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(*Z*)-3-(1*H*-Indol-3-yl)-2-(4-nitrophenyl)-acrylonitrile

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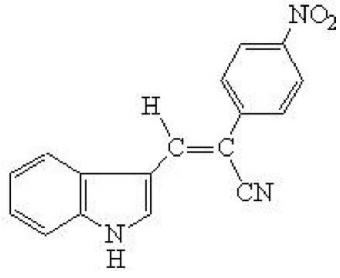
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.127; data-to-parameter ratio = 12.3.

The dihedral angle between the indole and benzene ring systems in the title compound, $C_{17}H_{11}N_3O_2$, is 4.37 (7) °. In the crystal structure, molecules are linked by N—H···N and C—H···O hydrogen bonds, resulting in the formation of layers. These layers are further interconnected through weak offset π–π stacking between the nitrophenyl and indole ring systems, with a centroid-to-centroid distance of 3.766 (2) Å and an interplanar distance of 3.524 Å.

Related literature

For related literature, see: Horton *et al.* (2003); Martino *et al.* (2004); Mei *et al.* (2006); Narayana *et al.* (2005); Rohrer *et al.* (1998); Smith *et al.* (2000).



Experimental

Crystal data

$C_{17}H_{11}N_3O_2$
M_r = 289.29
Monoclinic, $P2_1/c$
a = 7.6534 (7) Å
b = 12.7131 (14) Å
c = 14.3741 (19) Å
β = 92.329 (2)°
V = 1397.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.50 × 0.49 × 0.41 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.955, T_{max} = 0.963
6876 measured reflections
2457 independent reflections
1469 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.127
S = 1.03
2457 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.86	2.28	3.048 (3)	149
C8—H8···O2^{ii}	0.93	2.45	3.346 (3)	161

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 2000) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2224).

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supplementary materials

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(*Z*)-3-(1*H*-Indol-3-yl)-2-(4-nitrophenyl)acrylonitrile

B.-H. Qian, W.-W. Liu and H.-W. Hu

Comment

Owing to the utilization and development of acrylonitrile derivatives in electroluminescence material and medicine domain, the synthesis of such compounds has been a subject of considerable importance in both academic and industrial interest (Mei *et al.*, 2006). Indole and its derivatives are important heterocyclic nitrogen compounds which display a wide range of biological activity. Indole derivatives (Horton *et al.*, 2003) have been used as antitumor (Martino *et al.*, 2004), h5-$HT_{2\ A}$ antagonist (Smith *et al.*, 2000), the Agonists of the Somatostatin Receptor (Rohrer *et al.*, 1998) and also as anti-inflammatory activity (Narayana *et al.*, 2005). We report here the X-ray crystal structure of (*Z*)-2-(4-Nitrophenyl)-3-(3-indole)acrylonitrile, containing indole ring and acrylonitrile structure.

The molecule contains one benzene ring, C12—C17 (denoted A) and one indolizinyl ring C1—C8/N1 (denoted B) (Fig. 1). The dihedral angle between Ring A and B is 4.37 (7)°. The values of C10—C12 [1.477 (3) Å] and C2—C9 [1.433 (3) Å] bond length are shorter than the value for C—C single bond because of conjugation effect. The C9 ═ C10 bond length of 1.350 (3)Å is typical for C=C double bond; it links ring A and B to form a planar structure and extended conjugated system.

The occurrence of N—H···N and C—H···O weak hydrogen bonds results in the formation of layers (Table 1, Fig. 2). These layers are further interconnected through weak offset π···π stacking between nitrophenyl and indolyl rings with a centroid to centroid distance of 3.766 (2)Å and an interplanar distance of 3.524 Å.

Experimental

A solution of 3-indolealdehyde (0.837 g, 5.8 mmol), *p*-nitrophenyl acetonitrile (0.94 g, 5.8 mmol) in anhydrous methyl hydrate(20 ml) was stirred at 317 K for 0.5 h, the mixture of potassium hydroxide (0.325 g, 5.8 mmol)and methyl hydrate(10 ml) was added slowly, the reaction mass was stirred and kept at 317 K until all the substrate had disappeared (monitored by thin-layer chromatography). The resulting mixture was settled, the title compound was collected by filtration and desiccated *in vacuo*, the orange_ red single crystals of (I) suitable for *x*-raycrystallographic analysis were obtained by recrystallization from the mixture of alcohol and acetone.

Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.93 Å and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}(C or N).

