

Bis[2-hydroxy-3-(1*H*-imidazol-4-yl)propionato]-nickel(II)

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Key indicators

Single-crystal X-ray study

 $T = 296\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$ R factor = 0.019 wR factor = 0.057

Data-to-parameter ratio = 9.6

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

In the title compound, $[\text{Ni}(\text{C}_6\text{H}_7\text{N}_2\text{O}_3)_2]$, the Ni^{II} ion has a slightly distorted octahedral coordination geometry and lies on a twofold rotation axis. 2-Hydroxy-3-(1*H*-imidazol-4-yl)propionic acid ligates in a tridentate manner. Two carboxylate-O atoms and two hydroxyl-O atoms are coordinated in *cis* positions with respect to each other and form the equatorial plane, and two imidazole-N atoms are coordinated in axial positions. The molecules are held together by an intermolecular hydrogen-bonding network involving the carboxylate, imino and hydroxyl groups.

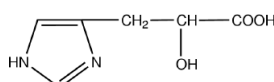
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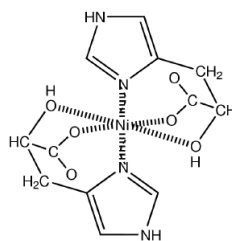
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Comment

2-Hydroxy-3-(1*H*-imidazol-4-yl)propionic acid [*L*- β -imidazolelactic acid, (I)] is one of the final catabolites of *L*-histidine. Patients with liver cirrhosis or histidinemia have high urinary concentrations of (I) (Dubovsky & Duvovska, 1965; Murray *et al.*, 1993). It also has an inhibitory action on cholinesterase and monoamine oxidase (Kurocochi *et al.*, 1956). Understanding the coordination ability and diversity of biologically important metal ions is helpful in clarifying their functions in biological systems. Hitherto the crystal structure of the Co^{II} complex has been determined (Okabe & Adachi, 1999). In this study, we have crystallized another metal complex, the Ni^{II} complex, (II), and its structure analysis has been undertaken.



(I)



(II)

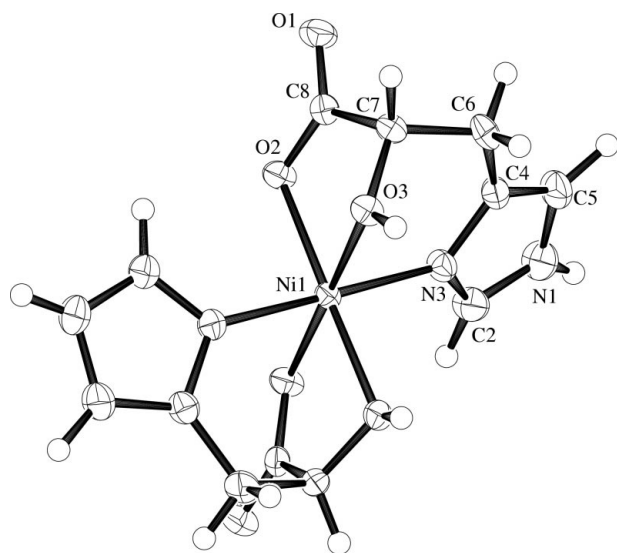


Figure 1
ORTEP (Johnson, 1976) drawing of the title compound, with the atomic numbering scheme. Ellipsoids for non-H atoms correspond to 50% probability.

(I) acts as a tridentate ligand and forms a distorted five-membered ring, which includes the Ni^{II} and the 2-hydroxyl- and carboxylate-O atoms. These O atoms bind to the Ni^{II} in *cis* positions with respect to each other in the equatorial plane. The imidazole-N atoms bind to nickel in the axial positions. No significant distortion is observed among the six coordination bonds of the complex: Ni1–O2 2.076 (2), Ni1–O3 2.066 (2) and Ni1–N3 2.066 (2) Å. This coordination mode is similar to that of the Co^{II} complex [Co1–O2 2.114 (2), Co1–O3 2.100 (2) and Co1–N3 2.103 (2) Å]. The ionized propionic acid side chain adopts a *gauche* conformation: C4–C6–C7–C8 –52.2 (2)°, which is also similar to the Co^{II} complex. Therefore, it is suggested that the coordination mode of (I) with transition metals is identical.

