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# (2-Chloroanilino)acetophenone

**Haleyur G. Anilkumar,[a] Hemmige S. Yathirajan,[a] Padmarajaiah Nagaraja[a] and Michael Bolte[b]***

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, and [b]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Strasse 11, 60439 Frankfurt/Main, Germany

Correspondence e-mail:
bolte@chemie.uni-frankfurt.de

The title compound, $C_{14}H_{12}ClNO$, is used in perfumery, as a catalyst for the polymerization of olefins, and in organic synthesis, especially as a photosensitizer and in the manufacture of dyes. The molecule is essentially planar and has a *trans* configuration. In this configuration, the Cl and O atoms shield the amino H atom, preventing the formation of an intermolecular hydrogen bond.

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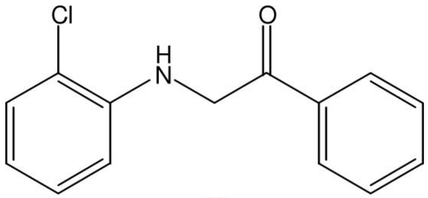
**Key indicators**

Single-crystal X-ray study
*T* = 173 K
Mean *σ*(C–C) = 0.007 Å
*R* factor = 0.050
*wR* factor = 0.146
Data-to-parameter ratio = 7.4

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

## Comment

The title compound, (I), is used in perfumery, as a catalyst for the polymerization of olefins. In organic synthesis, it is especially useful as a photosensitizer and in the manufacture of dyes (Epe *et al.*, 1993; da Silva *et al.*, 2001; Erian *et al.*, 2003).



(I)

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles are normal (Cambridge Crystallographic Database, Version 1.7; *MOGUL* Version 1.0.1; Allen, 2002). The molecule is essentially planar, the r.m.s. deviation for all non-H atoms being 0.023 Å. As a consequence of the *trans* configuration of the N1—C1 bond, the amino H atom is shielded by the Cl and the O atoms. As a result, an intermolecular hydrogen bond cannot be formed.

The crystal packing can be described as a herring-bone pattern (Fig. 2).

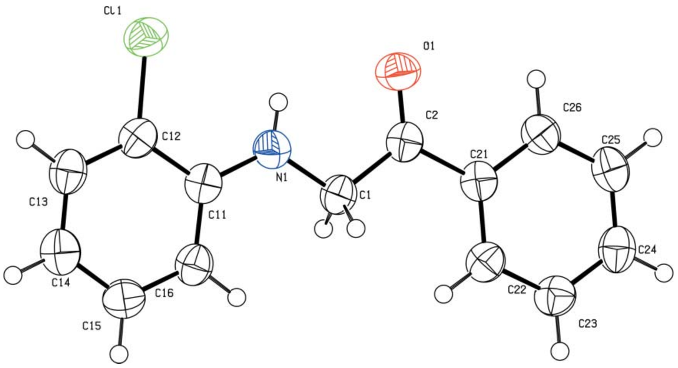


**Figure 1**
Perspective view of the title compound with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

## Experimental

A solution of phenacyl bromide (1.99 g, 10 mmol) in ethanol (5 ml) was added slowly to a solution of 2-chloroaniline (1.05 ml, 10 mmol) dissolved in ethanol (5 ml). The reaction mixture was warmed (333 K) on a water bath for 20 min until the colour of the mixture turned dark brown. Upon cooling the contents to room temperature, a brown precipitate was formed. The precipitate was filtered off and washed with ethanol (3 ml). The compound was recrystallized from ethanol to give pale-brown crystals of the title compound (yield 85%; m.p. 366 K). Analysis calculated: C 68.44, H 4.92, N 5.7%; found: C 68.26, H 4.87, N 5.78%.

### *Crystal data*

$C_{14}H_{12}ClNO$
$M_r = 245.70$
Orthorhombic, $Pca2_1$
$a = 18.363\ (4)$ Å
$b = 5.2852\ (14)$ Å
$c = 12.509\ (2)$ Å
$V = 1214.0\ (5)$ Å$^3$
$Z = 4$
$D_x = 1.344$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 7972 reflections
$\theta = 2.8$–$25.6^\circ$
$\mu = 0.30$ mm$^{-1}$
$T = 173\ (2)$ K
Needle, colourless
0.33 × 0.12 × 0.12 mm

### *Data collection*

Stoe IPDS-II two-circle diffractometer
$\omega$ scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
$T_{\min} = 0.909$, $T_{\max} = 0.945$
3857 measured reflections
1169 independent reflections
986 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.069$
$\theta_{\max} = 25.4^\circ$
$h = -18 \rightarrow 22$
$k = -6 \rightarrow 5$
$l = -15 \rightarrow 15$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.146$
$S = 1.04$
1169 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.096P)^2 + 0.1628P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.30$ e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.044 (8)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cl1—C12 | 1.734 (6) | N1—C11 | 1.372 (7) |
| O1—C2 | 1.210 (6) | N1—C1 | 1.439 (6) |
| C11—N1—C1—C2 | −178.5 (4) | | |

All H atoms were located in a difference map. Those bonded to carbon were positioned geometrically and refined with fixed individual displacement parameters (set to 1.2 times $U_{\rm eq}$ of the parent atom) using a riding model, with C—H = 0.95 and 0.99 Å for aromatic and methylene H atoms, respectively. The H atom bonded to nitrogen was refined freely. Friedel pairs were merged, since the Flack (1983) parameter refined to a meaningless value of −0.4 (2), despite the presence of a Cl atom in the molecule.

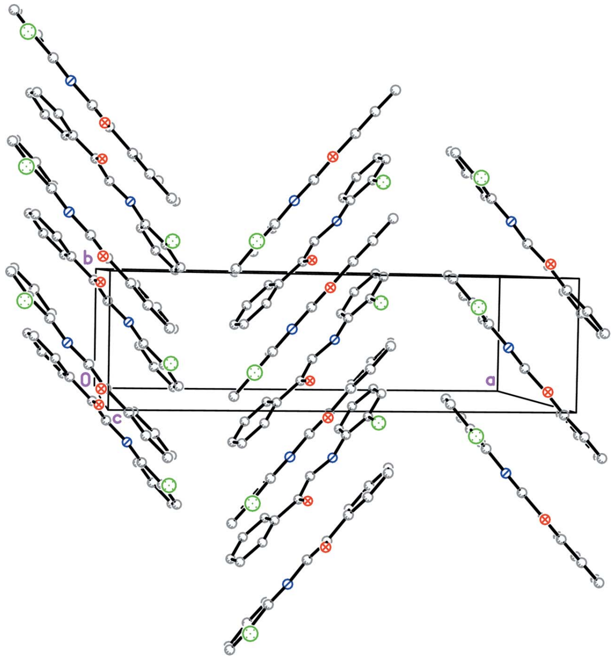


**Figure 2**
Packing diagram of the title compound, viewed approximately on to the *ab* plane. H atoms have been omitted.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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## References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Epe, B., Henzl, H., Adam, W. & Saha-Moller, C. R. (1993). *Nucleic Acids Res.* **21**, 863–869.
Erian, A. W., Sherif, S. M. & Gaber, H. M. (2003). *Molecules*, **8**, 793-865.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Silva, J. F. M. da, Garden, S. J. & Pinto, A. C. (2001). *J. Braz. Chem. Soc.* **12**, 273–324.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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