Table 2. *Geometric parameters* (Å, °)

O1—C1	1.309 (2)	C4—C5	1.496 (2)
O2—C1	1.205 (2)	C6—C7	1.350 (2)
O3—C5	1.190 (2)	C6—C9	1.399 (2)
O4—C5	1.340 (2)	C7—C8	1.421 (2)
O4—C6	1.404 (1)	C8—C8*	1.417 (2)
C1—C2	1.495 (2)	C8*—C10	1.411 (2)
C2—C3	1.514 (2)	C9—C10	1.366 (2)
C3—C4	1.512 (2)		
C5—O4—C6	120.5 (1)	O4—C5—C4	110.3 (1)
O1—C1—O2	122.3 (1)	O4—C6—C7	122.6 (1)
O1—C1—C2	113.9 (1)	O4—C6—C9	115.1 (1)
O2—C1—C2	123.8 (1)	C7—C6—C9	122.2 (1)
C1—C2—C3	112.7 (1)	C6—C7—C8	119.3 (1)
C2—C3—C4	112.4 (1)	C8*—C8—C7	119.5 (1)
C3—C4—C5	112.6 (1)	C8—C8*—C10	118.6 (1)
O3—C5—O4	122.9 (1)	C6—C9—C10	119.5 (1)
O3—C5—C4	126.8 (1)	C8*—C10—C9	120.9 (1)
C6—O4—C5—O3	6.9 (4)	C2—C3—C4—C5	173.4 (2)
C6—O4—C5—C4	−173.6 (2)	C3—C4—C5—O3	21.5 (4)
C5—O4—C6—C7	−63.9 (3)	C3—C4—C5—O4	−158.0 (2)
C5—O4—C6—C9	119.6 (2)	O4—C6—C7—C8	−175.9 (2)
O1—C1—C2—C3	177.1 (2)	C9—C6—C7—C8	0.3 (3)
O2—C1—C2—C3	−4.0 (3)	O4—C6—C9—C10	176.0 (4)
C1—C2—C3—C4	175.3 (2)	C7—C6—C9—C10	−0.5 (4)

Programs used to solve the structure: *SIR*88 (Burla, Camalli, Cascarano, Giacovazzo, Polidori, Spagna & Viterbo, 1989). Program used to refine the structure: *SDP* (Enraf-Nonius, 1985). Refinement by full-matrix least-squares methods. All programs were run on a MicroVAX computer.

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References

Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Polidori, G., Spagna, R. & Viterbo, D. (1989). *J. Appl. Cryst.* **22**, 389–393.

Centore, R., Ciajolo, M. R., Roviello, A., Sirigu, A. & Tuzi, A. (1990). *Mol. Cryst. Liq. Cryst.* **185**, 99–108.

Centore, R., Ciajolo, M. R., Roviello, A., Sirigu, A. & Tuzi, A. (1992). *Mol. Cryst. Liq. Cryst.* **214**, 105–115.

Centore, R., Roviello, A. & Sirigu, A. (1989). *Liq. Cryst.* **6**, 175–183.

Cotton, F. A. (1971). *Chemical Application of Group Theory*, 2nd ed., pp. 161–165. New York: Wiley-Interscience.

Enraf-Nonius (1985). *Structure Determination Package*. Enraf-Nonius, Delft, The Netherlands.

Hummel, J. P. & Flory, P. J. (1980). *Macromolecules*, **13**, 479–484.

Krigbaum, W. R., Watanabe, J. & Ishikawa, T. (1983). *Macromolecules*, **16**, 1271–1279.

Leiserowitz, L. (1976). *Acta Cryst.* B**32**, 775–802.

Trotter, J. (1986). *Acta Cryst.* C**42**, 351–353.

Watanabe, J., Ikeda, K. & Krigbaum, W. R. (1987). *J. Polym. Sci. Polym. Phys. Ed.* **25**, 19–30.

White, D. N. J., Carnduff, J., Guy, M. H. P. & Bovill, M. J. (1977). *Acta Cryst.* B**33**, 2982–2984.

