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# Diaquabis[1,2-bis(pyridin-4-yl)ethene]-bis[2-(4-carboxyphenyl)acetato]cobalt(II)

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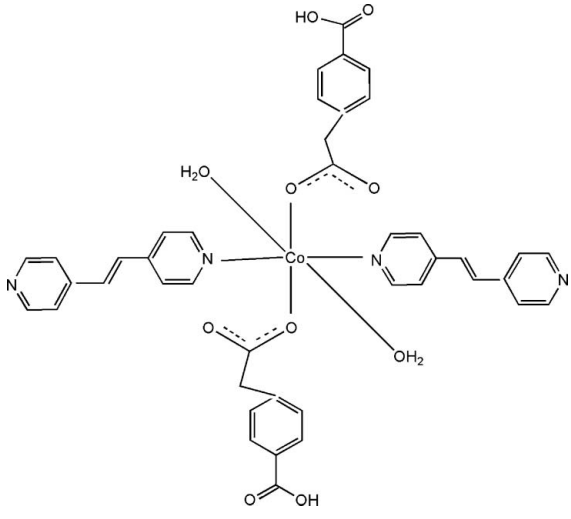
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.055; $wR$ factor = 0.105; data-to-parameter ratio = 13.6.

The asymmetric unit of the title compound, $[Co(C_9H_7O_4)_2(C_{12}H_{10}N_2)_2(H_2O)_2]$, consists of one $Co^{2+}$ ion, one monodeprotonated 2-(4-carboxylatophenyl)acetate carboxylic acid, one 1,2-bis(pyridin-4-yl)ethane molecule and one water molecule. The $Co^{II}$ atom is situated on a crystallographic center of inversion and is octahedrally coordinated by two O atoms from two anions, two N atoms of two 1,2-bis(pyridin-4-yl)-ethane molecules and two O atoms from two water molecules. A three-dimensional network is established by intermolecular O—H···O and O—H···N hydrogen bonds.

## Related literature

For general background to the design of metal-organic supramolecular solids with potential functionality, see: Moulton & Zaworotko (2001); Janiak (2003). For weak non-covalent interactions in supramolecular solids, see: Hosseini (2005); Nishio (2004). For metal-organic supramolecular frameworks based on organic connectors containing pyridyl and/or carboxylate groups, see: Brammer (2004).




## Experimental

### Crystal data

$[Co(C_9H_7O_4)_2(C_{12}H_{10}N_2)_2(H_2O)_2]$
$M_r$ = 817.69
Monoclinic, $P2_1/c$
$a$ = 21.349 (5) Å
$b$ = 5.6522 (12) Å
$c$ = 15.659 (4) Å
$\beta$ = 98.999 (4)°
$V$ = 1866.3 (7) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.53 mm$^{-1}$
$T$ = 293 K
0.40 × 0.30 × 0.10 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.850, $T_{max}$ = 0.874
9499 measured reflections
3635 independent reflections
2640 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.105
$S$ = 1.06
3635 reflections
268 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.71 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H5$C$···O1$^{i}$ | 0.73 (4) | 2.13 (4) | 2.822 (3) | 158 (4) |
| O5—H5$D$···O2$^{ii}$ | 0.98 (4) | 1.74 (4) | 2.610 (3) | 145 (3) |
| O3—H3···N2$^{iii}$ | 0.82 | 1.85 | 2.667 (3) | 173 |

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2300).

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# supporting information

*Acta Cryst.* (2011). E**67**, m999 [doi:10.1107/S1600536811024755]

## Diaquabis[1,2-bis(pyridin-4-yl)ethene]bis[2-(4-carboxyphenyl)acetato]cobalt(II)

**Wei-Hua Yu, Jian-Lan Liu and Xiao-Ming Ren**

### S1. Comment

During the past decade, the design of new metal-organic supramolecular solids has attracted ever-increasing focus in the fields of coordination chemistry and crystal engineering, for the sake of developing desired crystalline materials with potential functionality (Moulton & Zaworotko, 2001; Janiak *et al.*, 2003). Furthermore, it has been realised that weak noncovalent interactions such as hydrogen bonds, aromatic stacking, and van der Waals forces (Hosseini, 2005; Nishio, 2004) are crucial in the direction of such crystalline architectures. Hitherto, a variety of organic connectors containing pyridyl and/or carboxylate groups (Brammer, 2004) have been widely used to construct metal-organic supramolecular frameworks. Herein we report the crystal structure of the title compound (1).

