# metal-organic compounds

## *catena*-Poly[[[tetraaquacobalt(II)]-μ-4,4′-bipyridine-$\kappa^2 N$:$N'$] 2-[4-(2-carboxylato-ethyl)phenoxy]acetate]

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In the title complex, $\{[Co(C_{10}H_8N_2)(H_2O)_4](C_{11}H_{10}O_5)\}_n$, the unique $Co^{II}$ ion lies on an inversion center and is coordinated by two N atoms from two 4,4′-bipyridine ligands and four O atoms from four water molecules in a slightly distorted octahedral coordination geometry. The 4,4′-bipyridine ligands bridge $Co^{II}$ ions into a one-dimensional chain structure. In the crystal structure, intermolecular O—H···O hydrogen bonds link cations and anions into a three-dimensional network. The dianions are completely disordered about an inversion center.

## Related literature

For background to assembly of high-dimensional supra-molecular coordination polymers, see: Ye *et al.* (2005). For 3-(4-hydroxyphenyl)propanoic acid as a potential multidentate ligand and a good donor and acceptor of hydrogen bonds, see: Tan *et al.* (2007). 4,4′-Bipyridine is widely used as a spacer in the construction of supramolecular architectures, see: Tao *et al.* (2000); Cussen *et al.* (2002). For the analogous one-dimensional structure with a 3-carboxylatophenoxyacetate dianion, see: Zhao *et al.* (2005).
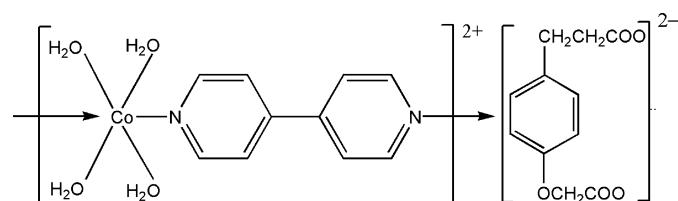


## Experimental

### Crystal data

| | |
|---|---|
| $[Co(C_{10}H_8N_2)(H_2O)_4](C_{11}H_{10}O_5)$ | $\gamma$ = 94.002 (1)° |
| $M_r$ = 509.37 | $V$ = 557.15 (13) Å³ |
| Triclinic, $P\bar{1}$ | $Z$ = 1 |
| $a$ = 7.1311 (10) Å | Mo $K\alpha$ radiation |
| $b$ = 7.6319 (10) Å | $\mu$ = 0.83 mm⁻¹ |
| $c$ = 10.4978 (14) Å | $T$ = 291 K |
| $\alpha$ = 91.930 (1)° | 0.50 × 0.41 × 0.21 mm |
| $\beta$ = 101.832 (1)° | |

### Data collection

| | |
|---|---|
| Bruker SMART CCD diffractometer | 4108 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 2036 independent reflections |
| | 2008 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.674, $T_{max}$ = 0.845 | $R_{int}$ = 0.011 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.036 | 364 restraints |
| $wR(F^2)$ = 0.085 | H-atom parameters constrained |
| $S$ = 1.06 | $\Delta\rho_{max}$ = 0.61 e Å⁻³ |
| 2036 reflections | $\Delta\rho_{min}$ = −0.63 e Å⁻³ |
| 176 parameters | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Co1—O1 | 2.0840 (16) | Co1—N1 | 2.1530 (17) |
| Co1—O2 | 2.1083 (16) | | |
| O1ⁱ—Co1—O1 | 180 | O2—Co1—N1 | 90.36 (7) |
| O1—Co1—O2ⁱ | 88.34 (7) | O1—Co1—N1ⁱ | 88.07 (7) |
| O1—Co1—O2 | 91.66 (7) | O2—Co1—N1ⁱ | 89.63 (7) |
| O2ⁱ—Co1—O2 | 180 | N1—Co1—N1ⁱ | 180 |
| O1—Co1—N1 | 91.93 (7) | | |

