Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaquabis[2-(3-benzoylphenyl)-propanoato-κ*O*]cobalt(II) monohydrate

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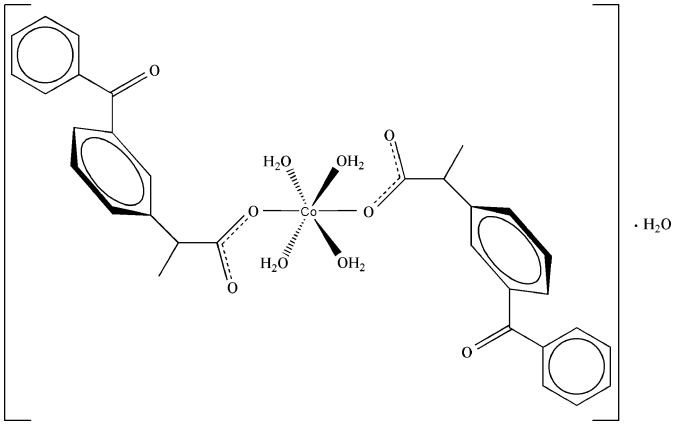
Received 27 April 2007; accepted 5 June 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.049; wR factor = 0.177; data-to-parameter ratio = 16.3.

The title compound, $[Co(C_{16}H_{13}O_3)_2(H_2O)_4]\cdot H_2O$, is a transition metal complex of ketoprofen [2-(3-benzoylphenyl)-propanoic acid], a well known nonsteroidal anti-inflammatory drug. The asymmetric unit consists of two half-complexes and one water molecule of crystallization. The Co^{II} atoms are located on inversion centers and show an octahedral coordination geometry, defined by two carboxylate O atoms from two ketoprofenate ligands and four water molecules. The molecules are connected *via* O—H···O hydrogen bonds into a three-dimensional network.

Related literature

For the only crystal structure of a ketoprofen complex, (ketoprofenato)trimethyltin(IV), see: Tahir *et al.* (1997).



Experimental

Crystal data

$[Co(C_{16}H_{13}O_3)_2(H_2O)_4]\cdot H_2O$
M_r = 655.54
Triclinic, $P\overline{1}$
a = 8.5966 (17) Å
b = 8.8939 (18) Å
c = 21.872 (4) Å
α = 92.08 (3)°
β = 99.69 (3)°
γ = 108.92 (3)°
V = 1551.9 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 295 (2) K
0.36 × 0.28 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.810, T_{max} = 0.892
15351 measured reflections
7032 independent reflections
4192 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.177
S = 1.05
7032 reflections
432 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2*W*	2.084 (3)	Co2—O4*W*	2.051 (3)
Co1—O3*W*	2.095 (2)	Co2—O4	2.064 (2)
Co1—O2	2.134 (2)	Co2—O5*W*	2.183 (2)
O2*W*—Co1—O3*W*	91.81 (11)	O4*W*—Co2—O4^{ii}	88.35 (12)
O2*W*—Co1—O3*W*^{i}	88.19 (11)	O4*W*—Co2—O5*W*^{ii}	89.34 (10)
O2*W*—Co1—O2^{i}	88.33 (10)	O4—Co2—O5*W*^{ii}	90.54 (10)
O3*W*—Co1—O2^{i}	86.82 (10)	O4*W*—Co2—O5*W*	90.66 (10)
O2*W*—Co1—O2	91.67 (10)	O4—Co2—O5*W*	89.46 (10)
O3*W*—Co1—O2	93.18 (10)	O4*W*—Co2—O4	91.65 (12)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*W*—H3*W*1···O1	0.85 (3)	1.82 (3)	2.646 (4)	164 (4)
O1*W*—H1*W*1···O1^{iii}	0.85 (4)	1.83 (4)	2.665 (4)	170 (4)
O2*W*—H2*W*1···O3	0.850 (10)	1.990 (15)	2.822 (4)	166 (4)
O2*W*—H2*W*2···O5*W*^{iv}	0.85 (3)	1.93 (3)	2.781 (4)	179 (4)
O3*W*—H3*W*2···O4^{iv}	0.85 (3)	2.107 (16)	2.920 (4)	161 (3)
O4*W*—H4*W*1···O2^{v}	0.85 (3)	1.826 (12)	2.660 (4)	169 (4)
O5*W*—H5*W*1···O3^{ii}	0.85 (3)	1.81 (3)	2.653 (4)	170 (4)
O1*W*—H1*W*2···O5^{v}	0.848 (10)	1.97 (2)	2.757 (4)	154 (4)
O4*W*—H4*W*2···O1*W*	0.85 (4)	1.867 (16)	2.675 (4)	159 (4)
O5*W*—H5*W*2···O1*W*	0.85 (3)	1.96 (3)	2.795 (4)	171 (4)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

We thank the Heilongjiang Province Natural Science Foundation (No. B200501), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (No. 1054 G036), Heilongjiang University and Harbin Medical University for supporting this work.

  doi:10.1107/S1600536807027572

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2071).

References

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.

Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.

Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

Tahir, M. N., Ülkü, D., Ali, S., Masood, T., Danish, M. & Mazhar, M. (1997). *Acta Cryst.* C**53**, 1574–1576.

supplementary materials

Acta Cryst. (2007). E**63**, m1900-m1901 [**doi:10.1107/S1600536807027572**]

Tetraaquabis[2-(3-benzoylphenyl)propanoato-*κO*]cobalt(II) monohydrate

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Comment

Crystal structure of only one metal complex of ketoprofen has been reported up till now. Ketoprofen forms with trimethyltin(IV)] a polymeric compound with the carboxylate group acting in a bidentate bridging mode (Tahir *et al.*, 1997). Here we report crystal structure of the first transition metal complex of ketoprofen.

As illustrated in Fig. 1, the crystal structure of the title compound consists of two independent neutral mononuclear Co^{II} complex molecules and one water of crystallization. The Co^{II} atoms of the two molecules lie on inversion centers and display an octahedral geometry defined by two carboxylate O atoms of two ketoprofenato ligands and four water molecules. The Co1—$O_{ketoprofenato}$ and Co2—$O_{ketoprofenato}$ bond lengths are 2.134 (2) and 2.064 (2) Å, respectively. The Co—O_{water} bond lengths range from 2.051 (3) to 2.183 (2) Å. In the ketoprofenato ligands, two benzene rings are not coplanar, the dihedral angles are 70.1 (3) and 121.7 (3) °. A three-dimensional supramolecular network structure is formed through the extended hydrogen bonding interactions between water molecules and carboxylate O atoms (Table 2).

Experimental

The title complex was prepared by the addition of cobalt diacetate trihydrate (2.31 g, 10 mmol) to a hot aqueous solution of 2-(3-benzoylphenyl)propanoic acid (3.65 g, 10 mmol); the pH was adjusted to 6 with 0.1*M* sodium hydroxide. The solution was allowed to evaporate at room temperature. Pink prismatic crystals separated from the filtered solution after several days. CH&N analysis. Calc. for $C_{32}H_{36}CoO_{11}$: C 58.63, H 5.54%. Found: C 58.54, H 5.64%.

Refinement

The H atoms were placed in calculated positions [C—H = 0.93 and 0.97 Å and U_{iso}(H) = 1.2U_{eq} (C) for aromatic H atoms and methine H atoms, respectively, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq} (C) for methyl group H atoms] and were included in the refinement in the riding-model approximation. The H atoms of water molecules were located in difference Fourier maps and refined with the O—H distance restrained to 0.85 (1) Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

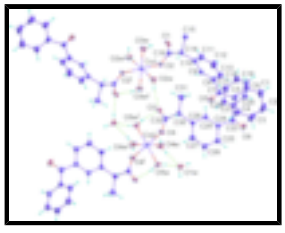


Fig. 1. Molecular structure of of the title compound with 30% probability ellipsoids for the non-H atoms.

