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Diaquadibromobis(1*H*-imidazole)nickel(II)

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Key indicators

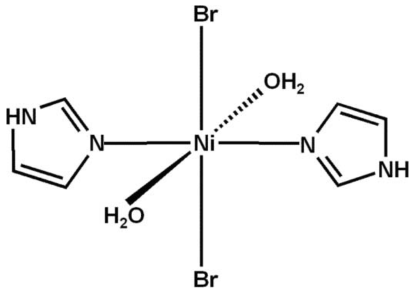
Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.003 Å
R factor = 0.020
wR factor = 0.051
Data-to-parameter ratio = 19.7

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

The structure of the title compound, $[NiBr_2(C_3H_4N_2)_2(H_2O)_2]$, consists of monomers with inversion symmetry. The three monodentate ligands (imidazole, bromine and aqua), together with their symmetry equivalents, define an almost perfect octahedral coordination. Hydrogen-bonding interactions *via* the NH group of imidazole, Br and aqua H atoms lead to a three-dimensional network.

Comment

The structure of the title compound, (I), is composed of monomeric units possessing a crystallographically imposed center of symmetry (Fig. 1). The coordination environment of nickel is almost perfect octahedral (Table 1), corresponding to that observed in $[NiCl_2(Him)_2(H_2O)_2]$ (Him is 1*H*-imidazole), (II) (Atria *et al.*, 2003). However, (I) and (II) crystallize in different space groups, *viz.* monoclinic $P2_1/c$ and orthorhombic *Pbca*, respectively.



(I)

In (I), the three potentially active H atoms, *viz.* imidazole H2 and aqua H1*W* and H2*W* atoms, are engaged in hydrogen bonds with the Br atom, which acts as the sole acceptor for all three interactions (Table 2). The O—H···Br hydrogen bonds

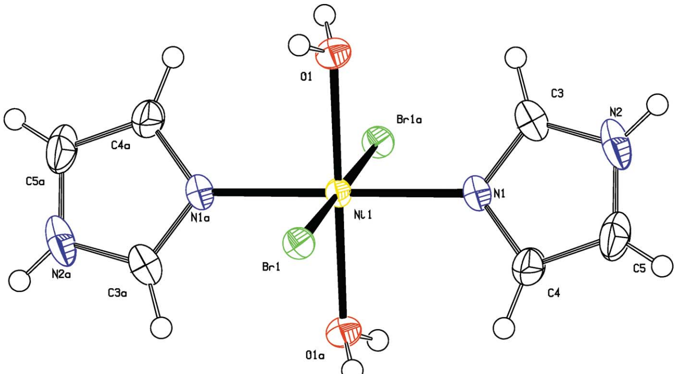


Figure 1
View of (I) shown with 50% probability displacement ellipsoids. Atoms labelled with the suffix a are at symmetry position ($\frac{1}{2} - x, -y, 2 - z$).

(Fig. 2, dashed red lines) link monomers along the *b* and *c* axes, thus defining two-dimensional arrays, which are further linked by the N—H···Br hydrogen bonds (Fig. 2, dashed blue lines), to form a three-dimensional network.

Experimental

Crystals of (I) were obtained from $NiBr_2\cdot 6H_2O$ (5 mmol) and 1*H*-imidazole (5 mmol) in aqueous solution (30 ml) at room temperature. After a few days, green prismatic crystals appeared.

Crystal data

$[NiBr_2(C_3H_4N_2)_2(H_2O)_2]$
$M_r = 390.69$
Monoclinic, $P2_1/c$
$a = 7.8000\ (18)$ Å
$b = 9.366\ (2)$ Å
$c = 8.474\ (2)$ Å
$\beta = 96.114\ (4)^\circ$
$V = 615.6\ (2)$ Å^3
$Z = 2$

$D_x = 2.108$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1538 reflections
$\theta = 2.6$–28.3°
$\mu = 8.05$ mm^{-1}
$T = 223\ (2)$ K
Prism, green
0.36 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS* in *SAINT*; Bruker, 1998)
$T_{min} = 0.16$, $T_{max} = 0.28$
8270 measured reflections

1538 independent reflections
1414 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 28.3^\circ$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.051$
$S = 1.05$
1538 reflections
78 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.0562P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	2.0557 (16)	Ni1—Br1	2.6184 (6)
Ni1—O1	2.0910 (15)		
N1—Ni1—O1	88.53 (6)	O1—Ni1—Br1	90.15 (5)
N1—Ni1—Br1	89.59 (5)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*W*···Br1^{i}	0.79 (3)	2.56 (3)	3.3356 (16)	168 (3)
O1—H2*W*···Br1^{ii}	0.81 (3)	2.55 (3)	3.3273 (17)	164 (2)
N2—H2···Br1^{iii}	0.87	2.64	3.4782 (19)	162

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{5}{2}$; (ii) $x, -y-\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x, -y, -z+2$.

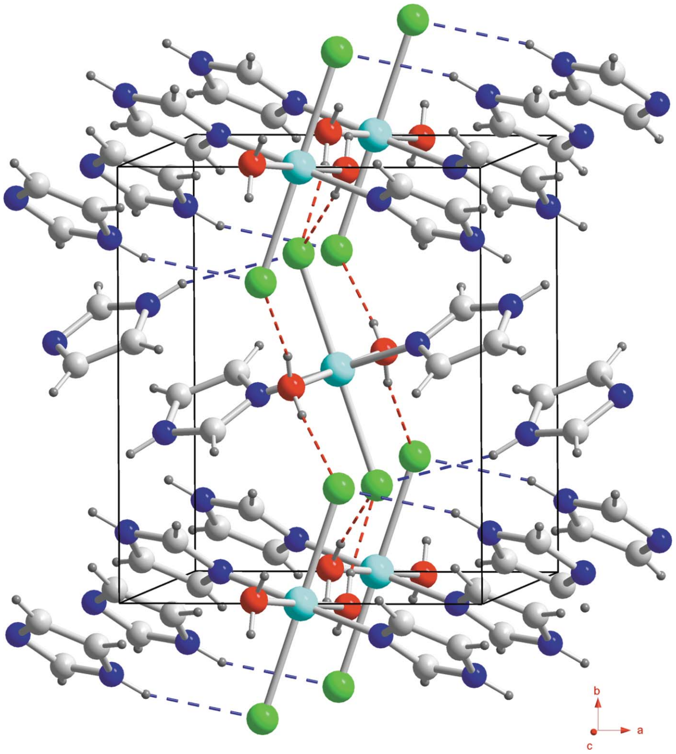


Figure 2
View of the crystal packing, showing the O—H···Br and N—H···Br hydrogen bonds as red and blue dashed lines, respectively.

The imidazole H atoms were constrained to an ideal geometry, with C—H and N—H distances of 0.94 and 0.87 Å, respectively. Aqua H atoms were located in a difference Fourier map and their positions were refined freely. All H atoms were treated as isotropic, with $U_{iso}(H) = 1.2U_{eq}(C,N,O)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

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