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4-Hydroxyindan-1-one

Che-Wei Chang, Sin-Kai Fang, Ming-Hui Luo, Hsing-Yang Tsai and Kew-Yu Chen*

Department of Chemical Engineering, Feng Chia University, 40724 Taichung, Taiwan
Correspondence e-mail: kyuchen@fcu.edu.tw

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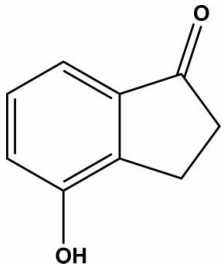
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.115; data-to-parameter ratio = 17.2.

The molecule of the title compound, $C_9H_8O_2$, is essentially planar except for the methylene H atoms [maximum deviation = 0.028 (1) Å]. In the crystal, the molecules are linked by classical O—H···O hydrogen bonds and weak C—H···O interactions into chains along [110] and [1$\bar{1}$0].

Related literature

For the preparation of the title compound, see: Gerasov *et al.* (2011). For applications of indanone derivatives, see: Tang *et al.* (2011); Borbone *et al.* (2011); Borge *et al.* (2010); Cai *et al.* (2005); Cui *et al.* (2009); Fu & Wang (2008); Li *et al.* (2009); Sousa *et al.* (2011); Yu *et al.* (2011). For related structures, see: Ali *et al.* (2010); Chen *et al.* (2011*a*,*b*). For graph-set theory, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_9H_8O_2$
M_r = 148.15
Monoclinic, $C2/c$
a = 13.5890 (6) Å
b = 8.6160 (3) Å
c = 13.9435 (6) Å
β = 116.738 (6)°
V = 1457.98 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 297 K
0.63 × 0.60 × 0.38 mm

Data collection

Bruker SMART CCD detector diffractometer
6305 measured reflections
1794 independent reflections
1289 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.06
1794 reflections
104 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2^{i}	0.94 (2)	1.75 (2)	2.6918 (18)	175 (2)
C2—H2A···O2^{i}	0.93	2.59	3.255 (2)	129

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

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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* publication routines (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5628).

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4-Hydroxyindan-1-one

Che-Wei Chang, Sin-Kai Fang, Ming-Hui Luo, Hsing-Yang Tsai and Kew-Yu Chen

S1. Comment

Indanone derivatives are some of the most widely used organic compounds (Tang *et al.*, 2011). Indanone derivatives are used as dyes and pigments (Cui *et al.*, 2009; Li *et al.*, 2009), intermediates in organic synthesis (Borbone *et al.*, 2011; Borge *et al.*, 2010; Fu & Wang, 2008; Yu *et al.*, 2011), and exhibit a wide variety of biological activities (Sousa *et al.*, 2011). In addition, 1-indanones were important precursors in the regiospecific synthesis of 2-fluoro-1-naphthols (Cai *et al.*, 2005).

The molecular structure of the title compound is shown in Figure 1. The molecule is essentially planar (the maximum deviation = 0.028 (1) Å), which is consistent with previous studies (Ali *et al.*, 2010; Chen *et al.*, 2011*a*,*b*). In the crystal (Fig. 2), molecules are linked by intermolecular O—H···O and C—H···O hydrogen bonds (Table 1) to form an infinite one-dimensional chain along and [1 1 0 and][1 -1 0], generating two different kinds of C(7) motifs (Bernstein *et al.*, 1995).

S2. Experimental

The title compound was synthesized by the hydrolation of 4-benzoyloxy-1-indanone with sodium hydroxide (Gerasov *et al.*, 2011). Colorless parallelepiped -shaped crystals suitable for the crystallographic studies reported here were isolated over a period of five weeks by slow evaporation from a ethyl acetate solution.

S3. Refinement

H atoms bonded to O and C atoms were located in a difference electron density map. The hydroxy H atom and the C_{sp3} H atoms were freely refined, and the C_{sp2} H atoms repositioned geometrically and refined using a riding model, [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)].

