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Dibenzoato-di(2-aminopyridine)nickel(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.095
Data-to-parameter ratio = 17.2

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

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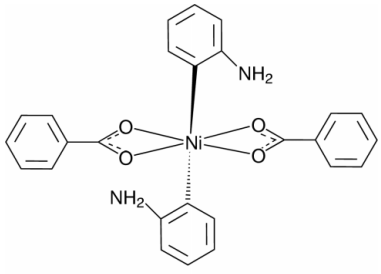
In the title compound, $[(C_7H_5O_2)_2(C_5H_6N_2)_2Ni]$, the Ni^{II} atom is six coordinated by four O atoms from two benzoate anions, and two pyridine N atoms from the two 2-aminopyridine ligands to give a distorted octahedral geometry. All of the O atoms and both the amine groups of the ligands contribute to form a one-dimensional chain consisting of intra- and intermolecular N—H···O hydrogen bonds.

Comment

The title complex, (I), is an electrically neutral compound. The Ni^{II} atom in the complex is six coordinated by two pyridine N atoms from two 2-aminopyridine ligands, and by four O atoms from two different benzoate anions, exhibiting a distorted octahedral configuration of the Ni^{II} atom. The Ni—N bond lengths of 2.0569 (14) and 2.0647 (15) Å, and the Ni—O distances, which range from 2.0716 (12) to 2.1750 (12) Å, are normal for this type of compound. The O1—Ni1—O2 [62.02 (4)°] and O3—Ni1—O4 [61.79 (4)°] angles are not unusual, and are comparable to that [61.9 (4)°] in a similar Ni^{II} complex with carboxylates (Zhu *et al.*, 1999). All the O atoms and the primary N atoms contribute to form a one-dimensional chain along [110], through N—H···O hydrogen bonds (see Fig. 2 and Table 2).



(I)

Experimental

Nickel benzoate and 2-aminopyridine were available commercially and were used without further purification. Nickel benzoate (1 mmol, 337 mg) and 2-aminopyridine (2.0 mmol, 188 mg) were dissolved in acetonitrile and water (v/v = 1: 1, 10 ml). The mixture was stirred for *ca*. 0.5 h to give a clear solution. After keeping the resulting solution in air for ten days, large blue prisms were formed. The crystals were isolated, washed with acetonitrile three times and dried in a vacuum desiccator using $CaCl_2$ (Yield 87%). Elemental analysis found: C, 59.11; H, 4.60; N, 11.28%. Calc. for $C_{24}H_{22}N_4NiO_4$: C, 58.93; H, 4.53; N, 11.45%.

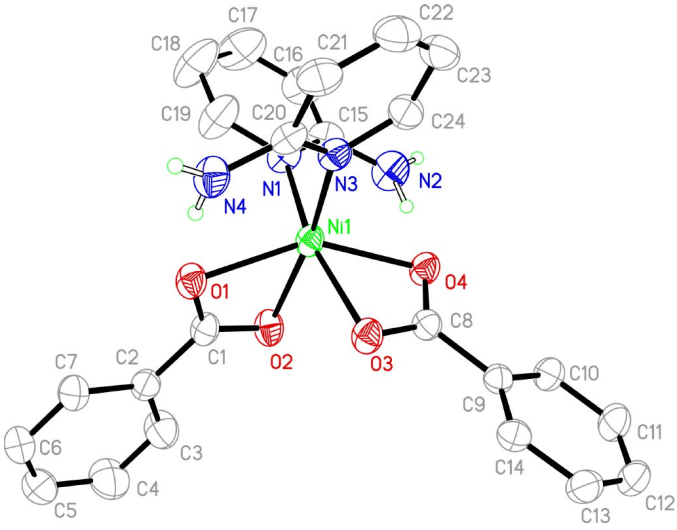


Figure 1
The structure of the title compound (I), showing 30% probability ellipsoids and the atom-numbering scheme. All H atoms, except those bonded to N, are omitted for clarity.

Crystal data

$[Ni(C_7H_5O_2)_2(C_5H_6N_2)_2]$
M_r = 489.17
Monoclinic, $C2/c$
a = 25.097 (5) Å
b = 10.991 (2) Å
c = 17.499 (3) Å
β = 101.28 (3)°
V = 4733.7 (15) Å^3
Z = 8
D_x = 1.373 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 19350 reflections
θ = 2.9–25.4°
μ = 0.86 mm^{-1}
T = 293 (2) K
Prism, blue
0.55 × 0.43 × 0.38 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.649, T_{max} = 0.722
19355 measured reflections
5137 independent reflections
4599 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 27.0°
$h = -14 \rightarrow 32$
$k = -13 \rightarrow 13$
$l = -22 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.095
S = 1.03
5137 reflections
299 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 1.3806P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.011
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N3	2.0569 (14)	Ni1—O2	2.1144 (14)
Ni1—N1	2.0647 (15)	Ni1—O1	2.1266 (11)
Ni1—O4	2.0716 (12)	Ni1—O3	2.1750 (12)
N3—Ni1—N1	90.56 (6)	O4—Ni1—O1	147.68 (4)
N3—Ni1—O4	96.27 (5)	O2—Ni1—O1	62.02 (4)
N1—Ni1—O4	104.78 (5)	N3—Ni1—O3	90.58 (5)
N3—Ni1—O2	168.76 (5)	N1—Ni1—O3	166.56 (5)
N1—Ni1—O2	94.23 (6)	O4—Ni1—O3	61.79 (4)
O4—Ni1—O2	92.34 (4)	O2—Ni1—O3	87.12 (5)
N3—Ni1—O1	107.32 (5)	O1—Ni1—O3	95.52 (5)
N1—Ni1—O1	96.92 (6)		

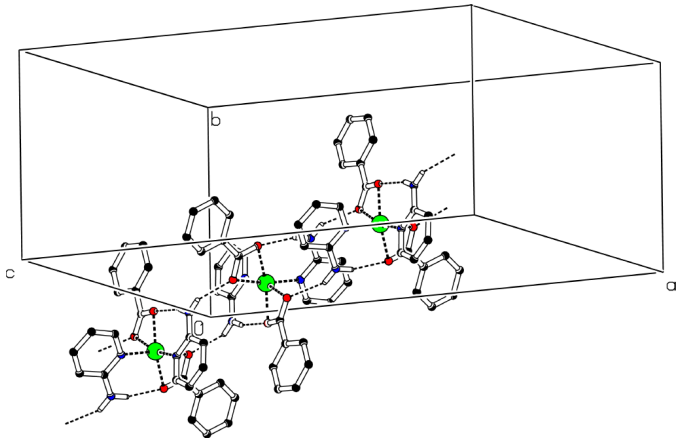


Figure 2
A one-dimensional chain of (I) along [110], showing the hydrogen-bonded interactions as dashed lines. Colour codes: green Zn, red O, blue O, black C.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.90	2.13	2.9187 (19)	146
N2—H2B···O4	0.90	1.99	2.850 (2)	161
N4—H4B···O3^{ii}	0.90	2.17	2.9790 (18)	149
N4—H4C···O1	0.90	2.08	2.954 (2)	164

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

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H and C—H distances of 0.90 Å and 0.96 Å, respectively. The U_{iso}(H) values were fixed at 0.08 Å^2. The U_{eq} values for C18 [0.1170 (12)], C17 [0.1132 (10)], C19 [0.0904 (8)], C16 [0.0887 (7)], C4 [0.0974 (8)], C5 [0.0883 (7)] and C6 [0.0822 (7) Å^2] are quite large, but these atoms were not considered to be disordered.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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