

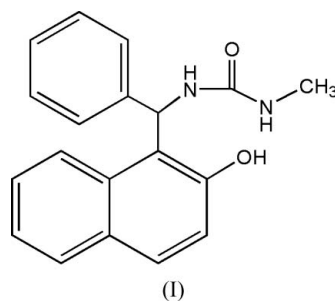
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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.045
 wR factor = 0.112
Data-to-parameter ratio = 12.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.1-[(2-Hydroxynaphthalen-1-yl)(phenyl)methyl]-
3-methylureaIntermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ and intramolecular
 $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds are effective in the stabilization of
the crystal structure of the title compound, $\text{C}_{19}\text{H}_{18}\text{N}_2\text{O}_2$.Received 9 August 2006
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Comment

Multi-component reactions (MCRs) are economically and
environmentally very advantageous because multi-step
syntheses produce considerable amounts of waste, mainly due
to a series of complex isolation procedures often involving
expensive, toxic and hazardous solvents after each step. MCRs
are perfectly suited for combinatorial laboratory synthesis,
and thus they are finding increasing use in the discovery
process for new drugs and agrochemicals (Domling & Ugi,
2000; Heck & Domling, 2000; Ugi *et al.*, 1994).The carbamate function is widely encountered in the
structure of biologically active compounds. These compounds
are generally prepared from phosgene (Nowick *et al.*, 1992),
phosgene derivatives (Majer & Randad, 1994; Batey *et al.*,
1998) or isocyanates (Ozaki, 1972), in reaction with amines.
None of these methods is environmentally benign. In the light
of the above, we have synthesized the title compound, (I),
under solvent-free conditions and characterized its structure.In the molecule of the title compound, (I) (Fig. 1), the bond
lengths and angles are within normal ranges (Allen *et al.*, 1987;
Bazgir *et al.*, 2006).The rings *A* (C4–C8/C13), *B* (C8–C13) and *C* (C14–C19)
are, of course, planar; the dihedral angles between them are $A/B = 2.93$ (3)°, $A/C = 79.4$ (3)° and $B/C = 82.4$ (4)°.As can be seen from the packing diagram (Fig. 2), inter-
molecular $\text{O}-\text{H}\cdots\text{O}$ [$\text{H}2b\cdots\text{O}1^i = 1.82$ (2), $\text{O}2\cdots\text{O}1^i = 2.689$ (1) Å and $\text{O}2-\text{H}2b\cdots\text{O}1^i = 175$ (2)°] and $\text{N}-\text{H}\cdots\text{O}$ [$\text{H}1d\cdots\text{O}1^{ii} = 2.111$ (19), $\text{N}1\cdots\text{O}1^{ii} = 2.992$ (2) Å and $\text{N}1-\text{H}1d\cdots\text{O}1^{ii} = 171$ (2)°] hydrogen bonds [symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + 2, -y, -z + 1$] link the molecules to form infinite chains. The intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ and intramolecular $\text{N}-\text{H}\cdots\text{O}$ [$\text{H}2a\cdots\text{O}2 = 2.185$ (18),

