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# Tetraaquabis(2-methyl-1*H*-benzimidazolium-1,3-diacetato-κ*O*)cobalt(II) tetrahydrate

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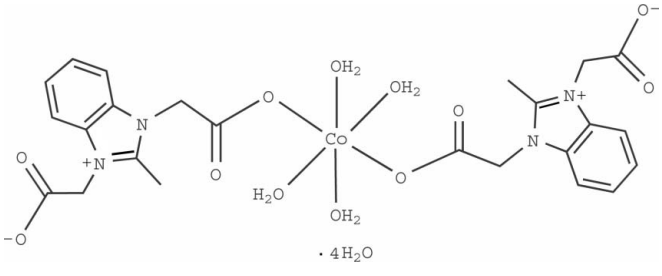
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean σ(C–C) = 0.004 Å; $R$ factor = 0.041; $wR$ factor = 0.103; data-to-parameter ratio = 12.7.

In the title compound, $[Co(C_{12}H_{11}N_2O_4)_2(H_2O)_4]\cdot 4H_2O$, the $Co^{II}$ atom lies on an inversion center and is octahedrally coordinated by six O atoms from four water molecules and two monodentate zwitterionic 2-methylbenzimidazolium-1,3-diacetate ligands. An intramolecular O—H···O hydrogen bond occurs. In the crystal, intermolecular O—H···O hydrogen bonds link the molecules into a three-dimensional network. π–π interactions between the imidazole and benzene rings [centroid–centroid distance = 3.9031 (17) Å] consolidate the crystal packing.

## Related literature

For general background to coordination polymers, see: Kitagawa *et al.* (2004); Robson (2000). For a related structure, see: Lian *et al.* (2009).




## Experimental

### Crystal data

$[Co(C_{12}H_{11}N_2O_4)_2(H_2O)_4]\cdot 4H_2O$ $M_r$ = 697.51
Monoclinic, $P2_1/n$
$a$ = 7.2930 (7) Å
$b$ = 21.240 (2) Å
$c$ = 9.8123 (11) Å
β = 104.907 (1)°
$V$ = 1468.8 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.67 mm$^{-1}$
$T$ = 298 K
0.30 × 0.21 × 0.14 mm

### Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.825, $T_{max}$ = 0.912
7434 measured reflections
2594 independent reflections
1922 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
$S$ = 0.96
2594 reflections
205 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.03 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H5$D$···O4$^{i}$ | 0.85 | 1.89 | 2.742 (3) | 180 |
| O5—H5$E$···O7$^{ii}$ | 0.85 | 1.86 | 2.706 (3) | 179 |
| O6—H6$C$···O4$^{iii}$ | 0.85 | 2.05 | 2.847 (3) | 156 |
| O6—H6$D$···O2 | 0.85 | 1.85 | 2.614 (2) | 149 |
| O7—H7$C$···O1$^{iv}$ | 0.85 | 2.02 | 2.859 (3) | 170 |
| O7—H7$D$···O8$^{v}$ | 0.85 | 1.96 | 2.797 (3) | 170 |
| O8—H8$F$···O4$^{i}$ | 0.85 | 1.96 | 2.793 (3) | 168 |
| O8—H8$G$···O3$^{vi}$ | 0.85 | 2.03 | 2.863 (3) | 169 |

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $-x+2, -y+1, -z+1$; (v) $x, y, z-1$; (vi) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (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: *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: HY2449).

## References

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# supporting information

*Acta Cryst.* (2011). E**67**, m1170 [doi:10.1107/S1600536811029059]

# Tetraaquabis(2-methyl-1*H*-benzimidazolium-1,3-diacetato-*κO*)cobalt(II) tetrahydrate

**Xiu-Ling Feng and Yu-Ping Zhang**

## S1. Comment

Coordination polymers have attracted much interest due to their potential applications in many areas such as catalysis, molecular adsorption, magnetism properties and non-linear optics (Kitagawa *et al.*, 2004; Robson, 2000). We report herein the structure of the title compound based on a flexible ligand 1-acetoxy-2-methylbenzimidazole-3-acetate acid (Lian *et al.*, 2009).

The asymmetric unit of the title compound (Fig. 1) contains half of the complex molecule and two uncoordinated water molecules. The $Co^{II}$ atom lies on an inversion center and is octahedrally coordinated by six O atoms from four water molecules and two 2-methylbenzimidazolium-1,3-diacetate ligands. In the crystal structure, intra- and intermolecular O—H···O hydrogen bonds link the molecules into a three-dimensional network (Fig. 2). *π*–*π* interactions between the imidazole and benzene rings [centroid–centroid distance = 3.9031 (17) Å] consolidate the crystal packing.