Tetraaquabis[2-(3-benzoylphenyl)propanoato-κ*O*]cobalt(II) monohydrate

Crystal data

$[Co(C_{16}H_{13}O_3)_2(H_2O)_4]\cdot H_2O$	$Z = 2$
$M_r = 655.54$	$F_{000} = 686$
Triclinic, $P\overline{1}$	$D_x = 1.403$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.5966$ (17) Å	Cell parameters from 9690 reflections
$b = 8.8939$ (18) Å	$\theta = 3.2$–27.5º
$c = 21.872$ (4) Å	$\mu = 0.61$ mm^{-1}
$\alpha = 92.08$ (3)º	$T = 295$ (2) K
$\beta = 99.69$ (3)º	Prism, pink
$\gamma = 108.92$ (3)º	0.36 × 0.28 × 0.19 mm
$V = 1551.9$ (6) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	7032 independent reflections
Radiation source: fine-focus sealed tube	4192 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.049$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295(2)$ K	$\theta_{min} = 3.2$º
ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -11 \rightarrow 11$
$T_{min} = 0.810$, $T_{max} = 0.892$	$l = -28 \rightarrow 28$
15351 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.177$	$w = 1/[\sigma^2(F_o^2) + (0.0981P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
7032 reflections	$\Delta\rho_{max} = 0.75$ e Å^{-3}
432 parameters	$\Delta\rho_{min} = -0.62$ e Å^{-3}
15 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.0000	0.5000	0.02863 (19)
Co2	0.0000	0.5000	0.5000	0.02836 (19)
O1	0.7225 (4)	−0.1111 (3)	0.61833 (13)	0.0555 (8)
O1W	−0.1286 (5)	0.6695 (4)	0.63546 (13)	0.0560 (8)
O2	0.7012 (3)	0.1050 (3)	0.57693 (10)	0.0336 (5)
O2W	0.3229 (3)	0.0047 (3)	0.55380 (13)	0.0405 (6)
O3W	0.4817 (3)	−0.2333 (3)	0.51952 (12)	0.0401 (6)
O3	0.2059 (3)	0.2647 (3)	0.56416 (12)	0.0432 (6)
O4	0.2168 (3)	0.5170 (3)	0.56140 (12)	0.0417 (6)
O4W	−0.1442 (4)	0.4111 (3)	0.56481 (13)	0.0457 (7)
O5W	0.0284 (3)	0.7437 (3)	0.53313 (12)	0.0364 (6)
O5	0.9239 (5)	0.6840 (4)	0.76371 (14)	0.0666 (10)
O6	0.3928 (5)	0.6321 (4)	0.91110 (14)	0.0765 (11)
C1	0.9958 (9)	0.6929 (7)	0.9782 (2)	0.0874 (19)
H1	1.0615	0.6735	1.0133	0.105*
C2	0.9025 (9)	0.7898 (7)	0.9845 (3)	0.090 (2)
H2	0.9021	0.8328	1.0238	0.108*
C3	0.8116 (9)	0.8226 (7)	0.9336 (3)	0.0860 (19)
H3	0.7489	0.8886	0.9381	0.103*
C4	0.8102 (7)	0.7592 (5)	0.8744 (2)	0.0638 (13)
H4	0.7498	0.7853	0.8395	0.077*
C5	0.8998 (6)	0.6566 (5)	0.86799 (19)	0.0469 (10)
C6	0.9929 (7)	0.6236 (6)	0.9199 (2)	0.0662 (14)
H6	1.0536	0.5553	0.9160	0.079*
C7	0.8989 (5)	0.5920 (5)	0.80391 (18)	0.0436 (9)
C8	0.8629 (5)	0.4175 (5)	0.78967 (17)	0.0412 (9)
C9	0.9120 (5)	0.3631 (4)	0.73750 (15)	0.0351 (8)
H9	0.9773	0.4365	0.7149	0.042*
C10	0.8645 (5)	0.2020 (4)	0.71943 (16)	0.0359 (8)
C11	0.7664 (6)	0.0951 (5)	0.75340 (19)	0.0531 (11)
H11	0.7331	−0.0139	0.7415	0.064*
C12	0.7169 (7)	0.1480 (5)	0.8050 (2)	0.0655 (14)
H12	0.6495	0.0747	0.8271	0.079*
C13	0.7674 (6)	0.3083 (5)	0.82348 (19)	0.0523 (11)
H13	0.7372	0.3434	0.8588	0.063*
C14	0.9233 (5)	0.1427 (4)	0.66370 (15)	0.0343 (8)
H14	0.9803	0.2361	0.6435	0.041*
C15	1.0479 (5)	0.0574 (5)	0.68472 (18)	0.0449 (10)
H15A	1.1453	0.1305	0.7115	0.067*
H15B	1.0799	0.0187	0.6489	0.067*
H15C	0.9969	−0.0309	0.7070	0.067*
C16	0.7703 (5)	0.0361 (4)	0.61625 (16)	0.0338 (8)
C17	0.2352 (7)	0.0842 (6)	0.8625 (2)	0.0667 (14)
H17	0.1514	−0.0046	0.8402	0.080*
C18	0.3483 (8)	0.0650 (7)	0.9110 (2)	0.0745 (16)