The molecular structure of (1) is illustrated in Fig. 1. Compound (1) crystallizes in the monoclinic space group $P2_1/c$. The structure of (1) is a single molecule, in which the $Co^{2+}$ center is situated on a crystallographic center of inversion. The coordination sphere of cobalt is a slightly distorted octahedron and consistes of by two O atoms from two mono-deprotonated (4-carboxyphenyl)acetate groups, two N atoms of two 1,2-di(pyridin-4-yl)ethane molecules and two O atoms from two water molecules. As shown in Fig. 2, a one-dimensional chain is formed by O–H···N hydrogen bonds. In addition, these one-dimensional chains are linked together by additional O—H···O hydrogen bonds between water molecules and the cobalt bound carboxylate group generating a three-dimensional framework.

### S2. Experimental

Cobalt chloride hexahydrate (1 mmol), 1,2-di(pyridin-4-yl)ethane (1 mmol) and (4-carboxyphenyl)acetic acid (1 mmol) in water (8 ml) were placed in a Teflon-lined stainless-steel Parr bomb that was heated to 433 K for 48 h. Red plate crystals were collected after the bomb was subsequently allowed to cool to room temperature (yield: 38%).

### S3. Refinement

C-bound H atoms were placed geometrically (C—H = 0.93, and 0.98 Å) and refined as riding atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C). O-bound H atoms were located in difference Fourier maps and refined as riding in their as-found relative positions (O—H =0.96 Å) with $U_{iso}$(H) = 1.5$U_{eq}$(C).

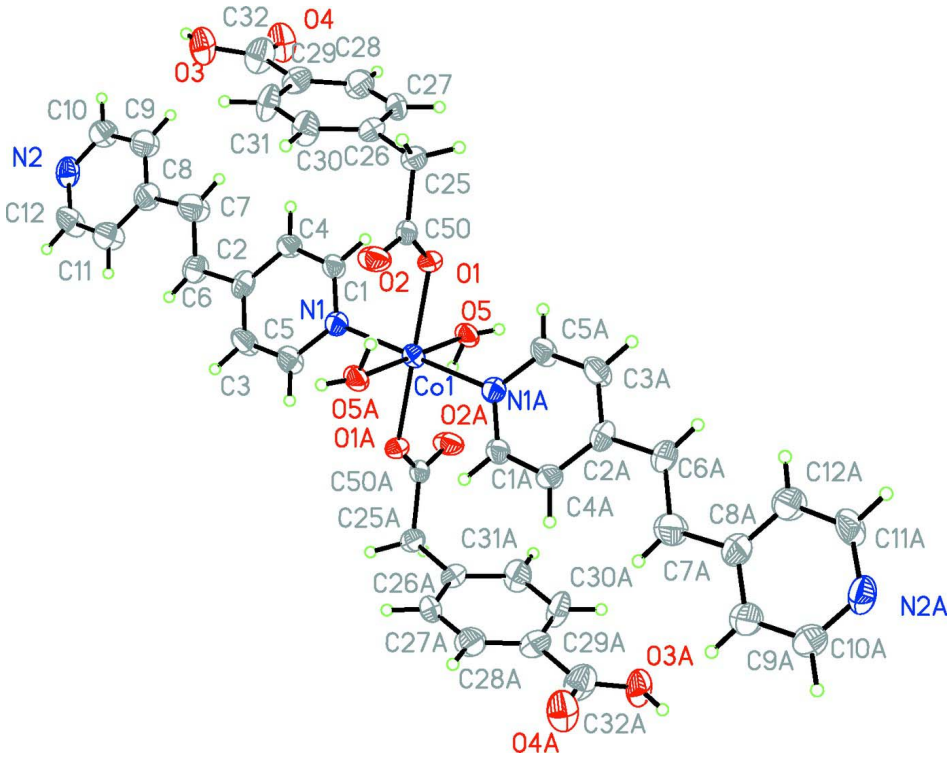


**Figure 1**

Molecular structure of (I), showing displacement ellipsoids at the 30% probability level.

