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

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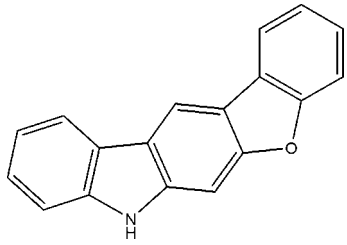
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.084; data-to-parameter ratio = 14.8.

In the title compound, $C_{18}H_{11}NO$, the carbazole and benzofuran rings are almost co-planar, making a dihedral angle of 3.31 (3)°. The crystal structure is stabilized by weak C—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

$C_{18}H_{11}NO$
M_r = 257.28
Orthorhombic, $Pca2_1$
a = 26.087 (3) Å
b = 5.9585 (8) Å
c = 7.8146 (10) Å
V = 1214.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.24 × 0.22 × 0.20 mm

Data collection

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

Refinement

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

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

*Cg*2, *Cg*3 and *Cg*4 are the centroids of the N1/C1/C6/C7/C12, C1–C6 and C7–C12 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots Cg4^{i}$	0.86	2.91	3.530 (2)	130
C5—H5$\cdots Cg2^{ii}$	0.93	2.70	3.449 (2)	138
C11—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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S1. 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.*, 2008*a*, 2008*b*). 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···π interactions (Table 1).

S2. 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 $ZnBr_2$ (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_2 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_2SO_4). 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.

S3. Refinement

All H atoms were positioned geometrically, with C—H = 0.93Å and N—H = 0.86Å and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C,N).

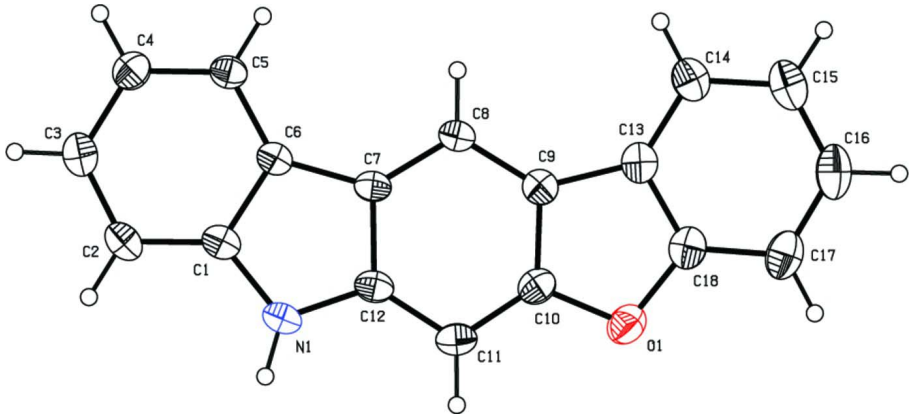

Figure 1

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

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

Crystal data

$C_{18}H_{11}NO$
$M_r = 257.28$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 26.087$ (3) Å
$b = 5.9585$ (8) Å
$c = 7.8146$ (10) Å
$V = 1214.7$ (3) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.407$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2246 reflections
$\theta = 1.6$–$28.3°$
$\mu = 0.09$ mm^{-1}
$T = 295$ K
Block, colourless
0.24 × 0.22 × 0.20 mm

Data collection

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

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.084$
$S = 1.05$
2700 reflections
182 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
$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.0541P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0083 (13)

Absolute structure: Flack (1983), 1086 Friedel pairs

Absolute structure parameter: 0.2 (15)

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

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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)

Geometric parameters (Å, º)

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 (Å, º)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···*Cg*4^{i}	0.86	2.91	3.530 (2)	130
C5—H5···*Cg*2^{ii}	0.93	2.70	3.449 (2)	138
C11—H11···*Cg*3^{i}	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.