H18	0.3432	−0.0370	0.9209	0.089*
C19	0.4708 (7)	0.1977 (6)	0.9453 (2)	0.0659 (14)
H19	0.5472	0.1844	0.9784	0.079*
C20	0.4789 (6)	0.3479 (6)	0.93060 (18)	0.0573 (12)
H20	0.5594	0.4365	0.9543	0.069*
C21	0.3676 (5)	0.3689 (5)	0.88030 (17)	0.0469 (10)
C22	0.2456 (6)	0.2351 (5)	0.84673 (19)	0.0543 (11)
H22	0.1699	0.2475	0.8132	0.065*
C23	0.3743 (6)	0.5346 (5)	0.86745 (19)	0.0522 (11)
C24	0.3617 (5)	0.5821 (4)	0.80224 (18)	0.0420 (9)
C25	0.3313 (6)	0.7258 (5)	0.7927 (2)	0.0541 (11)
H25	0.3137	0.7842	0.8254	0.065*
C26	0.3277 (6)	0.7794 (5)	0.7345 (2)	0.0608 (13)
H26	0.3070	0.8745	0.7282	0.073*
C27	0.3540 (6)	0.6956 (5)	0.6852 (2)	0.0524 (11)
H27	0.3514	0.7349	0.6464	0.063*
C28	0.3846 (5)	0.5518 (5)	0.69338 (17)	0.0412 (9)
C29	0.3868 (5)	0.4972 (5)	0.75199 (17)	0.0414 (9)
H29	0.4056	0.4011	0.7580	0.050*
C30	0.4215 (5)	0.4663 (5)	0.63817 (17)	0.0444 (10)
H30	0.5069	0.5487	0.6219	0.053*
C31	0.4963 (6)	0.3409 (6)	0.6545 (2)	0.0581 (12)
H31A	0.5943	0.3850	0.6866	0.087*
H31B	0.5268	0.3025	0.6183	0.087*
H31C	0.4163	0.2542	0.6693	0.087*
C32	0.2669 (5)	0.4081 (4)	0.58425 (16)	0.0351 (8)
H3W1	0.554 (4)	−0.213 (4)	0.5531 (11)	0.053*
H1W1	−0.185 (5)	0.732 (4)	0.6325 (16)	0.053*
H2W1	0.296 (4)	0.088 (2)	0.551 (2)	0.053*
H2W2	0.234 (3)	−0.076 (3)	0.5474 (19)	0.053*
H3W2	0.395 (3)	−0.311 (3)	0.5224 (16)	0.053*
H4W1	−0.202 (5)	0.3180 (18)	0.5707 (18)	0.053*
H5W1	−0.049 (4)	0.750 (5)	0.5046 (12)	0.053*
H1W2	−0.082 (5)	0.672 (5)	0.6731 (8)	0.053*
H4W2	−0.166 (5)	0.481 (3)	0.5861 (17)	0.053*
H5W2	−0.009 (4)	0.721 (5)	0.5663 (10)	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0258 (4)	0.0237 (3)	0.0323 (3)	0.0044 (3)	0.0025 (3)	0.0026 (3)
Co2	0.0252 (4)	0.0243 (3)	0.0320 (3)	0.0048 (3)	0.0028 (3)	0.0030 (3)
O1	0.0560 (19)	0.0321 (14)	0.0627 (18)	0.0085 (13)	−0.0203 (15)	0.0110 (13)
O1W	0.084 (3)	0.0487 (17)	0.0439 (16)	0.0372 (17)	0.0068 (15)	−0.0004 (14)
O2	0.0301 (14)	0.0295 (12)	0.0366 (12)	0.0082 (10)	−0.0028 (10)	0.0041 (10)
O2W	0.0346 (15)	0.0307 (13)	0.0545 (15)	0.0071 (11)	0.0122 (12)	−0.0009 (12)
O3W	0.0333 (15)	0.0288 (12)	0.0478 (15)	0.0002 (11)	−0.0007 (11)	0.0091 (11)
O3	0.0428 (16)	0.0380 (14)	0.0473 (15)	0.0152 (12)	0.0007 (12)	0.0059 (12)

O4	0.0341 (15)	0.0326 (13)	0.0513 (15)	0.0106 (11)	−0.0101 (12)	0.0044 (11)
O4W	0.0594 (19)	0.0279 (13)	0.0486 (16)	0.0049 (13)	0.0264 (13)	0.0047 (12)
O5W	0.0349 (15)	0.0288 (12)	0.0419 (14)	0.0063 (11)	0.0069 (11)	0.0012 (11)
O5	0.113 (3)	0.0494 (17)	0.0480 (17)	0.0370 (19)	0.0229 (18)	0.0081 (15)
O6	0.116 (3)	0.072 (2)	0.0417 (17)	0.037 (2)	0.0081 (18)	−0.0142 (16)
C1	0.122 (6)	0.082 (4)	0.044 (3)	0.019 (4)	0.004 (3)	0.002 (3)
C2	0.136 (6)	0.061 (3)	0.059 (3)	0.005 (4)	0.040 (4)	−0.017 (3)
C3	0.104 (5)	0.070 (3)	0.089 (4)	0.024 (3)	0.047 (4)	−0.016 (3)
C4	0.073 (4)	0.054 (3)	0.067 (3)	0.024 (3)	0.017 (2)	−0.006 (2)
C5	0.055 (3)	0.036 (2)	0.047 (2)	0.0096 (19)	0.0177 (19)	−0.0023 (18)
C6	0.085 (4)	0.069 (3)	0.047 (3)	0.028 (3)	0.011 (2)	0.004 (2)
C7	0.050 (3)	0.043 (2)	0.039 (2)	0.0201 (19)	0.0069 (17)	−0.0001 (18)
C8	0.039 (2)	0.043 (2)	0.0383 (19)	0.0115 (18)	0.0054 (16)	0.0009 (17)
C9	0.037 (2)	0.0393 (19)	0.0296 (17)	0.0146 (16)	0.0031 (14)	0.0029 (15)
C10	0.034 (2)	0.0374 (19)	0.0323 (18)	0.0091 (16)	0.0015 (15)	0.0004 (15)
C11	0.061 (3)	0.039 (2)	0.052 (2)	0.004 (2)	0.016 (2)	−0.0024 (19)
C12	0.082 (4)	0.049 (3)	0.057 (3)	0.002 (2)	0.033 (3)	0.003 (2)
C13	0.065 (3)	0.051 (2)	0.043 (2)	0.017 (2)	0.021 (2)	0.0014 (19)
C14	0.033 (2)	0.0337 (18)	0.0319 (17)	0.0084 (15)	0.0009 (14)	0.0011 (15)
C15	0.038 (2)	0.046 (2)	0.047 (2)	0.0157 (18)	−0.0043 (17)	−0.0044 (18)
C16	0.034 (2)	0.0297 (17)	0.0347 (18)	0.0071 (15)	0.0052 (15)	0.0020 (15)
C17	0.087 (4)	0.057 (3)	0.050 (3)	0.016 (3)	0.012 (2)	0.000 (2)
C18	0.122 (5)	0.067 (3)	0.048 (3)	0.046 (3)	0.027 (3)	0.013 (2)
C19	0.085 (4)	0.083 (4)	0.039 (2)	0.042 (3)	0.006 (2)	0.005 (2)
C20	0.062 (3)	0.073 (3)	0.034 (2)	0.023 (3)	0.0009 (19)	−0.005 (2)
C21	0.050 (3)	0.054 (2)	0.0337 (19)	0.017 (2)	0.0049 (17)	−0.0023 (18)
C22	0.059 (3)	0.059 (3)	0.039 (2)	0.018 (2)	−0.0022 (19)	−0.002 (2)
C23	0.052 (3)	0.057 (3)	0.041 (2)	0.015 (2)	0.0042 (18)	−0.010 (2)
C24	0.040 (2)	0.041 (2)	0.041 (2)	0.0141 (18)	0.0005 (16)	−0.0052 (17)
C25	0.061 (3)	0.054 (3)	0.050 (2)	0.027 (2)	0.003 (2)	−0.008 (2)
C26	0.077 (4)	0.049 (2)	0.060 (3)	0.033 (2)	0.002 (2)	−0.008 (2)
C27	0.063 (3)	0.049 (2)	0.046 (2)	0.025 (2)	0.002 (2)	0.0027 (19)
C28	0.043 (2)	0.045 (2)	0.0362 (19)	0.0198 (18)	−0.0018 (16)	−0.0020 (17)
C29	0.041 (2)	0.042 (2)	0.041 (2)	0.0170 (18)	0.0008 (16)	−0.0052 (17)
C30	0.048 (3)	0.050 (2)	0.0351 (19)	0.021 (2)	0.0001 (17)	0.0011 (17)
C31	0.048 (3)	0.075 (3)	0.054 (3)	0.030 (2)	−0.002 (2)	−0.006 (2)
C32	0.031 (2)	0.041 (2)	0.0337 (18)	0.0121 (16)	0.0086 (15)	0.0025 (16)

