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N-(4-Amino-2-methylphenyl)-4-chlorophthalimide

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Key indicators

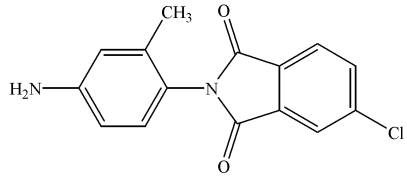
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.147
Data-to-parameter ratio = 20.3

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

In the title compound, $C_{15}H_{11}ClN_2O_2$, the benzene ring is twisted with respect to the phthalimide plane. The molecules are held together by intermolecular O···H—N hydrogen bonds, giving rise to a dimeric structure.

Comment

4-Chlorophthalimides serve as building blocks for the preparation of various 4-aminophthalimides, which have very interesting photophysical properties. The crystal structure of the title compound, (I), was determined to predict its reactivity and other useful properties. The isoindole ring and the benzene ring are almost perpendicular to each other [dihedral angle = 80.47 (9)°]. An intermolecular N2—H2*A*···O2 hydrogen bond connects the molecules into a dimer (Table 2). The packing diagram (Fig. 2) shows that the molecules are packed in layers.



(I)

Experimental

The title compound, (I), was obtained from Aldrich Chemicals. Crystals suitable for X-ray diffraction were grown by slow evaporation of a solution in chloroform.

Crystal data

$C_{15}H_{11}ClN_2O_2$
M_r = 286.71
Monoclinic, $C2/c$
a = 23.624 (11) Å
b = 7.779 (5) Å
c = 14.307 (14) Å
β = 90.72 (6)°
V = 2629 (3) Å^3
Z = 8
D_x = 1.449 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9.4–10.4°
μ = 0.29 mm^{-1}
T = 293 (2) K
Prism, yellow
0.56 × 0.48 × 0.28 mm

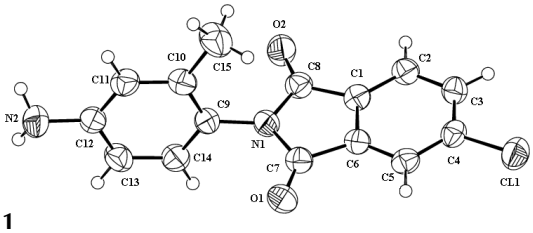


Figure 1
An *ORTEP*-3 (Farrugia, 1997) view of the molecular structure of (I), showing 50% displacement ellipsoids and the atom labelling of all non-H atoms.

Data collection

Enraf–Nonius MACH3 four-circle (CAD-4) diffractometer
Profile data from ω scans
Absorption correction: none
3897 measured reflections
3823 independent reflections
2136 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 30.0°$
$h = 0 \rightarrow 33$
$k = 0 \rightarrow 10$
$l = -20 \rightarrow 20$
3 standard reflections
frequency: 90 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.147$
$S = 1.01$
3823 reflections
188 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 1.5745P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C4	1.742 (3)	N2—C12	1.395 (3)
O2—C8	1.203 (3)	C1—C6	1.386 (3)
N1—C9	1.441 (3)		
C8—N1—C7	111.56 (19)	C5—C4—C3	122.9 (2)
C8—N1—C9	124.25 (19)	C11—C12—N2	120.5 (2)
C9—N1—C8—C1	170.6 (2)	C7—N1—C9—C10	96.5 (3)
C8—N1—C9—C14	106.0 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.90 (3)	2.27 (4)	3.167 (4)	174 (3)

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

H atoms attached to the amino N atom were located in a difference map and refined without any restraint, with the U_{iso} value set at U_{eq}(amino N). All aromatic and methyl H atoms were positioned geometrically and refined using a riding model, with C—H distances of 0.93 and 0.96 Å, respectively, and with U_{iso} values set at $1.2U_{eq}$(aromatic C) and $1.5U_{eq}$(methyl C).

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

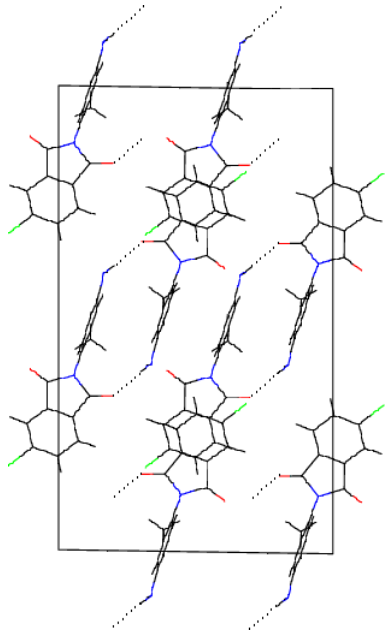


Figure 2
Packing diagram of (I), viewed along the *b* axis, illustrating the intermolecular hydrogen bonding, shown as dashed lines, between the amino and the carbonyl groups.

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