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catena-Poly[[[(4-aminobenzoato-κN)aqua(2,2′-diamino-4,4′-bithiazole-κ^2N,N')nickel(II)]-μ-4-aminobenzoato-κ^2N:O] monohydrate]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.015 Å
R factor = 0.059
wR factor = 0.217
Data-to-parameter ratio = 12.3

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

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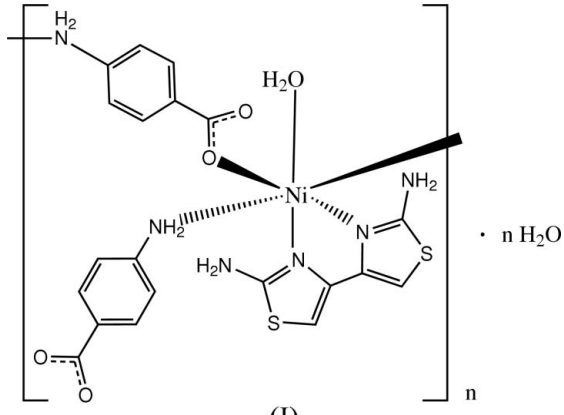
In the crystal structure of the title compound, $\{[Ni(C_7H_6NO_2)_2(C_6H_6N_4S_2)(H_2O)]\cdot H_2O\}_n$, the aminobenzoate anion bridges Ni^{II} ions through its terminal carboxylate and amino groups to form the polymeric Ni^{II} complex chain. π–π Stacking is observed between aminobenzoate and diaminobithiazole ligands.

Comment

As part of our ongoing investigation on the nature of π–π stacking in metal complexes (Liu *et al.*, 2004; Li *et al.*, 2005), the title Ni^{II} compound, (I), has been prepared and its crystal structure is presented here.



(I)

A segment of the polymeric structure of (I) is shown in Fig. 1. The Ni^{II} ion is coordinated by one diaminobithiazole (DABT) molecule, one water molecule and three aminobenzoate (ABA) monoanions in a distorted octahedral geometry (Table 1). Of the three ABA anions, one is coordinated in a monodentate manner to the Ni^{II} ion *via* a carboxyl O atom, and the others bridge neighboring Ni^{II} ions with the terminal carboxylate and amino groups, forming a polymeric complex chain extending along the *b* axis (Fig. 2). The two thiazole rings of DABT are twisted with respect to each other with a dihedral angle of 4.9 (6)°, which agrees with 4.6 (7)° found in Mn(DABT)(oxydiacetate) (Luo *et al.*, 2004) and 6.4 (2)° found in Cu(DABT)(oxydiacetate) (Wu *et al.*, 2003). It is notable that atoms N5 and N6 of the ABA anions deviate from the attached benzene planes by 0.219 (14) and 0.233 (15) Å, respectively, toward the Ni center.

The DABT unit is partially overlapped with the benzene rings of the ABA anions (Fig. 3). The distances of atoms C3 and C4 of DABT from the C22-containig benzene plane are 3.319 (12) and 3.334 (12) Å, respectively. The distances of

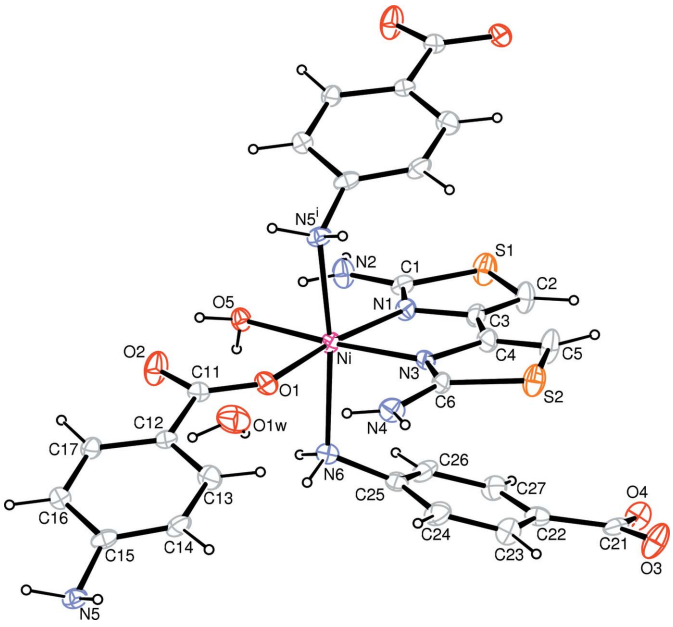


Figure 1
Part of the polymeric structure, with 30% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry code: (i) $x, 1 + y, z$].

