

catena-Poly[[aqua(2-iodobenzoato- κ O)-cobalt(II)]- μ -aqua- μ -2-iodobenzoato- κ^2 O:O']

Ömür Aydın,^a Nagihan Çaylak Delibaş,^b Hacı Necefoğlu^a and Tuncer Hökelek^{c*}

^aDepartment of Chemistry, Kafkas University, 36100 Kars, Turkey, ^bDepartment of Physics, Sakarya University, 54187 Esentepe, Sakarya, Turkey, and ^cDepartment of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey
Correspondence e-mail: merzifon@hacettepe.edu.tr

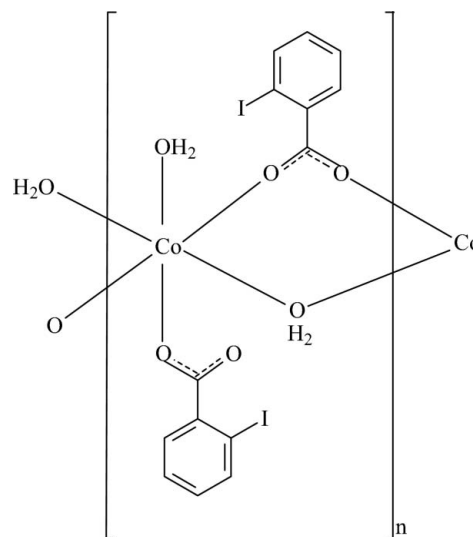
Received 29 March 2012; accepted 5 April 2012

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.020; wR factor = 0.051; data-to-parameter ratio = 19.3.

The asymmetric unit of the polymeric title compound, $[\text{Co}(\text{C}_7\text{H}_4\text{IO}_2)_2(\text{H}_2\text{O})_2]_n$, contains one Co^{II} cation, two iodobenzoate anions and two water molecules. One iodobenzoate anion and one water molecule bridge adjacent Co cations, forming a polymeric chain running along the a axis, while the other iodobenzoate anion and water molecule coordinate in a monodentate manner to the Co^{II} cation, completing the slightly distorted octahedral geometry. In the two independent anionic ligands, the carboxylate groups are twisted away from the attached benzene rings by 51.38 (18) and 39.89 (11)°, and the two benzene rings are nearly perpendicular to each other with a dihedral angle of 86.09 (10)°. Intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds between coordinating water molecules and adjacent carboxylate O atoms help to stabilize the molecular structure. In the crystal, weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the polymeric chains into a three-dimensional supramolecular network.

Related literature

For niacin, see: Krishnamachari (1974) and for information on the nicotinic acid derivative N,N -diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (2009, 2010a,b, 2011); Necefoğlu *et al.* (2011); Zaman *et al.* (2012). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[\text{Co}(\text{C}_7\text{H}_4\text{IO}_2)_2(\text{H}_2\text{O})_2]$
 $M_r = 588.97$
Orthorhombic, $P2_12_12_1$
 $a = 7.5051$ (3) Å
 $b = 10.5639$ (4) Å
 $c = 21.6723$ (9) Å

$V = 1718.25$ (12) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 4.62$ mm⁻¹
 $T = 100$ K
 $0.26 \times 0.23 \times 0.17$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.313$, $T_{\max} = 0.456$

30167 measured reflections
4313 independent reflections
4300 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$
 $wR(F^2) = 0.051$
 $S = 1.20$
4313 reflections
224 parameters
8 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.60$ e Å⁻³
 $\Delta\rho_{\min} = -1.03$ e Å⁻³
Absolute structure: Flack (1983), 1835 Friedel pairs
Flack parameter: 0.016 (19)

Table 1

Selected bond lengths (Å).