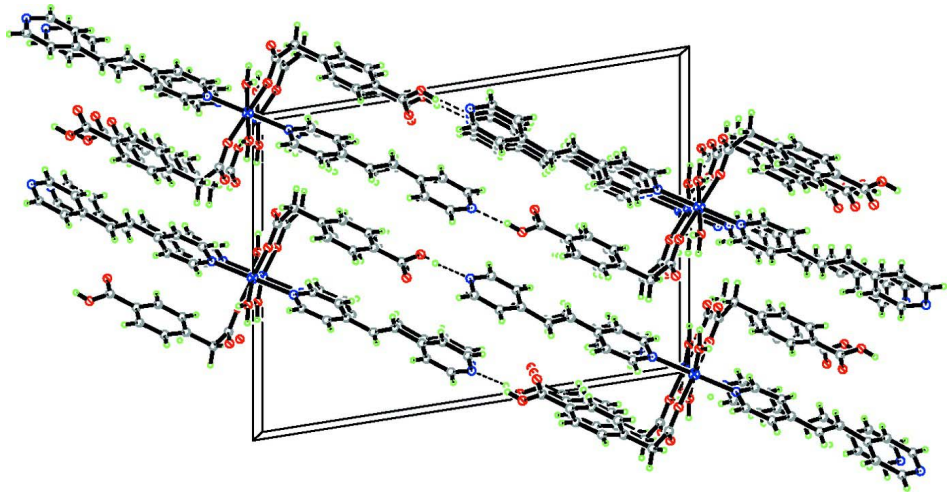

**Figure 2**

One-dimensional chain structure of (I).

**Diaquabis[1,2-bis(pyridin-4-yl)ethene]bis[2-(4- carboxylphenyl)acetato]cobalt(II)**

*Crystal data*

$[Co(C_9H_7O_4)_2(C_{12}H_{10}N_2)_2(H_2O)_2]$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

$a$ = 21.349 (5) Å
$b$ = 5.6522 (12) Å
$c$ = 15.659 (4) Å
$\beta$ = 98.999 (4)°

$V$ = 1866.3 (7) Å$^3$
$Z$ = 2
$F$(000) = 850
$D_x$ = 1.455 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 870 reflections

$\theta$ = 2.6–22.1°
$\mu$ = 0.53 mm$^{-1}$
$T$ = 293 K
Plate, red
0.40 × 0.30 × 0.10 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.850, $T_{max}$ = 0.874

9499 measured reflections
3635 independent reflections
2640 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 1.9°
$h$ = −26→23
$k$ = −6→6
$l$ = −19→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.105
$S$ = 1.06
3635 reflections
268 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.440P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.71 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.13939 (13) | 0.6024 (5) | 0.07330 (17) | 0.0285 (6) |
| H1 | 0.1308 | 0.7388 | 0.0404 | 0.034* |
| C2 | 0.21300 (13) | 0.3771 (6) | 0.16945 (19) | 0.0324 (7) |
| C3 | 0.16536 (14) | 0.2132 (6) | 0.1675 (2) | 0.0418 (8) |
| H3A | 0.1727 | 0.0750 | 0.1997 | 0.050* |
| C4 | 0.19847 (13) | 0.5792 (5) | 0.11978 (18) | 0.0305 (7) |
| H4 | 0.2287 | 0.6969 | 0.1183 | 0.037* |
| C5 | 0.10794 (14) | 0.2501 (5) | 0.11927 (19) | 0.0360 (7) |
| H5A | 0.0771 | 0.1338 | 0.1194 | 0.043* |
| C6 | 0.27478 (13) | 0.3325 (6) | 0.2271 (2) | 0.0446 (8) |

