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2-Chloro-*N*-[4-(dimethylamino)benzylidene]aniline

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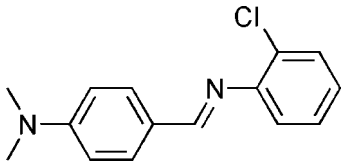
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.105; data-to-parameter ratio = 14.0.

In the title molecule, $C_{15}H_{15}ClN_2$, the dihedral angle between the aromatic is 64.1 (2)°.

Related literature

For a related compound, see: You *et al.* (2004).



Experimental

Crystal data

$C_{15}H_{15}ClN_2$
M_r = 258.74
Orthorhombic, $P2_12_12_1$
a = 7.7301 (8) Å
b = 12.2016 (18) Å
c = 14.047 (2) Å
V = 1325.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 298 (2) K
0.45 × 0.38 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.888, T_{max} = 0.923
5507 measured reflections
2318 independent reflections
1391 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.105
S = 1.02
2318 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack (1983), 1358 Friedel pairs
Flack parameter: −0.07 (10)

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2690).

References

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Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
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supporting information

Acta Cryst. (2008). E**64**, o2319 [doi:10.1107/S1600536808036386]

2-Chloro-*N*-[4-(dimethylamino)benzylidene]aniline

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S1. Comment

Schiff base compounds have been used as fine chemicals and medical substrates and they are important ligands in coordination chemistry due to their ease of preparation and their ability to be modified both electronically and sterically. In this paper, the structure of the title compound, (I), is reported. The molecular structure of (I) is illustrated in Fig. 1. The bond lengths and angles in the title molecule are similar to the related compound 4-chloro-*N*-[4-(dimethylamino)benzylidene]aniline (You *et al.*, 2004). The 4-(Dimethylamino)benzylidene system is nearly planar to within 0.035 (3) A°. 2-Chlorobenzenamine system is nearly planar to within 0.060 (3) A°. The dihedral angle between these two systems is 67.0 (2) °.

S2. Experimental

A mixture of 4-(dimethylamino)benzaldehyde (0.01 mol) and 2-chlorobenzenamine (0.01 mol) in ethanol (10 ml) was refluxed for 2 h. After cooling, filtration and drying, the title compound was obtained. 10 mg of (I) were dissolved in 15 ml of ethanol, and the solution was kept at room temperature for 5 d. Natural evaporation gave light yellow single crystals of the title compound, suitable for X-ray analysis.

S3. Refinement

H atoms were initially located from difference maps and then refined in a riding model with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

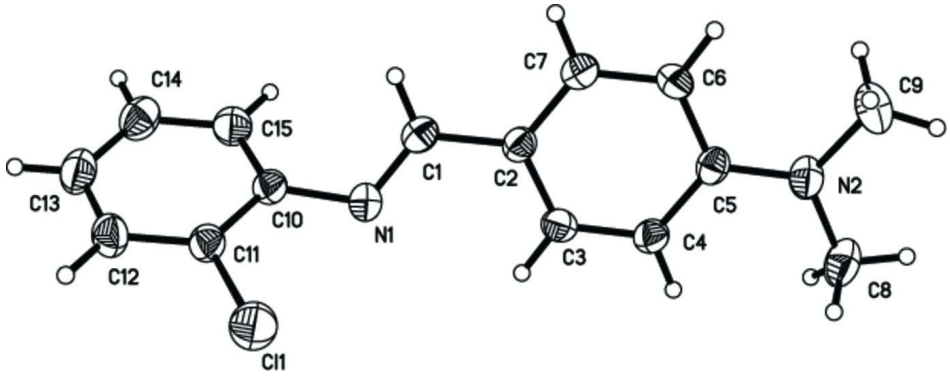

Figure 1

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

2-Chloro-*N*-[4-(dimethylamino)benzylidene]aniline

Crystal data

$C_{15}H_{15}ClN_2$
$M_r = 258.74$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 7.7301$ (8) Å
$b = 12.2016$ (18) Å
$c = 14.047$ (2) Å
$V = 1325.0$ (3) Å^3
$Z = 4$
$F(000) = 544$
$D_x = 1.297$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1182 reflections
$\theta = 2.9$–$20.1°$
$\mu = 0.27$ mm^{-1}
$T = 298$ K
Block, light yellow
0.45 × 0.38 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.888$, $T_{max} = 0.923$
5507 measured reflections
2318 independent reflections
1391 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 13$
$l = -9 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.105$
$S = 1.02$
2318 reflections
165 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Absolute structure: Flack (1983), 1358 Friedel pairs
Absolute structure parameter: −0.07 (10)

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	1.22788 (14)	1.11816 (8)	−0.13149 (7)	0.0753 (4)
N1	0.9918 (4)	0.9322 (2)	−0.09661 (18)	0.0513 (8)
N2	0.8770 (4)	0.7449 (2)	0.32629 (18)	0.0555 (8)

