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Diaquabis(D-valinato-κ^2N,O)nickel(II)

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Key indicators

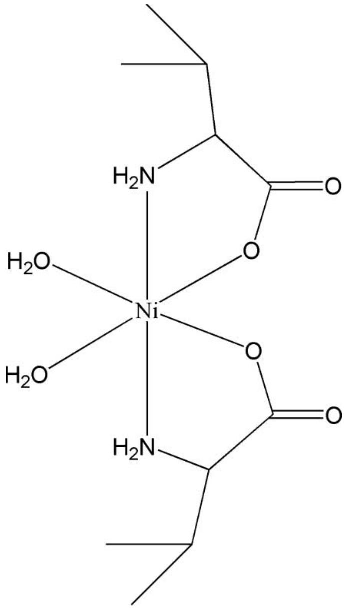
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.012 Å
R factor = 0.052
wR factor = 0.141
Data-to-parameter ratio = 13.0

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

In the title complex, diaquabis(2-amino-3-methylbutyrato-κ^2N,O)nickel(II), $[Ni(C_5H_{10}NO_2)_2(H_2O)_2]$, the Ni^{II} atom (site symmetry 2) is octahedrally coordinated by two N,O-bidenate valinate ions and two water molecules. A network of intermolecular hydrogen bonds links the complex molecules into a two-dimensional network.

Comment

As well as being the basic building blocks of proteins or enzymes, amino acids are versatile ligands showing flexible coordination modes (Lou *et al.*, 2005) and they can coordinate to metal ions by their carboxylate and/or amino groups. Amino acid–metal complexes and their derivatives are of great importance because of their biochemical and pharmacological properties (Patrick *et al.*, 2003). Valine is an essential amino acid (Ooiwa *et al.*, 1995), and it can chelate to metal ions *via* its amino N atom and carboxylate O atom (Zhou *et al.*, 2005). We report here the title compound, (I) (Fig. 1), a new chiral complex of Ni^{II} with valinate anions and water molecules.



(I)

The structure of (I) is formed of mononuclear diaquabis(D-valinato)nickel(II) units, in which the Ni^{II} ion (site symmetry 2) shows octahedral coordination geometry by binding to two bidentate valinate ions and two *cis* water molecules. Each valinate ion chelates to the metal ion through its amino N atom and one of the carboxylate O atoms. The Ni—O_c (c =

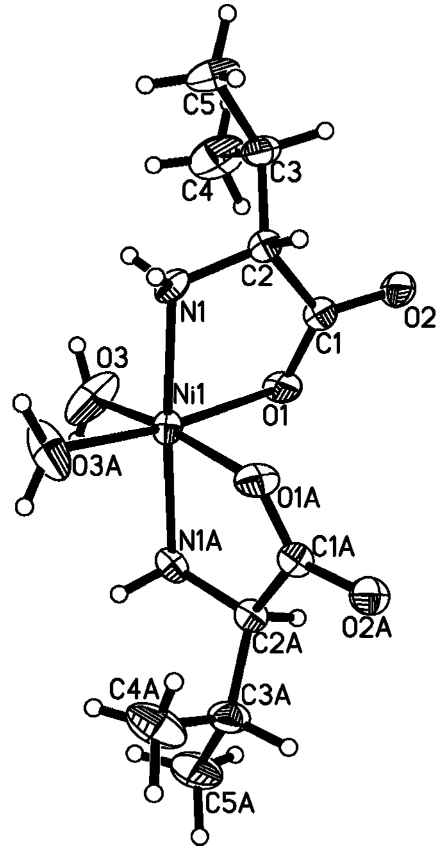


Figure 1
A view of the molecular structure of (I), showing the atom-numbering scheme and 30% displacement ellipsoids (arbitrary spheres for the H atoms). Atoms with the suffix A are generated by the symmetry operation $(1 - x, y, 1 - z)$.

