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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.028
 wR factor = 0.091
Data-to-parameter ratio = 10.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[*diaqua-di- μ -malonato-cobalt(II)disodium(I)*]

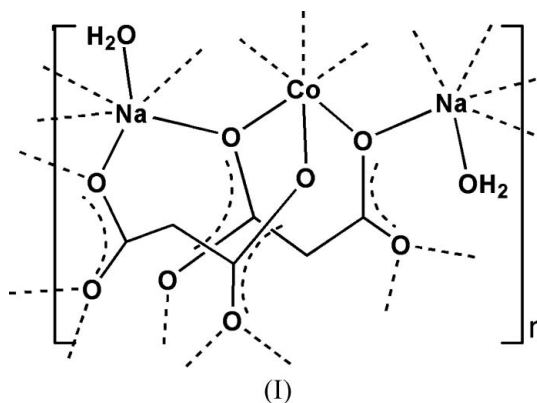
In the title compound, $[\text{CoNa}_2(\text{C}_3\text{H}_2\text{O}_4)_2(\text{H}_2\text{O})_2]_n$, a hetero-bimetallic malonate complex, both Co^{II} and Na^{I} ions have distorted octahedral coordination geometries. The Co^{II} ions are located on inversion centres and are surrounded only by carboxylate O atoms, while the Na^{I} ions are coordinated both by water and by carboxylate O atoms. The malonate dianions show an unusual heptadentate bridging mode.

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Comment

The malonate ion is known to be a versatile ligand since it can act as a monodentate or a multidentate ligand either in chelating or in bridging modes. Malonic acid has a wide use in many fields as a result of its excellent coordination ability. The complexes of malonic acid with lanthanide and transition metals have been used as fluorescent probes (Tsryuk *et al.*, 1977), solid fluorescent materials (Sun *et al.*, 1988) and magnetic materials (Ruiz-Perez, Sanchiz *et al.*, 2000; Ruiz-Perez, Hernandez-Molina *et al.*, 2000).



The title compound, (I) (Fig. 1), is isostructural with the previously reported diaquadisodiumdimalonatocopper(II) (Ghoshal *et al.*, 2005; Liu *et al.*, 2004; Deng *et al.*, 2002; Barnes & Weakley, 1997) and diaquadisodiumdimalonatozinc(II) (Lin *et al.*, 2003) complexes. The structure consists of an extended Co^{II} malonate network forming layers in the ab plane (Fig. 2). These layers are interlocked with the Na–water–malonate network, where the water molecules link the Na^{I} ions to form Na–O5(water)–Na zigzag chains. The Co^{II} and Na^{I} ions all have distorted octahedral coordination geometries (Table 1). The Co^{II} ions are located on inversion centres and are surrounded only by carboxylate O atoms, while the Na^{I} ions are coordinated both by water and by carboxylate O atoms. Each malonate dianion acts as a heptadentate ligand bridging two Co^{II} and four Na^{I} ions. The $\text{Co}\cdots\text{Na}$ shorter distance is

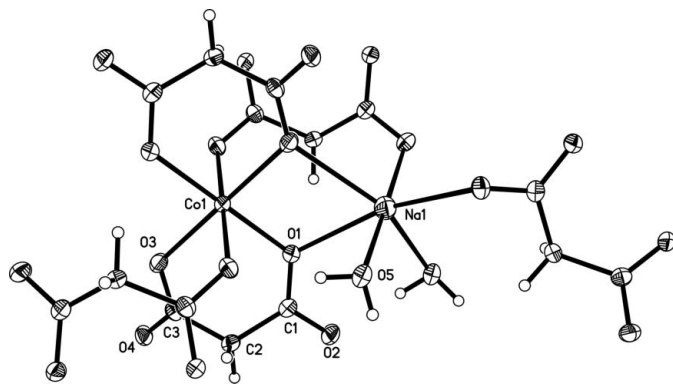


Figure 1
The asymmetric unit and selected symmetry-generated atoms, showing the coordination environments of the Co^{II} and Na^I ions.