## S2. Experimental

A methanol solution (6 ml) of $Co(CH_3COO)_2.4H_2O$ (0.6 mmol) was slowly added to an aqueous solution (8 ml) of 1-acetoxy-2-methylbenzimidazole-3-acetate acid (0.4 mmol) at room temperature. Red block crystals were obtained after two months in 30% yield based on Co.

## S3. Refinement

H atoms of water molecules were located in difference Fourier maps and refined as riding atoms, with a distance restraint of O—H = 0.85 Å and $U_{iso}$(H) = 1.2$U_{eq}$(O). H atoms bonded to C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97 (methylene) and 0.96 (methyl) Å and with $U_{iso}$(H) = 1.2(1.5 for methyl)$U_{eq}$(C). The highest residual electron density was found at 1.43 Å from H8F atom and the deepest hole at 0.80 Å from Co1 atom.

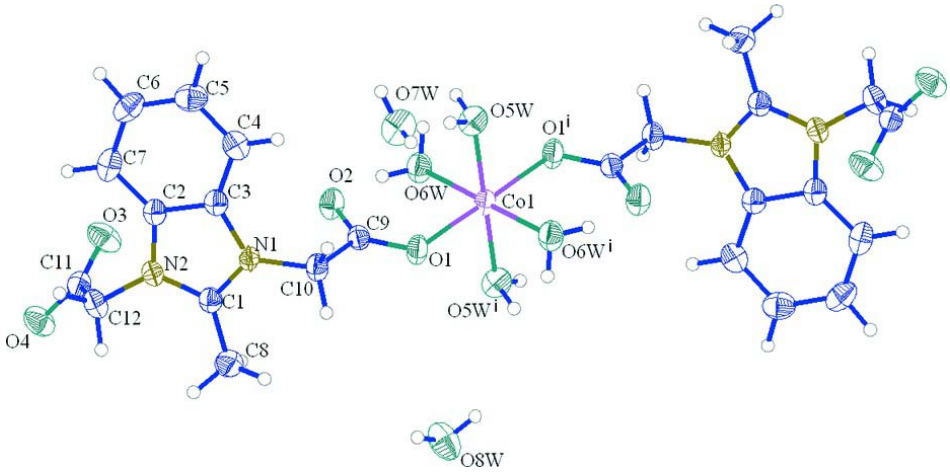


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) 1-x, 1-y, 1-z.]

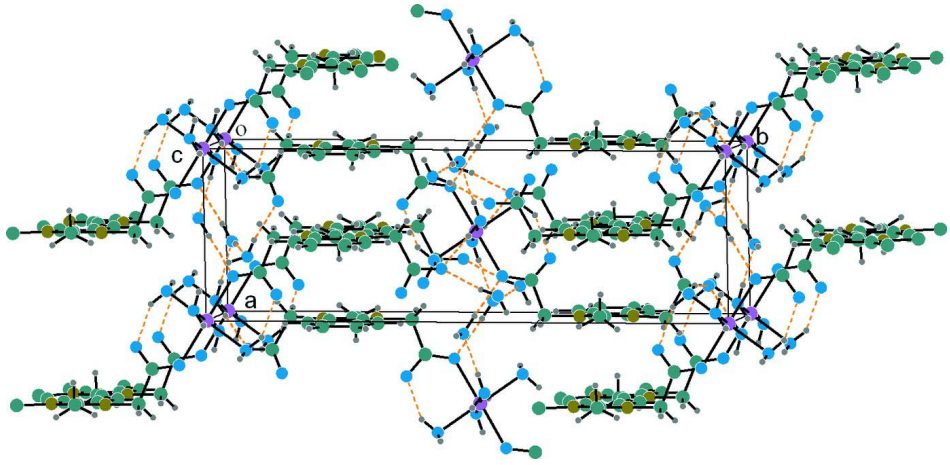


**Figure 2**

The packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

**Tetraaquabis(2-methyl-1*H*-benzimidazolium- 1,3-diacetato-$\kappa O$)cobalt(II) tetrahydrate**

*Crystal data*

$[Co(C_{12}H_{11}N_2O_4)_2(H_2O)_4]\cdot 4H_2O$
$M_r = 697.51$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.2930\ (7)$ Å
$b = 21.240\ (2)$ Å
$c = 9.8123\ (11)$ Å
$\beta = 104.907\ (1)°$
$V = 1468.8\ (3)$ Å$^3$
$Z = 2$
$F(000) = 730$
$D_x = 1.577$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2105 reflections
$\theta = 2.9–24.1°$
$\mu = 0.67$ mm$^{-1}$
$T = 298$ K
Block, red
0.30 × 0.21 × 0.14 mm

