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{[N,N'-Bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetato}bis(1H-imidazole-κN^3)nickel(II)

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In the title complex, $[Ni(C_{22}H_{26}N_2O_4)(C_3H_4N_2)_2]$, the Ni atom is in a distorted octahedral coordination environment defined by an N_4O_2 donor set. The asymmetric unit consists of two half-molecules; each Ni atom lies on a crystallographic twofold rotation axis. In the crystal structure, hydrogen bonds link two kinds of coordination geometry around the Ni atom.

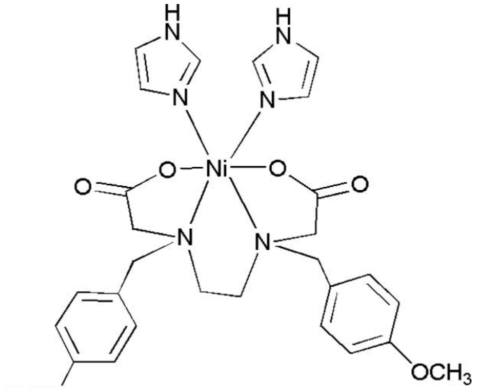
Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.005 Å
R factor = 0.050
wR factor = 0.131
Data-to-parameter ratio = 16.3

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

Comment

Much attention has been devoted to the study of acyclic ligands for their application in the design of DNA probes, but the exact coordination modes of this kind of ligand have received less attention. In this paper, we report the structure of a new Ni^{II} complex, $Ni(L_a)(L_b)_2$ {L_a = [N,N'-bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetate and L_b = imidazole}, (I). In (I) (Fig. 1), the Ni atom is six-coordinate in a slightly distorted octahedral configuration. The asymmetric unit consists of two half-molecules; each Ni atom lies on a crystallographic twofold rotation axis. In the crystal structure (Fig. 2), the coordination geometry around atoms Ni1 and Ni2 is different (Table 1). N—H···O and C—H···O hydrogen bonds (Table 2) consolidate the two units.



(I)

Experimental

The ligand [N,N'-bis(4-methoxybenzyl)ethane-1,2-diyldiimino]diacetic acid (H_2L) was synthesized according to a literature method (Xu *et al.*, 2004). When $Ni(CH_3COO)_2·4H_2O$ (0.22 g, 0.05 mmol) was added to a stirred solution (pH = 9) of H_2L (0.22 g, 0.05 mmol) (containing NaOH) in H_2O (15 ml), a blue precipitate formed immediately. After the pH of solution had been adjusted to pH 4–5 using dilute HCl, the resulting precipitate was filtered off and dried. Complex (I) was prepared by the reaction of imidazole (0.014 g, 0.2 mmol) with the precipitate NiL (0.048 g, 0.1 mmol) in a 2:1 molar ratio in MeOH (15 ml). Crystals were obtained by slow evaporation (three weeks) of a methanol solution.

Crystal data

$[Ni(C_{22}H_{26}N_2O_4)(C_3H_4N_2)_2]$
$M_r = 609.32$
Monoclinic, $C2/c$
$a = 26.0085\ (12)$ Å
$b = 16.4458\ (8)$ Å
$c = 15.0304\ (7)$ Å
$\beta = 105.7860\ (10)°$

$V = 6186.5\ (5)$ Å^3
$Z = 8$
Mo $K\alpha$ radiation
$\mu = 0.68$ mm^{-1}
$T = 297\ (2)$ K
$0.20 \times 0.10 \times 0.04$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{\min} = 0.823$, $T_{\max} = 0.967$

32089 measured reflections
6063 independent reflections
3702 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.089$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.131$
$S = 0.89$
6063 reflections

373 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.62$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O2	2.0655 (18)	Ni2—O6	2.0581 (18)
Ni1—N2	2.086 (2)	Ni2—N5	2.079 (2)
Ni1—N1	2.178 (2)	Ni2—N4	2.190 (2)
O2—Ni1—O2^{i}	175.98 (11)	O6—Ni2—O6^{ii}	174.46 (10)
O2—Ni1—N2	94.55 (8)	O6—Ni2—N5	95.36 (8)
O2^{i}—Ni1—N2	88.19 (8)	O6^{ii}—Ni2—N5	88.47 (8)
N2—Ni1—N2^{i}	94.21 (12)	N5—Ni2—N5^{ii}	92.59 (12)
O2—Ni1—N1^{i}	98.60 (8)	O6—Ni2—N4^{ii}	96.28 (8)
N2—Ni1—N1^{i}	165.24 (8)	N5—Ni2—N4^{ii}	167.05 (8)
O2—Ni1—N1	78.35 (8)	O6—Ni2—N4	79.53 (8)
N2—Ni1—N1	92.88 (8)	N5—Ni2—N4	93.36 (8)
N1^{i}—Ni1—N1	83.29 (12)	N4^{ii}—Ni2—N4	83.22 (12)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N3—H3$A\cdots$O3^{iii}	0.86	1.89	2.741 (3)	170
N6—H6$A\cdots$O5^{iii}	0.86	1.88	2.734 (3)	173
C12—H12$\cdots$O2^{i}	0.93	2.41	2.920 (3)	115
C26—H26$\cdots$O6^{ii}	0.93	2.45	2.933 (3)	113

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

H atoms bound to C atoms were included in calculated positions and allowed to ride during subsequent refinement, with C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for Csp^2, and C—H = 0.96 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for the methyl groups. H atoms bound to N atoms were located in a difference Fourier map and refined as riding, with N—H = 0.86 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm N})$.

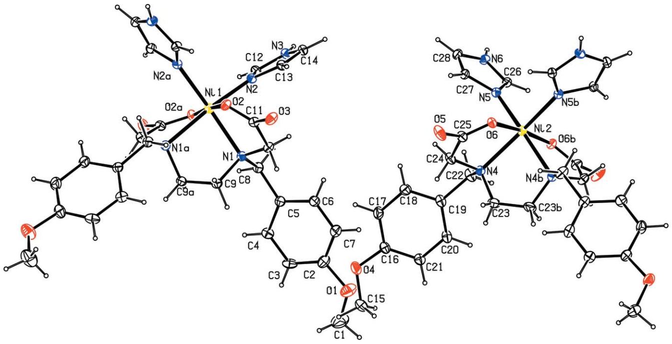


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. Unlabelled atoms in the Ni1 complex are related to labelled atoms by $(x+1, y, -z+\frac{1}{2})$. Unlabelled atoms in the Ni2 complex are related to labelled atoms by $(-x, y, -z+\frac{1}{2})$.

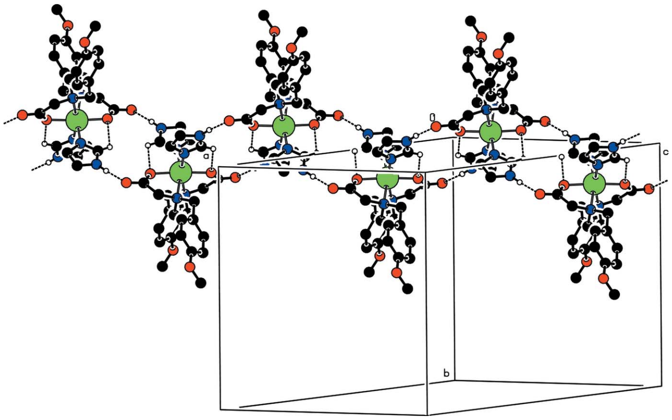


Figure 2
Part of the crystal structure of (I), showing the formation of a chain of rings along [010]. Dashed lines denote hydrogen bonds.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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