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# *catena*-Poly[[diaquacobalt(II)]-$\mu_2$-7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylato-$\kappa^4O^2,O^3,O^7:O^{2'}$]

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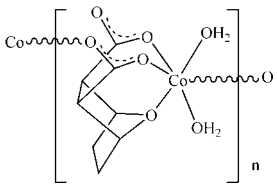
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.029; $wR$ factor = 0.088; data-to-parameter ratio = 12.6.

The polymeric title complex, $[\mathrm{Co(C_8H_8O_5)(H_2O)_2}]_n$ was synthesized by reaction of cobalt acetate with 7-oxabicyclo[2,2,1]heptane-2,3-dicarboxylic anhydride. The $\mathrm{Co^{II}}$ ion is six-coordinated in a distorted octahedral environment, binding to two water O atoms, to the ether O atom of the bicycloheptane unit, to two carboxylate O atoms from two different carboxylate groups of the same anion and to one carboxylate O atom from a symmetry-related anion. The bridging character of the dianion leads to the formation of ribbons along [001]. The ribbons are linked into a layered network parallel to (010) by several O—H⋯O hydrogen-bonding interactions involving the coordinating water molecules as donors and the carboxylate O atoms of neighbouring ribbons as acceptors. The crystal under investigation was an inversion twin.

## Related literature

For background to the applications of norcantharidin [systematic name: 7-oxabicyclo(2.2.1)heptane-2,3-dicarboxylic anhydride], see: Yang *et al.* (2002). For the isotypic Cu analogue, see: Wang *et al.* (2009*a*), and for a related Ni complex with monoclinic symmetry, see: Wang *et al.* (2009*b*).



## Experimental

### *Crystal data*

$[\mathrm{Co(C_8H_8O_5)(H_2O)_2}]$
$M_r$ = 279.11
Orthorhombic, $Iba2$
$a$ = 10.3794 (10) Å
$b$ = 18.983 (3) Å
$c$ = 10.5021 (12) Å
$V$ = 2069.3 (5) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.68 mm$^{-1}$
$T$ = 296 K
0.22 × 0.15 × 0.10 mm

### *Data collection*

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
$T_{\min}$ = 0.742, $T_{\max}$ = 0.851
13174 measured reflections
1837 independent reflections
1821 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}}$ = 0.025

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.088
$S$ = 1.00
1837 reflections
146 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.77 e Å$^{-3}$
Absolute structure: Flack (1983), 860 Friedel pairs
Flack parameter: 0.12 (3)

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| O1$W$—H1$WA$⋯O1$^{\mathrm{i}}$ | 0.85 | 1.98 | 2.832 (3) | 180 |
| O2$W$—H2$WB$⋯O4$^{\mathrm{i}}$ | 0.85 | 1.96 | 2.811 (3) | 180 |
| O1$W$—H1$WB$⋯O4$^{\mathrm{ii}}$ | 0.85 | 1.95 | 2.800 (3) | 180 |
| O2$W$—H2$WA$⋯O3$^{\mathrm{iii}}$ | 0.85 | 1.86 | 2.708 (3) | 180 |

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); 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, 2006); 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: WM2580).

## References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2006). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, Y.-Y., Hu, R.-D. & Wang, Y.-J. (2009*a*). *Acta Cryst.* E**65**, m169.
Wang, Y.-Y., Hu, R.-D., Zhu, W.-Z. & Lin, Q.-Y. (2009*b*). *Acta Cryst.* E**65**, m787.
Yang, L.-Q., Crans, D. C., Miller, S. M., Cour, A., Anderson, O. P., Kaszynski, P. M., Godzala, M. E., Austin, L. D. & Willsky, G. R. (2002). *Inorg. Chem.* **41**, 4859–4871.

