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Hexaaquanickel(II) bis[2-(4-carboxyphenoxy)-propionate] trihydrate

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In the title complex, $[Ni(H_2O)_6](C_{10}H_9O_5)_2\cdot 3H_2O$, two independent Ni atoms both lie on centers of symmetry and have an octahedral coordination. The cations and anions are linked by O—H$\cdots$O hydrogen bonds into a three-dimensional supramolecular framework.

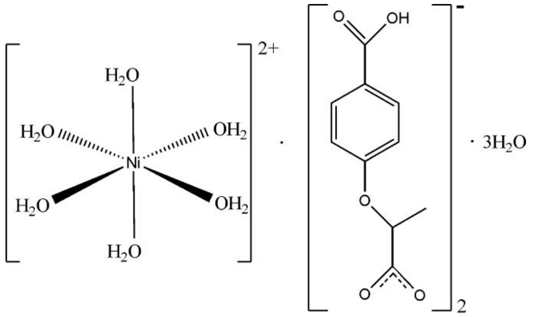
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
H-atom completeness 94%
Disorder in solvent or counterion
R factor = 0.036
wR factor = 0.105
Data-to-parameter ratio = 15.5

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

Comment

An earlier report (Deng *et al.*, 2007) detailed the synthesis and crystal structure of [2-(4-carboxylatophenoxy)propionato]-cobalt(II) hexahydrate. Replacing cobalt by nickel in a similar reaction leads to the formation of the title compound, (I) (Fig. 1), which is also a hexahydrated complex. The two Ni^{II} atoms both lie on centers of symmetry and are six-coordinate in an octahedral environment; the Ni—O bond lengths are somewhat shorter than the Co—O bond distances [2.0310 (17)–2.0685 (16) Å]. Similarly, the cations and anions are linked by extensive hydrogen bonds into a three-dimensional supramolecular network (Table 2).



(I)

Experimental

Nickel(II) acetate trihydrate (2.31 g, 10 mmol) was added to a hot aqueous solution of 2-(4-carboxyphenoxy)propionic acid (2.10 g, 10 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until the solution registered a pH of 6. The filtered solution was allowed to evaporate at room temperature, and green prismatic crystals of (I) were separated from the filtered solution after several days. Analysis calculated for $C_{40}H_{72}Ni_2O_{38}$: C 37.58, H 5.68%; found: C 37.63, H 5.66%.

Crystal data

$[Ni(H_2O)_6](C_{10}H_9O_5)_2\cdot 3H_2O$
M_r = 637.18
Monoclinic, $P2_1/n$
a = 7.9771 (16) Å
b = 13.265 (3) Å
c = 27.308 (6) Å
β = 96.17 (3)°
V = 2872.9 (10) Å^3
Z = 4
D_x = 1.473 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.76 mm^{-1}
T = 295 (2) K
Prism, green
0.36 × 0.24 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\rm min} = 0.772$, $T_{\rm max} = 0.863$

27742 measured reflections
6573 independent reflections
4873 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\rm max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.105$
$S = 1.08$
6573 reflections
424 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.9359P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.49$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.35$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O2*W*	2.0397 (14)	Ni2—O4*W*	2.0310 (17)
Ni1—O3*W*	2.0491 (14)	Ni2—O5*W*	2.0385 (17)
Ni1—O1*W*	2.0648 (15)	Ni2—O6*W*	2.0685 (16)
O2*W*—Ni1—O2*W*$^{\rm i}$	180	O4*W*—Ni2—O4*W*$^{\rm ii}$	180
O2*W*—Ni1—O3*W*	87.95 (6)	O4*W*—Ni2—O5*W*	89.59 (10)
O2*W*$^{\rm i}$—Ni1—O3*W*	92.05 (6)	O4*W*$^{\rm ii}$—Ni2—O5*W*	90.41 (10)
O3*W*—Ni1—O3*W*$^{\rm i}$	180	O5*W*—Ni2—O5*W*$^{\rm ii}$	180
O2*W*—Ni1—O1*W*$^{\rm i}$	86.29 (7)	O4*W*—Ni2—O6*W*	90.73 (8)
O3*W*—Ni1—O1*W*$^{\rm i}$	90.87 (6)	O4*W*$^{\rm ii}$—Ni2—O6*W*	89.27 (8)
O2*W*—Ni1—O1*W*	93.71 (7)	O5*W*—Ni2—O6*W*	90.18 (7)
O3*W*—Ni1—O1*W*	89.13 (6)	O5*W*$^{\rm ii}$—Ni2—O6*W*	89.82 (7)
O1*W*$^{\rm i}$—Ni1—O1*W*	180	O6*W*—Ni2—O6*W*$^{\rm ii}$	180

