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3-(1*H*-Indol-3-yl)-2-benzofuran-1(3*H*)-one

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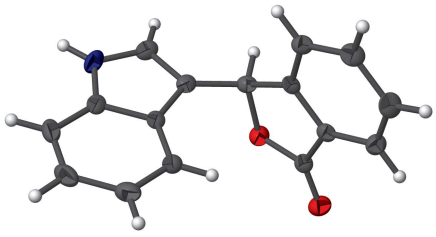
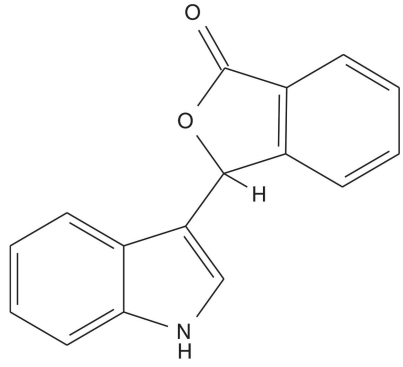
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{11}NO_2$, the benzofuran and indole ring systems are nearly orthogonal, subtending a dihedral angle of 86.55 (4)°. The crystal structure features an N—H···O hydrogen bond, which leads to the formation of chains propagating along the *a*-axis direction.

3D view



Chemical scheme



Structure description

The indole subunit is widely observed in a plethora of natural and synthetic compounds characterized by a variety of biological and pharmacological activities (Mahboobi *et al.*, 2006). Indole derivatives form the basis of a range of pharmaceuticals and a high level of activity continues in the search for new indole-based medicinal agents (Anil Kumar *et al.*, 2016*a*). In view of the broad spectrum of applications associated with indoles and as a part of our ongoing work on such molecules (Anil Kumar *et al.*, 2016*b*), we report herein the synthesis and crystal structure of the title compound.

The structure of the molecule is shown in Fig. 1. The dihedral angle value of 86.55 (4)° between the planes of the benzofuran and indole ring systems indicates that they are nearly orthogonal to one another. In the crystal, molecules are linked *via* N—H···O hydrogen bonds, forming chains propagating along the *a*-axis direction (Table 1, Fig. 2).

Synthesis and crystallization

The synthesis of the title compound was accomplished by condensation reaction between commercially available indole and 2-formylbenzoic acid in glacial acetic acid at room

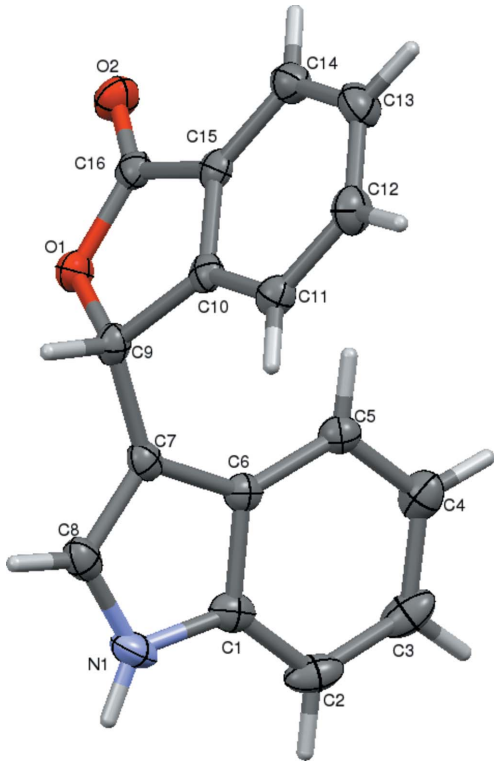


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for the non-H atoms are drawn at the 50% probability level.

temperature for 4–6 h. The resultant crude product was purified by recrystallization by using methanol as solvent to get colorless crystals. Yield: 83%, m.p. 174–176 °C.

Refinement

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

Acknowledgements

The authors are grateful to the Institution of Excellence, Vijnana Bhavana, University of Mysore, India, for providing the single-crystal X-ray diffractometer facility. RAK thanks UGC for financial assistance from BSR fellowship.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.07	2.8398 (16)	149

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{11}NO_2$
M_r	249.26
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, b, c (Å)	16.522 (3), 7.6439 (14), 19.331 (4)
V (Å^3)	2441.4 (8)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.73
Crystal size (mm)	0.30 × 0.28 × 0.25
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.811, 0.839
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11928, 1999, 1970
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.585
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.086, 1.09
No. of reflections	1999
No. of parameters	172
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.21