Geometric parameters (Å, °)

Co1—O2W	2.084 (3)	C9—H9	0.9300
Co1—O3W	2.095 (2)	C10—C11	1.382 (6)
Co1—O2	2.134 (2)	C10—C14	1.534 (5)
Co2—O4W	2.051 (3)	C11—C12	1.389 (6)
Co2—O4	2.064 (2)	C11—H11	0.9300
Co2—O5W	2.183 (2)	C12—C13	1.372 (6)
Co1—O2W^{i}	2.084 (3)	C12—H12	0.9300
Co1—O3W^{i}	2.095 (2)	C13—H13	0.9300

Co1—O2^{i}	2.134 (2)	C14—C15	1.524 (5)
Co2—O4W^{ii}	2.051 (3)	C14—C16	1.539 (5)
Co2—O4^{ii}	2.064 (2)	C14—H14	0.9800
Co2—O5W^{ii}	2.183 (2)	C15—H15A	0.9600
O1—C16	1.244 (4)	C15—H15B	0.9600
O1W—H1W1	0.85 (4)	C15—H15C	0.9600
O1W—H1W2	0.848 (10)	C17—C18	1.369 (7)
O2—C16	1.253 (4)	C17—C22	1.376 (7)
O2W—H2W1	0.850 (10)	C17—H17	0.9300
O2W—H2W2	0.85 (3)	C18—C19	1.389 (8)
O3W—H3W1	0.85 (3)	C18—H18	0.9300
O3W—H3W2	0.85 (3)	C19—C20	1.368 (7)
O3—C32	1.242 (4)	C19—H19	0.9300
O4—C32	1.268 (4)	C20—C21	1.392 (6)
O4W—H4W1	0.845 (10)	C20—H20	0.9300
O4W—H4W2	0.85 (4)	C21—C22	1.387 (6)
O5W—H5W1	0.85 (3)	C21—C23	1.495 (6)
O5W—H5W2	0.85 (3)	C22—H22	0.9300
O5—C7	1.221 (5)	C23—C24	1.499 (6)
O6—C23	1.220 (5)	C24—C29	1.396 (5)
C1—C2	1.370 (9)	C24—C25	1.401 (6)
C1—C6	1.390 (7)	C25—C26	1.375 (6)
C1—H1	0.9300	C25—H25	0.9300
C2—C3	1.347 (9)	C26—C27	1.379 (6)
C2—H2	0.9300	C26—H26	0.9300
C3—C4	1.389 (7)	C27—C28	1.399 (6)
C3—H3	0.9300	C27—H27	0.9300
C4—C5	1.389 (6)	C28—C29	1.386 (5)
C4—H4	0.9300	C28—C30	1.535 (5)
C5—C6	1.373 (6)	C29—H29	0.9300
C5—C7	1.494 (5)	C30—C31	1.484 (6)
C6—H6	0.9300	C30—C32	1.551 (5)
C7—C8	1.490 (5)	C30—H30	0.9800
C8—C13	1.380 (6)	C31—H31A	0.9600
C8—C9	1.403 (5)	C31—H31B	0.9600
C9—C10	1.379 (5)	C31—H31C	0.9600
O2W—Co1—O3W	91.81 (11)	C12—C11—H11	119.5
O2W—Co1—O3W^{i}	88.19 (11)	C13—C12—C11	120.0 (4)
O2W—Co1—O2^{i}	88.33 (10)	C13—C12—H12	120.0
O3W—Co1—O2^{i}	86.82 (10)	C11—C12—H12	120.0
O2W—Co1—O2	91.67 (10)	C12—C13—C8	120.1 (4)
O3W—Co1—O2	93.18 (10)	C12—C13—H13	120.0
O4W—Co2—O4^{ii}	88.35 (12)	C8—C13—H13	120.0
O4W—Co2—O5W^{ii}	89.34 (10)	C15—C14—C10	111.2 (3)
O4—Co2—O5W^{ii}	90.54 (10)	C15—C14—C16	112.2 (3)
O4W—Co2—O5W	90.66 (10)	C10—C14—C16	109.5 (3)
O4—Co2—O5W	89.46 (10)	C15—C14—H14	108.0

