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N-(4-Bromobenzylidene)-4-ethoxyaniline

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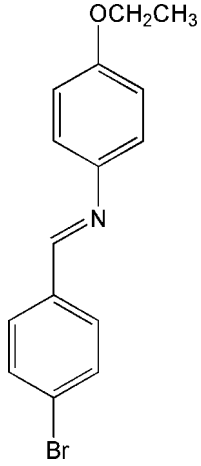
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.015 Å; R factor = 0.059; wR factor = 0.222; data-to-parameter ratio = 15.1.

In the title compound, $C_{15}H_{14}BrNO$, there are two molecules in the asymmetric unit with different conformations, as illustrated by the dihedral angles between the aromatic ring planes of 17.4 (5) and 9.7 (5)°.

Related literature

For related literature, see: Ma *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{14}BrNO$
M_r = 304.17
Triclinic, $P\overline{1}$
a = 8.0793 (10) Å
b = 8.5700 (11) Å
c = 10.3148 (13) Å
α = 88.390 (2)°
β = 85.615 (2)°
γ = 70.393 (2)°
V = 670.81 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.05 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.858, T_{max} = 0.913
(expected range = 0.783–0.833)
7771 measured reflections
4908 independent reflections
2957 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.222
S = 1.02
4908 reflections
325 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Absolute structure: Flack (1983), 1589 Friedel pairs
Flack parameter: −0.125 (19)

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: HB2572).

References

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Ma, R., Hou, Y., Yong, X. & Cen, Y. (2007). *Acta Cryst.* E**63**, o4188.
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supplementary materials

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N-(4-Bromobenzylidene)-4-ethoxyaniline

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Comment

As part of our onging studies of Schiff bases (Ma *et al.*, 2007) we now report the synthesis and structure of the title compound, (I), arising from the condensation of *p*-bromobenzaldehyde with 4-ethoxyaniline.

There are two molecules in the asymmetric unit of (I) (Fig. 1) with different conformations, as quantified by the dihedral angles between the armoatic ring planes of 17.4 (5)° and 9.7 (5)° for the C1 and C16 molecules, respectively.

Experimental

p-Ethoxyaniline (2.50 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 $C_{15}H_{14}Br_1N_1O_1$: C 59.23, H 4.64, N 4.60%; found: C 58.98, H 4.61, N 4.72%.

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

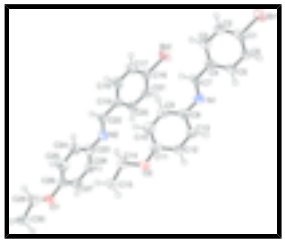

Fig. 1. Vew of the molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level (H atoms are drawn as spheres of arbitrary radius).

N-(4-Bromobenzylidene)-4-ethoxyaniline

Crystal data

$C_{15}H_{14}BrNO$	$Z = 2$
$M_r = 304.17$	$F_{000} = 308$
Triclinic, $P\overline{1}$	$D_x = 1.506$ Mg m^{-3}
Hall symbol: P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å

a = 8.0793 (10) Å	Cell parameters from 2326 reflections
b = 8.5700 (11) Å	θ = 2.5–24.4º
c = 10.3148 (13) Å	μ = 3.05 mm^{-1}
α = 88.390 (2)º	T = 293 (2) K
β = 85.615 (2)º	Block, colourless
γ = 70.393 (2)º	0.10 × 0.10 × 0.06 mm
V = 670.81 (15) $Å^3$	

Data collection

Bruker SMART CCD diffractometer	4908 independent reflections
Radiation source: fine-focus sealed tube	2957 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
T = 292(2) K	θ_{max} = 28.2º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -10 \rightarrow 10$
T_{min} = 0.858, T_{max} = 0.913	$k = -11 \rightarrow 11$
7771 measured reflections	$l = -13 \rightarrow 12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.059	$w = 1/[\sigma^2(F_o^2) + (0.1355P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.222	$(\Delta/\sigma)_{max} < 0.001$
S = 1.03	$\Delta\rho_{max}$ = 0.67 e $Å^{-3}$
4908 reflections	$\Delta\rho_{min}$ = −0.38 e $Å^{-3}$
325 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), 1589 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.125 (19)
Secondary atom site location: difference Fourier map	

