *R* indices and large peaks/deep holes in the difference Fourier map. The anisotropic displacement of the minor occupant was restrained to be nearly isotropic; the Co–Br distances were restrained to within 0.01 Å of each other.

The final difference Fourier map had a peak in the vicinity of Br2 and a hole in the vicinty of Br4. The magnitudes of both could be decreased by lowering the $2\theta$ limit to 50°.

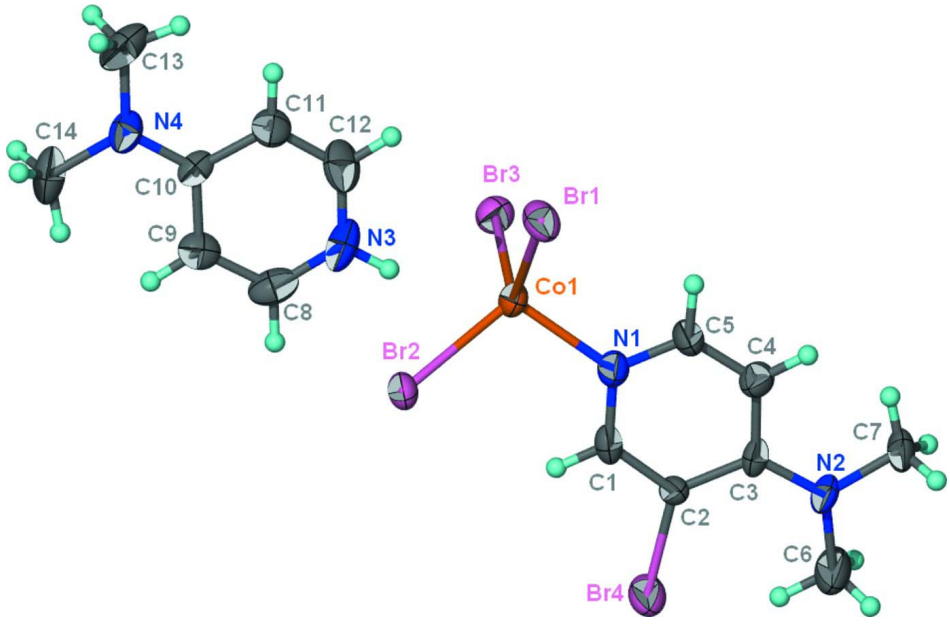


**Figure 1**

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 70% probability level. Minor disordered sites are omitted for clarity.

### 4-(Dimethylamino)pyridinium tribromido{3-[bromo/hydro(0.9/0.1)]-4- (dimethylamino)pyridine-$\kappa N^1$}cobaltate(II)

