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N-(4-Bromobenzylidene)-4-methoxyaniline

Rui Ma,[a]* Yubang Hou,[b] Xuejian Yong[b] and Yunbin Cen[b]

[a]Department of Materials Science and Chemical Engineering, China University of Geosciences, Wuhan 430074, People's Republic of China, and [b]Department of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China
Correspondence e-mail: marycandy@126.com

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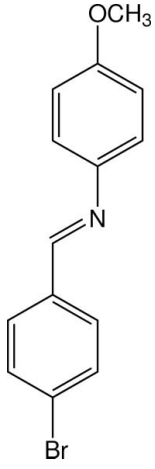
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.009 Å; R factor = 0.064; wR factor = 0.121; data-to-parameter ratio = 15.1.

In the title compound, $C_{14}H_{12}BrNO$, the torsion angle about the central C=N double bond is 170.4 (3)° and the dihedral angle between the aromatic rings is 9.6 (3)°.

Related literature

For related literature, see: Gao *et al.* (2004); Sun *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{12}BrNO$
M_r = 290.15
Orthorhombic, $Pca2_1$
a = 6.1510 (8) Å
b = 7.2726 (9) Å
c = 27.914 (4) Å
V = 1248.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.27 mm^{-1}
T = 292 (2) K
0.10 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.728, T_{max} = 0.822
8336 measured reflections
2349 independent reflections
1512 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.121
S = 1.06
2349 reflections
156 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 764 Friedel pairs
Flack parameter: 0.016 (18)

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2554).

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supplementary materials

Acta Cryst. (2007). E**63**, o4188 [**doi:10.1107/S1600536807046855**]

N-(4-Bromobenzylidene)-4-methoxyaniline

R. Ma, Y. Hou, X. Yong and Y. Cen

Comment

Schiff bases such as those derived from salicylaldehyde and aniline are readily synthesized. The Schiff base of *N*-(4-Bromobenzylidene)-3-nitroaniline had been reported before (Sun *et al.*, 2006). As part of a project to examine the catalytic activity of Schiff bases that in the form of their nickel complexes (Gao *et al.*, 2004), the title *p*-bromobenzaldehyde derivative, (I), was obtained by reaction with 4-methoxyaniline (Fig. 1). The molecule is not planar as the two aromatic rings are twisted about the double bond in order to relieve steric strain.

Experimental

p-Methoxyaniline (2.24 g, 18.2 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 8 h. Removal of the solvent followed by recrystallization from a 1:1 *v*/*v* ethanol/dichloromethane mixture (35 ml) gave the title compound in about 70% yield. Colourless blocks of (I) were grown from ethanol. Elemental analysis: calculated for $C_{14}H_{12}Br_1N_1O_1$: C 57.95, H 4.17, N 4.83%; found: C 57.80, H 4.01, N 5.02%.

Refinement

The H atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

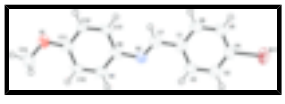

Fig. 1. Vew of (I), with displacement ellipsoids drawn at the 50% probability level. The H atoms are drawn as spheres of arbitrary radius.

N-(4-Bromobenzylidene)-4-methoxyaniline

Crystal data

$C_{14}H_{12}Br_1N_1O_1$	F_{000} = 584
M_r = 290.15	D_x = 1.543 Mg m^{-3}
Orthorhombic, *Pca*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 1585 reflections
a = 6.1510 (8) Å	θ = 2.1–28.3°
b = 7.2726 (9) Å	μ = 3.27 mm^{-1}
c = 27.914 (4) Å	*T* = 292 (2) K
V = 1248.7 (3) Å^3	Block, colorless

