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## Key indicators

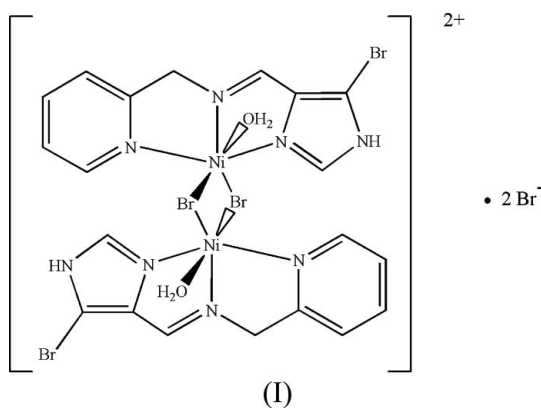
Single-crystal X-ray study  
*T* = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.015 \text{ \AA}$   
*R* factor = 0.043  
*wR* factor = 0.128  
Data-to-parameter ratio = 17.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Di- $\mu$ -bromo-bis{aqua[(5-bromo-1*H*-imidazol-4-yl-methylene)(2-pyridylmethyl)amine- $\kappa^3\text{N},\text{N}',\text{N}''$ ]-nickel(II)} dibromide

In the title compound,  $[\text{Ni}_2\text{Br}_2(\text{C}_{10}\text{H}_9\text{BrN}_4)_2(\text{H}_2\text{O})_2]\text{Br}_2$ , the asymmetric unit consists of one half-cation and one  $\text{Br}^-$  anion. The dinuclear cation is located on an inversion centre and each  $\text{Ni}^{\text{II}}$  ion is chelated by one tridentate (5-bromo-1*H*-imidazol-4-ylmethylene)(2-pyridylmethyl)amine (BIPI) ligand, one water molecule and two bridging  $\text{Br}^-$  ligands. The tridentate BIPI ligand is essentially planar. Hydrogen bonds involving the  $\text{Br}^-$  anions stabilize the crystal structure.

Received 29 August 2006  
Accepted 1 September 2006

## Comment

Biomimetic model studies of metalloproteins with active sites containing histidine often involve ligands bearing imidazole (Kirin *et al.*, 2004) or pyridine groups (Young *et al.*, 1995). However, only limited examples of ligands with both pyridyl and imidazolyl groups are available in the literature (Colacio *et al.*, 2000; Moriuchi *et al.*, 2001; Scarpellini *et al.*, 2004). As an extension of the work on the (4-imidazolylmethyl)(2-pyridylmethyl)amine (IPA) ligand, which we reported previously (Wang *et al.*, 2006), we have synthesized the bromo-substituted imine analogue of IPA, *viz.* the (5-bromo-1*H*-imidazol-4-ylmethylene)(2-pyridylmethyl)amine (BIPI) ligand. The BIPI ligand reacts with nickel dibromide to yield the title complex. We report here the structure of this  $\text{Ni}^{\text{II}}$  complex of BIPI, (I).



The asymmetric unit of (I) consists of one half-cation and one  $\text{Br}^-$  anion. The dinuclear cation possesses an inversion centre at the mid-point of the  $\text{Ni} \cdots \text{Ni}$  vector (Fig. 1). Each  $\text{Ni}^{\text{II}}$  ion is chelated by one BIPI ligand in the *mer* form, one water molecule and two bridging  $\text{Br}$  ligands, with a distorted octahedral coordination geometry (Table 1). The  $\text{Ni}-\text{N}2$  bond distance is significantly shorter than the  $\text{Ni}-\text{N}1$  and  $\text{Ni}-\text{N}3$  bond distances.

The tridentate BIPI ligand is essentially planar to within 0.08 Å. A related example of a dinuclear complex with a

multidentate ligand containing both pyridyl and imidazolyl groups is  $[\text{Cu}(\text{HL})(\text{Cl})_2][\text{ClO}_4]_2$  (HL = methylpyridylmethylideneaminoethylimidazole; Alves *et al.* 2003). In that complex, the chelating tridentate ligand is slightly puckered and the metal centre has no coordinated water. However, both complexes have an overall shape resembling a stairway.

There is extensive hydrogen bonding (Table 2), which stabilizes the crystal structure of (I).

## Experimental

BIPI was prepared by a condensation reaction, mixing 5-bromo-4-imidazolecarboxaldehyde (0.46 g, 2.63 mmol) and 2-aminomethylpyridine (0.27 ml, 2.63 mmol) in ethanol (25 ml) at room temperature for 4 h. Filtration gave the white powdery BIPI ligand in 86% yield. Compound (I) precipitated from the reaction of equimolar amounts of  $\text{NiBr}_2$  (0.11 g, 0.5 mmol) in acetonitrile (10 ml) and BIPI (0.13 g, 0.5 mmol) in methanol (10 ml) at room temperature after 4 h. Crystals of (I) were obtained by simple evaporation of a methanol solution of (I).

