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## Key indicators

Single-crystal X-ray study

T = 298 K

Mean  $\sigma(\text{C}-\text{C}) = 0.010 \text{ \AA}$ 

R factor = 0.047

wR factor = 0.113

Data-to-parameter ratio = 8.9

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

## Diaquadi(L-lactato)nickel(II)

The two L-lactate groups in diaquadi(L-lactato)nickel(II),  $[\text{Ni}(\text{C}_3\text{H}_5\text{O}_3)_2(\text{H}_2\text{O})_2]$ , chelate to the Ni atom through their carboxyl and hydroxy O atoms; the water molecules occupy *cis* positions in the coordination octahedron of the metal atom. The water molecules and hydroxy groups are engaged in hydrogen bonds, to furnish a tightly held three-dimensional network structure.

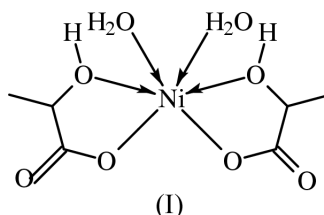
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## Comment

Lactic acid is a biologically important compound that binds strongly to metal ions. The crystal structures of a number of metal lactates and their complexes have been reported (Carballo *et al.*, 2002). Our interest in nickel lactate arises from our studies on the nickel derivatives of optically active carboxylic acids; we have recently reported the structure of the L-hydroxysuccinate (Zhou *et al.*, 2002). In this compound, the Ni atom is coordinated by two water molecules and the diaquanickel entity is linked by the dicarboxylate dianion into a helical chain. In the title compound, (I), however, the two L-lactate groups chelate to the Ni atom through the carboxyl and hydroxy O atoms; the water molecules occupy *cis* positions in the coordination octahedron of the Ni atom. The chelating mode of the anionic lactate group is also maintained in the bis(L-lactato)(*N,N,N',N'*-tetramethylenediamine)nickel(II) complex (Ahlgrén & Turpeinen, 1977).



In (I), an extensive hydrogen-bonding system involving all six 'active' H atoms (Table 2) links the molecules into a tightly held three-dimensional network structure.

## Experimental

Nickel lactate was prepared by the reaction of nickel chloride (2.38 g, 10 mmol) and L-lactic acid (1.80 g, 20 mmol). The reagents were dissolved in water; the pH of the solution was adjusted to 3 by the addition of 2 N sodium hydroxide solution. The solution was kept at 343 K for 24 h. The compound was isolated from solution in about 50% yield. CH analysis, found: C 26.0, H 5.0%; calculated for  $\text{C}_6\text{H}_{14}\text{NiO}_8$ : C 26.4, H 5.2%. UV-vis (reflectance):  $\lambda_{\text{max}}$  658 nm. IR (KBr plate):  $\nu_{\text{as}}(\text{COO})$  1598 (*br, s*);  $\nu_{\text{s}}(\text{COO})$  1485 (*m*), 1438 (*m*), 1413 (*s*);  $\nu(\text{Ni}-\text{O})$  800 (*m*)  $\text{cm}^{-1}$ .

## Crystal data

[Ni(C<sub>3</sub>H<sub>5</sub>O<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]  
*M<sub>r</sub>* = 272.88  
 Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>  
*a* = 6.033 (1) Å  
*b* = 11.805 (1) Å  
*c* = 14.354 (1) Å  
*V* = 1022.3 (2) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.773 Mg m<sup>-3</sup>

## Data collection

Enraf–Nonius CAD-4  
 diffractometer  
 $\omega$  scans  
 Absorption correction: empirical  
 via  $\psi$  scan (North *et al.*, 1968)  
*T<sub>min</sub>* = 0.611, *T<sub>max</sub>* = 0.698  
 1375 measured reflections  
 1375 independent reflections

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.047  
*wR*(*F*<sup>2</sup>) = 0.113  
*S* = 1.01  
 1375 reflections  
 154 parameters  
 H atoms treated by a mixture of  
 independent and constrained  
 refinement  
*w* = 1/[ $\sigma^2(F_o^2) + (0.0602P)^2$ ]  
 where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

Mo *K* $\alpha$  radiation  
 Cell parameters from 25  
 reflections  
 $\theta$  = 12.0–15.0°  
 $\mu$  = 1.92 mm<sup>-1</sup>  
*T* = 298 (2) K  
 Block, green  
 0.30 × 0.19 × 0.15 mm