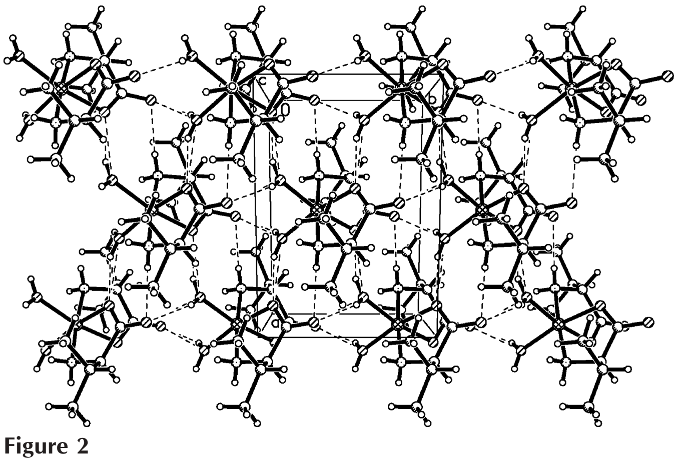


Figure 2
The packing for (I), viewed down [001], showing hydrogen bonds as dashed lines.

carboxylate), Ni—O$_w$ (w = water) and Ni—N bond distances (Table 1) agree well with published results for related complexes (Gong *et al.*, 1997). The C—O bond of the non-coordinated carboxylate O atom [C1—O2 = 1.244 (11) Å] is only slightly shorter than the coordinated bond to the Ni ion [C1—O1 = 1.261 (9) Å], suggesting the involvement of atom O2 in hydrogen bonding, as described below (Abdel-Rahmand *et al.*, 1996; Menabue *et al.*, 1998).

The crystal packing of (I) (Fig. 2) involves both N—H⋯O and O—H⋯O hydrogen bonds (Table 2). The coordinated carboxylate O1 atom accepts an intermolecular hydrogen bond from the O3 water molecule. The non-coordinated atom O2 accepts hydrogen bonds from the O3—H3*A* and N1—H1*B* groups of two different adjacent molecules. These interactions result in a two-dimensional network of hydrogen bonds.

Experimental

DL-Valine (0.1172 g, 1.0 mmol) was dissolved in water (5 ml), and a solution of $NiCl_2{\cdot}6H_2O$ (0.1188 g, 0.5 mmol) in water (5 ml) was added. The mixture was stirred at 353 K for 2 h and then cooled and filtered. The filtrate was allowed to evaporate slowly at room temperature. One month later, green block-shaped crystals of (I) were obtained.

Crystal data

$[Ni(C_5H_{10}NO_2)_2(H_2O)_2]$
$M_r = 327.02$
Monoclinic, $C2$
$a = 9.863$ (5) Å
$b = 6.458$ (3) Å
$c = 13.007$ (7) Å
$\beta = 111.199$ (8)°
$V = 772.3$ (7) Å^3
$Z = 2$
$D_x = 1.406$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 770 reflections
$\theta = 3.4$–23.4°
$\mu = 1.28$ mm^{-1}
$T = 293$ (2) K
Block, green
0.18 × 0.14 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.805$, $T_{max} = 0.881$
2215 measured reflections
1160 independent reflections
1014 reflections with $I > 2\sigma(I)$
$R_{int} = 0.065$
$\theta_{max} = 26.3°$
$h = -12 \rightarrow 11$
$k = -8 \rightarrow 4$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.141$
$S = 1.10$
1160 reflections
89 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0813P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.84$ e Å^{-3}
$\Delta\rho_{min} = -1.04$ e Å^{-3}
Absolute structure: Flack (1983), 305 Friedel pairs
Flack parameter: −0.03 (4)

Table 1
Selected bond lengths (Å).

Ni1—O1	2.046 (7)	Ni1—N1	2.076 (4)
Ni1—O3	2.059 (7)		

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*A*⋯O2^i	0.90	2.19	3.076 (7)	170
O3—H3*A*⋯O2^{ii}	0.85	1.95	2.644 (11)	138
O3—H3*B*⋯O1^{iii}	0.85	1.93	2.688 (10)	148

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

m2238 Bian *et al.* • $[Ni(C_5H_{10}NO_2)_2(H_2O)_2]$ *Acta Cryst.* (2005). E**61**, m2237–m2239

The chosen crystal of (I) has a well defined chiral structure. As the amino acid starting material was racemic, we must assume that crystallization resulted in a random mixture of enantiomers containing either the D or L forms of the valinate ion. The H atoms of the water molecules were located in a difference Fourier map, relocated in idealized positions (O—H = 0.85 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(O). H atoms on C and N atoms were positioned geometrically and refined using a riding model, with C—H = 0.96–0.98 Å, N—H = 0.90 Å and U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl carrier). The minimum electron-density peak is located 1.13 Å from atom Ni1.

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

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Acta Cryst. (2005). E**61**, m2237–m2239 Bian *et al.* • [Ni($C_5H_{10}NO_2$)$_2$(H_2O)$_2$] **m2239**