C1	1.0238 (4)	0.8391 (3)	−0.0595 (2)	0.0477 (9)
H1	1.0788	0.7861	−0.0962	0.057*
C2	0.9776 (4)	0.8127 (2)	0.0381 (2)	0.0436 (9)
C3	0.8837 (4)	0.8839 (3)	0.0949 (2)	0.0460 (9)
H3	0.8439	0.9491	0.0686	0.055*
C4	0.8472 (5)	0.8618 (3)	0.1884 (2)	0.0478 (9)
H4	0.7815	0.9112	0.2235	0.057*
C5	0.9077 (4)	0.7656 (3)	0.2319 (2)	0.0441 (9)
C6	0.9993 (5)	0.6920 (3)	0.1744 (2)	0.0498 (9)
H6	1.0379	0.6261	0.2002	0.060*
C7	1.0331 (5)	0.7156 (3)	0.0807 (2)	0.0510 (10)
H7	1.0949	0.6652	0.0445	0.061*
C8	0.7854 (5)	0.8221 (3)	0.3849 (2)	0.0719 (12)
H8A	0.8528	0.8878	0.3913	0.108*
H8B	0.7660	0.7908	0.4467	0.108*
H8C	0.6763	0.8394	0.3559	0.108*
C9	0.9648 (5)	0.6548 (3)	0.3736 (2)	0.0671 (11)
H9A	0.9342	0.5870	0.3432	0.101*
H9B	0.9305	0.6524	0.4393	0.101*
H9C	1.0876	0.6654	0.3696	0.101*
C10	1.0315 (5)	0.9502 (3)	−0.1928 (2)	0.0452 (9)
C11	1.1315 (4)	1.0405 (3)	−0.2197 (2)	0.0481 (9)
C12	1.1594 (5)	1.0664 (3)	−0.3137 (2)	0.0595 (10)
H12	1.2266	1.1269	−0.3298	0.071*
C13	1.0873 (5)	1.0020 (3)	−0.3841 (3)	0.0654 (11)
H13	1.1042	1.0197	−0.4478	0.078*
C14	0.9911 (5)	0.9125 (3)	−0.3600 (3)	0.0661 (11)
H14	0.9451	0.8682	−0.4075	0.079*
C15	0.9612 (5)	0.8869 (3)	−0.2650 (2)	0.0587 (10)
H15	0.8932	0.8266	−0.2497	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0818 (8)	0.0730 (7)	0.0711 (6)	−0.0204 (6)	−0.0003 (6)	−0.0069 (5)
N1	0.060 (2)	0.0516 (17)	0.0423 (16)	−0.0012 (18)	0.0060 (16)	0.0035 (14)
N2	0.053 (2)	0.069 (2)	0.0440 (17)	0.0048 (18)	0.0025 (15)	0.0064 (15)
C1	0.048 (3)	0.050 (2)	0.045 (2)	−0.0014 (19)	−0.0003 (19)	−0.0074 (17)
C2	0.046 (2)	0.0450 (19)	0.0397 (19)	−0.0033 (19)	0.0012 (18)	−0.0035 (16)
C3	0.049 (2)	0.0394 (18)	0.049 (2)	0.0003 (19)	−0.0047 (17)	0.0001 (18)
C4	0.050 (2)	0.048 (2)	0.045 (2)	0.0075 (17)	0.0021 (18)	−0.0034 (17)
C5	0.042 (2)	0.052 (2)	0.0386 (19)	−0.0057 (18)	−0.0011 (17)	−0.0029 (18)
C6	0.057 (3)	0.0407 (19)	0.051 (2)	0.005 (2)	−0.003 (2)	0.0055 (17)
C7	0.056 (3)	0.049 (2)	0.048 (2)	0.0044 (19)	0.0023 (19)	−0.0053 (18)
C8	0.076 (3)	0.095 (3)	0.045 (2)	0.004 (3)	0.012 (2)	−0.002 (2)
C9	0.062 (3)	0.078 (3)	0.061 (2)	−0.007 (2)	−0.004 (2)	0.024 (2)
C10	0.047 (2)	0.046 (2)	0.043 (2)	0.0044 (19)	0.0025 (19)	0.0001 (17)
C11	0.047 (2)	0.050 (2)	0.047 (2)	0.0046 (19)	0.0041 (19)	0.0020 (17)

C12	0.058 (3)	0.063 (2)	0.058 (2)	−0.002 (2)	0.014 (2)	0.009 (2)
C13	0.069 (3)	0.081 (3)	0.046 (2)	0.019 (2)	0.008 (2)	0.008 (2)
C14	0.068 (3)	0.080 (3)	0.050 (2)	0.007 (3)	−0.006 (2)	−0.007 (2)
C15	0.062 (3)	0.057 (2)	0.057 (2)	−0.003 (2)	0.000 (2)	−0.001 (2)