Co1—O2	2.118 (2)	Co1—O5	2.124 (2)
Co1—O3 ⁱ	2.021 (2)	Co1—O5 ⁱ	2.151 (2)
Co1—O4	2.016 (2)	Co1—O6	2.110 (2)

Symmetry code: (i) $x + \frac{1}{2}$, $-y + \frac{1}{2}$, $-z + 2$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H51 $\cdots$ O1 ⁱⁱ	0.86 (3)	1.64 (3)	2.486 (3)	167 (5)
O6—H61 $\cdots$ O2 ⁱ	0.86 (2)	1.92 (2)	2.742 (3)	161 (4)
C4—H4 $\cdots$ O1 ⁱⁱⁱ	0.95	2.56	3.364 (4)	142
C13—H13 $\cdots$ O4 ^{iv}	0.95	2.58	3.495 (4)	162

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

Data collection: *APEX2* (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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

The authors are indebted to Anadolu University and the Medicinal Plants and Medicine Research Centre of Anadolu University, Eskişehir, Turkey, for the use of X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5504).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bigoli, F., Braibanti, A., Pellinghelli, M. A. & Tiripicchio, A. (1972). *Acta Cryst. B28*, 962–966.
- Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Flack, H. D. (1983). *Acta Cryst. A39*, 876–881.
- Hökelek, T., Dal, H., Tercan, B., Çimen, E. & Necefoğlu, H. (2010a). *Acta Cryst. E66*, m734–m735.
- Hökelek, T., Dal, H., Tercan, B., Çimen, E. & Necefoğlu, H. (2010b). *Acta Cryst. E66*, m953–m954.
- Hökelek, T., Tercan, B., Şahin, E., Aktaş, V. & Necefoğlu, H. (2011). *Acta Cryst. E67*, m1057–m1058.
- Hökelek, T., Yılmaz, F., Tercan, B., Sertçelik, M. & Necefoğlu, H. (2009). *Acta Cryst. E65*, m1399–m1400.
- Krishnamachari, K. A. V. R. (1974). *Am. J. Clin. Nutr.* **27**, 108–111.
- Necefoğlu, H., Özbek, F. E., Öztürk, V., Tercan, B. & Hökelek, T. (2011). *Acta Cryst. E67*, m1003–m1004.
- Sheldrick, G. M. (2008). *Acta Cryst. A64*, 112–122.
- Spek, A. L. (2009). *Acta Cryst. D65*, 148–155.
- Zaman, İ. G., Çaylak Delibaş, N., Necefoğlu, H. & Hökelek, T. (2012). *Acta Cryst. E68*, m257–m258.

supporting information

Acta Cryst. (2012). E68, m601–m602 [https://doi.org/10.1107/S1600536812015115]

catena-Poly[[aqua(2-iodobenzoato- κ O)cobalt(II)]- μ -aqua- μ -2-iodobenzoato- κ^2 O:O']

Ömür Aydın, Nagihan Çaylak Delibaş, Hacali Necefoğlu and Tuncer Hökelek

S1. Comment

As a part of our ongoing investigations of transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N,N*-diethylnicotinamide (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

The asymmetric unit of the title compound, (I), contains one Co^{II} ion, two 2-iodobenzoate (IB) ligands and two water molecules (Fig. 1). In the crystal of the title compound, each Co^{II} ion is coordinated by one IB ligand, one water molecule, two symmetry related IB ligands and two symmetry related water molecules, while the symmetry related Co(II) ions are bridged by the two O atoms of the symmetry related IB ligands and the two O atoms of the two symmetry related water molecules forming a polymeric chain. The coordination around the Co(II) ion is a slightly distorted octahedral (Fig. 2).

