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Key indicators

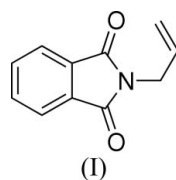
Single-crystal X-ray study
 $T = 100$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.039
 wR factor = 0.095
Data-to-parameter ratio = 11.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.***N*-Allylphthalimide: parallel ribbons of $R(10)$
motifs crosslinked by $\text{C}_{\text{vinyl}}-\text{H}\cdots\text{O}$ bonds**

In the title compound (systematic name: 2-allylisoindoline-1,3-dione), $\text{C}_{11}\text{H}_9\text{NO}_2$, the synperiplanar allyl substituent is orthogonal to the phthalimide ring plane. In the crystal structure, pairwise $\text{C}_{\text{aryl}}-\text{H}\cdots\text{O}=\text{C}$ bonds furnish ribbons of $R(10)$ motifs along the crystallographic b axis. Parallel layers of ribbons are crosslinked by additional $\text{C}_{\text{vinyl}}-\text{H}\cdots\text{O}$ bonds.

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Comment

N-Allylphthalimide (2-allylisoindoline-1,3-dione), (I) is a valuable masked allylamine synthon. Previously reported applications include its hydrocarbonylation en route to β - and γ -amino acid derivatives (Deloglu *et al.*, 1984), a Pd-catalysed approach to substituted 1,4-dienes (Kao *et al.*, 1982) and the synthesis of cinnamylamines *via* a Heck-type arylation procedure (Malek *et al.*, 1982).



We prepared the title compound, (I), in order to examine the influence of the allylic substituent on the photophysical and electrochemical properties of the phthalimide chromophore, which plays an important role as an electron acceptor in photo-induced electron-transfer reactions (Warzecha *et al.*, 2006).

The structure of (I) is shown in Fig. 1; relevant geometric parameters are summarized in Table 1. The allylic substituent at the imide N atom of the planar phthalimide adopts a synperiplanar conformation; a similar orientation has been reported for 1,4-diallylquinoxaline-2,3(1*H*,4*H*)-dione (Mustaphi *et al.*, 2001). In (I), the allyl group is orthogonal to the phthalimide ring plane.

In the crystal structure, each molecule features pairs of $\text{C}_{\text{aryl}}-\text{H}\cdots\text{O}=\text{C}$ bonds (Desiraju, 1991; Steiner, 2002) to its neighbours related by the symmetry operations $(1-x, -\frac{1}{2}+y, \frac{3}{2}-z)$ and $(1-x, \frac{1}{2}+y, \frac{3}{2}-z)$. These interactions lead to infinite ribbons of $R_2^2(10)$ motifs (Etter, 1990; Etter *et al.*, 1990), as illustrated in Fig. 2. The ribbons run in the direction of the crystallographic b axis and are staggered in a parallel fashion; the interplanar distance is 3.290 (1) Å.

The packing is further stabilized by additional interlayer $\text{C}-\text{H}\cdots\text{O}$ bonds perpendicular to the ribbon structure. In every molecule of (I), the carbonyl atom O2 is a bifurcated hydrogen-bond acceptor. In the crosslinking $\text{C}_{\text{vinyl}}-$

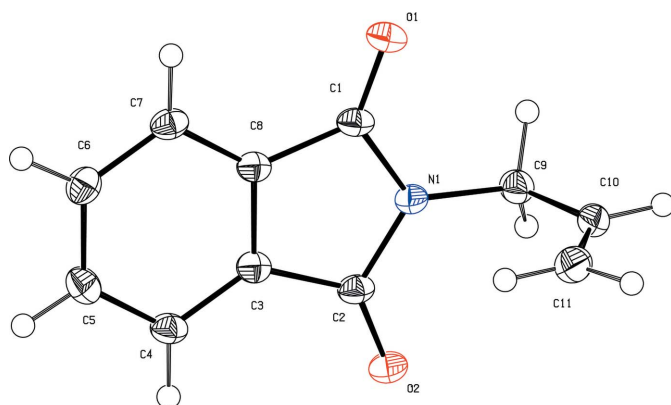


Figure 1
The molecular structure and the atom-labelling scheme for (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as circles of arbitrary size.

