organic compounds

7-Hydroxyindan-1-one

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In the title compound, $C_9H_8O_2$, an intramolecular O—H···O hydrogen bond generates an $S(6)$ ring. The dihedral angle between the mean plane of the $S(6)$ ring and the benzene ring is 1.89 (2)°. In the crystal, inversion-related molecules are linked by pairs of O—H···O hydrogen bonds, forming a cyclic dimers with $R_2^2(12)$ graph-set motif. Weak intermolecular C—H···$O_{carbonyl}$ and C—H···$O_{hydroxy}$ hydrogen bonds link the dimers into chains along [010], generating two $C(6)$ motifs that overlap three C atoms, forming $R_2^2(8)$ ring motifs.

Related literature

For the spectroscopy and the dynamic processes related to the intramolecular proton transfer of the title compound, see: Aquino et al. (2005); Chou et al. (1991); Nagaoka et al. (1984); Nishiya et al. (1986). For its preparation, see: Tadić et al. (1988). For related structures, see: Li et al. (2007); Saeed et al. (2007). For graph-set theory, see: Bernstein et al. (1995).
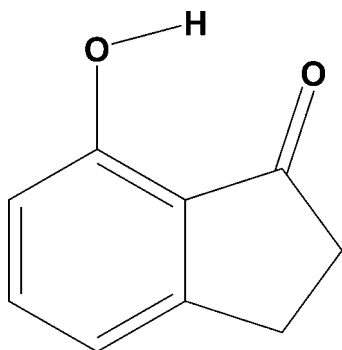
Experimental

Crystal data

$C_9H_8O_2$
$M_r = 148.15$

Monoclinic, $P2_1/n$
$a = 7.3457$ (3) Å
$b = 13.3767$ (5) Å
$c = 7.3693$ (3) Å
$\beta = 108.584$ (2)°
$V = 686.36$ (5) Å^3

$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 100$ K
$0.28 \times 0.24 \times 0.24$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2001)
$T_{min} = 0.676$, $T_{max} = 0.745$

5437 measured reflections
1400 independent reflections
1252 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.089$
$S = 1.04$
1400 reflections

133 parameters
All H-atom parameters refined
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.880 (17)	2.182 (18)	2.899 (1)	138 (1)
O2—H2···O1^i	0.880 (17)	2.219 (14)	2.864 (1)	130 (1)
C1—H1B···O2^{ii}	0.985 (14)	2.519 (14)	3.478 (1)	164 (1)
C4—H4···O1^{iii}	0.964 (16)	2.527 (16)	3.467 (1)	165 (1)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); 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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supporting information

7-Hydroxyindan-1-one

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S1. Comment

The excited-state intramolecular proton transfer (ESIPT) reaction of 7-hydroxy-1-indanone (7HIN) has been investigated for past decades (Aquino *et al.*, 2005; Nagaoka *et al.*, 1984; Nishiya *et al.*, 1986), which incorporates transfer of a hydroxy proton to the carbonyl oxygen through a intramolecular six-membered-ring hydrogen-bonding system (Chou *et al.*, 1991).

The *ORTEP* diagram of the title compound is shown in Figure 1. The indane moiety is essentially planar (r.m.s. deviation for the nine C atoms = 0.014 Å), which is consistent with previous studies (Li, *et al.*, 2007; Saeed *et al.*, 2007). 7HIN possesses a intramolecular six-membered ring hydrogen bond, which generates an $S(6)$ ring motif. The dihedral angle between the mean plane of the $S(6)$ ring and the mean plane of the benzene ring is 1.89 (2)°. This, together with 2.182 (18) Å of O2—H2···O1 distance and 138 (1)° of O2—H2—O1 (Table 1), strongly supports the $S(6)$ ring formation. (Bernstein *et al.*, 1995). In the crystal structure, two inversion related molecules are linked by dual O—H···O hydrogen bonds (black dashed line) to form a cyclic dimer of $R_2^2(12)$ ring system (Fig. 2). Furthermore, weak intermolecular C4—H4···O1 (green dashed line) and C1—H1B···O2 (blue dashed line) hydrogen bonds link the dimers into the chains along [0 1 0], generating two $C(6)$ motifs that overlap three C atoms (C2, C8 and C3) to form $R_2^2(8)$ ring motifs.