# supplementary materials

*Acta Cryst.* (2012). E**68**, m146    [ **doi:10.1107/S1600536812000554** ]

# *catena*-Poly[[diaquacobalt(II)]-$\mu_2$-7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylato-$\kappa^4 O^2,O^3,O^7:O^{2'}$]

**F. Zhang, Q.-Y. Lin, Y.-C. Wang and J.-D. He**

### Comment

7-oxabicyclo[2,2,1]heptane-2,3-dicarboxylic anhydride (norcantharidin), a traditional Chinese drug, has great anti-cancer activity. The coordination chemistry of cobalt has been important in biology mainly because of coenzyme $B_{12}$ (Yang *et al.*, 2002). Therefore studying the combination of norcantharidin and cobalt seemed interesting. In this communication, the polymeric title complex, $[Co(C_8H_8O_5)(H_2O)_2]_n$ is reported.

The isostructural cooper complex (Wang *et al.*, 2009*a*) and a similar nickel complex with monoclinic symmetry (Wang *et al.*, 2009*b*) of demethylcantharate have been reported previously. The coordination of the $Co^{2+}$ ion in the title complex is shown in Fig. 1. The $Co^{2+}$ ion is six-coordinated in a distorted octahedral coordination mode, binding to two water O atoms, to the bridging O atom of the bicycloheptane unit, to two carboxylate O atoms from different carboxylate groups and to one carboxylate O atom from a symmetry-related bridging anion. This leads to the formation of ribbons extending along [001] (Fig. 2).

As also shown in Fig. 2, the ribbons are linked into a two-dimensional network parallel to (010) by several O—H···O hydrogen-bonding interactions involving the coordinating water molecules as donors and the carboxylate O atoms of neighbouring ribbons as acceptors.

### Experimental

A mixture of 0.5 mmol norcantharidin, 0.5 mmol cobalt acetate and 15 mL distilled water was sealed in a 25 mL Teflon-lined stainless vessel and heated at 443 K for 3 d, then cooled slowly to room temperature. The solution was filtered and block red crystals were obtained.

### Refinement

H atoms bonded to C atoms were positioned geometrically and refined using a riding model [aliphatic tertiary carbon C—H = 0.98 Å, aliphatic secondary carbon C—H = 0.97 Å, both with $U_{iso}(H) = 1.2U_{eq}(C)$]. The H atoms bonded to the O atoms were located in a difference Fourier map and refined with O—H distance restraints of 0.85 (1) Å and $U_{iso}(H) = 1.5U_{eq}(O)$. The crystal under investigation was an inversion twin with a ratio of 0.88 (3):0.12 (3).

## Figures

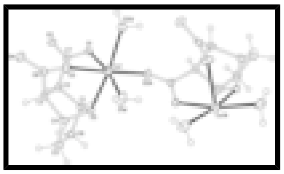

Fig. 1. The coordination of the $Co^{2+}$ ion with atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level. [[Symmetry code (A) x, -y+2, z-1/2].

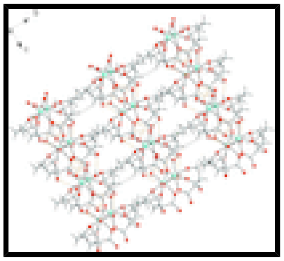

Fig. 2. The one-dimensional polymeric structure of the title complex along [001] with hydrogen bonding interactions (dotted lines).

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### *Crystal data*

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Orthorhombic, *Iba*2

Hall symbol: I 2 -2c

$a = 10.3794\ (10)$ Å

$b = 18.983\ (3)$ Å

$c = 10.5021\ (12)$ Å

$V = 2069.3\ (5)$ Å$^3$

$Z = 8$

$F(000) = 1144$

$D_x = 1.792$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9954 reflections

$\theta = 2.2$–$25.0°$

$\mu = 1.68$ mm$^{-1}$

$T = 296$ K

Block, red

0.22 × 0.15 × 0.10 mm

### *Data collection*

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

graphite

ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2006)

