6-Nitro-2-propyl-1*H*-indole

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There are two independent molecules in the asymmetric unit of the title compound, $C_{11}H_{12}N_2O_2$, which differ in the conformation of the propyl substituent. N—H···O, C—H···O and π–π interactions between inversion-related molecules result in a supramolecular assembly.

Comment

Indole compounds can be used as bioactive drugs (Stevenson *et al.*, 2000). Effective hydrogen-bonding interactions are observed in these compounds (Sonar *et al.*, 2004). Recently, we have carried out a large scale synthesis of a series of indole compounds. We report here the structure of the title compound, 6-nitro-2-propyl-1*H*-indole, (I).

(I)
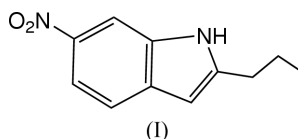
The asymmetric unit of (I) (Fig. 1) consists of pair of molecules (*A* and *B*) held together by C—H···π interactions (Table 2). In one molecule of the enantiomeric pair, the plane through the indole ring system forms a dihedral angle of 55.9 (2)° with the C2/C10—C12 plane [61.4 (3)° in the other molecule]. No significant differences are found between the corresponding bond distances and angles in these two molecules (see Table 1); the bond lengths in (I) are within normal ranges (Allen *et al.*, 1987). All the C—C bond distances in the indole ring system have typical Csp^2—Csp^2 values. The average C—C bond distances within the rings of the two independent indole moieties are 1.400 (3) and 1.398 (3) Å. In the five-membered rings, the intra-ring bond angles range from 106.3 (2) to 109.6 (2)°; the N1—C2 and N1—C9 bond lengths [average 1.375 (3) Å] are well within the range of the
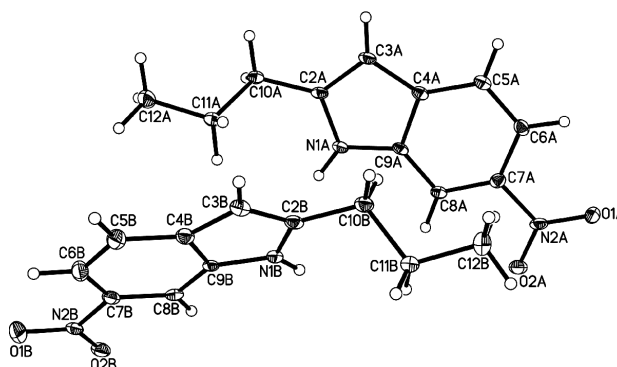

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme for the two independent molecules.
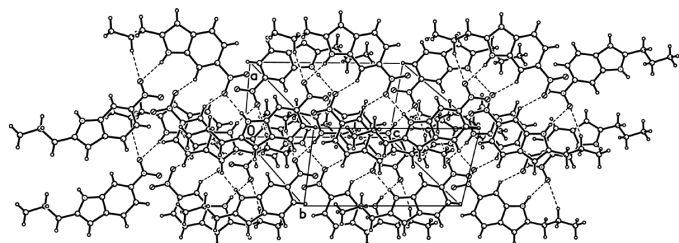
Figure 2
A view of the molecular packing, showing the network of hydrogen bonds as dashed lines.

Table 1
Selected geometric parameters (Å, °).

O1A—N2A	1.235 (2)	O1B—N2B	1.233 (2)
O2A—N2A	1.244 (3)	O2B—N2B	1.236 (2)
N1A—C9A	1.374 (3)	N1B—C2B	1.374 (3)
N1A—C2A	1.377 (3)	N1B—C9B	1.376 (3)
N2A—C7A	1.457 (3)	N2B—C7B	1.446 (3)
C9A—N1A—C2A	109.5 (2)	C2B—N1B—C9B	109.59 (19)
O1A—N2A—O2A	122.39 (19)	O1B—N2B—O2B	121.9 (2)
O1A—N2A—C7A	119.6 (2)	O1B—N2B—C7B	119.4 (2)
O2A—N2A—C7A	118.0 (2)	O2B—N2B—C7B	118.66 (19)
N1A—C2A—C3A	108.7 (2)	C3B—C2B—N1B	109.0 (2)
N1A—C2A—C10A	122.0 (2)	N1B—C2B—C10B	121.9 (2)
C8A—C7A—N2A	117.9 (2)	C8B—C7B—N2B	118.2 (2)
C6A—C7A—N2A	117.7 (2)	C6B—C7B—N2B	118.7 (2)
N1A—C9A—C8A	129.8 (2)	N1B—C9B—C8B	130.1 (2)
N1A—C9A—C4A	107.78 (19)	N1B—C9B—C4B	107.1 (2)

