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Key indicators

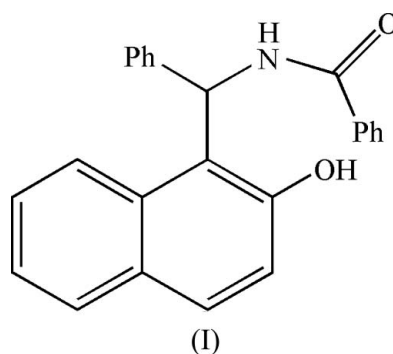
Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.080
 wR factor = 0.150
Data-to-parameter ratio = 12.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.***N*-[(2-Hydroxynaphthalen-1-yl)(phenyl)methyl]-
benzamide**Intermolecular O—H···O bonding and intramolecular N—
H···O hydrogen bonding are effective in the stabilization of
the crystal structure of the title compound, $\text{C}_{24}\text{H}_{19}\text{NO}_2$.

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Comment

Multi-component reactions (MCRs) (Hulme *et al.*, 2003; Ugi, 1962) involving at least three starting materials in a one-pot reaction remain the most efficient method of rapidly producing molecular diversity. As such, they have found widespread use in organic and diversity-oriented synthesis because of their ability to access highly functionalized molecules in simple and straightforward one-step transformations (Ugi, 2000). Compared to conventional multi-step organic syntheses, MCRs are advantageous owing to their greater atom efficiency, accessibility to large numbers of compounds and complex molecules, wide structural diversity and the simplicity of their one-pot procedures, making them amenable to combinatorial synthesis. The development and discovery of new MCRs is still in demand. Recently, we reported the syntheses and crystal structures of methyl *N*-[(2-hydroxynaphthalen-1-yl)(phenyl)methyl]carbamate (Bazgir *et al.*, 2006*a*) and 1-[(2-hydroxynaphthalen-1-yl)(phenyl)methyl]-3-methylurea (Bazgir *et al.*, 2006*b*). We now report the synthesis and structure of the title compound, (I).



The molecular structure of (I) is shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987; Bazgir *et al.*, 2006*a,b*). The crystal structure is stabilized by intramolecular N—H···O intermolecular O—H···O hydrogen bonding (Table 1), linking the molecules into a supramolecular chain (Fig. 2).

Experimental

2-Naphthol (1 mmol), benzaldehyde (1 mmol), benzamide (1 mmol) and 1-butyl-3-methylimidazolium bromide (1.4 mmol) were mixed

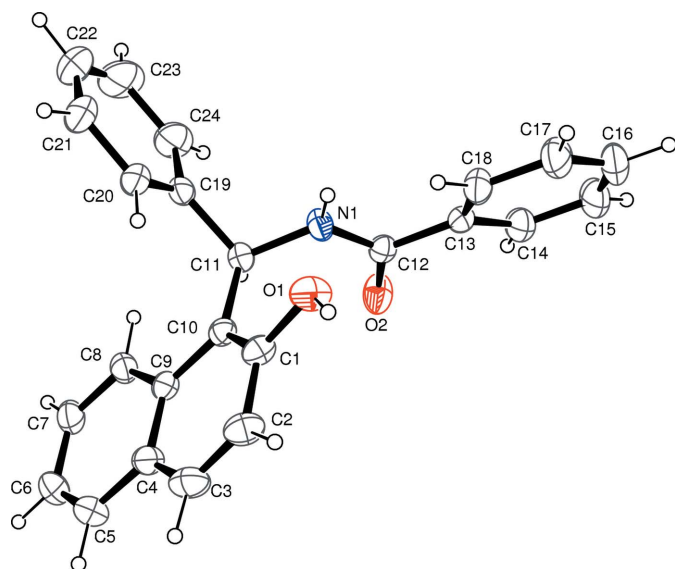


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

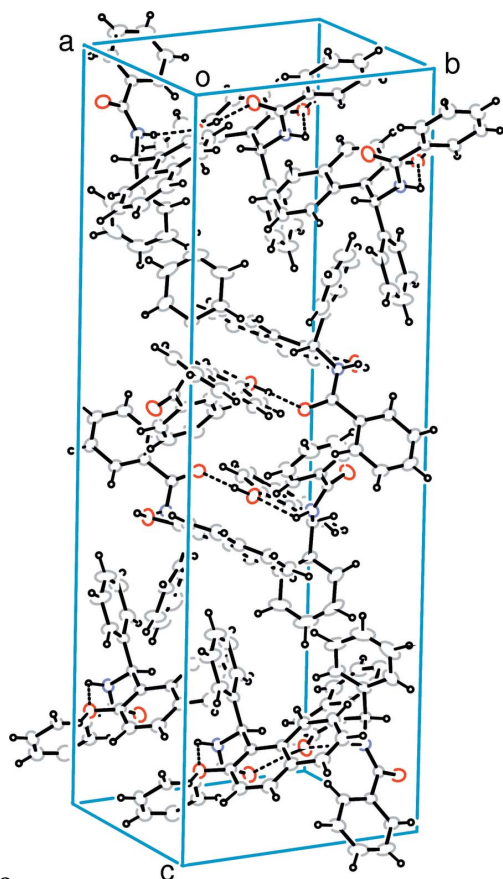


Figure 2
The packing of (I). Hydrogen bonds are shown as dashed lines.

and the reaction mixture was heated with stirring at 373 K for 2 h. After cooling, the reaction mixture was washed with water and then

recrystallized from EtOAc–hexane (1:3) to afford single crystals of (I) (yield 75%).

Crystal data

$C_{24}H_{19}NO_2$
 $M_r = 353.40$
Orthorhombic, $Pbca$
 $a = 9.8517 (17) \text{ \AA}$
 $b = 11.3516 (18) \text{ \AA}$
 $c = 33.451 (8) \text{ \AA}$
 $V = 3740.9 (12) \text{ \AA}^3$

$Z = 8$
 $D_x = 1.255 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
 $\mu = 0.08 \text{ mm}^{-1}$
 $T = 298 (2) \text{ K}$
Needle, colorless
 $0.6 \times 0.1 \times 0.05 \text{ mm}$

Data collection

Stoe IPDS-II diffractometer
 ω scans
Absorption correction: none
27152 measured reflections

4002 independent reflections
2906 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.147$
 $\theta_{max} = 27.1^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.080$
 $wR(F^2) = 0.150$
 $S = 1.18$
4002 reflections
320 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 2.1712P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.002$
 $\Delta\rho_{max} = 0.32 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.19 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1B \cdots O1$	0.90 (3)	2.31 (3)	2.633 (3)	101 (2)
$O1-H1A \cdots O2^i$	0.88 (4)	1.75 (4)	2.629 (3)	173 (4)

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

H atoms were located in a difference Fourier map and refined isotropically.

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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