$T_{min} = 0.742$, $T_{max} = 0.851$

13174 measured reflections

1837 independent reflections

1821 reflections with $I > 2\sigma(I)$

$R_{int} = 0.025$

$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$

$h = -12 \rightarrow 9$

$k = -22 \rightarrow 22$

$l = -12 \rightarrow 12$

### *Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

| | |
|---|---|
| $wR(F^2) = 0.088$ | $w = 1/[\sigma^2(F_o^2) + (0.0734P)^2 + 1.6545P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.00$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 1837 reflections | $\Delta\rho_{max} = 0.32$ e Å$^{-3}$ |
| 146 parameters | $\Delta\rho_{min} = -0.77$ e Å$^{-3}$ |
| 7 restraints | Absolute structure: Flack (1983), 860 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.12 (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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.23966 (4) | 0.966647 (19) | 0.74932 (8) | 0.02813 (16) |
| O1W | 0.1588 (3) | 0.91672 (15) | 0.5806 (2) | 0.0429 (6) |
| H1WA | 0.2080 | 0.9431 | 0.5369 | 0.064* |
| H1WB | 0.0843 | 0.8987 | 0.5727 | 0.064* |
| O1 | 0.3221 (2) | 0.99510 (11) | 0.9348 (2) | 0.0248 (4) |
| O2W | 0.1226 (2) | 1.06142 (12) | 0.7759 (2) | 0.0374 (6) |
| H2WA | 0.0483 | 1.0731 | 0.8026 | 0.056* |
| H2WB | 0.1121 | 1.0858 | 0.7089 | 0.056* |
| O2 | 0.3530 (2) | 0.96635 (11) | 1.1378 (2) | 0.0257 (5) |
| O3 | 0.1138 (2) | 0.90091 (11) | 0.8609 (2) | 0.0303 (5) |
| O4 | 0.0868 (2) | 0.85747 (12) | 1.0548 (2) | 0.0309 (5) |
| O5 | 0.37724 (17) | 0.87420 (9) | 0.76172 (19) | 0.0215 (4) |
| C1 | 0.4783 (3) | 0.87921 (15) | 0.8584 (3) | 0.0242 (6) |
| H1 | 0.5346 | 0.9202 | 0.8480 | 0.029* |
| C2 | 0.4010 (3) | 0.87971 (14) | 0.9824 (3) | 0.0201 (6) |
| H2 | 0.4522 | 0.8587 | 1.0510 | 0.024* |
| C3 | 0.2838 (3) | 0.82969 (15) | 0.9480 (3) | 0.0217 (6) |
| H3 | 0.2852 | 0.7878 | 1.0023 | 0.026* |
| C4 | 0.3196 (3) | 0.80965 (14) | 0.8104 (3) | 0.0258 (6) |
| H4 | 0.2465 | 0.7927 | 0.7597 | 0.031* |
| C5 | 0.4367 (4) | 0.75899 (17) | 0.8103 (4) | 0.0389 (8) |
| H5A | 0.4272 | 0.7223 | 0.8738 | 0.047* |
| H5B | 0.4492 | 0.7376 | 0.7273 | 0.047* |
| C6 | 0.5475 (3) | 0.80918 (18) | 0.8437 (3) | 0.0351 (7) |

