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Redetermination of *catena*-poly[diaqua(oxydiacetato-*O*,*O*′,*O*″)cobalt(II) monohydrate]

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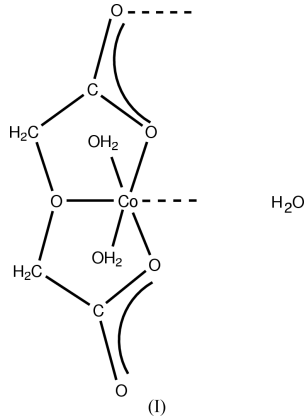
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.064
Data-to-parameter ratio = 13.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, *catena*-poly[[[diaquacobalt(II)]-μ-oxydiacetato-$\kappa^4O,O',O'':O'''$)cobalt(II)] monohydrate], $\{[Co(C_4H_4O_5)(H_2O)_2]\cdot H_2O\}_n$, (I), was first determined and reported by Hatfield *et al.* [*Proc. Indian Acad. Sci. Chem. Sci.* (1987), **98**, 23–31]. We present here a redetermination, with appreciably improved accuracy and successful location of H atoms. In the crystal structure, oxydiacetate plays the role of both chelating and bridging ligand, resulting in he formation of polymeric chains of complex molecules along the crystallographic *b* axis. Water molecules occupy the apical positions, thus completing the coordination octahedron of the Co^{II} atom. The polymeric chains are interlinked *via* intermolecular hydrogen bonding between carboxylate and water molecules, forming the three-dimensional supramolecular structure.



(I)

Experimental

A mixture of $CoCl_2$ (0.12 g, 0.5 mmol) and oxydiacetic acid monohydrate (0.076 g, 0.5 mmol) in acetonitrile (10 ml) was refluxed for several minutes until the solids had completely dissolved. A small amount of pyridine (80 µl) was introduced into the solution and a blue precipitate immediately appeared. Water (3 ml) was added dropwise, the blue precipitate gradually disappeared and the color of the solution changed to red. The red solution was refluxed for 30 min and then filtered. The filtrate was cooled and kept at room temperature. Red crystals were obtained after 2 d.

Crystal data

$[Co(C_4H_4O_5)(H_2O)_2]\cdot H_2O$
M_r = 245.05
Monoclinic, $P2_1/n$
a = 7.1220 (12) Å
b = 10.3935 (7) Å
c = 11.1259 (10) Å
β = 91.529 (10)°
V = 823.27 (17) Å^3
Z = 4
D_x = 1.977 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
θ = 5.0–10.3°
μ = 2.10 mm^{-1}
T = 298 (2) K
Prism, red
0.40 × 0.32 × 0.32 mm

Data collection

Rigaku AFC-7*S* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.451, T_{max} = 0.511
1757 measured reflections
1624 independent reflections
1458 reflections with $I > 2\sigma(I)$

R_{int} = 0.019
θ_{max} = 26.0°
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 12$
$l = -13 \rightarrow 13$
3 standard reflections
every 150 reflections
intensity decay: 0.7%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.064
S = 1.08
1624 reflections
118 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 0.4775P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected interatomic distances (Å).

Co—O1	2.1045 (14)	Co—O4	2.1041 (15)
Co—O2^{i}	2.0345 (14)	Co—O6	2.1213 (15)
Co—O3	2.0798 (15)	Co—O7	2.0841 (17)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H61···O4^{ii}	0.88	1.82	2.700 (2)	179
O6—H62···O5^{iii}	0.85	1.89	2.730 (2)	167
O7—H71···O5^{iv}	0.95	1.86	2.807 (2)	174
O7—H72···O8	0.86	1.87	2.687 (2)	158
O8—H81···O6^{v}	0.89	2.00	2.876 (2)	168
O8—H82···O1^{vi}	0.88	1.92	2.806 (2)	176

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

The H atoms of the methylene groups were placed in calculated positions, with C—H = 0.97 Å, and were included in the final cycles of refinement as riding, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atoms. The H atoms of the water molecule were located in a difference Fourier map and included in the structure-factor calculations with fixed positional and isotropic displacement parameters U_{iso} = 0.08 Å^2.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1985); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997).

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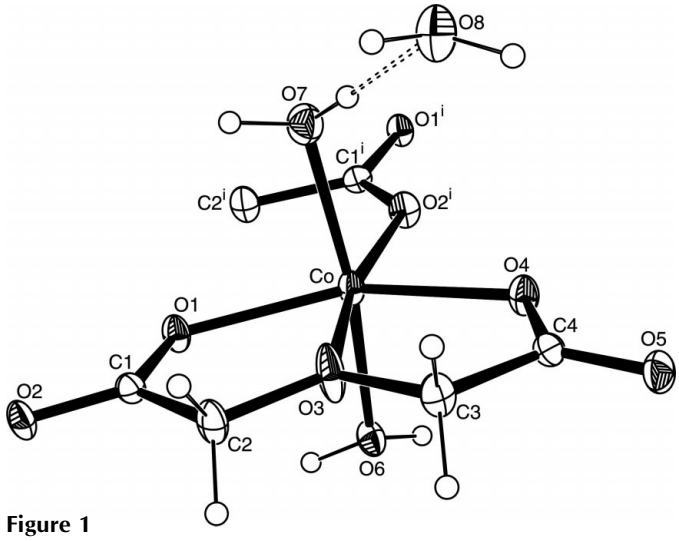

Figure 1
A section of the structure of the title compound, with 30% probability displacement ellipsoids, showing the Co-atom coordination environment (the symmetry code is as in Table 1).

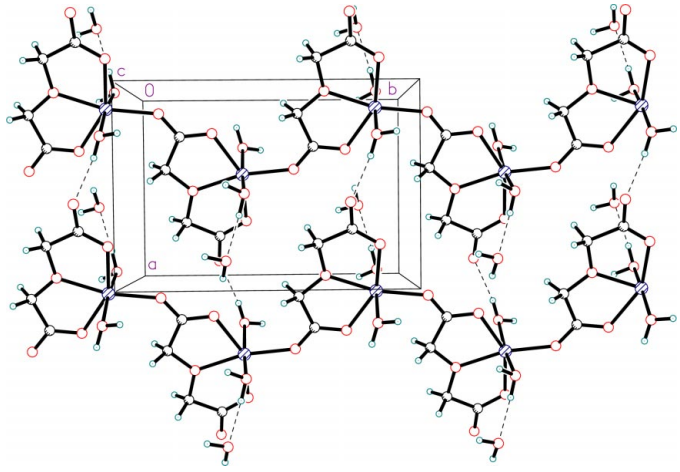

Figure 2
A packing diagram showing the polymeric chains linked by intermolecular hydrogen bonding between coordinated water and carboxylate groups.

References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hatfield, W. E., Helms, J. H., Rohrs, B. R., Singh, P., Wasson, J. R. & Weller R. R. (1987). *Proc. Indian Acad. Sci. Chem. Sci.* **98**, 23–31.
Molecular Structure Corporation (1985). *TEXSAN*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1992). *MSC/AFC Diffractometer Control Software*. Version 5.32. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.