Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Chloroanilino)-1-phenylethanone

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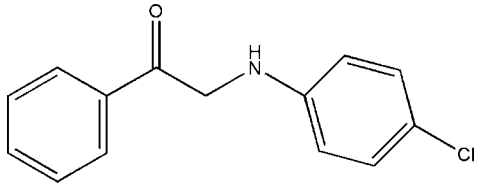
Received 16 February 2011; accepted 20 February 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.061; wR factor = 0.178; data-to-parameter ratio = 12.8.

In the title compound, $C_{14}H_{12}ClNO$, the planes of the two aromatic rings form a dihedral angle of 4.16 (1)°. The molecule is essentially planar with an r.m.s. deviation for all non-H atoms of 0.0372 Å.

Related literature

For a related structure, see: Anilkumar *et al.* (2005).



Experimental

Crystal data

$C_{14}H_{12}ClNO$
M_r = 245.70
Triclinic, $P\overline{1}$
a = 5.6500 (5) Å
b = 7.3921 (8) Å
c = 13.9769 (14) Å
α = 98.588 (2)°
β = 91.095 (1)°
γ = 97.590 (1)°
V = 571.70 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 298 K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.954, T_{max} = 0.969
2924 measured reflections
1971 independent reflections
1238 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.178
S = 1.03
1971 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5121).

References

Anilkumar, H. G., Yathirajan, H. S., Nagaraja, P. & Bolte, M. (2005). *Acta Cryst.* E**61**, o2551–o2552.
Bruker (2005). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o710 [doi:10.1107/S1600536811006404]

2-(4-Chloroanilino)-1-phenylethanone

Xing-Jun Yao and Qian Yuan

S1. Comment

The title compound, $C_{14}H_{12}ClNO$, is often used as catalyst for the polymerization of olefins and as a reactant in organic synthesis. The molecule of (I) is shown in Fig. 1. The bond lengths and angles are normal. The dihedral angle between the two benzene rings is 4.16 (1) °. The molecule is essentially planar, the r.m.s. deviation for all non-H atoms being 0.0372 Å.

S2. Experimental

The title compound was synthesized by the reaction of 4-chloroaniline (1 mmol, 127.6 mg) with 2-bromo-1-phenyl-ethanone (1 mmol, 199.0 mg) in ethanol (20 ml) under reflux conditions (338 K) for 3 h. The solvent was removed and the solid product recrystallized from ethanol. After six days brown crystals were obtained that were suitable for X-ray diffraction study.

S3. Refinement

All H atoms were placed in idealized positions (C—H = 0.93–0.97 Å, N—H = 0.86 Å) and refined as riding atoms. For those bound to C, U_{iso}(H) = 1.2 or 1.5 U_{eq}(C) whereas for those bound to N, U_{iso}(H) = 1.5 U_{eq}(N).

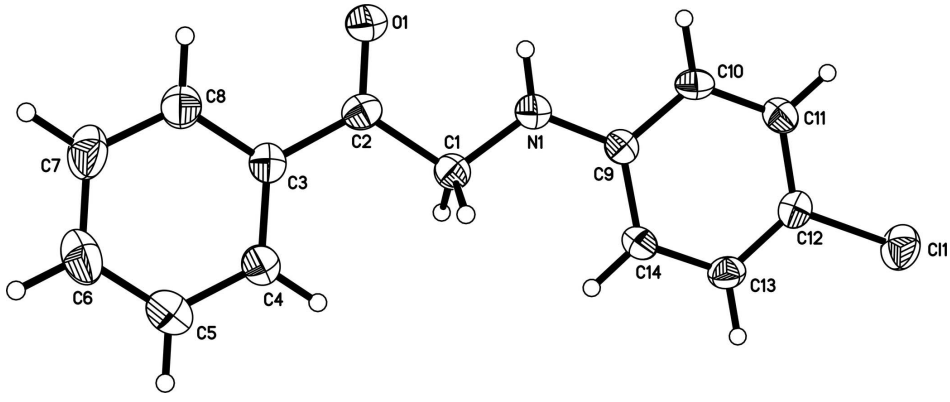


Figure 1

View of the title compound showing the atomic labeling and 30% probability displacement ellipsoids.