| | | | | |
|---|---|---|---|---|
| H6 | 0.2805 | 0.2017 | 0.2635 | 0.053* |
| C7 | 0.32607 (15) | 0.5046 (7) | 0.2236 (2) | 0.0542 (9) |
| H7 | 0.3213 | 0.6348 | 0.1868 | 0.065* |
| C8 | 0.38736 (14) | 0.4545 (6) | 0.2844 (2) | 0.0435 (8) |
| C9 | 0.43624 (15) | 0.6125 (7) | 0.2885 (2) | 0.0480 (9) |
| H9 | 0.4317 | 0.7491 | 0.2549 | 0.058* |
| C10 | 0.49294 (15) | 0.5670 (6) | 0.3433 (2) | 0.0418 (8) |
| H10 | 0.5263 | 0.6730 | 0.3439 | 0.050* |
| C11 | 0.45391 (15) | 0.2330 (6) | 0.3909 (2) | 0.0467 (9) |
| H11 | 0.4588 | 0.1017 | 0.4271 | 0.056* |
| C12 | 0.39688 (15) | 0.2605 (6) | 0.3370 (2) | 0.0476 (9) |
| H12 | 0.3651 | 0.1477 | 0.3363 | 0.057* |
| C25 | 0.09958 (12) | 0.8462 (5) | −0.19283 (18) | 0.0311 (6) |
| H25A | 0.1055 | 0.7968 | −0.2504 | 0.037* |
| H25B | 0.0775 | 0.9968 | −0.1978 | 0.037* |
| C26 | 0.16362 (13) | 0.8760 (5) | −0.13681 (18) | 0.0290 (6) |
| C27 | 0.17905 (14) | 1.0732 (5) | −0.0867 (2) | 0.0333 (7) |
| H27 | 0.1497 | 1.1953 | −0.0881 | 0.040* |
| C28 | 0.23634 (15) | 1.0942 (6) | −0.0351 (2) | 0.0422 (8) |
| H28 | 0.2446 | 1.2272 | −0.0002 | 0.051* |
| C29 | 0.28176 (14) | 0.9246 (6) | −0.0335 (2) | 0.0387 (7) |
| C30 | 0.26777 (14) | 0.7226 (6) | −0.0820 (2) | 0.0447 (8) |
| H30 | 0.2978 | 0.6031 | −0.0811 | 0.054* |
| C31 | 0.20875 (14) | 0.6992 (6) | −0.1321 (2) | 0.0408 (8) |
| H31 | 0.1992 | 0.5607 | −0.1635 | 0.049* |
| C32 | 0.34424 (16) | 0.9532 (6) | 0.0221 (2) | 0.0494 (9) |
| C50 | 0.05974 (12) | 0.6632 (5) | −0.15437 (17) | 0.0237 (6) |
| Co1 | 0.0000 | 0.5000 | 0.0000 | 0.02453 (15) |
| H5C | −0.0226 (18) | 0.907 (7) | 0.078 (3) | 0.057 (13)* |
| H5D | −0.0072 (15) | 0.719 (6) | 0.134 (2) | 0.049 (10)* |
| N1 | 0.09278 (10) | 0.4435 (4) | 0.07147 (14) | 0.0278 (5) |
| N2 | 0.50139 (12) | 0.3794 (5) | 0.39444 (17) | 0.0417 (6) |
| O1 | 0.03952 (8) | 0.7233 (3) | −0.08597 (11) | 0.0252 (4) |
| O2 | 0.05249 (10) | 0.4649 (4) | −0.18973 (14) | 0.0392 (5) |