O2W^{i}—Co1—O2W	180.000 (1)	C10—C14—H14	108.0
O2W^{i}—Co1—O3W	88.19 (11)	C16—C14—H14	108.0
O2W^{i}—Co1—O3W^{i}	91.81 (11)	C14—C15—H15A	109.5
O3W—Co1—O3W^{i}	180.00 (3)	C14—C15—H15B	109.5
O2W^{i}—Co1—O2^{i}	91.67 (10)	H15A—C15—H15B	109.5
O3W^{i}—Co1—O2^{i}	93.18 (10)	C14—C15—H15C	109.5
O2W^{i}—Co1—O2	88.33 (10)	H15A—C15—H15C	109.5
O3W^{i}—Co1—O2	86.82 (10)	H15B—C15—H15C	109.5
O2^{i}—Co1—O2	180.0	O1—C16—O2	123.7 (3)
O4W—Co2—O4W^{ii}	180.000 (1)	O1—C16—C14	119.4 (3)
O4W^{ii}—Co2—O4^{ii}	91.65 (12)	O2—C16—C14	116.9 (3)
O4W—Co2—O4	91.65 (12)	C18—C17—C22	119.9 (5)
O4W^{ii}—Co2—O4	88.35 (12)	C18—C17—H17	120.1
O4^{ii}—Co2—O4	180.000 (1)	C22—C17—H17	120.1
O4W^{ii}—Co2—O5W^{ii}	90.66 (10)	C17—C18—C19	120.1 (5)
O4^{ii}—Co2—O5W^{ii}	89.46 (10)	C17—C18—H18	119.9
O4W^{ii}—Co2—O5W	89.34 (10)	C19—C18—H18	119.9
O4^{ii}—Co2—O5W	90.54 (10)	C20—C19—C18	120.0 (5)
O5W^{ii}—Co2—O5W	180.00 (13)	C20—C19—H19	120.0
H1W1—O1W—H1W2	110 (2)	C18—C19—H19	120.0
C16—O2—Co1	128.2 (2)	C19—C20—C21	120.4 (4)
Co1—O2W—H2W1	113 (3)	C19—C20—H20	119.8
Co1—O2W—H2W2	116 (3)	C21—C20—H20	119.8
H2W1—O2W—H2W2	108 (2)	C22—C21—C20	118.8 (4)
Co1—O3W—H3W1	99 (3)	C22—C21—C23	122.0 (4)
Co1—O3W—H3W2	129 (3)	C20—C21—C23	119.0 (4)
H3W1—O3W—H3W2	111 (2)	C17—C22—C21	120.7 (4)
C32—O4—Co2	130.0 (2)	C17—C22—H22	119.6
Co2—O4W—H4W1	133 (2)	C21—C22—H22	119.6
Co2—O4W—H4W2	115 (2)	O6—C23—C21	118.9 (4)
H4W1—O4W—H4W2	111 (2)	O6—C23—C24	120.1 (4)
Co2—O5W—H5W1	94 (3)	C21—C23—C24	120.9 (3)
Co2—O5W—H5W2	96 (3)	C29—C24—C25	118.8 (4)
H5W1—O5W—H5W2	110 (2)	C29—C24—C23	124.3 (4)
C2—C1—C6	120.6 (6)	C25—C24—C23	116.8 (4)
C2—C1—H1	119.7	C26—C25—C24	119.2 (4)
C6—C1—H1	119.7	C26—C25—H25	120.4
C3—C2—C1	119.9 (5)	C24—C25—H25	120.4
C3—C2—H2	120.0	C25—C26—C27	121.7 (4)
C1—C2—H2	120.0	C25—C26—H26	119.1
C2—C3—C4	121.0 (6)	C27—C26—H26	119.1
C2—C3—H3	119.5	C26—C27—C28	120.3 (4)
C4—C3—H3	119.5	C26—C27—H27	119.9
C5—C4—C3	119.3 (5)	C28—C27—H27	119.9
C5—C4—H4	120.3	C29—C28—C27	118.0 (4)