*Crystal data*

$(C_7H_{11}N_2)[CoBr_3(C_7H_{9.1}Br_{0.9}N_2)]$
$M_r = 615.02$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.3768$ (2) Å
$b = 10.2622$ (2) Å
$c = 12.4691$ (3) Å
$\alpha = 99.028$ (2)°
$\beta = 98.927$ (1)°
$\gamma = 106.933$ (2)°
$V = 989.57$ (4) Å$^3$
$Z = 2$
$F(000) = 591.2$
$D_x = 2.064$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6987 reflections
$\theta = 2.4$–$28.3°$
$\mu = 8.74$ mm$^{-1}$
$T = 150$ K
Block, brown
0.40 × 0.20 × 0.10 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.128$, $T_{max} = 0.475$
7974 measured reflections
4451 independent reflections
3019 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.7°$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 13$
$l = -16 \rightarrow 16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.130$
$S = 0.97$
4451 reflections
221 parameters
7 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.29$ e Å$^{-3}$
$\Delta\rho_{min} = -1.04$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Br1 | 0.26488 (9) | 0.68358 (8) | 0.54136 (5) | 0.0375 (2) | |
| Br2 | 0.64945 (8) | 0.59464 (7) | 0.69989 (5) | 0.03080 (18) | |
| Br3 | 0.49021 (18) | 0.89737 (12) | 0.84679 (11) | 0.0315 (3) | 0.90 |
| Br3′ | 0.531 (2) | 0.8775 (13) | 0.8695 (11) | 0.068 (5) | 0.10 |
| Br4 | 0.30233 (9) | 0.25573 (8) | 0.96716 (6) | 0.0350 (2) | 0.90 |
| Co1 | 0.41492 (10) | 0.67837 (9) | 0.72097 (7) | 0.0271 (2) | |
| N1 | 0.2478 (6) | 0.5344 (5) | 0.7796 (4) | 0.0280 (12) | |
| N2 | −0.0965 (6) | 0.2792 (5) | 0.9321 (4) | 0.0276 (12) | |
| N3 | 0.6361 (7) | 0.7246 (6) | 0.4462 (5) | 0.0414 (15) | |
| H3 | 0.5580 | 0.6723 | 0.4751 | 0.050* | |
| N4 | 1.0006 (7) | 0.9742 (6) | 0.3157 (4) | 0.0318 (12) | |
| C1 | 0.2977 (8) | 0.4510 (6) | 0.8403 (5) | 0.0267 (13) | |
| H1 | 0.4135 | 0.4540 | 0.8492 | 0.032* | |
| C2 | 0.1936 (7) | 0.3618 (6) | 0.8904 (5) | 0.0226 (12) | |
| H2′ | 0.2368 | 0.3026 | 0.9293 | 0.027* | 0.10 |
| C3 | 0.0191 (7) | 0.3572 (6) | 0.8846 (5) | 0.0248 (13) | |
| C4 | −0.0282 (8) | 0.4425 (7) | 0.8152 (5) | 0.0320 (15) | |
| H4 | −0.1438 | 0.4404 | 0.8015 | 0.038* | |
| C5 | 0.0825 (8) | 0.5267 (7) | 0.7677 (6) | 0.0338 (15) | |
| H5 | 0.0420 | 0.5830 | 0.7239 | 0.041* | |
| C6 | −0.0620 (10) | 0.1971 (10) | 1.0125 (8) | 0.063 (3) | |
| H6A | 0.0449 | 0.2503 | 1.0660 | 0.094* | |
| H6B | −0.0516 | 0.1101 | 0.9737 | 0.094* | |
| H6C | −0.1559 | 0.1756 | 1.0518 | 0.094* | |
| C7 | −0.2699 (8) | 0.2868 (7) | 0.9146 (6) | 0.0377 (16) | |
| H7A | −0.3213 | 0.2596 | 0.8349 | 0.057* | |
| H7B | −0.2661 | 0.3824 | 0.9433 | 0.057* | |
| H7C | −0.3385 | 0.2234 | 0.9537 | 0.057* | |
| C8 | 0.7904 (10) | 0.7112 (7) | 0.4577 (5) | 0.0362 (16) | |
| H8 | 0.8148 | 0.6441 | 0.4962 | 0.043* | |
| C9 | 0.9138 (9) | 0.7919 (7) | 0.4155 (5) | 0.0320 (15) | |
| H9 | 1.0236 | 0.7811 | 0.4254 | 0.038* | |
| C10 | 0.8813 (7) | 0.8921 (6) | 0.3568 (4) | 0.0240 (13) | |
| C11 | 0.7136 (9) | 0.9012 (7) | 0.3454 (5) | 0.0360 (16) | |

