Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methoxy-*N*-(3-phenylallylidene)aniline

Ying Li, Xiao-Lian He and Xiao-Yan Yang*

College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China
Correspondence e-mail: qustchemistry@126.com

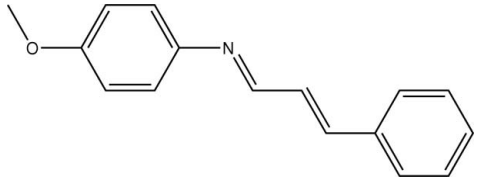
Received 27 October 2007; accepted 30 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.051; wR factor = 0.152; data-to-parameter ratio = 15.5.

In the molecule of the title compound, $C_{16}H_{15}NO$, all bond lengths and angles are within normal ranges. The dihedral angle between the two aromatic rings is of 62.80 (1)°. The crystal packing is stabilized by C—H$\cdots\pi$ interactions.

Related literature

For related literature, see: Yang *et al.* (2006); Allen *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{15}NO$
M_r = 237.29
Orthorhombic, *Pbca*
a = 7.2170 (9) Å
b = 6.3101 (8) Å
c = 57.061 (7) Å
V = 2598.6 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.43 × 0.35 × 0.16 mm

Data collection

Siemens SMART 1000 CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.988
13125 measured reflections
2545 independent reflections
2180 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.152
S = 1.09
2545 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C10–C15 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C15—H15$A\cdots Cg^{i}$	0.93	2.71	3.49	142

Symmetry code: (i) $-x-\frac{1}{2}, y-\frac{1}{2}, z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

This project was supported by the Natural Science Foundation of Shandong Province (grant Nos. Z2006B01 and Y2006B07).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2567).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS, Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-Ray Instruments, Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Yang, X.-Y., Li, Y., He, X.-L., Bi, S. & Zhang, S.-S. (2006). *Acta Cryst.* E**62**, o4070–o4071.

  doi:10.1107/S1600536807054542

supplementary materials

Acta Cryst. (2007). E**63**, o4546 [**doi:10.1107/S1600536807054542**]

4-Methoxy-*N*-(3-phenylallylidene)aniline

Y. Li, X.-L. He and X.-Y. Yang

Comment

Recently we have reported the structure of 4-methoxy-*N*-[3-(2-nitrophenyl)allylidene]aniline, (II) (Yang *et al.*, 2006). As part of our ongoing studies on push-pull Schiff base compounds, the title compound, (I), was synthesized and its structure is presented here.

In the molecule of the title compound, all bond lengths and angles show normal values (Allen *et al.*, 1987) and are comparable with those in (II). The whole molecule is non-planar, with a dihedral angle of 62.80 (1)° between the two aromatic rings, in contrast to that of 4.01 (1)° in (II). The crystal strucure is stabilized by a C—H···π interaction (C15—H15A···cg: H15A···*Cg* 2.708 Å, C15···cg 3.485 Å, C15—H15A···cg 141.6°; symmetry operator: 1/2 − *x*, 1/2 + *y*, *z*, cg is the centroid of the ring C10 to C15).

Experimental

The title compound was prepared according to the literature method of Yang *et al.* (2006). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of five days.

Refinement

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C) for methyl H atoms.

Figures

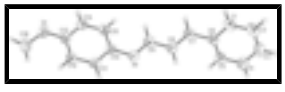


Fig. 1. The structure of the title compound showing 50% probability displacement ellipsoids and the atom numbering scheme.

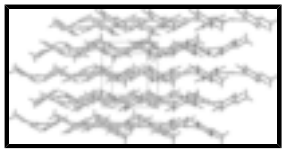


Fig. 2. A packing diagram of the title compound, viewed down the *c* axis.