Figures

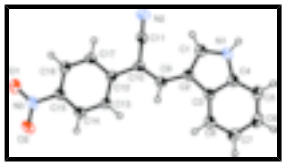

Fig. 1. A view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level and H atoms are represented as small spheres of arbitrary radii.

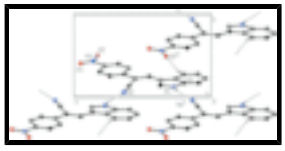

Fig. 2. Partial packing view showing the formation of the layer through N—H···N and C—H···O hydrogen bonds·Hydrogen bonds are indicated by dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) −*x*, *y* − 1:2, −*z* + 3/2; (ii) −*x* + 1, *y* − 1/2, −*z* + 1/2]

(*Z*)-3-(1*H*-Indol-3-yl)2-(4-nitrophenyl)acrylonitrile

Crystal data

$C_{17}H_{11}N_3O_2$	F_{000} = 600
M_r = 289.29	D_x = 1.375 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1699 reflections
a = 7.6534 (7) Å	θ = 2.7–25.8º
b = 12.7131 (14) Å	μ = 0.09 mm^{-1}
c = 14.3741 (19) Å	*T* = 298 (2) K
β = 92.329 (2)º	Block, orange-red
V = 1397.4 (3) Å^3	0.50 × 0.49 × 0.41 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2457 independent reflections
Radiation source: fine-focus sealed tube	1469 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −9→7
T_{min} = 0.955, T_{max} = 0.963	*k* = −15→15
6876 measured reflections	*l* = −15→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained

$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 0.4261P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2457 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.1143 (3)	0.27266 (15)	0.69809 (13)	0.0527 (6)
H1	0.0764	0.2570	0.7518	0.063*
N2	0.0515 (3)	0.63722 (16)	0.65436 (15)	0.0609 (6)
N3	0.4362 (3)	0.85849 (16)	0.25503 (15)	0.0540 (6)
O1	0.4104 (3)	0.95193 (13)	0.27196 (13)	0.0740 (6)
O2	0.5065 (3)	0.82885 (14)	0.18492 (13)	0.0743 (6)
C1	0.1351 (3)	0.37147 (17)	0.66547 (17)	0.0500 (6)
H1A	0.1104	0.4327	0.6979	0.060*
C2	0.1985 (3)	0.36808 (16)	0.57694 (15)	0.0389 (5)
C3	0.2169 (3)	0.25839 (17)	0.55554 (15)	0.0420 (6)
C4	0.1630 (3)	0.20133 (17)	0.63242 (16)	0.0467 (6)
C5	0.1642 (4)	0.09230 (19)	0.6352 (2)	0.0669 (8)
H5	0.1279	0.0554	0.6868	0.080*
C6	0.2209 (5)	0.0420 (2)	0.5588 (2)	0.0973 (12)
H6	0.2240	−0.0311	0.5585	0.117*
C7	0.2747 (5)	0.0964 (2)	0.4807 (2)	0.0980 (12)
H7	0.3126	0.0591	0.4296	0.118*
C8	0.2723 (4)	0.20418 (19)	0.47815 (19)	0.0642 (8)
H8	0.3071	0.2403	0.4257	0.077*
C9	0.2462 (3)	0.45127 (16)	0.51569 (15)	0.0394 (6)
H9	0.3063	0.4293	0.4642	0.047*
C10	0.2191 (3)	0.55609 (16)	0.51992 (14)	0.0373 (5)
C11	0.1267 (3)	0.59945 (17)	0.59569 (16)	0.0425 (6)
C12	0.2753 (3)	0.63297 (15)	0.45012 (15)	0.0371 (5)
C13	0.3487 (3)	0.60254 (17)	0.36748 (15)	0.0456 (6)