| O3 | 0.38617 (10) | 0.7984 (4) | 0.00934 (15) | 0.0448 (6) |
| H3 | 0.4191 | 0.8232 | 0.0426 | 0.067* |
| O4 | 0.35646 (11) | 1.1161 (4) | 0.07192 (15) | 0.0506 (6) |
| O5 | −0.00449 (10) | 0.7965 (4) | 0.07875 (14) | 0.0308 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0255 (14) | 0.0263 (14) | 0.0317 (15) | −0.0001 (11) | −0.0015 (11) | 0.0051 (12) |
| C2 | 0.0228 (15) | 0.0414 (18) | 0.0314 (15) | 0.0045 (12) | −0.0004 (12) | −0.0013 (13) |
| C3 | 0.0411 (17) | 0.0279 (17) | 0.052 (2) | −0.0034 (14) | −0.0078 (14) | 0.0124 (15) |
| C4 | 0.0254 (14) | 0.0280 (16) | 0.0360 (16) | −0.0053 (11) | −0.0017 (12) | 0.0017 (12) |
| C5 | 0.0329 (15) | 0.0323 (17) | 0.0372 (17) | −0.0017 (13) | −0.0112 (12) | 0.0083 (13) |
| C6 | 0.0238 (16) | 0.050 (2) | 0.056 (2) | 0.0032 (14) | −0.0049 (14) | 0.0141 (17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.0407 (18) | 0.056 (2) | 0.061 (2) | −0.0067 (18) | −0.0091 (15) | 0.023 (2) |
| C8 | 0.0303 (16) | 0.043 (2) | 0.055 (2) | −0.0009 (14) | −0.0020 (13) | 0.0019 (15) |
| C9 | 0.0383 (19) | 0.050 (2) | 0.053 (2) | −0.0036 (15) | −0.0021 (15) | 0.0131 (17) |
| C10 | 0.0357 (17) | 0.042 (2) | 0.0446 (19) | −0.0083 (14) | −0.0035 (14) | −0.0042 (14) |
| C11 | 0.0469 (19) | 0.0385 (19) | 0.0453 (19) | −0.0024 (15) | −0.0222 (15) | 0.0135 (15) |
| C12 | 0.0373 (18) | 0.051 (2) | 0.048 (2) | −0.0097 (16) | −0.0121 (15) | 0.0094 (17) |
| C25 | 0.0254 (14) | 0.0341 (17) | 0.0340 (15) | −0.0005 (12) | 0.0056 (12) | 0.0059 (13) |
| C26 | 0.0241 (14) | 0.0337 (16) | 0.0301 (15) | −0.0018 (12) | 0.0069 (11) | −0.0003 (12) |
| C27 | 0.0326 (16) | 0.0210 (16) | 0.0469 (18) | 0.0048 (11) | 0.0086 (13) | 0.0006 (12) |
| C28 | 0.0408 (19) | 0.0344 (18) | 0.054 (2) | −0.0039 (14) | 0.0135 (15) | −0.0099 (15) |
| C29 | 0.0296 (15) | 0.044 (2) | 0.0424 (17) | −0.0057 (13) | 0.0056 (13) | −0.0033 (14) |
| C30 | 0.0256 (15) | 0.052 (2) | 0.054 (2) | 0.0122 (15) | −0.0021 (13) | −0.0096 (17) |