4-Methoxy-*N*-(3-phenylallylidene)aniline

Crystal data

$C_{16}H_{15}NO$

M_r = 237.29

D_x = 1.213 Mg m^{-3}

Mo *K*α radiation

λ = 0.71073 Å

Orthorhombic, *Pbca*	Cell parameters from 4641 reflections
a = 7.2170 (9) Å	θ = 2.5–25.8º
b = 6.3101 (8) Å	μ = 0.08 mm^{-1}
c = 57.061 (7) Å	T = 293 (2) K
V = 2598.6 (6) $Å^3$	Block, yellow
Z = 8	0.43 × 0.35 × 0.16 mm
F_{000} = 1008	

Data collection

Siemens SMART 1000 CCD area detector diffractometer	2545 independent reflections
Radiation source: fine-focus sealed tube	2180 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 2.1º
ω scans	$h = -7 \rightarrow 8$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -7 \rightarrow 6$
T_{min} = 0.968, T_{max} = 0.988	$l = -70 \rightarrow 68$
13125 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.051	$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 1.0047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.152	$(\Delta/\sigma)_{max} < 0.001$
S = 1.09	$\Delta\rho_{max}$ = 0.17 e $Å^{-3}$
2545 reflections	$\Delta\rho_{min}$ = −0.18 e $Å^{-3}$
164 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0071 (11)
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 $F^2 > 2sigma(F^2)$ is used only for calculat-

ing *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}
C11	0.0834 (2)	0.1903 (3)	−0.15889 (3)	0.0406 (4)
H11A	0.1424	0.2640	−0.1469	0.049*
C13	0.0018 (2)	0.1614 (3)	−0.19944 (3)	0.0391 (4)
C14	−0.0944 (2)	−0.0240 (3)	−0.19445 (3)	0.0429 (4)
H14A	−0.1549	−0.0964	−0.2064	0.051*
C15	−0.1006 (2)	−0.1014 (3)	−0.17184 (3)	0.0421 (4)
H15A	−0.1650	−0.2259	−0.1687	0.051*
N1	−0.0165 (2)	−0.0590 (2)	−0.12986 (2)	0.0453 (4)
C5	−0.0877 (2)	−0.5033 (3)	−0.05198 (3)	0.0461 (4)
H5A	−0.1456	−0.3736	−0.0545	0.055*
C12	0.0924 (2)	0.2686 (3)	−0.18164 (3)	0.0417 (4)
H12A	0.1585	0.3917	−0.1849	0.050*
O1	−0.0046 (2)	0.2257 (2)	−0.22245 (2)	0.0548 (4)
C1	0.0695 (3)	−0.8103 (3)	−0.06647 (3)	0.0507 (5)
H1B	0.1167	−0.8889	−0.0789	0.061*
C8	−0.0343 (3)	−0.3294 (3)	−0.10091 (3)	0.0466 (4)
H8A	−0.0494	−0.2298	−0.0891	0.056*
C3	0.0120 (3)	−0.7744 (3)	−0.02546 (4)	0.0588 (6)
H3A	0.0222	−0.8262	−0.0103	0.071*
C4	−0.0749 (3)	−0.5832 (3)	−0.02956 (3)	0.0538 (5)
H4A	−0.1252	−0.5076	−0.0171	0.065*
C9	−0.0278 (3)	−0.2554 (3)	−0.12480 (3)	0.0458 (4)
H9A	−0.0319	−0.3540	−0.1369	0.055*
C2	0.0837 (3)	−0.8885 (3)	−0.04397 (4)	0.0580 (5)
H2A	0.1415	−1.0180	−0.0413	0.070*
C7	−0.0199 (3)	−0.5322 (3)	−0.09489 (3)	0.0471 (5)
H7A	−0.0125	−0.6304	−0.1070	0.057*
C6	−0.0146 (2)	−0.6149 (3)	−0.07092 (3)	0.0414 (4)
C10	−0.0111 (2)	0.0051 (3)	−0.15358 (3)	0.0376 (4)
C16	0.0889 (4)	0.4160 (4)	−0.22840 (4)	0.0744 (7)
H16A	0.0734	0.4439	−0.2448	0.112*
H16B	0.2183	0.4017	−0.2249	0.112*
H16C	0.0380	0.5313	−0.2195	0.112*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0415 (9)	0.0397 (9)	0.0404 (9)	−0.0017 (7)	−0.0034 (7)	−0.0053 (7)
C13	0.0384 (9)	0.0430 (9)	0.0360 (8)	0.0034 (7)	0.0013 (6)	0.0003 (7)
C14	0.0428 (9)	0.0435 (9)	0.0424 (9)	−0.0045 (7)	−0.0051 (7)	−0.0058 (7)
C15	0.0406 (9)	0.0391 (9)	0.0467 (9)	−0.0059 (7)	0.0008 (7)	0.0006 (7)
N1	0.0535 (9)	0.0450 (8)	0.0374 (8)	−0.0018 (7)	0.0009 (6)	0.0007 (6)

