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1-Hydroxy-11*H*-benzo[*b*]fluoren-11-one

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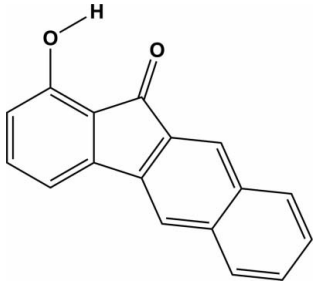
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.153; data-to-parameter ratio = 13.1.

The title compound, $C_{17}H_{10}O_2$, is nearly planar, the maximum atomic deviation being 0.053 (2) Å. In the molecule, an intramolecular O—H···O hydrogen bond generates an S(6) ring motif. In the crystal, inversion-related molecules are linked by pairs of weak C—H···O hydrogen bonds, forming dimers. π–π stacking is observed in the crystal structure, the closest centroid–centroid distance being 3.7846 (16) Å.

Related literature

For the spectroscopy and preparation of the title compound, see: Aquino *et al.* (2005); Tang *et al.* (2011). For applications of proton-transfer dyes, see: Chen & Pang (2009, 2010); Chuang *et al.* (2011); Han *et al.* (2010); Ito *et al.* (2011); Jung *et al.* (2009); Lim *et al.* (2011). For related structures, see: Chen *et al.* (2011*a*,*b*); Li *et al.* (2007); Saeed & Bolte (2007). For graph-set theory, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{10}O_2$
M_r = 246.25
Monoclinic, $P2_1/c$
a = 12.474 (2) Å
b = 6.4401 (12) Å
c = 15.601 (3) Å
β = 109.188 (3)°
V = 1183.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 297 K
0.42 × 0.22 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
6331 measured reflections
2310 independent reflections
1322 reflections with $I > 2\sigma(I)$
R_{int} = 0.087

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.153
S = 1.03
2310 reflections
176 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1	1.11 (4)	1.90 (4)	2.877 (3)	145 (3)
C3—H3A···O1^{i}	0.93	2.52	3.369 (3)	151

Symmetry code: (i) $-x+1, -y-1, -z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5365).

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supporting information

Acta Cryst. (2012). E**68**, o16 [doi:10.1107/S160053681104760X]

1-Hydroxy-11*H*-benzo[*b*]fluoren-11-one

Kew-Yu Chen, Ming-Jen Chang and Tzu-Chien Fang

S1. Comment

The excited-state intramolecular proton transfer (ESIPT) reaction of 7-hydroxy-1-indanone and its derivatives has been investigated for past years (Aquino *et al.*, 2005; Tang *et al.*, 2011), which incorporates transfer of a hydroxy proton to the carbonyl oxygen through a intramolecular six-membered-ring hydrogen-bonding system. The unusual photophysical property of the resulting proton-transfer tautomer has found many important applications (Chen *et al.*, 2009, 2010; Lim *et al.*, 2011; Ito *et al.*, 2011; Han *et al.*, 2010; Jung *et al.*, 2009).

The molecular structure of the title compound (HBO) comprises a 7-hydroxy-1-indanone unit having a naphthalene ring fused on one side (Figure 1). The molecule is nearly planar, which is consistent with previous studies (Chen *et al.*, 2011a; Li *et al.*, 2007; Saeed *et al.*, 2007). HBO possesses an intramolecular O—H···O hydrogen bond (Table 1), which generates an S(6) ring motif (Chen *et al.*, 2011b). In the crystal (Figure 2), inversion-related molceules are linked by a pair of weak C—H···O hydrogen bonds (Table 1), forming a cyclic dimers with $R_2^2(10)$ graph-set motif (Bernstein *et al.*, 1995). π—π stacking is observed between the tetracyclic plane and its adjacent one, the closest centroid-centroid distance being 3.7846 (16) Å [symmetry code: 1 - *x*, -*y*, 1 - *z*].

S2. Experimental

The title compound was synthesized according to the literature (Tang *et al.*, 2011). Yellow needle-shaped crystals suitable for the crystallographic studies reported here were isolated over a period of six weeks by slow evaporation from the chloroform solution.