$Z = 4$	0.10 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer	2349 independent reflections
Radiation source: fine-focus sealed tube	1512 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.063$
$T = 292(2)$ K	$\theta_{max} = 28.3°$
ω scans	$\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -7\rightarrow7$
$T_{min} = 0.728$, $T_{max} = 0.822$	$k = -9\rightarrow7$
8336 measured reflections	$l = -26\rightarrow36$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.121$	$(\Delta/\sigma)_{max} = 0.005$
$S = 1.06$	$\Delta\rho_{max} = 0.51$ e Å^{-3}
2349 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}
156 parameters	Extinction correction: ?
1 restraint	Extinction coefficient: ?
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 764 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.016 (18)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	−0.03907 (11)	0.72700 (9)	0.51664 (4)	0.0716 (3)
C1	0.2243 (10)	0.7455 (7)	0.3597 (2)	0.0396 (15)

C2	0.3529 (11)	0.8085 (8)	0.3978 (3)	0.0467 (16)
H2	0.4926	0.8518	0.3919	0.056*
C3	0.2744 (11)	0.8067 (9)	0.4438 (3)	0.0530 (17)
H3	0.3583	0.8526	0.4688	0.064*
C4	0.0688 (12)	0.7360 (8)	0.4527 (3)	0.0497 (17)
C5	−0.0597 (10)	0.6762 (8)	0.4166 (2)	0.0468 (16)
H5	−0.1985	0.6318	0.4230	0.056*
C6	0.0186 (11)	0.6820 (12)	0.3697 (3)	0.049 (2)
H6	−0.0700	0.6423	0.3447	0.059*
C7	0.3079 (11)	0.7367 (8)	0.3107 (3)	0.0463 (16)
H7	0.2108	0.7099	0.2862	0.056*
C8	0.5757 (9)	0.7501 (6)	0.2515 (2)	0.0350 (14)
C9	0.7727 (8)	0.8355 (7)	0.2403 (2)	0.0356 (14)
H9	0.8507	0.8937	0.2645	0.043*
C10	0.8535 (9)	0.8355 (7)	0.1949 (2)	0.0388 (14)
H10	0.9833	0.8956	0.1880	0.047*
C11	0.7415 (9)	0.7457 (7)	0.1590 (2)	0.0342 (13)
C12	0.5511 (10)	0.6601 (10)	0.1690 (2)	0.0375 (16)
H12	0.4771	0.6001	0.1446	0.045*
C13	0.4639 (9)	0.6596 (7)	0.2147 (2)	0.0381 (14)
H13	0.3331	0.6000	0.2209	0.046*
C14	1.0077 (11)	0.8162 (12)	0.0993 (3)	0.068 (2)
H14A	0.9931	0.9475	0.1005	0.102*
H14B	1.0472	0.7797	0.0674	0.102*
H14C	1.1186	0.7777	0.1213	0.102*
N1	0.5029 (8)	0.7632 (7)	0.3001 (2)	0.0428 (13)
O1	0.8083 (7)	0.7336 (5)	0.11189 (16)	0.0498 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0775 (5)	0.0926 (6)	0.0447 (4)	−0.0006 (3)	0.0177 (5)	−0.0023 (8)
C1	0.043 (4)	0.036 (4)	0.040 (4)	0.009 (3)	0.000 (3)	0.004 (3)
C2	0.038 (4)	0.050 (4)	0.052 (4)	−0.003 (3)	−0.004 (3)	0.003 (3)
C3	0.059 (5)	0.059 (4)	0.042 (4)	−0.011 (3)	−0.007 (3)	−0.004 (3)
C4	0.070 (5)	0.040 (4)	0.040 (4)	−0.002 (3)	0.012 (3)	−0.002 (3)
C5	0.043 (4)	0.049 (4)	0.049 (4)	−0.006 (3)	0.009 (3)	0.004 (3)
C6	0.041 (4)	0.055 (5)	0.052 (6)	−0.001 (3)	−0.012 (4)	−0.006 (4)
C7	0.048 (4)	0.045 (4)	0.046 (4)	−0.002 (3)	−0.007 (3)	−0.003 (3)
C8	0.038 (3)	0.024 (3)	0.043 (4)	0.003 (2)	−0.002 (3)	0.008 (3)
C9	0.033 (3)	0.035 (3)	0.039 (4)	0.002 (2)	−0.008 (3)	0.000 (3)
C10	0.032 (3)	0.032 (3)	0.052 (4)	−0.005 (2)	0.001 (3)	−0.004 (3)
C11	0.036 (3)	0.035 (3)	0.032 (3)	0.013 (3)	−0.003 (3)	0.005 (3)
C12	0.032 (3)	0.044 (4)	0.037 (4)	−0.005 (3)	−0.001 (3)	−0.006 (3)
C13	0.032 (3)	0.035 (3)	0.047 (4)	−0.008 (2)	0.003 (3)	0.000 (3)
C14	0.055 (5)	0.106 (6)	0.043 (5)	−0.005 (4)	0.004 (3)	0.014 (4)
N1	0.042 (3)	0.047 (3)	0.039 (3)	−0.007 (2)	−0.003 (2)	0.005 (2)
O1	0.048 (3)	0.063 (3)	0.039 (3)	−0.0046 (19)	0.003 (2)	0.004 (2)