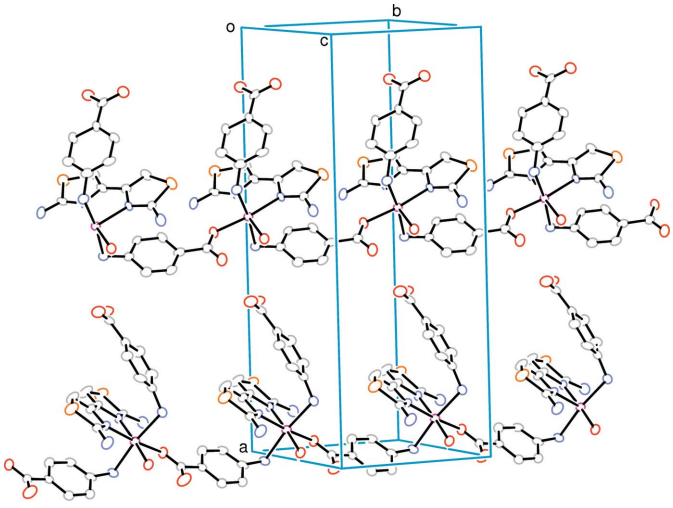


Figure 2
A packing diagram, showing polymeric complex chains extended along the b axis. H atoms have been omitted.

atoms C1^{viii} and N1^{viii} from the C12-containing benzene plane are 3.365 (10) and 2.888 (11) Å, respectively (symmetry code as in Fig. 3). These findings suggest the existence of π–π stacking between ABA and DABT in the crystal structure of (I).

The extensive hydrogen-bonding network (Table 2) helps to stabilize the crystal structure.

Experimental

An aqueous solution (20 ml) containing DABT (0.20 g, 1 mmol) and $NiCl_2$ (0.13 g, 1 mmol) was mixed with an aqueous solution (10 ml) of 4-aminobenzoic acid (0.28 g, 2 mmol) and NaOH (0.08 g, 2 mmol).

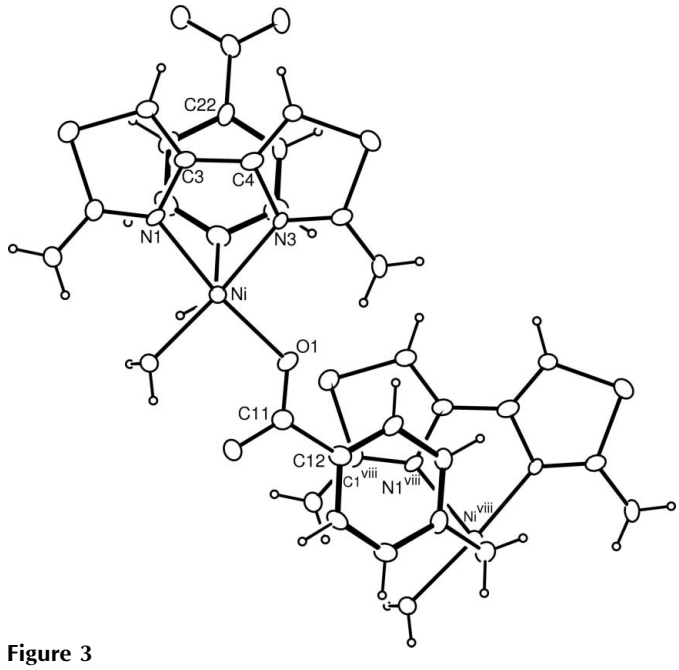


Figure 3
π–π Stacking between DABT and ABA [symmetry code: (viii) $x, -1 + y, z$].

Crystal data

$[Ni(C_7H_6NO_2)_2(C_6H_6N_4S_2)(H_2O)]\cdot H_2O$
$M_r = 565.27$
Orthorhombic, $Pna2_1$
$a = 23.383$ (3) Å
$b = 9.082$ (2) Å
$c = 10.929$ (2) Å
$V = 2320.9$ (7) Å^3
$Z = 4$
$D_x = 1.618$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.07$ mm^{-1}
$T = 295$ (2) K
Prism, yellow
0.33 × 0.26 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.732$, $T_{max} = 0.810$
3891 measured reflections
3891 independent reflections
2591 reflections with $I > 2\sigma(I)$
$\theta_{max} = 25.0°$
3 standard reflections
every 120 reflections
intensity decay: 1.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.217$
$S = 1.15$
3891 reflections
316 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1078P)^2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.77$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}
Absolute structure: Flack (1983), 1766 Friedel pairs
Flack parameter: 0.14 (4)

Table 1
Selected bond lengths (Å).

Ni—O1	2.078 (7)	Ni—N3	2.066 (7)
Ni—O5	2.066 (6)	Ni—N5^{i}	2.176 (7)
Ni—N1	2.116 (7)	Ni—N6	2.218 (8)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O5	0.86	2.30	3.061 (11)	147
N2—H2B···O3^{ii}	0.86	2.08	2.863 (13)	152
N4—H4A···O1	0.86	2.05	2.823 (11)	149
N4—H4B···O4^{iii}	0.86	1.99	2.808 (12)	157
N5—H5A···O4^{iv}	0.90	2.26	3.133 (9)	163
N5—H5B···O2^{v}	0.90	2.53	3.413 (12)	167
N6—H6B···O1W	0.90	2.19	3.052 (12)	161
O5—H5C···O2	0.81	2.03	2.584 (10)	125
O5—H5D···O1W	0.84	1.93	2.772 (11)	175
O1W—H1A···O4^{vi}	0.88	2.03	2.707 (12)	133
O1W—H1B···S2^{vii}	0.91	2.60	3.446 (9)	154

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

Water H atoms were located in a difference Fourier map and refined as riding in the as-found relative positions, with U_{iso}(H) = 1.5U_{eq}(O). H atoms on amino groups were placed in calculated positions with N—H = 0.90 (sp^3) or 0.86 Å (sp^2) and aromatic H atoms were placed in calculated positions with C—H = 0.93 Å; they were refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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