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trans-Bis(acetonitrile-*N*)tetraaquanickel(II) dibromide

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The structure of *trans*-$[Ni(CH_3CN)_2(H_2O)_4]Br_2$ has been determined at 153 K. The complex possesses C_i symmetry, with the Ni^{II} atom lying on an inversion center. The Ni atom is coordinated to four water molecules in the equatorial plane and to two *trans* acetonitrile molecules. In the crystal, a three-dimensional structure is formed by hydrogen bonding involving the lattice Br^- ions and the coordinated water molecules.

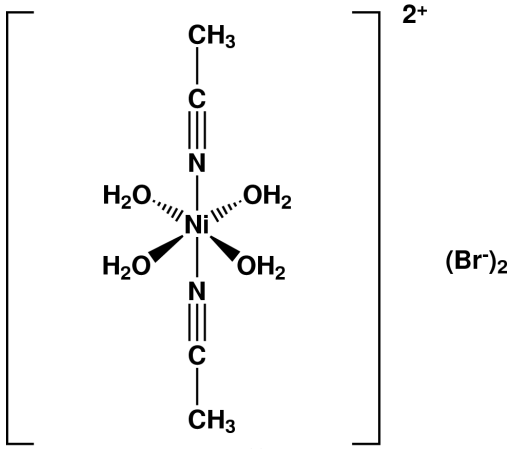
Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.008 Å
R factor = 0.040
wR factor = 0.112
Data-to-parameter ratio = 13.7

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

Comment

trans-$[Ni(CH_3CN)_2(H_2O)_4]Br_2$, (I), was prepared by accident. The structure is isomorphous with the cobalt(II) complex (Depree *et al.*, 2000).



(I)

Experimental

The title compound was prepared during attempts to synthesize an $NiBr_2$ complex of a substituted pyrazine ligand in acetonitrile.

Crystal data

$[Ni(C_2H_3N)_2(H_2O)_4]Br_2$
M_r = 372.70
Monoclinic, $P2_1/c$
a = 6.8839 (11) Å
b = 12.4630 (17) Å
c = 7.9173 (12) Å
β = 111.127 (18)°
V = 633.60 (16) Å^3
Z = 2
D_x = 1.954 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3712 reflections
θ = 3.2–26.0°
μ = 7.83 mm^{-1}
T = 153 (2) K
Block, blue–green
0.50 × 0.35 × 0.35 mm

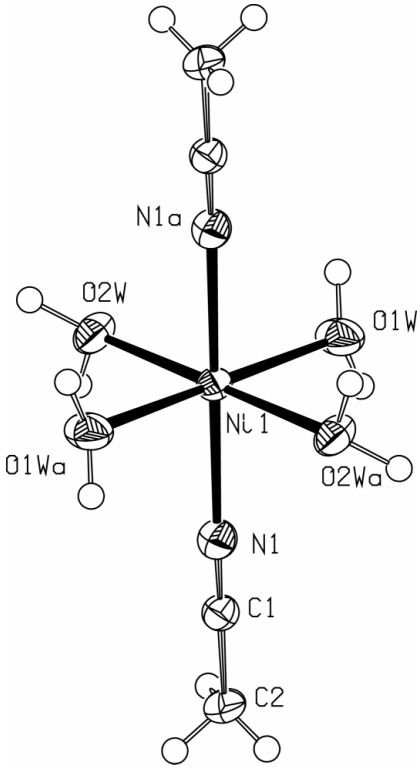


Figure 1
A perspective view of the $[Ni(CH_3CN)_2(H_2O)_4]^{2+}$ cation, showing the numbering scheme and displacement ellipsoids at the 50% probability level.

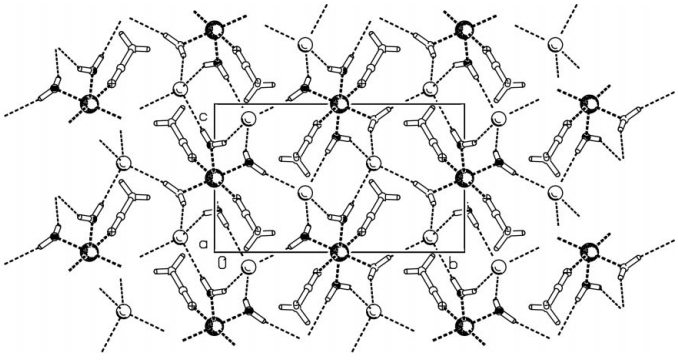


Figure 2
Packing diagram illustrating the O—H···Br bonds in the structure of *trans*-$[Ni(CH_3CN)_2(H_2O)_4]Br_2$ viewed down the *a* axis.

Data collection

Stoe Image Plate Diffraction System	1231 independent reflections
φ oscillation scans	1049 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*PLATON*; Spek, 1990)	$R_{int} = 0.079$
$T_{min} = 0.067$, $T_{max} = 0.214$	$\theta_{max} = 26.0°$
4033 measured reflections	$h = -8 \rightarrow 8$
	$k = -14 \rightarrow 15$
	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0727P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.112$	$\Delta\rho_{max} = 1.01$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -1.23$ e Å^{-3}
1231 reflections	Extinction correction: *SHELXL*97
90 parameters	Extinction coefficient: 0.021 (3)
All H-atom parameters refined	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*WA*···Br1^{i}	0.80 (9)	2.57 (9)	3.298 (4)	152 (8)
O1*W*—H1*WB*···Br1^{ii}	0.86 (8)	2.42 (8)	3.275 (4)	168 (6)
O2*W*—H2*WA*···Br1	0.83 (10)	2.48 (10)	3.275 (4)	162 (7)
O2*W*—H2*WB*···Br1^{iii}	0.89 (7)	2.46 (7)	3.339 (4)	170 (6)

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

The H atoms were located from difference Fourier maps and were refined isotropically. A semi-empirical absorption correction was applied using the *MULscanABS* routine in *PLATON*99 (Spek, 1990).

Data collection: *EXPOSE* (Stoe & Cie, 2000); cell refinement: *CELL* (Stoe & Cie, 2000); data reduction: *INTEGRATE* (Stoe & Cie, 2000); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXL*97.

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