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H4W···O4′ⁱⁱ | 0.83 | 2.00 | 2.796 (10) | 161 |
| O2—H4W···O4ⁱⁱ | 0.83 | 1.86 | 2.667 (10) | 165 |
| O2—H3W···O4ⁱⁱⁱ | 0.83 | 1.96 | 2.765 (14) | 163 |
| O2—H3W···O4′ⁱⁱⁱ | 0.83 | 1.86 | 2.678 (14) | 170 |
| O1—H2W···O3ⁱᵛ | 0.82 | 2.07 | 2.868 (16) | 164 |
| O1—H2W···O3′ⁱᵛ | 0.82 | 1.90 | 2.691 (16) | 161 |
| O1—H1W···O3ᵛ | 0.83 | 1.97 | 2.789 (13) | 169 |
| O1—H1W···O3′ᵛ | 0.83 | 1.79 | 2.612 (14) | 174 |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2836).

## References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Cussen, E. J., Claridge, J. B., Rosseinsky, M. J. & Kepert, C. J. (2002). *J. Am. Chem. Soc.* **124**, 9574–9581.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Tan, S., Wen, H., Liu, C., Peng, X. & Li, X. (2007). *Z. Kristallogr. New Cryst. Struct.* **222**, 137–138.

Tao, J., Tong, M. L. & Chen, X. M. (2000). *J. Chem. Soc. Dalton Trans.* p. 3669–3674.

Ye, B.-H., Tong, M.-L. & Chen, X.-M. (2005). *Coord. Chem. Rev.* **249**, 545–565.

Zhao, J.-G., Gu, C.-S., Gao, S., Huo, L.-H. & Liu, J.-W. (2005). *Acta Cryst.* E**61**, m33–m35.

# supporting information

# *catena*-Poly[[[tetraaquacobalt(II)]-*μ*-4,4′-bipyridine-*κ*²*N*:*N*′] 2-[4-(2-carboxylato-ethyl)phenoxy]acetate]

## Xi-Fang Wang, Chong-Bo Liu, De-He Huang and Zhi-Qiang Xiong

## S1. Comment

In recent years, assembly of high-dimensional supramolecular coordination polymers *via* coordination bonds, hydrogen bonds, and *π*···*π* stacks (Ye *et al.*, 2005) have received much attention and carboxylic acid compounds as good donors and acceptors of hydrogen bonds have been widely utilized as ligands. 3-(4-hydroxyphenyl)propanoic acid (Tan *et al.*, 2007) a pseudo-symmetric carboxylate acid is a potential multidentate ligand and a good donor and acceptor of hydrogen bonds, but its coordination polymers are less investigated. 4,4′-bipyridine is a neutral linear bifunctional ligand that is widely used as an excellent spacer in the construction of supramolecular architectures (Cussen *et al.*, 2002; Tao *et al.*, 2000). Here, we report the synthesis and crystals structure of a cobalt supramolecular complex formed using with 4,4′-bipyridine and 3-(4-(carboxymethoxy)phenyl)propanoic acid.

The asymmetric unit and some symmetry related atoms are shown in Fig. 1. The unique Co$^{II}$ ion lies on an invesion center and is coordinated by two nitrogen atoms from two 4,4′-bipyridine ligands and four oxygen atoms from four water molecules in a slightly distorted octahedral coordination geometry. The molecules of 3-(4-(carboxymethoxy)phenyl)-propanoic acid are completely deprotonated but remain uncoordinated, and the 4,4′-bipyridine ligands act as bridging to join the Co$^{II}$ ions into a one-dimensional chain structure, which is further linked to a 3-D network through intermolecular O—H···O hydrogen bonds.

