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# Poly[bis($\mu_2$-4,4′-bipyridine)bis(3-nitrobenzoato)cobalt(II)]

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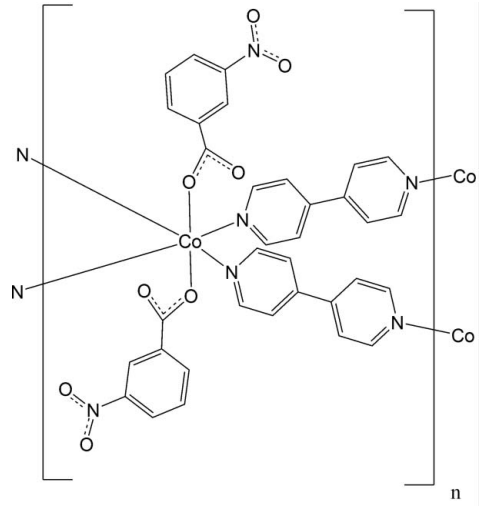
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.002 Å; disorder in main residue; $R$ factor = 0.030; $wR$ factor = 0.085; data-to-parameter ratio = 15.9.

The hydrothermal reaction of cobalt nitrate with 4,4′-bipyridine and 3-nitrobenzoic acid lead to the formation of the title complex, $[Co(C_7H_4NO_4)_2(C_{10}H_8N_2)_2]_n$. In the crystal structure, the $Co^{II}$ atoms are coordinated by two terminal carboxylate anions and four 4,4′-bipyridine ligands within slightly distorted octahedra. The $Co^{II}$ atom and one of the two independent 4,4′-bipyridine ligands are located on a twofold rotation axis, while the second independent 4,4′-bipyridine molecule is located on a centre of inversion. One of the two rings of one 4,4′-bipyridine ligand is disordered over two orientations and was refined using a split model [occupancy ratio 0.68 (2):0.32 (2)]. The $Co^{II}$ atoms are connected by the 4,4′-bipyridine ligands into layers, which are located parallel to the *ab* plane.

## Related literature

For background information on the solvothermal synthesis of coordination polymers with organic ligands, see: Kitagawa *et al.* (2004). For related structures, see: Biradha *et al.* (1999).



## Experimental

### Crystal data

$[Co(C_7H_4NO_4)_2(C_{10}H_8N_2)_2]$
$M_r$ = 703.52
Monoclinic, $C2/c$
$a$ = 18.2074 (15) Å
$b$ = 11.4717 (8) Å
$c$ = 15.0543 (12) Å
$\beta$ = 94.661 (2)°
$V$ = 3134.0 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.61 mm$^{-1}$
$T$ = 295 K
0.40 × 0.25 × 0.15 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.792, $T_{max}$ = 0.914
13056 measured reflections
3861 independent reflections
3389 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.085
$S$ = 1.03
3861 reflections
243 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2159).

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# supporting information

*Acta Cryst.* (2009). E**65**, m1302–m1303 [https://doi.org/10.1107/S1600536809039786]

## Poly[bis($\mu_2$-4,4′-bipyridine)bis(3-nitrobenzoato)cobalt(II)]

**Pei-Hsuan Chiang, Shih-Chen Hsu and Chia-Her Lin**

### S1. Comment

The synthesis of coordination polymers has been a subject of intense research owing to their interesting structural chemistry and potential applications. A large number of these compounds have been synthesized by the reactions of metal salts and organic dicarboxyl acids or bipyridines (Kitagawa *et al.* 2004). As a further study in this field, the structure of the title compound is reported.

The asymmetric unit of the title compound consists of one $Co^{II}$ atom, one 3-nitrobenzoate anion and two half 4,4′-bipyridine ligands (Figure 1). The octahedral metal ions are coordinated by four nitrogen atoms of two pairs of crystallographically independent 4,4′-bipyridine ligands and two oxygen atoms of two symmetry related 3-nitro benzoate anions. The Co—O bond length is 2.0557 (13) Å and the average Co—N distance amount to 2.1836 (19) Å. The metal centers are linked via the 4,4′-bipyridine ligands into layers and the anions are only terminal bonded to the $Co^{II}$ atoms (Figure 2). Thus, this structure is different from the analogous nickel compound with the same ligands (Biradha *et al.* 1999).

