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Methyl 1-hydroxy-2-naphthoate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.068
wR factor = 0.216
Data-to-parameter ratio = 14.6

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

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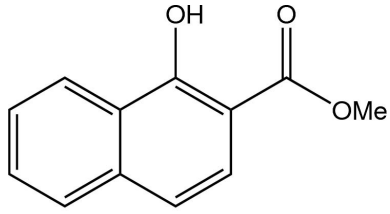
In the title compound, $C_{12}H_{10}O_3$, there are two independent molecules in the asymmetric unit. Both molecules are essentially planar and each features an intramolecular O—H···O hydrogen bond between the hydroxy H atom and the carbonyl O atom. The crystal structure is stabilized by π–π stacking interactions.

Comment

The title compound, (I), is an important material for the preparation of many compounds (Wang *et al.*, 2003; Kasibhatla *et al.*, 2001). Furthermore, 1-hydroxy-2-naphthoate and some of its derivatives also function as interesting ligands towards metal ions. These properties stimulated us to search for new methods to synthesize these types of molecules. In this paper, the X-ray crystal structure determination of (I) is reported.



(I)

The asymmetric unit contains two crystallographically independent molecules (Figs. 1 and 2). Bond lengths and angles in (I) are normal, and values for the two independent molecules agree well with each other (Table 1). Both of the independent molecules are essentially planar. For both molecules, an intramolecular hydrogen bond is observed between the hydroxy H atom and the carbonyl O atom (Table 2). The

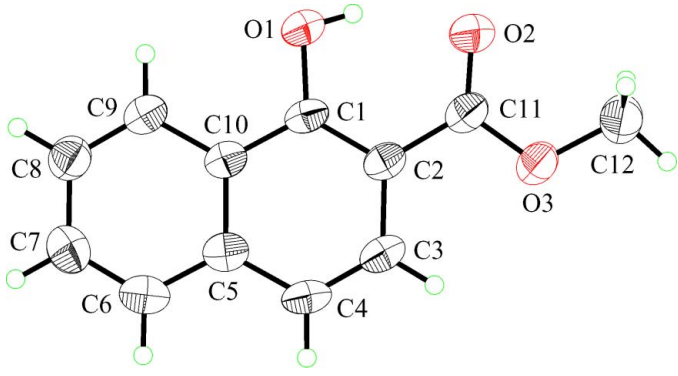


Figure 1
The first independent molecule of (I), showing 35% probability displacement ellipsoids.

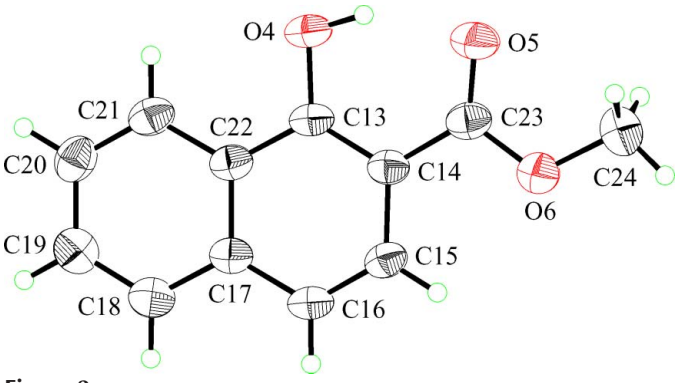


Figure 2
The second independent molecule of (I), showing 35% probability displacement ellipsoids.

crystal structure is stabilized by two types of π–π interactions. One is the centroid–centroid, $Cg3\cdots Cg3^{i}$ [$Cg3$ is the centroid of the C13–C17/C22 ring; symmetry code: (i) $-x, 2-y, -z$], separation of 3.5026 (17) Å. The other may be a face-to-face π–π stacking interaction between the independent molecules involving their respective inversion-related mate (Fig. 3), so that the perpendicular distances between the aromatic rings range from 3.41 to 3.57 Å, as observed in related structures (Du *et al.*, 2003; Xiao *et al.*, 2000).

Experimental

Compound (I) was synthesized according to a literature procedure (Gibney *et al.*, 1993). Single crystals suitable for X-ray analysis were grown from a saturated methanol solution, by slow evaporation at room temperature.

Crystal data

$C_{12}H_{10}O_3$
M_r = 202.20
Triclinic, $P\overline{1}$
a = 8.7325 (11) Å
b = 9.0677 (12) Å
c = 13.6287 (17) Å
α = 98.410 (2)°
β = 108.229 (2)°
γ = 102.689 (2)°
V = 972.7 (2) Å^3
Z = 4
D_x = 1.381 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1216 reflections
θ = 2.4–24.4°
μ = 0.10 mm^{-1}
T = 292 (2) K
Prism, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.971, T_{max} = 0.990
5729 measured reflections
4115 independent reflections
2602 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 27.0°
$h = -10 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -17 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.216
S = 1.04
4115 reflections
281 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0941P)^2 + 0.2807P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

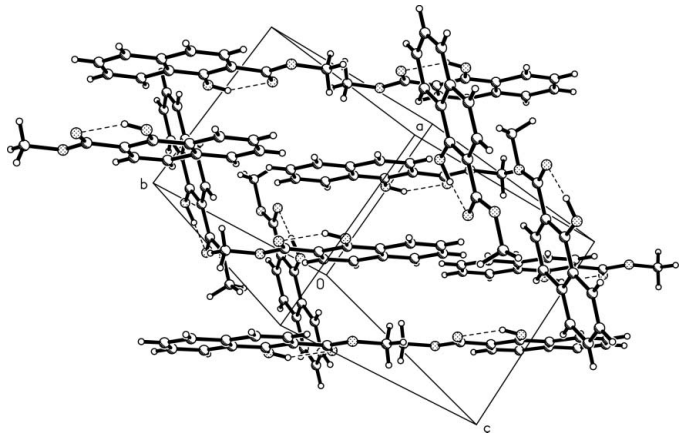


Figure 3
Packing diagram for (I). O—H···O hydrogen bonds are shown as dashed lines.

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.352 (3)	C13—O4	1.351 (3)
C2—C11	1.465 (4)	C14—C23	1.450 (4)
C11—O2	1.218 (3)	C23—O5	1.225 (3)
C11—O3	1.333 (3)	C23—O6	1.336 (3)
C12—O3	1.455 (4)	C24—O6	1.440 (4)
O1—C1—C2	122.6 (3)	O5—C23—O6	121.1 (3)
O2—C11—O3	121.8 (3)	O5—C23—C14	124.8 (3)
O2—C11—C2	124.5 (3)	C11—O3—C12	116.6 (2)
O4—C13—C14	122.6 (3)	C23—O6—C24	117.2 (2)
O1—C1—C10—C5	179.7 (2)	C15—C14—C23—O5	177.8 (3)
C3—C2—C11—O2	178.8 (3)	C2—C11—O3—C12	179.0 (3)
O4—C13—C22—C17	178.5 (2)	C14—C23—O6—C24	177.2 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.81 (3)	1.87 (3)	2.596 (3)	149 (3)
O4—H4···O5	0.94 (3)	1.74 (3)	2.594 (3)	149 (3)

The hydroxy H atoms were located in a difference Fourier map and refined isotropically. All other H atoms were placed in calculated positions, with C—H distances of 0.93 Å (Csp^2) and 0.96 Å (CH_3). They were included in the refinement in the riding-model approximation, with isotropic displacement parameters set to 1.2U_{eq} of the carrier atom (1.5U_{eq} for methyl H atoms).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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