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N-[(2-Hydroxynaphthalen-1-yl)(phenyl)methyl]-acetamide

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The crystal structure of the title compound, $C_{19}H_{17}N_1O_2$, obtained *via* a one-pot synthesis, is stabilized by intramolecular N—H···O and intermolecular O—H···O hydrogen bonds.

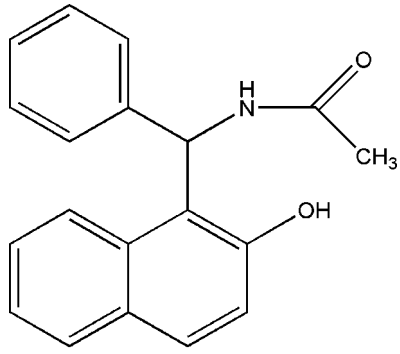
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.113
Data-to-parameter ratio = 13.2

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

Comment

Multi-component reactions (MCRs) have attracted considerable attention in terms of the saving of both energy and raw materials (Devi & Bhuyan, 2004). They have merits over multi-step reactions in several aspects, including the simplicity of a one-pot procedure, possible structural variations and in building up complex molecules (Domling & Ugi, 2000). Here we report the synthesis and crystal structure of the title compound (I) (Fig. 1), obtained by a three-component condensation reaction of 2-naphthol, benzaldehyde and acetamide under solvent-free conditions.



(I)

In the molecule of the title compound, (I) (Fig. 1), the bond distances and angles are within their normal ranges (Allen *et al.* 1987, Bazgir *et al.* 2006). The dihedral angles between the rings *A* (C14–C19), *B* (C4–C8/C13) and *C* (C8–C13) are *A*/*B* = 82.10 (2), *A*/*C* = 80.08 (3) and *B*/*C* = 2.25 (4)°. An intramolecular N—H···O interaction and an intermolecular O—H···O hydrogen bond (Table 1) help to establish the crystal packing (Fig. 2).

Experimental

2-Naphthol (1 mmol), benzaldehyde (1 mmol), acetamide (1.4 mmol) and *p*-toluenesulfonic acid (0.1 g) were mixed and the reaction mixture was placed in a screw-capped vial and heated at 373 K for 3 h. After cooling, the reaction mixture was washed with water and then recrystallized from EtOAc/hexane (1:2) to afford the pure product in 73% yield.

Crystal data

$C_{19}H_{17}NO_2$
M_r = 291.34
Monoclinic, $P2_1/n$
a = 11.835 (3) Å
b = 7.3428 (10) Å
c = 18.034 (3) Å
β = 106.958 (16)°
V = 1499.1 (5) Å^3
Z = 4
D_x = 1.291 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colorless
0.50 × 0.35 × 0.25 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: numerical (*X-RED32* and *X-SHAPE*; Stoe & Cie, 2005)
T_{min} = 0.960, T_{max} = 0.980
9203 measured reflections
3534 independent reflections
2932 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.9°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.114
S = 1.06
3534 reflections
267 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.3551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.889 (15)	2.118 (15)	2.7052 (16)	122.8 (13)
O2—H2···O1^{i}	0.87 (2)	1.82 (2)	2.6807 (16)	175 (3)

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

All of the H atoms were located in a difference sythesis and their positions and U_{iso} values were freely refined.

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; 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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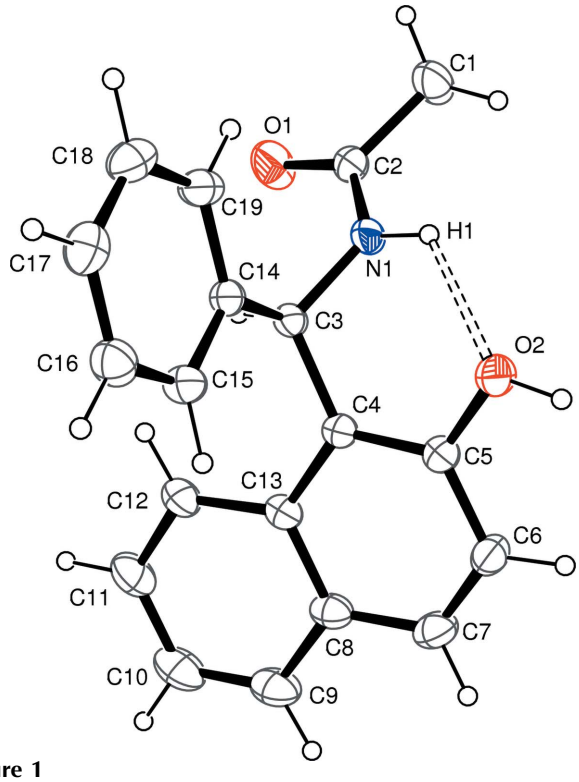

Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms). The double dashed line indicates a hydrogen bond.

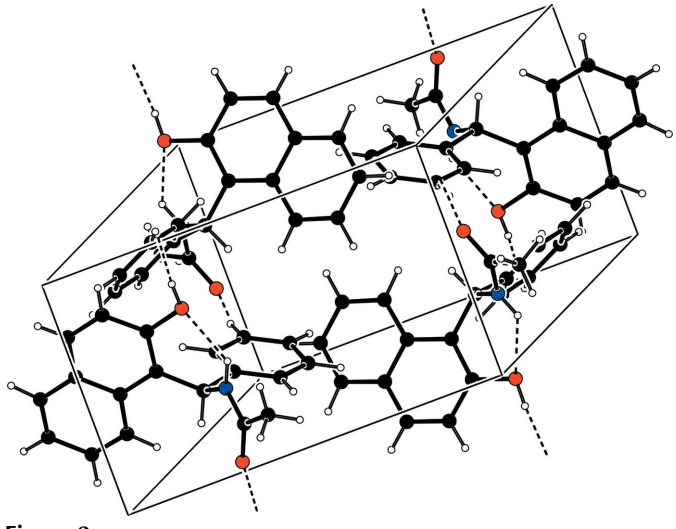

Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.