### S2. Experimental

The title compound was prepared by the reaction of 4,4′-bipyridine (0.0781 g, 0.5 mmol), 3-nitrobenzoic acid (0.0836 g, 0.5 mmol), $Co(NO_3)_2.6H_2O$ (0.1454 g, 0.5 mmol), $H_2O$ (12.0 ml) and $NH_4OH$ (0.1 ml) at a pH value of 9.28. The mixture was heated to 423 K for 2 days in a Teflon-lined autoclave with an internal volume of 23 ml followed by slow cooling at 6 K/h to room temperature. The title compound was obtained as orange crystals with a yield of 0.0284 g (7.7%, based on cobalt). Anal. found/calcd.: C, 58.11/58.06; N, 12.14/11.95; H, 3.46/3.44%.

### S3. Refinement

The hydrogen atoms of benzene rings are placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C). The C12 and C13 atoms are disordered and were refined using a split model with occupancies of 0.68 (2) and 0.32 (2).

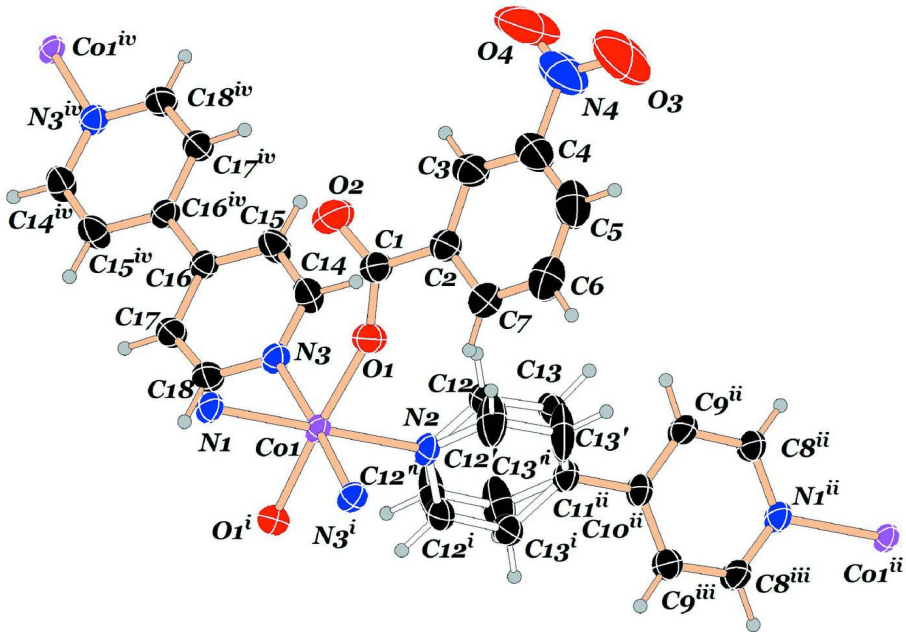


**Figure 1**

Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level. [symmetry codes: (i) -*x* + 1,*y*,-*z* + 5/2; (ii) *x*,*y* - 1,*z*; (iii) -*x* + 1,*y* + 1,-*z* + 5/2; (iv) -*x* + 1/2,-*y* + 5/2,-*z* + 2.]. The H atoms are omitted for clarity.