## S2. Experimental

A mixture of CoCl$_2$.2H$_2$O (0.1 mmol), 4,4′-bipyridine (0.1 mmol), 3-(4-(carboxymethoxy)phenyl)propanoic acid (0.1 mmol) and 10 ml water was placed in a tube and heated at 363 K for 6 h, then cooled to room temperature. Upon cooling to RT, a few red crystals were obtained. Anal. Calcd for C$_{21}$H$_{26}$N$_2$O$_9$Co (509.37): C, 49.47; H, 5.10; N, 5.50%; Found: C, 49.23; H, 4.98; N, 5.19%.

## S3. Refinement

The water H atoms were located in a difference Fourier map but were included in fixed positions in riding-model approximation with the O—H distances in the range 0.8245–0.8271 Å and $U_{iso}$(H) = 1.5$U_{eq}$(O); all other H atoms were placed in geometrically idealized positions with *C*—*H*(methylene) = 0.97 Å, C—H(aromatic) = 0.93 Å, and $U_{iso}$(H) = 1.2$U_{eq}$(C). The dianion is completely disordered over an inversion center. The SADI and EADP commands in SHELXL (Sheldrick, 2008) were used to model the disorder.
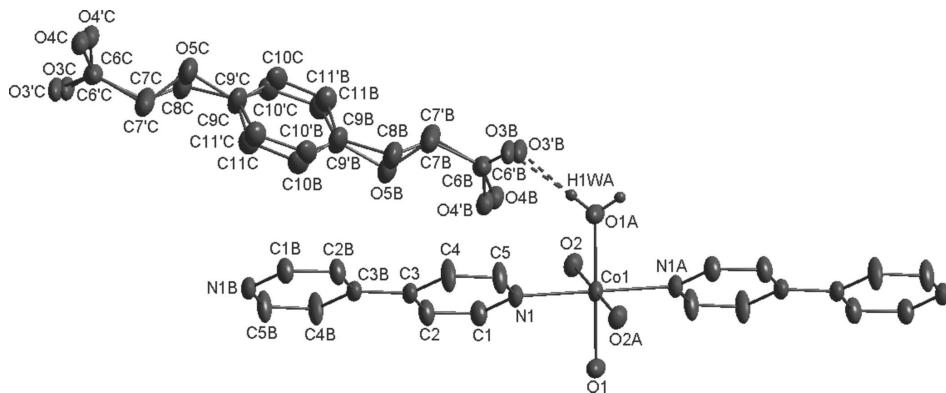
**Figure 1**

Part of the title complex (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30%
probability level and most H atoms are omitted for clarity. Primed atoms indicate one of the disorder components.
[Symmetry codes: (A) -x, -y, -z; (B) 1 - x, -y, 1 - z; (C) 1 + x, -1 + y, z.]

*catena*-Poly[[[tetraaquacobalt(II)]-*µ*-4,4′-bipyridine- $\kappa^2N:N'$] 2-[4-(2-carboxylatoethyl)phenoxy]acetate]

*Crystal data*
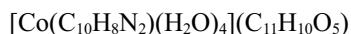
| | |
|---|---|
| [Co(C$_{10}$H$_8$N$_2$)(H$_2$O)$_4$](C$_{11}$H$_{10}$O$_5$) | $Z = 1$ |
| $M_r = 509.37$ | $F(000) = 265$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.518$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 7.1311$ (10) Å | Cell parameters from 3868 reflections |
| $b = 7.6319$ (10) Å | $\theta = 2.7–28.2°$ |
| $c = 10.4978$ (14) Å | $\mu = 0.83$ mm$^{-1}$ |
| $\alpha = 91.930$ (1)° | $T = 291$ K |
| $\beta = 101.832$ (1)° | Block, red |
| $\gamma = 94.002$ (1)° | $0.50 \times 0.41 \times 0.21$ mm |
| $V = 557.15$ (13) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 4108 measured reflections |
| Radiation source: fine-focus sealed tube | 2036 independent reflections |
| Graphite monochromator | 2008 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.011$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $\theta_{max} = 25.5°$, $\theta_{min} = 2.7°$ |
| | $h = -8 \rightarrow 8$ |
| | $k = -9 \rightarrow 9$ |
| $T_{min} = 0.674$, $T_{max} = 0.845$ | $l = -12 \rightarrow 12$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.085$ | |
| $S = 1.06$ | H-atom parameters constrained |
| 2036 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.7695P]$ |
| 176 parameters | where $P = (F_o^2 + 2F_c^2)/3$ |
| 364 restraints | $(\Delta/\sigma)_{max} < 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.61$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.63$ 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 (Å$^2$)*

