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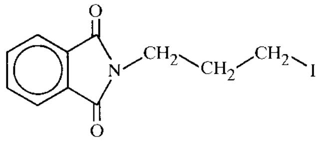
In the molecule of the title compound, $C_{11}H_{10}INO_2$, the phthalimide group is not exactly planar. The dihedral angle between the mean planes of the phthalimide and iodopropyl moieties is 76.6 (2)°. The structure is stabilized by intermolecular C—H···O and C—H···I interactions, and an intermolecular I···O interaction of 3.571 (4) Å, the latter linking the molecules into infinite chains.

Comment

N-Substituted phthalimides containing electron-donor and electron-acceptor fragments simultaneously are an important class of aromatic derivatives used in the synthesis of heat-resistant polymers (Magomedova *et al.*, 1980, 1981), many biological derivatives (Ribar *et al.*, 1974, 1976; Geita *et al.*, 1970; Benetollo *et al.*, 1993) and inclusion compounds (Herbstein & Kaftory, 1981; Kaftory, 1978). Their geometrical features play an important role in the synthesis process, and the X-ray analysis of the title compound, *N*-(3-iodopropyl)-pthalimide, (I), is a further step towards understanding their structural features, the effect of the substituents and the conformation changes in this class of compounds.



(I)

The phthalimide moiety is not exactly planar, the dihedral angle between the mean planes of the two individual rings being 2.8 (2)°. The iodopropyl and phthalimide groups are folded towards each other, making an angle of 76.6 (2)°, which is in good agreement with the corresponding angles found in 4-phthalimidobutanoic acid (67.4 and 65.5°; Feeder & Jones, 1996*a*) and 4-phthalimidoperoxybutanoic acid (82.8°; Feeder & Jones, 1996*b*).

An extensive three-dimensional network of C—H···I as well as C—H···O interactions are present in the structure, involving phenyl as well as propane C—H groups. An interesting feature of the title compound is the short intermolecular O···I contacts. The intermolecular I···O2^{i} distance is found to be 3.571 (4) Å [symmetry code: (i) $x-1, y, z-1$], which is slightly shorter than the O···I van der Waals sum of 3.67 Å (Bondi, 1964). Such oxygen–halogen interactions have been observed in many other structures (Hassel & Romming, 1962, 1967; Cody & Murray-Rust, 1984; Murray-Rust & Motherwell, 1979; Ramasubbu *et al.*, 1986). These O···I interactions link the molecule to form chains along the *c* axis, with the layers of the molecules plane-to-plane stacked in 'centrosymmetric dimers' and the maximum distance between the atoms in each plane being 3.8 Å. The intermolecular angles are C1═O2···I = 105.2 (3)° and C11—I···O2 = 166.0 (2)°, close to the ideal geometry (C═O···I = 120° and *R*—I···O = 180°) which has been proposed for this type of association (Leser & Rabinovich, 1978). Similar interactions have been reported for the structure of *N*,*N*-diiodoformamide (Pritzkow, 1974).

Experimental

The title compound was prepared as follows: 10 g of phthalimide (0.068 mol), 5.6 g of potassium carbonate and aliquat (catalytic amount) were taken in dry acetone and refluxed for 24 h, then 11.22 g of sodium iodide was added and reflux continued for another 12 h. The reaction mixture was filtered and concentrated. The product was recrystallized from ethanol.

Crystal data

$C_{11}H_{10}INO_2$
$M_r = 315.10$
Monoclinic, $P2_1/c$
$a = 7.582$ (1) Å
$b = 19.190$ (3) Å
$c = 8.143$ (1) Å
$\beta = 109.95$ (1)°
$V = 1113.7$ (3) Å^3
$Z = 4$
$D_x = 1.879$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 7$–16°
$\mu = 2.854$ mm^{-1}
$T = 293$ (2) K
Transparent cube, colourless
0.18 × 0.18 × 0.18 mm

Data collection

Siemens *R*3*m*/*V* diffractometer
$\omega/2\theta$ scans
Absorption correction: multi-scan (Sheldrick, 1991)
$T_{\min} = 0.560$, $T_{\max} = 0.589$
2350 measured reflections
2186 independent reflections
1784 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\max} = 26.04°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 22$
$l = -10 \rightarrow 9$
2 standard reflections every 98 reflections intensity decay: ≤1%

Refinement

Refinement on F^2
$R(F) = 0.036$
$wR(F^2) = 0.092$
$S = 1.183$
2186 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0440P)^2 + 1.5252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.36$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

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Table 1
Selected geometric parameters (Å, °).

I—C11	2.143 (6)	O1—C8	1.209 (6)
N—C8	1.390 (6)	O2—C1	1.203 (6)
N—C1	1.396 (6)	C1—C2	1.487 (6)
N—C9	1.471 (6)	C7—C8	1.479 (6)
C8—N—C1	112.0 (4)	O1—C8—N	124.0 (5)
C8—N—C9	122.1 (4)	O1—C8—C7	129.9 (5)
C1—N—C9	125.7 (4)	N—C8—C7	106.1 (4)
O2—C1—N	126.1 (5)	N—C9—C10	112.8 (4)
O2—C1—C2	127.8 (5)	C10—C11—I	112.1 (4)
N—C1—C2	106.1 (4)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O1^{i}	0.96 (1)	2.495 (7)	3.224 (6)	132.7 (2)
C9—H9*B*···O2^{ii}	0.96 (1)	2.773 (6)	3.368 (6)	120.9 (1)
C11—H11*B*···O2^{ii}	0.96 (1)	2.741 (7)	3.463 (7)	132.5 (1)
C4—H4*A*···I^{iii}	0.96 (1)	3.514 (5)	4.260 (5)	136.3 (1)
C5—H5*A*···I^{iv}	0.96 (1)	3.308 (5)	4.192 (5)	153.9 (1)
C6—H6*A*···I^{v}	0.96 (1)	3.241 (6)	4.185 (5)	168.3 (1)
C9—H9*B*···I^{vi}	0.96 (1)	3.211 (5)	3.969 (5)	137.2 (1)
C11—H11*A*···I^{vii}	0.96 (1)	3.793 (5)	4.225 (5)	110.4 (1)

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

H atoms were located from difference Fourier maps, positioned geometrically and included as riding atoms with fixed isotropic displacement parameters in the structure-factor calculations.

Data collection: *P*3 *Diffractometer Program* (Siemens, 1991); cell refinement and data reduction: *SHELXTL-Plus* (Sheldrick, 1991); program(s) used to solve structure: *SHELXTL-Plus*; program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993); software used to prepare material for publication: *SHELXL*93.

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