*Data collection*

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.825, $T_{max}$ = 0.912
7434 measured reflections
2594 independent reflections
1922 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.4°
$h$ = −8→8
$k$ = −22→25
$l$ = −9→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
$S$ = 0.96
2594 reflections
205 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
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.03 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.5000 | 0.5000 | 0.5000 | 0.02777 (17) |
| N1 | 0.9890 (3) | 0.69581 (10) | 0.5346 (2) | 0.0260 (5) |
| N2 | 0.9847 (3) | 0.79831 (10) | 0.5396 (2) | 0.0271 (5) |
| O1 | 0.7555 (2) | 0.55086 (8) | 0.57519 (19) | 0.0330 (5) |
| O2 | 0.6575 (2) | 0.63795 (9) | 0.4517 (2) | 0.0360 (5) |
| O3 | 0.6708 (3) | 0.87653 (10) | 0.4610 (2) | 0.0436 (5) |
| O4 | 0.8026 (3) | 0.94740 (9) | 0.6224 (2) | 0.0420 (5) |
| O5 | 0.4298 (3) | 0.51633 (9) | 0.6890 (2) | 0.0378 (5) |
| H5D | 0.5133 | 0.4951 | 0.7474 | 0.045* |
| H5E | 0.3210 | 0.5052 | 0.6967 | 0.045* |
| O6 | 0.3338 (2) | 0.57873 (8) | 0.4121 (2) | 0.0362 (5) |
| H6C | 0.2891 | 0.5705 | 0.3251 | 0.043* |
| H6D | 0.4099 | 0.6094 | 0.4164 | 0.043* |
| O7 | 0.9160 (3) | 0.52003 (10) | 0.2867 (2) | 0.0486 (6) |
| H7C | 1.0178 | 0.4993 | 0.3180 | 0.058* |
| H7D | 0.9076 | 0.5300 | 0.2014 | 0.058* |
| O8 | 0.8449 (3) | 0.56024 (10) | 1.0065 (2) | 0.0514 (6) |
| H8F | 0.8127 | 0.5261 | 0.9615 | 0.062* |
| H8G | 0.9424 | 0.5748 | 0.9852 | 0.062* |
| C1 | 0.9848 (4) | 0.74613 (12) | 0.6159 (3) | 0.0261 (6) |
| C2 | 0.9827 (4) | 0.78113 (12) | 0.4026 (3) | 0.0270 (6) |
| C3 | 0.9845 (4) | 0.71627 (12) | 0.3987 (3) | 0.0270 (6) |
| C4 | 0.9742 (4) | 0.68298 (14) | 0.2765 (3) | 0.0334 (7) |
| H4 | 0.9752 | 0.6392 | 0.2748 | 0.040* |
| C5 | 0.9624 (4) | 0.71819 (15) | 0.1572 (3) | 0.0391 (7) |