|  | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O3 | 0.7094 (13) | 0.448 (3) | 0.8766 (14) | 0.0419 (15) | 0.50 |
| O4 | 0.522 (2) | 0.2444 (14) | 0.9494 (9) | 0.0368 (16) | 0.50 |
| C8 | 0.3511 (11) | 0.4124 (10) | 0.6667 (8) | 0.0635 (11) | 0.50 |
| H8A | 0.4539 | 0.4806 | 0.6385 | 0.076* | 0.50 |
| H8B | 0.3700 | 0.2890 | 0.6533 | 0.076* | 0.50 |
| C6 | 0.5492 (16) | 0.370 (3) | 0.879 (3) | 0.0363 (9) | 0.50 |
| C7 | 0.3670 (11) | 0.4520 (12) | 0.8095 (7) | 0.0522 (14) | 0.50 |
| H7A | 0.2547 | 0.4010 | 0.8376 | 0.063* | 0.50 |
| H7B | 0.3781 | 0.5780 | 0.8285 | 0.063* | 0.50 |
| C9 | 0.1644 (19) | 0.451 (2) | 0.5829 (11) | 0.0583 (13) | 0.50 |
| C10 | 0.1182 (18) | 0.3869 (16) | 0.4541 (10) | 0.0612 (15) | 0.50 |
| H10 | 0.1933 | 0.3074 | 0.4232 | 0.073* | 0.50 |
| C11 | 0.0411 (14) | 0.5566 (15) | 0.6274 (14) | 0.0575 (17) | 0.50 |
| H11 | 0.0658 | 0.5913 | 0.7154 | 0.069* | 0.50 |
| O3′ | 0.7312 (13) | 0.450 (3) | 0.9043 (14) | 0.0419 (15) | 0.50 |
| O4′ | 0.513 (2) | 0.2290 (14) | 0.9156 (9) | 0.0368 (16) | 0.50 |
| C6′ | 0.5648 (17) | 0.374 (3) | 0.876 (3) | 0.0363 (9) | 0.50 |
| C7′ | 0.4168 (11) | 0.4553 (12) | 0.7713 (8) | 0.0522 (14) | 0.50 |
| H7′1 | 0.3503 | 0.5373 | 0.8153 | 0.063* | 0.50 |
| H7′2 | 0.4868 | 0.5234 | 0.7173 | 0.063* | 0.50 |
| O5 | 0.2825 (7) | 0.3461 (6) | 0.6915 (5) | 0.0635 (11) | 0.50 |
| C9′ | 0.1435 (18) | 0.435 (2) | 0.5964 (11) | 0.0583 (13) | 0.50 |
| C10′ | 0.1492 (18) | 0.4241 (16) | 0.4648 (9) | 0.0612 (15) | 0.50 |
| H10′ | 0.2554 | 0.3795 | 0.4403 | 0.073* | 0.50 |
| C11′ | −0.0013 (14) | 0.5223 (14) | 0.6328 (14) | 0.0575 (17) | 0.50 |
| H11′ | −0.0012 | 0.5453 | 0.7204 | 0.069* | 0.50 |
| Co1 | 0.0000 | 0.0000 | 0.0000 | 0.02210 (13) | |
| O1 | 0.0283 (2) | 0.2722 (2) | −0.01206 (18) | 0.0396 (4) | |
| H1W | −0.0701 | 0.3243 | −0.0349 | 0.059* | |
| H2W | 0.1207 | 0.3397 | 0.0241 | 0.059* | |
| O2 | 0.2400 (2) | −0.0305 (2) | −0.08486 (16) | 0.0338 (4) | |
| H3W | 0.3136 | 0.0561 | −0.0905 | 0.051* | |
| H4W | 0.2965 | −0.1087 | −0.0441 | 0.051* | |
| N1 | 0.1824 (3) | 0.0139 (3) | 0.19142 (17) | 0.0288 (4) | |
| C1 | 0.3560 (3) | 0.1002 (3) | 0.2175 (2) | 0.0341 (5) | |