| | | | | |
|---|---|---|---|---|
| H6A | 0.5895 | 0.7953 | 0.9224 | 0.042* |
| H6B | 0.6110 | 0.8110 | 0.7760 | 0.042* |
| C7 | 0.3557 (2) | 0.95301 (15) | 1.0216 (3) | 0.0179 (6) |
| C8 | 0.1514 (3) | 0.86588 (14) | 0.9561 (3) | 0.0211 (6) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0293 (2) | 0.0306 (3) | 0.0245 (2) | −0.00025 (14) | 0.0007 (2) | 0.0048 (2) |
| O1W | 0.0397 (14) | 0.0645 (17) | 0.0247 (11) | −0.0249 (12) | −0.0039 (11) | 0.0043 (12) |
| O1 | 0.0329 (11) | 0.0223 (10) | 0.0191 (9) | 0.0030 (8) | 0.0000 (9) | 0.0004 (8) |
| O2W | 0.0309 (12) | 0.0419 (12) | 0.0394 (14) | 0.0150 (10) | 0.0098 (10) | 0.0125 (10) |
| O2 | 0.0236 (12) | 0.0331 (10) | 0.0203 (10) | 0.0057 (8) | −0.0002 (9) | −0.0052 (7) |
| O3 | 0.0186 (10) | 0.0394 (12) | 0.0329 (12) | 0.0013 (9) | 0.0023 (9) | 0.0144 (10) |
| O4 | 0.0272 (11) | 0.0399 (12) | 0.0257 (11) | 0.0020 (9) | 0.0057 (9) | 0.0035 (9) |
| O5 | 0.0231 (9) | 0.0226 (9) | 0.0187 (10) | 0.0008 (7) | 0.0006 (8) | −0.0003 (8) |
| C1 | 0.0195 (13) | 0.0282 (14) | 0.0249 (15) | 0.0029 (11) | 0.0012 (12) | −0.0046 (11) |
| C2 | 0.0196 (13) | 0.0224 (14) | 0.0183 (13) | 0.0023 (11) | −0.0012 (11) | −0.0008 (11) |
| C3 | 0.0240 (13) | 0.0184 (13) | 0.0227 (14) | −0.0009 (12) | −0.0005 (12) | 0.0036 (11) |
| C4 | 0.0310 (16) | 0.0205 (13) | 0.0259 (14) | −0.0007 (11) | −0.0011 (13) | −0.0034 (11) |
| C5 | 0.051 (2) | 0.0250 (15) | 0.0408 (18) | 0.0140 (14) | 0.0077 (17) | −0.0045 (13) |
| C6 | 0.0303 (16) | 0.0438 (17) | 0.0312 (17) | 0.0170 (14) | 0.0038 (15) | −0.0048 (14) |
| C7 | 0.0125 (12) | 0.0237 (13) | 0.0174 (14) | −0.0020 (10) | −0.0001 (11) | −0.0046 (11) |
| C8 | 0.0200 (14) | 0.0196 (13) | 0.0238 (14) | −0.0038 (10) | −0.0011 (12) | −0.0001 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Co1—O2$^{\text{i}}$ | 2.091 (2) | C1—C6 | 1.519 (4) |
| Co1—O3 | 2.154 (2) | C1—C2 | 1.529 (4) |
| Co1—O1W | 2.178 (3) | C1—H1 | 0.9800 |
| Co1—O2W | 2.188 (2) | C2—C7 | 1.525 (4) |
| Co1—O1 | 2.194 (2) | C2—C3 | 1.585 (4) |
| Co1—O5 | 2.2664 (18) | C2—H2 | 0.9800 |
| O1W—H1WA | 0.8500 | C3—C8 | 1.539 (4) |
| O1W—H1WB | 0.8500 | C3—C4 | 1.540 (4) |
| O1—C7 | 1.262 (4) | C3—H3 | 0.9800 |
| O2W—H2WA | 0.8501 | C4—C5 | 1.550 (4) |
| O2W—H2WB | 0.8499 | C4—H4 | 0.9800 |
| O2—C7 | 1.246 (4) | C5—C6 | 1.534 (5) |
| O2—Co1$^{\text{ii}}$ | 2.091 (2) | C5—H5A | 0.9700 |
| O3—C8 | 1.262 (4) | C5—H5B | 0.9700 |
| O4—C8 | 1.244 (4) | C6—H6A | 0.9700 |
| O5—C4 | 1.456 (3) | C6—H6B | 0.9700 |
| O5—C1 | 1.462 (4) | | |
| O2$^{\text{i}}$—Co1—O3 | 176.84 (9) | C1—C2—C3 | 101.8 (2) |
| O2$^{\text{i}}$—Co1—O1W | 91.46 (10) | C7—C2—H2 | 109.9 |
| O3—Co1—O1W | 87.54 (10) | C1—C2—H2 | 109.9 |
| O2$^{\text{i}}$—Co1—O2W | 83.31 (9) | C3—C2—H2 | 109.9 |