| | | | | |
|---|---|---|---|---|
| H5A | 0.9547 | 0.6978 | 0.0721 | 0.047* |
| C6 | 0.9615 (4) | 0.78393 (15) | 0.1605 (3) | 0.0411 (8) |
| H6A | 0.9532 | 0.8061 | 0.0773 | 0.049* |
| C7 | 0.9727 (4) | 0.81696 (14) | 0.2830 (3) | 0.0367 (7) |
| H7 | 0.9734 | 0.8607 | 0.2853 | 0.044* |
| C8 | 0.9780 (4) | 0.74391 (14) | 0.7636 (3) | 0.0373 (7) |
| H8A | 1.0481 | 0.7787 | 0.8138 | 0.056* |
| H8B | 1.0329 | 0.7051 | 0.8054 | 0.056* |
| H8C | 0.8484 | 0.7464 | 0.7686 | 0.056* |
| C9 | 0.7804 (4) | 0.60450 (12) | 0.5301 (3) | 0.0259 (6) |
| C10 | 0.9814 (4) | 0.63010 (12) | 0.5744 (3) | 0.0294 (6) |
| H10A | 1.0296 | 0.6261 | 0.6758 | 0.035* |
| H10B | 1.0621 | 0.6054 | 0.5303 | 0.035* |
| C11 | 0.8025 (4) | 0.89776 (13) | 0.5524 (3) | 0.0303 (6) |
| C12 | 0.9927 (4) | 0.86308 (12) | 0.5904 (3) | 0.0319 (6) |
| H12A | 1.0823 | 0.8864 | 0.5519 | 0.038* |
| H12B | 1.0409 | 0.8628 | 0.6922 | 0.038* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0247 (3) | 0.0239 (3) | 0.0339 (3) | −0.0009 (2) | 0.0062 (2) | 0.0047 (2) |
| N1 | 0.0230 (11) | 0.0213 (12) | 0.0321 (13) | −0.0029 (9) | 0.0042 (10) | 0.0030 (9) |
| N2 | 0.0252 (12) | 0.0210 (12) | 0.0336 (13) | −0.0013 (9) | 0.0049 (10) | −0.0016 (9) |
| O1 | 0.0307 (10) | 0.0249 (11) | 0.0408 (11) | −0.0050 (8) | 0.0043 (9) | 0.0085 (8) |
| O2 | 0.0251 (10) | 0.0307 (11) | 0.0479 (12) | −0.0007 (9) | 0.0017 (9) | 0.0102 (9) |
| O3 | 0.0330 (11) | 0.0439 (13) | 0.0475 (13) | 0.0033 (10) | −0.0014 (10) | −0.0140 (10) |
| O4 | 0.0455 (12) | 0.0305 (12) | 0.0453 (13) | 0.0092 (9) | 0.0030 (10) | −0.0110 (9) |
| O5 | 0.0300 (11) | 0.0438 (13) | 0.0394 (12) | 0.0004 (9) | 0.0090 (9) | 0.0057 (9) |
| O6 | 0.0323 (11) | 0.0297 (11) | 0.0431 (12) | −0.0013 (9) | 0.0035 (9) | 0.0052 (8) |
| O7 | 0.0363 (12) | 0.0547 (14) | 0.0568 (14) | 0.0068 (10) | 0.0155 (11) | 0.0069 (11) |
| O8 | 0.0426 (13) | 0.0466 (14) | 0.0690 (16) | −0.0077 (11) | 0.0219 (11) | −0.0166 (11) |
| C1 | 0.0209 (14) | 0.0255 (15) | 0.0300 (15) | −0.0009 (11) | 0.0032 (11) | 0.0014 (11) |
| C2 | 0.0225 (14) | 0.0250 (15) | 0.0339 (15) | 0.0003 (11) | 0.0079 (11) | 0.0017 (11) |
| C3 | 0.0208 (14) | 0.0271 (15) | 0.0327 (15) | −0.0001 (11) | 0.0062 (11) | 0.0013 (11) |
| C4 | 0.0291 (15) | 0.0314 (17) | 0.0403 (17) | 0.0002 (12) | 0.0096 (13) | −0.0041 (13) |
| C5 | 0.0359 (17) | 0.050 (2) | 0.0338 (17) | 0.0012 (14) | 0.0128 (13) | −0.0035 (14) |
| C6 | 0.0379 (18) | 0.051 (2) | 0.0366 (18) | 0.0008 (15) | 0.0137 (14) | 0.0141 (14) |
| C7 | 0.0329 (16) | 0.0305 (17) | 0.0480 (19) | 0.0010 (13) | 0.0126 (14) | 0.0099 (13) |
| C8 | 0.0368 (17) | 0.0397 (18) | 0.0335 (17) | −0.0052 (13) | 0.0058 (13) | 0.0014 (13) |
| C9 | 0.0296 (15) | 0.0227 (15) | 0.0274 (14) | −0.0018 (12) | 0.0108 (12) | −0.0013 (11) |
| C10 | 0.0267 (15) | 0.0223 (15) | 0.0367 (16) | −0.0007 (11) | 0.0039 (12) | 0.0035 (11) |
| C11 | 0.0326 (16) | 0.0272 (16) | 0.0309 (16) | −0.0010 (12) | 0.0078 (13) | 0.0033 (12) |
| C12 | 0.0281 (15) | 0.0239 (15) | 0.0421 (17) | −0.0015 (12) | 0.0059 (12) | −0.0047 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co1—O5 | 2.0758 (19) | O8—H8F | 0.8500 |
| Co1—O5$^{i}$ | 2.0758 (19) | O8—H8G | 0.8501 |
| Co1—O6$^{i}$ | 2.1146 (17) | C1—C8 | 1.464 (4) |
| Co1—O6 | 2.1146 (17) | C2—C3 | 1.378 (4) |
| Co1—O1 | 2.1157 (17) | C2—C7 | 1.384 (4) |
| Co1—O1$^{i}$ | 2.1157 (17) | C3—C4 | 1.377 (4) |
| N1—C1 | 1.339 (3) | C4—C5 | 1.373 (4) |
| N1—C3 | 1.395 (3) | C4—H4 | 0.9300 |
| N1—C10 | 1.454 (3) | C5—C6 | 1.397 (4) |
| N2—C1 | 1.338 (3) | C5—H5A | 0.9300 |
| N2—C2 | 1.390 (3) | C6—C7 | 1.376 (4) |
| N2—C12 | 1.459 (3) | C6—H6A | 0.9300 |
| O1—C9 | 1.252 (3) | C7—H7 | 0.9300 |
| O2—C9 | 1.243 (3) | C8—H8A | 0.9600 |
| O3—C11 | 1.219 (3) | C8—H8B | 0.9600 |
| O4—C11 | 1.258 (3) | C8—H8C | 0.9600 |
| O5—H5D | 0.8500 | C9—C10 | 1.518 (3) |
| O5—H5E | 0.8500 | C10—H10A | 0.9700 |
| O6—H6C | 0.8500 | C10—H10B | 0.9700 |
| O6—H6D | 0.8500 | C11—C12 | 1.530 (4) |
| O7—H7C | 0.8500 | C12—H12A | 0.9700 |
| O7—H7D | 0.8501 | C12—H12B | 0.9700 |
| | | | |
| O5—Co1—O5$^{i}$ | 180.0 | C2—C3—N1 | 106.4 (2) |
| O5—Co1—O6$^{i}$ | 90.84 (7) | C5—C4—C3 | 116.1 (3) |
| O5$^{i}$—Co1—O6$^{i}$ | 89.16 (8) | C5—C4—H4 | 122.0 |
| O5—Co1—O6 | 89.16 (8) | C3—C4—H4 | 122.0 |
| O5$^{i}$—Co1—O6 | 90.84 (7) | C4—C5—C6 | 121.6 (3) |
| O6$^{i}$—Co1—O6 | 180.0 | C4—C5—H5A | 119.2 |
| O5—Co1—O1 | 90.03 (8) | C6—C5—H5A | 119.2 |
| O5$^{i}$—Co1—O1 | 89.97 (8) | C7—C6—C5 | 122.0 (3) |
| O6$^{i}$—Co1—O1 | 84.29 (7) | C7—C6—H6A | 119.0 |
| O6—Co1—O1 | 95.71 (7) | C5—C6—H6A | 119.0 |
| O5—Co1—O1$^{i}$ | 89.97 (8) | C6—C7—C2 | 116.0 (3) |
| O5$^{i}$—Co1—O1$^{i}$ | 90.03 (8) | C6—C7—H7 | 122.0 |
| O6$^{i}$—Co1—O1$^{i}$ | 95.71 (7) | C2—C7—H7 | 122.0 |
| O6—Co1—O1$^{i}$ | 84.29 (7) | C1—C8—H8A | 109.5 |
| O1—Co1—O1$^{i}$ | 180.00 (8) | C1—C8—H8B | 109.5 |
| C1—N1—C3 | 108.8 (2) | H8A—C8—H8B | 109.5 |
| C1—N1—C10 | 126.7 (2) | C1—C8—H8C | 109.5 |
| C3—N1—C10 | 124.2 (2) | H8A—C8—H8C | 109.5 |
| C1—N2—C2 | 108.8 (2) | H8B—C8—H8C | 109.5 |
| C1—N2—C12 | 126.5 (2) | O2—C9—O1 | 126.3 (2) |
| C2—N2—C12 | 124.6 (2) | O2—C9—C10 | 117.5 (2) |
| C9—O1—Co1 | 122.42 (16) | O1—C9—C10 | 116.2 (2) |
| Co1—O5—H5D | 102.5 | N1—C10—C9 | 111.6 (2) |