C3—C4—H4	120.3	C29—C28—C30	123.3 (3)
C6—C5—C4	119.7 (4)	C27—C28—C30	118.7 (4)
C6—C5—C7	121.8 (4)	C28—C29—C24	122.0 (4)
C4—C5—C7	118.5 (4)	C28—C29—H29	119.0
C5—C6—C1	119.5 (5)	C24—C29—H29	119.0
C5—C6—H6	120.3	C31—C30—C28	115.1 (3)
C1—C6—H6	120.3	C31—C30—C32	113.2 (3)
O5—C7—C8	121.4 (3)	C28—C30—C32	111.2 (3)
O5—C7—C5	118.6 (3)	C31—C30—H30	105.5
C8—C7—C5	120.0 (4)	C28—C30—H30	105.5
C13—C8—C9	119.5 (4)	C32—C30—H30	105.5
C13—C8—C7	120.6 (4)	C30—C31—H31A	109.5
C9—C8—C7	119.6 (4)	C30—C31—H31B	109.5
C10—C9—C8	120.7 (4)	H31A—C31—H31B	109.5
C10—C9—H9	119.7	C30—C31—H31C	109.5
C8—C9—H9	119.7	H31A—C31—H31C	109.5
C9—C10—C11	118.7 (3)	H31B—C31—H31C	109.5
C9—C10—C14	120.5 (3)	O3—C32—O4	124.3 (3)
C11—C10—C14	120.7 (3)	O3—C32—C30	120.3 (3)
C10—C11—C12	120.9 (4)	O4—C32—C30	115.3 (3)
C10—C11—H11	119.5		
O2W^{i}—Co1—O2—C16	−88.5 (3)	C15—C14—C16—O1	29.8 (5)
O2W—Co1—O2—C16	91.5 (3)	C10—C14—C16—O1	−94.1 (4)
O3W—Co1—O2—C16	−0.4 (3)	C15—C14—C16—O2	−149.8 (3)
O3W^{i}—Co1—O2—C16	179.6 (3)	C10—C14—C16—O2	86.3 (4)
O4W—Co2—O4—C32	67.1 (3)	C22—C17—C18—C19	1.7 (8)
O4W^{ii}—Co2—O4—C32	−112.9 (3)	C17—C18—C19—C20	−0.3 (8)
O5W^{ii}—Co2—O4—C32	−22.2 (3)	C18—C19—C20—C21	−1.6 (8)
O5W—Co2—O4—C32	157.8 (3)	C19—C20—C21—C22	1.9 (7)
C6—C1—C2—C3	−2.2 (10)	C19—C20—C21—C23	176.9 (4)
C1—C2—C3—C4	0.2 (10)	C18—C17—C22—C21	−1.3 (8)
C2—C3—C4—C5	2.0 (9)	C20—C21—C22—C17	−0.4 (7)
C3—C4—C5—C6	−2.2 (8)	C23—C21—C22—C17	−175.3 (5)
C3—C4—C5—C7	−179.0 (5)	C22—C21—C23—O6	133.1 (5)
C4—C5—C6—C1	0.2 (8)	C20—C21—C23—O6	−41.8 (7)
C7—C5—C6—C1	176.9 (5)	C22—C21—C23—C24	−48.1 (6)
C2—C1—C6—C5	2.0 (9)	C20—C21—C23—C24	137.1 (4)
C6—C5—C7—O5	−129.8 (5)	O6—C23—C24—C29	161.5 (4)
C4—C5—C7—O5	46.9 (6)	C21—C23—C24—C29	−17.4 (7)
C6—C5—C7—C8	52.0 (6)	O6—C23—C24—C25	−15.1 (7)
C4—C5—C7—C8	−131.3 (4)	C21—C23—C24—C25	166.1 (4)
O5—C7—C8—C13	−151.7 (4)	C29—C24—C25—C26	−0.3 (7)
C5—C7—C8—C13	26.4 (6)	C23—C24—C25—C26	176.5 (4)
O5—C7—C8—C9	21.7 (6)	C24—C25—C26—C27	−0.3 (8)
C5—C7—C8—C9	−160.1 (4)	C25—C26—C27—C28	0.3 (8)
C13—C8—C9—C10	0.6 (6)	C26—C27—C28—C29	0.2 (7)
C7—C8—C9—C10	−172.9 (3)	C26—C27—C28—C30	−177.1 (4)
C8—C9—C10—C11	0.5 (6)	C27—C28—C29—C24	−0.8 (6)

