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## Structure Reports

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7*H*-1-Benzofuro[2,3-*b*]carbazole

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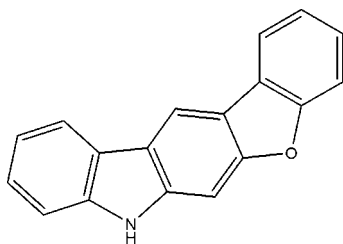
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Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.033;  $wR$  factor = 0.084; data-to-parameter ratio = 14.8.

In the title compound,  $\text{C}_{18}\text{H}_{11}\text{NO}$ , the carbazole and benzofuran rings are almost co-planar, making a dihedral angle of  $3.31$  (3)°. The crystal structure is stabilized by weak  $\text{C}-\text{H}\cdots\pi$  interactions.

## Related literature

For the biological activity of carbazole derivatives, see: Ramsewak *et al.* (1999); Diaz *et al.* (2002); Zhang *et al.* (2004). For the structures of closely related compounds, see: Chakkaravarthi *et al.* (2008*a,b*).



## Experimental

## Crystal data

$\text{C}_{18}\text{H}_{11}\text{NO}$	$V = 1214.7$ (3) Å <sup>3</sup>
$M_r = 257.28$	$Z = 4$
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation
$a = 26.087$ (3) Å	$\mu = 0.09$ mm <sup>-1</sup>
$b = 5.9585$ (8) Å	$T = 295$ K
$c = 7.8146$ (10) Å	$0.24 \times 0.22 \times 0.20$ mm

## Data collection

Bruker Kappa APEXII diffractometer	6591 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2700 independent reflections
$T_{\min} = 0.979$ , $T_{\max} = 0.983$	2331 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.022$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$	$\Delta\rho_{\text{max}} = 0.13$ e Å <sup>-3</sup>
$wR(F^2) = 0.084$	$\Delta\rho_{\text{min}} = -0.13$ e Å <sup>-3</sup>
$S = 1.05$	Absolute structure: Flack (1983),
2700 reflections	1086 Friedel pairs
182 parameters	Flack parameter: 0.2 (15)
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (Å, °).

$Cg2$ ,  $Cg3$  and  $Cg4$  are the centroids of the  $\text{N1}/\text{C1}/\text{C6}/\text{C7}/\text{C12}$ ,  $\text{C1}-\text{C6}$  and  $\text{C7}-\text{C12}$  rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots Cg4^i$	0.86	2.91	3.530 (2)	130
$\text{C5}-\text{H5}\cdots Cg2^{ii}$	0.93	2.70	3.449 (2)	138
$\text{C11}-\text{H11}\cdots Cg3^i$	0.93	2.79	3.526 (2)	137

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

The authors wish to acknowledge the SAIF, IIT, Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2122).

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**supplementary materials**

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## 7H-1-Benzofuro[2,3-b]carbazole

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### Comment

Carbazole derivatives exhibit anti-inflammatory and antimutagenic activities (Ramsewak *et al.*, 1999). A carbazole ring is easily functionalized and covalently linked to other molecules (Diaz *et al.*, 2002). This enables its use as a convenient building block for the design and synthesis of molecular glasses, which are widely studied as components of electroactive and photoactive materials (Zhang *et al.*, 2004).

We herewith report the crystal structure of the title compound (Fig. 1). The geometric parameters agree well with those of similar reported structures (Chakkaravarthi *et al.*, 2008a, 2008b). The benzofuran moiety (C9/C13-C18/O1/C10) is almost co-planar [dihedral angle 3.31 (3)°] with the carbazole ring (C1-C12/N1). The crystal structure is stabilized by weak intermolecular C-H... $\pi$  interactions (Table 1).

### Experimental

To a solution of tert-butyl-3-(2,2-di(ethoxycarbonyl)vinyl)-2-(bromomethyl)-1H-indole-1-carboxylate (0.5 g, 1.04 mmol) in dry 1,2-dichloroethane (15 mL), anhydrous ZnBr<sub>2</sub> (0.05 g, 0.22 mmol) and benzo[b]furan (0.13 mL, 1.27 mmol) were added. It was then stirred at room temperature for 2 h under N<sub>2</sub> atmosphere. The solvent was removed and the residue was quenched with ice-water (50 mL) containing 1 mL of conc. HCl, extracted with chloroform (2 x 10 mL) and dried (Na<sub>2</sub>SO<sub>4</sub>). Removal of solvent followed by flash column chromatography purification (n-hexane/ethyl acetate 80:20) led to the isolation of title compound as a colourless crystal suitable for X-Ray diffraction quality.