| | | | | |
|---|---|---|---|---|
| H11 | 0.6826 | 0.9655 | 0.3062 | 0.043* |
| C12 | 0.5987 (9) | 0.8172 (8) | 0.3908 (6) | 0.0405 (17) |
| H12 | 0.4871 | 0.8243 | 0.3831 | 0.049* |
| C13 | 0.9613 (11) | 1.0765 (8) | 0.2567 (6) | 0.051 (2) |
| H13A | 0.9162 | 1.1366 | 0.3038 | 0.076* |
| H13B | 0.8758 | 1.0282 | 0.1881 | 0.076* |
| H13C | 1.0654 | 1.1334 | 0.2384 | 0.076* |
| C14 | 1.1733 (9) | 0.9648 (8) | 0.3293 (6) | 0.048 (2) |
| H14A | 1.2214 | 0.9768 | 0.4084 | 0.073* |
| H14B | 1.2452 | 1.0380 | 0.2994 | 0.073* |
| H14C | 1.1689 | 0.8733 | 0.2893 | 0.073* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0327 (4) | 0.0541 (5) | 0.0345 (4) | 0.0205 (3) | 0.0109 (3) | 0.0188 (3) |
| Br2 | 0.0220 (3) | 0.0369 (4) | 0.0365 (4) | 0.0102 (3) | 0.0092 (3) | 0.0119 (3) |
| Br3 | 0.0321 (5) | 0.0292 (5) | 0.0328 (5) | 0.0089 (4) | 0.0070 (3) | 0.0071 (4) |
| Br3′ | 0.076 (9) | 0.060 (7) | 0.057 (7) | 0.001 (5) | 0.034 (6) | 0.001 (5) |
| Br4 | 0.0253 (4) | 0.0469 (5) | 0.0403 (4) | 0.0144 (3) | 0.0087 (3) | 0.0237 (4) |
| Co1 | 0.0236 (5) | 0.0288 (5) | 0.0310 (5) | 0.0068 (4) | 0.0110 (3) | 0.0108 (4) |
| N1 | 0.025 (3) | 0.030 (3) | 0.031 (3) | 0.008 (2) | 0.009 (2) | 0.011 (2) |
| N2 | 0.022 (3) | 0.031 (3) | 0.029 (3) | 0.003 (2) | 0.010 (2) | 0.013 (2) |
| N3 | 0.033 (3) | 0.047 (4) | 0.034 (3) | −0.005 (3) | 0.011 (3) | 0.007 (3) |
| N4 | 0.026 (3) | 0.038 (3) | 0.026 (3) | 0.002 (2) | 0.003 (2) | 0.010 (2) |
| C1 | 0.017 (3) | 0.033 (4) | 0.028 (3) | 0.007 (3) | 0.007 (2) | 0.002 (3) |
| C2 | 0.023 (3) | 0.023 (3) | 0.025 (3) | 0.009 (2) | 0.008 (2) | 0.010 (2) |
| C3 | 0.020 (3) | 0.025 (3) | 0.024 (3) | 0.000 (2) | 0.006 (2) | 0.000 (2) |
| C4 | 0.023 (3) | 0.035 (4) | 0.039 (4) | 0.007 (3) | 0.004 (3) | 0.015 (3) |
| C5 | 0.024 (3) | 0.039 (4) | 0.046 (4) | 0.014 (3) | 0.011 (3) | 0.020 (3) |
| C6 | 0.036 (5) | 0.085 (7) | 0.083 (6) | 0.017 (5) | 0.021 (4) | 0.058 (5) |
| C7 | 0.024 (4) | 0.042 (4) | 0.049 (4) | 0.008 (3) | 0.017 (3) | 0.010 (3) |
| C8 | 0.055 (5) | 0.029 (4) | 0.023 (3) | 0.011 (3) | 0.007 (3) | 0.007 (3) |
| C9 | 0.036 (4) | 0.031 (4) | 0.027 (3) | 0.012 (3) | 0.001 (3) | 0.002 (3) |
| C10 | 0.027 (3) | 0.025 (3) | 0.015 (3) | 0.003 (3) | 0.002 (2) | 0.003 (2) |
| C11 | 0.033 (4) | 0.045 (4) | 0.030 (4) | 0.014 (3) | 0.002 (3) | 0.013 (3) |
| C12 | 0.023 (4) | 0.059 (5) | 0.033 (4) | 0.007 (3) | 0.002 (3) | 0.008 (3) |
| C13 | 0.060 (5) | 0.035 (4) | 0.050 (5) | −0.001 (4) | 0.008 (4) | 0.022 (4) |
| C14 | 0.031 (4) | 0.056 (5) | 0.045 (5) | −0.003 (4) | 0.013 (3) | −0.002 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co1—Br1 | 2.4086 (11) | C4—H4 | 0.9500 |
| Co1—Br2 | 2.3958 (10) | C5—H5 | 0.9500 |
| Co1—Br3 | 2.3814 (13) | C6—H6A | 0.9800 |
| Co1—Br3′ | 2.376 (9) | C6—H6B | 0.9800 |
| Br4—C2 | 1.888 (6) | C6—H6C | 0.9800 |
| Co1—N1 | 2.032 (5) | C7—H7A | 0.9800 |

