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2-[(4-Bromophenyl)amino]-1-phenylethanone

Ishu Saraogi,[a] B. H. M. Mruthyunjayaswamy,[b] Omkar B. Ijare,[b] Y Jadegoud[b] and T. N. Guru Row[a]*

[a]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, India, and [b]Department of Chemistry, Gulbarga University, Gulbarga 585106, India

Correspondence e-mail: ssctng@sscu.iisc.ernet.in

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.054
wR factor = 0.100
Data-to-parameter ratio = 13.9

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

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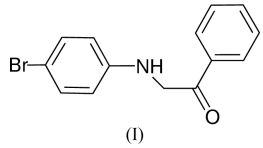
The crystal structure of the title compound, $C_{14}H_{12}BrNO$, has been determined in the triclinic space group $P\overline{1}$ at room temperature. The molecules pack in an all-*trans* conformation in the crystal structure which precludes the formation of any hydrogen bond. The shortest intermolecular contact between N and O in a neighbouring molecule is 3.411 Å.

Comment

The title compound, (I), provides the required starting material for the synthesis of 2,5-diphenyl-3,4-bis(*p*-bromoanilino)furan in good yield (Bryce *et al.*, 1965). It is interesting to note that the atoms C4—N1—C7—C8—C9 (Fig. 1) possess an all-*trans* conformation and the N1—H1···O1 intermolecular hydrogen bond which could be expected to form dimers across the centre of symmetry is absent (Fig. 2). The bond lengths and angles are as expected. The shortest intermolecular contact between N and O in a neighbouring molecule is 3.411 Å.



(I)

Experimental

To a solution of acetophenone in acetic acid, bromine in acetic acid was added and the contents were shaken for 10–15 min and allowed to stand for half an hour. Crushed ice was added to the mixture and the resulting solid was washed with absolute alcohol to yield phenacyl bromide. The latter was dissolved in ethanol and slowly added to an ethanol solution of *p*-bromoaniline. The reaction mixture was heated for 15–20 min until the colour changed to dark brown. The contents were cooled to room temperature. The solid obtained by filtration was crystallized from dry ethanol.

Crystal data

$C_{14}H_{12}BrNO$
M_r = 290.15
Triclinic, $P\overline{1}$
a = 5.7609 (9) Å
b = 7.5689 (11) Å
c = 14.227 (2) Å
α = 99.374 (2)°
β = 91.216 (2)°
γ = 96.778 (2)°
V = 607.27 (16) Å^3
Z = 2
D_x = 1.587 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 903 reflections
θ = 2.8–25.0°
μ = 3.37 mm^{-1}
T = 293 (2) K
Rod, pale yellow
0.40 × 0.06 × 0.02 mm

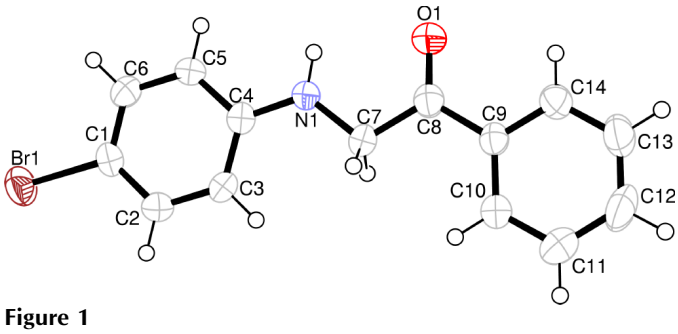


Figure 1
View of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

Data collection

Bruker SMART CCD area-detector diffractometer	1748 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.043$
Absorption correction: none	$\theta_{max} = 25.1^\circ$
5884 measured reflections	$h = -6 \rightarrow 6$
2133 independent reflections	$k = -9 \rightarrow 9$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.055$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.100$	$\Delta\rho_{max} = 0.38$ e Å^{-3}
$S = 1.15$	$\Delta\rho_{min} = -0.40$ e Å^{-3}
2133 reflections	Absolute structure: none
154 parameters	
H-atom parameters constrained	

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with U_{iso}(H) equal to U_{eq} of the parent atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993) in the suite *WinGX* (Farrugia, 1999); software used to prepare material for publication: *PLATON* (Spek, 1990).

We thank the Department of Science and Technology, India, for data collection on the CCD facility set up under the IRHPA–DST program and the Chairman, Department of Chemistry, Gulbarga University, for providing facilities to carry out the synthesis of the title compound.

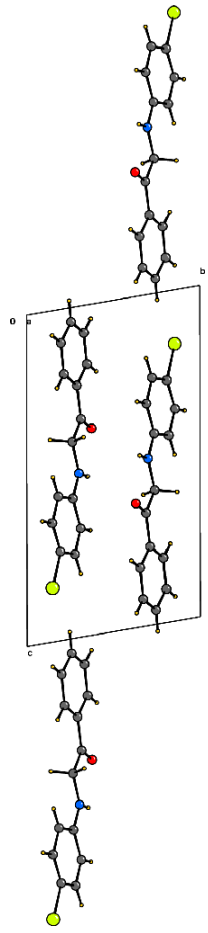


Figure 2
Packing diagram of the title compound, viewed down the *a* axis.

References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bryce, T., Proctor, G. R. & Rehman, M. A. (1965). *J. Chem. Soc.* pp. 7105–7109.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.
Watkin, D. M., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.