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Hexakis(imidazole-N^3)nickel(II) bis(4-methoxybenzoate)

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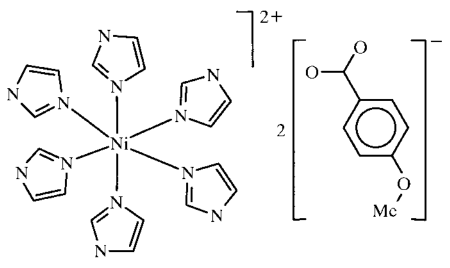
In the title complex of $[Ni(C_3H_4N_2)_6](C_8H_7O_3)_2$, the Ni atom is in an octahedral environment formed by the tertiary N atom of the imidazole moieties. The methoxybenzoate moieties act as a bridge connecting two hexakis(imidazole)nickel(II) molecules through N—H···O hydrogen bonds.

Comment

Imidazole is of considerable interest as a potential binding site for metal ions in many biological systems. It is a monodentate ligand and forms complexes with metal ions through its tertiary N atom. Some complexes of imidazole and its derivatives with transition metal ions have been reported (Brooks & Davidson, 1960; Davis & Smith, 1971). Complexes of copper(II) and cobalt(II) with carboxylate and imidazole ligands have been studied as models for metalloproteins since both contain functionalities in the side chain (Sigel, 1980; Bernarducci *et al.*, 1983; Abuhijleh & Woods, 1992). In addition, some of these copper(II) complexes were found to have a variety of pharmacological activities (Tamura *et al.*, 1987) and superoxide dismutase activities (Bhirud & Srivastava, 1990). Complexes of $[Co(RCOO)_2(Im)_2]$ (R = $-CH_3$, $-C_2H_5$) and model complexes for cobalt(II)-substituted zinc metalloenzymes, have been reported by Horrocks' group (Horrocks *et al.*, 1982).

The asymmetric unit of the title complex, (I), is formed by one half of the hexakis(imidazole)nickel(II) molecule; the other half is related by inversion symmetry through the Ni atom located at the inversion centre and one methoxybenzoate molecule. The Ni atom is in an octahedral environment formed by the tertiary N atom of the imidazole moieties. The bond distances involved in this octahedral geometry, (Ni1—N1, Ni1—N2 and Ni1—N3) ranging from 2.127 (2) to 2.141 (2) Å, are comparable with those found in the complex of hexakis(imidazole)nickel(II) disalicylate (Jian *et al.*, 1999). All the imidazole rings are individually planar. The methoxybenzoate moiety is planar with a maximum deviation of 0.111 (2) Å for the O3 atom.



(I)

In the solid state, intermolecular C—H···O(x, $y - 1$, z) interactions connect the methoxybenzoate with the NiN_6 chromophore. The complex forms a three-dimensional network through N—H···O intermolecular hydrogen bonds with the methoxybenzoate moieties acting as a bridge connecting the two hexakis(imidazole)nickel(II) molecules (Fig. 2). In addition, intra- and intermolecular C—H···π interactions contribute to the molecular packing [C3—H3A = 0.93, H3A···Cg1 = 2.77, C3···Cg1 = 3.48 Å and C3—H3···Cg1 = 134°; C16—H16C = 0.93, H16A···Cg2($1 - x$, $1 - y$, $1 - z$) = 2.84, C16···Cg2 = 3.66 Å and C16—H16···Cg2 = 145°; Cg1 is the centroid of the imidazole ring formed by

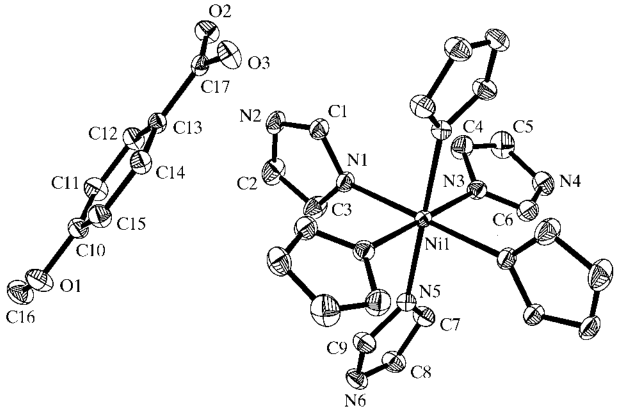


Figure 1
The molecular structure of the title complex. Displacement ellipsoids are shown at the 30% probability level. H atoms have been omitted for clarity.

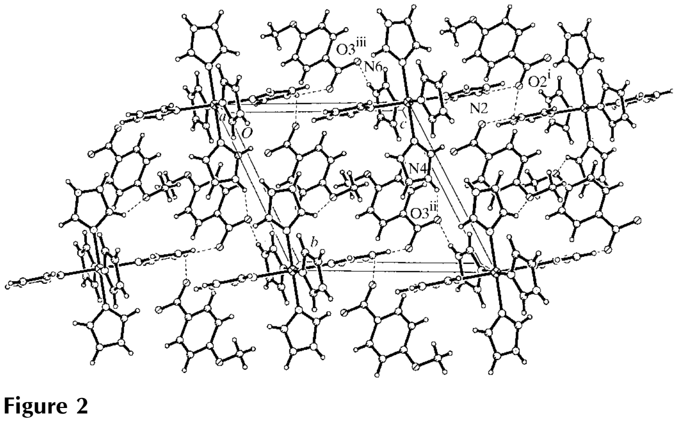


Figure 2
Part of the three-dimensional network of the title complex.

atoms N5, N6, C7–C9, and *Cg*2 is the centroid of the C10–C15 ring].

Experimental

The title complex was prepared by the reaction of imidazole (1 g, 15 mmol) with Ni(p-$CH_3O{\cdot}C_6H_4COO)_2{\cdot}4H_2O$ (Ephraim & Pfister, 1925) (1 g, 2.5 mmol) in warm ethanol (50 ml). Single crystals suitable for X-ray analysis were obtained by recrystallization from ethanol.

Crystal data

$[Ni(C_3H_4N_2)_6](C_8H_7O_3)_2$
$M_r = 769.48$
Triclinic, $P\overline{1}$
$a = 9.8185$ (4) Å
$b = 10.5191$ (4) Å
$c = 10.8556$ (5) Å
$\alpha = 61.474$ (1)°
$\beta = 76.764$ (1)°
$\gamma = 70.973$ (1)°
$V = 927.62$ (7) Å^3
$Z = 1$
$D_x = 1.377$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5621 reflections
$\theta = 2.74$–61.10°
$\mu = 0.584$ mm^{-1}
$T = 293$ (2) K
Parallelepiped, pale blue
0.50 × 0.24 × 0.14 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.759$, $T_{max} = 0.923$
6314 measured reflections
4138 independent reflections
3474 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.50°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 12$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.140$
$S = 1.00$
4140 reflections
241 parameters
H atoms constrained
$w = 1/[\sigma^2(F_o^2) + (0.0853P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -1.05$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N3	2.127 (2)	Ni1—N1	2.141 (2)
Ni1—N5	2.140 (2)		
N3—Ni1—N5	90.40 (7)	N5—Ni1—N1	88.57 (7)
N3—Ni1—N1	89.75 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.86	2.02	2.790 (3)	147
N4—H4A···O3^{ii}	0.86	2.04	2.803 (3)	147
N6—H6A···O3^{iii}	0.86	1.91	2.762 (3)	169

Symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $1 + x, y - 1, z$; (iii) $1 + x, y, z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1338). Services for accessing these data are described at the back of the journal.

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