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N-(2-Fluorophenyl)phthalimide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.037
wR factor = 0.104
Data-to-parameter ratio = 12.9

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

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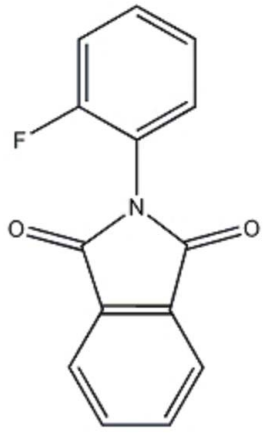
In the title compound, $C_{14}H_8FNO_2$, the dihedral angle between the two planar ring systems is 59.95 (4)°.

Comment

The crystal structure of the title compound, (I), has been determined in order to elucidate the molecular conformation. The dihedral angle between the benzene ring and the phthalimide plane is 59.95 (4)°.



(I)

Experimental

Compound (I) was prepared from phthalic anhydride and 2-fluoroaniline (Barchin *et al.*, 2002). An acetic acid solution of phthalic anhydride (14.8 g, 100 mmol) and 2-fluoroaniline (11.1 g, 100 mmol) was refluxed overnight, and then filtered. The crude product was washed with water three times, and dried. The compound (I) was recrystallized from ethyl acetate (m.p. 465 K).

Crystal data

$C_{14}H_8FNO_2$
M_r = 241.21
Orthorhombic, *Pbca*
a = 11.622 (3) Å
b = 7.8368 (16) Å
c = 24.017 (5) Å
V = 2187.5 (8) Å^3
Z = 8
D_x = 1.465 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 1794 reflections
θ = 2.4–22.5°
μ = 0.11 mm^{-1}
T = 294 (2) K
Prism, white
0.26 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.967, T_{max} = 0.983
11486 measured reflections
2240 independent reflections
1169 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 26.4°
h = −13 → 14
k = −7 → 9
l = −29 → 29

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 0.2748P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.104$	$\Delta\rho_{max} = 0.13$ e Å^{-3}
$S = 0.99$	$\Delta\rho_{min} = -0.12$ e Å^{-3}
2240 reflections	Extinction correction: *SHELXTL*
174 parameters	Extinction coefficient: 0.0218 (14)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

F1—C2	1.307 (2)	C4—C5	1.372 (3)
F1′—C6	1.344 (4)	C7—C8	1.475 (3)
N1—C1	1.426 (2)	C8—C13	1.382 (3)
C1—C2	1.374 (3)	C13—C14	1.489 (3)
C2—C1—N1	120.85 (18)	C10—C11—C12	120.9 (2)
F1—C2—C1	118.73 (19)	O2—C14—N1	125.17 (18)
C1—C2—C3	122.5 (2)	O2—C14—C13	129.19 (19)
F1′—C6—C1	114.4 (2)	N1—C14—C13	105.64 (16)

The F atom is disordered over two ortho positions with refined occupancies of 0.681 (3) and 0.319 (3). All H atoms were initially located in a difference Fourier map. All H atoms were then constrained to an ideal geometry, with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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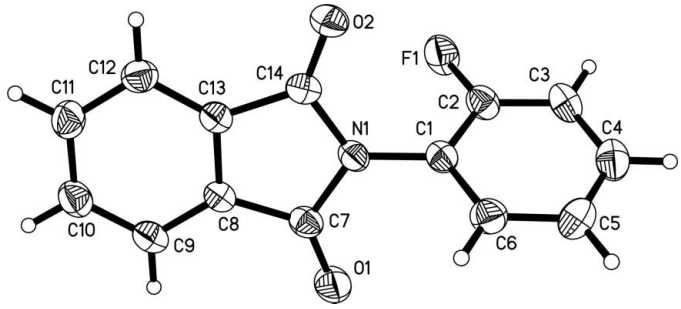

Figure 1
The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

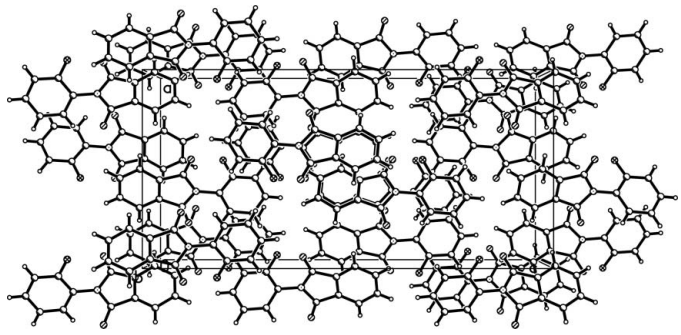

Figure 2
The crystal packing of (I), viewed along the *b* axis.

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