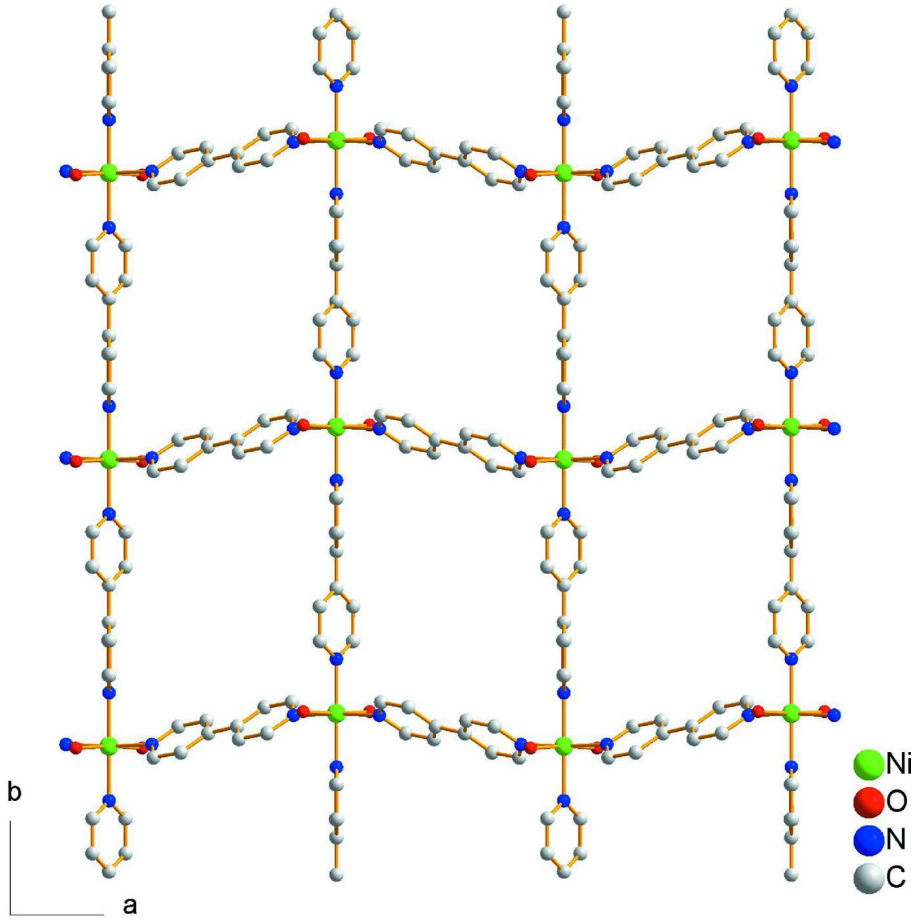


**Figure 2**

Crystal structure of the title compound in c-direction showing the layers. The H atoms and the disordered C atoms are not shown for clarity.

**Poly[bis($\mu_2$-4,4′-bipyridine)bis(3-nitrobenzoato)cobalt(II)]**

*Crystal data*

$[Co(C_7H_4NO_4)_2(C_{10}H_8N_2)_2]$
$M_r = 703.52$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 18.2074\ (15)$ Å
$b = 11.4717\ (8)$ Å
$c = 15.0543\ (12)$ Å
$\beta = 94.661\ (2)°$
$V = 3134.0\ (4)$ Å$^3$
$Z = 4$
$F(000) = 1444$
$D_x = 1.491$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6091 reflections
$\theta = 2.3–28.1°$
$\mu = 0.61$ mm$^{-1}$
$T = 295$ K
Columnar, pink
0.40 × 0.25 × 0.15 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.792$, $T_{max} = 0.914$
13056 measured reflections

3861 independent reflections
3389 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.1°$
$h = -24 \rightarrow 23$
$k = -8 \rightarrow 15$
$l = -19 \rightarrow 20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.085$
$S = 1.03$
3861 reflections
243 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 1.8393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.29$ e Å$^{-3}$
$\Delta\rho_{min} = -0.25$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Co1 | 0.5000 | 1.191582 (19) | 1.2500 | 0.02382 (8) | |
