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N-(4-Chlorobenzylidene)-4-methoxyaniline

 Xiao-Yan Ren,^a Yu-Feng Ding^b and Fang-Fang Jian^{a*}
^aMicroscale Science Institute, Weifang University, Weifang 261061, People's Republic of China, and ^bThe 7th Middle School, Weifang 261061, People's Republic of China

Correspondence e-mail: ffjian2008@163.com

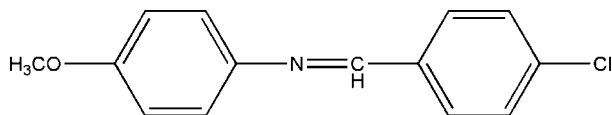
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.035; wR factor = 0.089; data-to-parameter ratio = 18.2.

The title compound, $\text{C}_{14}\text{H}_{12}\text{ClNO}$, was prepared by the reaction of 4-methoxyaniline and 4-chlorobenzaldehyde in ethanol at 367 K. The molecule is almost planar, with a dihedral angle between the two benzene rings of $9.1(2)^\circ$ and an r.m.s. deviation from the mean plane through all non-H atoms in the molecule of 0.167 Å.

Related literature

For applications of Schiff base compounds, see: Deschamps *et al.* (2003); Rozwadowski *et al.* (1999); Tarafder *et al.* (2000). For a related structure, see: Jian *et al.* (2006).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{12}\text{ClNO}$	$V = 1230.9(3) \text{ \AA}^3$
$M_r = 245.70$	$Z = 4$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 6.1055(9) \text{ \AA}$	$\mu = 0.29 \text{ mm}^{-1}$
$b = 7.3392(11) \text{ \AA}$	$T = 293(2) \text{ K}$
$c = 27.469(4) \text{ \AA}$	$0.20 \times 0.15 \times 0.11 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	2806 independent reflections
Absorption correction: none	2092 reflections with $I > 2\sigma(I)$
7232 measured reflections	$R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.088$	$\Delta\rho_{\text{max}} = 0.14 \text{ e \AA}^{-3}$
$S = 1.01$	$\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$
2806 reflections	Absolute structure: Flack (1983),
154 parameters	1450 Friedel pairs
1 restraint	Flack parameter: $-0.01(7)$

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2527).

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supporting information

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N-(4-Chlorobenzylidene)-4-methoxyaniline

Xiao-Yan Ren, Yu-Feng Ding and Fang-Fang Jian

S1. Comment

Schiff bases have been used extensively as ligands in the field of coordination chemistry (Jian *et al.*, 2006), and have antimicrobial (Tarafder *et al.*, 2000) and anticancer applications (Deschamps *et al.*, 2003). Additional recent interest in Schiff base compounds comes from their ability to form intramolecular hydrogen bonds by electron coupling between acid-base centers (Rozwadowski *et al.*, 1999). We report here the synthesis and structure of the title Schiff base compound, I, Fig. 1.

The molecule is almost planar with a dihedral angle between the C2...C7 and C9...C13 benzene rings of 9.1 (2)° and an rms deviation from the meanplane through all non-hydrogen atoms in the molecule of 0.167. The C=N bond distance (1.255 (2) Å) is in reasonable agreement with that observed in a similar compound (Jian *et al.*, 2006).

S2. Experimental

A mixture of 4-methoxyaniline 2.46 g (0.02 mol) and 4-chlorobenzaldehyde 2.8 g (0.02 mol) was stirred in ethanol (50 mL) at 367 K for 2 h, to give the title compound (3.9 g, yield 81%). Single crystals suitable for X-ray measurements were obtained by recrystallization from acetone and ethanol(1:1) at room temperature.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with $d(\text{C-H}) = 0.93 \text{ \AA}$, $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for aromatic and 0.96 \AA , $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ for CH_3 atoms.

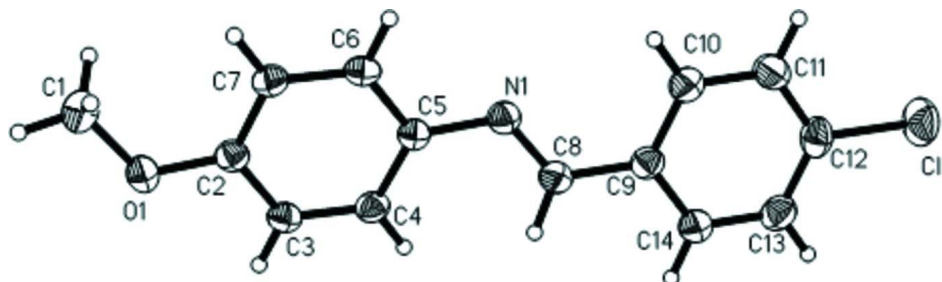


Figure 1

The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N-(4-Chlorobenzylidene)-4-methoxyaniline