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

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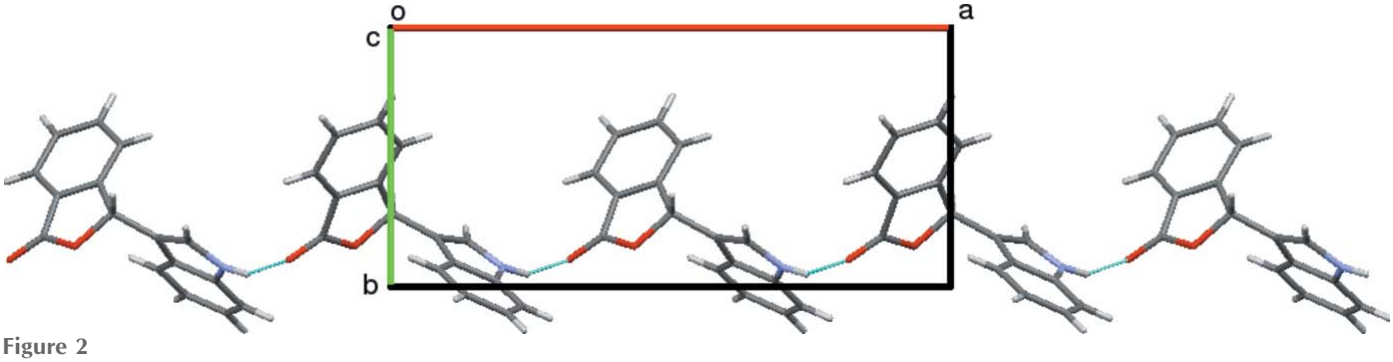

Figure 2
Packing of the molecules viewed along the c axis, with N—H···O hydrogen bonds drawn as blue lines.

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full crystallographic data

IUCrData (2017). **2**, x170107 [https://doi.org/10.1107/S2414314617001079]

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Crystal data

$C_{16}H_{11}NO_2$
M_r = 249.26
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 16.522 (3) Å
b = 7.6439 (14) Å
c = 19.331 (4) Å
V = 2441.4 (8) Å^3
Z = 8
F(000) = 1040
D_x = 1.356 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 1970 reflections
θ = 5.3–64.3°
μ = 0.73 mm^{-1}
T = 296 K
Rectangle, white
0.30 × 0.28 × 0.25 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.811, T_{max} = 0.839
11928 measured reflections
1999 independent reflections
1970 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 64.3°, θ_{min} = 5.3°
h = −18→18
k = −8→7
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.086
S = 1.09
1999 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 1.1739P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.43433 (5)	0.84507 (12)	0.28595 (4)	0.0232 (3)
O2	0.31751 (6)	0.89685 (13)	0.34137 (5)	0.0285 (3)
N1	0.70014 (7)	0.92519 (16)	0.26536 (6)	0.0284 (4)
C1	0.68634 (8)	0.97689 (17)	0.33228 (7)	0.0237 (4)
C2	0.73445 (8)	1.07594 (18)	0.37663 (8)	0.0310 (4)
C3	0.70652 (9)	1.10207 (19)	0.44267 (8)	0.0335 (4)
C4	0.63269 (8)	1.03069 (19)	0.46506 (8)	0.0297 (4)
C5	0.58456 (8)	0.93417 (17)	0.42091 (7)	0.0223 (4)
C6	0.61104 (8)	0.90567 (16)	0.35301 (7)	0.0194 (3)
C7	0.58029 (8)	0.80951 (17)	0.29459 (6)	0.0204 (3)
C8	0.63688 (8)	0.82481 (18)	0.24342 (7)	0.0253 (4)
C9	0.50181 (7)	0.71623 (17)	0.28822 (6)	0.0209 (4)
C10	0.47770 (8)	0.59775 (17)	0.34676 (6)	0.0192 (4)
C11	0.51687 (8)	0.45282 (17)	0.37444 (7)	0.0227 (4)
C12	0.47774 (9)	0.36276 (19)	0.42680 (7)	0.0275 (4)
C13	0.40181 (9)	0.41450 (19)	0.45134 (7)	0.0295 (4)
C14	0.36326 (8)	0.55958 (18)	0.42418 (7)	0.0251 (4)
C15	0.40316 (8)	0.65007 (17)	0.37214 (6)	0.0201 (4)
C16	0.37754 (8)	0.80699 (17)	0.33410 (6)	0.0213 (4)
H1	0.74200	0.95180	0.24110	0.0340*
H2	0.78360	1.12250	0.36210	0.0370*
H3	0.73720	1.16850	0.47330	0.0400*
H4	0.61590	1.04880	0.51040	0.0360*
H5	0.53540	0.88880	0.43600	0.0270*
H8	0.63280	0.77400	0.19980	0.0300*
H9	0.50180	0.64880	0.24510	0.0250*
H11	0.56740	0.41770	0.35840	0.0270*
H12	0.50260	0.26520	0.44620	0.0330*
H13	0.37700	0.35060	0.48630	0.0350*
H14	0.31270	0.59500	0.44010	0.0300*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0225 (5)	0.0239 (5)	0.0233 (5)	0.0029 (4)	−0.0018 (4)	0.0050 (4)
O2	0.0240 (5)	0.0306 (6)	0.0310 (5)	0.0070 (4)	−0.0031 (4)	0.0005 (4)
N1	0.0230 (6)	0.0315 (7)	0.0307 (6)	0.0013 (5)	0.0091 (5)	0.0100 (5)
C1	0.0221 (7)	0.0171 (6)	0.0320 (7)	0.0032 (5)	0.0024 (5)	0.0068 (6)
C2	0.0209 (7)	0.0194 (7)	0.0527 (9)	−0.0016 (6)	−0.0012 (6)	0.0034 (6)

