Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Hexaaquanickel(II) bis(6-hydroxypyridine-3-carboxylate)

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Received 3 May 2005
Accepted 10 May 2005
Online 21 May 2005

In the title compound, $[Ni(H_2O)_6](C_6H_4NO_3)_2$, the Ni^{II} atom lies on a special position of $2/m$ site symmetry in an octahedron made up of water molecules. The anions show orientational disorder over mirror planes and are linked together by a pair of N—H···O hydrogen bonds into a dianion. The complex cations and dianions are connected through O—H···O hydrogen bonds to form a three-dimensional network.

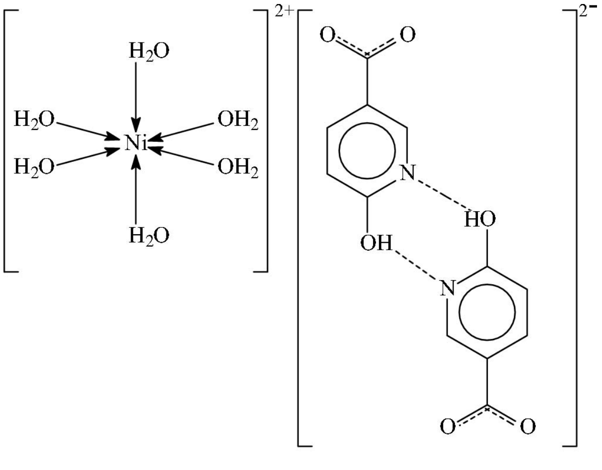
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(i–O) = 0.003 Å
Disorder in main residue
R factor = 0.041
wR factor = 0.111
Data-to-parameter ratio = 8.6

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

Comment

The title compound, (I), is isostructural with the Zn^{II} (Zhang *et al.*, 2005) and Co^{II} analogues (Zhang & Ng, 2005). The crystal structure of (I) consists of octahedral cations and hydrogen-bonded dianions (Fig. 1). Atom Ni1 lies on a position of $2/m$ site symmetry, and atom O2w also lies on the mirror plane, which bisects the O1w—Ni1—O1w^{iii} bond angle (for symmetry code see Fig. 1). In the anion, a crystallographic mirror plane passes through atom C6 and perpendicular to the carboxylate group. As a result, the hydroxypyridyl group of the anion shows orientational disorder. The cations and dianions are linked by hydrogen bonds (Table 2) to form a three-dimensional network.



(I)

Experimental

A mixture of nickel chloride hexahydrate (0.237 g, 1 mmol), 6-hydroxypyridyl-3-carboxylic acid (0.139 g, 1 mmol), sodium hydroxide (0.040 g, 1 mmol) and water (10 ml) was sealed in a 23 ml Teflon-lined stainless steel Parr bomb. The bomb was heated to 433 K for 2 d. It was then cooled to room temperature at 10 K h^{-1} to yield light-green crystals of (I).

Crystal data

$[Ni(H_2O)_6](C_6H_4NO_3)_2$
$M_r = 443.01$
Monoclinic, $C2/m$
$a = 11.556\ (1)$ Å
$b = 9.767\ (1)$ Å
$c = 7.5422\ (8)$ Å
$\beta = 91.320\ (2)^\circ$
$V = 851.1\ (2)$ Å^3
$Z = 2$
$D_x = 1.729$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1513 reflections
$\theta = 2.7$–27.4°
$\mu = 1.21$ mm^{-1}
$T = 295\ (2)$ K
Block, light green
$0.33 \times 0.28 \times 0.20$ mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.519$, $T_{\max} = 0.794$
2640 measured reflections
974 independent reflections
939 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 27.5^\circ$
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -7 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.111$
$S = 1.12$
974 reflections
113 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 1.687P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.44$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1*w*	2.015 (2)	Ni1—O2*w*	2.059 (4)
O1*w*—Ni1—O2*w*	91.2 (1)		
C1—C2—C6—O1	10.4 (5)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O1	0.84 (1)	1.83 (1)	2.659 (3)	169 (3)
O1*w*—H1*w*2···O1$^{\rm v}$	0.84 (1)	1.90 (1)	2.713 (3)	164 (3)
O2*w*—H2*w*1···O2$^{\rm vi}$	0.84 (1)	2.03 (2)	2.804 (5)	152 (3)
O2*w*—H2*w*1···O2$^{\rm vi}$	0.84 (1)	2.03 (2)	2.804 (5)	152 (3)
O2*w*—H2*w*2···O2$^{\rm vii}$	0.84 (1)	1.94 (1)	2.741 (6)	158 (1)
O2*w*—H2*w*2···O2$^{\rm viii}$	0.84 (1)	1.94 (1)	2.741 (6)	158 (1)
O2—H2o···N1$^{\rm iv}$	0.85	2.03	2.874 (7)	170

Symmetry codes: (iv) $-x+\frac{5}{2}, -y+\frac{3}{2}, -z+2$; (v) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$; (vi) $x-1, y, z-1$; (vii) $-x+2, -y+1, -z+1$; (viii) $-x+2, y, -z+1$.

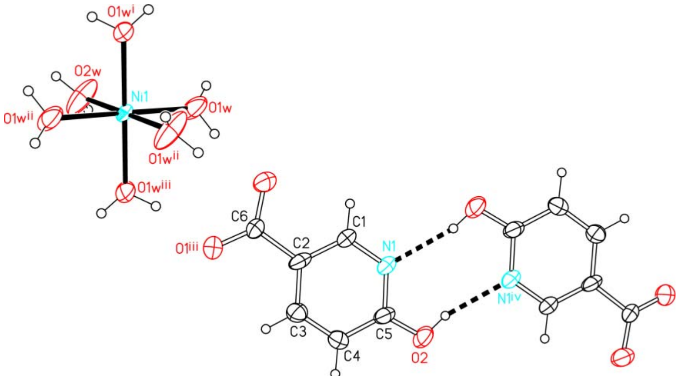


Figure 1
ORTEPII (Johnson, 1976) plot of (I), showing the numbering scheme. Atomic displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds. [Symmetry codes: (i) $1-x, y, 1-z$; (ii) $1-x, 1-y, 1-z$; (iii) $x, 1-y, z$; (iv) $\frac{5}{2}-x, \frac{3}{2}-y, 2-z$.]

Atoms C1–C5, N1 and O2 in the anion are disordered over two possible positions related by mirror symmetry. The C—C distances were restrained to 1.39 (1) Å, and the two N—C distances were restrained to within 0.01 Å of each other. Additionally, the ring was restrained to near planarity. C-bound H atoms were placed at calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{\rm iso}$(H) set to $1.2U_{\rm eq}$(C). The water H atoms were located in difference Fourier maps, and were refined with a distance restraint of O—H = 0.85 (1) Å. OH groups were allowed to rotate about the C—O bond to fit the electron density, with O—H constrained to 0.85 Å and C—O—H = 109.5°.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: atomic coordinates taken from the isostructural Zn analogue (Zhang *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

We thank the National Science Foundation of China (grant No. 29973059), Shenzhen University and the University of Malaya for supporting this study.

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