The crystal structures of some benzoate containing polymeric complexes of Mn^{II}, Zn^{II} and Pb^{II} ions, [Mn₂(C₈H₇O₂)₄(C₁₀H₁₄N₂O)₂(H₂O)]_n (Hökelek *et al.*, 2010a), [Mn(C₇H₄FO₂)₂(H₂O)₂]_n (Necefoğlu *et al.*, 2011), [Zn(C₈H₅O₃)₂(C₆H₆N₂O)]_n (Hökelek *et al.*, 2009), [Pb(C₈H₇O₂)₂(C₆H₆N₂O)]_n (Hökelek *et al.*, 2010b), {[Pb(C₉H₉O₂)₂(C₆H₆N₂O)]·H₂O}_n (Hökelek *et al.*, 2011), {[Pb(C₇H₅O₃)₂(C₆H₆N₂O)]·H₂O}_n (Zaman *et al.*, 2012) have also been reported.

In the title compound, the four O atoms (O2, O3', O4 and O6) in the equatorial plane around the Co^{II} ion form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two symmetry related O atoms of the water molecules (O5 and O5') in the axial positions. The near equalities of the C1—O1 [1.252 (4) Å], C1—O2 [1.267 (4) Å], C8—O3 [1.251 (4) Å] and C8—O4 [1.260 (4) Å] bonds in the carboxylate groups indicate delocalized bonding arrangement, rather than localized single and double bonds. The average Co—O bond lengths are 2.052 (2) Å (for benzoate oxygens) and 2.128 (2) Å (for water oxygens) (Table 1) close to standard values (Allen *et al.*, 1987). The Co atom is displaced out of the mean-planes of the carboxylate groups (O1/C1/O2) and (O3/C8/O4) by -0.5163 (4) and 0.3155 (4) Å, respectively. The dihedral angles between the planar carboxylate groups (O1/C1/O2) and (O3/C8/O4) and the adjacent benzene rings A (C2—C7) and B (C9—C14) are 51.38 (18) and 39.89 (11)°, respectively. The benzene rings are oriented at a dihedral angle of A/B = 86.09 (10)°.

In the crystal, O—H...O and weak C—H...O hydrogen bonds (Table 2) link the molecules into a three-dimensional supramolecular network. A weak C—H... π interaction is also found in the crystal structure.

S2. Experimental

The title compound was prepared by the reaction of CoSO₄·7H₂O (1.41 g, 5 mmol) in H₂O (100 ml) with sodium 2-iodobenzoate (2.70 g, 10 mmol) in H₂O (50 ml) at room temperature. The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving orange single crystals.

S3. Refinement

Atoms H51, H52, H61 and H62 (for H₂O) were located in a difference Fourier map and were refined by applying restraints. The C-bound H-atoms were positioned geometrically with C—H = 0.95 Å for aromatic H-atoms, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2 \times U_{\text{eq}}(\text{C})$.