C3	0.0274 (7)	0.0232 (7)	0.0498 (9)	0.0008 (6)	−0.0110 (7)	−0.0100 (7)
C4	0.0304 (7)	0.0278 (8)	0.0309 (7)	0.0055 (6)	−0.0038 (6)	−0.0082 (6)
C5	0.0213 (6)	0.0205 (7)	0.0251 (7)	0.0014 (5)	0.0005 (5)	−0.0005 (5)
C6	0.0195 (6)	0.0148 (6)	0.0238 (6)	0.0025 (5)	−0.0002 (5)	0.0040 (5)
C7	0.0230 (6)	0.0193 (6)	0.0188 (6)	0.0031 (5)	0.0011 (5)	0.0039 (5)
C8	0.0274 (7)	0.0271 (7)	0.0215 (6)	0.0062 (6)	0.0028 (5)	0.0055 (6)
C9	0.0232 (7)	0.0208 (7)	0.0187 (6)	0.0038 (5)	−0.0013 (5)	−0.0005 (5)
C10	0.0222 (6)	0.0186 (7)	0.0168 (6)	−0.0026 (5)	−0.0027 (5)	−0.0035 (5)
C11	0.0231 (7)	0.0220 (7)	0.0230 (7)	0.0025 (5)	−0.0018 (5)	−0.0017 (5)
C12	0.0327 (7)	0.0232 (7)	0.0265 (7)	0.0035 (6)	−0.0027 (6)	0.0047 (6)
C13	0.0335 (8)	0.0301 (8)	0.0248 (7)	−0.0030 (6)	0.0030 (6)	0.0065 (6)
C14	0.0239 (7)	0.0276 (7)	0.0239 (7)	−0.0008 (6)	0.0019 (5)	−0.0015 (6)
C15	0.0222 (6)	0.0195 (7)	0.0185 (6)	−0.0010 (5)	−0.0041 (5)	−0.0034 (5)
C16	0.0210 (6)	0.0232 (7)	0.0196 (6)	−0.0015 (6)	−0.0037 (5)	−0.0029 (5)

Geometric parameters (Å, º)

O1—C9	1.4882 (15)	C10—C11	1.3901 (19)
O1—C16	1.3533 (15)	C11—C12	1.384 (2)
O2—C16	1.2146 (17)	C12—C13	1.398 (2)
N1—C1	1.3717 (18)	C13—C14	1.382 (2)
N1—C8	1.3642 (18)	C14—C15	1.3875 (19)
N1—H1	0.8600	C15—C16	1.4692 (18)
C1—C2	1.393 (2)	C2—H2	0.9300
C1—C6	1.4159 (19)	C3—H3	0.9300
C2—C3	1.372 (2)	C4—H4	0.9300
C3—C4	1.405 (2)	C5—H5	0.9300
C4—C5	1.380 (2)	C8—H8	0.9300
C5—C6	1.4006 (19)	C9—H9	0.9800
C6—C7	1.4401 (18)	C11—H11	0.9300
C7—C9	1.4849 (18)	C12—H12	0.9300
C7—C8	1.3661 (18)	C13—H13	0.9300
C9—C10	1.5032 (18)	C14—H14	0.9300
C10—C15	1.3847 (19)		
C9—O1—C16	110.90 (9)	C10—C15—C16	108.34 (11)
C1—N1—C8	109.14 (11)	C14—C15—C16	129.27 (12)
C8—N1—H1	125.00	C10—C15—C14	122.38 (12)
C1—N1—H1	125.00	O2—C16—C15	129.72 (12)
C2—C1—C6	122.43 (13)	O1—C16—O2	121.61 (11)
N1—C1—C2	129.96 (13)	O1—C16—C15	108.67 (11)
N1—C1—C6	107.59 (11)	C1—C2—H2	121.00
C1—C2—C3	117.38 (13)	C3—C2—H2	121.00
C2—C3—C4	121.48 (14)	C2—C3—H3	119.00
C3—C4—C5	121.16 (14)	C4—C3—H3	119.00
C4—C5—C6	118.86 (12)	C3—C4—H4	119.00
C1—C6—C5	118.68 (12)	C5—C4—H4	119.00
C5—C6—C7	134.76 (12)	C4—C5—H5	121.00

