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Bis(η^3-2-*tert*-butyl-3-phenyl-1-trimethylsilyl-1-azaallyl)cobalt(II)

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Key indicators

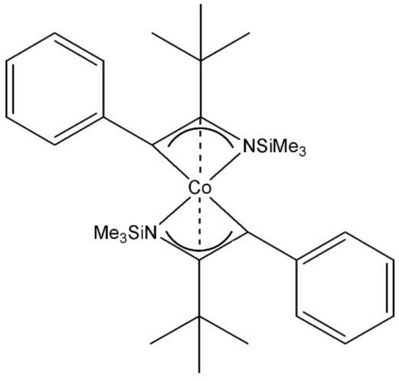
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.123
Data-to-parameter ratio = 16.6

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

The title compound, $[Co(C_{15}H_{24}NSi)_2]$, is a homoleptic metal–η^3-azaallyl complex, which has a center of symmetry. It contains two azaallyl ligands bound in an η^3-*N*,*C*,*C* mode to the Co atom.

Comment

Earlier work has shown that metal–η^3-allyl complexes can play an important part in many metal-mediated reactions (Blystone, 1989). Both amidinates and β-diketiminates have delocalized π-electrons produced from various addition reactions of nitriles with anions (Bourget-Merle *et al.*, 2002). Thermally stable η^3-1-azaallyl complexes of the *s*-, *p*-, *d*- and *f*-block metals in a variety of metal oxidation states have been prepared and characterized (Caro *et al.*, 2001). 1-Azaallyl ligands can play the role of spectator ligands by virtue of their strong binding ability to metals, their exceptional and tunable steric demands, and their diverse bonding modes (Leung *et al.*, 2004). Recently, a series of homoleptic late transition metal(II) 1-azaallyl compounds has been prepared by reactions of anhydrous late transition metal halides (metal = Fe, Co, Ni and Pd) with the appropriate lithium or potassium 1-azallyl in a 1:2 molar ratio (Avent *et al.*, 2004). An example of an η^3-azaallyl cobalt complex has been reported (Zhang *et al.*, 2006). In this paper, we report the synthesis of a similar Co–η^3-azaallyl complex, (I), by reaction of Li[η^3-N(SiMe$_3$)C(*t*-Bu)CH(C$_6$H$_5$)] or [Li(tmeda)] with CoCl$_2$ in a 2:1 ratio. X-ray crystal structure analysis revealed that the 1-azaallyl group is bonded to Co atom in an η^3-*N*,*C*,*C* mode, not in the κ^1-enamido fashion. Compound (I) contains an enlarged π-conjugation formed by an aryl ring and an η^3-azaallyl group.



(I)

The Co atom lies on an inversion center. A significant feature of compound (I) is that the central Co—C8 bond in the η^3-*N*,*C*,*C* mode is slightly shorter than the terminal Co—C7

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bond (Table 1). This is quite unusual in η^3-azaallyl complexes, but can be explained as a steric hindrance effect. The mode of bonding agrees with those of similar Co–η^3-azaallyl complexes (Avent *et al.*, 2004; Zhang *et al.*, 2006). Compound (I) has a non-planar four-membered ring (N1–C8–C7–Co). The dihedral angle between the N1—C7—Co and C8—C7—Co planes is 48.4 (3)°. Although the C and N atoms of the azaallyl group are sp^2-hybridized and involved in a conjugated system, the N1—C8 bond [1.353 (4) Å] has double-bond character.

Experimental

All experiments were performed under an atmosphere of pure argon using Schlenk apparatus and a vacuum line, unless otherwise stated. The solvents used were of reagent grade or better, and were freshly distilled under dry dinitrogen and degassed prior to use. Compound (I) was synthesized according to literature methods (Avent *et al.*, 2004). A solution of Li(tmeda) (1.853 g, 5 mmol) in hexane (ca 40 ml) was added slowly to a stirred suspension of $CoCl_2$ (0.325g, 2.5 mmol) in hexane (ca 10ml) at 195 K. After warming to room temperature and stirring for a further 12 h, a dark-red solution was obtained. The white precipitate was filtered off and the solution was carefully concentrated *in vacuo*, yielding dark-red single crystals of (I).

Crystal data

$[Co(C_{15}H_{24}NSi)_2]$
$M_r = 551.81$
Monoclinic, $P2_1/n$
$a = 10.3800\ (17)$ Å
$b = 9.2743\ (15)$ Å
$c = 16.588\ (3)$ Å
$\beta = 94.399\ (3)$°
$V = 1592.2\ (5)$ Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.63$ mm^{-1}
$T = 293\ (2)$ K
0.30 × 0.20 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.833$, $T_{max} = 0.884$
6427 measured reflections
2806 independent reflections
2322 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.123$
$S = 1.02$
2806 reflections
169 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Co—N1	1.874 (2)	Co—C7	2.089 (3)
Co—C8	2.034 (2)		

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for CH groups, and C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3 groups.

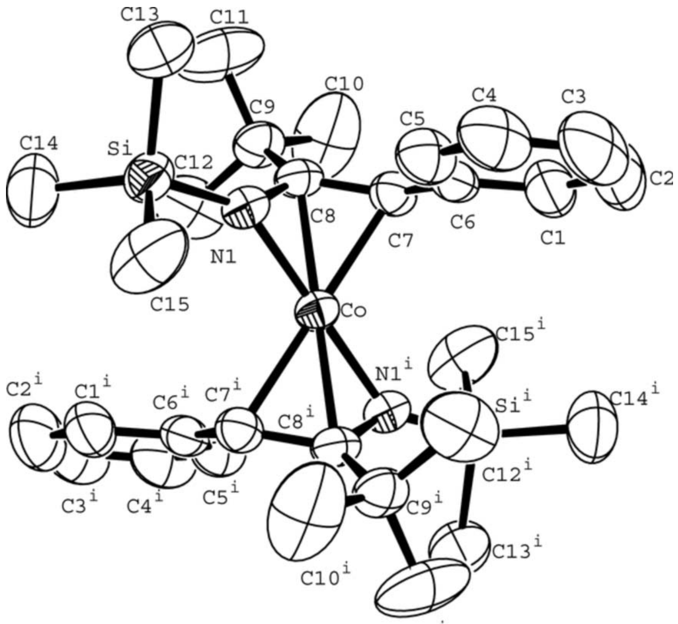

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $-x$, $-y$, $-z$.]

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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References

Avent, A. G., Hitchcock, P. B., Lappert, M. F., Sablong, R. & Severn, J. R. (2004). *Organometallics*, **23**, 2591–2600.
Blystone, S. L. (1989). *Chem. Rev.* **89**, 1663–1679.
Bourget-Merle, L., Lappert, M. F. & Severn, J. R. (2002). *Chem. Rev.* **102**, 3031–3065.
Caro, C. F., Lappert, M. F. & Merle, P. G. (2001). *Coord. Chem. Rev.* **219–221**, 605–663.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Leung, W.-P., Ip, Q. W.-Y., Lam, T.-W. & Mak, T. C. W. (2004). *Organometallics*, **23**, 1284–1291.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Zhang, Y., Tong, H.-B., Liu, D.-S., Zhou, M.-S. & Huang, S.-P. (2006). *Acta Cryst.* E**62**, m490–m491.

m1326 Yuan *et al.* • $[Co(C_{15}H_{24}NSi)_2]$ *Acta Cryst.* (2007). E**63**, m1325–m1326