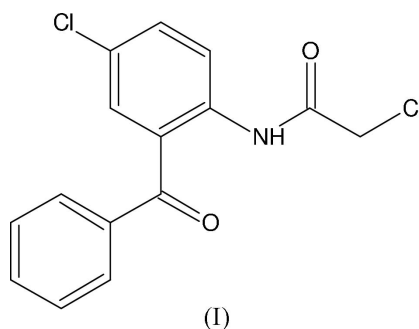


N*-(2-Benzoyl-4-chlorophenyl)-2-chloroacetamide*S. M. Malathy Sony,^a P. Charles,^a
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mnp2004@yahoo.com**Key indicators**Single-crystal X-ray study
T = 293 K
Mean σ (C–C) = 0.004 Å
R factor = 0.063
wR factor = 0.160
Data-to-parameter ratio = 16.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, C₁₅H₁₁Cl₂NO₂, the aromatic rings are twisted by 62.2 (1)° and the chloroacetamide moiety adopts an extended conformation. Intramolecular N–H···O and N–H···Cl interactions stabilize the structure and networks of intermolecular C–H···O hydrogen bonds stabilize the crystal packing in addition to C–H··· π and halogen–halogen interactions.

Comment

Phenylmethanones are a class of compounds having many pharmacological properties. 4-Aminobenzophenones have high anti-inflammatory activity (Ottosen *et al.*, 2003), a benzophenyl cyano derivative acts as a vasorelaxant (Duncan *et al.*, 2004) and the piperidinyl derivative produces analgesia (Colpaert *et al.*, 2004). Certain aminothiophenes of phenylmethanone are positive allosteric regulators of the human A1 adenosine receptor (Figler *et al.*, 2003) and biphenyl derivatives show moderate to high activity against Mycobacterium tuberculosis in *in vitro* studies (de Souza *et al.*, 1999). These factors prompted us to carry out the crystal structure determination of the title compound, (I).



The two benzene rings are planar and twisted by 62.2 (1)°. Atom O8 is displaced by 0.547 (2) Å from the plane of the C1–C6 benzene ring and by 0.969 (2) Å from the plane of the C9–C14 phenyl ring. In this conformation, atom O8 forms an intramolecular N–H···O hydrogen bond of pattern type *S*(6) with atom N15 (Table 2). The chloroacetamide moiety has an extended conformation, as indicated by the torsion angles around the C2–N15 [C1–C2–N15–C16 = 163.7 (3)°] and N15–C16 [C2–N15–C16–C18 = –178.1 (3)°] bonds. The sum of the angles around atom N15 (360°) suggests *sp*²-hybridization.

A one-dimensional C–H···O network of pattern type *C*(5) involving atoms C14 and O8(*x* – 1, *y*, *z*) is found in the crystal structure (Table 2). These chains interact forming dimers through C–H···O hydrogen bonds of type *R*₂²(12) (Bernstein

Received 17 December 2004

Accepted 21 January 2005

Online 12 February 2005

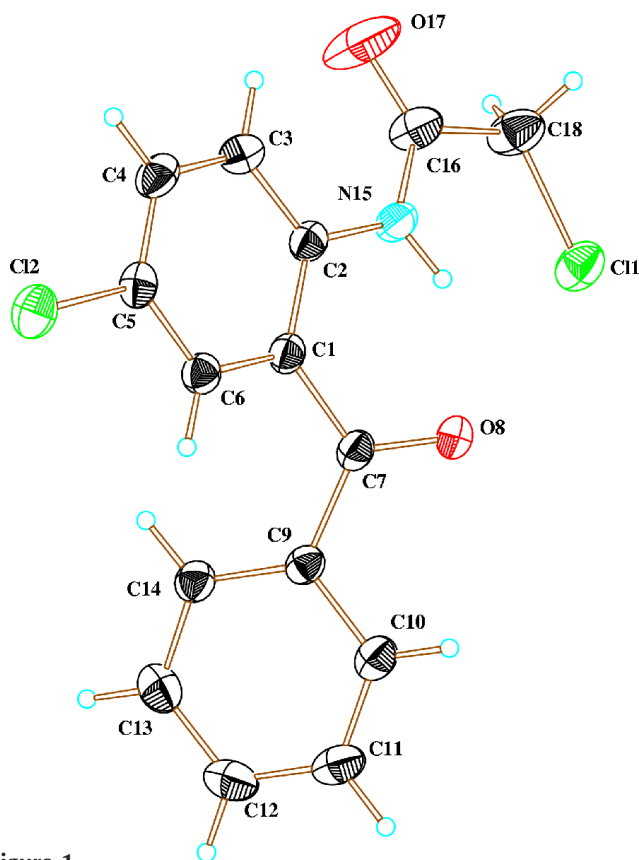


Figure 1
ZORTEP (Zsolnai, 1998) plot of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

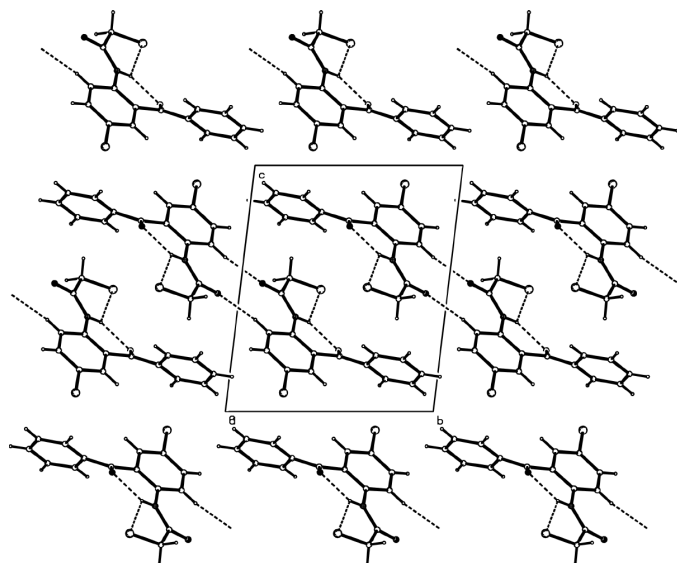


Figure 2
A packing diagram of the crystal structure, viewed down the *a* axis. Dashed lines represent hydrogen bonds.

