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1-[(2*E*)-3-Phenylprop-2-en-1-yl]-1*H*-indole-2,3-dione

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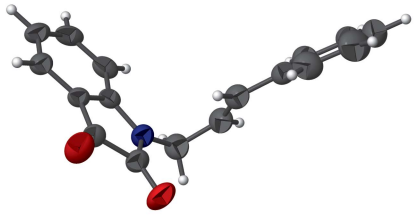
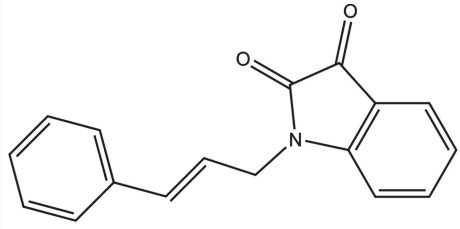
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{17}H_{13}NO_2$, the indole ring is essentially planar (r.m.s. deviation = 0.027 Å) and is oriented at an angle of 69.33 (7)° with respect to the phenyl ring. In the crystal, C—H···O hydrogen bonds link the molecules, forming zigzag chains propagating along the *a*-axis direction. Within the chains there are π–π stacking interactions [centroid–centroid distances = 3.7163 (8) and 3.7162 (8) Å] involving isatin groups of neighbouring molecules.

3D view



Chemical scheme



Structure description

The importance of the indole derivatives in different fields and, in particular, chemistry, biology and pharmacology, has prompted researchers to develop many synthetic methods for their preparation and to find new applications. Isatin (indoline-2,3-dione) has provoked tremendous interest due to its numerous biological and pharmacological activities. The growing importance of substituted isatins in the field of medicinal chemistry as potential chemotherapeutic agents and their implications for prodrug design have been reported (Matesic *et al.*, 2008; Wang *et al.*, 2008; Lane *et al.*, 2001; Patyna *et al.*, 2006). As a continuation of our research devoted to the development of isatin derivatives (Qachchachi *et al.*, 2014*a*,*b*), we report herein on the synthesis and crystal structure of a new indoline-2,3-dione derivative.

In the title compound, Fig. 1, the indole ring system is essentially planar, with an r.m.s. deviation of 0.027 Å, and is oriented at an angle of 69.33 (7) ° with respect to the phenyl ring.

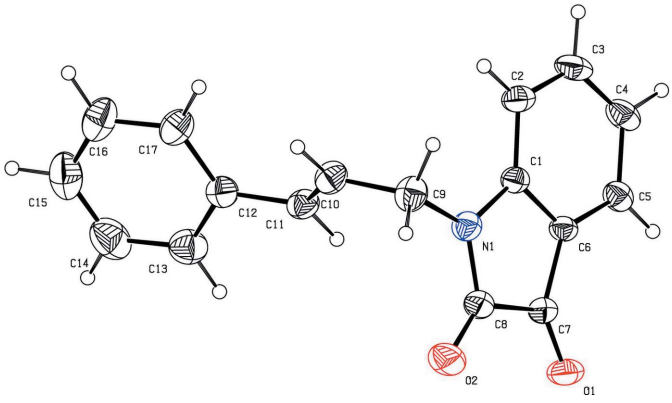


Figure 1
View of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

In the crystal, C—H···O hydrogen bonds link the molecules, and lead to the formation of zigzag chains parallel to the *a* axis (Table 1 and Fig. 2). There are weak π–π stacking [centroid–centroid separations = 3.7163 (8) and 3.7162 (8) Å] interactions present involving the six-membered rings (C1–C6) of the isatin groups of neighbouring molecules in the chain.

Synthesis and crystallization

To a solution of isatin (0.2 g, 1.4 mmol) dissolved in DMF(10 ml) was added potassium carbonate (0.33 g, 2.38 mmol), a catalytic quantity of tetra-*n*-butylammonium bromide (0.04 g, 0.11 mmol) and 3-bromo-1-phenyl-1-propene (0.3 g, 1.5 mmol). The mixture was stirred for 48 h; the reaction was monitored by thin layer chromatography. On completion of the reaction, the mixture was filtered and the solvent removed under vacuum. The solid obtained was recrystallized from ethanol to afford the title compound as orange crystals (yield 86%; m.p. = 413 K).