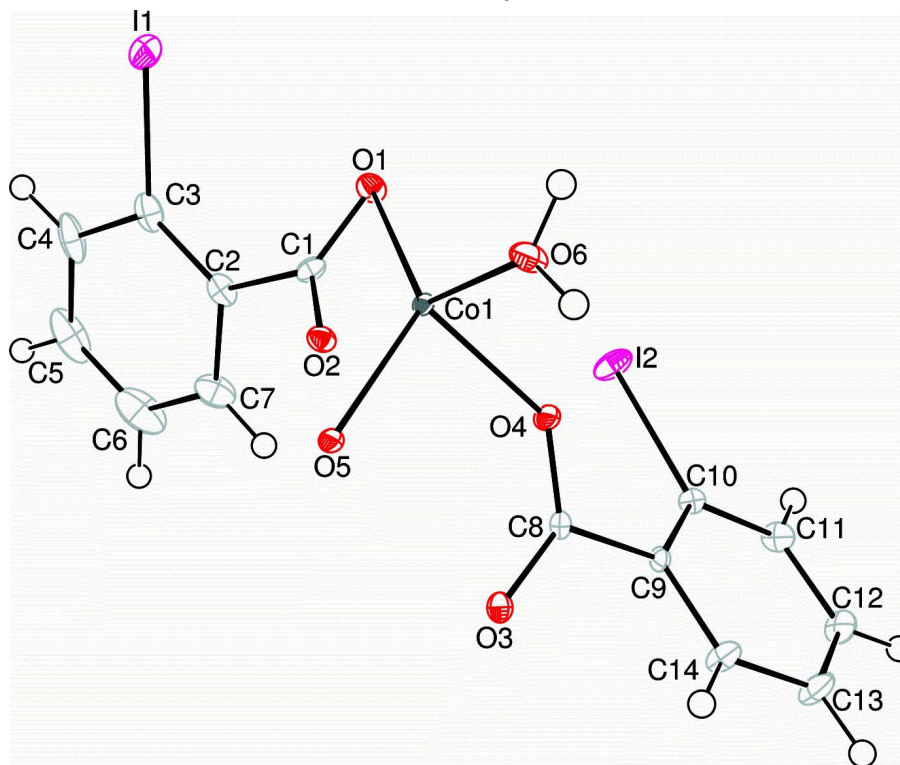


Figure 1

The asymmetric unit of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

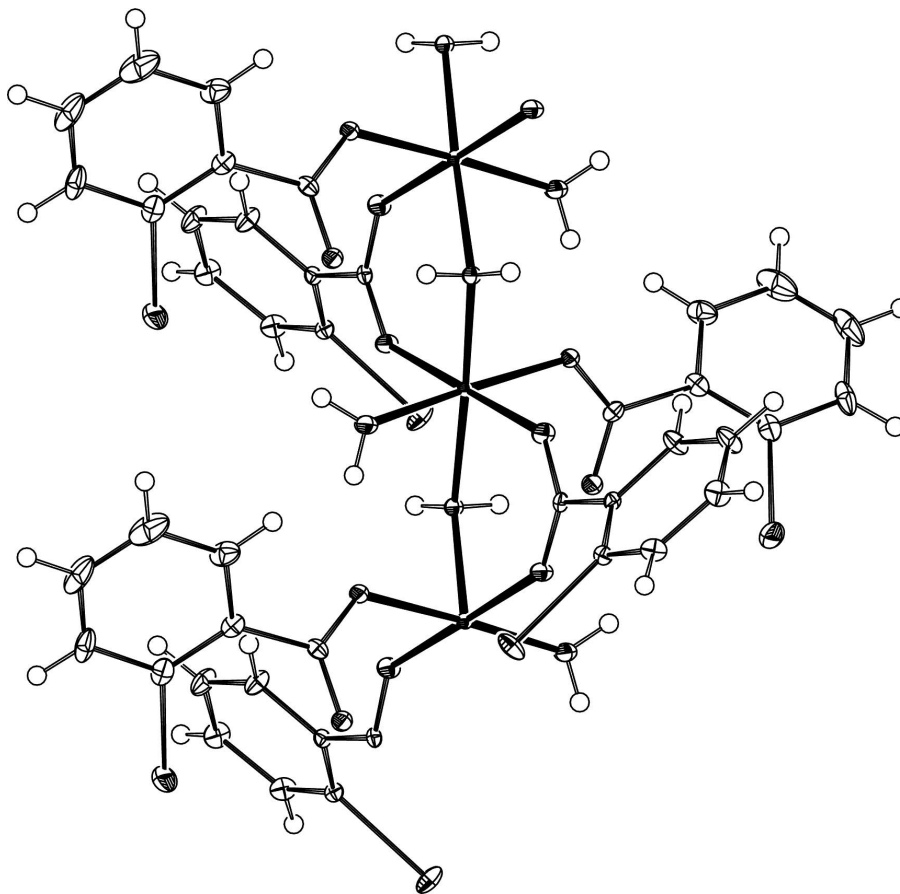


Figure 2

Part of the polymeric chain of the title compound.

catena-Poly[[aqua(2-iodobenzoato- κ O)cobalt(II)]- μ -aqua- μ -2-iodobenzoato- κ^2 O: O']

Crystal data

$[\text{Co}(\text{C}_7\text{H}_4\text{IO}_2)_2(\text{H}_2\text{O})_2]$

$M_r = 588.97$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 7.5051$ (3) Å