| | | | |
|---|---|---|---|
| O3—Co1—O2W | 94.03 (8) | C8—C3—C4 | 112.2 (2) |
| O1W—Co1—O2W | 104.34 (11) | C8—C3—C2 | 113.9 (2) |
| O2$^{i}$—Co1—O1 | 97.37 (9) | C4—C3—C2 | 100.2 (2) |
| O3—Co1—O1 | 84.03 (9) | C8—C3—H3 | 110.0 |
| O1W—Co1—O1 | 168.35 (9) | C4—C3—H3 | 110.0 |
| O2W—Co1—O1 | 84.31 (9) | C2—C3—H3 | 110.0 |
| O2$^{i}$—Co1—O5 | 98.56 (8) | O5—C4—C3 | 102.7 (2) |
| O3—Co1—O5 | 84.39 (7) | O5—C4—C5 | 101.5 (2) |
| O1W—Co1—O5 | 87.28 (10) | C3—C4—C5 | 110.1 (2) |
| O2W—Co1—O5 | 168.22 (10) | O5—C4—H4 | 113.8 |
| O1—Co1—O5 | 83.92 (8) | C3—C4—H4 | 113.8 |
| Co1—O1W—H1WA | 87.2 | C5—C4—H4 | 113.8 |
| Co1—O1W—H1WB | 127.2 | C6—C5—C4 | 101.7 (2) |
| H1WA—O1W—H1WB | 137.0 | C6—C5—H5A | 111.4 |
| C7—O1—Co1 | 126.40 (17) | C4—C5—H5A | 111.4 |
| Co1—O2W—H2WA | 139.4 | C6—C5—H5B | 111.4 |
| Co1—O2W—H2WB | 114.5 | C4—C5—H5B | 111.4 |
| H2WA—O2W—H2WB | 90.8 | H5A—C5—H5B | 109.3 |
| C7—O2—Co1$^{ii}$ | 133.2 (2) | C1—C6—C5 | 102.2 (3) |
| C8—O3—Co1 | 123.30 (19) | C1—C6—H6A | 111.3 |
| C4—O5—C1 | 96.1 (2) | C5—C6—H6A | 111.3 |
| C4—O5—Co1 | 114.38 (16) | C1—C6—H6B | 111.3 |
| C1—O5—Co1 | 116.19 (14) | C5—C6—H6B | 111.3 |
| O5—C1—C6 | 102.2 (2) | H6A—C6—H6B | 109.2 |
| O5—C1—C2 | 102.4 (2) | O2—C7—O1 | 124.9 (3) |
| C6—C1—C2 | 109.8 (2) | O2—C7—C2 | 117.2 (2) |
| O5—C1—H1 | 113.7 | O1—C7—C2 | 117.9 (2) |
| C6—C1—H1 | 113.7 | O4—C8—O3 | 124.1 (3) |
| C2—C1—H1 | 113.7 | O4—C8—C3 | 118.0 (3) |
| C7—C2—C1 | 113.4 (2) | O3—C8—C3 | 117.8 (3) |
| C7—C2—C3 | 111.8 (2) | | |

| | | | |
|---|---|---|---|
| O2$^{i}$—Co1—O1—C7 | −134.4 (2) | C7—C2—C3—C4 | 122.2 (2) |
| O3—Co1—O1—C7 | 48.5 (2) | C1—C2—C3—C4 | 0.9 (3) |
| O1W—Co1—O1—C7 | 4.6 (6) | C1—O5—C4—C3 | 57.7 (2) |
| O2W—Co1—O1—C7 | 143.1 (2) | Co1—O5—C4—C3 | −64.7 (2) |
| O5—Co1—O1—C7 | −36.5 (2) | C1—O5—C4—C5 | −56.1 (2) |
| O1W—Co1—O3—C8 | 131.9 (2) | Co1—O5—C4—C5 | −178.54 (17) |
| O2W—Co1—O3—C8 | −123.9 (2) | C8—C3—C4—O5 | 85.4 (3) |
| O1—Co1—O3—C8 | −40.0 (2) | C2—C3—C4—O5 | −35.8 (3) |
| O5—Co1—O3—C8 | 44.4 (2) | C8—C3—C4—C5 | −167.1 (2) |
| O2$^{i}$—Co1—O5—C4 | −167.10 (18) | C2—C3—C4—C5 | 71.7 (3) |
| O3—Co1—O5—C4 | 11.75 (19) | O5—C4—C5—C6 | 34.5 (3) |
| O1W—Co1—O5—C4 | −76.03 (19) | C3—C4—C5—C6 | −73.8 (3) |
| O2W—Co1—O5—C4 | 94.6 (4) | O5—C1—C6—C5 | −35.0 (3) |
| O1—Co1—O5—C4 | 96.32 (19) | C2—C1—C6—C5 | 73.2 (3) |
| O2$^{i}$—Co1—O5—C1 | 82.24 (18) | C4—C5—C6—C1 | 0.3 (3) |
| O3—Co1—O5—C1 | −98.90 (18) | Co1$^{ii}$—O2—C7—O1 | 27.9 (4) |