Crystal data

$\text{C}_{14}\text{H}_{12}\text{ClNO}$

$M_r = 245.70$

Orthorhombic, $Pna2_1$

Hall symbol: P 2c -2n

$a = 6.1055 (9) \text{ \AA}$

$b = 7.3392 (11) \text{ \AA}$

$c = 27.469$ (4) Å
 $V = 1230.9$ (3) Å³
 $Z = 4$
 $F(000) = 512$
 $D_x = 1.326$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2092 reflections

$\theta = 2.9$ – 28.3°
 $\mu = 0.29$ mm⁻¹
 $T = 293$ K
 Block, yellow
 $0.20 \times 0.15 \times 0.11$ mm

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 7232 measured reflections
 2806 independent reflections

2092 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$
 $\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 2.9^\circ$
 $h = -8 \rightarrow 4$
 $k = -9 \rightarrow 9$
 $l = -36 \rightarrow 33$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.088$
 $S = 1.01$
 2806 reflections
 154 parameters
 1 restraint
 Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map

Hydrogen site location: inferred from
 neighbouring sites

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.0836P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³

Absolute structure: Flack (1983), 1450 Friedel
 pairs
 Absolute structure parameter: -0.01 (7)

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.77772 (12)	0.00540 (10)	0.23599 (3)	0.0862 (2)
O1	-0.0611 (2)	-0.01368 (19)	0.64134 (5)	0.0560 (4)
N1	0.2457 (3)	0.0122 (2)	0.45058 (6)	0.0463 (4)
C1	-0.2589 (4)	0.0731 (4)	0.65469 (10)	0.0750 (7)
H1B	-0.2859	0.0539	0.6887	0.112*
H1C	-0.3775	0.0230	0.6361	0.112*
H1D	-0.2475	0.2014	0.6483	0.112*
C2	0.0048 (3)	-0.0027 (2)	0.59389 (7)	0.0421 (4)
C3	0.1994 (3)	-0.0915 (2)	0.58341 (7)	0.0446 (4)
H3A	0.2739	-0.1522	0.6081	0.053*

C4	0.2838 (3)	-0.0909 (3)	0.53699 (7)	0.0456 (4)
H4A	0.4144	-0.1513	0.5305	0.055*
C5	0.1737 (3)	0.0005 (2)	0.49944 (7)	0.0395 (4)
C6	-0.0225 (3)	0.0856 (3)	0.51062 (6)	0.0436 (4)
H6A	-0.0996	0.1442	0.4860	0.052*
C7	-0.1074 (3)	0.0862 (2)	0.55747 (7)	0.0451 (4)
H7A	-0.2384	0.1458	0.5642	0.054*
C8	0.4424 (3)	-0.0157 (2)	0.43961 (7)	0.0475 (5)
H8A	0.5407	-0.0439	0.4644	0.057*
C9	0.5235 (3)	-0.0060 (2)	0.38958 (8)	0.0456 (4)
C10	0.3951 (4)	0.0631 (3)	0.35228 (7)	0.0537 (5)
H10A	0.2559	0.1075	0.3592	0.064*
C11	0.4712 (4)	0.0666 (3)	0.30525 (8)	0.0595 (6)
H11A	0.3842	0.1133	0.2804	0.071*
C12	0.6790 (4)	0.0000 (3)	0.29508 (8)	0.0572 (6)
C13	0.8091 (3)	-0.0666 (3)	0.33165 (8)	0.0579 (5)
H13A	0.9480	-0.1115	0.3247	0.069*
C14	0.7321 (3)	-0.0665 (3)	0.37880 (7)	0.0534 (5)
H14A	0.8221	-0.1079	0.4038	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0943 (5)	0.1126 (5)	0.0517 (3)	-0.0069 (4)	0.0194 (4)	-0.0127 (3)
O1	0.0570 (9)	0.0702 (10)	0.0409 (7)	0.0069 (7)	0.0025 (7)	-0.0003 (6)
N1	0.0453 (10)	0.0487 (10)	0.0448 (10)	0.0027 (7)	-0.0005 (7)	-0.0006 (7)
C1	0.0614 (15)	0.104 (2)	0.0598 (14)	0.0089 (13)	0.0097 (11)	-0.0055 (13)
C2	0.0414 (9)	0.0408 (9)	0.0440 (10)	-0.0062 (7)	-0.0034 (9)	-0.0031 (8)
C3	0.0429 (9)	0.0450 (10)	0.0459 (11)	0.0016 (8)	-0.0062 (8)	0.0036 (8)
C4	0.0396 (10)	0.0457 (10)	0.0516 (11)	0.0073 (8)	-0.0017 (8)	0.0024 (8)
C5	0.0408 (10)	0.0361 (9)	0.0417 (9)	-0.0022 (7)	-0.0009 (7)	-0.0013 (7)
C6	0.0409 (10)	0.0411 (10)	0.0487 (11)	0.0043 (8)	-0.0080 (8)	0.0020 (8)
C7	0.0397 (10)	0.0444 (9)	0.0511 (11)	0.0048 (8)	-0.0023 (8)	-0.0014 (8)
C8	0.0453 (11)	0.0527 (11)	0.0446 (10)	-0.0005 (9)	-0.0036 (9)	-0.0018 (9)
C9	0.0435 (10)	0.0449 (10)	0.0484 (10)	-0.0041 (8)	-0.0011 (9)	-0.0025 (8)
C10	0.0479 (11)	0.0593 (12)	0.0540 (12)	0.0032 (10)	0.0019 (9)	-0.0013 (9)
C11	0.0598 (14)	0.0688 (14)	0.0498 (12)	0.0060 (11)	-0.0051 (10)	0.0013 (9)
C12	0.0660 (14)	0.0581 (13)	0.0476 (12)	-0.0085 (11)	0.0123 (10)	-0.0092 (10)
C13	0.0473 (12)	0.0646 (13)	0.0617 (14)	0.0032 (10)	0.0059 (10)	-0.0055 (11)
C14	0.0473 (12)	0.0620 (13)	0.0508 (12)	0.0043 (9)	-0.0002 (9)	0.0018 (9)