The molecules of (II) are linked by intermolecular hydrogen bonds between carboxylate, imino and hydroxyl groups. No stacking interactions between imidazole rings are observed in (II).

Experimental

Light-blue pillar-shaped crystals of the title compound were obtained by the slow evaporation, at room temperature, of an aqueous solution of 2-hydroxy-3-(1*H*-imidazol-4-yl)propionic acid and ammonium nickel(II) sulfate hexahydrate (molar ratio 2:1), adjusted to pH 10 with dilute aqueous ammonia.

Crystal data

[Ni(C₆H₇N₂O₃)₂]
M_r = 368.96
 Orthorhombic, *P*2₁2₁
a = 10.631 (3) Å
b = 13.283 (3) Å
c = 5.214 (3) Å
V = 736.3 (4) Å³
Z = 2
D_x = 1.664 Mg m⁻³

Mo *K*α radiation
 Cell parameters from 25 reflections
 θ = 24.7–25.0°
 μ = 1.36 mm⁻¹
T = 296.2 K
 Pillar, light blue
 0.50 × 0.30 × 0.30 mm

Data collection

Rigaku AFC-5R diffractometer
 ω -2 θ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 T_{\min} = 0.621, T_{\max} = 0.666
 1018 measured reflections
 1018 independent reflections
 991 reflections with $I > 2\sigma(I)$

θ_{\max} = 27.5°
 $h = 0 \rightarrow 13$
 $k = 0 \rightarrow 17$
 $l = 0 \rightarrow 6$
 3 standard reflections
 every 150 reflections
 intensity decay: 0.5%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.057$
 $S = 1.10$
 1018 reflections
 106 parameters
 H-atom parameters not refined
 $w = 1/[\sigma^2(F_o^2) + (0.0370P)^2 + 0.1736P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.32 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.31 \text{ e } \text{Å}^{-3}$
 Extinction correction: *SHELXL*
 Extinction coefficient: 0.0230
 Absolute structure: Flack (1983),
 1016 Friedel pairs
 Flack parameter = –0.03 (3)

Table 1

Selected geometric parameters (Å, °).

Ni1–O2	2.076 (2)	N1–C5	1.369 (3)
Ni1–O3	2.066 (2)	N3–C2	1.322 (3)
Ni1–N3	2.067 (2)	N3–C4	1.388 (3)
O1–C8	1.229 (3)	C4–C5	1.361 (3)
O2–C8	1.283 (3)	C4–C6	1.493 (3)
O3–C7	1.425 (3)	C6–C7	1.531 (3)
N1–C2	1.343 (3)	C7–C8	1.533 (3)
O2–Ni1–O3	76.78 (6)	N3–C4–C6	122.8 (2)
O2–Ni1–N3	86.96 (8)	C5–C4–C6	128.7 (2)
O3–Ni1–N3	88.71 (7)	N1–C5–C4	106.7 (2)
Ni1–O2–C8	113.2 (1)	C4–C6–C7	113.9 (2)
Ni1–O3–C7	108.7 (1)	O3–C7–C6	111.4 (2)
C2–N1–C5	107.6 (2)	O3–C7–C8	107.2 (2)
Ni1–N3–C2	126.4 (1)	C6–C7–C8	110.8 (2)
Ni1–N3–C4	126.7 (1)	O1–C8–O2	124.6 (2)
C2–N3–C4	106.1 (2)	O1–C8–C7	118.7 (2)
N1–C2–N3	111.0 (2)	O2–C8–C7	116.6 (2)
N3–C4–C5	108.6 (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>
N1–H1...O1 ⁱ	0.88	2.01	2.808 (3)	150
O3–H7...O2 ⁱⁱ	0.75	1.91	2.642 (2)	167

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

H atoms were located in a difference Fourier map and were not refined.

Data collection: *MSC/AF*C Diffractometer Control Software (Molecular Structure Corporation, 1992); cell refinement: *MSC/AF*C Diffractometer Control Software; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku, 1999); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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