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	−0.22363 (11)	−0.10639 (12)	0.46304 (9)	0.0755 (5)
Br2	0.24929 (11)	0.45540 (12)	0.45854 (9)	0.0746 (5)
C7	0.2988 (14)	0.1021 (14)	0.7530 (13)	0.051 (3)
H7A	0.4005	0.1089	0.7082	0.061*
C2	0.0784 (14)	−0.0185 (13)	0.4837 (10)	0.058 (3)
H2A	0.0932	−0.0340	0.3942	0.070*
C22	0.8171 (15)	0.5733 (14)	0.7634 (10)	0.044 (3)
H22A	0.9347	0.5187	0.7372	0.053*
C9	0.5246 (13)	0.2394 (11)	0.8860 (9)	0.046 (2)
H9A	0.5330	0.2558	0.7966	0.055*
C8	0.4014 (12)	0.1767 (12)	0.9370 (10)	0.044 (2)
C24	1.0866 (13)	0.5919 (12)	0.9241 (11)	0.050 (2)
H24A	1.1293	0.5046	0.8655	0.060*
N2	0.7844 (11)	0.6655 (10)	0.8580 (8)	0.0442 (18)
C21	0.3703 (14)	0.6083 (11)	0.6459 (9)	0.047 (2)
H21A	0.2520	0.6685	0.6654	0.056*
O1	1.2500 (11)	0.7989 (10)	1.1729 (8)	0.051 (2)
C28	0.8533 (12)	0.8233 (11)	1.0187 (9)	0.044 (2)
H28A	0.7351	0.8890	1.0263	0.053*
C17	0.5989 (12)	0.4026 (12)	0.5183 (10)	0.053 (2)
H17A	0.6299	0.3270	0.4503	0.064*
C6	−0.0879 (12)	−0.0166 (12)	0.6807 (9)	0.047 (2)
H6A	−0.1858	−0.0312	0.7259	0.057*
O2	0.7400 (10)	0.2858 (10)	1.1812 (7)	0.048 (2)
C10	0.6409 (13)	0.2811 (11)	0.9618 (10)	0.048 (2)
H10A	0.7214	0.3268	0.9223	0.058*
C25	1.1941 (15)	0.6240 (13)	1.0027 (12)	0.058 (3)
H25A	1.3106	0.5540	1.0005	0.070*
C13	0.3944 (13)	0.1517 (10)	1.0740 (8)	0.042 (2)
H13A	0.3115	0.1082	1.1126	0.051*
C4	0.1760 (13)	0.0553 (12)	0.6805 (11)	0.048 (2)
C23	0.9093 (15)	0.6902 (12)	0.9303 (11)	0.046 (3)
C27	0.9710 (12)	0.8582 (10)	1.0945 (8)	0.043 (2)
H27A	0.9325	0.9502	1.1488	0.052*
C26	1.1393 (15)	0.7604 (12)	1.0900 (10)	0.042 (2)
N1	0.2768 (12)	0.1336 (10)	0.8706 (8)	0.0482 (19)
C11	0.6364 (15)	0.2543 (11)	1.0960 (10)	0.041 (2)
C15	0.9732 (15)	0.3761 (15)	1.2359 (10)	0.058 (3)
H15A	1.0599	0.4229	1.2012	0.088*
H15B	1.0309	0.2702	1.2742	0.088*
H15C	0.8965	0.4487	1.3009	0.088*
C30	1.5091 (16)	0.7643 (12)	1.2688 (9)	0.054 (3)
H30A	1.6314	0.6997	1.2725	0.082*
H30B	1.4484	0.7624	1.3523	0.082*
H30C	1.4980	0.8765	1.2459	0.082*