1138 reflections with *I* > 2 $\sigma$ (*I*)  
 $\theta_{\max}$  = 27.5°  
*h* = 0 → 7  
*k* = 0 → 15  
*l* = 0 → 18  
 3 standard reflections  
 frequency: 60 min  
 intensity decay: none

( $\Delta/\sigma$ )<sub>max</sub> = 0.001  
 $\Delta\rho_{\max}$  = 0.78 e Å<sup>-3</sup>  
 $\Delta\rho_{\min}$  = -0.57 e Å<sup>-3</sup>  
 Absolute structure: Flack &  
 Schwarzenbach (1988), no Friedel  
 pairs; the absolute configuration  
 is in agreement with known  
 L-lactate  
 Flack parameter for absolute  
 structure determination = 0.00 (4)

Table 1

Selected geometric parameters (Å, °).

Ni1–O1	2.075 (5)	Ni1–O6	2.046 (4)
Ni1–O3	2.017 (4)	Ni1–O1w	2.077 (5)
Ni1–O5	2.025 (4)	Ni1–O2w	2.031 (4)
O1–Ni1–O3	78.7 (2)	O3–Ni1–O2w	91.8 (2)
O1–Ni1–O5	91.8 (2)	O5–Ni1–O6	78.5 (2)
O1–Ni1–O6	98.5 (2)	O5–Ni1–O1w	88.3 (2)
O1–Ni1–O1w	171.6 (2)	O5–Ni1–O2w	175.5 (2)
O1–Ni1–O2w	91.0 (2)	O6–Ni1–O1w	89.7 (2)
O3–Ni1–O5	92.2 (2)	O6–Ni1–O2w	97.6 (2)
O3–Ni1–O6	170.3 (2)	O1w–Ni1–O2w	89.4 (2)
O3–Ni1–O1w	92.9 (2)		

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O1w–H1w1...O1 <sup>i</sup>	0.85 (1)	2.11 (3)	2.911 (6)	158 (7)
O1w–H1w2...O5 <sup>ii</sup>	0.85 (1)	1.93 (2)	2.778 (7)	174 (7)
O2w–H2w2...O2 <sup>i</sup>	0.85 (1)	1.92 (2)	2.735 (7)	162 (7)
O2w–H2w1...O4 <sup>iii</sup>	0.85 (1)	1.85 (2)	2.687 (7)	170 (7)
O3–H3o...O4 <sup>ii</sup>	0.85 (1)	1.81 (1)	2.657 (7)	176 (8)
O6–H6o...O2 <sup>iv</sup>	0.85 (1)	1.91 (4)	2.658 (6)	147 (7)

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

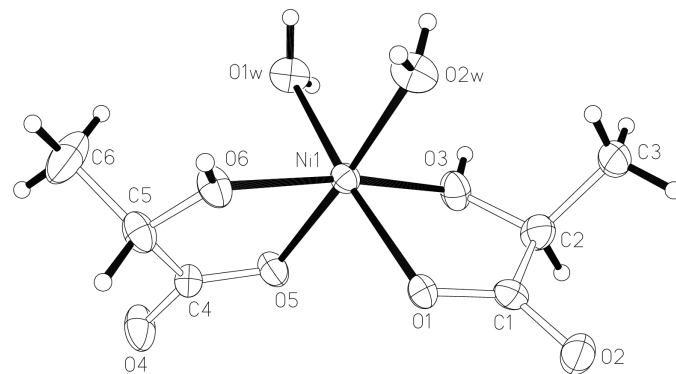


Figure 1

ORTEP II (Johnson, 1976) plot of the title complex, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

The hydroxyl and water H atoms were located and refined, subject to the following constraints: O–H = 0.85 ± 0.01 Å and H...H = 1.39 ± 0.01 Å; *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(O). The methyl and methine H atoms were generated geometrically and were allowed to ride on their parent C atoms, with *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub> for methyl and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub> for methine H atoms.

Data collection: CAD-4 VAX/PC (Enraf–Nonius, 1988); cell refinement: CAD-4 VAX/PC; data reduction: NRCVAX (Gabe *et al.*, 1989); 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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