C5	0.0493 (10)	0.0436 (10)	0.0454 (9)	0.0041 (8)	−0.0012 (8)	0.0023 (8)
C12	0.0431 (9)	0.0366 (9)	0.0453 (9)	−0.0059 (7)	0.0007 (7)	−0.0003 (7)
O1	0.0682 (9)	0.0590 (8)	0.0373 (7)	−0.0089 (7)	−0.0028 (6)	0.0052 (6)
C1	0.0504 (11)	0.0397 (10)	0.0618 (11)	0.0012 (8)	0.0061 (9)	0.0000 (8)
C8	0.0550 (11)	0.0466 (10)	0.0383 (9)	−0.0034 (8)	0.0010 (8)	−0.0004 (8)
C3	0.0630 (13)	0.0591 (12)	0.0543 (12)	−0.0064 (10)	−0.0098 (9)	0.0171 (10)
C4	0.0611 (12)	0.0581 (12)	0.0422 (9)	−0.0018 (10)	−0.0017 (8)	0.0006 (8)
C9	0.0494 (10)	0.0483 (10)	0.0398 (9)	−0.0001 (8)	0.0034 (7)	−0.0011 (8)
C2	0.0553 (12)	0.0423 (10)	0.0763 (14)	0.0025 (9)	−0.0055 (10)	0.0158 (9)
C7	0.0526 (11)	0.0466 (10)	0.0422 (9)	−0.0018 (8)	0.0039 (8)	−0.0038 (8)
C6	0.0407 (9)	0.0387 (9)	0.0447 (9)	−0.0031 (7)	−0.0005 (7)	0.0012 (7)
C10	0.0373 (9)	0.0386 (8)	0.0368 (8)	0.0040 (7)	0.0019 (6)	−0.0007 (7)
C16	0.0997 (19)	0.0715 (15)	0.0522 (12)	−0.0198 (14)	−0.0039 (12)	0.0215 (11)

Geometric parameters (Å, °)

C11—C10	1.386 (2)	C1—C2	1.379 (3)
C11—C12	1.390 (2)	C1—C6	1.397 (2)
C11—H11A	0.9300	C1—H1B	0.9300
C13—O1	1.3752 (19)	C8—C7	1.329 (3)
C13—C12	1.384 (2)	C8—C9	1.442 (2)
C13—C14	1.390 (2)	C8—H8A	0.9300
C14—C15	1.380 (2)	C3—C2	1.379 (3)
C14—H14A	0.9300	C3—C4	1.380 (3)
C15—C10	1.398 (2)	C3—H3A	0.9300
C15—H15A	0.9300	C4—H4A	0.9300
N1—C9	1.275 (2)	C9—H9A	0.9300
N1—C10	1.413 (2)	C2—H2A	0.9300
C5—C4	1.378 (2)	C7—C6	1.465 (2)
C5—C6	1.394 (2)	C7—H7A	0.9300
C5—H5A	0.9300	C16—H16A	0.9600
C12—H12A	0.9300	C16—H16B	0.9600
O1—C16	1.418 (3)	C16—H16C	0.9600
C10—C11—C12	121.79 (15)	C2—C3—H3A	120.1
C10—C11—H11A	119.1	C4—C3—H3A	120.1
C12—C11—H11A	119.1	C5—C4—C3	120.52 (19)
O1—C13—C12	124.90 (16)	C5—C4—H4A	119.7
O1—C13—C14	115.29 (15)	C3—C4—H4A	119.7
C12—C13—C14	119.79 (15)	N1—C9—C8	122.08 (17)
C15—C14—C13	120.35 (15)	N1—C9—H9A	119.0
C15—C14—H14A	119.8	C8—C9—H9A	119.0
C13—C14—H14A	119.8	C3—C2—C1	119.89 (18)
C14—C15—C10	120.78 (16)	C3—C2—H2A	120.1
C14—C15—H15A	119.6	C1—C2—H2A	120.1
C10—C15—H15A	119.6	C8—C7—C6	125.90 (17)
C9—N1—C10	119.80 (15)	C8—C7—H7A	117.0
C4—C5—C6	120.64 (17)	C6—C7—H7A	117.0
C4—C5—H5A	119.7	C5—C6—C1	117.99 (16)
C6—C5—H5A	119.7	C5—C6—C7	122.28 (16)