S3. Refinement

Hydroxy H atom was located in a Fourier map and refined isotropically. Other H atoms ware placed geometrically and refined using a riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

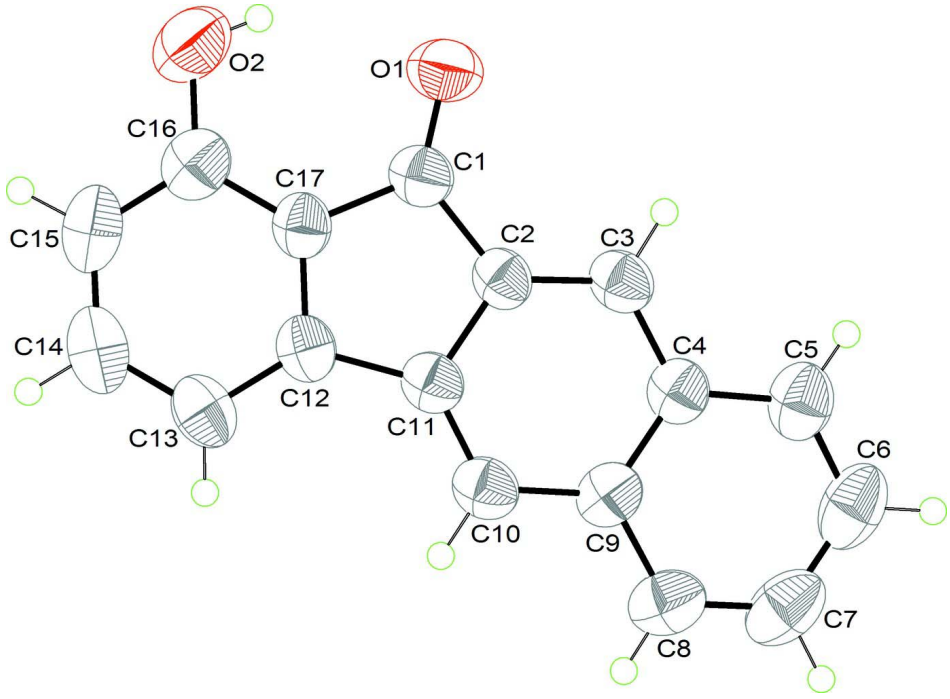

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

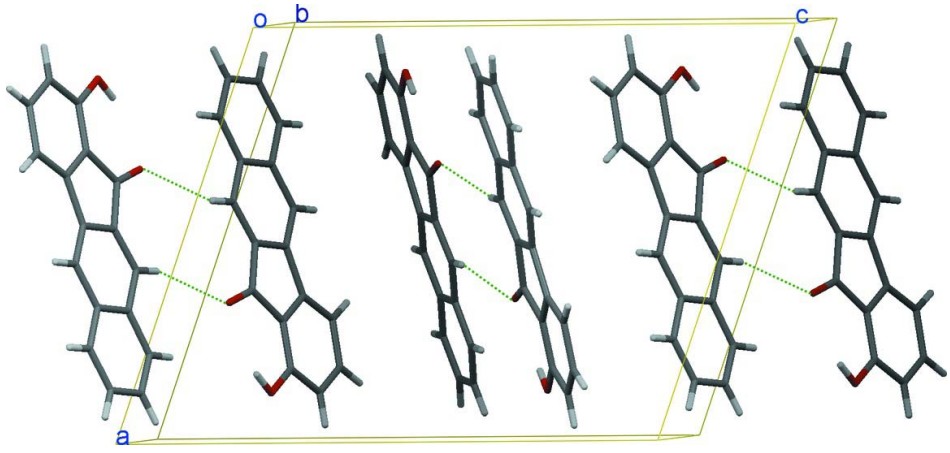

Figure 2

A section of the crystal packing of the title compound, viewed down the *b* axis. Green dashed lines denote the intermolecular C—H···O hydrogen bonds.