0108-2701/92/122257-02$06.00

Acta Cryst. (1992). C**48**, 2257–2258

Structure of 4-[(4-Methoxyphenylimino)-methyl]phenol

GUAN-YEOW YEAP

School of Chemical Sciences, Universiti Sains Malaysia, Minden, 11800 *Penang, Malaysia*

HOONG-KUN FUN

School of Physics, Universiti Sains Malaysia, Minden, 11800 *Penang, Malaysia*

SIANG-GUAN TEOH* AND SOON-BENG TEO

School of Chemical Sciences, Universiti Sains Malaysia, Minden, 11800 *Penang, Malaysia*

K. CHINNAKALI† AND BOON-CHUAN YIP

School of Physics, Universiti Sains Malaysia, Minden, 11800 *Penang, Malaysia*

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Abstract

The benzylideneaniline moiety adopts a non-planar conformation with a dihedral angle of 51.0 (1)° between the two phenyl rings. The methoxy substituent is twisted from the aniline ring by 4.1 (5)°.

Comment

Benzylideneaniline normally adopts a non-planar conformation minimizing steric hindrance (Bürgi & Dunitz, 1970; Bernstein, Engel & Hagler, 1981) but disorder can give rise to a nominally planar conformation (Bar & Bernstein, 1983). An almost planar conformation, stabilized by an intramolecular hydrogen bond, is observed in some of its derivatives (Yeap, Fun, Teo & Teoh, 1992). The title compound, which was prepared according to Srivastava & Chauhan (1977), exhibits a non-planar conformation [C(7)—N—C(8)—C(9) −147.4 (4), C(8)—N—C(7)—C(1) −170.5 (4) and N—C(7)—C(1)—C(2) 14.7 (4)°]. The methoxy substitutent is nearly coplanar with the phenyl ring having a torsion angle of 4.1 (5)° about O(2)—C(11). The widening of the angle O(2)—C(11)—C(10) [124.6 (3)°] and the narrowing of O(2)—C(11)—C(12) [115.4 (3)°] are due to steric interactions between C(10) and C(14).

† Post Doctoral Research Fellow. Permanent address: Physics Division, Department of Chemical Engineering, AC Tech. Campus, Anna University, Madras 600025, India.

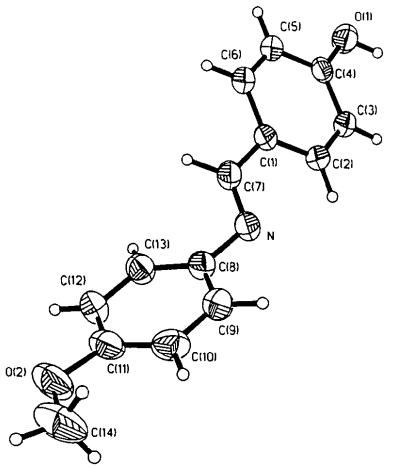

Fig. 1. A view of the molecule showing the labelling of the non-H atoms. Thermal ellipsoids are shown at 50% probability levels.

Experimental

Crystal data

$C_{14}H_{13}NO_2$
M_r = 227.3
Orthorhombic
Pbcn
a = 22.521 (6) Å
b = 10.809 (3) Å
c = 9.509 (2) Å
V = 2314.9 (10) Å^3
Z = 8
D_x = 1.304 Mg m^{-3}
D_m = 1.310 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 7.5–17.5°
μ = 0.088 mm^{-1}
T = 298 K
Needle
2 × 0.2 × 0.1 mm
Yellow

Data collection

Siemens *P*4 diffractometer
$2\theta/\theta$ scans
Absorption correction: none
2681 measured reflections
2681 independent reflections
1171 observed reflections [$F>4.0\sigma(F)$]

θ_{max} = 55.0°
h = 0 → 29
k = 0 → 14
l = 0 → 12
2 standard reflections monitored every 100 reflections
intensity variation: none

Refinement

Refinement on F
Final R = 0.0454
wR = 0.0493
S = 1.00
1171 reflections
206 parameters

