

Harry Adams, Scott Clunas and
David E. Fenton*Department of Chemistry, Dainton Building,
University of Sheffield, Sheffield S7 3HF,
EnglandCorrespondence e-mail:
d.fenton@sheffield.ac.uk

Key indicators

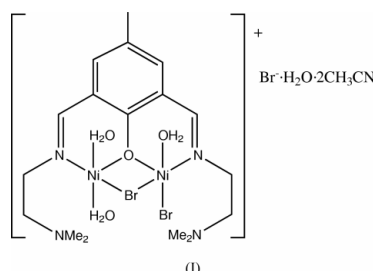
Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.041
 wR factor = 0.087
Data-to-parameter ratio = 16.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.A dinuclear nickel(II) complex of the ligand
2,6-bis[2-(dimethylamino)ethyliminomethyl]-
4-methylphenol

In the title complex, triqua[μ -2,6-bis[2-(dimethylamino)ethyliminomethyl]-4-methylphenolato]- μ -bromo-bromodinicel(II) bromide monohydrate acetonitrile disolvate, $[\text{Ni}_2\text{Br}_2(\text{C}_{17}\text{H}_{27}\text{N}_4\text{O})(\text{H}_2\text{O})_3]\text{Br}\cdot\text{H}_2\text{O}\cdot 2\text{C}_2\text{H}_3\text{N}$, the Ni^{II} atoms are octahedrally coordinated and the donor groups are different ($\text{N}_2\text{O}_3\text{Br}$ and $\text{N}_2\text{O}_2\text{Br}_2$), with an intermetallic separation of 3.2346 (9) Å.

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Comment

Hydrolysis of the imine function has been observed in the reaction of asymmetric Schiff base compartmental ligands with Ni^{II} salts (Adams *et al.*, 2000; Adams, Clunas & Fenton, 2002). The reaction of the symmetric compartmental ligand 2,6-bis[2-(dimethylamino)ethyliminomethyl]-4-methylphenol with nickel(II) bromide gave the title complex, $[\text{Ni}_2\text{Br}_2\text{L}(\text{H}_2\text{O})_3]\text{Br}\cdot\text{H}_2\text{O}\cdot 2\text{CH}_3\text{CN}$, (I), in which the integrity of the imine functions is retained. The Ni atoms are octahedrally coordinated and the donor groups are different ($\text{N}_2\text{O}_3\text{Br}$ and $\text{N}_2\text{O}_2\text{Br}_2$; Satcher *et al.*, 1995). The intermetallic separation of 3.2346 (9) Å is comparable with those found in related Ni^{II} complexes of asymmetric Schiff base compartmental ligands (Adams, Clunas, Fenton & Spey, 2002). The Ni atoms are doubly bridged, by the phenolate O atom of the ligand and by a bromide anion.



Experimental

The complex was prepared from the ligand and nickel(II) bromide by the method of Sakiyama *et al.* (2000). The reaction mixture was allowed to evaporate in air, yielding crystals suitable for crystallographic study.

Crystal data

$[\text{Ni}_2\text{Br}_2(\text{C}_{17}\text{H}_{27}\text{N}_4\text{O})(\text{H}_2\text{O})_3]\text{Br}\cdot\text{H}_2\text{O}\cdot 2\text{C}_2\text{H}_3\text{N}$
 $M_r = 814.75$
Monoclinic, $P2_1/n$
 $a = 10.5662$ (13) Å
 $b = 11.8911$ (15) Å
 $c = 25.158$ (3) Å
 $\beta = 100.039$ (2)°
 $V = 3112.5$ (7) Å³
 $Z = 4$

$D_x = 1.739$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 4188 reflections
 $\theta = 4.5$ – 55.9 °
 $\mu = 5.1$ mm⁻¹
 $T = 150$ (2) K
Block, green
 $0.25 \times 0.18 \times 0.10$ mm

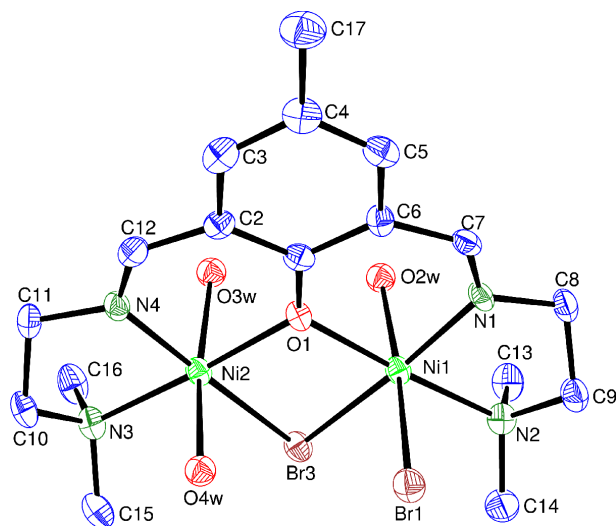


Figure 1
View of the $[\text{Ni}_2\text{BrL}(\text{H}_2\text{O})_3]^+$ cation, with 50% probability displacement ellipsoids. H atoms have been omitted.

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 ω scans
Absorption correction: multi-scan (SADABS; Bruker, 1997)
 $T_{\min} = 0.344$, $T_{\max} = 0.600$
14 837 measured reflections

5468 independent reflections
3844 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.102$
 $\theta_{\max} = 25^\circ$
 $h = -12 \rightarrow 12$
 $k = -13 \rightarrow 14$
 $l = -14 \rightarrow 29$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.088$
 $S = 0.87$
5468 reflections
336 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0396P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.79 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.68 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1W}-\text{H1WA}\cdots\text{Br2}^{\text{i}}$	0.85	2.44	3.256 (3)	162
$\text{O1W}-\text{H1WB}\cdots\text{Br1}^{\text{i}}$	0.85	2.55	3.398 (3)	173
$\text{O2W}-\text{H2WA}\cdots\text{O3W}$	0.85	2.07	2.868 (4)	157
$\text{O2W}-\text{H2WB}\cdots\text{O1W}$	0.85	1.86	2.707 (4)	172
$\text{O3W}-\text{H3WA}\cdots\text{N5}^{\text{ii}}$	0.85	2.03	2.880 (5)	180
$\text{O3W}-\text{H3WB}\cdots\text{Br2}^{\text{ii}}$	0.85	2.42	3.270 (3)	180
$\text{O4W}-\text{H4WA}\cdots\text{Br2}^{\text{iii}}$	0.85	2.41	3.260 (3)	180
$\text{O4W}-\text{H4WB}\cdots\text{Br1}$	0.85	2.42	3.266 (3)	180

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

H atoms for the solvent water molecules were calculated by difference Fourier. All other H atoms were placed geometrically and refined with a riding model (including torsional freedom for methyl groups) and with U_{iso} constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom.

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

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