metal-organic papers

Diaquabis(4-formylbenzoato-κO)bis(1H-imidazole-κN³)nickel(II)

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The title compound, [Ni(C₈H₅O₃)₂(C₃H₄N₂)₂(H₂O)₂], is isostructural with the manganese analogue. The Ni atom, which lies on a centre of inversion, is coordinated by two imidazole and two water ligands, as well as by the formylbenzoate groups, in an all-*trans* octahedral geometry.

Comment

The first example of a metal derivative of 4-formylbenzoic acid is the manganese derivative, which was characterized as the diaquabisimidazole complex (Deng *et al.*, 2006), where the metal shows an all-*trans* octahedral coordination. The title nickel analogue, (I), is isostructural (Fig. 1); the bond dimensions in the two complexes are nearly identical. Similarly, the coordinated water molecules engage in hydrogen bonding (Table 2) to furnish the same type of three-dimensional network as formed by the Mn complex.

(I)
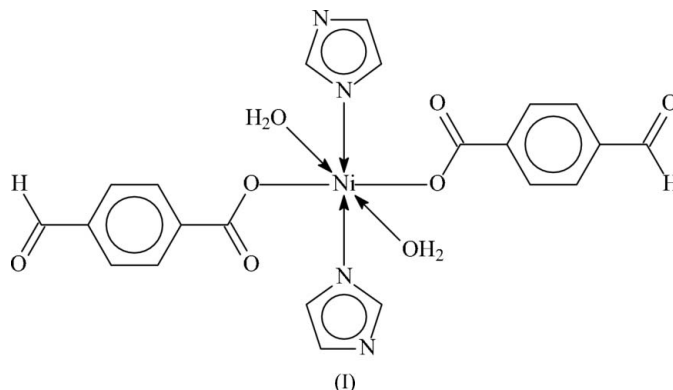
Experimental

Manganese diacetate tetrahydrate (0.125 g, 0.5 mmol) was added to an aqueous solution (10 ml) of 4-formylbenzoic acid (0.15 g, 1 mmol) and imidazole (0.068 g, 1 mmol). The pH value of the mixture was about 5. The solution was allowed to evaporate at room temperature; green prismatic crystals separated from the filtered solution after several days. CH&N elemental analysis calculated for C₂₂H₂₂N₄NiO₈: C 49.9, H 4.2, N 10.6%. Found: C 49.9, H 4.2, N 10.7%.

Crystal data

[Ni(C₈H₅O₃)₂(C₃H₄N₂)₂(H₂O)₂]	$V = 557.14$ (4) Å³
$M_r = 529.15$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 1.577$ Mg m⁻³
$a = 5.6143$ (2) Å	Mo $K\alpha$ radiation
$b = 8.0757$ (4) Å	$\mu = 0.93$ mm⁻¹
$c = 12.8208$ (5) Å	$T = 295$ (2) K
$\alpha = 73.995$ (1)°	Prism, green
$\beta = 86.114$ (1)°	$0.35 \times 0.26 \times 0.18$ mm
$\gamma = 87.038$ (1)°	

Data collection

Rigaku R-AXIS RAPID IP
    diffractometer
ω scans
Absorption correction: multi-scan
    (*ABSCOR*; Higashi, 1995)
    $T_{min} = 0.729$, $T_{max} = 0.851$

5506 measured reflections
2542 independent reflections
2334 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.093$
$S = 1.21$
2542 reflections
182 parameters
H atoms treated by a mixture of
    independent and constrained
    refinement

$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.0472P]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	2.071 (2)	Ni1—O1w	2.093 (1)
Ni1—O1	2.125 (1)		
N1—Ni1—O1	92.51 (5)	N1—Ni1—O1w^i	88.23 (6)
N1—Ni1—O1^i	87.49 (5)	O1—Ni1—O1w	86.61 (5)
N1—Ni1—O1w	91.77 (6)	O1—Ni1—O1w^i	93.39 (5)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1w—H1a···O1^{ii}	0.84 (1)	2.10 (1)	2.868 (2)	153 (2)
O1w—H1b···O2^i	0.84 (1)	1.81 (1)	2.636 (2)	169 (3)
N2—H2n···O2^{iii}	0.85 (1)	2.33 (2)	3.061 (2)	144 (3)
N2—H2n···O3^{iv}	0.85 (1)	2.45 (3)	3.041 (3)	127 (3)

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

The formyl group is disordered over two sets of atom positions; the site occupancy factors refined to 0.679 (7):0.311 (6). The carbon-bound H atoms were positioned geometrically (C—H = 0.93 Å) and
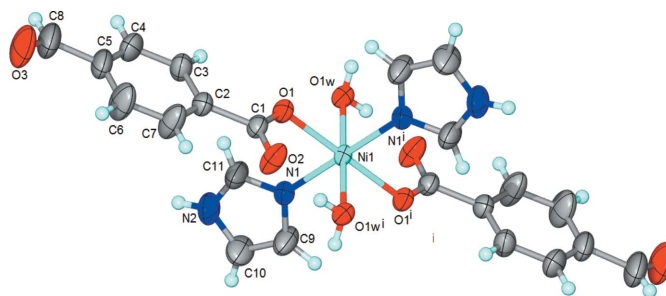

Figure 1
The molecular structure. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. The minor disorder component is not shown. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$.]

were included in the refinement in the riding-model approximation, with $U_{iso}(H)$ set to $1.2U_{eq}(C)$. The amino and water H atoms were located in a difference Fourier map, and were refined with a distance restraint of N—H = O—H = 0.85 (1) Å.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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