| | | | |
|---|---|---|---|
| N1—C1 | 1.340 (8) | C7—H7B | 0.9800 |
| N1—C5 | 1.347 (8) | C7—H7C | 0.9800 |
| N2—C3 | 1.343 (7) | C8—C9 | 1.356 (9) |
| N2—C6 | 1.454 (9) | C8—H8 | 0.9500 |
| N2—C7 | 1.461 (8) | C9—C10 | 1.416 (8) |
| N3—C8 | 1.328 (9) | C9—H9 | 0.9500 |
| N3—C12 | 1.338 (9) | C10—C11 | 1.421 (9) |
| N3—H3 | 0.8800 | C11—C12 | 1.353 (9) |
| N4—C10 | 1.333 (7) | C11—H11 | 0.9500 |
| N4—C13 | 1.456 (9) | C12—H12 | 0.9500 |
| N4—C14 | 1.463 (9) | C13—H13A | 0.9800 |
| C1—C2 | 1.368 (8) | C13—H13B | 0.9800 |
| C1—H1 | 0.9500 | C13—H13C | 0.9800 |
| C2—C3 | 1.439 (8) | C14—H14A | 0.9800 |
| C2—H2′ | 0.9500 | C14—H14B | 0.9800 |
| C3—C4 | 1.415 (9) | C14—H14C | 0.9800 |
| C4—C5 | 1.350 (9) | | |

| | | | |
|---|---|---|---|
| N1—Co1—Br3′ | 105.5 (5) | N2—C6—H6A | 109.5 |
| N1—Co1—Br3 | 107.98 (15) | N2—C6—H6B | 109.5 |
| Br3′—Co1—Br3 | 12.5 (4) | H6A—C6—H6B | 109.5 |
| N1—Co1—Br2 | 106.97 (14) | N2—C6—H6C | 109.5 |
| Br3′—Co1—Br2 | 104.7 (4) | H6A—C6—H6C | 109.5 |
| Br3—Co1—Br2 | 114.67 (5) | H6B—C6—H6C | 109.5 |
| N1—Co1—Br1 | 105.94 (15) | N2—C7—H7A | 109.5 |
| Br3′—Co1—Br1 | 123.1 (4) | N2—C7—H7B | 109.5 |
| Br3—Co1—Br1 | 111.17 (5) | H7A—C7—H7B | 109.5 |
| Br2—Co1—Br1 | 109.64 (4) | N2—C7—H7C | 109.5 |
| C1—N1—C5 | 116.2 (5) | H7A—C7—H7C | 109.5 |
| C1—N1—Co1 | 122.3 (4) | H7B—C7—H7C | 109.5 |
| C5—N1—Co1 | 121.2 (4) | N3—C8—C9 | 121.1 (6) |
| C3—N2—C6 | 125.9 (5) | N3—C8—H8 | 119.5 |
| C3—N2—C7 | 119.4 (5) | C9—C8—H8 | 119.5 |
| C6—N2—C7 | 114.3 (5) | C8—C9—C10 | 120.9 (6) |
| C8—N3—C12 | 120.3 (6) | C8—C9—H9 | 119.5 |
| C8—N3—H3 | 119.9 | C10—C9—H9 | 119.5 |
| C12—N3—H3 | 119.9 | N4—C10—C9 | 122.3 (6) |
| C10—N4—C13 | 120.2 (6) | N4—C10—C11 | 121.8 (6) |
| C10—N4—C14 | 121.2 (6) | C9—C10—C11 | 115.9 (6) |
| C13—N4—C14 | 118.6 (6) | C12—C11—C10 | 119.2 (6) |
| N1—C1—C2 | 124.6 (5) | C12—C11—H11 | 120.4 |
| N1—C1—H1 | 117.7 | C10—C11—H11 | 120.4 |
| C2—C1—H1 | 117.7 | N3—C12—C11 | 122.6 (6) |
| C1—C2—C3 | 120.5 (5) | N3—C12—H12 | 118.7 |
| C1—C2—Br4 | 114.0 (4) | C11—C12—H12 | 118.7 |
| C3—C2—Br4 | 125.5 (4) | N4—C13—H13A | 109.5 |
| C1—C2—H2′ | 119.8 | N4—C13—H13B | 109.5 |
| C3—C2—H2′ | 119.8 | H13A—C13—H13B | 109.5 |

