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Disodium diaquabis(malonato-κ^2O,O')-cobalt(II) monohydrate

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In the title compound, $Na_2[Co(C_3H_2O_4)_2(H_2O)_2]\cdot H_2O$, the Co atom and two crystallographically independent Na^+ ions lie on twofold rotation axes. The Co atom is coordinated by four O atoms from two malonate ligands and two water molecules in a distorted octahedral geometry [Co—O = 1.595 (3)–2.219 (4) Å]. The two independent Na^+ ions are coordinated by six and eight O atoms, respectively [Na—O = 2.268 (4)–2.844 (3) Å]. A two-dimensional hydrogen-bonding network formed by O—H···O hydrogen bonds stabilizes the crystal structure.

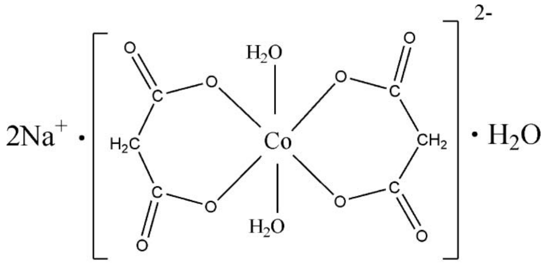
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.114
Data-to-parameter ratio = 14.2

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

Comment

Malonate is an important ligand for building metal-organic frameworks (MOFs) (Lightfoot & Snedden, 1999; Muro *et al.*, 1999; Wang *et al.*, 2004). Recently, we have reported the crystal structure of trisodium diaquabis(malonato-κ^2O,O')nickelate(II) chloride hexahydrate (Li *et al.*, 2006). Here we present the crystal structure of the title compound, (I).



(I)

In (I) (Fig.1), the Co atom lies on a twofold axis and is coordinated by the four O atoms from two malonate ligands and two water molecules in a distorted octahedral geometry (Table 1). Interestingly, the Co1—O6 bond length of 1.595 (3) Å is distinctly shorter than the other Co—O bonds (Table 1). Two crystallographically independent Na^+ ions are both located on twofold rotation axes and have different chemical environments. Na1 is coordinated by four O atoms from four malonate ligands and two O atoms from two water molecules. Na2 is coordinated by six O atoms from four malonate ligands and two O atoms from two water molecues. A two-dimensional hydrogen-bonding network formed by O—H···O hydrogen bonds (Table 2) stabilizes the crystal structure.

Experimental

Malonic acid and $CoCl_2\cdot 6H_2O$ of analytical grade were used without further purification. Malonic acid (2.08 g, 20 mmol) and $CoCl_2\cdot 6H_2O$

(2.38 g, 10 mmol) were dissolved in water (30 ml), and the pH was adjusted to about 5 using an NaOH solution (0.1 *M*) with stirring. The mixture was stirred for another hour and then filtered. The filtrate was allowed to stand at room temperature for several weeks, giving brown block-shaped crystals.

Crystal data

$Na_2[Co(C_3H_2O_4)_2(H_2O)_2]\cdot H_2O$
$M_r = 363.05$
Orthorhombic, $C222_1$
$a = 7.2503\ (15)$ Å
$b = 15.952\ (3)$ Å
$c = 10.371\ (2)$ Å
$V = 1199.5\ (4)$ Å^3
$Z = 4$
$D_x = 2.010$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.56$ mm^{-1}
$T = 295\ (2)$ K
Block, brown
$0.43 \times 0.41 \times 0.38$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.557$, $T_{max} = 0.590$ (expected range = 0.522–0.553)
5787 measured reflections
1348 independent reflections
1312 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.114$
$S = 1.25$
1348 reflections
95 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0723P)^2 + 1.3726P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.85$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-3}
Absolute structure: Flack (1983), 543 Friedel pairs
Flack parameter: 0.17 (3)

Table 1
Selected geometric parameters (Å, °).

Co1—O6	1.595 (3)	Na1—O7	2.321 (3)
Co1—O1	1.995 (2)	Na1—O4^{ii}	2.507 (3)
Co1—O3	2.016 (2)	Na2—O2^{iii}	2.418 (3)
Co1—O5	2.219 (4)	Na2—O4^{iv}	2.493 (3)
Na1—O6	2.268 (4)	Na2—O7	2.6917 (8)
Na1—O2^{i}	2.321 (2)	Na2—O3^{v}	2.844 (3)
O6—Co1—O1	98.32 (9)	O1—Co1—O3	88.62 (11)
O1^{vi}—Co1—O1	163.36 (18)	O3^{vi}—Co1—O3	159.50 (15)
O6—Co1—O3^{vi}	100.25 (7)	O6—Co1—O5	180.0
O1—Co1—O3^{vi}	88.43 (11)	O1—Co1—O5	81.68 (9)
O6—Co1—O3	100.25 (7)	O3—Co1—O5	79.75 (7)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O4^{vii}	0.85	1.90	2.743 (4)	176
O7—H3···O1^{iii}	0.85	1.98	2.797 (3)	162

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

C-bound H atoms were positioned geometrically (C—H = 0.97 Å) and treated as riding on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. The water H atoms were initially located in a difference Fourier map, but were idealized and refined as riding on their parent atoms, with O—H = 0.85 Å, H···H = 1.37 Å and $U_{iso}(H) = 1.5U_{eq}(O)$. The value of the Flack parameter suggests some inversion twinning.

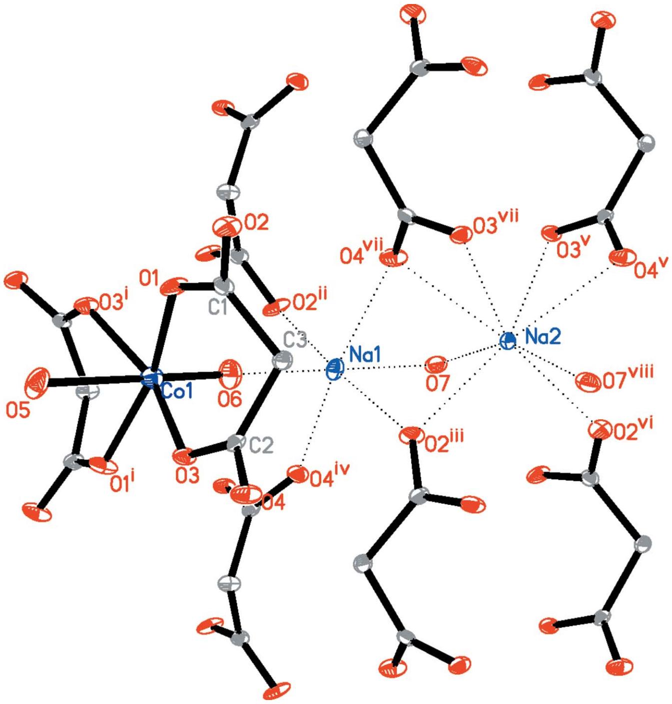


Figure 1
The structure of the title compound, showing the atom-labelling scheme [symmetry codes: (i) $-x+1, y, -z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (iv) $-x+\frac{3}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (vi) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (vii) $x-\frac{1}{2}, y+\frac{1}{2}, z$; (viii) $-x+1, -y+1, z+\frac{1}{2}$]. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

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: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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