C8—C9—C10—C14	−177.9 (3)	C30—C28—C29—C24	176.4 (4)
C9—C10—C11—C12	−0.3 (7)	C25—C24—C29—C28	0.8 (6)
C14—C10—C11—C12	178.1 (4)	C23—C24—C29—C28	−175.7 (4)
C10—C11—C12—C13	−0.9 (8)	C29—C28—C30—C31	−12.9 (6)
C11—C12—C13—C8	2.1 (8)	C27—C28—C30—C31	164.3 (4)
C9—C8—C13—C12	−1.9 (7)	C29—C28—C30—C32	117.4 (4)
C7—C8—C13—C12	171.6 (4)	C27—C28—C30—C32	−65.4 (5)
C9—C10—C14—C15	110.7 (4)	Co2—O4—C32—O3	14.4 (6)
C11—C10—C14—C15	−67.7 (5)	Co2—O4—C32—C30	−169.4 (2)
C9—C10—C14—C16	−124.8 (4)	C31—C30—C32—O3	8.2 (5)
C11—C10—C14—C16	56.8 (5)	C28—C30—C32—O3	−123.1 (4)
Co1—O2—C16—O1	−4.6 (6)	C31—C30—C32—O4	−168.2 (4)
Co1—O2—C16—C14	174.9 (2)	C28—C30—C32—O4	60.5 (5)

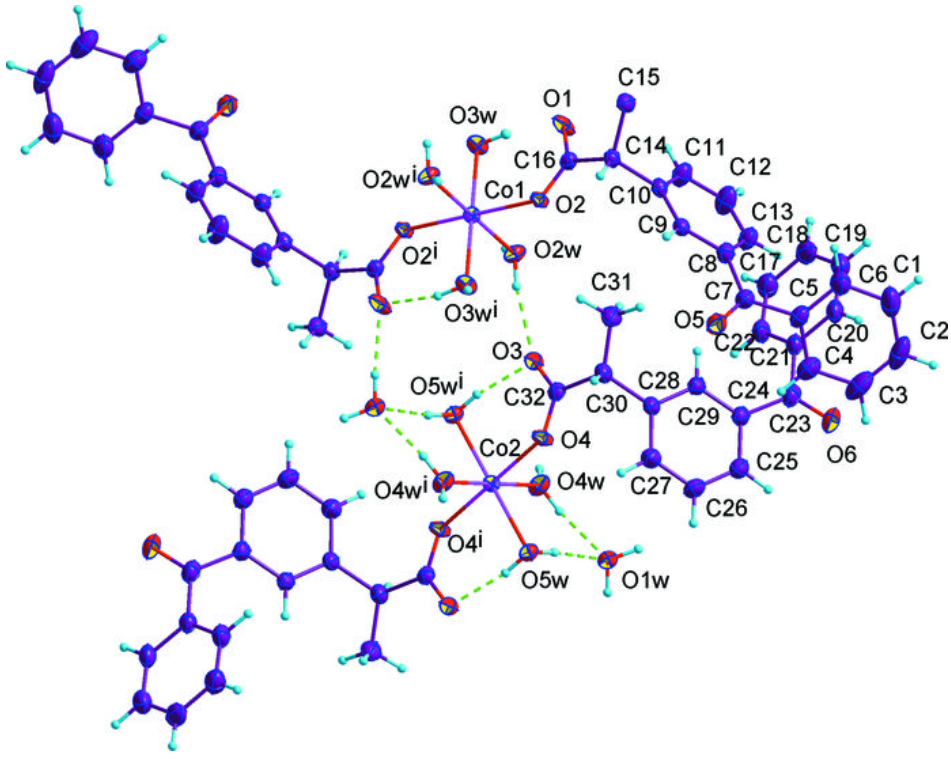
Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3W—H3W1···O1	0.85 (3)	1.82 (3)	2.646 (4)	164 (4)
O1W—H1W1···O1^{iii}	0.85 (4)	1.83 (4)	2.665 (4)	170 (4)
O2W—H2W1···O3	0.850 (10)	1.990 (15)	2.822 (4)	166 (4)
O2W—H2W2···O5W^{iv}	0.85 (3)	1.93 (3)	2.781 (4)	179 (4)
O3W—H3W2···O4^{iv}	0.85 (3)	2.107 (16)	2.920 (4)	161 (3)
O4W—H4W1···O2^{v}	0.85 (3)	1.826 (12)	2.660 (4)	169 (4)
O5W—H5W1···O3^{ii}	0.85 (3)	1.81 (3)	2.653 (4)	170 (4)
O1W—H1W2···O5^{v}	0.848 (10)	1.97 (2)	2.757 (4)	154 (4)
O4W—H4W2···O1W	0.85 (4)	1.867 (16)	2.675 (4)	159 (4)
O5W—H5W2···O1W	0.85 (3)	1.96 (3)	2.795 (4)	171 (4)

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

Fig. 1


C15
O1
O3w
C14
C11
C16
C12
O2wi
Co1
O2
C10
C13
C9
C18
C19
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O2w
C8
C17
C1
C31
C7
C5
C6
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O5
C22
C20
C2
O3
C21
C4
O5wi
C28
C24
C32
C30
C29
C3
C23
Co2
O4
O6
C25
O4wi
O4w
C27
C26
O4i
O5w
O1w