et al., 1995) occurring between atoms C3 and O17. It is interesting to note that the dimers interact along the *b* axis through halogen–halogen intermolecular contacts [$\text{Cl1}\cdots\text{Cl1}^{\text{iv}}$ = 3.346 (1) Å; symmetry code: (iv) $1 - x, 1 - y, 1 - z$]. A weak C–H $\cdots\pi$ interaction is observed along the *c* axis

involving atom C18 and the symmetry-related C9–C14 phenyl ring at $(-x, 1 - y, 1 - z)$, the distance between H18B and the centroid of the ring being 2.81 Å.

Experimental

Benzoyl chloride (0.01 *M*) with 2-chloro-*N*-(4-chlorophenyl)acetamide (0.01 *M*) was placed in a dry vessel. Finely powdered anhydrous AlCl_3 was added to the reaction mixture and the resulting mixture was stirred vigorously for 10 min. The reaction mixture was placed on a water bath and refluxed for 3 h until HCl was no longer evolved; it was then poured on to crushed ice under warm conditions. Concentrated HCl (100 ml) was added to the mixture, which was then washed with aqueous NaOH solution. The product was separated and recrystallized by slow evaporation of a solution in benzene.

Crystal data

$\text{C}_{15}\text{H}_{11}\text{Cl}_2\text{NO}_2$
 $M_r = 308.15$
Triclinic, $P\bar{1}$
 $a = 5.9991$ (15) Å
 $b = 10.052$ (3) Å
 $c = 12.161$ (3) Å
 $\alpha = 81.391$ (4)°
 $\beta = 76.933$ (4)°
 $\gamma = 81.214$ (4)°
 $V = 700.9$ (3) Å³

$Z = 2$
 $D_x = 1.460$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 7815 reflections
 $\theta = 1.7\text{--}28.1^\circ$
 $\mu = 0.46$ mm⁻¹
 $T = 293$ (2) K
Block, colorless
 $0.30 \times 0.25 \times 0.22$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
Absorption correction: none
7815 measured reflections
3135 independent reflections

2362 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$
 $\theta_{\text{max}} = 28.1^\circ$
 $h = -7 \rightarrow 7$
 $k = -13 \rightarrow 13$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.063$
 $wR(F^2) = 0.160$
 $S = 1.08$
3135 reflections
185 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2 + 0.2942P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

H atoms treated by a mixture of independent and constrained refinement

Table 1

Selected geometric parameters (Å, °) for (I).

Cl1–C18	1.769 (3)	C7–C9	1.487 (4)
Cl2–C5	1.739 (3)	N15–C16	1.355 (4)
C1–C7	1.488 (4)	N15–H15	0.87 (3)
C2–N15	1.400 (3)	C16–O17	1.200 (4)
C7–O8	1.225 (3)	C16–C18	1.507 (4)
O8–C7–C1	120.9 (2)	C2–N15–H15	114.5 (18)
O8–C7–C9	118.2 (2)	O17–C16–N15	125.5 (3)
C1–C7–C9	120.9 (2)	O17–C16–C18	117.3 (3)
C16–N15–C2	128.6 (3)	N15–C16–C18	117.2 (3)
C16–N15–H15	116.9 (18)	C16–C18–C11	116.5 (2)
C6–C1–C7–O8	–149.3 (3)	C1–C7–C9–C14	39.6 (4)
C2–C1–C7–O8	28.8 (4)	C1–C2–N15–C16	163.7 (3)
C6–C1–C7–C9	32.0 (4)	C3–C2–N15–C16	–15.9 (5)
C2–C1–C7–C9	–150.0 (3)	O17–C16–C18–C11	–169.6 (3)
O8–C7–C9–C14	–139.2 (3)	N15–C16–C18–C11	11.6 (4)

Table 2
Hydrogen-bonding geometry (Å, °) for (I).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N15—H15 \cdots C11	0.87 (3)	2.46 (3)	2.954 (2)	117 (2)
N15—H15 \cdots O8	0.87 (3)	1.97 (3)	2.686 (3)	138 (2)
C3—H3 \cdots O17 ⁱ	0.93	2.46	3.236 (4)	141
C14—H14 \cdots O8 ⁱⁱ	0.93	2.69	3.474 (3)	142
C18—H18B \cdots Cg ⁱⁱⁱ	0.97	2.81	3.593 (5)	138

Symmetry codes: (i) $-1-x, 2-y, 1-z$; (ii) $x-1, y, z$; (iii) $-x, 1-y, 1-z$. Cg is the centroid of the C9–C14 ring.

All H atoms bonded to C atoms were positioned geometrically ($C-H = 0.93-0.98$ Å) and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2$ or 1.5 times $U_{eq}(C)$. The H atom on atom N15 was identified in a difference Fourier map and refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003), *ORTEP-3* (Farrugia, 1997) and *ZORTEP* (Zsolnai, 1998); software used to prepare material for publication: *PLATON*.

SMMS acknowledges the Council of Scientific and Industrial Research for financial support. The authors also thank the Department of Science and Technology, India, for data collection on the CCD Facility set up at IISc, Bangalore, India, under the IRHPA–DST programme.

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