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N-(3-Thienylmethyl)-1,8-naphthalimide

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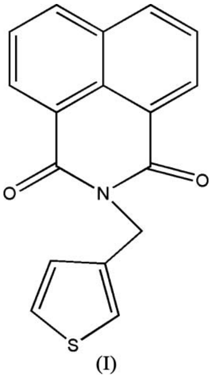
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.097
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, $C_{17}H_{11}NO_2S$, is a new fluorescent 1,8-naphthalimide derivative. The dihedral angle between the thiophene ring and the plane of the naphthalimide is 77.2 (3)°. In the crystal structure, π–π stacking interactions stabilize the structure



(I)

Experimental

1,8-Naphthalimide (1.97 g, 10 mmol) and anhydrous potassium carbonate (1.38 g, 10 mmol) were added to dry DMF (50 ml). The mixture was stirred at room temperature for 30 min and freshly distilled 3-thienyl bromide (0.88 g, 5 mmol) added under nitrogen. The solution was refluxed lightly for 10 h. After cooling, the mixture was poured into water. The precipitate was separated by filtration, washed with water, vacuum dried and chromatograped on silica gel, eluted with dichloromethane to give the title compound. Recrystallization from ethanol afforded pure (I) as colourless crystals (yield: 73%, m.p. 481 K). A translucent single crystal suitable for X-ray

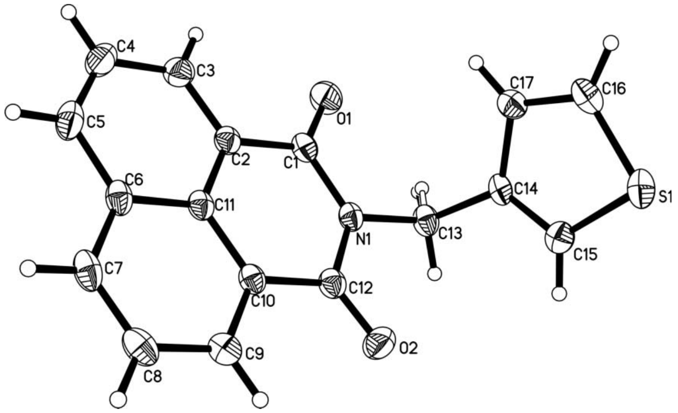


Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Only one major disorder component of the thiophene ring is shown.

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analysis was obtained by slow evaporation of an ethyl acetate–petroleum ether (2:1) solution at room temperature over a period of 3 d. Analysis calculated for $C_{17}H_{11}NO_2S$: C 69.61, H 3.78, N 4.77%; found: C 69.60%, H 3.76%, N 4.78%.

Crystal data

$C_{17}H_{11}NO_2S$
$M_r = 293.33$
Monoclinic, $P2_1/n$
$a = 8.6904$ (15) Å
$b = 13.096$ (2) Å
$c = 11.590$ (2) Å
$\beta = 93.961$ (3)°
$V = 1315.9$ (4) Å^3

$Z = 4$
$D_x = 1.481$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.25$ mm^{-1}
$T = 294$ (2) K
Plate, colourless
0.24 × 0.18 × 0.06 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.943$, $T_{\max} = 0.985$

7239 measured reflections
2687 independent reflections
1822 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.097$
$S = 1.01$
2687 reflections
206 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.1904P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C12	1.399 (2)	C17—C16	1.340 (7)
N1—C1	1.401 (2)	S1—C16	1.712 (8)
N1—C13	1.484 (2)	C14′—C15′	1.327 (9)
C13—C14′	1.502 (9)	C14′—C17′	1.470 (9)
C13—C14	1.505 (6)	C17′—C16′	1.344 (9)
C14—C15	1.326 (6)	C15′—S1′	1.697 (9)
C14—C17	1.462 (7)	S1′—C16′	1.716 (9)
C15—S1	1.695 (6)		
C12—N1—C1	124.94 (14)	C15—C14—C13	123.2 (9)
C12—N1—C13	117.28 (14)	C17—C14—C13	123.9 (9)
C1—N1—C13	117.67 (14)	C15′—C14′—C13	122.8 (13)
N1—C13—C14′	106.1 (8)	C17′—C14′—C13	125.5 (14)
N1—C13—C14	115.4 (5)		

The atoms of the thiophene ring are disordered over two positions; site-occupancy factors were refined and converged to 0.608 (2) and 0.392 (2). The C—S and C═C distances were restrained to C—S = 1.70 (1) Å and C═C = 1.34 (1) Å. All H atoms were initially located in a difference Fourier map and were then constrained to an ideal geometry using a riding model, with C—H = 0.93–0.96 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

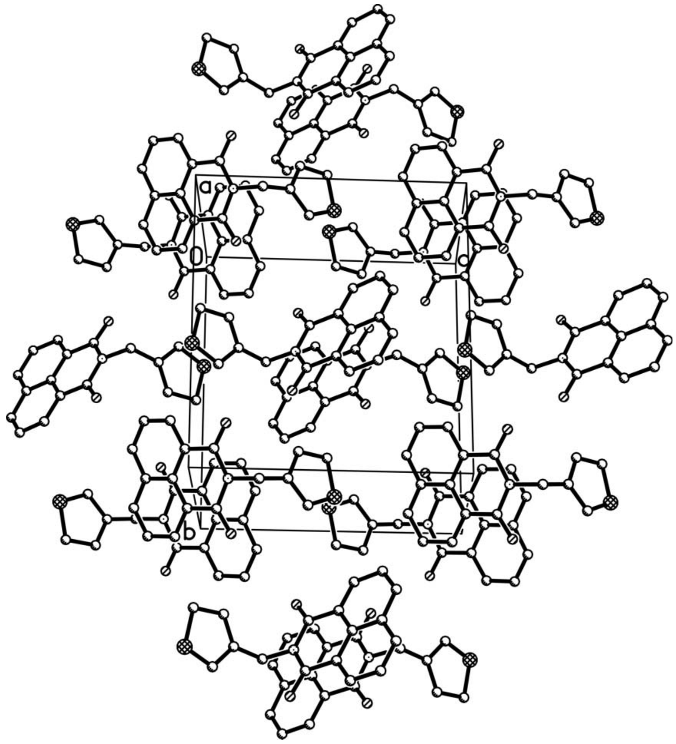

Figure 2
The molecular packing of (I), viewed approximately along the *a* axis. H atoms have been omitted. Only one disorder component is shown.

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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