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catena-Poly[[diaquabis(1*H*-benzimidazole-κN^3)nickel(II)]-μ-succinato-κ^2O:O']

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Key indicators

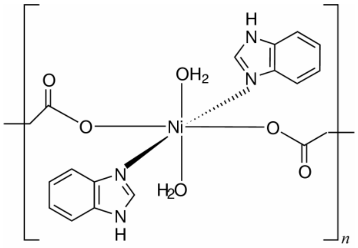
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.074
Data-to-parameter ratio = 15.3

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

The crystal structure of the title compound, $[Ni(C_4H_4O_4)(C_7H_6N_2)_2(H_2O)_2]_n$, consists of a polymeric Ni^{II} complex bridged by succinate dianions. The Ni atom is located at a crystallographic inversion center. Both carboxyl groups of the succinate coordinate, in monodentate fashion, to the neighboring Ni^{II} atoms to form one-dimensional chains, and the chains link to each other *via* hydrogen bonds between the benzimidazole and carboxyl group to form a two-dimensional supramolecular structure. The overlapped arrangement of parallel benzimidazole ligands, with a separation of 3.350 (3) Å, suggests the existence of π–π-stacking interactions between adjacent chains.

Comment

A series of transition metal complexes bridged by dicarboxylate, such as fumarate, succinate, *etc*., has been prepared in the laboratory. Their crystal structures show versatile coordination modes of the carboxyl groups (Chen *et al.*, 2003). As part of this research, the structure of the title nickel(II) complex, (I), bridged by succinate has been determined by X-ray diffraction methods.



(I)

The crystal structure consists of polymeric Ni^{II} complex molecules. The coordination environment around the Ni^{II} atom is illustrated in Fig. 1. The Ni^{II} atom is located at a crystallographic inversion center. Together with two water molecules, two O atoms from different succinate ligands and two imidazole N atoms coordinate the Ni^{II} atom in an octahedral geometry (see Table 1). The carboxyl groups of the succinate coordinate in monodentate fashion; the uncoordinated carboxyl O atoms form hydrogen bonds with the neighboring coordinated water.

The bridging succinate groups also lie on inversion centers. The planar carbon skeleton makes a dihedral angle of 56.6 (2)° with each carboxyl group. Carboxyl groups of the succinate coordinate to neighboring Ni^{II} atoms to form one-dimensional polymeric chains. Adjacent chains link to each other *via* hydrogen bonds between benzimidazole N and carboxyl O atoms, forming the two-dimensional supramolecular structure shown in Fig. 2 and detailed in Table 2.

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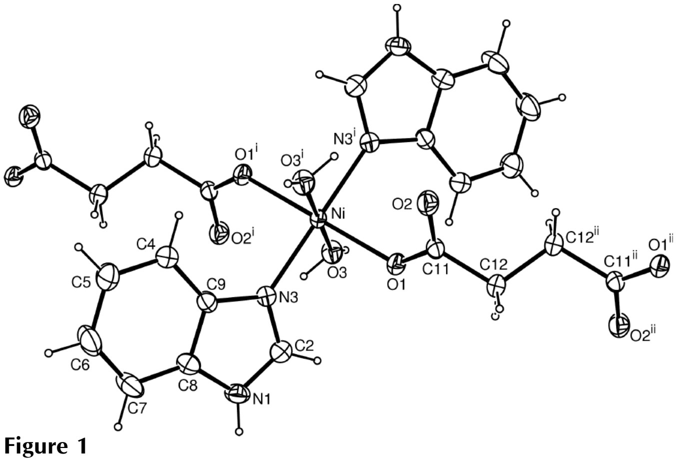

Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $-x, -y, 1 - z$.]

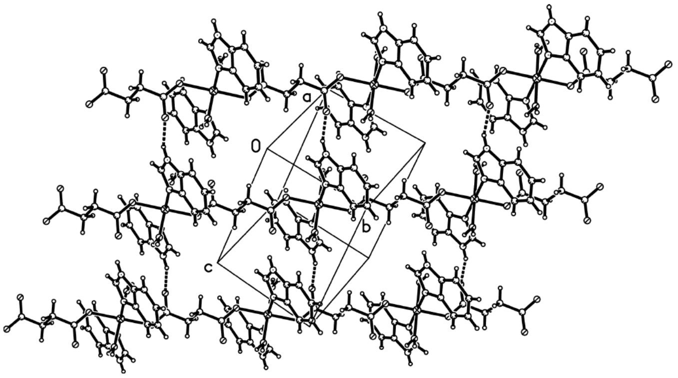

Figure 2
The molecular packing; dashed lines denote hydrogen bonds.

An overlapped arrangement of parallel benzimidazole ligands is observed in the crystal structure. Neighboring benzimidazole ligands, related by the symmetry transformation ($-x$, $1 - y$, $-z$), are separated by 3.350 (3) Å. These findings suggest the existence of π–π-stacking interactions between adjacent polymeric chains.

Experimental

$NiCl_2{\cdot}6H_2O$ (0.48 g, 2 mmol) was added to an aqueous solution (10 ml) containing succinic acid (0.24 g, 2 mmol) and NaOH (0.16 g, 4 mmol). After the mixture was refluxed for 30 min, an ethanol solution (10 ml) of benzimidazole (0.24 g, 2 mmol) was added to the above solution with continuous stirring. The solution was refluxed for 3 h, until the color changed to pale green. The reaction mixture was cooled to room temperature and filtered. Pale green single crystals were obtained from the filtrate after one week.

Crystal data

$[Ni(C_4H_4O_4)(C_7H_6N_2)_2(H_2O)_2]$
$M_r = 447.08$
Triclinic, $P\overline{1}$
$a = 7.0244$ (7) Å
$b = 8.5982$ (11) Å
$c = 8.7399$ (5) Å
$\alpha = 100.248$ (6)°
$\beta = 111.981$ (7)°
$\gamma = 104.734$ (9)°
$V = 450.91$ (9) Å^3
$Z = 1$
$D_x = 1.646$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2206 reflections
$\theta = 2.6$–27.4°
$\mu = 1.12$ mm^{-1}
$T = 298$ (2) K
Prism, green
0.39 × 0.19 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.64$, $T_{max} = 0.88$
4252 measured reflections
2036 independent reflections
1913 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 27.5°$
$h = -8 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.074$
$S = 1.11$
2036 reflections
133 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 0.2892P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Selected geometric parameters (Å).

Ni—O1	2.0733 (12)	O2—C11	1.274 (2)
Ni—N3	2.0774 (14)	C11—C12	1.519 (2)
Ni—O3	2.1028 (13)	C12—C12^{ii}	1.523 (3)
O1—C11	1.255 (2)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O2^{iii}	0.86	2.06	2.871 (2)	156
O3—H13$\cdots$O2^{iv}	0.85	2.09	2.878 (2)	153
O3—H23$\cdots$O2^{i}	0.86	2.24	2.688 (2)	112

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

The H atoms on C atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement as riding, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atoms. H atoms of water were placed in calculation positions (Nardelli, 1993), and were included in the final cycles of refinement with fixed coordinates and isotropic displacement parameters of 0.08 Å^2.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC and Rigaku, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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