### Crystal data

$[\text{Ni}_2\text{Br}_2(\text{C}_{10}\text{H}_9\text{BrN}_4)_2(\text{H}_2\text{O})_2]\text{Br}_2$	$V = 755.1 (3) \text{ \AA}^3$
$M_r = 1003.24$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 2.207 \text{ Mg m}^{-3}$
$a = 8.4833 (17) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.4187 (19) \text{ \AA}$	$\mu = 9.22 \text{ mm}^{-1}$
$c = 10.748 (2) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\alpha = 90.16 (3)^\circ$	Prism, green
$\beta = 107.77 (3)^\circ$	$0.2 \times 0.15 \times 0.15 \text{ mm}$
$\gamma = 111.40 (3)^\circ$	

### Data collection

Rigaku AFC-7S diffractometer	1603 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$R_{\text{int}} = 0.039$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$\theta_{\text{max}} = 26.0^\circ$
$T_{\text{min}} = 0.196$ , $T_{\text{max}} = 0.252$	3 standard reflections
3189 measured reflections	every 150 reflections
2977 independent reflections	intensity decay: 0.5%

### Refinement

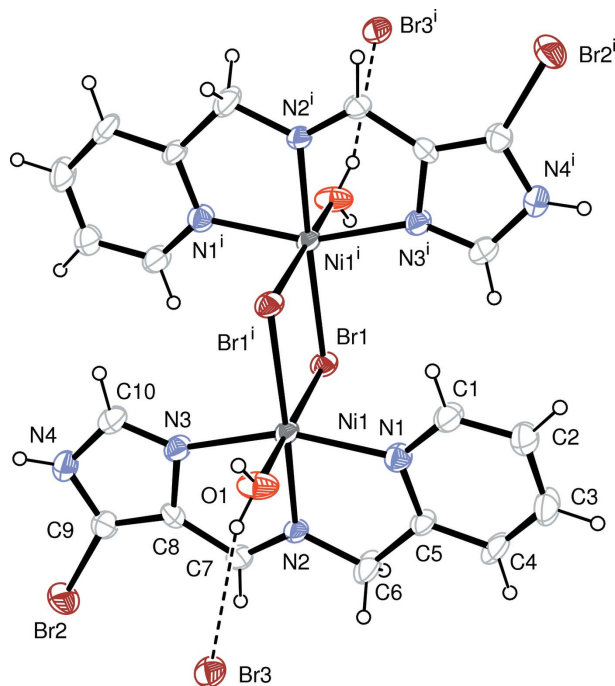
Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2]$
$wR(F^2) = 0.128$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2977 reflections	$\Delta\rho_{\text{max}} = 0.71 \text{ e \AA}^{-3}$
172 parameters	$\Delta\rho_{\text{min}} = -0.85 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ni1—N2	2.017 (6)	Ni1—N3	2.099 (7)
Ni1—N1	2.071 (7)	Ni1—Br1 <sup>i</sup>	2.5157 (17)
Ni1—O1	2.082 (6)	Ni1—Br1	2.5884 (16)
N2—Ni1—N1	79.7 (3)	N2—Ni1—Br1	92.0 (2)
N2—Ni1—O1	91.5 (3)	N1—Ni1—Br1	90.9 (2)
N1—Ni1—O1	87.5 (3)	O1—Ni1—Br1	175.78 (18)
N2—Ni1—N3	79.4 (3)	N3—Ni1—Br1	93.5 (2)
N1—Ni1—N3	158.8 (3)	Br1 <sup>i</sup> —Ni1—Br1	88.01 (5)
O1—Ni1—N3	89.4 (3)		

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



**Figure 1**

The molecular structure of (I), with 30% probability displacement ellipsoids (spheres of arbitrary radii for H atoms). Dashed lines indicate hydrogen bonds. [Symmetry code: (i)  $-x, -y, -z$ .]

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1W $\cdots$ Br3	0.80	2.54	3.306 (6)	161
O1—H2W $\cdots$ Br3 <sup>ii</sup>	0.87	2.46	3.315 (6)	168
N4—H4A $\cdots$ Br3 <sup>iii</sup>	0.86	2.43	3.266 (7)	165

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

Water H atoms were located in a difference map and refined in riding mode, with  $O-H = 0.80$  and  $0.87 \text{ \AA}$ , and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ . All other H atoms were placed in calculated positions, with  $C-H = 0.93 \text{ \AA}$  (aromatic) or  $0.97 \text{ \AA}$  (methylene), and  $N-H = 0.86 \text{ \AA}$ , and refined in riding mode, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ .

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1985); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); 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).

This work was supported by the National Science Council of Taiwan (grant No. NSC94-2113-M-110-009).

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