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Chloro[η^5-1-(dimethylaminoethyl)indenyl]-(triphenylphosphine)nickel(II) diethyl ether hemisolvate

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.007 Å
R factor = 0.048
wR factor = 0.118
Data-to-parameter ratio = 10.6

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

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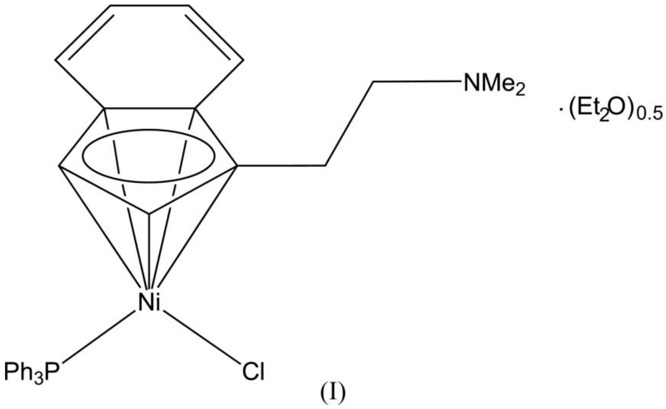
The title complex, $[\mathrm{Ni(C_{13}H_{16}N)Cl(C_{18}H_{15}P)]\cdot 0.5C_4H_{10}O}$, consists of an $\mathrm{Ni^{II}}$ center coordinated by a dimethylaminoethyl-substituted indenyl ligand, a triphenylphosphine ligand and a chloride ion. The asymmetric unit includes two very similar molecules that show only small conformational differences in the indenyl side chain.

Comment

The crystallographic study of the title compound, (I), was undertaken during the course of our studies on substituted indenyl complexes. The asymmetric unit contains two independent complex molecules and a diethyl ether molecule. One of the two complex molecules is represented in Fig. 1. The other has the same structure with minor differences in the conformation of the side chain.



(I)

Crystal structures of two solvent-free polymorphs of the same complex have already been published by our group (Groux *et al.*, 2000; Groux & Zargarian, 2001). All three crystal structures display a similar coordination environment around the Ni atom and spacial orientations for the indenyl group, the amine side chain, and the phenyl rings of the triphenylphosphine ligand. The solvent-free materials show disorder in the side chain, but there is no evidence of such disorder in the present structure.

Experimental

The preparation of the main title complex has already been published (Groux *et al.*, 2000). The single crystals of (I) obtained in the present study were grown from a solution of the complex in diethyl ether/hexanes.

Crystal data

$[Ni(C_{13}H_{16}N)Cl(C_{18}H_{15}P)]\cdot$-
$0.5C_4H_{10}O$
$M_r = 579.77$
Triclinic, $P\bar{1}$
$a = 12.7839$ (5) Å
$b = 12.9973$ (6) Å
$c = 18.0683$ (8) Å
$\alpha = 100.725$ (2)°
$\beta = 98.363$ (2)°
$\gamma = 90.364$ (2)°
$V = 2916.6$ (2) Å^3
$Z = 4$
$D_x = 1.320$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 5841 reflections
$\theta = 3.5$–55.1°
$\mu = 2.50$ mm^{-1}
$T = 100$ (2) K
Block, red
0.20 × 0.15 × 0.12 mm

Data collection

Bruker SMART2000 diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.600$, $T_{max} = 0.770$
36298 measured reflections
7196 independent reflections
4733 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 55.2°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.118$
$S = 0.95$
7196 reflections
682 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.009$
$\Delta\rho_{max} = 0.77$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni—C3	2.045 (4)	Ni1—C13	2.014 (4)
Ni—C2	2.068 (4)	Ni1—C12	2.059 (5)
Ni—C1	2.142 (4)	Ni1—C11	2.168 (4)
Ni—C3a	2.332 (5)	Ni1—C13a	2.306 (4)
Ni—C7a	2.366 (5)	Ni1—C17a	2.361 (4)
Ni—P	2.1758 (14)	Ni1—P1	2.1846 (14)
Ni—Cl	2.1976 (13)	Ni1—Cl1	2.1925 (13)

The H atoms were placed in calculated positions (C—H = 0.93–0.98 Å) and refined as riding with the constraint $U_{iso}(H) = 1.2U_{eq}$(carrier) or $1.5U_{eq}$(methyl carrier) applied.

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, 1997); software used to prepare material for publication: *UdMX* (Maris, 2004).

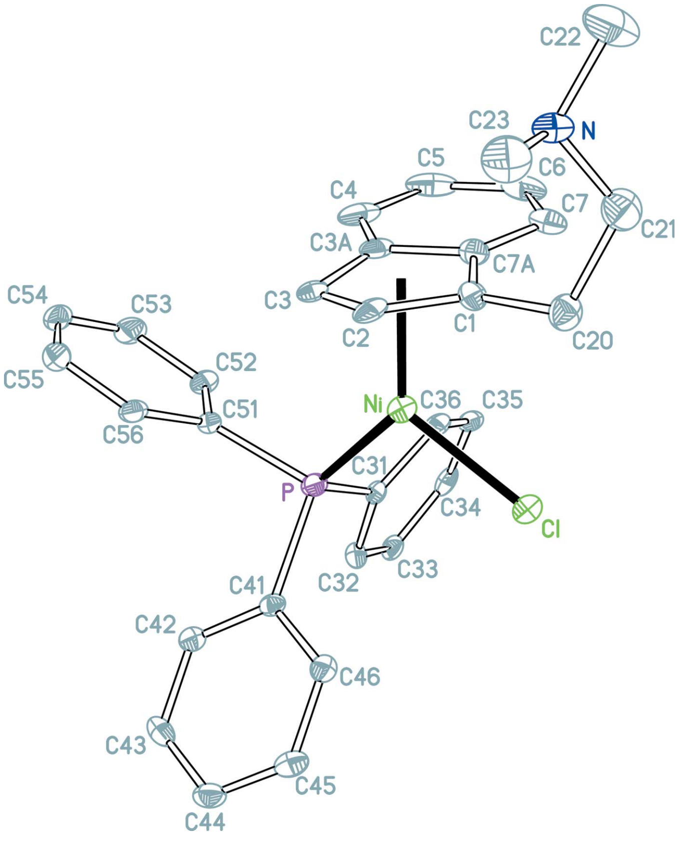


Figure 1
View of one of the Ni-containing molecules in (I), showing 30% displacement ellipsoids. H atoms have been omitted for clarity and the interaction between Ni and the centroid of the five-membered ring is shown. The second molecule has a very similar structure.

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