# N-(4-Chlorobenzylidene)-4-methoxy-aniline

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The title compound, $C_{14}H_{12}ClNO$, 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)° 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).
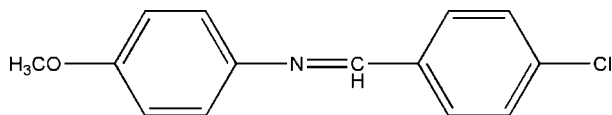


## Experimental

### Crystal data

| | |
|---|---|
| $C_{14}H_{12}ClNO$ | $V = 1230.9\ (3)\ \text{Å}^3$ |
| $M_r = 245.70$ | $Z = 4$ |
| Orthorhombic, $Pna2_1$ | Mo $K\alpha$ radiation |
| $a = 6.1055\ (9)\ \text{Å}$ | $\mu = 0.29\ \text{mm}^{-1}$ |
| $b = 7.3392\ (11)\ \text{Å}$ | $T = 293\ (2)\ \text{K}$ |
| $c = 27.469\ (4)\ \text{Å}$ | $0.20 \times 0.15 \times 0.11$ 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 | $R_{int} = 0.021$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.035$ | H-atom parameters constrained |
| $wR(F^2) = 0.088$ | $\Delta\rho_{max} = 0.14\ \text{e Å}^{-3}$ |
| $S = 1.01$ | $\Delta\rho_{min} = -0.16\ \text{e Å}^{-3}$ |
| 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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**supplementary materials**

## *N*-(4-Chlorobenzylidene)-4-methoxyaniline

### X.-Y. Ren, Y.-F. Ding and F.-F. Jian

### 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).

### 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.

### Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C-H) = 0.93Å, $U_{iso}$=1.2$U_{eq}$(C) for aromatic and 0.96Å, $U_{iso}$ = 1.5$U_{eq}$(C) for CH$_3$ atoms.

### Figures
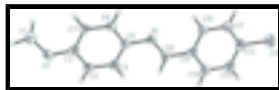


Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

**N-(4-Chlorobenzylidene)-4-methoxyaniline**

*Crystal data*

| | |
|---|---|
| C$_{14}$H$_{12}$ClNO | $F_{000} = 512$ |
| $M_r = 245.70$ | $D_x = 1.326$ Mg m$^{-3}$ |
| Orthorhombic, *Pna*2$_1$ | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: P 2c -2n | Cell parameters from 2092 reflections |
| $a = 6.1055$ (9) Å | θ = 2.9–28.3° |
| $b = 7.3392$ (11) Å | μ = 0.29 mm$^{-1}$ |

| | |
|---|---|
| $c = 27.469\ (4)$ Å | $T = 293\ (2)$ K |
| $V = 1230.9\ (3)$ Å$^3$ | Block, yellow |
| $Z = 4$ | $0.20 \times 0.15 \times 0.11$ mm |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2092 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.022$ |
| Monochromator: graphite | $\theta_{max} = 28.3°$ |
| $T = 293(2)$ K | $\theta_{min} = 2.9°$ |
| φ and ω scans | $h = -8 \rightarrow 4$ |
| Absorption correction: none | $k = -9 \rightarrow 9$ |
| 7232 measured reflections | $l = -36 \rightarrow 33$ |
| 2806 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.035$ | $w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.0836P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.088$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $S = 1.01$ | $\Delta\rho_{max} = 0.14$ e Å$^{-3}$ |
| 2806 reflections | $\Delta\rho_{min} = -0.16$ e Å$^{-3}$ |
| 154 parameters | Extinction correction: none |
| 1 restraint | Absolute structure: Flack (1983), 1450 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: −0.01 (7) |
| 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 $F^2 > \sigma(F^2)$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 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 ($Å^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 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, °)*

| Cl1—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—Cl1 | 119.55 (17) |
| C5—C4—H4A | 119.9 | C11—C12—Cl1 | 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) | | |

**Fig. 1**