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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
 R factor = 0.040
 wR factor = 0.088
 Data-to-parameter ratio = 18.5

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

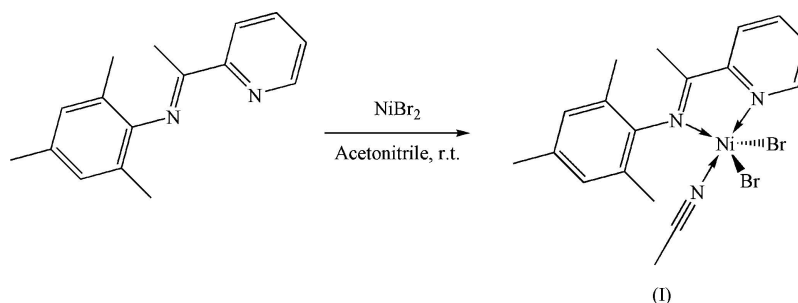
(Acetonitrile)dibromo{(E)-2,4,6-trimethyl-N-[1-(pyridin-2-yl)ethylidene]aniline- $\kappa^2\text{N},\text{N}'$]nickel(II)}

The title complex, $[\text{NiBr}_2(\text{C}_2\text{H}_3\text{N})(\text{C}_{16}\text{H}_{18}\text{N}_2)]$, contains a slightly distorted trigonal bipyramidal Ni(II) center bound to two Br atoms and three N atoms from an *N,N*-bidentate ligand backbone and an acetonitrile molecule.

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Comment

Pyridylimine-coordinated nickel(II) complexes (Benito *et al.*, 2005; Köppl & Alt, 2000) have shown good catalytic activity in the polymerization of olefins (Gibson & Spitzmesser, 2003; Ittel *et al.*, 2000), yielding ethylene oligomers and polyethylene (PE) from linear to hyperbranched or even dendritic microstructures. The linearity of the PE can be controlled precisely by tuning of the ancillary ligands. Furthermore, copolymerization of olefins with acrylamide (Marques *et al.*, 2000) or vinyl monomers (Marques *et al.*, 2001) can be achieved by α -diimine-Ni(II)-type complexes in the presence of methylaluminumoxane as cocatalyst. We report here the structure of a nickel-mediated *N,N*-bidentate complex.



The solid state structure of (I) shows a monomeric nickel(II) complex (Fig. 1) in which the Ni atom is bound to three N atoms (imine, pyridine and acetonitrile) and two Br atoms. Bond lengths around the Ni atom are comparable to the corresponding values observed in pyridinylimine-based Ni(II) complexes (Laine *et al.*, 2000). The geometry around Ni can be regarded as slightly deformed trigonal bipyramidal; the equatorial plane includes the nitrogen of the imino group in the ligand (N2) and the terminal bromine atoms; the nickel center is slightly displaced from the triangular plane [0.1075 (11) Å]. The pyridine nitrogen (N1) and the acetonitrile nitrogen (N3) occupy the axial coordination sites (Table 1). The dihedral angle between the pyridine and benzene rings is 86.8 (4)°.

Experimental

The title compound was prepared by the reaction of (E)-2,4,6-trimethyl-N-(1-(pyridin-2-yl)ethylidene)benzenamine (4 mmol) with

nickel(II) bromide (4 mmol) at room temperature in acetonitrile (10 ml). The resulting green mixture was stirred for 24 h and then dried *in vacuo*. The residue was extracted with acetonitrile (30 ml) and filtered. The filtrate was concentrated to *ca* 10 ml. Green crystals suitable for X-ray structure determination were obtained at room temperature in 3 days. Yield: 1.81 g (91%).

Crystal data

[NiBr₂(C₂H₃N)(C₁₆H₁₈N₂)]
M_r = 497.91
 Monoclinic, *P*2₁/*c*
a = 14.4149 (17) Å
b = 8.8331 (11) Å
c = 16.0753 (19) Å
 β = 92.626 (3)°
V = 2044.7 (4) Å³

Z = 4
D_x = 1.617 Mg m⁻³
 Mo *K*α radiation
 μ = 4.86 mm⁻¹
T = 298 (2) K
 Parallelepiped, green
 0.37 × 0.36 × 0.22 mm

Data collection

Bruker SMART 1000 CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
SADABS, Sheldrick (1996)
T_{min} = 0.595, *T_{max}* = 1.000
 (expected range = 0.204–0.343)

11307 measured reflections
 4005 independent reflections
 2294 reflections with *I* > 2σ(*I*)
R_{int} = 0.047
 θ_{\max} = 26.0°

Refinement

Refinement on *F*²
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.088$
S = 1.06
 4005 reflections
 217 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.03P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.50 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.30 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ni–N2	2.020 (3)	Ni–Br1	2.4225 (8)
Ni–N3	2.034 (4)	Ni–Br2	2.4592 (7)
Ni–N1	2.046 (3)		
N2–Ni–N3	95.42 (14)	N1–Ni–Br1	90.69 (10)
N2–Ni–N1	79.10 (14)	N2–Ni–Br2	111.37 (9)
N3–Ni–N1	174.50 (15)	N3–Ni–Br2	91.61 (11)
N2–Ni–Br1	111.17 (9)	N1–Ni–Br2	90.03 (9)
N3–Ni–Br1	91.70 (11)	Br1–Ni–Br2	136.79 (3)

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C–H distances of 0.96 Å and *U_{iso}*(H) = 1.5*U_{eq}*(C). All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H distances in the range 0.95–1.00 Å and *U_{iso}*(H) = 1.2*U_{eq}*(C).

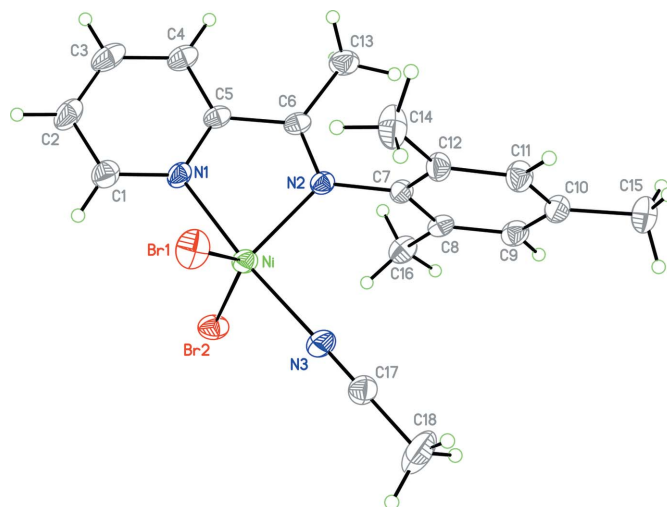


Figure 1

A view of the molecular structure of (I), with displacement ellipsoids drawn at the 20% probability level. H atoms are represented by circles of arbitrary size.

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: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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