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**Key indicators**

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma(C-C)$  = 0.008 Å  
 H-atom completeness 94%  
 Disorder in solvent or counterion  
 R factor = 0.054  
 wR factor = 0.143  
 Data-to-parameter ratio = 13.5

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

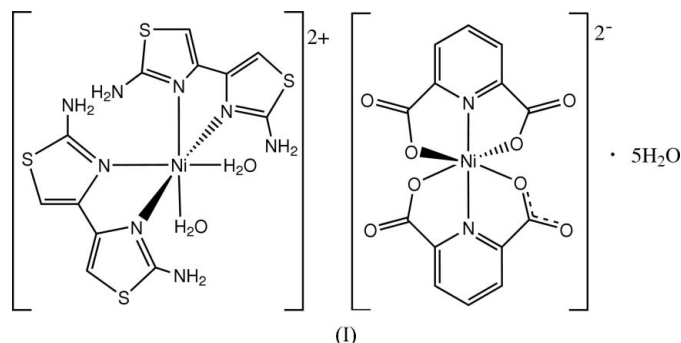
**Diaqua(2,2'-diamino-4,4'-bi-1,3-thiazole- $\kappa^2N^3,N^{3'}$ )nickel(II) (pyridine-2,6-dicarboxylato- $\kappa^3O,N,O'$ )nickelate(II) pentahydrate**

The crystal structure of the title compound,  $[Ni(C_6H_6N_4S_2)_2(H_2O)_2][Ni(C_7H_3NO_4)_2] \cdot 5H_2O$ , consists of Ni<sup>II</sup> complex cations, Ni<sup>II</sup> complex anions and five uncoordinated water molecules. In both the complex cation and anion, the Ni<sup>II</sup> ions assume a distorted octahedral coordination. There is extensive hydrogen bonding between water molecules, complex cations and complex anions.

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**Comment**

Transition metal complexes of 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown potential application in the field of soft magnetic materials (Sun *et al.*, 1997). As part of a series of structural investigations of metal complexes with DABT (Liu *et al.*, 2003), the title Ni<sup>II</sup> complex was recently prepared.



The structure of (I) consists of Ni<sup>II</sup> complex cations, Ni<sup>II</sup> complex anions and five uncoordinated water molecules (Fig. 1). Within the complex cation, the Ni<sup>II</sup> ion is coordinated by two DABT ligands and two water molecules in a distorted octahedral geometry. Two planar DABT ligands are approximately perpendicular to each other, the dihedral angle being 83.69 (9)°. The C–N bond distances between thiazole rings and amino groups range from 1.319 (7) to 1.350 (7) Å, suggesting electron delocalization between the amino groups and thiazole rings. In the complex anion, the Ni<sup>II</sup> ion is chelated by two pyridinedicarboxylate (pdc) dianions with a distorted octahedral geometry (Table 1). The two pdc ligands are nearly perpendicular to each other, the dihedral angle being 87.39 (7)°.

Extensive hydrogen bonding between coordinated water molecules, complex cations and complex anions helps to stabilize the crystal structure (Table 2).

**Experimental**

An aqueous solution (20 ml) containing DABT (1 mmol) and NiCl<sub>2</sub> (1 mmol) was mixed with an aqueous solution (10 ml) of pyridine-2,6-

dicarboxylic acid (1 mmol) and NaOH (2 mmol). The mixture was refluxed for 5 h. After cooling to room temperature, the solution was filtered. Single crystals of (I) were obtained from the filtrate after 20 d.

#### Crystal data

$[\text{Ni}(\text{C}_6\text{H}_6\text{N}_4\text{S}_2)_2(\text{H}_2\text{O})_2] \cdot$   
 $[\text{Ni}(\text{C}_7\text{H}_3\text{NO}_4)_2] \cdot 5\text{H}_2\text{O}$   
 $M_r = 970.28$   
 Monoclinic,  $P2_1/n$   
 $a = 11.7980$  (11) Å  
 $b = 18.5558$  (17) Å  
 $c = 17.6429$  (17) Å  
 $\beta = 92.964$  (2)°

$V = 3857.2$  (6) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.671$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 1.27$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 Prism, green  
 $0.23 \times 0.20 \times 0.18$  mm

#### Data collection

Rigaku R-Axis RAPID  
 diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.740$ ,  $T_{\max} = 0.800$

20280 measured reflections  
 6988 independent reflections  
 4180 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.070$   
 $\theta_{\text{max}} = 25.2^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.054$   
 $wR(F^2) = 0.143$   
 $S = 1.05$   
 6988 reflections  
 517 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.3071P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.003$   
 $\Delta\rho_{\text{max}} = 0.77$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.49$  e Å<sup>-3</sup>