1-Hydroxy-11*H*-benzo[*b*]fluoren-11-one

Crystal data

$C_{17}H_{10}O_2$
M_r = 246.25
Monoclinic, $P2_1/c$
Hall symbol: -p 2ybc
a = 12.474 (2) Å
b = 6.4401 (12) Å
c = 15.601 (3) Å
β = 109.188 (3)°
V = 1183.6 (4) Å^3
Z = 4
$F(000)$ = 512
D_x = 1.382 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1918 reflections
θ = 2.7–24.7°
μ = 0.09 mm^{-1}
T = 297 K
Parallelepiped, yellow
0.42 × 0.22 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
6331 measured reflections
2310 independent reflections
1322 reflections with $I > 2\sigma(I)$
R_{int} = 0.087
θ_{max} = 26.0°, θ_{min} = 1.7°
h = −14→15
k = −7→7
l = −19→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.153
S = 1.03
2310 reflections
176 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 0.2285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.66186 (16)	−0.4250 (3)	0.11797 (12)	0.0730 (6)
O2	0.88146 (17)	−0.3141 (4)	0.24218 (14)	0.0836 (6)
H2A	0.816 (3)	−0.412 (6)	0.194 (3)	0.147 (15)*
C1	0.6346 (2)	−0.2548 (4)	0.14017 (15)	0.0515 (6)
C2	0.52192 (19)	−0.1511 (3)	0.10894 (14)	0.0466 (6)
C3	0.4220 (2)	−0.2150 (4)	0.04737 (15)	0.0527 (6)
H3A	0.4171	−0.3429	0.0187	0.063*
C4	0.3259 (2)	−0.0847 (4)	0.02760 (14)	0.0505 (6)
C5	0.2190 (2)	−0.1414 (5)	−0.03430 (16)	0.0656 (7)
H5A	0.2111	−0.2688	−0.0638	0.079*
C6	0.1281 (2)	−0.0144 (6)	−0.05160 (18)	0.0764 (9)
H6A	0.0587	−0.0549	−0.0928	0.092*