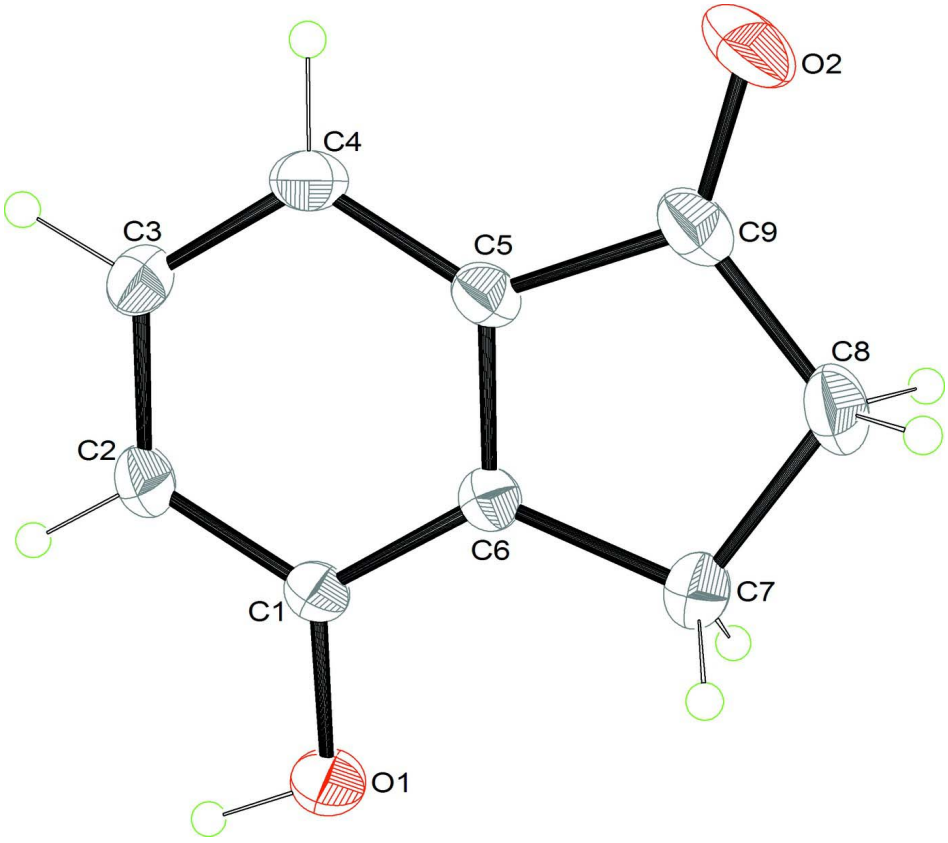

Figure 1

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

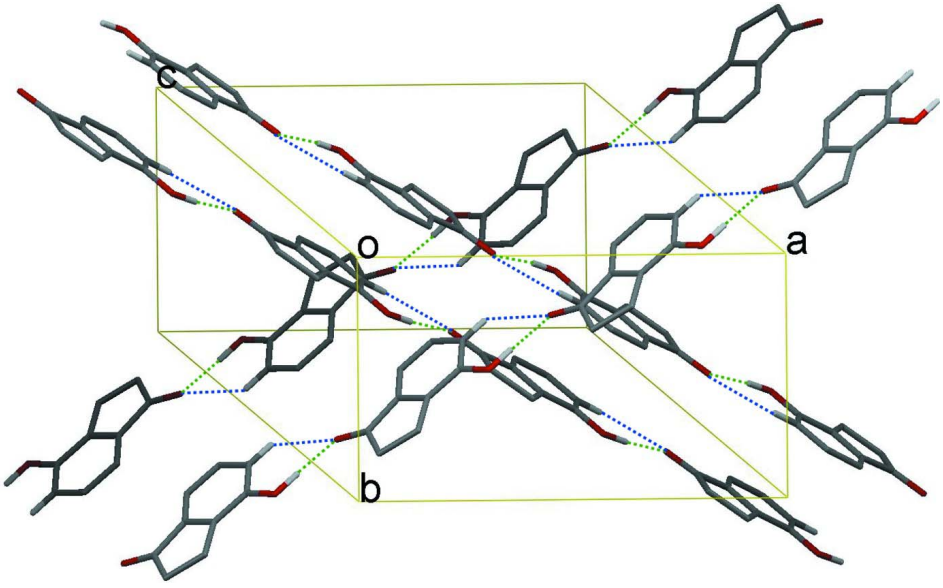

Figure 2

A section of the crystal packing of the title compound, viewed along the *c* axis. Green and blue dashed lines denote the intermolecular O1—H1A···O2 and C2—H2A···O2 hydrogen bonds, respectively. For clarity, hydrogen atoms not involved in hydrogen bonding have been omitted.

4-Hydroxyindan-1-one

Crystal data

$C_9H_8O_2$
$M_r = 148.15$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 13.5890\ (6)$ Å
$b = 8.6160\ (3)$ Å
$c = 13.9435\ (6)$ Å
$\beta = 116.738\ (6)°$
$V = 1457.98\ (13)$ Å^3
$Z = 8$
$F(000) = 624$
$D_x = 1.350$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3232 reflections
$\theta = 2.8–29.2°$
$\mu = 0.10$ mm^{-1}
$T = 297$ K
Parallelepiped, colorless
0.63 × 0.60 × 0.38 mm

Data collection

Bruker SMART CCD detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6305 measured reflections
1794 independent reflections
1289 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 29.2°$, $\theta_{min} = 2.9°$
$h = -18\rightarrow18$
$k = -11\rightarrow11$
$l = -19\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.115$
$S = 1.06$
1794 reflections
104 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
$w = 1/[\sigma^2(F_o^2) + (0.0704P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.21183 (9)	0.05958 (13)	0.03489 (8)	0.0607 (3)
H1A	0.1454 (17)	0.116 (3)	0.0012 (17)	0.101 (6)*
O2	0.51759 (9)	−0.29276 (13)	−0.06930 (10)	0.0714 (4)
C1	0.24288 (9)	0.01208 (14)	−0.04004 (9)	0.0373 (3)