C1—C6—C7	106.52 (11)	C6—C5—H5	121.00
C6—C7—C9	128.19 (11)	N1—C8—H8	125.00
C6—C7—C8	106.42 (12)	C7—C8—H8	125.00
C8—C7—C9	125.36 (11)	O1—C9—H9	109.00
N1—C8—C7	110.33 (12)	C7—C9—H9	109.00
O1—C9—C7	109.81 (10)	C10—C9—H9	109.00
C7—C9—C10	117.28 (10)	C10—C11—H11	121.00
O1—C9—C10	102.85 (9)	C12—C11—H11	121.00
C9—C10—C15	109.17 (11)	C11—C12—H12	119.00
C11—C10—C15	120.52 (12)	C13—C12—H12	119.00
C9—C10—C11	130.28 (12)	C12—C13—H13	120.00
C10—C11—C12	117.41 (12)	C14—C13—H13	120.00
C11—C12—C13	121.76 (13)	C13—C14—H14	121.00
C12—C13—C14	120.76 (13)	C15—C14—H14	121.00
C13—C14—C15	117.15 (12)		

C16—O1—C9—C7	−127.15 (10)	C6—C7—C9—O1	69.43 (16)
C16—O1—C9—C10	−1.57 (12)	C6—C7—C9—C10	−47.42 (19)
C9—O1—C16—O2	179.41 (11)	C8—C7—C9—O1	−108.12 (14)
C9—O1—C16—C15	0.14 (13)	C8—C7—C9—C10	135.03 (13)
C8—N1—C1—C2	178.09 (14)	O1—C9—C10—C11	−179.29 (13)
C8—N1—C1—C6	−0.05 (14)	O1—C9—C10—C15	2.50 (13)
C1—N1—C8—C7	0.51 (16)	C7—C9—C10—C11	−58.72 (18)
N1—C1—C2—C3	−177.39 (14)	C7—C9—C10—C15	123.07 (12)
C6—C1—C2—C3	0.5 (2)	C9—C10—C11—C12	−176.83 (13)
N1—C1—C6—C5	177.48 (12)	C15—C10—C11—C12	1.21 (19)
N1—C1—C6—C7	−0.40 (14)	C9—C10—C15—C14	176.57 (12)
C2—C1—C6—C5	−0.8 (2)	C9—C10—C15—C16	−2.51 (14)
C2—C1—C6—C7	−178.71 (12)	C11—C10—C15—C14	−1.9 (2)
C1—C2—C3—C4	0.5 (2)	C11—C10—C15—C16	179.07 (12)
C2—C3—C4—C5	−1.3 (2)	C10—C11—C12—C13	−0.1 (2)
C3—C4—C5—C6	0.9 (2)	C11—C12—C13—C14	−0.5 (2)
C4—C5—C6—C1	0.09 (19)	C12—C13—C14—C15	−0.1 (2)
C4—C5—C6—C7	177.22 (14)	C13—C14—C15—C10	1.2 (2)
C1—C6—C7—C8	0.70 (14)	C13—C14—C15—C16	−179.89 (13)
C1—C6—C7—C9	−177.22 (12)	C10—C15—C16—O1	1.51 (14)
C5—C6—C7—C8	−176.68 (15)	C10—C15—C16—O2	−177.68 (13)
C5—C6—C7—C9	5.4 (2)	C14—C15—C16—O1	−177.49 (13)
C6—C7—C8—N1	−0.75 (15)	C14—C15—C16—O2	3.3 (2)
C9—C7—C8—N1	177.24 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.07	2.8398 (16)	149

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