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Diaquaiminodiacetatonickel(II)

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Key indicators

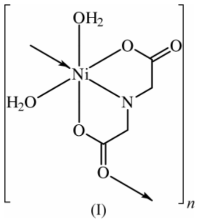
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.054
wR factor = 0.105
Data-to-parameter ratio = 13.0

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

The iminodiacetate dianion in diaquaiminodiacetatonickel(II), [Ni($C_4H_5NO_4$)(H_2O)$_2$], chelates to the Ni atom through two carboxyl O and one imino N atoms; the six-fold coordination coordination environment comprises these three atoms, the water molecules and the carbonyl O atom of an adjacent dianionic group. The dative Ni← O linkage leads to the formation of a helical chain running along the *a* axis of the orthorhombic crystal; adjacent chains are held in a network motif by hydrogen bonds.

Comment

Unlike iminodiacetatocopper(II), a compound that forms a large number of coordination complexes, as well as complexes with metal salts (Román-Alpiste *et al.*, 1999), the nickel(II) analog is much less studied, and the crystal structure of iminodiacetatonickel(II) has not been reported. The limited number of derivatives of this compound comprise the trihydrated 1:1 complex of dipotassium bis(iminodiacetato)-nickelate (Agre *et al.*, 1984), caesium bis(iminodiacetato)nickelate tetrahydrate (Mammano *et al.*, 1977), lithium bis(iminodiacetato)nickelate tetrahydrate (Kramarenko *et al.*, 1974; Mammano *et al.*, 1977) and the only *N*-heterocycle adduct, tris(imidazole)iminodiacetatonickel hydrate (Polyakova *et al.*, 2000).



(I)

Iminodiacetatonickel crystallizes as a dihydrate, (I), in which the Ni atom exists in an octahedral environment; this comprises the *O,N,O′*-chelating iminodiacetate ligand, the two water molecules and the carbonyl O atom of an adjacent molecule. The dative Ni← O linkage [2.011 (4) Å] leads to the formation of a helical chain running along the *a* axis of the orthorhombic crystal (Fig. 2). The other carbonyl O atom does not participate in bonding to the Ni atom but is, instead, engaged in hydrogen bonding with a water molecule and the imino N atom of an adjacent molecule. The extensive hydrogen bonds consolidate the structure into a tightly held network.

Experimental

Nickel nitrate hexahydrate (0.29 g, 1 mmol) dissolved in water (2 ml) was reacted with iminodiacetic acid (0.13 g, 1 mmol) dissolved in

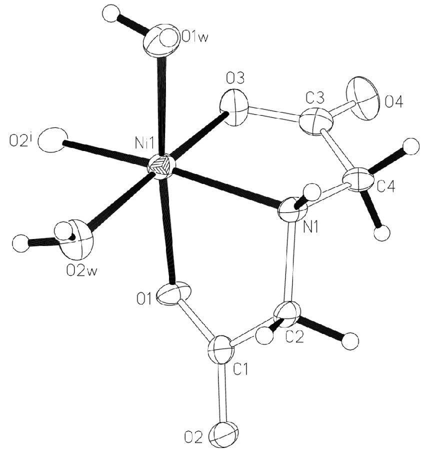


Figure 1
*ORTEP*II (Johnson, 1976) plot of the repeat unit of diaquaiminodiacetatonickel, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

