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Bis(2-methylphenylamino)phenylborane

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Key indicators

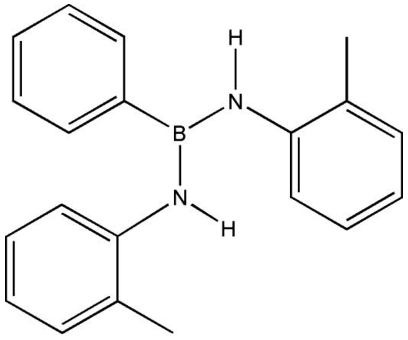
Single-crystal X-ray study
T = 213 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.098
Data-to-parameter ratio = 14.4

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

In the title compound, $C_{20}H_{21}BN_2$, the B and N atoms show trigonal planar geometry. The B—N bond lengths of 1.4177 (19) and 1.418 (2) Å indicate covalent partial double bonds.

Comment

Among the group 3 elements B, Al, Ga, In and Tl, the organometallic chemistry of boron and aluminium clearly predominates. Organoboron chemistry is of interest from many perspectives, including electronic and structural, as well as its heterocyclic chemistry (Elschenbroich & Salzer, 1992). Recently, we have reported the synthesis and structure of two five-membered heterocyclic compounds incorporating boron in which the coordination around the B atom was distorted tetrahedral with B—N bond lengths in the range 1.685 (4)–1.734 (4) Å (Tong *et al.*, 2002, 2004).



(I)

In the title molecule, bis(2-methylphenylamino)phenylborane, (I), in which the B and N atoms show trigonal planar geometry (Fig. 1), the two B—N bonds of 1.4177 (19) and 1.418 (2) Å are significantly shorter than in the two above-mentioned compounds, indicating their covalent partial double-bond character. The observed B–N bond lengths in (I) compare well with the values reported for similar compounds (Chivers *et al.*, 2004). Atom B1 lies 0.032 (2) Å out of the plane defined by the C and two N atoms bonded to it.

Experimental

All manipulations were carried out under argon using standard Schlenk techniques. Diethyl ether was dried by distillation over sodium, and CH_2Cl_2 was distilled from CaH_2. *n*-Butyllithium was added dropwise, in an equimolar ratio, to a stirred solution of 2-methylphenylaniline in diethyl ether at ca. 273 K. The resulting mixture was slowly warmed to room temperature and stirred for 5 h. Subsequently, two molar equivalents of dichlorophenylborane were added at 273 K, and the mixture was warmed to room temperature and stirred for an additional 12 h to give a white precipitate (LiCl). The mixture was filtered, the solvent evaporated with a vacuum pump and the residue extracted with CH_2Cl_2. The CH_2Cl_2 solution of (I) was concentrated carefully under vacuum, yielding colourless crystals of the title compound.

Crystal data

$C_{20}H_{21}BN_2$
$M_r = 300.20$
Monoclinic, $P2_1/c$
$a = 9.607$ (3) Å
$b = 17.454$ (5) Å
$c = 10.307$ (3) Å
$\beta = 93.272$ (5)°
$V = 1725.6$ (8) Å^3
$Z = 4$
$D_x = 1.156$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 213$ (2) K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.980$, $T_{\max} = 0.987$
7056 measured reflections
3030 independent reflections
2112 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.038$
$\theta_{\max} = 25.0$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.099$
$S = 0.92$
3030 reflections
210 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.14$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

B1—N1	1.4177 (19)	N1—C7	1.4090 (17)
B1—N2	1.418 (2)	N2—C14	1.4059 (17)
B1—C1	1.560 (2)		
N1—B1—N2	119.45 (14)	C7—N1—B1	132.18 (13)
N1—B1—C1	116.59 (14)	C14—N2—B1	130.97 (12)
N2—B1—C1	123.81 (13)		

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(C,N) or $1.5U_{\rm eq}$(methyl C). A torsion parameter was refined for the methyl group.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

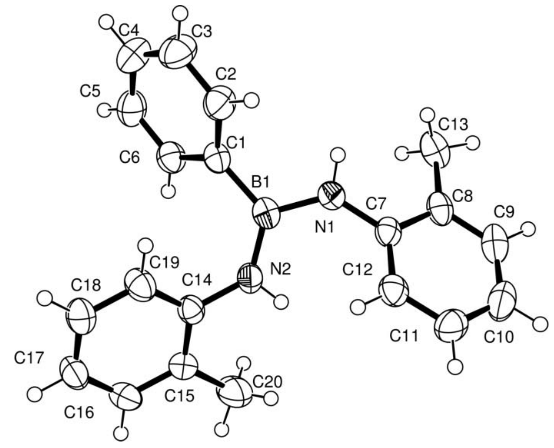


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. Amine H atoms are represented by small spheres of arbitrary radii and C-bound H atoms have been omitted for clarity.

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