Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Bromobenzylidene)-3-nitroaniline

Shao-Fa Sun,[a] Rong-Ming Ma[a] and Seik Weng Ng[b]*

[a]Department of Chemistry and Life Science, Xianning College, Xianning, Hubei 437005, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.007 Å
R factor = 0.059
wR factor = 0.145
Data-to-parameter ratio = 16.2

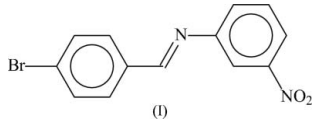
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 25 July 2006
Accepted 26 July 2006

N-(4-Bromobenzylidene)-3-nitroaniline, $C_{13}H_9BrN_2O_2$, is a non-planar molecule whose two aromatic rings are twisted about the C=N double bond in order to relieve strain [dihedral angle = 17.8 (2)°].

Comment

The structures of several Schiff bases have been determined (Gao *et al.*, 2005; Gui *et al.*, 2005) because their complexes with nickel(II) exhibit superior activity as catalysts in polymerizations (Gao *et al.*, 2004; Gui *et al.*, 2006). Schiff bases such as those derived from salicylaldehyde and aniline are readily synthesized. The Schiff bases that will be examined for their catalytic activity in the form of their nickel compounds include the present *p*-bromosalicyldehyde derivative, (I), that is obtained by reaction with *m*-nitroaniline (Fig. 1). Other Schiff bases from this aldehyde whose crystal structures are known include the *m*-chloroaniline (Navon & Bernstein, 1997), the *p*-chloroaniline (Bar & Bernstein, 1987), the *m*-bromoaniline (Navon & Bernstein, 1997), the *p*-bromoaniline (Bernstein & Izak, 1975) and the *p*-cyanoaniline (Ojala *et al.*, 2001) derivatives. The principal features of the title compound, (I), *i.e.*, the C=N and C—Br bond distances, are similar to those in reported compounds. The molecule is not planar as the two aromatic rings are twisted about the double bond in order to relieve steric strain [dihedral angle = 17.8 (2)°].



(I)

Experimental

m-Nitroaniline (2.50 g, 18.1 mmol) and *p*-bromobenzaldehyde (3.33 g, 18.0 mmol) were dissolved in ethanol (35 ml) along with 1 ml of formic acid. The solution was refluxed for 6 h. Removal of the solvent followed by recrystallization from a 1:1 ethanol/dichloromethane mixture (35 ml) gave the compound in about 75% yield. Crystals were grown from ethanol. Elemental analysis calculated for $C_{13}H_9BrN_2O_2$: C 51.17, H 2.97, N 9.18%; found: C 51.20, H 3.01, N 9.10%.

Crystal data

$C_{13}H_9BrN_2O_2$
M_r = 305.13
Monoclinic, $P2_1/n$
a = 13.501 (2) Å
b = 3.9390 (5) Å
c = 22.433 (3) Å
β = 98.016 (2)°
V = 1181.3 (3) Å^3
Z = 4
D_x = 1.716 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.47 mm^{-1}
T = 292 (2) K
Needle, light yellow
0.30 × 0.10 × 0.06 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.422, T_{max} = 0.819
7663 measured reflections
2648 independent reflections
1545 reflections with $I > 2\sigma(I)$
R_{int} = 0.108
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.145
S = 0.95
2648 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0665P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

H atoms were placed in calculated positions [C—H = 0.93 Å and $U = 1.2U_{eq}$(C)] and were included in the refinement in the riding-model approximation.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

We thank Xianning College and the University of Malaya for supporting this study.

References

Bar, I. & Bernstein, J. (1987). *Tetrahedron*, **43**, 1299–1305.
Bernstein, J. & Izak, I. (1975). *J. Cryst. Mol. Struct.* **5**, 257–266.

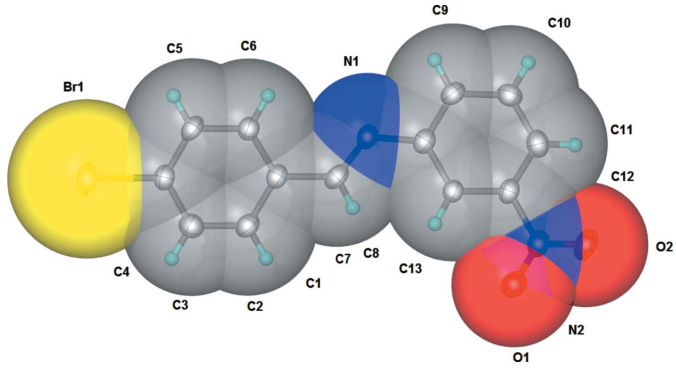


Figure 1
The molecular structure of (I), with van der Waals surfaces. Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radii.

Bruker (2003). *SAINT* (Version 6.54A) and *SMART* (Version 6.54A). Bruker AXS Inc., Madison, Wisconsin, USA.
Gao, H.-Y., Guo, W.-J., Bao, F., Gui, G.-Q., Zhang, J.-K., Zhu, F.-M. & Wu, Q. (2004). *Organometallics*, **23**, 6273–6280.
Gao, H.-Y., Lü, X.-Q., Bao, F., Wu, Q. & Ng, S. W. (2005). *Acta Cryst.* E**61**, o1068–o1069.
Gui, G.-Q., Bao, F., Gao, H.-Y., Zhu, F.-M. & Wu, Q. (2006). *J. Coord. Chem.* **59**, 107–118.
Gui, G.-Q., Bao, F., Lü, X.-Q., Wu, Q. & Ng, S. W. (2005). *Acta Cryst.* E**61**, o1070–o1071.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Navon, O. & Bernstein, J. (1997). *Struct. Chem.* **8**, 3–11.
Ojala, C. R., Ojala, W. H., Gleason, W. B. & Britton, D. (2001). *J. Chem. Crystallogr.* **31**, 377–386.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.