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# Diaquadi(L-lactato)nickel(II)

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**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.010 Å
*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.



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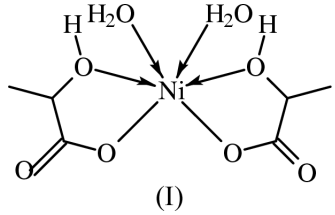
The two L-lactate groups in diaquadi(L-lactato)nickel(II), $[Ni(C_3H_5O_3)_2(H_2O)_2]$, chelate to the Ni atom through their carboxyl and hydroxy O atoms; the water molecules occupy *cis* positions in the coordination octahedron of the metal atom. The water molecules and hydroxy groups are engaged in hydrogen bonds, to furnish a tightly held three-dimensional network structure.

## 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).




(I)

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 $C_6H_{14}NiO_8$: C 26.4, H 5.2%. UV-vis (reflectance): $\lambda_{max}$ 658 nm. IR (KBr plate): $\nu_{as}$(COO) 1598 (*br*, *s*); $\nu_s$(COO) 1485 (*m*), 1438 (*m*), 1413 (*s*); $\nu$(Ni—O) 800 (*m*) cm$^{-1}$.

*Crystal data*

$[Ni(C_3H_5O_3)_2(H_2O)_2]$
$M_r$ = 272.88
Orthorhombic, $P2_12_12_1$
$a$ = 6.033 (1) Å
$b$ = 11.805 (1) Å
$c$ = 14.354 (1) Å
$V$ = 1022.3 (2) Å$^3$
$Z$ = 4
$D_x$ = 1.773 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 12.0–15.0°
$\mu$ = 1.92 mm$^{-1}$
$T$ = 298 (2) K
Block, green
0.30 × 0.19 × 0.15 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega$ scans
Absorption correction: empirical *via* $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.611, $T_{max}$ = 0.698
1375 measured reflections
1375 independent reflections
1138 reflections with $I > 2\sigma(I)$
$\theta_{max}$ = 27.5°
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 15$
$l = 0 \rightarrow 18$
3 standard reflections
frequency: 60 min
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.78 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.57 e Å$^{-3}$
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—O1*w* | 2.077 (5) |
| Ni1—O5 | 2.025 (4) | Ni1—O2*w* | 2.031 (4) |
| | | | |
| O1—Ni1—O3 | 78.7 (2) | O3—Ni1—O2*w* | 91.8 (2) |
| O1—Ni1—O5 | 91.8 (2) | O5—Ni1—O6 | 78.5 (2) |
| O1—Ni1—O6 | 98.5 (2) | O5—Ni1—O1*w* | 88.3 (2) |
| O1—Ni1—O1*w* | 171.6 (2) | O5—Ni1—O2*w* | 175.5 (2) |
| O1—Ni1—O2*w* | 91.0 (2) | O6—Ni1—O1*w* | 89.7 (2) |
| O3—Ni1—O5 | 92.2 (2) | O6—Ni1—O2*w* | 97.6 (2) |
| O3—Ni1—O6 | 170.3 (2) | O1*w*—Ni1—O2*w* | 89.4 (2) |
| O3—Ni1—O1*w* | 92.9 (2) | | |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*w*—H1*w*1···O1$^{i}$ | 0.85 (1) | 2.11 (3) | 2.911 (6) | 158 (7) |
| O1*w*—H1*w*2···O5$^{ii}$ | 0.85 (1) | 1.93 (2) | 2.778 (7) | 174 (7) |
| O2*w*—H2*w*2···O2$^{i}$ | 0.85 (1) | 1.92 (2) | 2.735 (7) | 162 (7) |
| O2*w*—H2*w*1···O4$^{iii}$ | 0.85 (1) | 1.85 (2) | 2.687 (7) | 170 (7) |
| O3—H3*o*···O4$^{ii}$ | 0.85 (1) | 1.81 (1) | 2.657 (7) | 176 (8) |
| O6—H6*o*···O2$^{iv}$ | 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) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$.

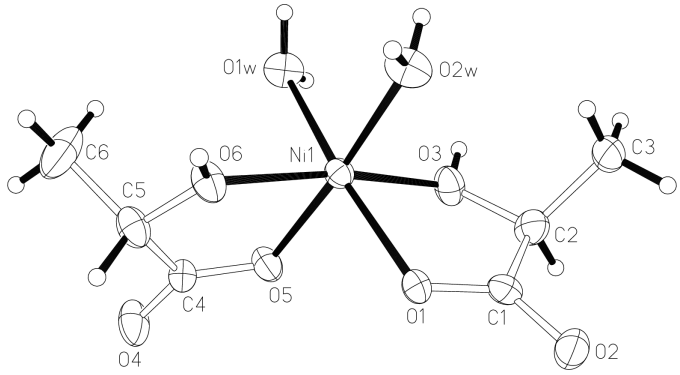



**Figure 1**
*ORTEP*II (Johnson, 1976) plot of the title complex, with displacement ellispoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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; $U_{iso}$(H) = 1.2$U_{eq}$(O). The methyl and methine H atoms were generated geometrically and were allowed to ride on their parent C atoms, with $U_{iso}$(H) = 1.5$U_{eq}$ for methyl and $U_{iso}$(H) = 1.2$U_{eq}$ 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: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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