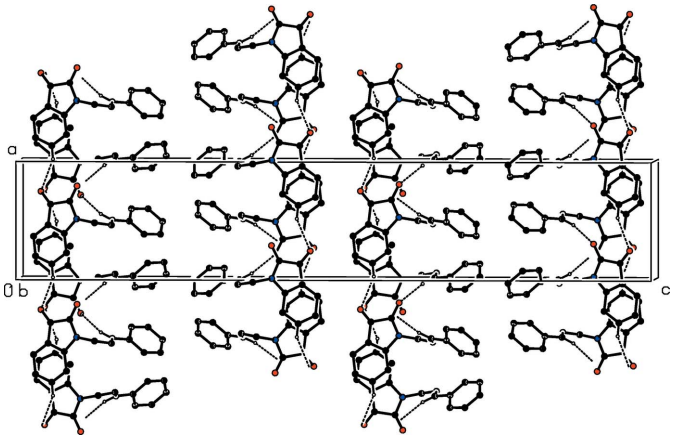


Figure 2
View along the *b* axis of the crystal packing of the title compound. Dashed lines indicate hydrogen bonds (see Table 1).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.947 (17)	2.539 (17)	3.3642 (17)	145.8 (13)
C11—H11···O2^{ii}	0.990 (17)	2.585 (16)	3.5281 (18)	159.2 (13)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{13}NO_2$
M_r	263.28
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, *b*, *c* (Å)	8.2585 (2), 7.2677 (1), 44.4667 (8)
V (Å^3)	2668.90 (9)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.60 × 0.25 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.689, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23607, 4060, 2571
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.127, 1.04
No. of reflections	4060
No. of parameters	233
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.17

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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Crystal data

$C_{17}H_{13}NO_2$
M_r = 263.28
Orthorhombic, *Pbca*
a = 8.2585 (2) Å
b = 7.2677 (1) Å
c = 44.4667 (8) Å
V = 2668.90 (9) Å^3
Z = 8
F(000) = 1104
D_x = 1.310 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 5160 reflections
θ = 2.6–26.3°
μ = 0.09 mm^{-1}
T = 296 K
Prism, orange
0.60 × 0.25 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.689, T_{max} = 0.746
23607 measured reflections
4060 independent reflections
2571 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 30.5°, θ_{min} = 3.1°
h = −11→11
k = −9→10
l = −62→62

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.127
S = 1.04
4060 reflections
233 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.4017P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.60603 (15)	0.50695 (16)	0.42372 (3)	0.0383 (3)
C2	0.77082 (17)	0.51765 (19)	0.42004 (4)	0.0477 (3)
C3	0.86641 (17)	0.4597 (2)	0.44390 (4)	0.0552 (4)
C4	0.80102 (18)	0.3924 (2)	0.47026 (4)	0.0530 (4)
C5	0.63530 (17)	0.37805 (19)	0.47351 (3)	0.0449 (3)
C6	0.53775 (14)	0.43512 (17)	0.44995 (3)	0.0370 (3)
C7	0.36259 (15)	0.43553 (19)	0.44613 (3)	0.0429 (3)
C8	0.33388 (16)	0.5264 (2)	0.41483 (3)	0.0468 (3)
C9	0.5122 (2)	0.6473 (2)	0.37450 (3)	0.0544 (4)
C10	0.53530 (19)	0.5127 (2)	0.34949 (3)	0.0519 (4)
C11	0.49844 (17)	0.3365 (2)	0.35012 (3)	0.0485 (3)
C12	0.51148 (17)	0.2088 (2)	0.32464 (3)	0.0478 (3)
C13	0.4109 (2)	0.0559 (2)	0.32305 (4)	0.0661 (4)
C14	0.4145 (3)	−0.0586 (3)	0.29827 (5)	0.0850 (6)
C15	0.5194 (3)	−0.0252 (3)	0.27504 (5)	0.0813 (6)
C16	0.6240 (3)	0.1213 (3)	0.27678 (4)	0.0736 (5)
C17	0.6202 (2)	0.2371 (2)	0.30122 (3)	0.0593 (4)
H2	0.816 (2)	0.566 (2)	0.4016 (4)	0.063 (5)*
H3	0.980 (2)	0.473 (2)	0.4419 (4)	0.067 (5)*
H4	0.873 (2)	0.355 (2)	0.4865 (4)	0.070 (5)*
H5	0.5861 (17)	0.328 (2)	0.4922 (3)	0.051 (4)*
H10	0.5754 (18)	0.565 (2)	0.3313 (4)	0.061 (4)*
H11	0.4492 (19)	0.285 (2)	0.3686 (4)	0.067 (4)*
H13	0.336 (2)	0.031 (3)	0.3395 (4)	0.089 (6)*
H14	0.342 (3)	−0.158 (3)	0.2971 (5)	0.102 (7)*
H15	0.526 (3)	−0.104 (3)	0.2577 (5)	0.109 (7)*
H16	0.703 (2)	0.141 (3)	0.2607 (4)	0.087 (6)*
H17	0.695 (2)	0.338 (3)	0.3020 (4)	0.074 (5)*
H9A	0.6096 (18)	0.722 (2)	0.3761 (3)	0.051 (4)*
H9B	0.417 (2)	0.725 (2)	0.3698 (4)	0.072 (5)*
N1	0.48280 (13)	0.56265 (16)	0.40353 (2)	0.0449 (3)
O1	0.25550 (12)	0.37772 (17)	0.46186 (2)	0.0631 (3)
O2	0.20406 (12)	0.55750 (18)	0.40305 (2)	0.0681 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0342 (6)	0.0341 (6)	0.0464 (6)	0.0005 (5)	0.0018 (5)	−0.0056 (5)
C2	0.0378 (7)	0.0413 (7)	0.0640 (8)	−0.0042 (6)	0.0111 (6)	−0.0084 (6)
C3	0.0284 (7)	0.0471 (8)	0.0902 (11)	0.0016 (6)	−0.0010 (7)	−0.0154 (7)
C4	0.0394 (7)	0.0489 (8)	0.0707 (9)	0.0074 (6)	−0.0167 (7)	−0.0063 (7)
C5	0.0425 (7)	0.0428 (7)	0.0495 (7)	0.0021 (6)	−0.0061 (6)	−0.0019 (6)
C6	0.0296 (6)	0.0378 (6)	0.0436 (6)	0.0017 (5)	0.0001 (5)	−0.0026 (5)
C7	0.0329 (6)	0.0530 (8)	0.0428 (6)	0.0010 (6)	0.0017 (5)	−0.0018 (6)
C8	0.0369 (7)	0.0580 (8)	0.0456 (7)	0.0039 (6)	−0.0028 (5)	−0.0008 (6)