Geometric parameters (Å, °)

Br1—C4	1.905 (7)	C8—C13	1.400 (9)
C1—C6	1.376 (9)	C8—N1	1.431 (9)
C1—C2	1.404 (9)	C9—C10	1.363 (7)
C1—C7	1.461 (9)	C9—H9	0.9300
C2—C3	1.370 (9)	C10—C11	1.379 (8)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.388 (9)	C11—C12	1.356 (8)
C3—H3	0.9300	C11—O1	1.381 (7)
C4—C5	1.352 (10)	C12—C13	1.383 (9)
C5—C6	1.397 (10)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—O1	1.411 (8)
C7—N1	1.251 (8)	C14—H14A	0.9600
C7—H7	0.9300	C14—H14B	0.9600
C8—C9	1.397 (7)	C14—H14C	0.9600
C6—C1—C2	118.3 (7)	C10—C9—C8	121.6 (6)
C6—C1—C7	119.9 (6)	C10—C9—H9	119.2
C2—C1—C7	121.7 (6)	C8—C9—H9	119.2
C3—C2—C1	120.6 (7)	C9—C10—C11	119.6 (5)
C3—C2—H2	119.7	C9—C10—H10	120.2
C1—C2—H2	119.7	C11—C10—H10	120.2
C2—C3—C4	119.5 (7)	C12—C11—C10	119.9 (6)
C2—C3—H3	120.2	C12—C11—O1	115.1 (6)
C4—C3—H3	120.2	C10—C11—O1	124.9 (5)
C5—C4—C3	121.2 (7)	C11—C12—C13	121.8 (6)
C5—C4—Br1	118.9 (5)	C11—C12—H12	119.1
C3—C4—Br1	119.9 (6)	C13—C12—H12	119.1
C4—C5—C6	119.2 (6)	C12—C13—C8	119.0 (5)
C4—C5—H5	120.4	C12—C13—H13	120.5
C6—C5—H5	120.4	C8—C13—H13	120.5
C1—C6—C5	121.2 (7)	O1—C14—H14A	109.5
C1—C6—H6	119.4	O1—C14—H14B	109.5
C5—C6—H6	119.4	H14A—C14—H14B	109.5
N1—C7—C1	123.6 (6)	O1—C14—H14C	109.5
N1—C7—H7	118.2	H14A—C14—H14C	109.5
C1—C7—H7	118.2	H14B—C14—H14C	109.5
C9—C8—C13	118.2 (6)	C7—N1—C8	121.0 (6)
C9—C8—N1	116.9 (5)	C11—O1—C14	118.0 (5)
C13—C8—N1	124.9 (5)		

Fig. 1