# Diaquabis[malonato(1−)-$\kappa^2O,O'$]cobalt(II)

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**Key indicators**

Single-crystal X-ray study

$T = 292$ K

Mean $\sigma$(C–C) = 0.002 Å

$R$ factor = 0.031

$wR$ factor = 0.077

Data-to-parameter ratio = 13.3

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

The title complex, [Co($C_3H_3O_4$)$_2$($H_2O$)$_2$], is isostructural with its iron, zinc and magnesium analogues. The molecule has inversion symmetry. The molecules are linked together *via* O—H···O hydrogen bonds, leading to a three-dimensional network.

## Comment

The title complex, [Co(Hmal)$_2$($H_2O$)$_2$] ($H_2$mal is malonic acid), (I), is isostructural with its iron(II) (Ravi *et al.*, 1982), zinc (Sinha & Ojha, 1980) and magnesium (Briggman & Oskarsson, 1978) analogues. A compound with the same formula as (I) and a similar unit cell was reported by Walter-Levy *et al.* (1973), but no atomic coordinates were established.



(I)
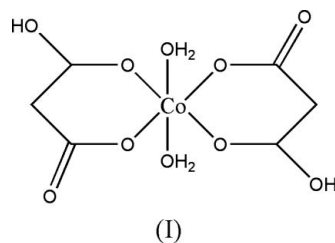
The complete molecule of (I) is generated by inversion symmetry (Fig. 1), resulting in a slightly distorted Co$^{II}$O$_6$ octahedron arising from two bidentate HMal ligands and two water molecules (Table 1). The fact that the Co1—O3 bond is significantly shorter than the Co1—O2 bond might be rationalized in terms of the formal negative charge shared between atoms O3 and O4, resulting in a stronger electrostatic attraction between atoms Co1 and O3 than between atoms Co1 and O2.
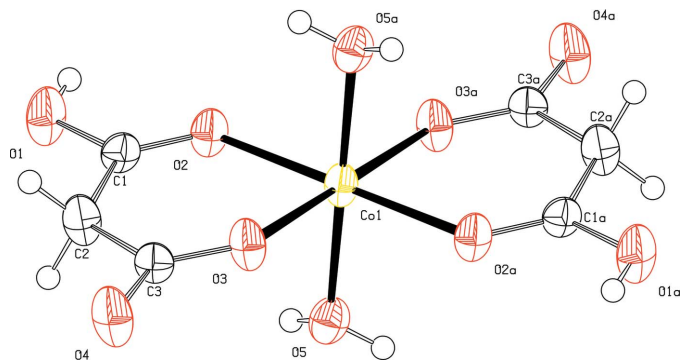


**Figure 1**

The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. Atoms with the suffix a are generated by the symmetry operation (−x, 1 − y, 1 − z).
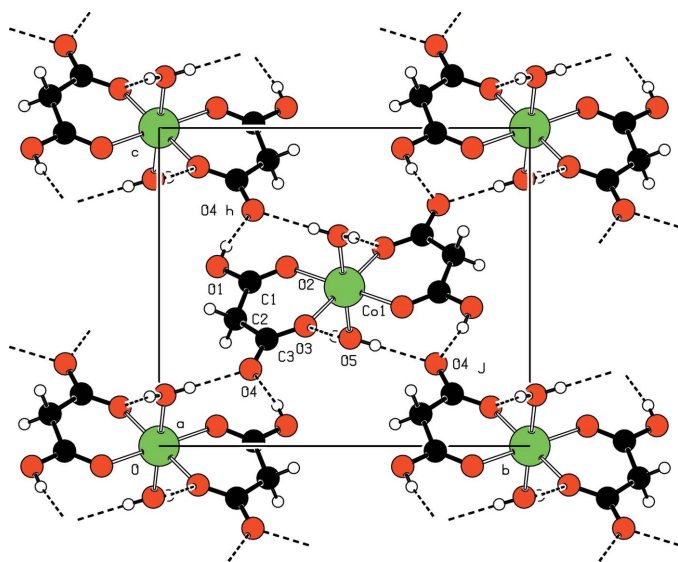
**Figure 2**
The crystal packing in (I), viewed down the *a* axis of the unit cell, showing hydrogen bonds as dashed lines. [Symmetry codes: (h) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (j) $x, \frac{1}{2} + y, \frac{1}{2} + z$.]