C7	0.1378 (2)	0.1778 (6)	−0.00777 (19)	0.0774 (9)
H7A	0.0747	0.2637	−0.0195	0.093*
C8	0.2396 (2)	0.2395 (4)	0.05214 (17)	0.0655 (7)
H8A	0.2452	0.3682	0.0803	0.079*
C9	0.33640 (19)	0.1115 (4)	0.07200 (14)	0.0516 (6)
C10	0.4427 (2)	0.1731 (4)	0.13508 (15)	0.0538 (6)
H10A	0.4497	0.3015	0.1637	0.065*
C11	0.53325 (19)	0.0456 (3)	0.15340 (14)	0.0478 (6)
C12	0.65335 (19)	0.0694 (4)	0.21356 (13)	0.0485 (6)
C13	0.7106 (2)	0.2252 (4)	0.26996 (16)	0.0631 (7)
H13A	0.6733	0.3451	0.2778	0.076*
C14	0.8266 (2)	0.1985 (5)	0.31532 (18)	0.0714 (8)
H14A	0.8664	0.3039	0.3533	0.086*
C15	0.8842 (2)	0.0228 (5)	0.30603 (18)	0.0714 (8)
H15A	0.9617	0.0115	0.3366	0.086*
C16	0.8262 (2)	−0.1378 (4)	0.25083 (16)	0.0602 (7)
C17	0.71100 (19)	−0.1116 (4)	0.20486 (14)	0.0490 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0818 (13)	0.0622 (12)	0.0679 (12)	0.0176 (10)	0.0151 (10)	−0.0086 (9)
O2	0.0615 (12)	0.1010 (16)	0.0844 (14)	0.0228 (12)	0.0186 (10)	0.0023 (12)
C1	0.0613 (15)	0.0508 (14)	0.0419 (12)	0.0043 (12)	0.0163 (11)	0.0011 (10)
C2	0.0527 (14)	0.0471 (13)	0.0392 (11)	0.0003 (11)	0.0140 (10)	−0.0014 (10)
C3	0.0620 (15)	0.0513 (14)	0.0431 (12)	0.0013 (12)	0.0151 (11)	−0.0029 (10)
C4	0.0537 (14)	0.0595 (15)	0.0379 (11)	0.0019 (11)	0.0146 (10)	0.0028 (10)
C5	0.0568 (16)	0.0860 (19)	0.0495 (14)	−0.0037 (15)	0.0114 (12)	0.0012 (13)
C6	0.0502 (16)	0.116 (3)	0.0570 (16)	0.0029 (17)	0.0098 (13)	0.0123 (17)
C7	0.0581 (18)	0.108 (3)	0.0659 (18)	0.0236 (17)	0.0205 (14)	0.0195 (18)
C8	0.0675 (18)	0.0757 (18)	0.0571 (15)	0.0177 (14)	0.0256 (14)	0.0093 (13)
C9	0.0511 (14)	0.0645 (16)	0.0410 (12)	0.0086 (12)	0.0174 (11)	0.0086 (11)
C10	0.0636 (16)	0.0537 (14)	0.0463 (13)	0.0024 (13)	0.0211 (11)	−0.0014 (11)
C11	0.0539 (14)	0.0511 (14)	0.0402 (12)	0.0016 (11)	0.0177 (10)	0.0006 (10)
C12	0.0541 (14)	0.0552 (14)	0.0371 (11)	−0.0062 (11)	0.0161 (10)	0.0012 (10)
C13	0.0717 (19)	0.0627 (16)	0.0529 (14)	−0.0096 (14)	0.0176 (13)	−0.0059 (12)
C14	0.0688 (19)	0.080 (2)	0.0587 (16)	−0.0256 (16)	0.0121 (14)	−0.0024 (14)
C15	0.0489 (15)	0.101 (2)	0.0588 (16)	−0.0135 (16)	0.0096 (12)	0.0049 (16)
C16	0.0574 (16)	0.0745 (18)	0.0506 (14)	0.0049 (14)	0.0202 (12)	0.0085 (13)
C17	0.0492 (14)	0.0589 (15)	0.0384 (11)	−0.0019 (11)	0.0137 (10)	0.0009 (10)

Geometric parameters (Å, º)

O1—C1	1.231 (3)	C7—H7A	0.9300
O2—C16	1.358 (3)	C8—C9	1.409 (3)
O2—H2A	1.11 (4)	C8—H8A	0.9300
C1—C17	1.465 (3)	C9—C10	1.423 (3)
C1—C2	1.486 (3)	C10—C11	1.349 (3)

C2—C3	1.364 (3)	C10—H10A	0.9300
C2—C11	1.429 (3)	C11—C12	1.492 (3)
C3—C4	1.412 (3)	C12—C13	1.370 (3)
C3—H3A	0.9300	C12—C17	1.400 (3)
C4—C5	1.413 (3)	C13—C14	1.397 (4)
C4—C9	1.426 (3)	C13—H13A	0.9300
C5—C6	1.352 (4)	C14—C15	1.374 (4)
C5—H5A	0.9300	C14—H14A	0.9300
C6—C7	1.399 (4)	C15—C16	1.387 (4)
C6—H6A	0.9300	C15—H15A	0.9300
C7—C8	1.365 (4)	C16—C17	1.390 (3)