### Refinement

All H atoms were positioned geometrically, with C—H = 0.93 Å and N—H = 0.86 Å and allowed to ride on their parent atoms, with U<sub>iso</sub>(H) = 1.2 U<sub>eq</sub>(C,N).

### Figures

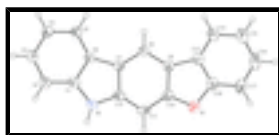


Fig. 1. The molecular structure of the title compound with atom labels and 30% probability displacement ellipsoids for non-H atoms.

## 7H-1-Benzofuro[2,3-b]carbazole

### Crystal data

C<sub>18</sub>H<sub>11</sub>NO

$F(000) = 536$

# supplementary materials

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$M_r = 257.28$	$D_x = 1.407 \text{ Mg m}^{-3}$
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: P 2c -2ac	Cell parameters from 2246 reflections
$a = 26.087 (3) \text{ \AA}$	$\theta = 1.6\text{--}28.3^\circ$
$b = 5.9585 (8) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 7.8146 (10) \text{ \AA}$	$T = 295 \text{ K}$
$V = 1214.7 (3) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.24 \times 0.22 \times 0.20 \text{ mm}$

## Data collection

Bruker Kappa APEXII diffractometer	2700 independent reflections
Radiation source: fine-focus sealed tube graphite	2331 reflections with $I > 2\sigma(I)$
$\omega$ and $\varphi$ scans	$R_{\text{int}} = 0.022$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 28.3^\circ$ , $\theta_{\text{min}} = 1.6^\circ$
$T_{\text{min}} = 0.979$ , $T_{\text{max}} = 0.983$	$h = -33 \rightarrow 34$
6591 measured reflections	$k = -7 \rightarrow 7$
	$l = -7 \rightarrow 10$

## Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.0541P]$
$wR(F^2) = 0.084$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2700 reflections	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
182 parameters	$\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL</i> , $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0083 (13)
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), 1086 Friedel pairs
	Flack parameter: 0.2 (15)

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.95422 (6)	0.1951 (2)	0.5133 (2)	0.0412 (3)
C2	0.90187 (6)	0.2333 (3)	0.5252 (2)	0.0481 (4)
H2	0.8802	0.1313	0.5790	0.058*
C3	0.88330 (6)	0.4286 (3)	0.4541 (2)	0.0526 (4)
H3	0.8484	0.4587	0.4602	0.063*
C4	0.91550 (6)	0.5822 (3)	0.3733 (2)	0.0491 (4)
H4	0.9017	0.7122	0.3262	0.059*

