metal-organic papers

Bis(2-formylphenolato-$\kappa^2 O,O'$)nickel(II)

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The title compound, [Ni(C$_7$H$_5$O$_2$)$_2$], exhibits a mononuclear structure in which the central Ni^{II} atom is located on an inversion centre and is coordinated by four O atoms from two salicylaldehyde ligands in a distorted square-planar geometry. The complex was obtained by the reaction of salicylaldehyde and nickel(II) nitrate hexahydrate in ethanol, using 3-amino-1,2-propanediol as a growth-directing reagent.

Comment

Research effort has been devoted to the study of substituted bis(salicylaldehydato)nickel(II) complexes, due to their catalytic activity in the dimerization of propylene and in olefin oligomerization when used together with an aluminium co-catalyst and/or phosphine ligand (Wu & Lu, 2003). Crystal structure analysis showed that the central Ni^{II} atom has an octahedral configuration in diaquabis(salicylaldehydato)-nickel(II) (Stewart *et al.*, 1961). Interest in the magnetic properties of transition metal complexes encouraged us to prepare the title mononuclear complex, (I). As the Ni^{II} atom in a square-planar configuration has two available coordination positions for further bonding with metals, we intend to use this compound for synthesizing other heteropolynuclear complexes.

(I)
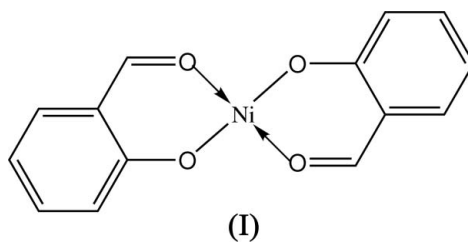
In compound (I), the Ni^{II} atom lies on an inversion centre and is coordinated by a pair of O atoms from the two salicylaldehyde ligands (Fig. 1). The bond distance between the Ni^{II} atom and the phenolic O atom is shorter than that between the Ni^{II} atom and the aldehyde O atom.

The IR spectrum of (I) shows a strong band at 1619 cm^{-1}, which is assigned to the stretching frequency of the bonded aldehyde group (Gupta *et al.*, 1999). A medium strong band appears at 1219 cm^{-1}, which is assigned to the C—O stretching frequency.

Experimental

An aqueous solution (5 ml) containing nickel(II) nitrate hexahydrate (0.19 g, 0.41 mmol) was added to a hot ethanol solution (10 ml) containing salicylaldehyde (0.10 g, 0.80 mmol) and 3-amino-1,2-

propanediol (0.09 g, 0.80 mmol). Aqueous ammonia (0.5 mol l^{-1}) was added until the pH of the mixture was 7. The mixture was stirred for 10 min to give a precipitate that was collected and washed with ethanol. After being air-dried for a day, the compound was recrystallized from dimethylformamide–cyclohexane (1:10 v/v). Red crystals of (I) suitable for X-ray analysis separated after 3 d in about 5% yield.

Crystal data

[Ni(C$_7$H$_5$O$_2$)$_2$]	$Z = 2$
$M_r = 300.93$	$D_x = 1.644$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 12.934$ (3) Å	$\mu = 1.60$ mm^{-1}
$b = 5.827$ (1) Å	$T = 293$ (2) K
$c = 8.108$ (2) Å	Block, red
$\beta = 95.67$ (3)°	$0.24 \times 0.21 \times 0.16$ mm
$V = 608.1$ (2) Å^3	

Data collection

Siemens $R3m$ diffractometer	856 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.033$
Absorption correction: ψ scan	$\theta_{max} = 27.0°$
(Kopfmann & Huber, 1968)	2 standard reflections
$T_{min} = 0.688$, $T_{max} = 0.774$	every 200 reflections
2151 measured reflections	intensity decay: none
1224 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0158P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.046$	$+ 1.3629P]$
$wR(F^2) = 0.100$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.032$
1224 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
89 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL97*
	(Sheldrick, 1997)
	Extinction coefficient: 0.001 (2)

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.832 (2)	Ni1—O2	1.853 (3)
O1^i—Ni1—O2	85.83 (12)	O1—Ni1—O2	94.17 (12)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

H atoms of the salicylaldehyde groups were placed in calculated positions and allowed to ride on their respective parent atoms, with
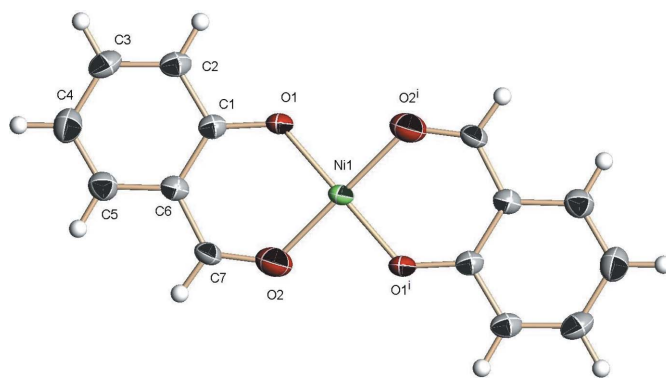

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level. [Symmetry code: (i) $1 - x$, $1 - y$, $1 - z$.]

C—H = 0.96 Å, and were assigned fixed isotropic displacement parameters of 0.080 Å^2.

Data collection: *XSCANS* (Siemens, 1990); cell refinement: *XSCANS*; data reduction: *SHELXTL-Plus* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXL97*.

References

Bruker (1998). *SHELXTL-Plus*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Gupta, T., Saha, M. K., Sen, S., Mitra, S., Edwards, A. J. & Clegg, W. (1999). *Polyhedron*, **18**, 197–201.
Kopfmann, G. & Huber, R. (1968). *Acta Cryst.* A**24**, 348–351.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1990). *XSCANS User's Manual*. Version 4.2. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Stewart, J. M., Lingafelter, E. C. & Breazeale, J. D. (1961). *Acta Cryst.* **14**, 888–891.
Wu, S. & Lu, S. (2003). *J. Mol. Catal. A Chem.* **198**, 29–38.