$b = 10.5639$ (4) Å

$c = 21.6723$ (9) Å

$V = 1718.25$ (12) Å³

$Z = 4$

$F(000) = 1108$

$D_x = 2.277$ Mg m⁻³

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

Cell parameters from 9972 reflections

$\theta = 2.7\text{--}28.4^\circ$

$\mu = 4.62$ mm⁻¹

$T = 100$ K

Block, orange

$0.26 \times 0.23 \times 0.17$ mm

Data collection

Bruker Kappa APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.313$, $T_{\max} = 0.456$

30167 measured reflections

4313 independent reflections

4300 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -10 \rightarrow 10$

$k = -13 \rightarrow 14$

$l = -29 \rightarrow 28$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.020$ $wR(F^2) = 0.051$ $S = 1.20$

4313 reflections

224 parameters

8 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0209P)^2 + 2.2878P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.002$ $\Delta\rho_{\max} = 0.60 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -1.03 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack (1983), 1835 Friedel
pairs

Absolute structure parameter: 0.016 (19)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
I1	1.14075 (3)	0.58295 (2)	0.834432 (12)	0.02259 (6)
I2	0.86998 (3)	−0.04434 (2)	0.858655 (9)	0.01608 (6)
Co1	0.81243 (5)	0.25155 (4)	0.997594 (19)	0.00670 (8)
O1	1.0232 (3)	0.2952 (2)	0.86860 (10)	0.0128 (5)
O2	0.7492 (3)	0.3161 (2)	0.90771 (10)	0.0107 (4)
O3	0.4106 (3)	0.0744 (2)	0.98386 (11)	0.0136 (5)
O4	0.7100 (3)	0.0786 (2)	0.98080 (11)	0.0122 (4)
O5	0.5662 (3)	0.3202 (2)	1.03253 (11)	0.0093 (4)
H51	0.562 (7)	0.289 (4)	1.0690 (12)	0.030 (14)*
H52	0.561 (7)	0.4004 (18)	1.037 (2)	0.034 (14)*
O6	0.8845 (3)	0.1971 (2)	1.08789 (11)	0.0148 (5)
H61	0.993 (3)	0.190 (5)	1.100 (2)	0.021 (12)*
H62	0.824 (6)	0.151 (5)	1.113 (2)	0.048 (17)*
C1	0.8667 (5)	0.3361 (3)	0.86686 (13)	0.0104 (5)
C2	0.8126 (4)	0.4134 (3)	0.81193 (14)	0.0125 (6)
C3	0.9090 (5)	0.5170 (3)	0.79051 (15)	0.0161 (7)
C4	0.8484 (6)	0.5875 (4)	0.74032 (16)	0.0229 (8)
H4	0.9116	0.6607	0.7273	0.027*
C5	0.6959 (6)	0.5502 (5)	0.70965 (16)	0.0311 (10)
H5	0.6560	0.5967	0.6748	0.037*
C6	0.6007 (6)	0.4452 (5)	0.72940 (19)	0.0329 (10)
H6	0.4969	0.4192	0.7078	0.040*