| | | | |
|---|---|---|---|
| Co1—O5—H5E | 118.9 | N1—C10—H10A | 109.3 |
| H5D—O5—H5E | 108.4 | C9—C10—H10A | 109.3 |
| Co1—O6—H6C | 106.2 | N1—C10—H10B | 109.3 |
| Co1—O6—H6D | 106.7 | C9—C10—H10B | 109.3 |
| H6C—O6—H6D | 106.5 | H10A—C10—H10B | 108.0 |
| H7C—O7—H7D | 108.6 | O3—C11—O4 | 127.0 (3) |
| H8F—O8—H8G | 108.7 | O3—C11—C12 | 119.6 (2) |
| N2—C1—N1 | 108.9 (2) | O4—C11—C12 | 113.4 (2) |
| N2—C1—C8 | 125.9 (2) | N2—C12—C11 | 114.6 (2) |
| N1—C1—C8 | 125.2 (2) | N2—C12—H12A | 108.6 |
| C3—C2—C7 | 121.7 (3) | C11—C12—H12A | 108.6 |
| C3—C2—N2 | 106.9 (2) | N2—C12—H12B | 108.6 |
| C7—C2—N2 | 131.4 (3) | C11—C12—H12B | 108.6 |
| C4—C3—C2 | 122.6 (2) | H12A—C12—H12B | 107.6 |
| C4—C3—N1 | 130.9 (3) | | |