| C31 | 0.0404 (17) | 0.0326 (17) | 0.0480 (19) | 0.0022 (14) | 0.0024 (14) | −0.0182 (14) |
| C32 | 0.0381 (18) | 0.053 (2) | 0.054 (2) | −0.0008 (16) | −0.0024 (15) | −0.0161 (18) |
| C50 | 0.0207 (12) | 0.0236 (15) | 0.0258 (13) | 0.0028 (11) | 0.0003 (10) | 0.0029 (11) |
| Co1 | 0.0269 (3) | 0.0223 (3) | 0.0237 (3) | 0.0004 (2) | 0.00182 (19) | 0.0014 (2) |
| N1 | 0.0252 (12) | 0.0271 (13) | 0.0307 (12) | 0.0007 (9) | 0.0033 (9) | 0.0002 (9) |
| N2 | 0.0315 (14) | 0.0433 (16) | 0.0461 (16) | 0.0071 (12) | −0.0069 (12) | −0.0035 (13) |
| O1 | 0.0242 (9) | 0.0268 (10) | 0.0264 (10) | −0.0013 (8) | 0.0093 (8) | 0.0018 (8) |
| O2 | 0.0491 (13) | 0.0258 (12) | 0.0478 (13) | −0.0078 (10) | 0.0238 (10) | −0.0055 (9) |
| O3 | 0.0347 (12) | 0.0444 (14) | 0.0466 (13) | 0.0077 (11) | −0.0200 (10) | −0.0051 (11) |
| O4 | 0.0511 (15) | 0.0463 (14) | 0.0473 (14) | 0.0075 (11) | −0.0141 (11) | −0.0127 (12) |
| O5 | 0.0390 (11) | 0.0199 (11) | 0.0365 (12) | 0.0029 (9) | 0.0150 (9) | 0.0008 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.338 (3) | C25—H25A | 0.9700 |
| C1—C4 | 1.360 (4) | C25—H25B | 0.9700 |
| C1—H1 | 0.9300 | C26—C27 | 1.373 (4) |
| C2—C3 | 1.373 (4) | C26—C31 | 1.382 (4) |
| C2—C4 | 1.389 (4) | C27—C28 | 1.362 (4) |
| C2—C6 | 1.498 (4) | C27—H27 | 0.9300 |
| C3—C5 | 1.352 (4) | C28—C29 | 1.361 (4) |
| C3—H3A | 0.9300 | C28—H28 | 0.9300 |
| C4—H4 | 0.9300 | C29—C30 | 1.378 (5) |
| C5—N1 | 1.335 (4) | C29—C32 | 1.483 (4) |
| C5—H5A | 0.9300 | C30—C31 | 1.383 (4) |
| C6—C7 | 1.472 (5) | C30—H30 | 0.9300 |
| C6—H6 | 0.9300 | C31—H31 | 0.9300 |
| C7—C8 | 1.520 (4) | C32—O4 | 1.209 (4) |
| C7—H7 | 0.9300 | C32—O3 | 1.290 (4) |
| C8—C12 | 1.367 (5) | C50—O2 | 1.249 (3) |
| C8—C9 | 1.367 (5) | C50—O1 | 1.262 (3) |
| C9—C10 | 1.394 (4) | Co1—O5 | 2.092 (2) |
| C9—H9 | 0.9300 | Co1—O5$^{i}$ | 2.092 (2) |
| C10—N2 | 1.324 (4) | Co1—O1$^{i}$ | 2.1149 (17) |
| C10—H10 | 0.9300 | Co1—O1 | 2.1149 (17) |
| C11—N2 | 1.303 (4) | Co1—N1$^{i}$ | 2.141 (2) |