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

Cg1 and Cg2 denote the centroids of the five-membered rings in molecules A and B, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1A—H1$AA\cdots$O2B^{i}	0.88	2.10	2.965 (3)	167
N1B—H1$BA\cdots$O2A^{ii}	0.88	2.07	2.948 (3)	173
C8A—H8$AA\cdots$O2A^{ii}	0.95	2.53	3.203 (3)	128
C11A—H11$B\cdots$O2B^{i}	0.99	2.54	3.448 (3)	153
C10B—H10$D\cdots Cg$1	0.99	2.78	3.726 (3)	161
C11A—H11$A\cdots Cg$2	0.99	2.72	3.346 (3)	121

Symmetry codes: (i) $2-x, 1-y, 2-z$; (ii) $2-x, 1-y, 1-z$.

values normally considered standard for C—N (1.47 Å) and C=N (1.28 Å) bonds, which indicates that the geometry around N1 is normal sp^2 coordination, as expected for π-conjugation of the indole ring (Sonar *et al.*, 2004; Du & Zhao, 2003). The sums of the angles around atoms N2 show planar configurations, with an average N=O bond length of 1.237 (2) Å. In both molecules, the NO₂ fragment is almost coplanar with the indole ring system.

In the crystal structure, inversion-related molecules are linked by N—H$\cdots$O and weak C—H$\cdots$O interactions (Table 2), forming a supramolecular layered architecture (Fig. 2). The crystal packing is further stabilized by π–π stacking interactions between the indole ring systems of molecule A at (x, y, z) and ($1-x, 1-y, 1-z$), with their centroids separated by 3.568 (2) Å.

Experimental

The title compound was synthesized by a modification of the method previously described for the Sonogashira coupling reaction (Rodriguez *et al.*, 2000) of 2-amino-3-nitrophenol and 1-n-pentaacetylene under the catalysis of Pd(PPh₃)₄, CuI and n-Bu₄NI in DMF. Light yellow crystals of (I) were obtained by slow evaporation of an ethanol solution at 277 K.

Crystal data

C₁₁H₁₂N₂O₂	$Z = 4$
$M_r = 204.23$	$D_x = 1.300$ Mg m⁻³
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.229$ (2) Å	Cell parameters from 1705
$b = 11.828$ (3) Å	reflections
$c = 12.088$ (3) Å	$\theta = 2.8$–27.4°
$\alpha = 67.403$ (4)°	$\mu = 0.09$ mm⁻¹
$\beta = 86.940$ (4)°	$T = 100$ (2) K
$\gamma = 74.256$ (4)°	Block, light yellow
$V = 1043.8$ (5) Å³	0.40 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3980 independent reflections
	2616 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.038$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	$\theta_{max} = 26.0°$
	$h = -8 \rightarrow 10$
$T_{min} = 0.68$, $T_{max} = 1.00$	$k = -14 \rightarrow 14$
7051 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.052$	$w = 1/[\sigma^2(F_o^2) + (0.0899P)^2]$
$wR(F^2) = 0.142$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{max} < 0.001$
3980 reflections	$\Delta\rho_{max} = 0.38$ e Å⁻³
271 parameters	$\Delta\rho_{min} = -0.33$ e Å⁻³

H atoms were placed in calculated positions (C—H = 0.95–0.99 Å and N—H = 0.88 Å) and were allowed to ride on their parent atoms. The U_{iso}(H) values were set to $1.5U_{eq}$(parent) for the methyl H atoms and $1.2U_{eq}$(C) for other H atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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