| | | | |
|---|---|---|---|
| O5—Co1—O1—C9 | −107.6 (2) | C10—N1—C3—C4 | −0.6 (4) |
| O5$^{i}$—Co1—O1—C9 | 72.4 (2) | C1—N1—C3—C2 | 1.6 (3) |
| O6$^{i}$—Co1—O1—C9 | 161.6 (2) | C10—N1—C3—C2 | 176.4 (2) |
| O6—Co1—O1—C9 | −18.4 (2) | C2—C3—C4—C5 | 0.1 (4) |
| C2—N2—C1—N1 | 1.9 (3) | N1—C3—C4—C5 | 176.7 (3) |
| C12—N2—C1—N1 | −175.9 (2) | C3—C4—C5—C6 | 0.2 (4) |
| C2—N2—C1—C8 | −177.1 (3) | C4—C5—C6—C7 | 0.1 (4) |
| C12—N2—C1—C8 | 5.1 (4) | C5—C6—C7—C2 | −0.7 (4) |
| C3—N1—C1—N2 | −2.2 (3) | C3—C2—C7—C6 | 1.0 (4) |
| C10—N1—C1—N2 | −176.8 (2) | N2—C2—C7—C6 | −176.0 (3) |
| C3—N1—C1—C8 | 176.8 (2) | Co1—O1—C9—O2 | 9.4 (4) |
| C10—N1—C1—C8 | 2.2 (4) | Co1—O1—C9—C10 | −169.50 (17) |
| C1—N2—C2—C3 | −0.9 (3) | C1—N1—C10—C9 | 95.3 (3) |
| C12—N2—C2—C3 | 177.0 (2) | C3—N1—C10—C9 | −78.6 (3) |
| C1—N2—C2—C7 | 176.4 (3) | O2—C9—C10—N1 | 9.7 (3) |
| C12—N2—C2—C7 | −5.7 (4) | O1—C9—C10—N1 | −171.3 (2) |
| C7—C2—C3—C4 | −0.8 (4) | C1—N2—C12—C11 | −102.4 (3) |
| N2—C2—C3—C4 | 176.8 (2) | C2—N2—C12—C11 | 80.1 (3) |
| C7—C2—C3—N1 | −178.1 (2) | O3—C11—C12—N2 | −15.7 (4) |
| N2—C2—C3—N1 | −0.5 (3) | O4—C11—C12—N2 | 164.9 (2) |
| C1—N1—C3—C4 | −175.4 (3) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5*D*···O4$^{ii}$ | 0.85 | 1.89 | 2.742 (3) | 180 |
| O5—H5*E*···O7$^{i}$ | 0.85 | 1.86 | 2.706 (3) | 179 |
| O6—H6*C*···O4$^{iii}$ | 0.85 | 2.05 | 2.847 (3) | 156 |
| O6—H6*D*···O2 | 0.85 | 1.85 | 2.614 (2) | 149 |
| O7—H7*C*···O1$^{iv}$ | 0.85 | 2.02 | 2.859 (3) | 170 |

| | | | | |
|---|---|---|---|---|
| O7—H7*D*···O8$^{v}$ | 0.85 | 1.96 | 2.797 (3) | 170 |
| O8—H8*F*···O4$^{ii}$ | 0.85 | 1.96 | 2.793 (3) | 168 |
| O8—H8*G*···O3$^{vi}$ | 0.85 | 2.03 | 2.863 (3) | 169 |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iii) *x*−1/2, −*y*+3/2, *z*−1/2; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*, *y*, *z*−1; (vi) *x*+1/2, −*y*+3/2, *z*+1/2.