All H-atom parameters refined
$w = 1.0/[\sigma^2(F)+0.001F^2]$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
N	0.3305 (1)	0.5219 (2)	0.1597 (3)	0.038 (1)
O(1)	0.1366 (1)	0.7434 (2)	−0.2745 (3)	0.051 (1)
O(2)	0.4661 (1)	0.1609 (2)	0.4301 (3)	0.068 (1)
C(1)	0.2442 (1)	0.5609 (3)	0.0125 (3)	0.034 (1)
C(2)	0.2631 (1)	0.6721 (3)	−0.0480 (3)	0.036 (1)
C(3)	0.2281 (1)	0.7347 (3)	−0.1422 (3)	0.037 (1)
C(4)	0.1725 (1)	0.6878 (3)	−0.1795 (3)	0.036 (1)
C(5)	0.1529 (1)	0.5778 (3)	−0.1191 (4)	0.043 (1)
C(6)	0.1879 (1)	0.5160 (3)	−0.0253 (4)	0.042 (1)
C(7)	0.2818 (1)	0.4861 (3)	0.1026 (3)	0.039 (1)
C(8)	0.3667 (1)	0.4318 (3)	0.2274 (3)	0.038 (1)
C(9)	0.4000 (1)	0.4636 (3)	0.3431 (3)	0.046 (1)
C(10)	0.4339 (2)	0.3765 (3)	0.4152 (4)	0.053 (1)
C(11)	0.4354 (1)	0.2559 (3)	0.3665 (4)	0.049 (1)
C(12)	0.4052 (2)	0.2243 (3)	0.2462 (4)	0.049 (1)
C(13)	0.3710 (1)	0.3106 (3)	0.1762 (4)	0.043 (1)
C(14)	0.4953 (3)	0.1857 (7)	0.5594 (5)	0.081 (2)

Table 2. *Bond lengths* (Å) *and angles* (°)

N—C(7)	1.283 (4)	C(9)—C(8)	1.375 (4)
N—C(8)	1.424 (4)	C(9)—C(10)	1.393 (5)
O(1)—C(4)	1.352 (4)	C(3)—C(2)	1.372 (4)
C(4)—C(5)	1.392 (4)	O(2)—C(11)	1.377 (4)
C(4)—C(3)	1.397 (4)	O(2)—C(14)	1.420 (6)
C(5)—C(6)	1.365 (5)	C(13)—C(8)	1.400 (4)
C(1)—C(6)	1.405 (4)	C(13)—C(12)	1.380 (5)
C(1)—C(7)	1.450 (4)	C(11)—C(12)	1.374 (5)
C(1)—C(2)	1.398 (4)	C(11)—C(10)	1.383 (5)
C(7)—N—C(8)	118.3 (2)	N—C(7)—C(1)	125.5 (3)
O(1)—C(4)—C(5)	117.8 (3)	C(8)—C(13)—C(12)	120.2 (3)
O(1)—C(4)—C(3)	122.9 (3)	N—C(8)—C(9)	120.1 (3)
C(5)—C(4)—C(3)	119.3 (3)	N—C(8)—C(13)	121.5 (3)
C(4)—C(5)—C(6)	120.3 (3)	C(9)—C(8)—C(13)	118.3 (3)
C(6)—C(1)—C(7)	119.0 (3)	C(1)—C(2)—C(3)	121.2 (3)
C(6)—C(1)—C(2)	117.8 (3)	O(2)—C(11)—C(12)	115.4 (3)
C(7)—C(1)—C(2)	123.0 (3)	O(2)—C(11)—C(10)	124.6 (3)
C(8)—C(9)—C(10)	121.5 (3)	C(12)—C(11)—C(10)	120.0 (3)
C(4)—C(3)—C(2)	120.2 (3)	C(13)—C(12)—C(110	120.6 (3)
C(5)—C(6)—C(1)	121.3 (3)	C(9)—C(10)—C(11)	119.1 (3)
C(11)—O(2)—C(14)	118.1 (4)		

The data were collected using a variable scan speed of 5.33–29.3° min^{-1} in ω. The structure was solved by direct methods and refined by full-matrix least squares. *SHELXTL/PC* (Siemens Crystallographic Research Systems, 1990) was used for all calculations.

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References

Bar, I. & Bernstein, J. (1983). *Acta Cryst.* B**39**, 266–272.
Bernstein, J., Engel, Y. M. & Hagler, A. T. (1981). *J. Chem. Phys.* **75**, 2346–2353.
Bürgi, H. B. & Dunitz, J. D. (1970). *Helv. Chim. Acta,* **52**, 1747–1750.
Siemens Crystallographic Research Systems (1990). *SHELXTL/PC.* Release 4.1. Siemens Crystallographic Research Systems, Madison, Wisconsin, USA.
Srivastava, T. N. & Chauhan, A. K. S. (1977). *J. Inorg. Nucl. Chem.* **39**, 371–373.
Yeap, G. Y., Fun, H. K., Teo, S. B. & Teoh, S. G. (1992). *Acta Cryst.* C**48**, 1109–1110.