C7	0.6571 (5)	0.3786 (4)	0.78044 (16)	0.0201 (7)
H7	0.5897	0.3082	0.7945	0.024*
C8	0.5602 (4)	0.0274 (3)	0.97274 (13)	0.0082 (5)
C9	0.5600 (4)	−0.1065 (3)	0.94894 (14)	0.0081 (5)
C10	0.6767 (4)	−0.1532 (3)	0.90444 (13)	0.0088 (6)
C11	0.6674 (4)	−0.2780 (3)	0.88547 (15)	0.0134 (6)
H11	0.7435	−0.3072	0.8535	0.016*
C12	0.5480 (5)	−0.3607 (3)	0.91279 (16)	0.0157 (7)
H12	0.5450	−0.4471	0.9006	0.019*
C13	0.4330 (5)	−0.3169 (3)	0.95795 (18)	0.0183 (7)
H13	0.3521	−0.3733	0.9774	0.022*
C14	0.4365 (5)	−0.1903 (3)	0.97459 (15)	0.0137 (6)
H14	0.3531	−0.1599	1.0040	0.016*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Il	0.01863 (11)	0.01494 (11)	0.03419 (13)	−0.00281 (9)	0.00237 (10)	0.00476 (9)
I2	0.01887 (10)	0.01658 (10)	0.01281 (9)	−0.00775 (9)	0.00753 (8)	−0.00351 (8)
Co1	0.00702 (19)	0.00527 (16)	0.00782 (16)	−0.00060 (14)	−0.00006 (14)	−0.00093 (15)
O1	0.0111 (11)	0.0154 (11)	0.0118 (11)	0.0016 (9)	0.0016 (8)	0.0024 (9)
O2	0.0092 (11)	0.0128 (11)	0.0102 (10)	0.0004 (9)	0.0007 (8)	0.0018 (8)
O3	0.0117 (11)	0.0071 (10)	0.0221 (12)	0.0017 (8)	0.0011 (8)	−0.0025 (9)
O4	0.0091 (10)	0.0069 (10)	0.0208 (11)	−0.0004 (8)	0.0004 (9)	−0.0025 (9)
O5	0.0088 (10)	0.0056 (10)	0.0135 (11)	−0.0002 (8)	−0.0002 (8)	−0.0014 (8)
O6	0.0092 (11)	0.0205 (12)	0.0146 (11)	0.0002 (10)	−0.0005 (9)	0.0039 (9)
C1	0.0114 (13)	0.0107 (13)	0.0092 (13)	−0.0034 (12)	0.0005 (12)	−0.0020 (10)
C2	0.0144 (15)	0.0163 (15)	0.0067 (13)	0.0044 (12)	0.0008 (11)	−0.0022 (11)
C3	0.0202 (17)	0.0169 (17)	0.0111 (14)	0.0077 (13)	0.0059 (12)	0.0005 (12)
C4	0.032 (2)	0.0222 (17)	0.0145 (16)	0.0163 (17)	0.0104 (15)	0.0081 (13)
C5	0.039 (2)	0.044 (3)	0.0107 (15)	0.023 (2)	0.0014 (15)	0.0072 (16)
C6	0.028 (2)	0.053 (3)	0.0177 (17)	0.012 (2)	−0.0096 (15)	−0.0045 (19)
C7	0.0167 (17)	0.0296 (19)	0.0139 (15)	0.0014 (15)	−0.0035 (13)	−0.0010 (13)
C8	0.0106 (13)	0.0065 (14)	0.0075 (12)	0.0013 (11)	0.0005 (10)	0.0006 (10)
C9	0.0093 (13)	0.0054 (13)	0.0096 (13)	0.0005 (11)	−0.0006 (11)	−0.0011 (10)
C10	0.0101 (14)	0.0111 (15)	0.0052 (12)	−0.0006 (11)	0.0000 (10)	−0.0003 (10)
C11	0.0139 (16)	0.0139 (15)	0.0124 (14)	0.0004 (12)	0.0018 (12)	−0.0059 (11)
C12	0.0186 (17)	0.0083 (15)	0.0202 (16)	−0.0011 (13)	0.0010 (13)	−0.0066 (12)
C13	0.0198 (17)	0.0116 (16)	0.0235 (17)	−0.0066 (14)	0.0052 (14)	−0.0014 (13)
C14	0.0161 (15)	0.0118 (15)	0.0132 (14)	−0.0038 (13)	0.0063 (12)	−0.0041 (12)

Geometric parameters (Å, °)