| O1 | 0.57262 (6) | 1.18588 (9) | 1.15246 (7) | 0.0354 (2) | |
| O2 | 0.55038 (8) | 1.25715 (13) | 1.01478 (8) | 0.0558 (3) | |
| O3 | 0.81068 (14) | 1.0206 (2) | 0.83179 (16) | 0.1227 (9) | |
| O4 | 0.70904 (15) | 1.1028 (2) | 0.79153 (13) | 0.1102 (8) | |
| N1 | 0.5000 | 1.38167 (14) | 1.2500 | 0.0311 (3) | |
| N2 | 0.5000 | 0.99916 (13) | 1.2500 | 0.0300 (3) | |
| N3 | 0.40427 (7) | 1.19830 (9) | 1.15518 (8) | 0.0298 (2) | |
| N4 | 0.75458 (14) | 1.06877 (18) | 0.84869 (16) | 0.0765 (6) | |
| C1 | 0.58770 (8) | 1.20319 (12) | 1.07270 (10) | 0.0330 (3) | |
| C2 | 0.66071 (9) | 1.15062 (13) | 1.05012 (10) | 0.0347 (3) | |
| C3 | 0.67493 (10) | 1.13700 (14) | 0.96153 (11) | 0.0427 (4) | |
| H3A | 0.6406 | 1.1601 | 0.9158 | 0.051* | |
| C4 | 0.74128 (12) | 1.08841 (15) | 0.94287 (13) | 0.0517 (5) | |
| C5 | 0.79520 (11) | 1.05707 (17) | 1.00796 (16) | 0.0590 (5) | |
| H5A | 0.8399 | 1.0267 | 0.9930 | 0.071* | |
| C6 | 0.78115 (11) | 1.07189 (17) | 1.09553 (15) | 0.0548 (5) | |
| H6A | 0.8169 | 1.0522 | 1.1407 | 0.066* | |
| C7 | 0.71369 (9) | 1.11618 (14) | 1.11679 (12) | 0.0435 (4) | |
| H7A | 0.7039 | 1.1229 | 1.1762 | 0.052* | |
| C8 | 0.49826 (9) | 1.44210 (12) | 1.17370 (10) | 0.0359 (3) | |

