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## Key indicators

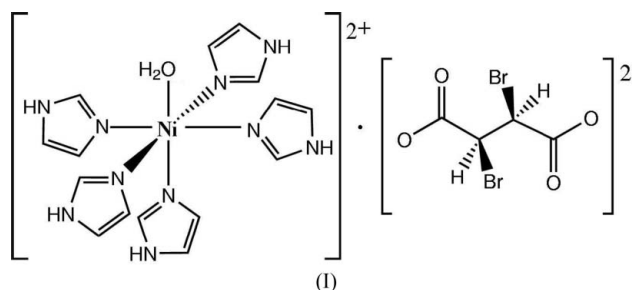
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$   
Disorder in main residue  
 $R$  factor = 0.050  
 $wR$  factor = 0.155  
Data-to-parameter ratio = 17.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Aquapentakis(1*H*-imidazole- $\kappa N^3$ )nickel(II)  
dibromosuccinate

The title compound,  $[\text{Ni}(\text{C}_3\text{H}_4\text{N}_2)_5(\text{H}_2\text{O})](\text{C}_4\text{H}_2\text{Br}_2\text{O}_4)$ , consists of  $\text{Ni}^{\text{II}}$  complex cations and dibromosuccinate anions. The Ni atom, water O atom and one imidazole N atom of the complex cation lie on a twofold axis. The anion lies on an inversion centre. The crystal packing is reinforced by  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, but there are no  $\pi-\pi$  stacking interactions even though the complex contains five aromatic imidazole rings. The compound is isostructural with its cobalt analogue.

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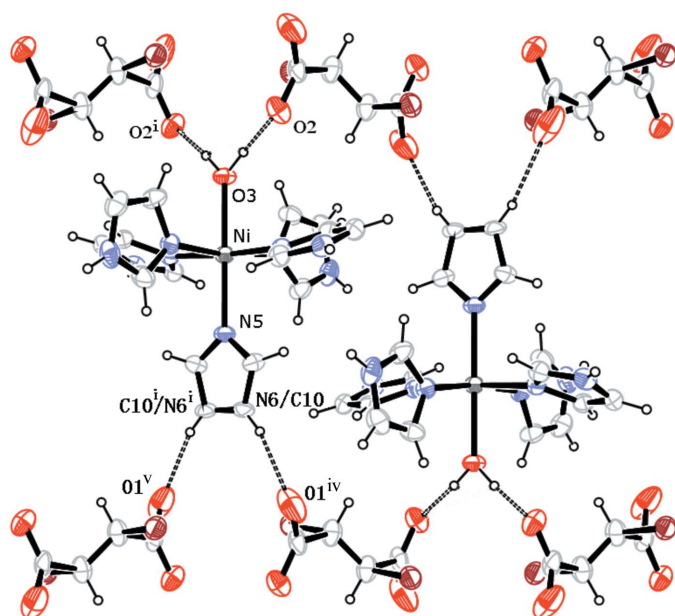
## Comment

As  $\pi-\pi$  stacking plays an important role in some biological processes (Deisenhofer & Michel, 1989), the nature of these stacking interactions has attracted our attention. A series of metal complexes incorporating different aromatic ligands has been prepared and their structures determined to compare the effect of the size of the aromatic ring on  $\pi-\pi$  stacking. The research results show that not all complexes containing aromatic rings display  $\pi-\pi$  stacking interactions. The title  $\text{Ni}^{\text{II}}$  complex, (I), with imidazole ligands and dibromosuccinate anions, has been prepared, but its crystal structure shows no  $\pi-\pi$  stacking.