C13—C12—C11	119.29 (16)	C1—C6—C7	119.72 (16)
C13—C12—H12A	120.4	C11—C10—C15	118.00 (15)
C11—C12—H12A	120.4	C11—C10—N1	117.67 (14)
C13—O1—C16	117.53 (15)	C15—C10—N1	124.29 (15)
C2—C1—C6	121.14 (18)	O1—C16—H16A	109.5
C2—C1—H1B	119.4	O1—C16—H16B	109.5
C6—C1—H1B	119.4	H16A—C16—H16B	109.5
C7—C8—C9	123.60 (17)	O1—C16—H16C	109.5
C7—C8—H8A	118.2	H16A—C16—H16C	109.5
C9—C8—H8A	118.2	H16B—C16—H16C	109.5
C2—C3—C4	119.80 (18)		
O1—C13—C14—C15	−178.76 (15)	C9—C8—C7—C6	176.14 (17)
C12—C13—C14—C15	0.2 (3)	C4—C5—C6—C1	0.7 (3)
C13—C14—C15—C10	0.2 (3)	C4—C5—C6—C7	−177.93 (17)
O1—C13—C12—C11	177.96 (16)	C2—C1—C6—C5	−1.4 (3)
C14—C13—C12—C11	−0.9 (2)	C2—C1—C6—C7	177.27 (18)
C10—C11—C12—C13	1.2 (3)	C8—C7—C6—C5	23.2 (3)
C12—C13—O1—C16	0.1 (3)	C8—C7—C6—C1	−155.4 (2)
C14—C13—O1—C16	179.01 (18)	C12—C11—C10—C15	−0.8 (2)
C6—C5—C4—C3	0.6 (3)	C12—C11—C10—N1	−178.40 (15)
C2—C3—C4—C5	−1.2 (3)	C14—C15—C10—C11	0.1 (2)
C10—N1—C9—C8	−179.82 (16)	C14—C15—C10—N1	177.50 (16)
C7—C8—C9—N1	−170.2 (2)	C9—N1—C10—C11	−150.54 (18)
C4—C3—C2—C1	0.5 (3)	C9—N1—C10—C15	32.0 (3)
C6—C1—C2—C3	0.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15A···Cg^{i}	0.93	2.71	3.49	142

Symmetry codes: (i) −*x*−1/2, *y*−1/2, *z*.

Fig. 1

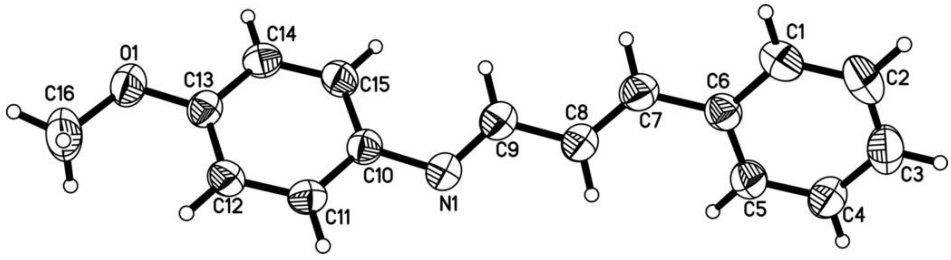


Fig. 2