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Key indicators

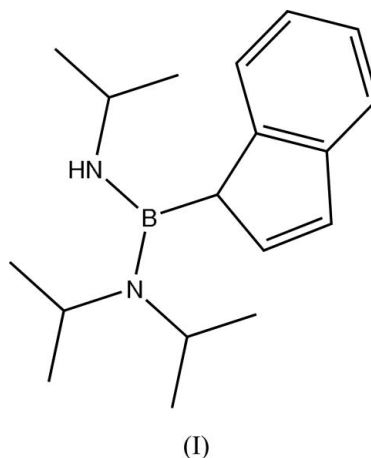
Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.045
 wR factor = 0.114
Data-to-parameter ratio = 17.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.***rac*-(Diisopropylamino)(1-indenyl)(isopropyl-
amino)borane**In the racemic title compound, $\text{C}_{18}\text{H}_{29}\text{BN}_2$, the B and the N atoms are virtually trigonal-planar coordinated and the presence of B=N partial double bonding is confirmed by the B–N bond lengths of 1.4154 (18) and 1.4178 (18) Å.

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Comment

Ligand precursors related to the title compound *rac*-(diisopropylamino)(1-indenyl)(isopropylamino)borane, (I), have been previously employed for the synthesis of boron-bridged constrained-geometry complexes. These complexes exhibit activity for the polymerization of ethene and higher α -olefins when activated with MAO (methylaluminumoxane) (Braunschweig *et al.*, 2000, 2004). In comparative studies, a strong influence of the ligand substitution patterns in corresponding complexes has been demonstrated on both catalyst activity and polymerization characteristics (Stevens 1994), justifying the synthesis of a series of boron-bridged analogues.

The structure of (I) (Fig. 1) in the solid state largely resembles that of its corresponding *N*-phenyl-substituted counterpart ($\eta^1\text{-C}_9\text{H}_7$)B(NⁱPr₂)N(H)Ph (Braunschweig *et al.*, 2003). Compound (I) adopts C_1 symmetry in the crystal structure. The crystal structure confirms the constitution assumed by NMR spectroscopy, with boron being attached to the sp^3 -hybridized C atom of the indenyl system. The B1 and N2 centres adopt trigonal-planar geometries, with the central atoms lying only 0.015 (B1) and 0.025 Å (N2) out of the planes of their respective substituents. These two trigonal planes are virtually coplanar with torsion angles of 176.35 (12) (C16–N2–B1–N1) and 0.2 (2)° (C13–N2–B1–N1). The B1–N1 and B1–N2 bond lengths of 1.4154 (18) and 1.4178 (18) Å, respectively, are equivalent within experimental error, indicating equal π -contributions from both amino groups. The N2–

bound isopropyl group *syn* to the indenyl moiety (which is coplanar to within 0.007 Å) is oriented such that the methine proton is directed towards the middle of the five-membered ring, a conformation also seen in the corresponding compound (C₉H₇)B(NⁱPr₂)N(H)Ph) with H— π distances to the centres of the C₂=C₃ olefinic and C₁=C₉ aromatic bonds of 2.446 and 2.509 Å, respectively. No short intermolecular contacts were observed.

Experimental

The title compound was prepared by a modified literature procedure (Braunschweig *et al.*, 2003) by sequential reaction of ⁱPr₂NBCl₂ (2.16 g, 11.9 mmol) with lithium indenide (1.45 g, 11.9 mmol) and lithium isopropylamide (0.77 g, 11.9 mmol) in a hexane–toluene mixture. Recrystallization from hexane at 243 K afforded (I) exclusively as the 1-indenyl isomer in 35% yield in the form of pale-yellow crystals suitable for single-crystal X-ray diffraction.

Crystal data

C ₁₈ H ₂₉ BN ₂	$D_x = 1.078 \text{ Mg m}^{-3}$
$M_r = 284.24$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 4341 reflections
$a = 8.1029 (8) \text{ \AA}$	$\theta = 2.6\text{--}26.1^\circ$
$b = 14.0352 (14) \text{ \AA}$	$\mu = 0.06 \text{ mm}^{-1}$
$c = 15.6679 (15) \text{ \AA}$	$T = 173 (2) \text{ K}$
$\beta = 100.503 (2)^\circ$	Tablet, yellow
$V = 1752.0 (3) \text{ \AA}^3$	$0.25 \times 0.20 \times 0.09 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3471 independent reflections
φ and ω scans	2751 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$R_{\text{int}} = 0.032$
$T_{\text{min}} = 0.972$, $T_{\text{max}} = 0.99$	$\theta_{\text{max}} = 26.1^\circ$
16287 measured reflections	$h = -10 \rightarrow 10$
	$k = -17 \rightarrow 17$
	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 0.4773P]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.114$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
3471 reflections	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$
196 parameters	
H-atom parameters constrained	

H atoms were visible in difference Fourier maps and were subsequently placed at idealized positions and treated as riding atoms, with C—H = 0.98 (CH₃), 0.95 (aromatic CH) and 1.00 Å (aliphatic CH), and N—H = 0.88 Å. U_{iso} values for primary H atoms were fixed at 1.5 times and tertiary H atoms at 1.2 times $U_{\text{eq}}(\text{C})$.

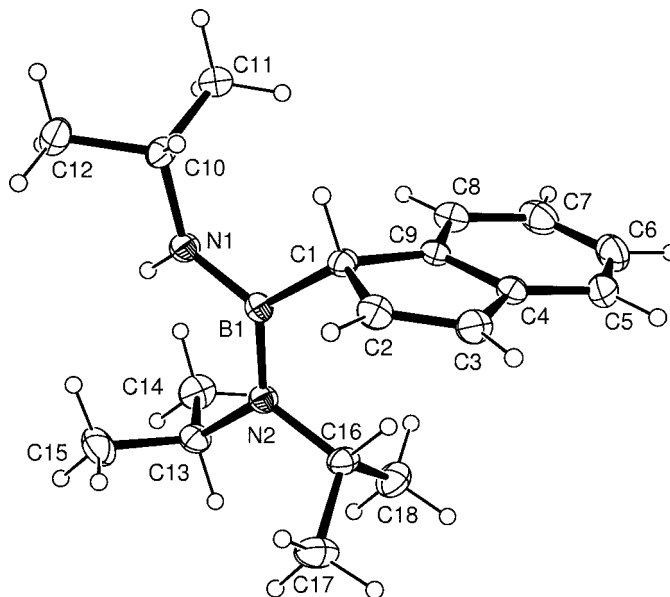


Figure 1
A view of (I), with displacement ellipsoids drawn at the 30% probability level.

Data collection: SMART-NT (Bruker, 2001); cell refinement: SAINT-Plus-NT (Bruker, 2001); data reduction: SAINT-Plus-NT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: XP in SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: XP in SHELXTL.

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