Geometric parameters (Å, °)

C11—C12	1.732 (2)	C6—C7	1.387 (2)
O1—C2	1.366 (2)	C6—H6A	0.9300
O1—C1	1.414 (3)	C7—H7A	0.9300
N1—C8	1.255 (2)	C8—C9	1.463 (3)
N1—C5	1.415 (3)	C8—H8A	0.9300

C1—H1B	0.9600	C9—C14	1.381 (3)
C1—H1C	0.9600	C9—C10	1.386 (3)
C1—H1D	0.9600	C10—C11	1.373 (3)
C2—C7	1.377 (3)	C10—H10A	0.9300
C2—C3	1.386 (2)	C11—C12	1.388 (3)
C3—C4	1.375 (2)	C11—H11A	0.9300
C3—H3A	0.9300	C12—C13	1.371 (3)
C4—C5	1.402 (3)	C13—C14	1.378 (3)
C4—H4A	0.9300	C13—H13A	0.9300
C5—C6	1.386 (3)	C14—H14A	0.9300
C2—O1—C1	118.19 (17)	C2—C7—H7A	120.4
C8—N1—C5	121.00 (17)	C6—C7—H7A	120.4
O1—C1—H1B	109.5	N1—C8—C9	122.78 (18)
O1—C1—H1C	109.5	N1—C8—H8A	118.6
H1B—C1—H1C	109.5	C9—C8—H8A	118.6
O1—C1—H1D	109.5	C14—C9—C10	118.7 (2)
H1B—C1—H1D	109.5	C14—C9—C8	119.87 (19)
H1C—C1—H1D	109.5	C10—C9—C8	121.40 (17)
O1—C2—C7	125.07 (16)	C11—C10—C9	120.7 (2)
O1—C2—C3	115.02 (17)	C11—C10—H10A	119.6
C7—C2—C3	119.91 (18)	C9—C10—H10A	119.6
C4—C3—C2	120.82 (17)	C10—C11—C12	119.5 (2)
C4—C3—H3A	119.6	C10—C11—H11A	120.3
C2—C3—H3A	119.6	C12—C11—H11A	120.3
C3—C4—C5	120.27 (17)	C13—C12—C11	120.5 (2)
C3—C4—H4A	119.9	C13—C12—C11	119.55 (17)
C5—C4—H4A	119.9	C11—C12—C11	119.92 (19)
C6—C5—C4	117.86 (18)	C12—C13—C14	119.42 (18)
C6—C5—N1	116.83 (16)	C12—C13—H13A	120.3
C4—C5—N1	125.31 (16)	C14—C13—H13A	120.3
C5—C6—C7	122.00 (17)	C13—C14—C9	121.1 (2)
C5—C6—H6A	119.0	C13—C14—H14A	119.5
C7—C6—H6A	119.0	C9—C14—H14A	119.5
C2—C7—C6	119.11 (17)		
