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N-Ethyl-5-(pyrrol-1-yl)-1,8-naphthalimide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.089
Data-to-parameter ratio = 7.0

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

The title pyrrole derivative, $C_{18}H_{14}N_2O_2$, is a new fluorescent compound, the molecular structure of which is stabilized by a conjugated system.

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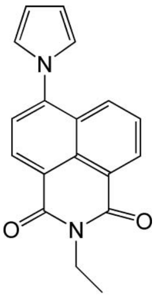
Comment

Pyrrole and its derivatives have been widely investigated because of their easy electrosynthesis, good stability and excellent conductivity in the oxidized state (Grimshaw & Petera, 1989). In the course of our investigation of characterizations of pyrrole derivatives, we determined the crystal structure of the title compound, (I).



(I)

In the pyrrole ring, the bond lengths of 1.359 (4) Å for C13=C14 and 1.360 (3) Å for C15=C16 are significantly longer than the normal C=C bond (1.34 Å; Pauling, 1960), because of the existence of a conjugate system. The dihedral angle between the pyrrole ring and the naphthalimide plane (the maximum deviation is 0.114 (2) Å for atom C8) is 51.08 (7) ° (Fig. 1). In the crystal structure, molecules are linked through weak intermolecular C—H···O hydrogen bonds (Table 2), forming a layer parallel to the (010) plane (Fig. 2).

Experimental

The title fluorescent compound was synthesized from pyrrole and 4-bromo-*N*-ethyl-1,8-naphthalimide using solid–liquid phase-transfer catalysis. Potassium *tert*-isobutylate (1.12 g, 10 mmol) was added to a solution of 25 ml anhydrous tetrahydrofuran and distilled pyrrole (0.67 g, 10 mmol). The mixture was stirred at room temperature for 30 min. 18-Crown-6 ether (0.26 g, 1 mmol) and 4-bromo-*N*-ethylnaphthalimide (1.52 g, 5 mmol) were then added, and the mixture was stirred for 7 h. The solution was poured into ice water and the solid was separated, and then washed with water. The product was purified by passing through a silica-gel column (yield: 75%). A yellow single crystal suitable for X-ray analysis was obtained by slow evaporation at room temperature for 2 d. Analysis calculated for $C_{18}H_{14}N_2O_2$: C 74.47, H 4.86, N 9.65%; found: C 74.45, H 4.83, N 9.66%.

Crystal data

$C_{18}H_{14}N_2O_2$
$M_r = 290.31$
Monoclinic, Cc
$a = 10.257\ (4)$ Å
$b = 23.040\ (8)$ Å
$c = 7.424\ (3)$ Å
$\beta = 127.771\ (4)°$
$V = 1386.7\ (9)$ Å^3
$Z = 4$

$D_x = 1.391$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2040 reflections
$\theta = 2.7–26.3°$
$\mu = 0.09$ mm^{-1}
$T = 294\ (2)$ K
Prism, yellow
0.32 × 0.22 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.962$, $T_{\max} = 0.989$
3830 measured reflections

1401 independent reflections
1240 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 26.3°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 28$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.089$
$S = 1.06$
1401 reflections
200 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 0.2346P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C5	1.392 (4)	C3—C9	1.428 (3)
N1—C1	1.394 (3)	C6—C7	1.402 (3)
N2—C13	1.378 (3)	C7—C8	1.380 (3)
N2—C16	1.385 (3)	C8—C9	1.424 (4)
O1—C1	1.222 (3)	C13—C14	1.359 (4)
C1—C2	1.480 (3)	C14—C15	1.415 (4)
C2—C6	1.374 (3)	C15—C16	1.360 (3)
C2—C3	1.413 (3)		
C5—N1—C1	124.4 (2)	C3—C4—C5	120.1 (2)
C5—N1—C17	117.5 (2)	C7—C8—C9	120.5 (2)
C13—N2—C8	125.8 (2)	C10—C11—C12	120.3 (2)
C16—N2—C8	124.3 (2)	C13—C14—C15	108.1 (2)
C6—C2—C1	120.3 (2)	C15—C16—N2	108.1 (2)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C7—H7$\cdots$O2$^{\rm i}$	0.93	2.51	3.413 (4)	164
C16—H16$\cdots$O1$^{\rm ii}$	0.93	2.46	3.392 (3)	177

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

All H atoms were initially located in a difference Fourier map and then constrained to an ideal geometry, with C—H distances of 0.93–0.97 Å and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). In the absence of significant anomalous scattering effects, Friedel pairs were merged before the final refinement.

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*.

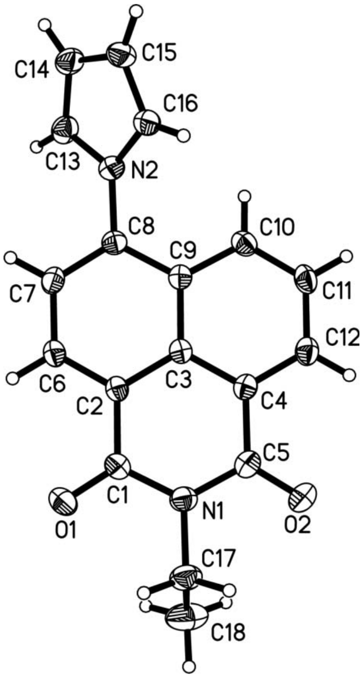


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

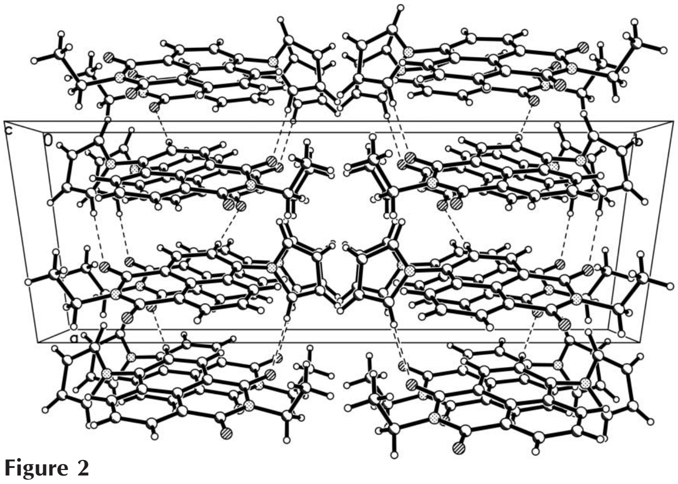


Figure 2
The molecular packing of (I) viewed along the c axis. Dashed lines indicate hydrogen bonds.

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References

Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Grimshaw J. & Petera, S. D. (1989). *J. Electroanal. Chem.* **265**, 335–339.
Pauling, L. (1960). *The Nature of the Chemical Bond*, 3rd ed., p. 239 Ithaca: Cornell University Press.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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