Geometric parameters (Å, º)

Cl1—C11	1.728 (3)	C7—H7	0.9300
N1—C1	1.274 (3)	C8—H8A	0.9600
N1—C10	1.403 (4)	C8—H8B	0.9600
N2—C5	1.371 (4)	C8—H8C	0.9600
N2—C8	1.438 (4)	C9—H9A	0.9600
N2—C9	1.453 (4)	C9—H9B	0.9600
C1—C2	1.453 (4)	C9—H9C	0.9600
C1—H1	0.9300	C10—C15	1.385 (4)
C2—C3	1.385 (4)	C10—C11	1.398 (4)
C2—C7	1.395 (4)	C11—C12	1.376 (4)
C3—C4	1.369 (4)	C12—C13	1.379 (5)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.404 (4)	C13—C14	1.364 (5)
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.400 (4)	C14—C15	1.390 (4)
C6—C7	1.373 (4)	C14—H14	0.9300
C6—H6	0.9300	C15—H15	0.9300
C1—N1—C10	119.4 (3)	N2—C8—H8C	109.5
C5—N2—C8	121.2 (3)	H8A—C8—H8C	109.5
C5—N2—C9	120.1 (3)	H8B—C8—H8C	109.5
C8—N2—C9	117.6 (3)	N2—C9—H9A	109.5
N1—C1—C2	122.5 (3)	N2—C9—H9B	109.5
N1—C1—H1	118.8	H9A—C9—H9B	109.5
C2—C1—H1	118.8	N2—C9—H9C	109.5
C3—C2—C7	116.5 (3)	H9A—C9—H9C	109.5
C3—C2—C1	122.2 (3)	H9B—C9—H9C	109.5
C7—C2—C1	121.2 (3)	C15—C10—C11	117.3 (3)
C4—C3—C2	122.5 (3)	C15—C10—N1	122.2 (3)
C4—C3—H3	118.7	C11—C10—N1	120.2 (3)
C2—C3—H3	118.7	C12—C11—C10	121.8 (3)
C3—C4—C5	120.9 (3)	C12—C11—Cl1	119.7 (3)
C3—C4—H4	119.6	C10—C11—Cl1	118.5 (3)
C5—C4—H4	119.6	C11—C12—C13	119.6 (3)
N2—C5—C6	121.8 (3)	C11—C12—H12	120.2
N2—C5—C4	121.2 (3)	C13—C12—H12	120.2
C6—C5—C4	117.0 (3)	C14—C13—C12	119.9 (3)
C7—C6—C5	121.0 (3)	C14—C13—H13	120.0
C7—C6—H6	119.5	C12—C13—H13	120.0
C5—C6—H6	119.5	C13—C14—C15	120.6 (4)
C6—C7—C2	122.1 (3)	C13—C14—H14	119.7

C6—C7—H7	119.0	C15—C14—H14	119.7
C2—C7—H7	119.0	C10—C15—C14	120.8 (3)
N2—C8—H8A	109.5	C10—C15—H15	119.6
N2—C8—H8B	109.5	C14—C15—H15	119.6
H8A—C8—H8B	109.5		

C10—N1—C1—C2	−176.5 (3)	C3—C2—C7—C6	−1.0 (5)
N1—C1—C2—C3	5.2 (5)	C1—C2—C7—C6	176.2 (3)
N1—C1—C2—C7	−171.9 (3)	C1—N1—C10—C15	58.8 (5)
C7—C2—C3—C4	0.5 (5)	C1—N1—C10—C11	−127.5 (4)
C1—C2—C3—C4	−176.7 (3)	C15—C10—C11—C12	0.1 (5)
C2—C3—C4—C5	1.4 (5)	N1—C10—C11—C12	−173.9 (3)
C8—N2—C5—C6	178.9 (3)	C15—C10—C11—Cl1	−177.6 (2)
C9—N2—C5—C6	10.8 (5)	N1—C10—C11—Cl1	8.4 (4)
C8—N2—C5—C4	−1.6 (5)	C10—C11—C12—C13	0.1 (5)
C9—N2—C5—C4	−169.6 (3)	Cl1—C11—C12—C13	177.7 (3)
C3—C4—C5—N2	177.6 (3)	C11—C12—C13—C14	−1.0 (6)
C3—C4—C5—C6	−2.8 (5)	C12—C13—C14—C15	1.6 (6)
N2—C5—C6—C7	−178.1 (3)	C11—C10—C15—C14	0.6 (5)
C4—C5—C6—C7	2.3 (5)	N1—C10—C15—C14	174.4 (3)
C5—C6—C7—C2	−0.4 (5)	C13—C14—C15—C10	−1.5 (6)