| | | | | | |
|---|---|---|---|---|---|
| H8A | 0.4975 | 1.4011 | 1.1203 | 0.043* | |
| C9 | 0.49748 (9) | 1.56253 (12) | 1.17056 (10) | 0.0370 (3) | |
| H9A | 0.4953 | 1.6012 | 1.1161 | 0.044* | |
| C10 | 0.5000 | 1.62512 (16) | 1.2500 | 0.0317 (4) | |
| C11 | 0.5000 | 1.75431 (16) | 1.2500 | 0.0314 (4) | |
| C12 | 0.5282 (4) | 0.9374 (4) | 1.1858 (3) | 0.0383 (11) | 0.68 (2) |
| H12 | 0.5490 | 0.9779 | 1.1406 | 0.046* | 0.68 (2) |
| C13 | 0.5285 (4) | 0.8176 (4) | 1.1825 (3) | 0.0402 (11) | 0.68 (2) |
| H13 | 0.5477 | 0.7793 | 1.1351 | 0.048* | 0.68 (2) |
| C12′ | 0.5517 (9) | 0.9382 (10) | 1.2151 (18) | 0.060 (4) | 0.32 (2) |
| H12′ | 0.5890 | 0.9784 | 1.1896 | 0.071* | 0.32 (2) |
| C13′ | 0.5538 (10) | 0.8169 (9) | 1.2143 (19) | 0.068 (5) | 0.32 (2) |
| H13′ | 0.5920 | 0.7785 | 1.1892 | 0.082* | 0.32 (2) |
| C14 | 0.40078 (8) | 1.15400 (14) | 1.07344 (10) | 0.0362 (3) | |
| H14A | 0.4399 | 1.1087 | 1.0574 | 0.043* | |
| C15 | 0.34177 (8) | 1.17185 (14) | 1.01086 (10) | 0.0369 (3) | |
| H15A | 0.3422 | 1.1395 | 0.9543 | 0.044* | |
| C16 | 0.28195 (7) | 1.23815 (12) | 1.03276 (9) | 0.0281 (3) | |
| C17 | 0.28502 (9) | 1.28120 (15) | 1.11918 (10) | 0.0386 (3) | |
| H17A | 0.2458 | 1.3239 | 1.1381 | 0.046* | |
| C18 | 0.34630 (9) | 1.26053 (15) | 1.17697 (10) | 0.0381 (3) | |
| H18A | 0.3474 | 1.2915 | 1.2341 | 0.046* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.02889 (14) | 0.01737 (12) | 0.02410 (13) | 0.000 | −0.00451 (9) | 0.000 |
| O1 | 0.0408 (6) | 0.0355 (5) | 0.0300 (5) | −0.0014 (4) | 0.0041 (4) | 0.0005 (4) |
| O2 | 0.0581 (8) | 0.0690 (9) | 0.0398 (7) | 0.0156 (7) | 0.0004 (6) | 0.0141 (6) |
| O3 | 0.1288 (19) | 0.144 (2) | 0.1065 (16) | 0.0236 (16) | 0.0775 (15) | −0.0159 (14) |
| O4 | 0.137 (2) | 0.150 (2) | 0.0493 (10) | 0.0023 (16) | 0.0364 (12) | −0.0075 (12) |
| N1 | 0.0420 (9) | 0.0187 (7) | 0.0316 (8) | 0.000 | −0.0024 (7) | 0.000 |
| N2 | 0.0347 (8) | 0.0192 (7) | 0.0354 (9) | 0.000 | −0.0011 (7) | 0.000 |
| N3 | 0.0314 (6) | 0.0275 (6) | 0.0293 (6) | 0.0021 (4) | −0.0044 (5) | −0.0009 (4) |
| N4 | 0.0978 (16) | 0.0672 (12) | 0.0717 (13) | −0.0167 (11) | 0.0522 (13) | −0.0103 (10) |
| C1 | 0.0392 (7) | 0.0287 (7) | 0.0307 (7) | −0.0045 (6) | 0.0006 (6) | 0.0000 (5) |
| C2 | 0.0435 (8) | 0.0259 (6) | 0.0352 (7) | −0.0049 (6) | 0.0064 (6) | 0.0022 (6) |
| C3 | 0.0555 (10) | 0.0350 (8) | 0.0389 (8) | −0.0080 (7) | 0.0121 (7) | 0.0018 (6) |
| C4 | 0.0668 (12) | 0.0365 (8) | 0.0559 (11) | −0.0120 (8) | 0.0305 (9) | −0.0021 (7) |
| C5 | 0.0527 (11) | 0.0418 (9) | 0.0863 (15) | 0.0012 (8) | 0.0290 (11) | 0.0038 (10) |
| C6 | 0.0469 (10) | 0.0475 (10) | 0.0699 (13) | 0.0050 (8) | 0.0040 (9) | 0.0080 (9) |