H13	0.3632	0.5313	0.3553	0.055*
C14	0.4004 (3)	0.67492 (17)	0.30336 (16)	0.0479 (6)
H14	0.4497	0.6530	0.2485	0.057*
C15	0.3787 (3)	0.77990 (17)	0.32110 (15)	0.0429 (6)
C16	0.3045 (4)	0.81272 (18)	0.40089 (18)	0.0628 (8)
H16	0.2884	0.8841	0.4120	0.075*
C17	0.2539 (4)	0.73956 (18)	0.46449 (17)	0.0576 (7)
H17	0.2039	0.7623	0.5188	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0708 (14)	0.0472 (12)	0.0416 (11)	−0.0023 (11)	0.0192 (10)	0.0083 (10)
N2	0.0813 (16)	0.0562 (13)	0.0468 (13)	0.0071 (12)	0.0221 (12)	−0.0053 (11)
N3	0.0631 (14)	0.0485 (13)	0.0515 (13)	0.0008 (11)	0.0158 (11)	0.0109 (11)
O1	0.1092 (16)	0.0399 (10)	0.0750 (13)	−0.0022 (10)	0.0293 (12)	0.0121 (9)
O2	0.0973 (15)	0.0686 (12)	0.0600 (12)	0.0114 (11)	0.0421 (11)	0.0157 (10)
C1	0.0620 (17)	0.0387 (13)	0.0503 (15)	0.0003 (12)	0.0156 (13)	0.0027 (11)
C2	0.0412 (13)	0.0374 (12)	0.0387 (13)	−0.0001 (10)	0.0091 (10)	0.0026 (10)
C3	0.0464 (14)	0.0368 (12)	0.0437 (13)	−0.0009 (11)	0.0113 (11)	0.0025 (11)
C4	0.0523 (15)	0.0392 (12)	0.0492 (15)	−0.0015 (11)	0.0114 (12)	0.0052 (12)
C5	0.095 (2)	0.0410 (14)	0.0665 (18)	−0.0017 (14)	0.0274 (16)	0.0116 (14)
C6	0.167 (4)	0.0342 (15)	0.094 (2)	−0.0020 (18)	0.055 (2)	0.0029 (16)
C7	0.173 (4)	0.0404 (16)	0.085 (2)	0.0000 (19)	0.065 (2)	−0.0074 (16)
C8	0.095 (2)	0.0415 (14)	0.0583 (17)	−0.0034 (14)	0.0312 (15)	0.0034 (12)
C9	0.0429 (14)	0.0381 (12)	0.0380 (12)	−0.0006 (10)	0.0110 (10)	−0.0003 (10)
C10	0.0430 (13)	0.0362 (12)	0.0331 (12)	−0.0010 (10)	0.0086 (10)	−0.0031 (10)
C11	0.0554 (15)	0.0363 (12)	0.0365 (13)	−0.0020 (11)	0.0095 (12)	0.0027 (11)
C12	0.0404 (13)	0.0328 (11)	0.0388 (13)	−0.0008 (10)	0.0077 (10)	−0.0014 (10)
C13	0.0612 (16)	0.0325 (11)	0.0442 (14)	0.0043 (11)	0.0166 (12)	−0.0027 (11)
C14	0.0586 (16)	0.0444 (13)	0.0419 (14)	0.0081 (12)	0.0189 (12)	0.0034 (11)
C15	0.0498 (14)	0.0385 (12)	0.0413 (13)	0.0013 (11)	0.0135 (11)	0.0078 (11)
C16	0.100 (2)	0.0317 (13)	0.0594 (17)	0.0011 (13)	0.0329 (16)	−0.0001 (12)
C17	0.091 (2)	0.0380 (13)	0.0467 (14)	−0.0012 (13)	0.0338 (14)	−0.0036 (12)

Geometric parameters (Å, °)

N1—C1	1.353 (3)	C7—C8	1.370 (4)
N1—C4	1.371 (3)	C7—H7	0.9300
N1—H1	0.8600	C8—H8	0.9300
N2—C11	1.146 (3)	C9—C10	1.350 (3)
N3—O2	1.221 (2)	C9—H9	0.9300
N3—O1	1.230 (2)	C10—C11	1.433 (3)
N3—C15	1.459 (3)	C10—C12	1.477 (3)
C1—C2	1.381 (3)	C12—C17	1.382 (3)
C1—H1A	0.9300	C12—C13	1.390 (3)
C2—C9	1.433 (3)	C13—C14	1.372 (3)
C2—C3	1.436 (3)	C13—H13	0.9300
C3—C8	1.390 (3)	C14—C15	1.370 (3)

