O3—C15	1.313 (3)	C10—C18	1.525 (3)
O3—C16	1.461 (4)	C10—C15	1.535 (4)
O4—C18	1.194 (3)	C11—C12	1.358 (4)
O5—C18	1.320 (3)	C12—C13	1.412 (4)
O5—C19	1.467 (4)	C13—C14	1.346 (5)
N—C7	1.377 (4)	C16—C17	1.470 (7)
N—C6	1.434 (3)	C19—C20	1.489 (7)
N—C10	1.470 (3)		
C14—S—C11	92.3 (2)	N—C10—C15	110.2 (2)
C15—O3—C16	118.0 (3)	C18—C10—C15	112.1 (2)
C18—O5—C19	116.0 (2)	N—C10—C9	101.2 (2)
C7—N—C10	113.0 (2)	C18—C10—C9	109.9 (2)
C6—N—C10	125.6 (2)	C15—C10—C9	111.3 (2)
C5—C6—N	119.2 (2)	C12—C11—C9	129.3 (2)
O1—C7—N	124.4 (3)	C12—C11—S	110.3 (2)
N—C7—C8	108.2 (2)	C9—C11—S	120.4 (2)
C7—C8—C9	104.4 (2)	C11—C12—C13	112.8 (3)
C11—C9—C8	115.4 (2)	C14—C13—C12	113.1 (4)
C8—C9—C10	103.0 (2)	C13—C14—S	111.5 (3)
N—C10—C18	111.7 (2)		
C10—N—C7—C8	4.0 (3)	C8—C9—C10—N	30.8 (3)
N—C7—C8—C9	17.0 (3)	N—C10—C15—O2	98.5 (3)
C7—C8—C9—C10	−29.4 (3)	N—C10—C18—O4	−17.0 (4)
C7—N—C10—C9	−22.2 (3)		

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	1.00 (3)	2.57 (3)	3.366 (3)	137 (3)
C12—H12···O4^{ii}	0.91 (4)	2.52 (4)	3.351 (5)	153 (3)
C14—H14···O1^{iii}	0.92 (5)	2.58 (5)	3.433 (6)	154 (4)

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

The title structure was solved by direct methods and refined by full-matrix least-squares techniques. All H atoms were located from a difference Fourier map and refined isotropically.

Programs used for data collection, cell refinement and data reduction: *XSCANS* (Siemens, 1994); for structure solution and molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); for structure refinement: *SHELXL*93 (Sheldrick, 1993); for geometrical calculations: *PARST* (Nardelli, 1983*b*).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: MU1338). Services for accessing these data are described at the back of the journal.

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2-Acetyl-5,8-dihydronaphthalen-1-ol

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Abstract

The heavy-atom skeleton of the title molecule, $C_{12}H_{12}O_2$, is planar to within ±0.023 (2) Å and an O—H···O intramolecular hydrogen bond contributes to this planarity.

Comment

Dihydronaphthalene derivatives are widely used as intermediates in the synthesis of several polycyclic phenols which are useful antifibrillatory agents, disinfectants and water softeners (Hauck *et al.*, 1977). Furthermore, hydroxy–ketone derivatives of naphthalene are useful in synthesizing the sub-units of daunomycinone and adiramycin, which are important anticancer drugs (Crouse *et al.*, 1981).

The title molecule, (I), as a whole, is planar within ±0.023 (2) Å. The planarity is stabilized by an O—H···O intramolecular hydrogen bond involving atoms O1 and O2 [O1···O2 2.546 (2), H1O2···O1 1.65 (2) Å and O2—H1O2···O1 154 (2)°]. In the dihydrobenzene ring, the C_{sp^2}—C_{sp^3} distances C5—C6 [1.481 (2) Å] and C9—C10 [1.491 (2) Å] are longer than the C6—C7 [1.465 (2) Å] and C8—C9 [1.461 (3) Å] distances because of the steric interactions caused by the planarity of the dihydrobenzene ring. The C5—C6—C7 [115.1 (2)°] and C8—C9—C10 [115.5 (2)°] angles are also widened

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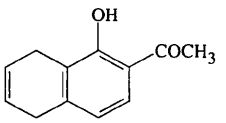
from ideal tetrahedral values due to these interactions. The length of the C7—C8 bond [1.327 (2)°] shows its double-bond nature.



(I)

In the crystal, molecules related by inversion lie in parallel planes 3.505 (1) Å apart, an optimum distance for π–π stacking interactions. These two sets of planes are nearly orthogonal [dihedral angle 85.36 (2)°] and are separated by a minimum non-bonding distance of 3.630 (2) Å between C6 and C2(x, $\frac{1}{2}-y$, $\frac{1}{2}+z$). This geometry indicates a possible side-on interaction. These pairs extend along the [011] direction to form infinite parallel chains.

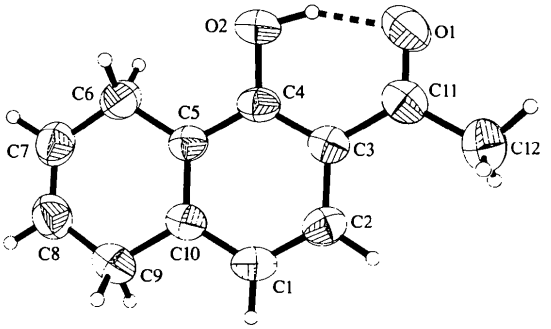


Fig. 1. The structure of title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms are displayed as small circles with an arbitrary radius.

Experimental

5,8-Dihydronaphthyl acetate was prepared by acylation of 5,8-dihydronaphthol using acetyl chloride and pyridine in dry benzene. Irradiation of 5,8-dihydronaphthyl acetate at 254 nm in dry ethyl acetate furnished the title compound (Sriraghavan & Ramakrishnan, 1997). Single crystals were obtained by slow concentration of a methanol solution of the compound.

Crystal data

$C_{12}H_{12}O_2$
M_r = 188.22
Monoclinic
$P2_1/c$
a = 8.9674 (8) Å
b = 9.0604 (9) Å
c = 11.8823 (11) Å
β = 96.087 (8)°
V = 960.0 (2) Å^3
Z = 4
D_x = 1.302 Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 33 reflections
θ = 5.5–12.5°
μ = 0.088 mm^{-1}
T = 293 (2) K
Rectangular
0.48 × 0.36 × 0.22 mm
Colourless

Data collection

Siemens $P4$ diffractometer
$\theta/2\theta$ scans
Absorption correction: none
2944 measured reflections
2207 independent reflections
1203 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.50°
$h = -1 \rightarrow 11$
$k = -1 \rightarrow 11$
$l = -15 \rightarrow 15$
3 standard reflections every 97 reflections
intensity decay: <3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.124
S = 0.881
2207 reflections
176 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.012 (4)
Scattering factors from *International Tables for Crystallography* (Vol. C)

The structure was solved by direct methods and refined by full-matrix least-squares techniques. All H atoms were located from a difference Fourier map and refined isotropically. S.u.'s on C—C distances do not exceed 0.003 Å.

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC*. Software used to prepare material for publication: *SHELXTL/PC*. Program used for molecular geometry: *PARST* (Nardelli, 1983).

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