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+1, -y+1, -z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O5$^{\rm i}$	0.827 (9)	1.968 (10)	2.792 (2)	175 (2)
O1*W*—H1*W*2···O8*W*	0.831 (19)	1.975 (10)	2.801 (2)	173 (3)
O2*W*—H2*W*1···O9*W*$^{\rm iii}$	0.81 (2)	1.939 (13)	2.726 (2)	162 (3)
O2*W*—H2*W*2···O2$^{\rm iv}$	0.811 (9)	1.943 (12)	2.738 (2)	166 (3)
O3*W*—H3*W*1···O4	0.837 (9)	1.805 (11)	2.636 (2)	171 (2)
O3*W*—H3*W*2···O9$^{\rm v}$	0.83 (2)	2.079 (13)	2.862 (2)	158 (2)
O4*W*—H4*W*1···O7$^{\rm vi}$	0.821 (10)	1.965 (11)	2.781 (2)	173 (4)
O4*W*—H4*W*2···O9*W*$^{\rm ii}$	0.820 (10)	1.98 (3)	2.766 (2)	160 (3)
O6*W*—H6*W*1···O10	0.83 (3)	1.851 (10)	2.675 (2)	174 (3)
O6*W*—H6*W*2···O5	0.821 (9)	2.452 (18)	3.135 (2)	141 (2)
O8*W*—H8*W*1···O7$^{\rm iv}$	0.83 (3)	1.96 (3)	2.788 (2)	176 (3)
O8*W*—H8*W*2···O2$^{\rm iv}$	0.83 (3)	1.991 (10)	2.809 (2)	170 (3)
O9*W*—H9*W*1···O5	0.841 (9)	1.922 (11)	2.750 (2)	168 (3)
O9*W*—H9*W*2···O9	0.85 (2)	1.894 (10)	2.737 (2)	172 (3)
O1—H1*O*···O4$^{\rm vii}$	0.818 (10)	1.827 (11)	2.6401 (19)	172 (3)
O6—H6*O*···O10$^{\rm viii}$	0.810 (10)	1.847 (11)	2.6522 (19)	173 (3)

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

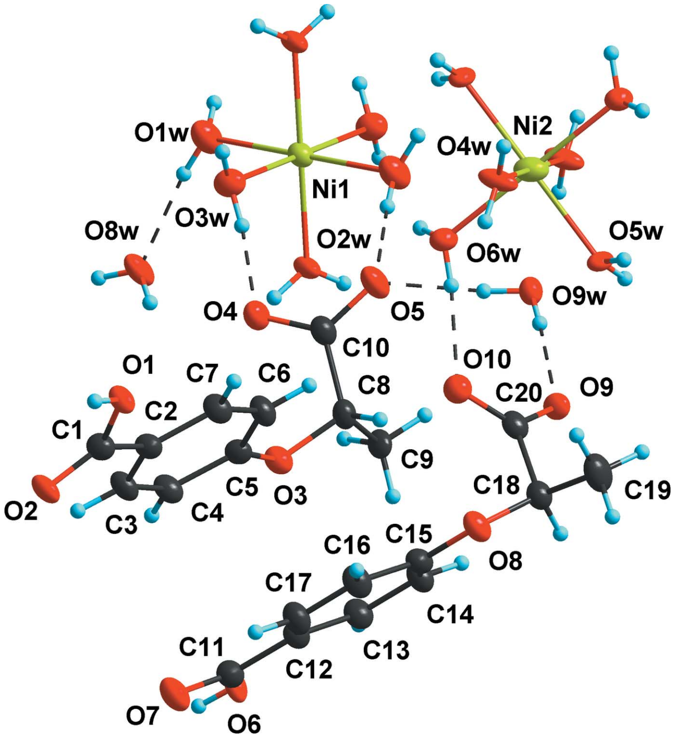


Figure 1
The structure of the independent components of (I). The disordered water molecule is not shown. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius. Hydrogen bonds are shown as dashed lines. Unlabeled atoms in the Ni1 cation are related to labeled atoms by $(-x, -y, -z)$. Unlabeled atoms in the Ni2 cation are related to labeled atoms by $(1-x, 1-y, -z)$.

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.93–0.97Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl or $1.2U_{\rm eq}({\rm C})$ for other H atoms, and were refined in the riding-model approximation. The uncoordinated water molecule O7*W* is disordered over two positions; the occupancies of O7*W* and O7*W*′ refined to 0.755 (3) and 0.245 (3), respectively. H atoms could not be placed in any chemical sensible positions owing to the disorder. Other H atoms of the water molecules and hydroxyl groups were located in a difference Fourier map and refined with O—H and H···H distance restraints of 0.82 (1) and 1.39 (1) Å, respectively, and with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

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: *ORTEP*-II (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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