| | | | |
|---|---|---|---|
| N2—C3—C4 | 120.3 (5) | N4—C13—H13C | 109.5 |
| N2—C3—C2 | 127.4 (6) | H13A—C13—H13C | 109.5 |
| C4—C3—C2 | 112.2 (5) | H13B—C13—H13C | 109.5 |
| C5—C4—C3 | 123.4 (6) | N4—C14—H14A | 109.5 |
| C5—C4—H4 | 118.3 | N4—C14—H14B | 109.5 |
| C3—C4—H4 | 118.3 | H14A—C14—H14B | 109.5 |
| N1—C5—C4 | 122.9 (6) | N4—C14—H14C | 109.5 |
| N1—C5—H5 | 118.6 | H14A—C14—H14C | 109.5 |
| C4—C5—H5 | 118.6 | H14B—C14—H14C | 109.5 |

| | | | |
|---|---|---|---|
| Br3′—Co1—N1—C1 | −83.8 (6) | Br4—C2—C3—C4 | −176.4 (5) |
| Br3—Co1—N1—C1 | −96.6 (5) | N2—C3—C4—C5 | 177.9 (6) |
| Br2—Co1—N1—C1 | 27.3 (5) | C2—C3—C4—C5 | −5.0 (9) |
| Br1—Co1—N1—C1 | 144.2 (4) | C1—N1—C5—C4 | 1.3 (9) |
| Br3′—Co1—N1—C5 | 90.1 (7) | Co1—N1—C5—C4 | −173.0 (5) |
| Br3—Co1—N1—C5 | 77.3 (5) | C3—C4—C5—N1 | 1.8 (11) |
| Br2—Co1—N1—C5 | −158.8 (5) | C12—N3—C8—C9 | 1.0 (10) |
| Br1—Co1—N1—C5 | −41.9 (5) | N3—C8—C9—C10 | −0.6 (10) |
| C5—N1—C1—C2 | −0.6 (9) | C13—N4—C10—C9 | −179.5 (6) |
| Co1—N1—C1—C2 | 173.6 (5) | C14—N4—C10—C9 | 0.0 (9) |
| N1—C1—C2—C3 | −3.0 (9) | C13—N4—C10—C11 | −0.2 (9) |
| N1—C1—C2—Br4 | 178.6 (5) | C14—N4—C10—C11 | 179.3 (6) |
| C6—N2—C3—C4 | −174.2 (7) | C8—C9—C10—N4 | 179.1 (6) |
| C7—N2—C3—C4 | −2.0 (9) | C8—C9—C10—C11 | −0.3 (9) |
| C6—N2—C3—C2 | 9.1 (10) | N4—C10—C11—C12 | −178.6 (6) |
| C7—N2—C3—C2 | −178.7 (6) | C9—C10—C11—C12 | 0.7 (9) |
| C1—C2—C3—N2 | −177.7 (6) | C8—N3—C12—C11 | −0.5 (10) |
| Br4—C2—C3—N2 | 0.5 (9) | C10—C11—C12—N3 | −0.3 (11) |
| C1—C2—C3—C4 | 5.4 (8) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···Br1 | 0.88 | 2.74 | 3.434 (6) | 137 |