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1-(2,4-Dichlorophenyl)-2-phthalimidoethanone

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Key indicators

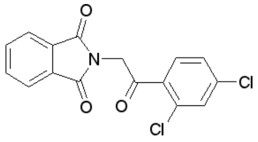
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.111
Data-to-parameter ratio = 13.0

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

The title compound, $C_{16}H_9Cl_2NO_3$, contains two planar ring systems and, in the crystal structure, there are intermolecular π–π stacking interactions between neighboring benzene rings of the phthalimide groups.

Comment

Phthalimides are of particular biological interest and have been reported as antipsychotics (Norman *et al.*, 1996), anti-inflammatory agents (Collin *et al.*, 2001), herbicides and insecticides. In addition, some phthalimide derivatives have been designed as electron acceptors in the formation of supramolecular assemblies (Nilotpal *et al.*, 2003). Some interesting crystal structures involving phthalimide groups have been published (Barrett *et al.*, 1995). The title compound, hitherto unreported, is an intermediate in the preparation of 2-amino-1-(2,4-dichlorophenyl)ethanone, an important primary amine.



(I)

In the molecule of the title compound, (I), all atoms of the phthalimide moiety are coplanar, as are all atoms of the 2,4-dichlorophenyl moiety and the keto group. The dihedral angle between the two ring systems is 88.4 (1)°.

The bond lengths and angles (Table 1) are similar to those in other phthalimides. The C—Cl, C—C, C═O and C—N bond lengths [C1—Cl1 = 1.7371 (18) Å, C3—Cl2 = 1.7243 (19) Å, C7—C8 = 1.521 (3) Å, C7—C4 = 1.496 (2) Å, C10═O2 = 1.208 (2) Å, C9═O3 = 1.205 (2) Å, C9—N1 = 1.388 (2) Å and C10—N1 = 1.394(2) Å] are within normal ranges for phthalimides.

As in other phthalimides (Barrett *et al.*, 1995), there are intermolecular π–π stacking interactions between the benzene rings of adjacent phthalimide moieties in different molecules; the face-to-face separation is 3.367 Å.

Experimental

The title compound was synthesized from potassium phthalimide and 2,2′,4′-trichloroacetophenone by the Gabriel reaction (Gabriel, 1887). Single crystals suitable for X-ray data collection were obtained by slow evaporation of a benzene/toluene (1:2) solution (m.p. 427–428 K). Spectroscopic analysis: IR (KBr, ν cm^{-1}): 1774, 1705, 1108; ^{1}H NMR (CDCl$_3$, δ): 7.95 (*m*, 2H), 7.76 (*m*, 2H), 7.70 (*d*, 1H, J = 8.4 Hz), 7.52 (*s*, 1H), 7.30 (*d*, 1H, J = 8.4 Hz), 5.08 (*s*, 2H).

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Crystal data

$C_{16}H_9Cl_2NO_3$
$M_r = 334.14$
Monoclinic, $P2_1/c$
$a = 12.9211 (5)$ Å
$b = 14.0305 (5)$ Å
$c = 8.0488 (3)$ Å
$\beta = 99.341 (2)°$
$V = 1439.81 (9)$ Å^3
$Z = 4$
$D_x = 1.541$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 684 reflections
$\theta = 2.4$–$21.4°$
$\mu = 0.46$ mm^{-1}
$T = 273 (2)$ K
Block, colorless
0.39 × 0.34 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.840$, $T_{max} = 0.905$
7571 measured reflections
2592 independent reflections
2226 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.2°$
$h = -15 \rightarrow 15$
$k = -16 \rightarrow 16$
$l = -8 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.111$
$S = 1.08$
2592 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.1986P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C1	1.7371 (18)	C4—C5	1.394 (3)
Cl2—C3	1.7243 (19)	C4—C7	1.496 (2)
O1—C7	1.209 (2)	C5—C6	1.379 (3)
O2—C10	1.208 (2)	C7—C8	1.521 (3)
O3—C9	1.205 (2)	C9—C16	1.489 (2)
N1—C9	1.388 (2)	C10—C11	1.485 (2)
N1—C10	1.394 (2)	C11—C12	1.375 (2)
N1—C8	1.438 (2)	C11—C16	1.395 (2)
C1—C2	1.375 (3)	C12—C13	1.381 (3)
C1—C6	1.379 (3)	C13—C14	1.386 (3)
C2—C3	1.385 (3)	C14—C15	1.387 (3)
C3—C4	1.401 (2)	C15—C16	1.378 (2)
C9—N1—C10	112.58 (15)	C10—N1—C8	123.98 (15)
C9—N1—C8	123.10 (15)		

All H atoms were initially located in a difference Fourier map and were placed in geometrically idealized positions. They were constrained to ride on their parent atoms, with Csp^2—H = 0.93 Å, Csp^3—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

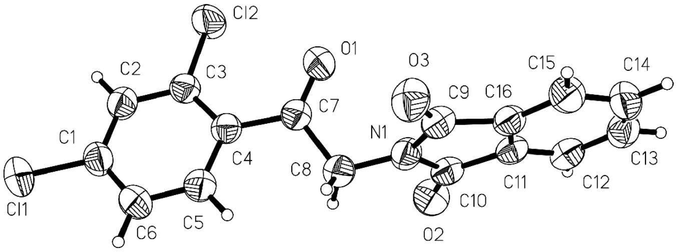

Figure 1
The structure of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 50% probability level.

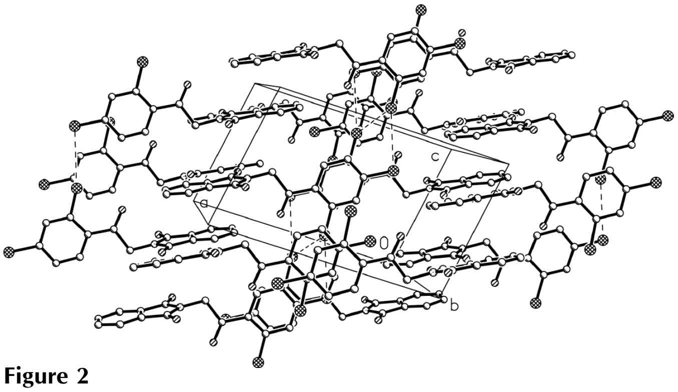

Figure 2
A packing diagram for (I), viewed down the *c* axis. The dashed lines indicate possible weak interactions.

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