2-(4-Chloroanilino)-1-phenylethanone

Crystal data

$C_{14}H_{12}ClNO$	a = 5.6500 (5) Å
M_r = 245.70	b = 7.3921 (8) Å
Triclinic, $P\overline{1}$	c = 13.9769 (14) Å
Hall symbol: -P 1	α = 98.588 (2)°

β = 91.095 (1)°
γ = 97.590 (1)°
V = 571.70 (10) Å^3
Z = 2
F(000) = 256
D_x = 1.427 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 945 reflections
θ = 2.8–24.4°
μ = 0.31 mm^{-1}
T = 298 K
Block, brown
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.954, T_{max} = 0.969

2924 measured reflections
1971 independent reflections
1238 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.1°, θ_{min} = 2.8°
h = −6→6
k = −7→8
l = −13→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.178
S = 1.03
1971 reflections
154 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.0005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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	−0.43122 (17)	0.65041 (13)	0.83483 (7)	0.0650 (4)
N1	0.1395 (5)	0.7998 (4)	0.5053 (2)	0.0506 (8)
H1	0.2852	0.8498	0.5179	0.061*
O1	0.4464 (4)	0.8715 (3)	0.37523 (18)	0.0598 (7)
C1	0.0566 (6)	0.7594 (4)	0.4079 (2)	0.0413 (8)
H1A	−0.0764	0.8266	0.3988	0.050*
H1B	−0.0005	0.6285	0.3920	0.050*
C2	0.2487 (6)	0.8107 (4)	0.3420 (2)	0.0415 (8)

C3	0.1916 (5)	0.7858 (4)	0.2383 (2)	0.0405 (8)
C4	−0.0282 (6)	0.7083 (4)	0.1998 (2)	0.0533 (9)
H4	−0.1467	0.6676	0.2399	0.064*
C5	−0.0752 (7)	0.6900 (5)	0.1028 (3)	0.0706 (12)
H5	−0.2255	0.6365	0.0769	0.085*
C6	0.0965 (8)	0.7495 (5)	0.0435 (3)	0.0737 (12)
H6	0.0634	0.7377	−0.0228	0.088*
C7	0.3167 (8)	0.8265 (5)	0.0813 (3)	0.0700 (12)
H7	0.4348	0.8671	0.0410	0.084*
C8	0.3635 (6)	0.8438 (4)	0.1780 (2)	0.0536 (10)
H8	0.5146	0.8959	0.2036	0.064*
C9	0.0012 (5)	0.7637 (4)	0.5807 (2)	0.0363 (7)
C10	0.0950 (6)	0.8121 (4)	0.6740 (2)	0.0424 (8)
H10	0.2520	0.8695	0.6842	0.051*
C11	−0.0353 (6)	0.7783 (4)	0.7514 (2)	0.0446 (8)
H11	0.0313	0.8129	0.8139	0.054*
C12	−0.2643 (6)	0.6932 (4)	0.7368 (2)	0.0412 (8)
C13	−0.3618 (6)	0.6439 (4)	0.6462 (3)	0.0449 (8)
H13	−0.5185	0.5854	0.6369	0.054*
C14	−0.2313 (6)	0.6795 (4)	0.5679 (2)	0.0445 (8)
H14	−0.3004	0.6466	0.5057	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0711 (7)	0.0651 (7)	0.0599 (7)	0.0021 (5)	0.0184 (5)	0.0176 (5)
N1	0.0441 (17)	0.0607 (19)	0.0426 (18)	−0.0048 (14)	0.0015 (13)	0.0045 (14)
O1	0.0500 (16)	0.0705 (18)	0.0540 (16)	−0.0095 (13)	−0.0005 (13)	0.0097 (13)
C1	0.0433 (19)	0.0377 (19)	0.042 (2)	0.0048 (15)	0.0009 (16)	0.0047 (15)
C2	0.044 (2)	0.0269 (17)	0.053 (2)	0.0003 (15)	0.0030 (17)	0.0074 (14)
C3	0.050 (2)	0.0285 (17)	0.043 (2)	0.0070 (15)	0.0045 (16)	0.0044 (14)
C4	0.054 (2)	0.060 (2)	0.044 (2)	0.0007 (18)	0.0003 (18)	0.0076 (17)
C5	0.069 (3)	0.082 (3)	0.057 (3)	0.003 (2)	−0.011 (2)	0.006 (2)
C6	0.099 (4)	0.077 (3)	0.045 (2)	0.009 (3)	−0.001 (2)	0.015 (2)
C7	0.091 (3)	0.062 (3)	0.057 (3)	−0.003 (2)	0.020 (2)	0.018 (2)
C8	0.063 (2)	0.044 (2)	0.051 (2)	−0.0021 (17)	0.0072 (18)	0.0044 (16)
C9	0.0419 (18)	0.0278 (17)	0.0393 (19)	0.0074 (14)	0.0003 (15)	0.0032 (13)
C10	0.0364 (17)	0.0358 (19)	0.053 (2)	−0.0030 (14)	−0.0031 (16)	0.0059 (15)
C11	0.050 (2)	0.044 (2)	0.0389 (19)	0.0025 (16)	−0.0033 (16)	0.0058 (15)
C12	0.046 (2)	0.0348 (18)	0.045 (2)	0.0078 (15)	0.0086 (16)	0.0104 (14)
C13	0.0369 (18)	0.041 (2)	0.054 (2)	−0.0004 (15)	0.0013 (16)	0.0021 (16)
C14	0.043 (2)	0.048 (2)	0.0388 (19)	0.0025 (16)	−0.0054 (16)	−0.0010 (15)