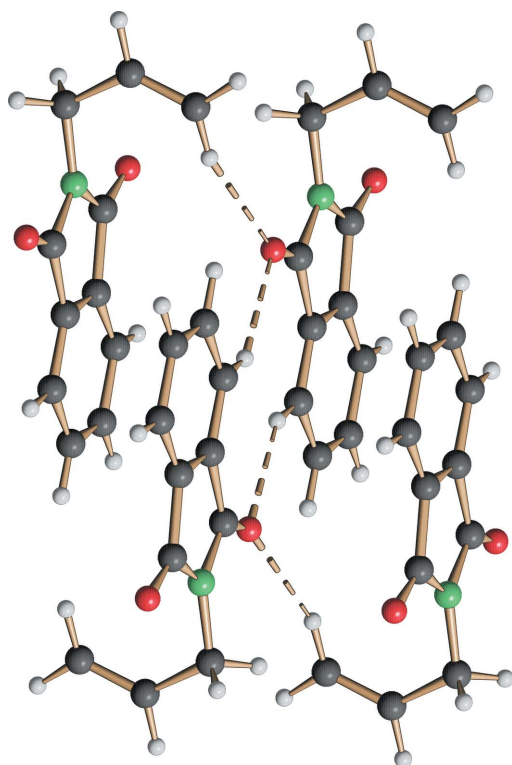


Figure 2
C—H...O hydrogen bonds (dashed lines) in the crystal structure of (I), forming cross-linked ribbons of $R(10)$ motifs.

H...O=C bonds, C11—H11a of a molecule related by $(x, -y + \frac{1}{2}, z - \frac{1}{2})$, *i.e.* from a neighbouring ribbon, serves as a donor group.

Experimental

Phthalic anhydride (Acros) and allylamine (Merck) were used as received. A mixture of 3.7 g (25 mmol) phthalic anhydride and 2.15 g (38 mmol) allylamine was heated to reflux for 3 h. Recrystallization of the resulting crude material from ethanol furnished colourless blocks of the title compound (4.97 g, 20 mmol, 80%; m.p. 345 K) suitable for X-ray diffraction.

Crystal data

$C_{11}H_9NO_2$
 $M_r = 187.19$
Monoclinic, $P2_1/c$
 $a = 9.3914 (3) \text{ \AA}$
 $b = 14.1284 (5) \text{ \AA}$
 $c = 7.1083 (2) \text{ \AA}$
 $\beta = 106.094 (1)^\circ$
 $V = 906.20 (5) \text{ \AA}^3$

$Z = 4$
 $D_x = 1.372 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
 $\mu = 0.10 \text{ mm}^{-1}$
 $T = 100 (2) \text{ K}$
Block, colourless
 $0.55 \times 0.35 \times 0.18 \text{ mm}$

Data collection

Nonius KappaCCD diffractometer
 φ and ω scans
Absorption correction: none
4595 measured reflections
1949 independent reflections
1330 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.052$
 $\theta_{max} = 27.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.095$
 $S = 1.01$
1949 reflections
165 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.005$
 $\Delta\rho_{max} = 0.27 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.18 \text{ e \AA}^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.033 (6)

Table 1

Selected bond and torsion angles ($^\circ$).

N1—C9—C10	113.56 (10)	C11—C10—C9	126.28 (13)
N1—C9—C10—C11	5.3 (2)	C10—C9—N1—C2	−84.85 (15)
C10—C9—N1—C1	93.13 (14)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

D—H...A	D—H	H...A	D...A	D—H...A
C4—H4...O1 ⁱ	0.952 (14)	2.411 (14)	3.3568 (17)	172.0 (10)
C7—H7...O2 ⁱⁱ	0.951 (14)	2.451 (14)	3.3933 (18)	171.2 (10)
C11—H11a...O2 ⁱⁱⁱ	0.963 (14)	2.597 (13)	3.4914 (17)	154.6 (10)

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

H atoms were located in a difference map and their parameters refined freely [range of refined C—H distances = 0.93 (2)–1.00 (2) \AA].

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SCHAKAL99* (Keller, 1999); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *enCIFer* (Allen *et al.*, 2004).

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