C9	0.0663 (10)	0.0498 (8)	0.0472 (8)	−0.0036 (8)	0.0045 (7)	0.0080 (6)
C10	0.0582 (9)	0.0546 (9)	0.0429 (7)	−0.0022 (7)	0.0059 (6)	0.0099 (6)
C11	0.0465 (8)	0.0546 (8)	0.0443 (7)	−0.0021 (6)	0.0055 (6)	0.0087 (6)
C12	0.0474 (8)	0.0493 (7)	0.0467 (7)	0.0030 (6)	−0.0022 (6)	0.0079 (6)
C13	0.0619 (10)	0.0590 (10)	0.0775 (11)	−0.0042 (8)	0.0033 (9)	0.0013 (8)
C14	0.0801 (14)	0.0678 (12)	0.1070 (16)	−0.0065 (11)	−0.0166 (13)	−0.0168 (11)
C15	0.1023 (16)	0.0746 (13)	0.0671 (11)	0.0209 (12)	−0.0208 (11)	−0.0169 (10)
C16	0.0950 (14)	0.0745 (12)	0.0512 (9)	0.0218 (11)	0.0070 (9)	0.0037 (8)
C17	0.0674 (10)	0.0591 (10)	0.0512 (8)	0.0032 (8)	0.0089 (7)	0.0060 (7)
N1	0.0429 (6)	0.0507 (6)	0.0410 (5)	0.0005 (5)	0.0012 (4)	0.0036 (5)
O1	0.0364 (5)	0.0969 (9)	0.0560 (6)	−0.0069 (5)	0.0069 (5)	0.0103 (6)
O2	0.0440 (6)	0.0988 (9)	0.0614 (6)	0.0094 (6)	−0.0131 (5)	0.0108 (6)

Geometric parameters (Å, º)

C1—C2	1.3730 (19)	C9—H9A	0.972 (15)
C1—C6	1.3968 (17)	C9—H9B	0.987 (18)
C1—N1	1.4162 (16)	C10—C11	1.316 (2)
C2—C3	1.388 (2)	C10—H10	0.952 (16)
C2—H2	0.967 (17)	C11—C12	1.469 (2)
C3—C4	1.380 (2)	C11—H11	0.990 (16)
C3—H3	0.950 (18)	C12—C13	1.389 (2)
C4—C5	1.380 (2)	C12—C17	1.390 (2)
C4—H4	0.976 (18)	C13—C14	1.381 (3)
C5—C6	1.3850 (18)	C13—H13	0.98 (2)
C5—H5	0.994 (14)	C14—C15	1.370 (3)
C6—C7	1.4565 (17)	C14—H14	0.94 (2)
C7—O1	1.2033 (15)	C15—C16	1.374 (3)
C7—C8	1.5583 (19)	C15—H15	0.96 (2)
C8—O2	1.2146 (16)	C16—C17	1.375 (2)
C8—N1	1.3545 (17)	C16—H16	0.98 (2)
C9—N1	1.4504 (18)	C17—H17	0.959 (19)
C9—C10	1.494 (2)		
C2—C1—C6	121.40 (12)	H9A—C9—H9B	110.9 (13)
C2—C1—N1	128.35 (12)	C11—C10—C9	126.28 (13)
C6—C1—N1	110.25 (11)	C11—C10—H10	119.1 (10)
C1—C2—C3	117.09 (14)	C9—C10—H10	114.5 (10)
C1—C2—H2	120.5 (10)	C10—C11—C12	125.53 (13)
C3—C2—H2	122.4 (10)	C10—C11—H11	118.5 (10)
C4—C3—C2	122.29 (13)	C12—C11—H11	115.7 (10)
C4—C3—H3	120.1 (10)	C13—C12—C17	117.78 (15)
C2—C3—H3	117.5 (10)	C13—C12—C11	120.06 (13)
C3—C4—C5	120.26 (14)	C17—C12—C11	122.14 (14)
C3—C4—H4	119.2 (10)	C14—C13—C12	120.66 (18)
C5—C4—H4	120.5 (10)	C14—C13—H13	120.0 (12)
C4—C5—C6	118.35 (14)	C12—C13—H13	119.3 (12)
C4—C5—H5	121.4 (8)	C15—C14—C13	120.5 (2)