| | | | | |
|---|---|---|---|---|
| H1 | 0.3934 | 0.1655 | 0.1524 | 0.041* |
| C2 | 0.4835 (3) | 0.0981 (3) | 0.3358 (2) | 0.0356 (6) |
| H2 | 0.6033 | 0.1601 | 0.3483 | 0.043* |
| C3 | 0.4332 (3) | 0.0036 (3) | 0.4357 (2) | 0.0285 (5) |
| C4 | 0.2514 (4) | −0.0850 (5) | 0.4090 (3) | 0.0557 (9) |
| H4 | 0.2096 | −0.1502 | 0.4726 | 0.067* |
| C5 | 0.1325 (4) | −0.0761 (4) | 0.2877 (3) | 0.0532 (8) |
| H5 | 0.0114 | −0.1361 | 0.2725 | 0.064* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O3 | 0.0288 (17) | 0.0355 (10) | 0.050 (5) | −0.0043 (18) | −0.0169 (18) | 0.009 (3) |
| O4 | 0.0306 (14) | 0.0374 (17) | 0.038 (4) | 0.0015 (14) | −0.005 (3) | 0.010 (3) |
| C8 | 0.053 (2) | 0.056 (2) | 0.067 (2) | 0.0142 (17) | −0.0250 (18) | 0.0040 (18) |
| C6 | 0.0301 (17) | 0.0288 (13) | 0.0428 (15) | 0.0016 (14) | −0.0095 (18) | 0.0037 (10) |
| C7 | 0.044 (3) | 0.0434 (16) | 0.059 (3) | 0.006 (2) | −0.016 (2) | 0.011 (2) |
| C9 | 0.044 (2) | 0.058 (2) | 0.065 (2) | 0.0198 (19) | −0.0110 (16) | −0.0018 (17) |
| C10 | 0.042 (3) | 0.063 (3) | 0.072 (2) | 0.020 (3) | −0.0052 (19) | −0.016 (2) |
| C11 | 0.047 (3) | 0.063 (3) | 0.059 (2) | 0.010 (3) | 0.001 (2) | −0.001 (2) |
| O3′ | 0.0288 (17) | 0.0355 (10) | 0.050 (5) | −0.0043 (18) | −0.0169 (18) | 0.009 (3) |
| O4′ | 0.0306 (14) | 0.0374 (17) | 0.038 (4) | 0.0015 (14) | −0.005 (3) | 0.010 (3) |
| C6′ | 0.0301 (17) | 0.0288 (13) | 0.0428 (15) | 0.0016 (14) | −0.0095 (18) | 0.0037 (10) |
| C7′ | 0.044 (3) | 0.0434 (16) | 0.059 (3) | 0.006 (2) | −0.016 (2) | 0.011 (2) |