C2	0.18722 (10)	0.05169 (14)	−0.14805 (10)	0.0405 (3)
H2A	0.1252	0.1147	−0.1716	0.049*
C3	0.22258 (10)	−0.00108 (14)	−0.22117 (9)	0.0414 (3)
H3A	0.1839	0.0273	−0.2930	0.050*
C4	0.31337 (10)	−0.09427 (14)	−0.18965 (10)	0.0404 (3)
H4A	0.3372	−0.1300	−0.2386	0.049*
C5	0.36864 (9)	−0.13348 (13)	−0.08148 (9)	0.0350 (3)
C6	0.33542 (9)	−0.08162 (13)	−0.00686 (9)	0.0341 (3)
C7	0.40960 (11)	−0.13665 (16)	0.10481 (10)	0.0470 (3)
H7A	0.3686	−0.1952	0.1343	0.056*
H7B	0.4457	−0.0499	0.1519	0.056*
C8	0.49369 (11)	−0.24025 (16)	0.09019 (12)	0.0499 (4)
H8A	0.5681	−0.2036	0.1346	0.060*
H8B	0.4879	−0.3465	0.1100	0.060*
C9	0.46657 (10)	−0.23041 (14)	−0.02658 (11)	0.0445 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0637 (7)	0.0832 (8)	0.0452 (6)	0.0363 (6)	0.0333 (5)	0.0071 (5)
O2	0.0529 (6)	0.0864 (8)	0.0794 (8)	0.0316 (6)	0.0337 (6)	−0.0066 (6)
C1	0.0363 (6)	0.0424 (6)	0.0357 (6)	0.0098 (5)	0.0186 (5)	0.0002 (5)
C2	0.0350 (6)	0.0421 (7)	0.0416 (7)	0.0121 (5)	0.0149 (5)	0.0066 (5)
C3	0.0460 (7)	0.0437 (7)	0.0305 (6)	0.0028 (5)	0.0135 (5)	0.0024 (5)
C4	0.0442 (7)	0.0446 (7)	0.0373 (6)	0.0016 (5)	0.0226 (6)	−0.0067 (5)
C5	0.0305 (6)	0.0354 (6)	0.0398 (6)	0.0029 (5)	0.0162 (5)	−0.0040 (4)
C6	0.0315 (6)	0.0365 (6)	0.0327 (6)	0.0047 (5)	0.0130 (5)	−0.0003 (4)
C7	0.0428 (7)	0.0557 (8)	0.0357 (7)	0.0110 (6)	0.0118 (6)	0.0040 (5)
C8	0.0353 (7)	0.0491 (7)	0.0532 (8)	0.0116 (6)	0.0091 (6)	0.0054 (6)
C9	0.0329 (6)	0.0425 (7)	0.0559 (8)	0.0069 (5)	0.0181 (6)	−0.0051 (6)

Geometric parameters (Å, º)

O1—C1	1.3542 (13)	C4—H4A	0.9300
O1—H1A	0.94 (2)	C5—C6	1.3814 (15)
O2—C9	1.2229 (14)	C5—C9	1.4622 (16)
C1—C6	1.3869 (15)	C6—C7	1.5011 (16)
C1—C2	1.3899 (17)	C7—C8	1.5341 (18)
C2—C3	1.3848 (16)	C7—H7A	0.9700
C2—H2A	0.9300	C7—H7B	0.9700
C3—C4	1.3683 (16)	C8—C9	1.501 (2)
C3—H3A	0.9300	C8—H8A	0.9700
C4—C5	1.3906 (16)	C8—H8B	0.9700
C1—O1—H1A	109.4 (12)	C1—C6—C7	127.94 (10)
O1—C1—C6	117.97 (10)	C5—C6—C7	112.62 (10)
O1—C1—C2	123.73 (11)	C6—C7—C8	103.81 (10)
C6—C1—C2	118.30 (10)	C6—C7—H7A	111.0

C1—C2—C3	121.15 (11)	C8—C7—H7A	111.0
C1—C2—H2A	119.4	C6—C7—H7B	111.0
C3—C2—H2A	119.4	C8—C7—H7B	111.0
C4—C3—C2	121.17 (11)	H7A—C7—H7B	109.0
C4—C3—H3A	119.4	C9—C8—C7	106.09 (10)
C2—C3—H3A	119.4	C9—C8—H8A	110.5
C3—C4—C5	117.38 (10)	C7—C8—H8A	110.5
C3—C4—H4A	121.3	C9—C8—H8B	110.5
C5—C4—H4A	121.3	C7—C8—H8B	110.5
C4—C5—C6	122.57 (10)	H8A—C8—H8B	108.7
C4—C5—C9	128.81 (10)	O2—C9—C5	125.30 (13)
C6—C5—C9	108.63 (10)	O2—C9—C8	125.95 (12)
C1—C6—C5	119.44 (10)	C5—C9—C8	108.75 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2^{i}	0.94 (2)	1.75 (2)	2.6918 (18)	175 (2)
C2—H2*A*···O2^{i}	0.93	2.59	3.255 (2)	129

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