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4-[(4-Chlorophenyl)iminomethyl]-2-methoxyphenol

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The title compound, $C_{14}H_{12}ClNO_2$,was prepared from 4-hydroxy-3-methoxybenzaldehyde and 4-chlorophenylamine. The two aromatic substituents lie trans to each other across the C═N bond, with a dihedral angle of 44.40 (8)° between the two rings

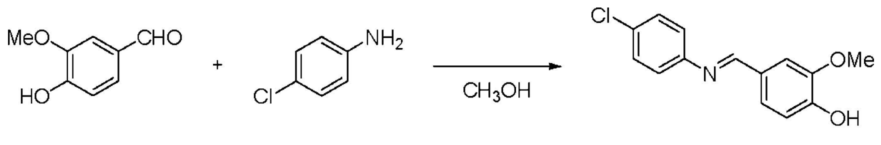
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.130
Data-to-parameter ratio = 15.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Shiff bases are important intermediates in organic chemistry, and can be used to prepare β-lactams (Hart *et al.*, 1983; van der Veen *et al.*, 1989). The title compound, (I), was synthesized from 4-hydroxy-3-methoxybenzaldehyde reacted with 4-chlorophenylamine in methanol.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The structure contains two aromatic rings, which are bridged by a C═N unit and are *trans* to each other; the aromatic rings make an angle of 44.40 (8)°.

Experimental

4-Hydroxy-3-methoxybenzaldehyde (1.52 g, 10 mmol) and 4-chlorophenylamine (1.28 g, 10 mmol) were added to methanol (30 ml). The mixture was heated and kept at reflux temperature for 3 h. After completion of the reaction, monitored by thin-layer chromatography,

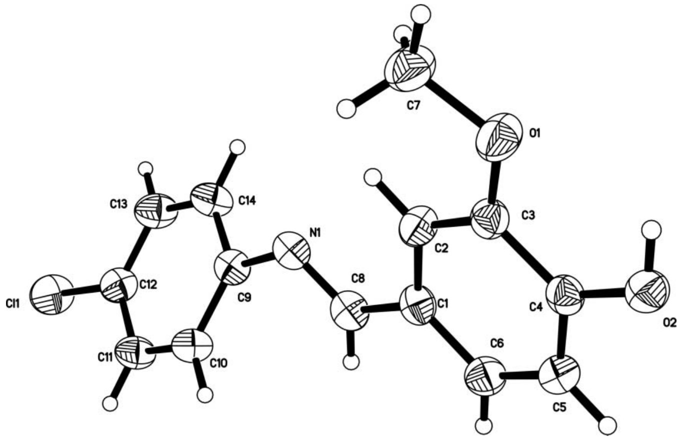


Figure 1
The molecular structure of (I), drawn with 30% probability displacement ellipsoids.

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the reaction mixture was cooled and filtered. The product obtained was dissolved in methanol (100 ml) at room temperature and the solution was kept at room temperature for 15 d. By natural evaporation, colourless single crystals of (I) were formed, which were suitable for X-ray diffraction analysis.

Crystal data

$C_{14}H_{12}ClNO_2$
$M_r = 261.70$
Monoclinic, $P2_1/c$
$a = 6.3411$ (13) Å
$b = 10.263$ (2) Å
$c = 19.803$ (4) Å
$\beta = 90.157$ (4)°
$V = 1288.8$ (5) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.29$ mm^{-1}
$T = 294$ (2) K
0.24 × 0.22 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{\min} = 0.934$, $T_{\max} = 0.945$
14787 measured reflections
2617 independent reflections
1575 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.130$
$S = 1.00$
2617 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.37$ e Å^{-3}

The hydroxy H atom was initially located in a difference map. In the final refinement, all H atoms were positioned geometrically, with C—H = 0.93–0.96 Å and O—H = 0.82 Å, and refined using a riding model, with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(parent) for methyl C and hydroxy O or 1.2$U_{\rm eq}$(parent) for the remaining atoms.

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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