Il—C3	2.102 (4)	C3—C4	1.395 (5)
I2—C10	2.100 (3)	C4—C5	1.381 (7)
Co1—O2	2.118 (2)	C4—H4	0.9500
Co1—O3 ⁱ	2.021 (2)	C5—C6	1.387 (7)
Co1—O4	2.016 (2)	C5—H5	0.9500

Co1—O5	2.124 (2)	C6—C7	1.377 (5)
Co1—O5 ⁱ	2.151 (2)	C6—H6	0.9500
Co1—O6	2.110 (2)	C7—C2	1.400 (5)
O1—C1	1.252 (4)	C7—H7	0.9500
O2—C1	1.267 (4)	C8—C9	1.506 (4)
O3—Co1 ⁱⁱ	2.021 (2)	C9—C10	1.393 (4)
O3—C8	1.251 (4)	C9—C14	1.397 (4)
O4—C8	1.260 (4)	C11—C10	1.382 (4)
O5—Co1 ⁱⁱ	2.151 (2)	C11—H11	0.9500
O5—H51	0.855 (19)	C12—C11	1.385 (5)
O5—H52	0.855 (18)	C12—H12	0.9500
O6—H61	0.854 (18)	C13—C12	1.385 (5)
O6—H62	0.86 (2)	C13—H13	0.9500
C2—C1	1.499 (4)	C14—C13	1.385 (4)
C3—C2	1.392 (5)	C14—H14	0.9500
O2—Co1—O5	91.32 (9)	C4—C3—I1	116.5 (3)
O2—Co1—O5 ⁱ	91.88 (9)	C5—C4—C3	119.5 (4)
O3 ⁱ —Co1—O6	88.28 (10)	C5—C4—H4	120.2
O3 ⁱ —Co1—O2	88.37 (10)	C3—C4—H4	120.2
O3 ⁱ —Co1—O5	86.32 (9)	C4—C5—C6	120.5 (3)
O3 ⁱ —Co1—O5 ⁱ	93.32 (9)	C4—C5—H5	119.8
O4—Co1—O2	92.32 (9)	C6—C5—H5	119.8
O4—Co1—O3 ⁱ	178.57 (10)	C7—C6—C5	119.8 (4)
O4—Co1—O5	92.41 (9)	C7—C6—H6	120.1
O4—Co1—O5 ⁱ	87.92 (9)	C5—C6—H6	120.1
O4—Co1—O6	91.04 (10)	C6—C7—C2	120.9 (4)
O5—Co1—O5 ⁱ	176.77 (4)	C6—C7—H7	119.5
O6—Co1—O2	176.58 (10)	C2—C7—H7	119.5
O6—Co1—O5	89.15 (9)	O3—C8—O4	127.2 (3)
O6—Co1—O5 ⁱ	87.63 (9)	O3—C8—C9	116.0 (3)
C1—O2—Co1	122.7 (2)	O4—C8—C9	116.8 (3)
C8—O3—Co1 ⁱⁱ	136.6 (2)	C10—C9—C8	124.7 (3)
C8—O4—Co1	139.0 (2)	C10—C9—C14	117.9 (3)
Co1—O5—Co1 ⁱⁱ	122.81 (10)	C14—C9—C8	117.3 (3)
Co1—O5—H51	103 (3)	C9—C10—I2	124.6 (2)
Co1 ⁱⁱ —O5—H51	97 (4)	C11—C10—I2	114.6 (2)
Co1—O5—H52	115 (4)	C11—C10—C9	120.8 (3)
Co1 ⁱⁱ —O5—H52	110 (4)	C10—C11—C12	120.5 (3)
H51—O5—H52	106 (4)	C10—C11—H11	119.8
Co1—O6—H61	123 (3)	C12—C11—H11	119.8
Co1—O6—H62	127 (4)	C11—C12—H12	120.2
H61—O6—H62	106 (4)	C13—C12—C11	119.6 (3)
O1—C1—O2	125.1 (3)	C13—C12—H12	120.2
O1—C1—C2	117.8 (3)	C12—C13—H13	120.1
O2—C1—C2	117.2 (3)	C14—C13—C12	119.7 (3)
C3—C2—C1	123.5 (3)	C14—C13—H13	120.1
C3—C2—C7	118.5 (3)	C9—C14—H14	119.3