C3	0.1990 (14)	0.0285 (13)	0.5487 (10)	0.057 (2)
H3A	0.2965	0.0420	0.5021	0.068*
C14	0.8666 (13)	0.3548 (12)	1.1279 (9)	0.051 (2)
H14A	0.8084	0.4612	1.0882	0.061*
H14B	0.9433	0.2821	1.0615	0.061*
C19	0.6839 (15)	0.5442 (12)	0.6899 (9)	0.044 (2)
C20	0.5079 (13)	0.6343 (12)	0.7134 (10)	0.046 (2)
H20A	0.4764	0.7165	0.7766	0.056*
C29	1.4326 (13)	0.6951 (14)	1.1719 (10)	0.052 (2)
H29A	1.4922	0.6965	1.0868	0.062*
H29B	1.4422	0.5817	1.1938	0.062*
C18	0.7266 (13)	0.4298 (12)	0.5881 (11)	0.057 (3)
H18A	0.8445	0.3701	0.5665	0.068*
C1	−0.0611 (15)	−0.0413 (13)	0.5533 (11)	0.057 (3)
C12	0.5048 (12)	0.1892 (11)	1.1491 (9)	0.043 (2)
H12A	0.4949	0.1722	1.2384	0.051*
C5	0.0303 (13)	0.0308 (12)	0.7459 (11)	0.049 (2)
H5A	0.0119	0.0466	0.8354	0.059*
C16	0.4229 (14)	0.4914 (12)	0.5527 (9)	0.048 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0730 (10)	0.0956 (11)	0.0752 (9)	−0.0457 (10)	−0.0265 (8)	−0.0109 (9)
Br2	0.0686 (10)	0.0923 (11)	0.0770 (9)	−0.0416 (9)	−0.0176 (7)	−0.0163 (9)
C7	0.029 (5)	0.053 (6)	0.070 (8)	−0.008 (4)	−0.021 (5)	−0.025 (5)
C2	0.060 (6)	0.074 (7)	0.048 (6)	−0.031 (5)	0.002 (5)	−0.020 (5)
C22	0.043 (6)	0.062 (6)	0.031 (6)	−0.020 (5)	−0.007 (5)	−0.002 (5)
C9	0.047 (6)	0.043 (5)	0.042 (6)	−0.008 (4)	−0.005 (5)	−0.001 (4)
C8	0.033 (5)	0.042 (5)	0.048 (6)	0.002 (4)	−0.007 (4)	−0.014 (4)
C24	0.038 (5)	0.040 (5)	0.068 (7)	−0.005 (4)	−0.008 (5)	−0.020 (5)
N2	0.040 (4)	0.044 (4)	0.051 (5)	−0.016 (4)	−0.005 (4)	−0.004 (4)
C21	0.054 (6)	0.048 (5)	0.039 (5)	−0.018 (4)	−0.003 (4)	0.008 (4)
O1	0.053 (5)	0.057 (4)	0.048 (4)	−0.023 (4)	−0.008 (4)	−0.017 (3)
C28	0.037 (5)	0.035 (5)	0.048 (5)	0.006 (4)	−0.006 (4)	−0.004 (4)
C17	0.041 (5)	0.055 (6)	0.065 (7)	−0.015 (4)	−0.010 (5)	−0.021 (5)
C6	0.032 (5)	0.068 (6)	0.048 (6)	−0.026 (4)	0.003 (4)	−0.012 (4)
O2	0.053 (5)	0.063 (4)	0.036 (4)	−0.028 (4)	−0.008 (3)	−0.008 (3)
C10	0.053 (6)	0.036 (5)	0.057 (6)	−0.015 (4)	−0.005 (5)	0.003 (4)
C25	0.045 (6)	0.037 (5)	0.082 (8)	0.005 (5)	−0.016 (6)	−0.019 (5)
C13	0.054 (6)	0.043 (5)	0.033 (5)	−0.022 (4)	−0.002 (4)	−0.002 (4)
C4	0.041 (5)	0.046 (5)	0.058 (6)	−0.013 (4)	−0.003 (5)	−0.014 (4)
C23	0.040 (6)	0.035 (5)	0.055 (7)	−0.004 (4)	−0.007 (5)	−0.004 (4)
C27	0.048 (5)	0.036 (4)	0.040 (5)	−0.007 (4)	0.000 (4)	−0.007 (4)
C26	0.042 (5)	0.041 (5)	0.040 (5)	−0.007 (4)	−0.008 (4)	−0.007 (4)
N1	0.053 (5)	0.050 (5)	0.042 (5)	−0.017 (4)	−0.003 (4)	−0.014 (4)
C11	0.052 (5)	0.028 (4)	0.037 (5)	−0.004 (4)	−0.003 (4)	0.000 (3)
C15	0.061 (7)	0.083 (8)	0.044 (6)	−0.040 (6)	−0.009 (5)	−0.002 (5)