C5	0.96747 (6)	0.5437 (2)	0.3624 (2)	0.0414 (3)
H5	0.9889	0.6474	0.3093	0.050*
C6	0.98745 (5)	0.3475 (2)	0.43203 (19)	0.0370 (3)
C7	1.03818 (5)	0.2503 (2)	0.43841 (19)	0.0366 (3)
C8	1.08582 (5)	0.3196 (2)	0.37727 (18)	0.0386 (3)
H8	1.0899	0.4576	0.3233	0.046*
C9	1.12697 (6)	0.1751 (2)	0.4000 (2)	0.0412 (3)
C10	1.11930 (6)	-0.0328 (2)	0.4815 (2)	0.0439 (4)
C11	1.07375 (6)	-0.1066 (3)	0.5477 (2)	0.0464 (4)
H11	1.0703	-0.2431	0.6042	0.056*
C12	1.03323 (6)	0.0405 (2)	0.5230 (2)	0.0403 (3)
C13	1.18108 (6)	0.1825 (3)	0.3568 (2)	0.0458 (4)
C14	1.21349 (6)	0.3394 (3)	0.2832 (2)	0.0525 (4)
H14	1.2009	0.4763	0.2444	0.063*
C15	1.26512 (6)	0.2873 (4)	0.2688 (3)	0.0617 (5)
H15	1.2874	0.3903	0.2192	0.074*
C16	1.28401 (7)	0.0836 (4)	0.3275 (3)	0.0666 (6)
H16	1.3188	0.0533	0.3169	0.080*
C17	1.25258 (7)	-0.0744 (3)	0.4009 (2)	0.0624 (5)
H17	1.2652	-0.2110	0.4403	0.075*
C18	1.20141 (6)	-0.0194 (3)	0.4131 (2)	0.0508 (4)
N1	0.98259 (5)	0.0150 (2)	0.57102 (18)	0.0443 (3)
H1	0.9706	-0.0965	0.6283	0.053*
O1	1.16449 (4)	-0.15463 (18)	0.48849 (17)	0.0557 (3)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0493 (8)	0.0409 (7)	0.0336 (8)	-0.0090 (6)	-0.0002 (7)	-0.0032 (6)
C2	0.0450 (8)	0.0557 (9)	0.0434 (9)	-0.0134 (7)	0.0036 (7)	-0.0009 (8)
C3	0.0419 (8)	0.0659 (11)	0.0501 (10)	-0.0015 (7)	0.0016 (7)	-0.0052 (8)
C4	0.0511 (8)	0.0487 (8)	0.0474 (10)	0.0039 (7)	-0.0041 (8)	-0.0009 (8)
C5	0.0470 (7)	0.0383 (7)	0.0389 (8)	-0.0052 (6)	-0.0007 (7)	-0.0001 (6)
C6	0.0421 (7)	0.0381 (7)	0.0309 (7)	-0.0070 (5)	-0.0014 (6)	-0.0026 (6)
C7	0.0472 (7)	0.0313 (6)	0.0312 (7)	-0.0050 (6)	-0.0010 (6)	-0.0018 (6)
C8	0.0453 (7)	0.0350 (7)	0.0354 (8)	-0.0054 (6)	0.0002 (6)	0.0013 (6)
C9	0.0446 (7)	0.0402 (7)	0.0387 (9)	-0.0026 (6)	-0.0001 (6)	-0.0059 (6)
C10	0.0506 (8)	0.0386 (7)	0.0425 (9)	0.0033 (6)	-0.0040 (7)	-0.0048 (6)
C11	0.0596 (9)	0.0343 (7)	0.0452 (9)	-0.0023 (6)	-0.0016 (7)	0.0021 (7)
C12	0.0513 (8)	0.0347 (7)	0.0349 (8)	-0.0080 (6)	-0.0018 (6)	-0.0020 (6)
C13	0.0454 (8)	0.0519 (9)	0.0402 (9)	-0.0008 (7)	-0.0024 (7)	-0.0100 (7)
C14	0.0483 (9)	0.0633 (10)	0.0459 (10)	-0.0072 (7)	-0.0015 (8)	-0.0075 (8)
C15	0.0482 (9)	0.0839 (13)	0.0529 (12)	-0.0106 (9)	0.0043 (9)	-0.0151 (10)
C16	0.0451 (9)	0.0932 (15)	0.0616 (13)	0.0072 (10)	0.0007 (8)	-0.0240 (11)
C17	0.0550 (9)	0.0677 (10)	0.0645 (14)	0.0147 (9)	-0.0031 (9)	-0.0143 (10)
C18	0.0500 (8)	0.0540 (9)	0.0485 (11)	0.0034 (7)	-0.0025 (7)	-0.0109 (8)
N1	0.0505 (7)	0.0391 (6)	0.0432 (8)	-0.0106 (5)	0.0034 (6)	0.0053 (6)
O1	0.0558 (6)	0.0471 (6)	0.0643 (9)	0.0090 (5)	-0.0031 (6)	-0.0019 (5)

## supplementary materials

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### *Geometric parameters (Å, °)*

C1—N1	1.380 (2)	C10—C11	1.369 (2)
C1—C2	1.388 (2)	C10—O1	1.3856 (18)
C1—C6	1.407 (2)	C11—C12	1.387 (2)
C2—C3	1.377 (2)	C11—H11	0.9300
C2—H2	0.9300	C12—N1	1.3817 (19)
C3—C4	1.394 (2)	C13—C14	1.385 (2)
C3—H3	0.9300	C13—C18	1.386 (2)
C4—C5	1.378 (2)	C14—C15	1.387 (2)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.391 (2)	C15—C16	1.388 (3)
C5—H5	0.9300	C15—H15	0.9300
C6—C7	1.445 (2)	C16—C17	1.374 (3)
C7—C8	1.3940 (19)	C16—H16	0.9300
C7—C12	1.4202 (19)	C17—C18	1.378 (2)
C8—C9	1.388 (2)	C17—H17	0.9300
C8—H8	0.9300	C18—O1	1.387 (2)
C9—C10	1.407 (2)	N1—H1	0.8600
C9—C13	1.452 (2)		
N1—C1—C2	129.30 (14)	O1—C10—C9	110.99 (13)
N1—C1—C6	108.61 (13)	C10—C11—C12	113.97 (14)
C2—C1—C6	122.09 (14)	C10—C11—H11	123.0
C3—C2—C1	117.21 (15)	C12—C11—H11	123.0
C3—C2—H2	121.4	N1—C12—C11	128.43 (13)
C1—C2—H2	121.4	N1—C12—C7	108.07 (13)
C2—C3—C4	121.72 (15)	C11—C12—C7	123.50 (14)
C2—C3—H3	119.1	C14—C13—C18	118.94 (15)
C4—C3—H3	119.1	C14—C13—C9	135.24 (15)
C5—C4—C3	120.78 (15)	C18—C13—C9	105.78 (14)
C5—C4—H4	119.6	C13—C14—C15	118.36 (17)
C3—C4—H4	119.6	C13—C14—H14	120.8
C4—C5—C6	118.98 (14)	C15—C14—H14	120.8
C4—C5—H5	120.5	C14—C15—C16	120.92 (18)
C6—C5—H5	120.5	C14—C15—H15	119.5
C5—C6—C1	119.21 (13)	C16—C15—H15	119.5
C5—C6—C7	133.90 (13)	C17—C16—C15	121.69 (16)
C1—C6—C7	106.87 (13)	C17—C16—H16	119.2
C8—C7—C12	120.09 (13)	C15—C16—H16	119.2
C8—C7—C6	133.30 (13)	C16—C17—C18	116.36 (18)
C12—C7—C6	106.59 (12)	C16—C17—H17	121.8
C9—C8—C7	117.52 (12)	C18—C17—H17	121.8
C9—C8—H8	121.2	C17—C18—C13	123.72 (17)
C7—C8—H8	121.2	C17—C18—O1	124.33 (16)
C8—C9—C10	119.61 (13)	C13—C18—O1	111.91 (14)
C8—C9—C13	134.72 (14)	C1—N1—C12	109.77 (12)
C10—C9—C13	105.67 (13)	C1—N1—H1	125.1
C11—C10—O1	123.74 (14)	C12—N1—H1	125.1