| C7 | 0.0486 (9) | 0.0386 (8) | 0.0434 (9) | 0.0020 (7) | 0.0042 (7) | 0.0044 (7) |
| C8 | 0.0541 (9) | 0.0223 (6) | 0.0304 (7) | 0.0012 (6) | −0.0016 (6) | −0.0023 (5) |
| C9 | 0.0573 (9) | 0.0219 (6) | 0.0315 (7) | 0.0014 (6) | 0.0009 (6) | 0.0038 (5) |
| C10 | 0.0404 (10) | 0.0184 (8) | 0.0361 (10) | 0.000 | 0.0026 (8) | 0.000 |
| C11 | 0.0418 (10) | 0.0178 (8) | 0.0342 (10) | 0.000 | 0.0010 (8) | 0.000 |
| C12 | 0.058 (3) | 0.0214 (12) | 0.0374 (18) | −0.0007 (16) | 0.0131 (15) | 0.0017 (11) |
| C13 | 0.063 (3) | 0.0222 (13) | 0.0373 (18) | 0.0007 (16) | 0.0180 (15) | −0.0022 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12′ | 0.052 (6) | 0.024 (3) | 0.107 (12) | −0.001 (4) | 0.035 (7) | 0.009 (6) |
| C13′ | 0.062 (7) | 0.024 (3) | 0.126 (14) | 0.012 (4) | 0.050 (8) | 0.008 (6) |
| C14 | 0.0291 (7) | 0.0399 (8) | 0.0382 (8) | 0.0062 (6) | −0.0050 (6) | −0.0108 (6) |
| C15 | 0.0316 (7) | 0.0464 (8) | 0.0315 (7) | 0.0052 (6) | −0.0048 (6) | −0.0132 (6) |
| C16 | 0.0278 (6) | 0.0288 (6) | 0.0270 (6) | 0.0008 (5) | −0.0028 (5) | 0.0014 (5) |
| C17 | 0.0379 (8) | 0.0490 (9) | 0.0281 (7) | 0.0165 (7) | −0.0030 (6) | −0.0023 (6) |
| C18 | 0.0414 (8) | 0.0461 (8) | 0.0254 (7) | 0.0123 (7) | −0.0055 (6) | −0.0040 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co1—O1 | 2.0553 (11) | C7—H7A | 0.9300 |
| Co1—O1$^{i}$ | 2.0553 (11) | C8—C9 | 1.3824 (19) |
| Co1—N3 | 2.1627 (12) | C8—H8A | 0.9300 |
| Co1—N3$^{i}$ | 2.1627 (12) | C9—C10 | 1.3925 (17) |
| Co1—N1 | 2.1807 (16) | C9—H9A | 0.9300 |
| Co1—N2 | 2.2074 (16) | C10—C9$^{i}$ | 1.3925 (17) |
| O1—C1 | 1.2689 (18) | C10—C11 | 1.482 (3) |
| O2—C1 | 1.2283 (19) | C11—C13′$^{ii}$ | 1.359 (12) |
| O3—N4 | 1.206 (3) | C11—C13′$^{iii}$ | 1.359 (11) |
| O4—N4 | 1.210 (3) | C11—C13$^{iii}$ | 1.384 (5) |
| N1—C8 | 1.3398 (16) | C11—C13$^{ii}$ | 1.384 (5) |
| N1—C8$^{i}$ | 1.3398 (16) | C12—C13 | 1.375 (7) |
| N2—C12′ | 1.315 (12) | C12—H12 | 0.9300 |
| N2—C12′$^{i}$ | 1.315 (12) | C13—C11$^{iv}$ | 1.384 (5) |
| N2—C12$^{i}$ | 1.334 (5) | C13—H13 | 0.9300 |
| N2—C12 | 1.334 (5) | C12′—C13′ | 1.392 (16) |
| N3—C14 | 1.3280 (18) | C12′—H12′ | 0.9300 |
| N3—C18 | 1.3370 (19) | C13′—C11$^{iv}$ | 1.359 (11) |
| N4—C4 | 1.475 (3) | C13′—H13′ | 0.9300 |
| C1—C2 | 1.523 (2) | C14—C15 | 1.385 (2) |
| C2—C3 | 1.388 (2) | C14—H14A | 0.9300 |
| C2—C7 | 1.392 (2) | C15—C16 | 1.390 (2) |
| C3—C4 | 1.380 (3) | C15—H15A | 0.9300 |
| C3—H3A | 0.9300 | C16—C17 | 1.388 (2) |
| C4—C5 | 1.377 (3) | C16—C16$^{v}$ | 1.488 (2) |
| C5—C6 | 1.374 (3) | C17—C18 | 1.379 (2) |
| C5—H5A | 0.9300 | C17—H17A | 0.9300 |
| C6—C7 | 1.390 (2) | C18—H18A | 0.9300 |
| C6—H6A | 0.9300 | | |