S2. Experimental

7-hydroxy-1-indanone was purchased from Sigma-Aldrich (>97% purity) and used as received without further purification. White needle-shaped crystals suitable for the crystallographic studies reported here were isolated over a period of two weeks by slow evaporation from a cyclohexane solution.

S3. Refinement

H atoms bonded to O and C atoms were located in a difference electron density map and refined freely with respective distances of 0.88 (2) Å for O—H, and for C—H in the range 0.95 (2) - 1.01 (1) Å. The freely refined U_{iso}(H) were found in ranges between 0.019 (3) and 0.024 (4) Å^{-2} (bound to C atoms), for the hydroxy H atom a value of 0.044 (5) Å^{-2} was observed.
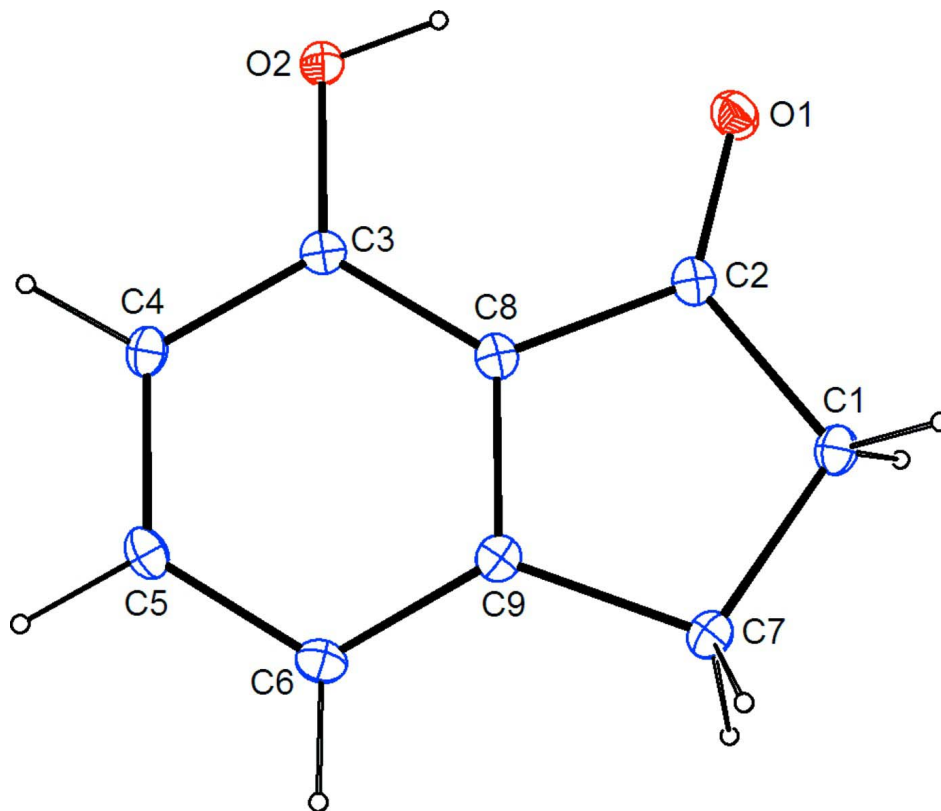
Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.
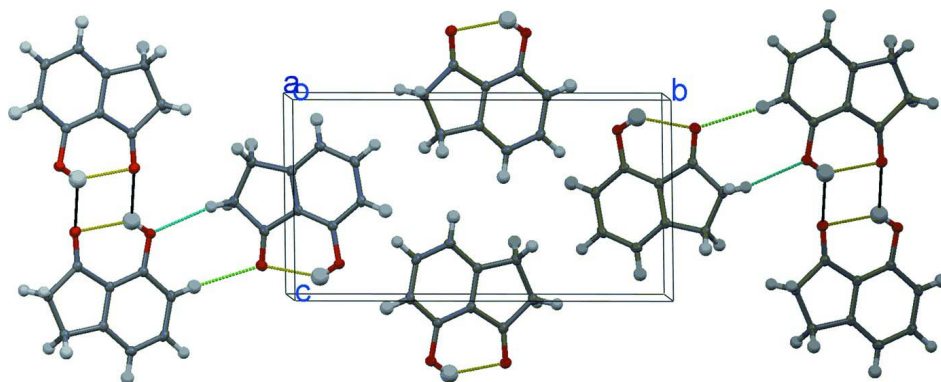
Figure 2

A section of the crystal packing of the title compound, viewed down the *a* axis.