C11—C10—C9	125.27 (14)	C10—O1—C18	105.64 (12)
N1—C1—C2—C3	-179.31 (16)	C8—C7—C12—N1	179.51 (13)
C6—C1—C2—C3	-0.1 (2)	C6—C7—C12—N1	-2.04 (16)
C1—C2—C3—C4	0.0 (3)	C8—C7—C12—C11	-1.0 (2)
C2—C3—C4—C5	-0.3 (3)	C6—C7—C12—C11	177.49 (15)
C3—C4—C5—C6	0.6 (2)	C8—C9—C13—C14	3.5 (3)
C4—C5—C6—C1	-0.7 (2)	C10—C9—C13—C14	-176.81 (17)
C4—C5—C6—C7	177.28 (15)	C8—C9—C13—C18	-179.06 (17)
N1—C1—C6—C5	179.83 (13)	C10—C9—C13—C18	0.64 (18)
C2—C1—C6—C5	0.5 (2)	C18—C13—C14—C15	0.1 (2)
N1—C1—C6—C7	1.33 (16)	C9—C13—C14—C15	177.25 (18)
C2—C1—C6—C7	-178.01 (15)	C13—C14—C15—C16	-0.4 (3)
C5—C6—C7—C8	0.4 (3)	C14—C15—C16—C17	0.4 (3)
C1—C6—C7—C8	178.59 (16)	C15—C16—C17—C18	0.0 (3)
C5—C6—C7—C12	-177.74 (17)	C16—C17—C18—C13	-0.3 (3)
C1—C6—C7—C12	0.44 (16)	C16—C17—C18—O1	-177.71 (17)
C12—C7—C8—C9	1.1 (2)	C14—C13—C18—C17	0.3 (3)
C6—C7—C8—C9	-176.87 (15)	C9—C13—C18—C17	-177.67 (16)
C7—C8—C9—C10	0.3 (2)	C14—C13—C18—O1	177.98 (13)
C7—C8—C9—C13	179.98 (16)	C9—C13—C18—O1	0.04 (19)
C8—C9—C10—C11	-2.1 (2)	C2—C1—N1—C12	176.60 (17)
C13—C9—C10—C11	178.14 (16)	C6—C1—N1—C12	-2.68 (17)
C8—C9—C10—O1	178.64 (14)	C11—C12—N1—C1	-176.56 (16)
C13—C9—C10—O1	-1.11 (17)	C7—C12—N1—C1	2.94 (17)
O1—C10—C11—C12	-178.66 (15)	C11—C10—O1—C18	-178.14 (15)
C9—C10—C11—C12	2.2 (2)	C9—C10—O1—C18	1.13 (17)
C10—C11—C12—N1	178.80 (15)	C17—C18—O1—C10	176.98 (17)
C10—C11—C12—C7	-0.6 (2)	C13—C18—O1—C10	-0.71 (18)

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

Cg2, Cg3 and Cg4 are the centroids of the N1/C1/C6/C7/C12, C1—C6 and C7—C12 rings, respectively.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 $\cdots$ Cg4 <sup>i</sup>	0.86	2.91	3.530 (2)	130
C5—H5 $\cdots$ Cg2 <sup>ii</sup>	0.93	2.70	3.449 (2)	138
C11—H11 $\cdots$ Cg3 <sup>i</sup>	0.93	2.79	3.526 (2)	137

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

Fig. 1