The molecules of (I) are linked together *via* O—H···O hydrogen bonds, leading to a three-dimensional network (Fig. 2, Table 2).

## Experimental

Solid cobalt basic carbonate (1.11 mmol, 0.593 g) was added to an aqueous solution (20 ml) of malonic acid (5.0 mmol, 0.520 g) under continuous stirring until a pink solution resulted. The solution was filtered and left at room temperature. After slow evaporation of the solvent over a period of a week, large pink crystals of (I) were formed (40% yield, based on Co). Analysis, found: C 23.98, H 3.42%; calculated for $C_6H_{10}CoO_{10}$: C 23.91, H 3.32%.

*Crystal data*

| | |
|---|---|
| $[Co(C_3H_3O_4)_2(H_2O)_2]$ | $D_x = 1.857$ Mg m$^{-3}$ |
| $M_r = 301.07$ | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1/c$ | Cell parameters from 2256 |
| $a = 4.9331$ (16) Å | reflections |
| $b = 11.276$ (4) Å | $\theta = 2.8$–28.0° |
| $c = 9.682$ (3) Å | $\mu = 1.64$ mm$^{-1}$ |
| $\beta = 90.018$ (1)° | $T = 292$ (2) K |
| $V = 538.6$ (3) Å$^3$ | Block, pink |
| $Z = 2$ | $0.30 \times 0.20 \times 0.10$ mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 1170 independent reflections |
| | 1070 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.061$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001) | $\theta_{max} = 27.0°$ |
| | $h = -6 \rightarrow 6$ |
| $T_{min} = 0.639$, $T_{max} = 0.853$ | $k = -10 \rightarrow 14$ |
| 3190 measured reflections | $l = -12 \rightarrow 11$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0457P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.031$ | $+ 0.0555P]$ |
| $wR(F^2) = 0.077$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1170 reflections | $\Delta\rho_{max} = 0.32$ e Å$^{-3}$ |
| 88 parameters | $\Delta\rho_{min} = -0.40$ e Å$^{-3}$ |
| H atoms treated by a mixture of independent and constrained refinement | |

**Table 1**
Selected geometric parameters (Å).

| | | | |
|---|---|---|---|
| Co1—O3 | 2.0488 (11) | C1—O2 | 1.2170 (19) |
| Co1—O2 | 2.0815 (12) | C3—O3 | 1.249 (2) |
| Co1—O5 | 2.0825 (15) | C3—O4 | 1.2492 (19) |
| C1—O1 | 1.3067 (19) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O4$^i$ | 0.82 | 1.80 | 2.6099 (17) | 168 |
| O5—H5$A$···O4$^{ii}$ | 0.81 (1) | 1.94 (1) | 2.747 (2) | 172 (2) |
| O5—H5$B$···O3$^{iii}$ | 0.82 (1) | 1.96 (1) | 2.767 (2) | 171 (2) |

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

H atoms bonded to C and carboxylate O atoms were placed in idealized positions (C—H = 0.97 Å and O—H = 0.82 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(carboxylate O). The water H atoms were found in a difference Fourier map and were refined with restraints on the O—H distance [0.811 (9)–0.815 (9) Å].

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

## References

Briggman, B. & Oskarsson, Å. (1978). *Acta Cryst.* B**34**, 3357–3359.
Bruker (2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Ravi, N., Jagannathan, R., Rao, B. B. & Hussain, M. R. (1982). *Inorg. Chem.* **21**, 1019–1022.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sinha, U. C. & Ojha, S. (1980). *Z. Kristallogr.* **152**, 157.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Walter-Levy, L., Perroyey, J. & Visser, J. W. (1973). *C. R. Acad. Sci. Ser. C*, **277**, 1351–1354.