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2-[2-(5-Ethoxy-4-methoxy-2-nitrophenyl)-vinyl]-1*H*-indole

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In the title compound, $C_{19}H_{18}N_2O_4$, the indole moiety is planar and the dihedral angle between it and the substituted phenyl ring is 24.38 (5)°. In the solid state, inversion-related molecules are linked to form N—H···O hydrogen-bonded dimers. The molecular packing is stabilized by C—H···π interactions.

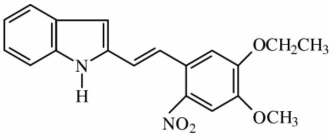
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.061
wR factor = 0.189
Data-to-parameter ratio = 18.0

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

Comment

Substituted indole compounds have gained much importance in past years, since they are present in a number of natural products, many of which are found to possess antibacterial (Okabe & Adachi, 1998), antitumour (Schollmeyer *et al.*, 1995), antidepressant (Grinev *et al.*, 1984), antimicrobial (El-Sayed *et al.*, 1986; Gadaginamath & Patil, 1999) and anti-inflammatory (Rodriguez *et al.*, 1985) activities. The interaction of a phenylsulfonyl indole with calf-thymus DNA has been reported (Sivaraman *et al.*, 1996). Indoles have been proved to display high aldose reductose inhibitory activity (Rajeswaran *et al.*, 1999). 2-Aroylindole derivatives are found to possess high cytotoxicity and are used as antimitotic agents (Mahboobi *et al.*, 2001). The structure determination of the title compound, (I), was undertaken as part of our studies on indole derivatives.



(I)

The bond lengths and angles observed in the indole ring system show normal values. The Csp^2—Csp^2 single bond distances, C2—C10 [1.444 (3) Å] and C11—C12 [1.466 (2) Å], and Csp^2—Csp^2 double-bond distance C10═C11 [1.331 (3) Å] are comparable with the corresponding mean value of 1.455 (11) and 1.330 (14) Å, reported by Allen *et al.* (1987). These bond distances indicate conjugation along C3—C2—C9—C10—C11—C12. The C2—C10 bond is *trans* to C10—C11 [C2—C10—C11—C12 = −178.0 (2)°]. The dihedral angle between the indole plane and substituted phenyl ring is 24.38 (5)°; the N1—C2—C10—C11 and C10—C11—C12—C13 torsion angles are 4.7 (3) and −30.5 (3)°, respectively.

The NO_2 group is twisted away from the attached aromatic ring, with C12—C17—N21—O3 and C16—C17—N21—O4 torsion angles of −25.2 (3) and −24.3 (3)°, respectively. The rotation of the NO_2 group is restricted by a weak C11—H11···O3 interaction. The N—O distances in the nitro group agree with the mean value of 1.217 (11) Å (Allen *et al.*, 1987). The coplanarity of the methoxy carbon with the aromatic ring

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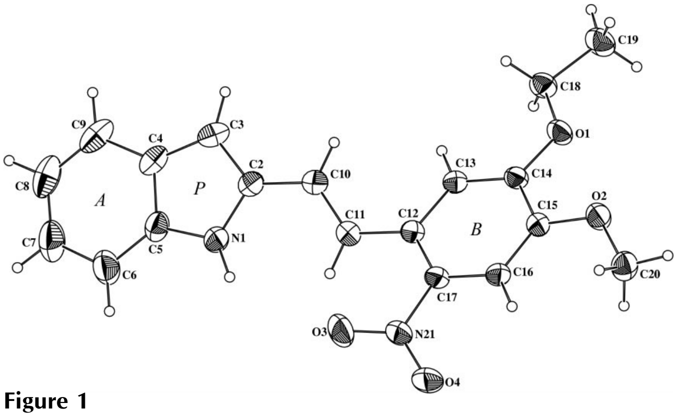

Figure 1
The molecular structure of the title compound, showing 35% probability displacement ellipsoids and the atom-numbering scheme.

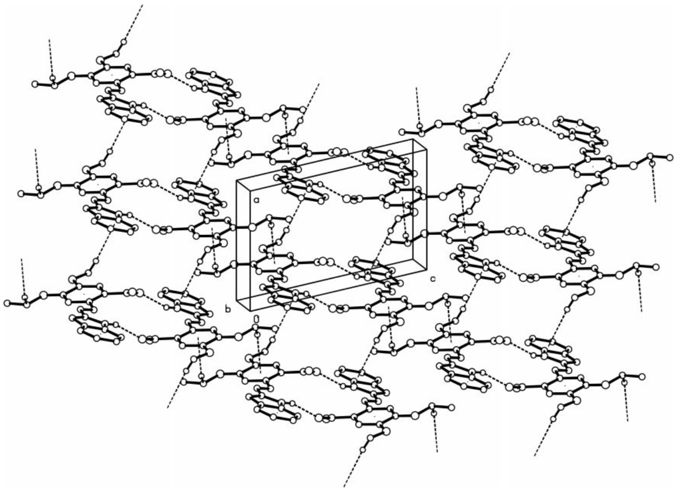

Figure 2
The molecular packing of the title compound, viewed down the *b* axis. For clarity, H atoms not involved in hydrogen bonding have been omitted.