Geometric parameters (Å, º)

Cl1—C12	1.723 (3)	C6—C7	1.360 (5)
N1—C9	1.361 (4)	C6—H6	0.9300
N1—C1	1.407 (4)	C7—C8	1.356 (5)

N1—H1	0.8600	C7—H7	0.9300
O1—C2	1.204 (4)	C8—H8	0.9300
C1—C2	1.485 (4)	C9—C14	1.374 (4)
C1—H1A	0.9700	C9—C10	1.376 (5)
C1—H1B	0.9700	C10—C11	1.355 (4)
C2—C3	1.457 (4)	C10—H10	0.9300
C3—C4	1.362 (4)	C11—C12	1.359 (5)
C3—C8	1.367 (4)	C11—H11	0.9300
C4—C5	1.360 (4)	C12—C13	1.350 (5)
C4—H4	0.9300	C13—C14	1.370 (4)
C5—C6	1.359 (4)	C13—H13	0.9300
C5—H5	0.9300	C14—H14	0.9300

C9—N1—C1	123.4 (3)	C8—C7—C6	119.8 (3)
C9—N1—H1	118.3	C8—C7—H7	120.1
C1—N1—H1	118.3	C6—C7—H7	120.1
N1—C1—C2	111.2 (3)	C7—C8—C3	120.9 (3)
N1—C1—H1A	109.4	C7—C8—H8	119.6
C2—C1—H1A	109.4	C3—C8—H8	119.6
N1—C1—H1B	109.4	N1—C9—C14	122.6 (3)
C2—C1—H1B	109.4	N1—C9—C10	119.6 (3)
H1A—C1—H1B	108.0	C14—C9—C10	117.8 (3)
O1—C2—C3	121.9 (3)	C11—C10—C9	121.8 (3)
O1—C2—C1	119.4 (3)	C11—C10—H10	119.1
C3—C2—C1	118.7 (3)	C9—C10—H10	119.1
C4—C3—C8	119.0 (3)	C10—C11—C12	119.3 (3)
C4—C3—C2	122.2 (3)	C10—C11—H11	120.3
C8—C3—C2	118.9 (3)	C12—C11—H11	120.3
C5—C4—C3	120.3 (3)	C13—C12—C11	120.4 (3)
C5—C4—H4	119.9	C13—C12—Cl1	120.0 (3)
C3—C4—H4	119.9	C11—C12—Cl1	119.6 (3)
C6—C5—C4	120.3 (4)	C12—C13—C14	120.4 (3)
C6—C5—H5	119.9	C12—C13—H13	119.8
C4—C5—H5	119.9	C14—C13—H13	119.8
C5—C6—C7	119.9 (4)	C13—C14—C9	120.3 (3)
C5—C6—H6	120.1	C13—C14—H14	119.9
C7—C6—H6	120.1	C9—C14—H14	119.9

C9—N1—C1—C2	−178.9 (3)	C2—C3—C8—C7	−178.8 (3)
N1—C1—C2—O1	2.6 (4)	C1—N1—C9—C14	1.8 (5)
N1—C1—C2—C3	−177.4 (2)	C1—N1—C9—C10	−178.3 (3)
O1—C2—C3—C4	176.5 (3)	N1—C9—C10—C11	−179.7 (3)
C1—C2—C3—C4	−3.5 (4)	C14—C9—C10—C11	0.1 (5)
O1—C2—C3—C8	−4.2 (4)	C9—C10—C11—C12	0.5 (5)
C1—C2—C3—C8	175.8 (2)	C10—C11—C12—C13	−0.4 (5)
C8—C3—C4—C5	−0.3 (2)	C10—C11—C12—Cl1	−179.8 (2)
C2—C3—C4—C5	179.0 (3)	C11—C12—C13—C14	−0.2 (5)
C3—C4—C5—C6	−0.2 (2)	Cl1—C12—C13—C14	179.2 (2)

C4—C5—C6—C7	0.5 (4)	C12—C13—C14—C9	0.8 (5)
C5—C6—C7—C8	−0.2 (5)	N1—C9—C14—C13	179.0 (3)
C6—C7—C8—C3	−0.4 (5)	C10—C9—C14—C13	−0.8 (5)
C4—C3—C8—C7	0.6 (4)		