7-Hydroxyindan-1-one

Crystal data

$C_9H_8O_2$	$c = 7.3693$ (3) Å
$M_r = 148.15$	$\beta = 108.584$ (2)°
Monoclinic, $P2_1/n$	$V = 686.36$ (5) Å^3
Hall symbol: -P 2yn	$Z = 4$
$a = 7.3457$ (3) Å	$F(000) = 312$
$b = 13.3767$ (5) Å	$D_x = 1.434$ Mg m^{-3}

Mo *Kα* radiation, *λ* = 0.71073 Å

Cell parameters from 2865 reflections

θ = 3.3–26.4°

μ = 0.10 mm⁻¹

T = 100 K

Prism, colourless

0.28 × 0.24 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer	5437 measured reflections
Radiation source: fine-focus sealed tube	1400 independent reflections
Graphite monochromator	1252 reflections with $I > 2\sigma(I)$
φ and *ω* scans	R_{int} = 0.022
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	θ_{max} = 26.4°, θ_{min} = 3.1°
T_{min} = 0.676, T_{max} = 0.745	$h = -9 \rightarrow 9$
	$k = -16 \rightarrow 16$
	$l = -9 \rightarrow 7$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.033

$wR(F^2)$ = 0.089

S = 1.04

1400 reflections

133 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

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 0.2373P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.28 e Å⁻³

$\Delta\rho_{min}$ = −0.18 e Å⁻³

Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc²λ³/sin(2θ)]⁻¹ᐟ⁴

Extinction coefficient: 0.014 (4)

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	0.08166 (12)	0.42309 (6)	0.66091 (12)	0.0198 (2)
O2	0.23230 (12)	0.62427 (6)	0.67482 (12)	0.0187 (2)
C1	0.13603 (16)	0.35050 (9)	0.97988 (17)	0.0164 (3)
C2	0.14647 (15)	0.42957 (8)	0.83566 (17)	0.0147 (3)
C3	0.28549 (15)	0.60687 (8)	0.86582 (17)	0.0141 (3)
C4	0.38227 (16)	0.68108 (9)	0.99239 (17)	0.0158 (3)
C5	0.43377 (16)	0.66351 (9)	1.18845 (17)	0.0168 (3)
C6	0.39144 (16)	0.57428 (9)	1.26467 (17)	0.0168 (3)
C7	0.23864 (17)	0.39569 (9)	1.17926 (18)	0.0170 (3)
C8	0.24541 (15)	0.51652 (8)	0.94170 (16)	0.0139 (3)
C9	0.29761 (15)	0.49992 (8)	1.13835 (17)	0.0143 (3)