| O5 | 0.053 (2) | 0.056 (2) | 0.067 (2) | 0.0142 (17) | −0.0250 (18) | 0.0040 (18) |
| C9′ | 0.044 (2) | 0.058 (2) | 0.065 (2) | 0.0198 (19) | −0.0110 (16) | −0.0018 (17) |
| C10′ | 0.042 (3) | 0.063 (3) | 0.072 (2) | 0.020 (3) | −0.0052 (19) | −0.016 (2) |
| C11′ | 0.047 (3) | 0.063 (3) | 0.059 (2) | 0.010 (3) | 0.001 (2) | −0.001 (2) |
| Co1 | 0.0185 (2) | 0.0246 (2) | 0.0200 (2) | 0.00069 (15) | −0.00368 (15) | 0.00413 (15) |
| O1 | 0.0309 (9) | 0.0260 (8) | 0.0538 (11) | −0.0002 (7) | −0.0092 (8) | 0.0043 (8) |
| O2 | 0.0249 (8) | 0.0398 (9) | 0.0356 (9) | 0.0033 (7) | 0.0029 (7) | 0.0085 (7) |
| N1 | 0.0246 (9) | 0.0354 (10) | 0.0226 (9) | 0.0004 (8) | −0.0041 (7) | 0.0048 (8) |
| C1 | 0.0307 (12) | 0.0427 (14) | 0.0248 (11) | −0.0057 (10) | −0.0024 (9) | 0.0090 (10) |
| C2 | 0.0279 (12) | 0.0450 (14) | 0.0281 (12) | −0.0084 (10) | −0.0052 (9) | 0.0073 (10) |
| C3 | 0.0280 (11) | 0.0307 (11) | 0.0229 (11) | 0.0029 (9) | −0.0044 (9) | 0.0025 (9) |
| C4 | 0.0417 (15) | 0.084 (2) | 0.0310 (14) | −0.0249 (15) | −0.0109 (11) | 0.0275 (14) |
| C5 | 0.0352 (14) | 0.079 (2) | 0.0348 (14) | −0.0234 (14) | −0.0105 (11) | 0.0218 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O3—C6 | 1.257 (6) | C10′—H10′ | 0.9300 |
| O4—C6 | 1.257 (6) | C11′—C10′i | 1.41 (2) |
| C8—C9 | 1.491 (13) | C11′—H11′ | 0.9300 |
| C8—C7 | 1.499 (11) | Co1—O1ii | 2.0840 (16) |
| C8—H8A | 0.9700 | Co1—O1 | 2.0840 (16) |
| C8—H8B | 0.9700 | Co1—O2ii | 2.1083 (16) |
| C6—C7 | 1.540 (8) | Co1—O2 | 2.1083 (16) |
| C7—H7A | 0.9700 | Co1—N1 | 2.1530 (17) |