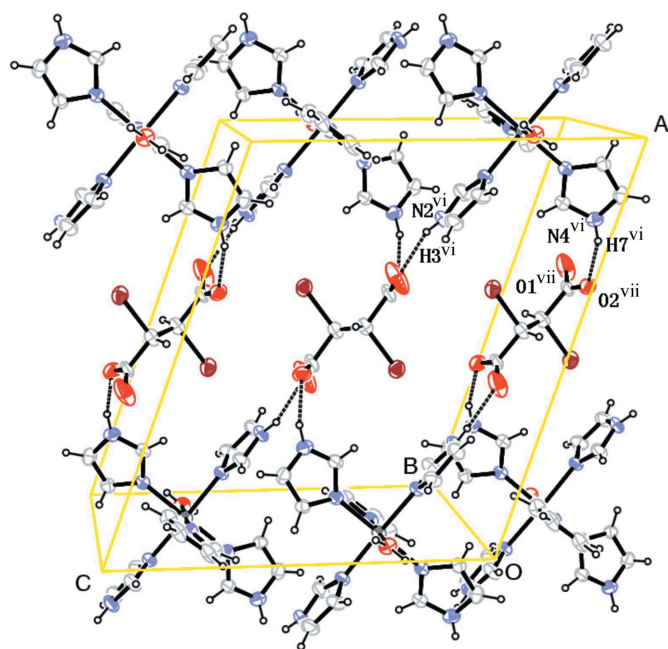


The crystal structure of (I) consists of  $\text{Ni}^{\text{II}}$  complex cations and dibromosuccinate anions (DBrS), as shown in Fig. 1. The compound is isostructural with the corresponding  $\text{Co}^{\text{II}}$  complex (Li *et al.*, 2004). The  $\text{Ni}^{\text{II}}$  atom, located on a twofold axis, is coordinated by five imidazole ligands and one water molecule in an octahedral geometry. The coordinated water O atom and the N5-containing imidazole ligand are also located on the twofold axis. Thus, the N5-imidazole is disordered, with atoms N6 and C10 occupying the same site, each with 0.5 occupancy. The N5-imidazole is linked to the carboxyl group of DBrS via a disordered  $\text{N6}-\text{H11}\cdots\text{O1}^i$  or  $\text{C10}-\text{H11}\cdots\text{O1}^i$  hydrogen bond [Table 2; symmetry code: (i)  $x, 1 + y, z$ ].

The DBrS anion lies on an inversion centre. Each carboxyl group participates in similar hydrogen-bond linkages with the  $\text{N2}^{\text{iii}}$ -imidazole, the  $\text{N4}^{\text{iii}}$ -imidazole and the O3 water molecule

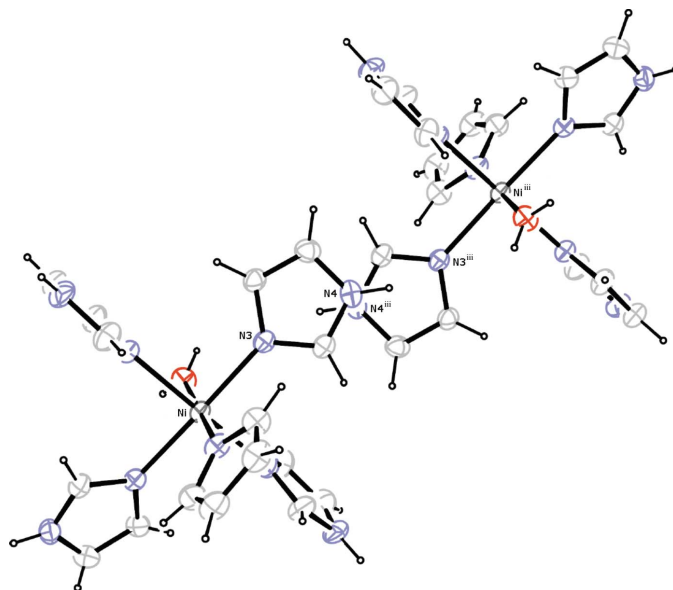

**Figure 1**

The molecular structure of (I), with 30% probability displacement ellipsoids. The atomic label of N6/C10 indicates two different atoms occupying the same site within the N5-imidazole ligand. Hydrogen bonds are shown as dashed lines. [Symmetry codes: (i)  $1 - x, y, \frac{1}{2} - z$ ; (iv)  $x, 1 + y, z$ ; (v)  $1 - x, 1 + y, \frac{1}{2} - z$ .]


**Figure 2**

The crystal packing of (I). Dashed lines indicate the hydrogen bonding between imidazole ligands and carboxyl groups. [Symmetry codes: (vi)  $\frac{3}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$ ; (vii)  $x, 1 + y, -\frac{1}{2} - z$ .]

