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Azido{2-bromo-4-chloro-6-[2-(diethylamino)-ethyliminomethyl]phenolato}nickel(II)

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Key indicators

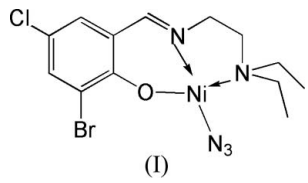
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.096
Data-to-parameter ratio = 18.6

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

In the title compound, $[Ni(C_{13}H_{17}BrClN_2O)(N_3)]$, the Ni atom is four-coordinated by one Schiff base ligand and by one terminal azide anion in a square-planar geometry.

Comment

Nickel(II) complexes play an important role in both bioinorganic chemistry and coordination chemistry (Suh *et al.*, 1996; Dey *et al.*, 2004; Angulo *et al.*, 2001; Ramadevi *et al.*, 2005; Edison *et al.*, 2004). As part of a further study of the structures of such complexes, the title mononuclear nickel(II) complex, (I), is reported in this paper.



(I)

The Ni atom in (I) is four-coordinated by one O atom and two N atoms of the Schiff base ligand, 2-bromo-4-chloro-6-[2-(diethylamino)ethyliminomethyl]phenol, and by one N atom of the terminal azide anion, forming a square-planar geometry (Fig. 1). The bond lengths and angles (Table 1) subtended at atom Ni1 are within normal ranges and are comparable with the corresponding values observed in other similar nickel(II) complexes (Zhu *et al.*, 2004; Wang, 2006; Wang & Wei, 2006; Liu *et al.*, 2006; Zhang, 2006). No hydrogen-bonding interactions are observed in the crystal structure.

Experimental

3-Bromo-5-chloro-2-hydroxybenzaldehyde (0.2 mmol, 47.7 mg), *N*,*N*-diethyl-1,2-diaminoethane (0.2 mmol, 23.2 mg) and sodium azide (0.2 mmol, 11.2 mg) were dissolved in methanol (10 ml). To the mixture was added dropwise a methanol solution (5 ml) of nickel(II) nitrate hexahydrate (0.2 mmol, 58.2 mg) with stirring. The resulting solution was allowed to stand in air for two weeks, yielding red block-shaped crystals of (I).

Crystal data

$[Ni(C_{13}H_{17}BrClN_2O)(N_3)]$
M_r = 433.39
Monoclinic, $P2_1/c$
a = 16.306 (2) Å
b = 9.934 (1) Å
c = 10.148 (2) Å
β = 95.170 (2)°
V = 1637.1 (4) Å^3
Z = 4
D_x = 1.758 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.80 mm^{-1}
T = 298 (2) K
Block, red
0.32 × 0.30 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.376, T_{max} = 0.427
(expected range = 0.316–0.359)
13675 measured reflections
3731 independent reflections
2532 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.096
S = 1.01
3731 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.836 (2)	Ni1—N3	1.890 (3)
Ni1—N1	1.848 (3)	Ni1—N2	1.959 (3)
O1—Ni1—N1	93.73 (11)	O1—Ni1—N2	178.72 (10)
O1—Ni1—N3	89.36 (13)	N1—Ni1—N2	86.85 (12)
N1—Ni1—N3	176.86 (13)	N3—Ni1—N2	90.05 (13)

H atoms were constrained to ideal geometries, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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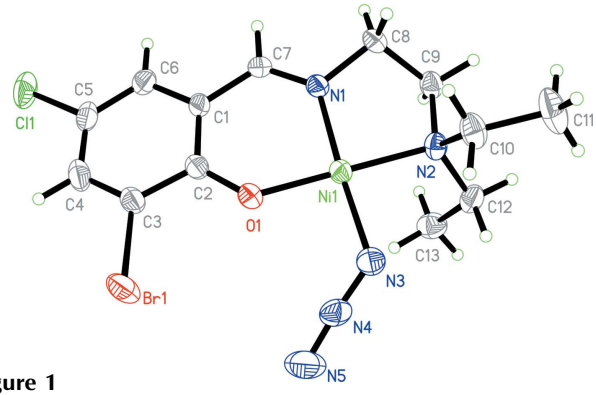

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

References

Angulo, I. M., Bouwman, E., Lutz, M., Mul, W. P. & Spek, A. L. (2001). *Inorg. Chem.* **40**, 2073–2082.
Bruker (2002). *SAINT* (Version 5.60) and *SMART* (Version 5.60). Bruker AXS Inc., Madison, Wisconsin, USA.
Dey, S. K., Mondal, N., El Fallah, M. S., Vicente, R., Escuer, A., Solans, X., Font-Bardia, M., Matsushita, T., Gramlich, V. & Mitra, S. (2004). *Inorg. Chem.* **43**, 2427–2434.
Edison, S. E., Krause Bauer, J. A. & Baldwin, M. J. (2004). *Acta Cryst.* E**60**, m1930–m1932.
Liu, H.-Y., Gao, F., Lu, Z.-S. & Wang, H.-Y. (2006). *Acta Cryst.* E**62**, m1306–m1308.
Ramadevi, P., Kumaresan, S. & Muir, K. W. (2005). *Acta Cryst.* E**61**, m1749–m1751.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Suh, M. P., Oh, K. Y., Lee, J. W. & Bae, Y. Y. (1996). *J. Am. Chem. Soc.* **118**, 777–783.
Wang, C. (2006). *Acta Cryst.* E**62**, m1754–m1755.
Wang, F.-W. & Wei, Y.-J. (2006). *Acta Cryst.* E**62**, m599–m600.
Zhang, Y.-L. (2006). *Acta Cryst.* E**62**, m2111–m2112.
Zhu, B., Ruang, W. & Zhu, Z. (2004). *Acta Cryst.* E**60**, m634–m636.