**Table 1**

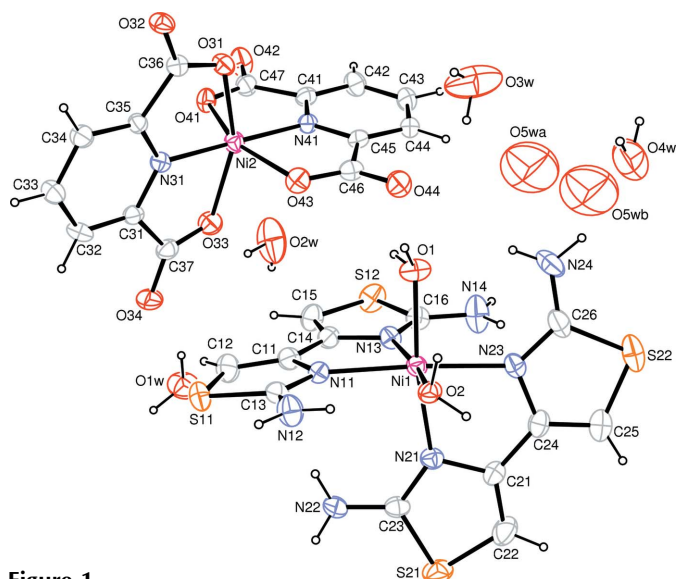
Selected bond lengths (Å).

Ni1—O1	2.107 (3)	Ni2—O31	2.109 (3)
Ni1—O2	2.104 (3)	Ni2—O33	2.137 (4)
Ni1—N11	2.097 (4)	Ni2—O41	2.187 (4)
Ni1—N13	2.083 (4)	Ni2—O43	2.104 (4)
Ni1—N21	2.110 (4)	Ni2—N31	1.952 (4)
Ni1—N23	2.125 (4)	Ni2—N41	1.961 (4)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1A $\cdots$ O42 <sup>i</sup>	0.89	1.83	2.672 (5)	155
O1—H1B $\cdots$ O44	0.87	1.98	2.700 (5)	139
O2—H2A $\cdots$ O41 <sup>i</sup>	0.94	1.78	2.702 (5)	165
O2—H2B $\cdots$ O32 <sup>ii</sup>	0.89	1.85	2.686 (5)	156
O1W—H1WA $\cdots$ O34	0.96	1.76	2.676 (6)	159
O1W—H1WB $\cdots$ O42 <sup>iii</sup>	0.92	1.92	2.831 (6)	171
O2W—H2WA $\cdots$ O33	0.93	1.97	2.739 (7)	138
O2W—H2WB $\cdots$ O5WB <sup>iv</sup>	0.94	1.95	2.89 (3)	174
O3W—H3WA $\cdots$ O1W <sup>v</sup>	0.82	2.12	2.720 (8)	130
O3W—H3WB $\cdots$ O5WA	0.88	2.52	3.09 (3)	123
O3W—H3WB $\cdots$ O44	0.88	2.23	2.942 (8)	139
O4W—H4A $\cdots$ O5WA <sup>iv</sup>	0.94	1.98	2.77 (2)	139
O4W—H4A $\cdots$ O5WB <sup>iv</sup>	0.94	2.16	2.91 (2)	135
O4W—H4B $\cdots$ O1W	0.92	2.33	2.900 (7)	120
N12—H12A $\cdots$ O2	0.86	2.13	2.891 (5)	147
N12—H12B $\cdots$ O3W <sup>iii</sup>	0.86	2.16	2.975 (8)	158
N14—H14A $\cdots$ N23	0.86	2.34	3.111 (6)	149
N14—H14B $\cdots$ O2W <sup>iv</sup>	0.86	2.20	2.865 (8)	134
N22—H22A $\cdots$ N11	0.86	2.36	3.111 (6)	146
N22—H22B $\cdots$ O31 <sup>iii</sup>	0.86	2.48	3.225 (6)	145
N22—H22B $\cdots$ O32 <sup>iii</sup>	0.86	2.16	2.975 (6)	157



**Figure 1**

The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Both disorder components are shown.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N24—H24A $\cdots$ O1	0.86	2.14	2.913 (6)	149
N24—H24B $\cdots$ O4W <sup>v</sup>	0.86	2.13	2.893 (8)	148

Symmetry codes: (i)  $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (ii)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (iii)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (iv)  $-x + 1, -y + 1, -z + 1$ ; (v)  $x - 1, y, z$ .

Atom O5W is disordered over two sites (O5WA and O5WB); occupancies for the disordered components were set at 0.5 and atomic displacement parameters were constrained to be the same. The H atoms of this disordered water molecule were not located. H atoms on the ordered water molecules were located in a difference Fourier map and refined as riding in their as-found relative positions, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . Other H atoms were placed in calculated positions, with  $C-H = 0.93$  Å and  $N-H = 0.86$  Å, and refined in riding mode, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ .

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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