

2-(4-Chloroanilino)-1-phenylethanone

Xing-Jun Yao^{a*} and Qian Yuan^b

^aCollege of Chemistry and Chemical Engineering, Liaocheng University, 252059 Liaocheng, Shandong, People's Republic of China, and ^bGuodian Liaocheng Power Co. Ltd, 252033 Liaocheng, Shandong, People's Republic of China
Correspondence e-mail: y_xingjun01@163.com

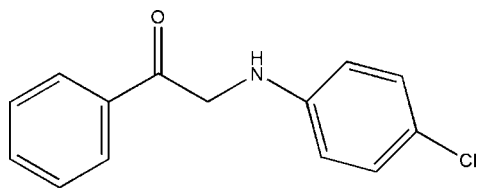
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.061; wR factor = 0.178; data-to-parameter ratio = 12.8.

In the title compound, $\text{C}_{14}\text{H}_{12}\text{ClNO}$, the planes of the two aromatic rings form a dihedral angle of $4.16(1)^\circ$. 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

$\text{C}_{14}\text{H}_{12}\text{ClNO}$
 $M_r = 245.70$
 Triclinic, $P\bar{1}$
 $a = 5.6500(5)$ Å
 $b = 7.3921(8)$ Å
 $c = 13.9769(14)$ Å
 $\alpha = 98.588(2)^\circ$
 $\beta = 91.095(1)^\circ$
 $\gamma = 97.590(1)^\circ$
 $V = 571.70(10)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.31$ mm⁻¹
 $T = 298$ K
 $0.15 \times 0.12 \times 0.10$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

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.* **E61**, o2551–o2552.
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supplementary materials

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X.-J. Yao and Q. Yuan

Comment

The title compound, C₁₄H₁₂ClNO, 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.

Experimental

The title compound was synthesized by the reaction of 4-chloroaniline (1 mmol, 127.6 mg) with 2-bromo-1-phenylethanone (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.

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, $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C})$ whereas for those bound to N, $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{N})$.

Figures

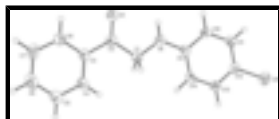


Fig. 1. View of the title compound showing the atomic labeling and 30% probability displacement ellipsoids.

2-(4-Chloroanilino)-1-phenylethanone

Crystal data

C₁₄H₁₂ClNO

$M_r = 245.70$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 5.6500$ (5) Å

$b = 7.3921$ (8) Å

$c = 13.9769$ (14) Å

$\alpha = 98.588$ (2)°

$\beta = 91.095$ (1)°

$\gamma = 97.590$ (1)°

$V = 571.70$ (10) Å³

$Z = 2$

$F(000) = 256$

$D_x = 1.427$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 945 reflections

$\theta = 2.8$ – 24.4 °

$\mu = 0.31$ mm⁻¹

$T = 298$ K

Block, brown

$0.15 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART APEX diffractometer	1971 independent reflections
Radiation source: fine-focus sealed tube graphite	1238 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.032$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$\theta_{\text{max}} = 25.1^\circ$, $\theta_{\text{min}} = 2.8^\circ$
$T_{\text{min}} = 0.954$, $T_{\text{max}} = 0.969$	$h = -6 \rightarrow 6$
2924 measured reflections	$k = -7 \rightarrow 8$
	$l = -13 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.061$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.178$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.0005P]$
1971 reflections	where $P = (F_o^2 + 2F_c^2)/3$
154 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.44 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.36 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	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)

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C14 0.043 (2) 0.048 (2) 0.0388 (19) 0.0025 (16) -0.0054 (16) -0.0010 (15)

Geometric parameters (Å, °)

C11—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—H13	120.0 (3)
C3—C4—H4	119.9	C11—C12—H13	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)

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C1—C2—C3—C8	175.8 (2)	C10—C11—C12—C13	-0.4 (5)
C8—C3—C4—C5	-0.3 (2)	C10—C11—C12—C11	-179.8 (2)
C2—C3—C4—C5	179.0 (3)	C11—C12—C13—C14	-0.2 (5)
C3—C4—C5—C6	-0.2 (2)	C11—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)		

Fig. 1