H1A	0.001 (2)	0.3364 (10)	0.9591 (19)	0.019 (3)*
H1B	0.1971 (19)	0.2884 (10)	0.9566 (19)	0.019 (3)*
H2	0.164 (2)	0.5745 (14)	0.609 (2)	0.044 (5)*
H4	0.414 (2)	0.7437 (12)	0.945 (2)	0.026 (4)*
H5	0.5008 (19)	0.7159 (10)	1.2762 (19)	0.019 (3)*
H6	0.425 (2)	0.5649 (11)	1.398 (2)	0.024 (4)*
H7A	0.154 (2)	0.3975 (11)	1.264 (2)	0.024 (4)*
H7B	0.354 (2)	0.3563 (10)	1.250 (2)	0.021 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0216 (5)	0.0187 (5)	0.0167 (5)	−0.0005 (3)	0.0025 (4)	−0.0018 (3)
O2	0.0228 (5)	0.0171 (4)	0.0146 (5)	−0.0036 (3)	0.0038 (3)	0.0006 (3)
C1	0.0153 (6)	0.0142 (6)	0.0200 (6)	0.0005 (4)	0.0061 (5)	0.0003 (5)
C2	0.0113 (5)	0.0144 (6)	0.0187 (6)	0.0021 (4)	0.0051 (4)	−0.0008 (4)
C3	0.0117 (5)	0.0157 (6)	0.0151 (6)	0.0024 (4)	0.0043 (4)	0.0009 (4)
C4	0.0140 (5)	0.0130 (5)	0.0204 (7)	0.0002 (4)	0.0057 (5)	0.0005 (4)
C5	0.0143 (5)	0.0153 (6)	0.0195 (6)	0.0006 (4)	0.0035 (5)	−0.0044 (5)
C6	0.0159 (6)	0.0198 (6)	0.0141 (6)	0.0024 (4)	0.0037 (5)	−0.0003 (5)
C7	0.0178 (6)	0.0154 (6)	0.0180 (6)	0.0008 (4)	0.0059 (5)	0.0019 (5)
C8	0.0110 (5)	0.0140 (5)	0.0170 (6)	0.0017 (4)	0.0050 (4)	−0.0010 (4)
C9	0.0118 (5)	0.0145 (6)	0.0173 (6)	0.0033 (4)	0.0054 (4)	0.0007 (4)

Geometric parameters (Å, º)

O1—C2	1.2255 (14)	C4—C5	1.3919 (17)
O2—C3	1.3556 (14)	C4—H4	0.962 (16)
O2—H2	0.883 (19)	C5—C6	1.3958 (17)
C1—C2	1.5185 (16)	C5—H5	0.974 (14)
C1—C7	1.5448 (17)	C6—C9	1.3864 (16)
C1—H1A	0.976 (15)	C6—H6	0.945 (15)
C1—H1B	0.984 (14)	C7—C9	1.5184 (16)
C2—C8	1.4594 (15)	C7—H7A	1.011 (14)
C3—C4	1.3922 (16)	C7—H7B	0.993 (14)
C3—C8	1.4017 (16)	C8—C9	1.3937 (16)
C3—O2—H2	111.7 (11)	C4—C5—H5	118.7 (8)
C2—C1—C7	105.96 (9)	C6—C5—H5	118.6 (8)
C2—C1—H1A	107.5 (8)	C9—C6—C5	118.04 (11)
C7—C1—H1A	112.9 (8)	C9—C6—H6	121.0 (9)
C2—C1—H1B	109.8 (8)	C5—C6—H6	120.9 (9)
C7—C1—H1B	112.6 (8)	C9—C7—C1	104.72 (9)
H1A—C1—H1B	107.9 (11)	C9—C7—H7A	111.8 (8)
O1—C2—C8	125.41 (11)	C1—C7—H7A	112.6 (8)
O1—C2—C1	126.65 (10)	C9—C7—H7B	110.0 (8)
C8—C2—C1	107.94 (10)	C1—C7—H7B	111.6 (8)
O2—C3—C4	119.33 (10)	H7A—C7—H7B	106.3 (11)

O2—C3—C8	122.32 (10)	C9—C8—C3	121.94 (10)
C4—C3—C8	118.35 (11)	C9—C8—C2	110.78 (10)
C5—C4—C3	119.14 (11)	C3—C8—C2	127.28 (11)
C5—C4—H4	120.3 (9)	C6—C9—C8	119.80 (11)
C3—C4—H4	120.5 (9)	C6—C9—C7	129.62 (11)
C4—C5—C6	122.71 (11)	C8—C9—C7	110.57 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.880 (17)	2.182 (18)	2.899 (1)	138 (1)
O2—H2···O1ⁱ	0.880 (17)	2.219 (14)	2.864 (1)	130 (1)
C1—H1*B*···O2ⁱⁱ	0.985 (14)	2.519 (14)	3.478 (1)	164 (1)
C4—H4···O1ⁱⁱⁱ	0.964 (16)	2.527 (16)	3.467 (1)	165 (1)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iii) −*x*+1/2, *y*+1/2, −*z*+3/2.