C3—C4	1.398 (3)	C14—H14	0.9300
C4—C5	1.387 (3)	C15—C16	1.366 (3)
C5—C6	1.357 (4)	C16—C17	1.371 (3)
C5—H5	0.9300	C16—H16	0.9300
C6—C7	1.395 (4)	C17—H17	0.9300
C6—H6	0.9300		
C1—N1—C4	109.66 (19)	C7—C8—H8	120.7
C1—N1—H1	125.2	C3—C8—H8	120.7
C4—N1—H1	125.2	C10—C9—C2	131.1 (2)
O2—N3—O1	122.7 (2)	C10—C9—H9	114.5
O2—N3—C15	118.7 (2)	C2—C9—H9	114.5
O1—N3—C15	118.5 (2)	C9—C10—C11	119.7 (2)
N1—C1—C2	109.9 (2)	C9—C10—C12	124.95 (19)
N1—C1—H1A	125.0	C11—C10—C12	115.34 (18)
C2—C1—H1A	125.0	N2—C11—C10	177.6 (2)
C1—C2—C9	130.6 (2)	C17—C12—C13	117.1 (2)
C1—C2—C3	105.60 (19)	C17—C12—C10	120.54 (19)
C9—C2—C3	123.73 (19)	C13—C12—C10	122.38 (19)
C8—C3—C4	119.0 (2)	C14—C13—C12	121.7 (2)
C8—C3—C2	133.5 (2)	C14—C13—H13	119.2
C4—C3—C2	107.44 (19)	C12—C13—H13	119.2
N1—C4—C5	130.0 (2)	C15—C14—C13	119.2 (2)
N1—C4—C3	107.35 (19)	C15—C14—H14	120.4
C5—C4—C3	122.6 (2)	C13—C14—H14	120.4
C6—C5—C4	116.7 (3)	C16—C15—C14	120.8 (2)
C6—C5—H5	121.6	C16—C15—N3	119.0 (2)
C4—C5—H5	121.6	C14—C15—N3	120.3 (2)
C5—C6—C7	122.2 (3)	C15—C16—C17	119.4 (2)
C5—C6—H6	118.9	C15—C16—H16	120.3
C7—C6—H6	118.9	C17—C16—H16	120.3
C8—C7—C6	120.8 (3)	C16—C17—C12	121.8 (2)
C8—C7—H7	119.6	C16—C17—H17	119.1
C6—C7—H7	119.6	C12—C17—H17	119.1
C7—C8—C3	118.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.86	2.28	3.048 (3)	149
C8—H8···O2^{ii}	0.93	2.45	3.346 (3)	161

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+3/2; (ii) −*x*+1, *y*−1/2, −*z*+1/2.

Fig. 1

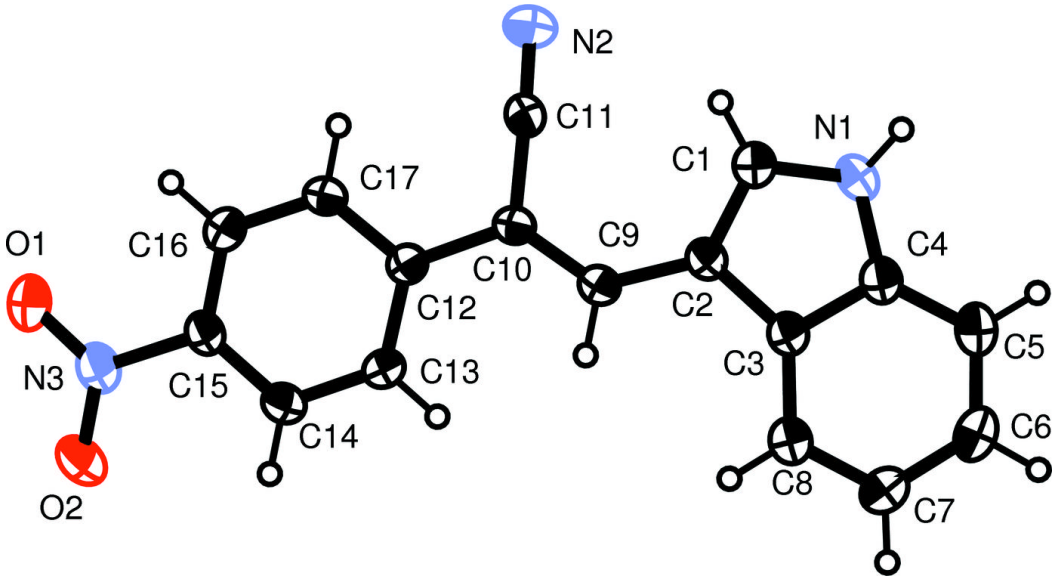
N2
C11
N1
C1
C17
C16
O1
C9
C4
C10
C12
C2
C5
N3
C15
C13
C3
C6
C14
C8
C7
O2

Fig. 2