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1,4-Bis(benzylamino)benzene

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The molecule of 1,4-bis(benzylamino)benzene, $C_{20}H_{20}N_2$, lies on a center of inversion in its crystal structure; adjacent pyramidal amino groups are linked by hydrogen bonds into a layer motif.

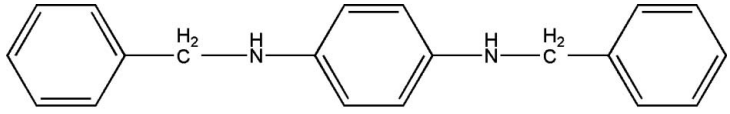
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.105
Data-to-parameter ratio = 12.9

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

Comment

The title compound, (I), is a spacer ligand used in the synthesis of coordination polymers (Diskin-Posner *et al.*, 2001). The molecule is an *N*-substituted *o*-phenylenediamine. The molecule lies on an inversion site; the amino group is pyramidal (Fig. 1). Adjacent molecules are linked into a layer structure by a weak hydrogen bond [N···N = 3.328 (1) Å].



(I)

Experimental

p-Phenylenediamine (1 mmol, 0.108 g) was dissolved in methanol (6 ml) and to the solution was added benzaldehyde (2 mmol, 0.212 g) dissolved in the same solvent (6 ml). The mixture was stirred for 3 h, and then treated with sodium borohydride in methanol at 273 K for 20 h. The reduced product was separated and recrystallized from methanol.

Crystal data

$C_{20}H_{20}N_2$
M_r = 288.38
Monoclinic, $P2_1/c$
a = 11.912 (1) Å
b = 5.5402 (8) Å
c = 11.895 (1) Å
β = 93.47 (1)°
V = 783.5 (2) Å^3
Z = 2
D_x = 1.222 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 295 (2) K
Plate, colorless
0.44 × 0.34 × 0.14 mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: none
6428 measured reflections
1800 independent reflections
1420 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 1.05
1800 reflections
140 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 0.0816P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

The amino and carbon-bound H atoms were located in a difference Fourier map, and were refined with distance restraints of N—H = 0.85 (1) Å and C—H = 0.95 (1) Å; their displacement parameters were freely refined.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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References

Bruker (2004). *SMART* (Version 7.12A) and *SAINT* (Version 7.12A). Bruker AXS Inc., Madison, Wisconsin, USA.

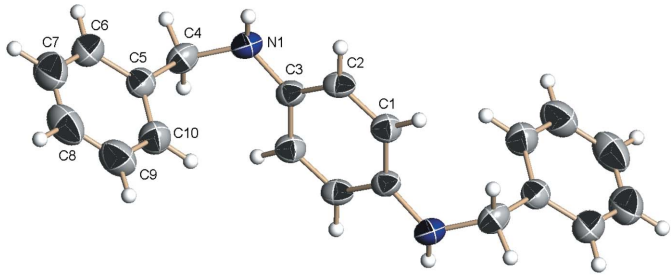

Figure 1
Plot of the title compound, with displacement ellipsoids drawn at the 50% probability level and H atoms as spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by $(\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z)$.

Diskin-Posner, Y., Patra, G. K. & Goldberg, I. (2001). *J. Chem. Soc. Dalton Trans*. pp. 2775–2782.
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