[symmetry codes: (ii)  $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$ ; (iii)  $\frac{3}{2} - x, \frac{3}{2} - y, 1 - z$ ], as shown in Fig. 2. No  $\pi$ - $\pi$  stacking is observed in (I). The nearest distance between imidazole rings of neighbouring complex cations is 3.284 (6) Å (N4 $\cdots$ N4<sup>iii</sup>; Fig.3).


**Figure 3**

The nearest contact between imidazole rings of neighbouring complex cations of (I) [symmetry code: (iii)  $\frac{3}{2} - x, \frac{3}{2} - y, 1 - z$ ].

## Experimental

An ethanol–water solution (5 ml, 1:1) of NiCl<sub>2</sub>·6H<sub>2</sub>O (0.24 g, 1 mmol) was mixed with an aqueous solution (4 ml) containing DBrSH<sub>2</sub> (0.55 g, 2 mmol) and Na<sub>2</sub>CO<sub>3</sub> (0.21 g, 2 mmol). The mixture was refluxed for 4 h and filtered. After cooling to room temperature, imidazole (0.20 g, 3 mmol) was added to the filtrate and green single crystals of (I) were obtained after 4 d.

### Crystal data

[Ni(C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>)<sub>5</sub>(H<sub>2</sub>O)](C<sub>4</sub>H<sub>2</sub>Br<sub>2</sub>O<sub>4</sub>)  
*M<sub>r</sub>* = 690.97  
 Monoclinic, C2/c  
*a* = 15.8702 (11) Å  
*b* = 12.9262 (11) Å  
*c* = 13.9436 (11) Å  
 $\beta$  = 109.468 (3)°  
*V* = 2696.9 (4) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.702 Mg m<sup>-3</sup>  
 Mo K $\alpha$  radiation  
 Cell parameters from 175 reflections  
 $\theta$  = 2.5–24.5°  
 $\mu$  = 3.73 mm<sup>-1</sup>  
*T* = 298 (2) K  
 Prism, green  
 0.36 × 0.24 × 0.22 mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1999)  
*T<sub>min</sub>* = 0.355, *T<sub>max</sub>* = 0.440  
 5513 measured reflections

3000 independent reflections  
 2048 reflections with  $I > 2\sigma(I)$   
*R<sub>int</sub>* = 0.020  
 $\theta_{\max}$  = 27.2°  
*h* = -20 → 20  
*k* = -16 → 16  
*l* = -17 → 17

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.050  
*wR* (*F*<sup>2</sup>) = 0.156  
*S* = 1.05  
 3000 reflections  
 175 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0964P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.67 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.66 \text{ e \AA}^{-3}$

**Table 1**  
Selected geometric parameters (Å, °).

Ni—N3	2.147 (3)	Ni—N1	2.185 (3)
Ni—O3	2.183 (4)	Ni—N5	2.217 (5)
N3—Ni—N3 <sup>i</sup>	176.24 (17)	N1 <sup>i</sup> —Ni—N1	172.14 (19)
N3—Ni—O3	88.12 (9)	N3—Ni—N5	91.88 (9)
N3—Ni—N1	89.13 (14)	O3—Ni—N5	180.000 (1)
N3 <sup>i</sup> —Ni—N1	90.61 (14)	N1 <sup>i</sup> —Ni—N5	93.93 (10)
O3—Ni—N1	86.07 (10)		

Symmetry code: (i)  $-x + 1, y, -z + \frac{1}{2}$ .**Table 2**  
Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O3—H12...O2	0.92	1.85	2.743 (5)	165
N2—H3...O1 <sup>ii</sup>	0.86	2.04	2.773 (9)	143
N4—H7...O2 <sup>iii</sup>	0.86	1.95	2.771 (6)	158
N6—H11...O1 <sup>iv</sup>	0.84	2.55	3.372 (8)	167
C10—H11...O1 <sup>iv</sup>	0.84	2.55	3.372 (8)	167

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

The water H atoms were located in a difference Fourier map and included in the final cycles of refinement with fixed positional and

displacement parameters, with O—H = 0.92 Å and  $U_{\text{iso}}(\text{H}) = 0.05 \text{ \AA}^2$ . Other H atoms were placed in calculated positions, with C—H = 0.93 Å (aromatic) or 0.98 Å (methine), and included in the final cycles of refinement in the riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  or  $1.5U_{\text{eq}}$  of the carrier atoms.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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