C6—C5—H5	120.3 (8)	C15—C14—H14	119.7 (14)
C5—C6—C1	120.58 (12)	C13—C14—H14	119.7 (14)
C5—C6—C7	131.81 (12)	C14—C15—C16	119.52 (19)
C1—C6—C7	107.61 (11)	C14—C15—H15	122.3 (14)
O1—C7—C6	131.40 (12)	C16—C15—H15	118.1 (14)
O1—C7—C8	123.73 (12)	C15—C16—C17	120.31 (19)
C6—C7—C8	104.85 (10)	C15—C16—H16	119.7 (12)
O2—C8—N1	127.24 (13)	C17—C16—H16	120.0 (12)
O2—C8—C7	126.76 (13)	C16—C17—C12	121.11 (18)
N1—C8—C7	106.00 (10)	C16—C17—H17	118.9 (11)
N1—C9—C10	113.96 (13)	C12—C17—H17	119.9 (11)
N1—C9—H9A	107.9 (8)	C8—N1—C1	111.20 (10)
C10—C9—H9A	108.3 (8)	C8—N1—C9	124.38 (12)
N1—C9—H9B	107.2 (9)	C1—N1—C9	124.42 (12)
C10—C9—H9B	108.5 (10)		

C6—C1—C2—C3	−2.10 (19)	C10—C11—C12—C13	−152.41 (16)
N1—C1—C2—C3	177.52 (12)	C10—C11—C12—C17	26.2 (2)
C1—C2—C3—C4	0.6 (2)	C17—C12—C13—C14	−3.0 (2)
C2—C3—C4—C5	1.0 (2)	C11—C12—C13—C14	175.72 (16)
C3—C4—C5—C6	−0.9 (2)	C12—C13—C14—C15	1.2 (3)
C4—C5—C6—C1	−0.60 (19)	C13—C14—C15—C16	1.4 (3)
C4—C5—C6—C7	178.91 (13)	C14—C15—C16—C17	−2.0 (3)
C2—C1—C6—C5	2.17 (19)	C15—C16—C17—C12	0.2 (3)
N1—C1—C6—C5	−177.51 (11)	C13—C12—C17—C16	2.3 (2)
C2—C1—C6—C7	−177.44 (12)	C11—C12—C17—C16	−176.36 (15)
N1—C1—C6—C7	2.88 (14)	O2—C8—N1—C1	−179.96 (15)
C5—C6—C7—O1	−4.3 (3)	C7—C8—N1—C1	−0.20 (15)
C1—C6—C7—O1	175.27 (15)	O2—C8—N1—C9	0.0 (2)
C5—C6—C7—C8	177.60 (13)	C7—C8—N1—C9	179.73 (12)
C1—C6—C7—C8	−2.84 (14)	C2—C1—N1—C8	178.67 (13)
O1—C7—C8—O2	3.3 (2)	C6—C1—N1—C8	−1.67 (15)
C6—C7—C8—O2	−178.36 (14)	C2—C1—N1—C9	−1.3 (2)
O1—C7—C8—N1	−176.42 (13)	C6—C1—N1—C9	178.39 (12)
C6—C7—C8—N1	1.88 (14)	C10—C9—N1—C8	−92.71 (18)
N1—C9—C10—C11	15.3 (2)	C10—C9—N1—C1	87.21 (18)
C9—C10—C11—C12	175.49 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.947 (17)	2.539 (17)	3.3642 (17)	145.8 (13)
C11—H11···O2^{ii}	0.990 (17)	2.585 (16)	3.5281 (18)	159.2 (13)

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