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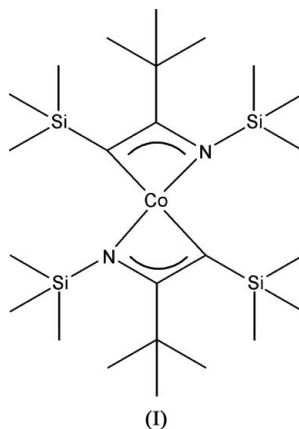
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.064
 wR factor = 0.127
Data-to-parameter ratio = 18.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis[η^3 -2-*tert*-butyl-1,3-bis(trimethylsilyl)-
1-azaallyl]cobalt(II)

The title compound, $[\text{Co}(\text{C}_{12}\text{H}_{27}\text{NSi}_2)_2]$, is a homoleptic metal- η^3 -azaallyl complex, which has a center of symmetry. The Co—C bond distances are 2.100 (4) and 2.068 (4) Å, and the Co—N bond distance is 1.878 (3) Å.

Comment

Metal- η^3 -allyl complexes are well known to play an important role in many metal-mediated reactions (Blystone *et al.*, 1989). Recently, metal 1-azaallyl complexes have attracted attention because of their synthetic utility in C—C bond formation (Caro *et al.*, 2001). As part of an investigation of the chemical and physical properties of metal- η^3 -azaallyl complexes, we have prepared the title complex, (I), and present its structure here (Fig. 1). The structure of the related compound, a homoleptic Co- η^3 -allyl complex, bis[1,3-bis(trimethylsilyl)allyl]cobalt(II), was reported by Smith *et al.* (2004).



The centrosymmetric title complex contains two azaallyl ligands bound in an η^3 manner to the Co^{II} atom, with Co—C bond lengths of 2.100 (4) and 2.068 (4) Å, and a Co—N bond length of 1.878 (3) Å (Table 1). The ligand forms a non-planar four-membered ring (N1/C1/C6/Co); the dihedral angle between the N1/C1/Co and C6/C1/Co planes is 47.2 (3)°. Although the C and N atoms of the azaallyl group are sp^2 -hybridized and involved in a conjugated system, the N1—C1 bond [1.352 (5) Å] has double-bond character.

Experimental

The title complex was synthesized according to literature methods (Hitchcock *et al.*, 2000, 2003; Avent *et al.*, 2004). To a solution of trimethylsilylmethyl lithium (6 mmol) in diethyl ether (20 ml) distilled over sodium, *tert*-butyl nitrile (6 mmol) was added at *ca* 273 K and the solution was stirred for 15 min and then for 5 h at room temperature.

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To the solution, CoCl_2 (3 mmol) was added at *ca* 200 K and the suspension was stirred for 15 min and then for 5 h at room temperature. The suspension was filtered and the filtrate was concentrated under a vacuum until red crystals of the title compound appeared. All experiments were performed under an argon atmosphere using Schlenk apparatus.

Crystal data

$[\text{Co}(\text{C}_{12}\text{H}_{27}\text{NSi}_2)_2]$
 $M_r = 544.00$
 Monoclinic, $C2/c$
 $a = 15.744$ (3) Å
 $b = 11.599$ (2) Å
 $c = 17.684$ (4) Å
 $\beta = 90.85$ (3)°
 $V = 3229.0$ (11) Å³
 $Z = 4$

$D_x = 1.115$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 2965 reflections
 $\theta = 2.2$ – 25.7 °
 $\mu = 0.69$ mm⁻¹
 $T = 293$ (2) K
 Block, red
 $0.20 \times 0.20 \times 0.10$ mm

Data collection

Siemens SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.874$, $T_{\max} = 0.934$
 6478 measured reflections

2846 independent reflections
 2406 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$
 $\theta_{\max} = 25.0$ °
 $h = -18 \rightarrow 18$
 $k = -13 \rightarrow 13$
 $l = -21 \rightarrow 15$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.064$
 $wR(F^2) = 0.127$
 $S = 1.19$
 2846 reflections
 151 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0001P)^2 + 17.1263P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.51$ e Å⁻³
 $\Delta\rho_{\min} = -0.50$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co–N1	1.878 (3)	Si2–N1	1.730 (4)
Co–C1	2.100 (4)	N1–C1	1.352 (5)
Co–C6	2.068 (4)	C1–C6	1.427 (6)
Si1–C6	1.861 (4)		

All H atoms were positioned geometrically, with C–H = 0.96–0.98 Å, and refined as riding, allowing for free rotation of the methyl groups. The $U_{\text{iso}}(\text{H})$ values were set at $1.5U_{\text{eq}}(\text{C})$.

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.

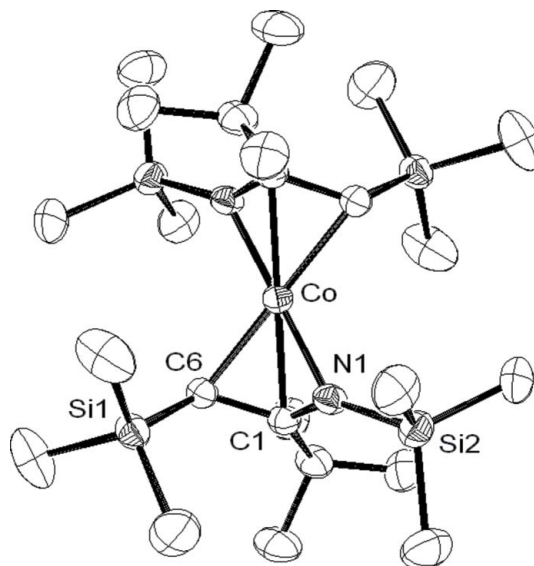


Figure 1

A molecular view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. Unlabeled atoms are related to labeled atoms by $\frac{1}{2} - x, \frac{3}{2} - y, 1 - z$.

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