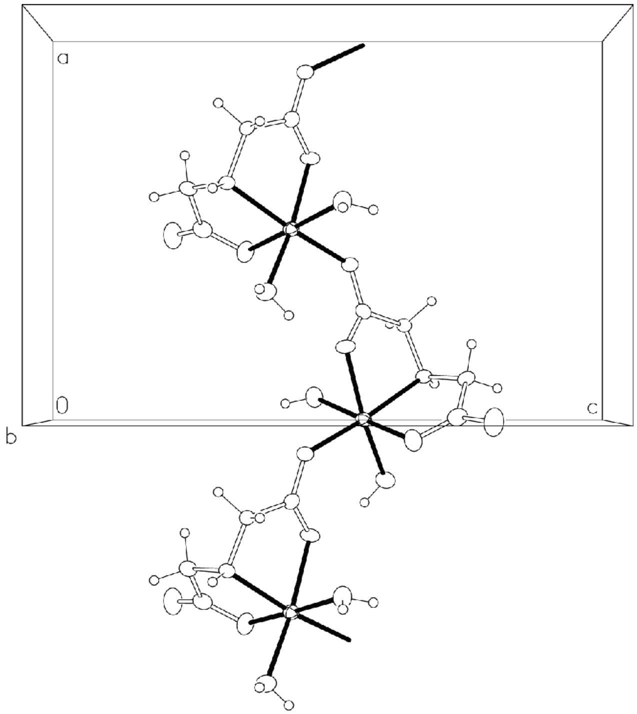


Figure 2
*ORTEP*II (Johnson, 1976) plot depicting the helical chain propagating along the *a* axis.

ethanol (8 ml). The pH of the solution was adjusted to 5 by the addition of aqueous sodium hydroxide. The solution was then sealed in a Teflon-lined Parr stainless-steel vessel, which was heated to 433 K for 2 h. The title compound separated as plates.

Crystal data

$[Ni(C_4H_5NO_4)(H_2O)_2]$
$M_r = 225.83$
Orthorhombic, $P2_1ca$
$a = 9.7610 (3)$ Å
$b = 5.2219 (2)$ Å
$c = 14.1713 (4)$ Å
$V = 722.32 (4)$ Å^3
$Z = 4$
$D_x = 2.08$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 1988 reflections
$\theta = 2.9–28.3°$
$\mu = 2.68$ mm^{-1}
$T = 298 (2)$ K
Plate, green
0.34 × 0.07 × 0.04 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.728$, $T_{max} = 0.898$
4084 measured reflections

1613 independent reflections
1585 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 28.3°$
$h = -12 \rightarrow 12$
$k = -6 \rightarrow 2$
$l = -16 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.105$
$S = 1.25$
1613 reflections
124 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 0.7011P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -1.03$ e Å^{-3}
Absolute structure: Flack (1983), 718 Friedel pairs
Flack parameter = 0.12 (3)

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.123 (4)	Ni1—O1*w*	2.087 (4)
Ni1—O2^i	2.011 (4)	Ni1—O2*w*	2.112 (4)
Ni1—O3	2.027 (4)	Ni1—N1	2.055 (5)
O1—Ni1—O2^i	90.5 (2)	O2^i—Ni1—O2*w*	91.7 (2)
O1—Ni1—O3	92.8 (2)	O3—Ni1—O1*w*	92.7 (2)
O1—Ni1—O1*w*	169.0 (2)	O3—Ni1—N1	83.6 (2)
O1—Ni1—O2*w*	85.7 (2)	O3—Ni1—O2*w*	178.5 (2)
O1—Ni1—N1	79.1 (2)	O1*w*—Ni1—O2*w*	88.8 (2)
O2^i—Ni1—O3	88.2 (2)	O1*w*—Ni1—N1	92.0 (2)
O2^i—Ni1—N1	166.4 (2)	O2*w*—Ni1—N1	96.2 (2)
O2^i—Ni1—O1*w*	99.2 (2)		

Symmetry code: (i) $x - \frac{1}{2}, -y, 1 - z$.

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 (5)	2.05 (5)	2.837 (6)	154 (5)
O1*w*—H1*w*2···O3^{ii}	0.85 (2)	2.10 (4)	2.863 (6)	150 (2)
O2*w*—H2*w*1···O2^{iii}	0.85 (2)	2.19 (4)	2.994 (6)	159 (2)
O2*w*—H2*w*2···O4^{iv}	0.85 (3)	1.86 (3)	2.673 (6)	160 (3)
N1—H1*n*···O4^{ii}	0.85 (5)	2.11 (5)	2.913 (7)	157 (3)

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

The H atoms of the imino N and water O atoms were located and refined, subject to O—H = N—H = 0.85 (1) Å; for the water H atoms, H···H = 1.39 (1) Å. The C-bound H atoms were generated geometrically and constrained with a riding model (C—H = 0.97 Å). The displacement parameters of all H atoms were set to 1.2 times U_{eq} of their parent atoms. The largest peak in the final difference map was about 1 Å from Ni1 and the deepest hole about 1 Å from C3. The structure was refined in the setting the data were commected on. The matrix $(00\overline{1},010,100)$ transforms the cell into the standard $Pca2_1$ setting.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); 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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