[C20—O2—C15—C16 = 4.9 (3)°] results in H16···H20*A* (2.30 Å) and H16···H20*C* (2.34 Å) short contacts. These contacts cause the widening of O2—C15—C16 [125.3 (2)°] and narrowing of O2—C15—C14 [116.0 (2)°] angles from 120°. Similar features have been reported in structures containing methoxy substituents (Chandrakantha *et al.*, 1990; Wakahara *et al.*, 1972; Falkenberg & Carlström, 1971; Sakaki *et al.*, 1975). The ethoxy group is also coplanar with the aromatic ring with C14—O1—C18—C19 = −179.1 (2) and C18—O1—C14—C13 = −2.8 (3)°; the resultant H13···H18*A* [2.31 Å] and H13···H18*B* [2.36 Å] short contacts cause the widening of C13—C14—O1 [125.5 (2)°] and narrowing of C15—C14—O1 [114.6 (2)°] angles, as reported in the literature (Chandrakantha *et al.*, 1998; Sakaki *et al.*, 1976).

One of the nitro group O atoms, O3, is involved in an intramolecular C11—H11···O3 interaction. The other O atom, O4, is involved in the formation of centrosymmetrically N1—H1···O4(−*x*, 1 − *y*, 1 − *z*) hydrogen-bonded dimers, in the solid state. In addition to these interactions, the molecular packing is also stabilized by C—H···π interactions (Table 2 and Fig. 2).

Experimental

1-(Indol-2-yl)-2-(6-nitroveratryl)ethene (0.68 g, 2 mmol) and sodium ethoxide (0.24 g, 5 mmol) were added to dry THF (40 ml) and refluxed for 6 h. The solution was cooled and poured over crushed ice. The precipitated solid was filtered, washed with water (2 × 5 ml) and dried over $CaCl_2$. The title compound was recrystallized from ethanol.

Crystal data

$C_{19}H_{18}N_2O_4$
$M_r = 338.35$
Triclinic, $P\overline{1}$
$a = 7.5949\ (4)$ Å
$b = 10.0887\ (6)$ Å
$c = 11.5777\ (7)$ Å
$\alpha = 85.298\ (1)°$
$\beta = 76.924\ (1)°$
$\gamma = 86.166\ (1)°$
$V = 860.14\ (9)$ Å^3
$Z = 2$
$D_x = 1.306$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3349 reflections
$\theta = 1.8$–$28.3°$
$\mu = 0.09$ mm^{-1}
$T = 293\ (2)$ K
Plate, red
0.44 × 0.28 × 0.16 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
5992 measured reflections
4109 independent reflections
2759 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\rm max} = 28.3°$
$h = -8 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.189$
$S = 1.02$
4109 reflections
228 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1036P)^2 + 0.0867P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.23$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C14	1.348 (2)	N1—C5	1.374 (2)
O1—C18	1.436 (2)	N1—C2	1.375 (3)
O2—C15	1.357 (2)	C2—C10	1.444 (3)
O2—C20	1.429 (2)	C10—C11	1.331 (3)
O3—N21	1.214 (2)	C11—C12	1.466 (2)
O4—N21	1.215 (2)	C17—N21	1.461 (2)
O1—C14—C13	125.5 (2)	O2—C15—C16	125.3 (2)
O1—C14—C15	114.6 (2)	O2—C15—C14	116.0 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O3	0.93	2.35	2.771 (3)	107
N1—H1···O4$^{\rm i}$	0.86	2.11	2.919 (2)	156
C18—H18*A*···*CgB*$^{\rm ii}$	0.97	2.84	3.714 (2)	150
C20—H20*A*···*CgA*$^{\rm iii}$	0.96	2.81	3.770 (3)	175

Symmetry codes: (i) −*x*, 1 − *y*, 1 − *z*; (ii) 1 − *x*, 1 − *y*, −*z*; (iii) 1 + *x*, *y* − 1, *z*. *CgA* and *CgB* denote the centroids of the rings *A* and *B*, respectively.

The H atoms were geometrically positioned and were treated as riding on the parent atoms, with C—H distances in the range 0.93–0.97 Å and N—H distance of 0.86 Å. Rotating group refinement was used for the methyl groups.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997) and *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXL*97 and *PARST* (Nardelli, 1995).

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