| | | | |
|---|---|---|---|
| O1—Co1—O1$^{i}$ | 176.35 (6) | C5—C6—H6A | 119.9 |
| O1—Co1—N3 | 93.46 (5) | C7—C6—H6A | 119.9 |
| O1$^{i}$—Co1—N3 | 86.68 (5) | C2—C7—C6 | 120.74 (17) |
| O1—Co1—N3$^{i}$ | 86.67 (5) | C2—C7—H7A | 119.6 |
| O1$^{i}$—Co1—N3$^{i}$ | 93.46 (5) | C6—C7—H7A | 119.6 |
| N3—Co1—N3$^{i}$ | 175.92 (6) | N1—C8—C9 | 123.08 (14) |
| O1—Co1—N1 | 91.82 (3) | N1—C8—H8A | 118.5 |
| O1$^{i}$—Co1—N1 | 91.82 (3) | C9—C8—H8A | 118.5 |

| | | | |
|---|---|---|---|
| N3—Co1—N1 | 87.96 (3) | C8—C9—C10 | 119.11 (14) |
| N3$^{i}$—Co1—N1 | 87.96 (3) | C8—C9—H9A | 120.4 |
| O1—Co1—N2 | 88.18 (3) | C10—C9—H9A | 120.4 |
| O1$^{i}$—Co1—N2 | 88.18 (3) | C9—C10—C9$^{i}$ | 117.92 (17) |
| N3—Co1—N2 | 92.04 (3) | C9—C10—C11 | 121.04 (9) |
| N3$^{i}$—Co1—N2 | 92.04 (3) | C9$^{i}$—C10—C11 | 121.04 (9) |
| N1—Co1—N2 | 180.000 (1) | C13′$^{ii}$—C11—C13′$^{iii}$ | 116.3 (9) |
| C1—O1—Co1 | 150.73 (10) | C13′$^{ii}$—C11—C13$^{iii}$ | 109.8 (6) |
| C8—N1—C8$^{i}$ | 117.69 (17) | C13′$^{iii}$—C11—C13$^{ii}$ | 109.8 (6) |
| C8—N1—Co1 | 121.16 (8) | C13$^{iii}$—C11—C13$^{ii}$ | 116.7 (4) |
| C8$^{i}$—N1—Co1 | 121.16 (8) | C13′$^{ii}$—C11—C10 | 121.9 (4) |
| C12′—N2—C12′$^{i}$ | 115.7 (10) | C13′$^{iii}$—C11—C10 | 121.9 (5) |
| C12′—N2—C12$^{i}$ | 109.7 (5) | C13$^{iii}$—C11—C10 | 121.7 (2) |
| C12′$^{i}$—N2—C12 | 109.7 (5) | C13$^{ii}$—C11—C10 | 121.7 (2) |
| C12$^{i}$—N2—C12 | 115.9 (4) | N2—C12—C13 | 124.0 (4) |
| C12′—N2—Co1 | 122.1 (5) | N2—C12—H12 | 118.0 |
| C12′$^{i}$—N2—Co1 | 122.1 (5) | C13—C12—H12 | 118.0 |
| C12$^{i}$—N2—Co1 | 122.1 (2) | C12—C13—C11$^{iv}$ | 119.7 (4) |
| C12—N2—Co1 | 122.1 (2) | C12—C13—H13 | 120.2 |
| C14—N3—C18 | 116.89 (12) | C11$^{iv}$—C13—H13 | 120.2 |
| C14—N3—Co1 | 124.98 (10) | N2—C12′—C13′ | 123.8 (10) |
| C18—N3—Co1 | 117.84 (9) | N2—C12′—H12′ | 118.1 |
| O3—N4—O4 | 122.7 (2) | C13′—C12′—H12′ | 118.1 |
| O3—N4—C4 | 118.7 (3) | C11$^{iv}$—C13′—C12′ | 120.2 (9) |
| O4—N4—C4 | 118.5 (2) | C11$^{iv}$—C13′—H13′ | 119.9 |
| O2—C1—O1 | 126.93 (15) | C12′—C13′—H13′ | 119.9 |
| O2—C1—C2 | 118.91 (14) | N3—C14—C15 | 123.34 (13) |
| O1—C1—C2 | 114.15 (13) | N3—C14—H14A | 118.3 |
| C3—C2—C7 | 119.26 (15) | C15—C14—H14A | 118.3 |
| C3—C2—C1 | 119.56 (14) | C14—C15—C16 | 119.93 (13) |
| C7—C2—C1 | 121.18 (14) | C14—C15—H15A | 120.0 |
| C4—C3—C2 | 118.41 (17) | C16—C15—H15A | 120.0 |
| C4—C3—H3A | 120.8 | C17—C16—C15 | 116.37 (12) |
| C2—C3—H3A | 120.8 | C17—C16—C16$^{v}$ | 121.74 (15) |
| C3—C4—C5 | 123.09 (18) | C15—C16—C16$^{v}$ | 121.89 (16) |
| C3—C4—N4 | 118.2 (2) | C18—C17—C16 | 119.94 (13) |
| C5—C4—N4 | 118.7 (2) | C18—C17—H17A | 120.0 |
| C6—C5—C4 | 118.21 (18) | C16—C17—H17A | 120.0 |
| C6—C5—H5A | 120.9 | N3—C18—C17 | 123.48 (14) |
| C4—C5—H5A | 120.9 | N3—C18—H18A | 118.3 |
| C5—C6—C7 | 120.21 (19) | C17—C18—H18A | 118.3 |

Symmetry codes: (i) −*x*+1, *y*, −*z*+5/2; (ii) *x*, *y*+1, *z*; (iii) −*x*+1, *y*+1, −*z*+5/2; (iv) *x*, *y*−1, *z*; (v) −*x*+1/2, −*y*+5/2, −*z*+2.