C7—C2—C1	118.0 (3)	C13—C14—C9	121.4 (3)
C2—C3—I1	122.7 (2)	C13—C14—H14	119.3
C2—C3—C4	120.7 (4)		
O3 ⁱ —Co1—O2—C1	72.6 (2)	C4—C3—C2—C1	−177.9 (3)
O4—Co1—O2—C1	−108.6 (2)	C4—C3—C2—C7	2.4 (5)
O5—Co1—O2—C1	158.9 (2)	I1—C3—C4—C5	−179.4 (3)
O5 ⁱ —Co1—O2—C1	−20.6 (2)	C2—C3—C4—C5	−3.3 (5)
O2—Co1—O4—C8	−70.4 (3)	C3—C4—C5—C6	1.6 (6)
O5—Co1—O4—C8	21.0 (3)	C4—C5—C6—C7	0.9 (6)
O5 ⁱ —Co1—O4—C8	−162.2 (3)	C5—C6—C7—C2	−1.7 (6)
O6—Co1—O4—C8	110.2 (3)	C6—C7—C2—C1	−179.6 (3)
O2—Co1—O5—Co1 ⁱⁱ	63.36 (13)	C6—C7—C2—C3	0.1 (5)
O3 ⁱ —Co1—O5—Co1 ⁱⁱ	151.65 (14)	O3—C8—C9—C10	142.8 (3)
O4—Co1—O5—Co1 ⁱⁱ	−29.01 (13)	O3—C8—C9—C14	−38.8 (4)
O6—Co1—O5—Co1 ⁱⁱ	−120.02 (13)	O4—C8—C9—C10	−39.0 (4)
Co1—O2—C1—O1	16.8 (4)	O4—C8—C9—C14	139.4 (3)
Co1—O2—C1—C2	−164.0 (2)	C8—C9—C10—I2	−2.7 (4)
Co1 ⁱⁱ —O3—C8—O4	14.0 (5)	C8—C9—C10—C11	179.7 (3)
Co1 ⁱⁱ —O3—C8—C9	−168.0 (2)	C14—C9—C10—I2	178.9 (2)
Co1—O4—C8—O3	−13.8 (5)	C14—C9—C10—C11	1.4 (5)
Co1—O4—C8—C9	168.2 (2)	C8—C9—C14—C13	−176.5 (3)
C3—C2—C1—O1	−51.1 (4)	C10—C9—C14—C13	2.0 (5)
C3—C2—C1—O2	129.7 (3)	C12—C11—C10—I2	178.7 (3)
C7—C2—C1—O1	128.6 (3)	C12—C11—C10—C9	−3.5 (5)
C7—C2—C1—O2	−50.7 (4)	C13—C12—C11—C10	2.2 (5)
I1—C3—C2—C1	−2.0 (4)	C14—C13—C12—C11	1.1 (6)
I1—C3—C2—C7	178.3 (2)	C9—C14—C13—C12	−3.2 (6)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H51 $\cdots$ O1 ⁱⁱ	0.86 (3)	1.64 (3)	2.486 (3)	167 (5)
O6—H61 $\cdots$ O2 ⁱ	0.86 (2)	1.92 (2)	2.742 (3)	161 (4)
C4—H4 $\cdots$ O1 ⁱⁱⁱ	0.95	2.56	3.364 (4)	142
C13—H13 $\cdots$ O4 ^{iv}	0.95	2.58	3.495 (4)	162

Symmetry codes: (i) $x+1/2, -y+1/2, -z+2$; (ii) $x-1/2, -y+1/2, -z+2$; (iii) $-x+2, y+1/2, -z+3/2$; (iv) $x-1/2, -y-1/2, -z+2$.