C30	0.086 (8)	0.051 (6)	0.030 (5)	−0.025 (6)	−0.019 (5)	0.006 (4)
C3	0.059 (6)	0.068 (6)	0.053 (6)	−0.031 (5)	−0.003 (5)	−0.015 (5)
C14	0.048 (6)	0.060 (6)	0.049 (6)	−0.026 (5)	0.003 (5)	−0.002 (5)
C19	0.063 (7)	0.044 (5)	0.031 (5)	−0.024 (5)	0.000 (5)	−0.002 (4)
C20	0.043 (6)	0.048 (5)	0.047 (6)	−0.013 (4)	0.001 (5)	−0.018 (4)
C29	0.045 (6)	0.070 (7)	0.042 (6)	−0.020 (5)	−0.011 (5)	0.003 (5)
C18	0.043 (5)	0.052 (5)	0.075 (7)	−0.012 (4)	−0.005 (5)	−0.023 (5)
C1	0.054 (6)	0.053 (6)	0.065 (7)	−0.015 (5)	−0.025 (5)	−0.010 (5)
C12	0.046 (5)	0.049 (5)	0.031 (5)	−0.013 (4)	−0.001 (4)	−0.007 (4)
C5	0.043 (5)	0.057 (6)	0.052 (6)	−0.019 (4)	−0.005 (5)	−0.020 (5)
C16	0.062 (7)	0.054 (6)	0.041 (5)	−0.034 (5)	−0.018 (5)	0.007 (4)

Geometric parameters (Å, °)

Br1—C1	1.900 (10)	C6—H6A	0.9300
Br2—C16	1.877 (9)	O2—C11	1.350 (12)
C7—N1	1.237 (14)	O2—C14	1.415 (12)
C7—C4	1.449 (13)	C10—C11	1.397 (14)
C7—H7A	0.9300	C10—H10A	0.9300
C2—C1	1.356 (16)	C25—C26	1.423 (14)
C2—C3	1.392 (13)	C25—H25A	0.9300
C2—H2A	0.9300	C13—C12	1.346 (12)
C22—N2	1.228 (13)	C13—H13A	0.9300
C22—C19	1.453 (14)	C4—C3	1.374 (15)
C22—H22A	0.9300	C4—C5	1.386 (14)
C9—C8	1.349 (15)	C27—C26	1.335 (14)
C9—C10	1.405 (13)	C27—H27A	0.9300
C9—H9A	0.9300	C11—C12	1.426 (14)
C8—N1	1.410 (12)	C15—C14	1.509 (13)
C8—C13	1.423 (13)	C15—H15A	0.9600
C24—C25	1.329 (15)	C15—H15B	0.9600
C24—C23	1.395 (14)	C15—H15C	0.9600
C24—H24A	0.9300	C30—C29	1.451 (13)
N2—C23	1.373 (13)	C30—H30A	0.9600
C21—C16	1.347 (14)	C30—H30B	0.9600
C21—C20	1.437 (14)	C30—H30C	0.9600
C21—H21A	0.9300	C3—H3A	0.9300
O1—C26	1.404 (12)	C14—H14A	0.9700
O1—C29	1.444 (13)	C14—H14B	0.9700
C28—C27	1.387 (12)	C19—C20	1.378 (14)
C28—C23	1.410 (14)	C19—C18	1.400 (14)
C28—H28A	0.9300	C20—H20A	0.9300
C17—C18	1.386 (13)	C29—H29A	0.9700
C17—C16	1.392 (14)	C29—H29B	0.9700
C17—H17A	0.9300	C18—H18A	0.9300
C6—C1	1.327 (14)	C12—H12A	0.9300
C6—C5	1.379 (13)	C5—H5A	0.9300
N1—C7—C4	124.2 (12)	O1—C26—C25	124.5 (11)
N1—C7—H7A	117.9	C7—N1—C8	122.0 (10)

