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Disodium diaquabis(malonato-κ^2O,O')nickelate(II) dihydrate

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In the title compound, $Na_2[Ni(C_3H_2O_4)_2(H_2O)_2]\cdot 2H_2O$, the Ni atom is coordinated by four O atoms from two malonate ligands and two water molecules in a distorted octahedral geometry. The two independent Na^+ ions are coordinated by five and six O atoms, respectively. The crystal structure is stabilized by the three-dimensional hydrogen-bonding network formed by O—H···O hydrogen bonds.

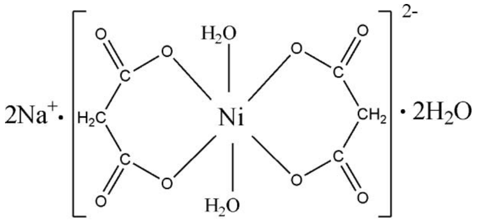
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.035
wR factor = 0.082
Data-to-parameter ratio = 15.0

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

Comment

Malonic acid has been widely used to build up supramolecular networks (Hemamalini *et al.*, 2006; Lightfoot & Snedden, 1999; Muro *et al.*, 1999). Recently, we have reported the crystal structures of trisodium diaquabis(malonato-κ^2O,O')nickel-')nickelate(II) chloride hexahydrate (Li *et al.*, 2006) and disodium diaquabis(malonato-κ^2O,O')cobaltate(II) monohydrate (Ye *et al.*, 2007). In our attempt to synthesize a nickel complex with malonic acid, we obtained two differently coloured crystals – colourless and green. We report here the crystal structure of the green title compound, (I).



(I)

In (I) (Fig. 1), the Ni atom is coordinated by four O atoms from two malonate ligands and two water molecules in a distorted octahedral geometry (Table 1). The two crystallographically independent Na^+ ions have different chemical environments. Na1 is coordinated by three O atoms from three malonate ligands and three O atoms from three water molecules. Na2 is coordinated by five O atoms from three malonate ligands and two O atoms from two water molecues. The three-dimensional hydrogen-bonding network formed by O—H···O hydrogen bonds (Table 2) stabilizes the crystal structure.

Experimental

Malonic acid and $NiBr_2\cdot 6H_2O$ of analytical grade were used without further purification. Malonic acid (1.04 g, 10 mmol) dissolved in dimethyl sulfoxide (10 ml) and $NiBr_2\cdot 6H_2O$ (1.64 g, 5 mmol) dissolved in water (10 ml) were mixed; the pH was adjusted to 5 by NaOH solution (0.1 *M*) with stirring. The mixture was heated with stirring for 0.5 h and then cooled to room temperature. The filtrate was allowed to stand overnight, yielding colourless and green block-shaped crystals.

Crystal data

$Na_2[Ni(C_3H_2O_4)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 380.85$
Orthorhombic, $P2_12_12_1$
$a = 7.287$ (3) Å
$b = 10.070$ (5) Å
$c = 17.646$ (10) Å
$V = 1294.9$ (11) Å^3
$Z = 4$
$D_x = 1.954$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.63$ mm^{-1}
$T = 291$ (2) K
Block, green
0.30 × 0.29 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.639$, $T_{\max} = 0.712$
11928 measured reflections
2858 independent reflections
2678 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.082$
$S = 1.01$
2858 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.94$ e Å^{-3}
$\Delta\rho_{\min} = -0.49$ e Å^{-3}
Absolute structure: Flack (1983), 1134 Friedel pairs
Flack parameter: −0.009 (15)

Table 1
Selected geometric parameters (Å, °).

Na1—O1^{i}	2.406 (3)	Na2—O11	2.468 (3)
Na1—O10	2.415 (3)	Na2—O12	2.572 (8)
Na1—O12	2.434 (6)	Na2—O6^{iii}	2.703 (4)
Na1—O11	2.458 (3)	Ni1—O5	2.009 (2)
Na1—O3	2.481 (3)	Ni1—O7	2.021 (2)
Na1—O12*A*	2.486 (12)	Ni1—O1	2.022 (2)
Na1—O5^{i}	2.494 (3)	Ni1—O3	2.032 (2)
Na2—O12*A*	2.178 (13)	Ni1—O10	2.088 (2)
Na2—O2^{ii}	2.339 (3)	Ni1—O9	2.091 (2)
Na2—O8	2.345 (4)		
O5—Ni1—O7	92.01 (9)	O1—Ni1—O10	89.85 (9)
O5—Ni1—O1	86.36 (8)	O3—Ni1—O10	85.49 (9)
O7—Ni1—O1	177.04 (10)	O5—Ni1—O9	90.58 (9)
O5—Ni1—O3	175.94 (9)	O7—Ni1—O9	89.99 (10)
O7—Ni1—O3	90.57 (9)	O1—Ni1—O9	92.49 (9)
O1—Ni1—O3	90.93 (9)	O3—Ni1—O9	92.55 (9)
O5—Ni1—O10	91.48 (9)	O10—Ni1—O9	176.97 (9)
O7—Ni1—O10	87.72 (10)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O9—H5···O4^{iv}	0.85	1.83	2.669 (3)	170
O9—H6···O8^{v}	0.85	1.83	2.677 (4)	171
O10—H8···O4^{vi}	0.85	1.79	2.614 (3)	165
O10—H7···O6^{i}	0.85	1.90	2.746 (4)	178
O11—H9···O2^{i}	0.85	1.99	2.813 (4)	162
O11—H10···O9^{vii}	0.85	2.17	3.004 (4)	164

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

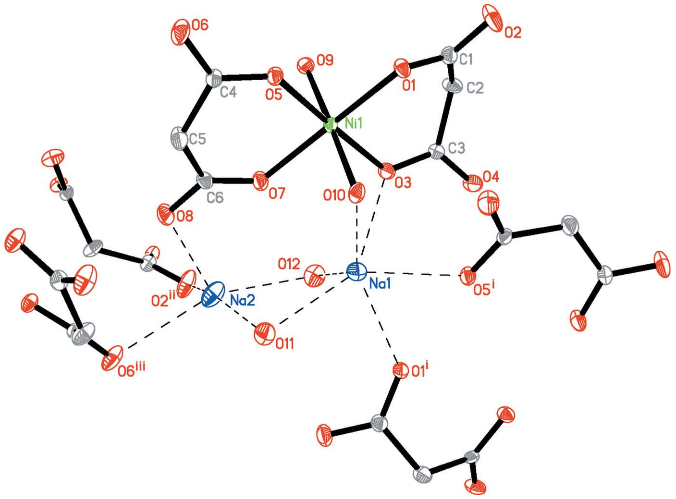


Figure 1
Part of the structure of the title complex with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Only the major component of the disordered atom O12 is shown. H atoms have been omitted. [Symmetry codes: (i) $1-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{3}{2}, 2-y, z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}$, 2 - z.].

C-bound H atoms were positioned geometrically (C—H = 0.97 Å) and refined as riding on their parent atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The uncoordinated water molecule was treated as disordered between two positions with refined occupancies of 0.616 (19) and 0.384 (19). The disordered atoms O12 and O12*A* were refined isotropically. 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 and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

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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