| | | | |
|---|---|---|---|
| C7—H7B | 0.9700 | Co1—N1ⁱⁱ | 2.1531 (17) |
| C9—C11 | 1.375 (6) | O1—H1W | 0.8271 |
| C9—C10 | 1.387 (7) | O1—H2W | 0.8245 |
| C10—C11ⁱ | 1.379 (19) | O2—H3W | 0.8262 |
| C10—H10 | 0.9300 | O2—H4W | 0.8251 |
| C11—C10ⁱ | 1.379 (19) | N1—C1 | 1.333 (3) |
| C11—H11 | 0.9300 | N1—C5 | 1.334 (3) |
| O3′—C6′ | 1.258 (6) | C1—C2 | 1.382 (3) |
| O4′—C6′ | 1.255 (6) | C1—H1 | 0.9300 |
| C6′—C7′ | 1.537 (7) | C2—C3 | 1.385 (3) |
| C7′—O5 | 1.352 (10) | C2—H2 | 0.9300 |
| C7′—H7′1 | 0.9700 | C3—C4 | 1.390 (3) |
| C7′—H7′2 | 0.9700 | C3—C3ⁱⁱⁱ | 1.489 (4) |
| O5—C9′ | 1.475 (13) | C4—C5 | 1.384 (3) |
| C9′—C11′ | 1.377 (6) | C4—H4 | 0.9300 |
| C9′—C10′ | 1.391 (7) | C5—H5 | 0.9300 |
| C10′—C11′ⁱ | 1.41 (2) | | |
| | | | |
| C9—C8—C7 | 114.6 (7) | C9′—C11′—H11′ | 120.6 |
| C9—C8—H8A | 108.6 | C10′ⁱ—C11′—H11′ | 120.6 |
| C7—C8—H8A | 108.6 | O1ⁱⁱ—Co1—O1 | 180 |
| C9—C8—H8B | 108.6 | O1ⁱⁱ—Co1—O2ⁱⁱ | 91.66 (7) |
| C7—C8—H8B | 108.6 | O1—Co1—O2ⁱⁱ | 88.34 (7) |
| H8A—C8—H8B | 107.6 | O1ⁱⁱ—Co1—O2 | 88.33 (7) |
| O3—C6—O4 | 125.4 (9) | O1—Co1—O2 | 91.66 (7) |
| O3—C6—C7 | 118.0 (7) | O2ⁱⁱ—Co1—O2 | 180 |
| O4—C6—C7 | 115.7 (8) | O1ⁱⁱ—Co1—N1 | 88.07 (7) |
| C8—C7—C6 | 106.0 (13) | O1—Co1—N1 | 91.93 (7) |
| C8—C7—H7A | 110.5 | O2ⁱⁱ—Co1—N1 | 89.64 (7) |
| C6—C7—H7A | 110.5 | O2—Co1—N1 | 90.36 (7) |
| C8—C7—H7B | 110.5 | O1ⁱⁱ—Co1—N1ⁱⁱ | 91.93 (7) |
| C6—C7—H7B | 110.5 | O1—Co1—N1ⁱⁱ | 88.07 (7) |
| H7A—C7—H7B | 108.7 | O2ⁱⁱ—Co1—N1ⁱⁱ | 90.36 (7) |
| C11—C9—C10 | 118.6 (7) | O2—Co1—N1ⁱⁱ | 89.63 (7) |
| C11—C9—C8 | 121.7 (6) | N1—Co1—N1ⁱⁱ | 180 |
| C10—C9—C8 | 119.5 (5) | Co1—O1—H1W | 118.4 |
| C11ⁱ—C10—C9 | 119.0 (12) | Co1—O1—H2W | 126.8 |
| C11ⁱ—C10—H10 | 120.5 | H1W—O1—H2W | 112.0 |
| C9—C10—H10 | 120.5 | Co1—O2—H3W | 119.7 |
| C9—C11—C10ⁱ | 122.2 (12) | Co1—O2—H4W | 104.4 |
| C9—C11—H11 | 118.9 | H3W—O2—H4W | 112.1 |
| C10ⁱ—C11—H11 | 118.9 | C1—N1—C5 | 116.50 (19) |
| O4′—C6′—O3′ | 125.8 (9) | C1—N1—Co1 | 122.27 (15) |
| O4′—C6′—C7′ | 116.6 (7) | C5—N1—Co1 | 121.02 (16) |
| O3′—C6′—C7′ | 117.2 (6) | N1—C1—C2 | 123.7 (2) |
| O5—C7′—C6′ | 118.2 (10) | N1—C1—H1 | 118.2 |
| O5—C7′—H7′1 | 107.8 | C2—C1—H1 | 118.2 |
| C6′—C7′—H7′1 | 107.8 | C1—C2—C3 | 120.1 (2) |