C4—C7—H7A	117.9	O2—C11—C10	127.5 (9)
C1—C2—C3	118.9 (9)	O2—C11—C12	116.5 (8)
C1—C2—H2A	120.6	C10—C11—C12	116.0 (9)
C3—C2—H2A	120.6	C14—C15—H15A	109.5
N2—C22—C19	124.2 (11)	C14—C15—H15B	109.5
N2—C22—H22A	117.9	H15A—C15—H15B	109.5
C19—C22—H22A	117.9	C14—C15—H15C	109.5
C8—C9—C10	123.0 (9)	H15A—C15—H15C	109.5
C8—C9—H9A	118.5	H15B—C15—H15C	109.5
C10—C9—H9A	118.5	C29—C30—H30A	109.5
C9—C8—N1	127.6 (9)	C29—C30—H30B	109.5
C9—C8—C13	116.7 (9)	H30A—C30—H30B	109.5
N1—C8—C13	115.7 (9)	C29—C30—H30C	109.5
C25—C24—C23	119.5 (11)	H30A—C30—H30C	109.5
C25—C24—H24A	120.3	H30B—C30—H30C	109.5
C23—C24—H24A	120.3	C4—C3—C2	120.9 (10)
C22—N2—C23	124.6 (11)	C4—C3—H3A	119.5
C16—C21—C20	115.9 (9)	C2—C3—H3A	119.5
C16—C21—H21A	122.0	O2—C14—C15	108.5 (8)
C20—C21—H21A	122.0	O2—C14—H14A	110.0
C26—O1—C29	119.2 (8)	C15—C14—H14A	110.0
C27—C28—C23	121.3 (9)	O2—C14—H14B	110.0
C27—C28—H28A	119.4	C15—C14—H14B	110.0
C23—C28—H28A	119.4	H14A—C14—H14B	108.4
C18—C17—C16	118.3 (8)	C20—C19—C18	116.3 (10)
C18—C17—H17A	120.8	C20—C19—C22	121.2 (10)
C16—C17—H17A	120.8	C18—C19—C22	122.4 (10)
C1—C6—C5	119.6 (9)	C19—C20—C21	123.6 (9)
C1—C6—H6A	120.2	C19—C20—H20A	118.2
C5—C6—H6A	120.2	C21—C20—H20A	118.2
C11—O2—C14	116.0 (8)	O1—C29—C30	105.8 (9)
C11—C10—C9	120.5 (9)	O1—C29—H29A	110.6
C11—C10—H10A	119.8	C30—C29—H29A	110.6
C9—C10—H10A	119.8	O1—C29—H29B	110.6
C24—C25—C26	123.1 (11)	C30—C29—H29B	110.6
C24—C25—H25A	118.4	H29A—C29—H29B	108.7
C26—C25—H25A	118.4	C17—C18—C19	122.1 (9)
C12—C13—C8	121.7 (9)	C17—C18—H18A	119.0
C12—C13—H13A	119.1	C19—C18—H18A	119.0
C8—C13—H13A	119.1	C6—C1—C2	121.9 (10)
C3—C4—C5	117.4 (10)	C6—C1—Br1	119.8 (9)
C3—C4—C7	123.1 (10)	C2—C1—Br1	118.2 (8)
C5—C4—C7	119.5 (10)	C13—C12—C11	122.0 (8)
N2—C23—C24	124.9 (10)	C13—C12—H12A	119.0
N2—C23—C28	117.5 (9)	C11—C12—H12A	119.0
C24—C23—C28	117.6 (11)	C6—C5—C4	121.2 (10)
C26—C27—C28	120.3 (8)	C6—C5—H5A	119.4
C26—C27—H27A	119.8	C4—C5—H5A	119.4
C28—C27—H27A	119.8	C21—C16—C17	123.5 (9)

C27—C26—O1	117.5 (9)	C21—C16—Br2	117.8 (8)
C27—C26—C25	118.0 (10)	C17—C16—Br2	118.5 (7)

Fig. 1