| | | | |
|---|---|---|---|
| C11—C12 | 1.378 (4) | Co1—N1 | 2.141 (2) |
| C11—H11 | 0.9300 | O3—H3 | 0.8200 |
| C12—H12 | 0.9300 | O5—H5C | 0.73 (4) |
| C25—C26 | 1.514 (4) | O5—H5D | 0.98 (4) |
| C25—C50 | 1.522 (4) | | |

| | | | |
|---|---|---|---|
| N1—C1—C4 | 124.8 (3) | C28—C27—C26 | 121.5 (3) |
| N1—C1—H1 | 117.6 | C28—C27—H27 | 119.2 |
| C4—C1—H1 | 117.6 | C26—C27—H27 | 119.2 |
| C3—C2—C4 | 116.3 (3) | C29—C28—C27 | 121.4 (3) |
| C3—C2—C6 | 118.6 (3) | C29—C28—H28 | 119.3 |
| C4—C2—C6 | 125.0 (3) | C27—C28—H28 | 119.3 |
| C5—C3—C2 | 120.8 (3) | C28—C29—C30 | 118.7 (3) |
| C5—C3—H3A | 119.6 | C28—C29—C32 | 120.5 (3) |
| C2—C3—H3A | 119.6 | C30—C29—C32 | 120.8 (3) |
| C1—C4—C2 | 119.1 (3) | C29—C30—C31 | 119.5 (3) |
| C1—C4—H4 | 120.5 | C29—C30—H30 | 120.3 |
| C2—C4—H4 | 120.5 | C31—C30—H30 | 120.3 |
| N1—C5—C3 | 124.0 (3) | C26—C31—C30 | 121.8 (3) |
| N1—C5—H5A | 118.0 | C26—C31—H31 | 119.1 |
| C3—C5—H5A | 118.0 | C30—C31—H31 | 119.1 |
| C7—C6—C2 | 117.1 (3) | O4—C32—O3 | 122.1 (3) |
| C7—C6—H6 | 121.4 | O4—C32—C29 | 123.0 (3) |
| C2—C6—H6 | 121.4 | O3—C32—C29 | 114.7 (3) |
| C6—C7—C8 | 115.2 (3) | O2—C50—O1 | 125.6 (2) |
| C6—C7—H7 | 122.4 | O2—C50—C25 | 118.2 (2) |
| C8—C7—H7 | 122.4 | O1—C50—C25 | 116.1 (2) |
| C12—C8—C9 | 117.1 (3) | O5—Co1—O5$^{i}$ | 180.00 (10) |
| C12—C8—C7 | 124.0 (3) | O5—Co1—O1$^{i}$ | 92.48 (8) |
| C9—C8—C7 | 118.9 (3) | O5$^{i}$—Co1—O1$^{i}$ | 87.52 (8) |
| C8—C9—C10 | 119.4 (3) | O5—Co1—O1 | 87.52 (8) |
| C8—C9—H9 | 120.3 | O5$^{i}$—Co1—O1 | 92.48 (8) |
| C10—C9—H9 | 120.3 | O1$^{i}$—Co1—O1 | 180.00 (7) |
| N2—C10—C9 | 122.9 (3) | O5—Co1—N1$^{i}$ | 93.70 (9) |
| N2—C10—H10 | 118.5 | O5$^{i}$—Co1—N1$^{i}$ | 86.30 (9) |
| C9—C10—H10 | 118.5 | O1$^{i}$—Co1—N1$^{i}$ | 89.61 (8) |
| N2—C11—C12 | 124.1 (3) | O1—Co1—N1$^{i}$ | 90.39 (8) |
| N2—C11—H11 | 117.9 | O5—Co1—N1 | 86.30 (9) |
| C12—C11—H11 | 117.9 | O5$^{i}$—Co1—N1 | 93.70 (9) |
| C8—C12—C11 | 119.6 (3) | O1$^{i}$—Co1—N1 | 90.39 (8) |
| C8—C12—H12 | 120.2 | O1—Co1—N1 | 89.61 (8) |
| C11—C12—H12 | 120.2 | N1$^{i}$—Co1—N1 | 180.00 (13) |
| C26—C25—C50 | 110.9 (2) | C5—N1—C1 | 115.0 (2) |
| C26—C25—H25A | 109.5 | C5—N1—Co1 | 122.57 (19) |
| C50—C25—H25A | 109.5 | C1—N1—Co1 | 122.36 (19) |
| C26—C25—H25B | 109.5 | C11—N2—C10 | 116.8 (3) |
| C50—C25—H25B | 109.5 | C50—O1—Co1 | 127.08 (17) |
| H25A—C25—H25B | 108.1 | C32—O3—H3 | 109.5 |

| | | | |
|---|---|---|---|
| C27—C26—C31 | 117.0 (3) | Co1—O5—H5C | 138 (3) |
| C27—C26—C25 | 122.4 (3) | Co1—O5—H5D | 100 (2) |
| C31—C26—C25 | 120.6 (3) | H5C—O5—H5D | 107 (3) |

Symmetry code: (i) −*x*, −*y*+1, −*z*.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5*C*···O1$^{ii}$ | 0.73 (4) | 2.13 (4) | 2.822 (3) | 158 (4) |
| O5—H5*D*···O2$^{i}$ | 0.98 (4) | 1.74 (4) | 2.610 (3) | 145 (3) |
| O3—H3···N2$^{iii}$ | 0.82 | 1.85 | 2.667 (3) | 173 |

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