C16—O2—H2A	105 (2)	C10—C9—C4	119.9 (2)
O1—C1—C17	125.3 (2)	C8—C9—C4	118.4 (2)
O1—C1—C2	128.8 (2)	C11—C10—C9	120.1 (2)
C17—C1—C2	105.9 (2)	C11—C10—H10A	119.9
C3—C2—C11	122.1 (2)	C9—C10—H10A	119.9
C3—C2—C1	130.0 (2)	C10—C11—C2	119.6 (2)
C11—C2—C1	107.90 (19)	C10—C11—C12	132.0 (2)
C2—C3—C4	119.3 (2)	C2—C11—C12	108.37 (19)
C2—C3—H3A	120.4	C13—C12—C17	119.8 (2)
C4—C3—H3A	120.4	C13—C12—C11	133.1 (2)
C3—C4—C5	122.5 (2)	C17—C12—C11	107.16 (19)
C3—C4—C9	119.0 (2)	C12—C13—C14	118.0 (3)
C5—C4—C9	118.5 (2)	C12—C13—H13A	121.0
C6—C5—C4	121.4 (3)	C14—C13—H13A	121.0
C6—C5—H5A	119.3	C15—C14—C13	122.6 (3)
C4—C5—H5A	119.3	C15—C14—H14A	118.7
C5—C6—C7	120.3 (3)	C13—C14—H14A	118.7
C5—C6—H6A	119.8	C14—C15—C16	119.7 (2)
C7—C6—H6A	119.8	C14—C15—H15A	120.2
C8—C7—C6	120.3 (3)	C16—C15—H15A	120.2
C8—C7—H7A	119.9	O2—C16—C17	121.5 (2)
C6—C7—H7A	119.9	O2—C16—C15	120.5 (2)
C7—C8—C9	121.1 (3)	C17—C16—C15	118.0 (3)
C7—C8—H8A	119.4	C16—C17—C12	121.9 (2)
C9—C8—H8A	119.4	C16—C17—C1	127.4 (2)
C10—C9—C8	121.7 (2)	C12—C17—C1	110.7 (2)

O1—C1—C2—C3	−1.4 (4)	C3—C2—C11—C12	−178.2 (2)
C17—C1—C2—C3	178.4 (2)	C1—C2—C11—C12	−0.1 (2)
O1—C1—C2—C11	−179.3 (2)	C10—C11—C12—C13	0.7 (4)
C17—C1—C2—C11	0.5 (2)	C2—C11—C12—C13	179.2 (2)
C11—C2—C3—C4	−1.0 (3)	C10—C11—C12—C17	−179.0 (2)
C1—C2—C3—C4	−178.6 (2)	C2—C11—C12—C17	−0.5 (2)
C2—C3—C4—C5	−179.0 (2)	C17—C12—C13—C14	1.7 (3)
C2—C3—C4—C9	0.7 (3)	C11—C12—C13—C14	−178.0 (2)
C3—C4—C5—C6	179.5 (2)	C12—C13—C14—C15	−0.6 (4)

C9—C4—C5—C6	−0.1 (3)	C13—C14—C15—C16	−1.0 (4)
C4—C5—C6—C7	−0.3 (4)	C14—C15—C16—O2	−178.8 (2)
C5—C6—C7—C8	0.7 (4)	C14—C15—C16—C17	1.5 (4)
C6—C7—C8—C9	−0.7 (4)	O2—C16—C17—C12	179.8 (2)
C7—C8—C9—C10	−179.3 (2)	C15—C16—C17—C12	−0.5 (3)
C7—C8—C9—C4	0.3 (4)	O2—C16—C17—C1	−2.8 (4)
C3—C4—C9—C10	0.0 (3)	C15—C16—C17—C1	176.9 (2)
C5—C4—C9—C10	179.7 (2)	C13—C12—C17—C16	−1.2 (3)
C3—C4—C9—C8	−179.6 (2)	C11—C12—C17—C16	178.5 (2)
C5—C4—C9—C8	0.1 (3)	C13—C12—C17—C1	−178.9 (2)
C8—C9—C10—C11	179.1 (2)	C11—C12—C17—C1	0.8 (2)
C4—C9—C10—C11	−0.4 (3)	O1—C1—C17—C16	1.4 (4)
C9—C10—C11—C2	0.2 (3)	C2—C1—C17—C16	−178.4 (2)
C9—C10—C11—C12	178.5 (2)	O1—C1—C17—C12	179.0 (2)
C3—C2—C11—C10	0.6 (3)	C2—C1—C17—C12	−0.8 (2)
C1—C2—C11—C10	178.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O1	1.11 (4)	1.90 (4)	2.877 (3)	145 (3)
C3—H3*A*···O1^{i}	0.93	2.52	3.369 (3)	151

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