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# 1-(1-Hydroxy-2-naphthyl)ethanone

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**Key indicators**

Single-crystal X-ray study
*T* = 296 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.060
*wR* factor = 0.171
Data-to-parameter ratio = 13.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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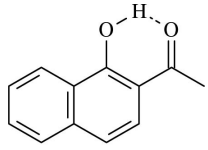
The molecule of the title compound, $C_{12}H_{10}O_2$, is planar, with an intramolecular O—H···O hydrogen bond between the hydroxy group and the carbonyl O atom. The structure is stabilized by intermolecular C—H···π and offset π–π stacking interactions.

## Comment

Some acetylnaphthalene derivatives have potential as pharmacologically active compounds (Walker *et al.*, 1981; Çalış *et al.*, 1988; Gupta & Singh, 1991; Karakurt *et al.*, 2001). In this study, we aimed to investigate the intra- and/or intermolecular interactions and the conformation of the title compound, (I), by X-ray crystallography.




(I)

In (I), the hydrogen-bonded ring *A* (O1/C2/C3/C12/O2/H2), and aromatic rings *B* (C3/C4/C5/C6/C11/C12) and *C* (C6/C7/C8/C9/C10/C11), are planar, with dihedral angles of 1.30 (1)° for *A*/*B*, 1.18 (1)° for *A*/*C* and 1.15 (1)° for *B*/*C* (Fig. 1). A significant intramolecular interaction is noted, involving hydroxy atom H1 and carbonyl atom O1, such that a six-membered ring is formed (Table 1). The bond lengths and angles are in normal ranges, and comparable with those in 2-bromo-1-(1-hydroxynaphthalen-2-yl)ethanone (Köysal *et al.*, 2004) and in our previous work on *o*-hydroxyaldehydes (Odabaşoğlu *et al.*, 2006; Odabaşoğlu & Büyükgüngör, 2006). The C2—O1 bond distance in (I) is also consistent with the value of the C=O double bond in carbonyl compounds (Loudon, 2002).

The structure of (I) is stabilized by C—H···π intermolecular interactions (Table 1, Fig. 2). There are also weak offset π—π stacking interactions between the *B* and *C* rings of symmetry-related molecules, with a plane-to-plane separation of 3.481 Å and a centroid-to-centroid distance of 3.821 Å, resulting in an angle between the ring normal and the centroid-to-centroid vector of 24° (Fig. 2).

## Experimental

1-(1-Hydroxynaphthalen-2-yl)ethanone, purchased from Avocado Research Chemicals Ltd. (99%), was dissolved in dimethylsulfoxide (393 K), and well shaped crystals of (I) were obtained from this hot solution (m.p. 372–373 K).

*Crystal data*

$C_{12}H_{10}O_2$
$M_r$ = 186.20
Monoclinic, $P2_1/c$
$a$ = 7.6259 (10) Å
$b$ = 7.0348 (7) Å
$c$ = 18.755 (3) Å
$\beta$ = 111.502 (10)°
$V$ = 936.1 (2) Å$^3$
$Z$ = 4
$D_x$ = 1.321 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 10250 reflections
$\theta$ = 2.3–27.1°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 (2) K
Prismatic stick, pale yellow
0.72 × 0.34 × 0.14 mm

*Data collection*

Stoe IPDS-2 diffractometer
$\omega$ scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min}$ = 0.548, $T_{max}$ = 0.946
10250 measured reflections
1692 independent reflections
1015 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.100
$\theta_{max}$ = 25.3°
$h = -9 \rightarrow 9$
$k = -8 \rightarrow 8$
$l = -22 \rightarrow 22$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.172
$S$ = 0.99
1692 reflections
129 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0964P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1$A$···$Cg2^{i}$ | 0.96 | 2.79 | 3.593 (3) | 142 |
| O2—H2···O1 | 0.82 | 1.80 | 2.524 (3) | 146 |

Symmetry code: (i) $-x+2, -y+1, -z+1$. $Cg2$ is the centroid of atoms C6–C11

All H atoms were introduced in calculated positions and treated as riding on their parent atoms, with O—H = 0.82 Å, and C—H = 0.93 Å ($C_{aromatic}$) and 0.96 Å ($CH_3$), and with $U_{iso}$(H) = 1.2$U_{eq}$($C_{aromatic}$,O) or $U_{iso}$(H) = 1.5$U_{eq}$($CH_3$).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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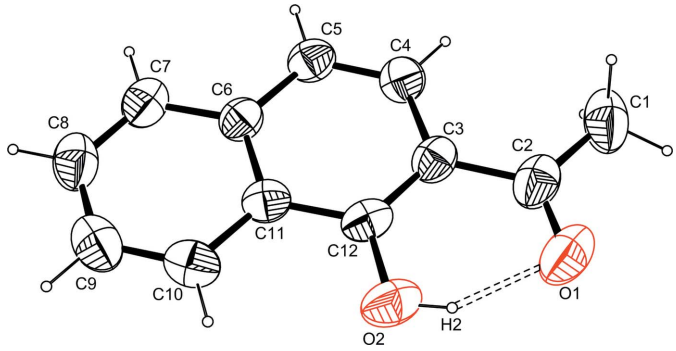


**Figure 1**
A view of (I), with the atomic numbering scheme. The intramolecular hydrogen bond is shown as a dashed line. Displacement ellipsoids are drawn at the 30% probability level.

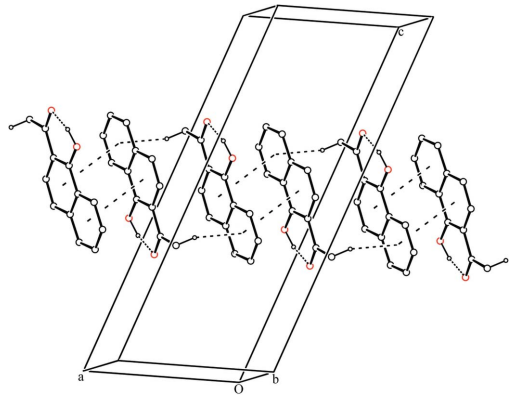


**Figure 2**
A partial packing diagram for (I). The intramolecular hydrogen bonds are shown as short dashed lines, and the C—H···$\pi$ and $\pi$–$\pi$ stacking interactions are shown as long dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.


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