| | | | |
|---|---|---|---|
| O1W—Co1—O5—C1 | 173.31 (19) | Co1$^{\rm ii}$—O2—C7—C2 | −151.0 (2) |
| O2W—Co1—O5—C1 | −16.1 (5) | Co1—O1—C7—O2 | −149.7 (2) |
| O1—Co1—O5—C1 | −14.33 (18) | Co1—O1—C7—C2 | 29.1 (3) |
| C4—O5—C1—C6 | 57.0 (3) | C1—C2—C7—O2 | −144.6 (3) |
| Co1—O5—C1—C6 | 178.01 (18) | C3—C2—C7—O2 | 101.0 (3) |
| C4—O5—C1—C2 | −56.8 (2) | C1—C2—C7—O1 | 36.5 (3) |
| Co1—O5—C1—C2 | 64.2 (2) | C3—C2—C7—O1 | −77.9 (3) |
| O5—C1—C2—C7 | −86.2 (3) | Co1—O3—C8—O4 | 142.1 (2) |
| C6—C1—C2—C7 | 165.7 (2) | Co1—O3—C8—C3 | −39.6 (3) |
| O5—C1—C2—C3 | 34.1 (3) | C4—C3—C8—O4 | 149.2 (3) |
| C6—C1—C2—C3 | −74.0 (3) | C2—C3—C8—O4 | −97.8 (3) |
| C7—C2—C3—C8 | 2.2 (3) | C4—C3—C8—O3 | −29.2 (3) |
| C1—C2—C3—C8 | −119.1 (2) | C2—C3—C8—O3 | 83.8 (3) |

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

### *Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1W—H1WA···O1$^{\rm i}$ | 0.85 | 1.98 | 2.832 (3) | 180. |
| O2W—H2WB···O4$^{\rm i}$ | 0.85 | 1.96 | 2.811 (3) | 180. |
| O1W—H1WB···O4$^{\rm iii}$ | 0.85 | 1.95 | 2.800 (3) | 180. |
| O2W—H2WA···O3$^{\rm iv}$ | 0.85 | 1.86 | 2.708 (3) | 180. |

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

**Fig. 1**

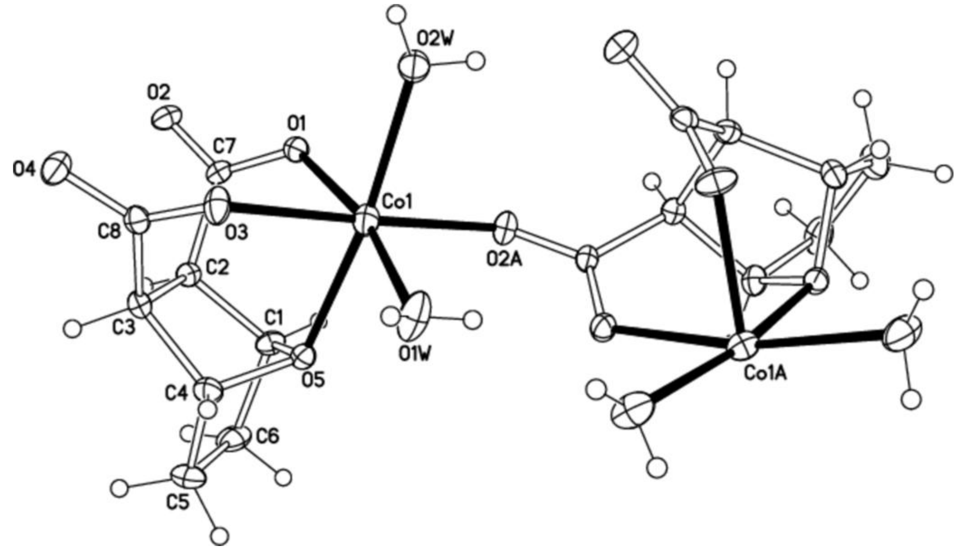

Fig. 2