3.5498 (16) Å and the Naⁱ··Naⁱⁱ distance is 3.7465 (19) Å [symmetry code (ii): $\frac{1}{2} + x, y, \frac{1}{2} - z$]. The Naⁱ··Naⁱ distance is shorter than those observed in the zinc and copper analogues [3.7751 (11) and 3.7860 (9) Å, respectively]. The coordinated water molecules donate their H atoms to neighbouring carboxylate groups, further strengthening the crystal cohesion (Table 2). In diaquadisodiumdimalonatocopper(II), a weak ferromagnetic interaction between the metal ions, mediated through the non-magnetic malonate ligands, was observed (Ghoshal *et al.*, 2005).

Experimental

All reagents and solvents were used as obtained without further purification. Malonic acid (21 mg) and sodium hydroxide (16 mg) were mixed in water (5 ml) and cobalt(II) chloride hexahydrate (24 mg) was added to afford a pink solution. After several days pink needles were obtained in 60% yield. Analysis calculated for C₆H₈CoNa₂O₁₀: C 20.89, H 2.34%; found: C 20.57, H 2.58%.

Crystal data

[CoNa ₂ (C ₃ H ₂ O ₄) ₂ (H ₂ O) ₂]	Z = 4
$M_r = 345.03$	$D_x = 2.190 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 6.7815 (16) \text{ \AA}$	$\mu = 1.77 \text{ mm}^{-1}$
$b = 9.348 (2) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 16.509 (4) \text{ \AA}$	Needles, pink
$V = 1046.6 (4) \text{ \AA}^3$	$0.18 \times 0.15 \times 0.11 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	4916 measured reflections
ϕ and ω scans	921 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	682 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.741, T_{\max} = 0.829$	$R_{\text{int}} = 0.038$
	$\sigma_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 0.1861P]$
$R[F^2 > 2\sigma(F^2)] = 0.028$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.091$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
921 reflections	$\Delta\rho_{\text{min}} = -0.35 \text{ e \AA}^{-3}$
88 parameters	
H-atom parameters constrained	

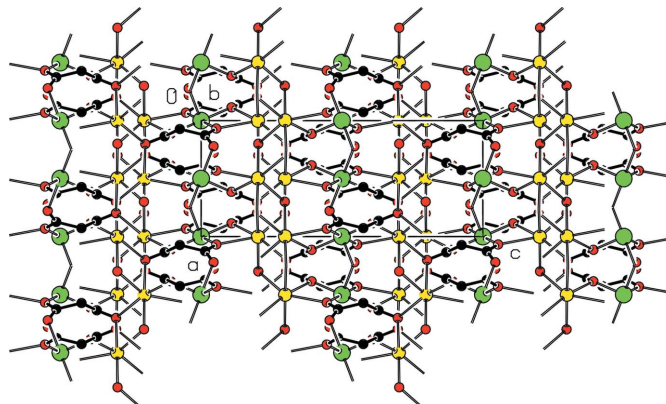


Figure 2
The three-dimensional network of the title compound. H atoms have been omitted for clarity.

Table 1

Selected bond lengths (Å).

Co1—O1	2.035 (2)	Na1—O5 ⁱⁱ	2.406 (3)
Co1—O3	2.101 (2)	Na1—O2 ⁱ	2.418 (3)
Co1—O4 ⁱ	2.205 (2)	Na1—O2 ⁱⁱⁱ	2.509 (3)
Na1—O5	2.359 (3)	Na1—O3 ^{iv}	2.553 (2)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H2···O4 ^v	0.85	1.95	2.777 (3)	163
O5—H1···O2 ^{vi}	0.85	1.86	2.706 (3)	174

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

Water H atoms were located in difference Fourier maps and refined as riding with an O—H distance of 0.85 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The remaining H atoms were placed in calculated positions and refined as riding with C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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