| | | | |
|---|---|---|---|
| O5—C7′—H7′2 | 107.8 | C1—C2—H2 | 119.9 |
| C6′—C7′—H7′2 | 107.8 | C3—C2—H2 | 119.9 |
| H7′1—C7′—H7′2 | 107.1 | C2—C3—C4 | 116.2 (2) |
| C7′—O5—C9′ | 114.6 (8) | C2—C3—C3ⁱⁱⁱ | 121.9 (3) |
| C11′—C9′—C10′ | 117.9 (7) | C4—C3—C3ⁱⁱⁱ | 121.9 (3) |
| C11′—C9′—O5 | 121.8 (6) | C5—C4—C3 | 120.0 (2) |
| C10′—C9′—O5 | 120.2 (6) | C5—C4—H4 | 120.0 |
| C9′—C10′—C11′ⁱ | 122.8 (12) | C3—C4—H4 | 120.0 |
| C9′—C10′—H10′ | 118.6 | N1—C5—C4 | 123.5 (2) |
| C11′ⁱ—C10′—H10′ | 118.6 | N1—C5—H5 | 118.2 |
| C9′—C11′—C10′ⁱ | 118.8 (12) | C4—C5—H5 | 118.2 |
| | | | |
| C9—C8—C7—C6 | 168.9 (10) | O1—Co1—N1—C1 | −51.9 (2) |
| O3—C6—C7—C8 | 76 (3) | O2ⁱⁱ—Co1—N1—C1 | −140.20 (19) |
| O4—C6—C7—C8 | −114 (2) | O2—Co1—N1—C1 | 39.80 (19) |
| C7—C8—C9—C11 | 17.1 (18) | N1ⁱⁱ—Co1—N1—C1 | 66 (3) |
| C7—C8—C9—C10 | −167.0 (13) | O1ⁱⁱ—Co1—N1—C5 | −46.4 (2) |
| C11—C9—C10—C11ⁱ | 5 (2) | O1—Co1—N1—C5 | 133.6 (2) |
| C8—C9—C10—C11ⁱ | −170.8 (13) | O2ⁱⁱ—Co1—N1—C5 | 45.3 (2) |
| C10—C9—C11—C10ⁱ | −5 (2) | O2—Co1—N1—C5 | −134.7 (2) |
| C8—C9—C11—C10ⁱ | 170.5 (13) | N1ⁱⁱ—Co1—N1—C5 | −109 (3) |
| O4′—C6′—C7′—O5 | −27 (3) | C5—N1—C1—C2 | 1.0 (4) |
| O3′—C6′—C7′—O5 | 146 (2) | Co1—N1—C1—C2 | −173.7 (2) |
| C6′—C7′—O5—C9′ | 178.6 (13) | N1—C1—C2—C3 | −0.5 (4) |
| C7′—O5—C9′—C11′ | −74.6 (15) | C1—C2—C3—C4 | −0.2 (4) |
| C7′—O5—C9′—C10′ | 109.2 (15) | C1—C2—C3—C3ⁱⁱⁱ | 179.5 (3) |
| C11′—C9′—C10′—C11′ⁱ | −8 (2) | C2—C3—C4—C5 | 0.3 (5) |
| O5—C9′—C10′—C11′ⁱ | 168.0 (12) | C3ⁱⁱⁱ—C3—C4—C5 | −179.4 (3) |
| C10′—C9′—C11′—C10′ⁱ | 8 (2) | C1—N1—C5—C4 | −0.9 (5) |
| O5—C9′—C11′—C10′ⁱ | −168.3 (12) | Co1—N1—C5—C4 | 173.9 (3) |
| O1ⁱⁱ—Co1—N1—C1 | 128.1 (2) | C3—C4—C5—N1 | 0.3 (6) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H4*W*···O4′ⁱⁱⁱ | 0.83 | 2.00 | 2.796 (10) | 161 |
| O2—H4*W*···O4ⁱⁱⁱ | 0.83 | 1.86 | 2.667 (10) | 165 |
| O2—H3*W*···O4ⁱᵛ | 0.83 | 1.96 | 2.765 (14) | 163 |
| O2—H3*W*···O4′ⁱᵛ | 0.83 | 1.86 | 2.678 (14) | 170 |
| O1—H2*W*···O3ᵛ | 0.82 | 2.07 | 2.868 (16) | 164 |
| O1—H2*W*···O3′ᵛ | 0.82 | 1.90 | 2.691 (16) | 161 |
| O1—H1*W*···O3ᵛⁱ | 0.83 | 1.97 | 2.789 (13) | 169 |
| O1—H1*W*···O3′ᵛⁱ | 0.83 | 1.79 | 2.612 (14) | 174 |

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