N,N-Dibenzoyl-4-chloroaniline

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Key indicators

Single-crystal X-ray study
$T = 183$ K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.131
Data-to-parameter ratio = 13.4

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

In the title compound, $C_{20}H_{14}ClNO_2$, the three aromatic rings are almost orthogonal to one another. The molecular packing is stabilized by weak C—H···π interactions and van der Waals forces.

Comment

Photoinduced electron transfer (PET) reactions of organic compounds have been receiving extensive investigation in recent years (Scheinbaum, 1964; Kavarnos & Turro, 1986; D'Auria *et al.*, 1996). However, PET reactions of nitroaromatic compounds, as electron acceptors, with different types of donors have not been much investigated. As a part of our ongoing research interest in PET reactions of various electron donor–acceptor combinations (Xue *et al.*, 2000, 2001; Zhang *et al.*, 2000), we have recently investigated the photo-induced reactions between nitroaromatic compounds and electron-rich alkenes, such as 1,2-diphenylacetylene. The title compound, (I), a dibenzoylaniline derivative, was isolated from the photoreaction of 4-chloronitrobenzene with 1,2-diphenyl-acetylene.
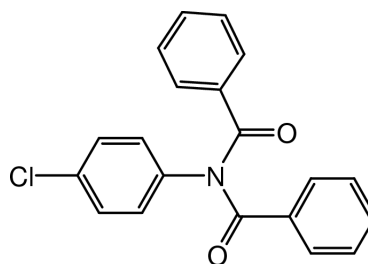
(I)

The bond lengths and angles in (I) have normal values (Allen *et al.*, 1987). The three aromatic rings *A* (C1–C6), *B* (C8–C13) and *C* (C15–C20) are almost orthogonal to one another (Fig. 1). The dihedral angles between *A* and *B*, *A* and *C*, *B* and *C* are 74.7 (1), 89.8 (1) and 81.6 (1)°, respectively. The O1/C7/C8/N1 amide plane is twisted by an angle of 30.2 (1)° from the benzoyl phenyl ring *B*, whereas the other amide plane, O2/C14/C15/N1, is twisted by 19.9 (1)° from ring *C*. The molecular packing in the crystal is stabilized by weak C—H···π interactions involving aromatic rings *B* and *C* (Table 2). In Table 2, C*g*(*B*) and C*g*(*C*) denote the centroids of rings *B* and *C*, respectively.

Experimental

The title compound was prepared by the photo-induced reaction of an acetonitrile solution of 4-chloronitrobenzene with an excess
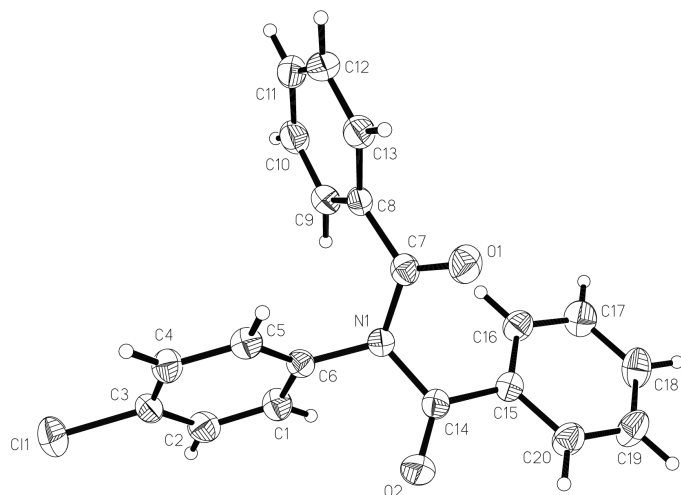
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Figure 1
The structure of the compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

amount of 1,2-diphenylacetylene and was isolated by column chromatography on silica gel. Single crystals of the compound were obtained by slow evaporation from a petroleum ether–ethyl acetate (2:1) solvent system.

Crystal data

$C_{20}H_{14}ClNO_2$	$D_x = 1.337$ Mg m^{-3}
$M_r = 335.77$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3800
$a = 10.2697$ (2) Å	reflections
$b = 9.0419$ (2) Å	$\theta = 2.2$–$29.6°$
$c = 17.9903$ (4) Å	$\mu = 0.24$ mm^{-1}
$\beta = 92.877$ (1)°	$T = 183$ (2) K
$V = 1668.4$ (1) Å^3	Block, colorless
$Z = 4$	$0.46 \times 0.20 \times 0.12$ mm

Data collection

Siemens SMART CCD area-detector diffractometer	2911 independent reflections
	1684 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.087$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -12 \rightarrow 12$
$T_{min} = 0.898$, $T_{max} = 0.972$	$k = -10 \rightarrow 10$
8993 measured reflections	$l = -21 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.131$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.89$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
2911 reflections	$\Delta\rho_{min} = -0.28$ e Å^{-3}
218 parameters	Extinction correction: *SHELXTL*
H-atom parameters constrained	Extinction coefficient: 0.036 (3)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.221 (3)	N1—C6	1.445 (3)
O2—C14	1.207 (3)	C7—C8	1.483 (4)
N1—C7	1.413 (3)	C14—C15	1.490 (4)
N1—C14	1.430 (3)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C1—H1$\cdots Cg(B^i)$	0.93	2.72	3.597 (2)	158
C10—H10$\cdots Cg(C^i)$	0.93	2.85	3.489 (2)	127

Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.

The H atoms were fixed geometrically and were treated as riding on their parent C atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

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