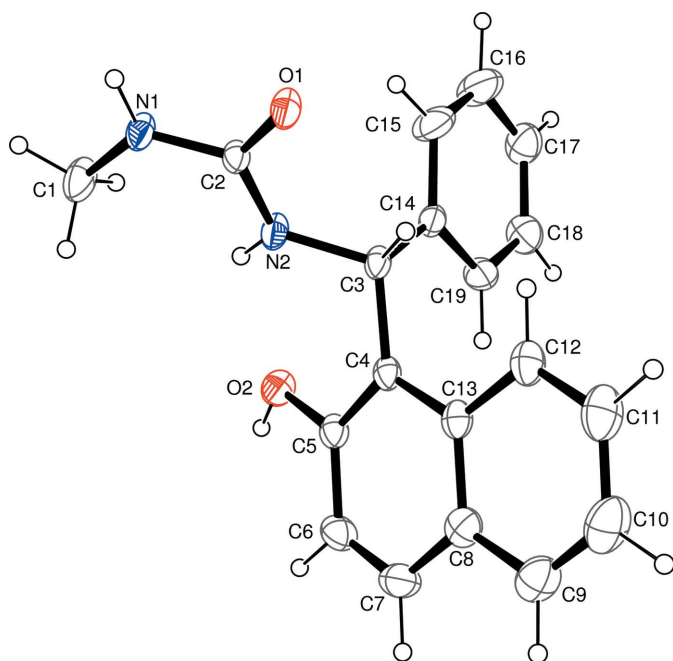


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

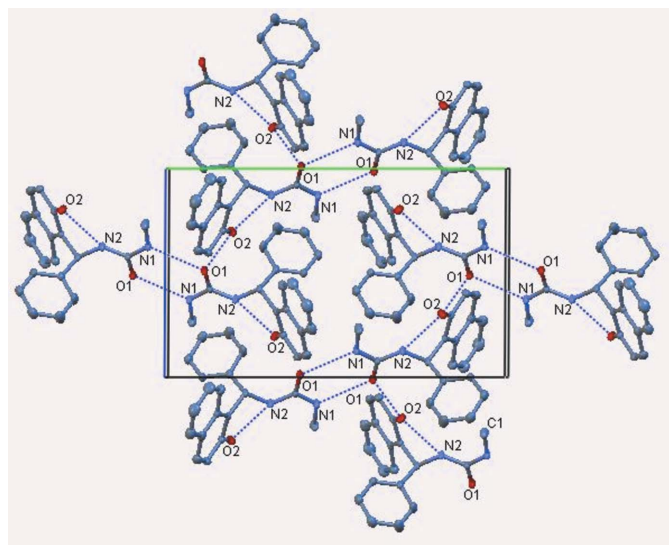


Figure 2
A packing diagram of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

$N2 \cdots O2 = 2.742(2) \text{ \AA}$ and $N2-H2a \cdots O2 = 122(2)^\circ$] hydrogen bonds seem to be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are effective in the molecular packing.

Experimental

2-Naphthol (1 mmol), benzaldehyde (1 mmol), *N*-methylurea (1.5 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 (1:3) to afford the pure product (yield 54%).

Crystal data

$C_{19}H_{18}N_2O_2$
 $M_r = 306.35$
Monoclinic, $P2_1/n$
 $a = 9.463(2) \text{ \AA}$
 $b = 16.550(3) \text{ \AA}$
 $c = 10.607(2) \text{ \AA}$
 $\beta = 107.191(16)^\circ$
 $V = 1587.0(6) \text{ \AA}^3$

$Z = 4$
 $D_x = 1.282 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
 $\mu = 0.08 \text{ mm}^{-1}$
 $T = 294(2) \text{ K}$
Block, colorless
 $0.35 \times 0.3 \times 0.2 \text{ mm}$

Data collection

Stoe IPDS-II diffractometer
 ω scans
Absorption correction: numerical
(shape of crystal determined optically) (*X-SHAPE*; Stoe & Cie, 2005)
 $T_{\min} = 0.971$, $T_{\max} = 0.983$

12022 measured reflections
3365 independent reflections
2827 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\max} = 26.7^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.112$
 $S = 1.09$
3365 reflections
280 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.4305P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 0.18 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$

H atoms were located in a difference synthesis and refined isotropically [$O-H = 0.88(2) \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 0.070(6) \text{ \AA}^2$; $N-H = 0.859(19)–0.889(19) \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 0.048(5)–0.050(5) \text{ \AA}^2$; $C-H = 0.94(3)–1.03(3) \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 0.035(4)–0.113(9) \text{ \AA}^2$].

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-STEP32* (Stoe & Cie, 2000); software used to prepare material for publication: *SHELXL97*.

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References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Batey, R. A., Santhakumar, V., Yoshina-Ishii, C. & Taylor, S. D. (1998). *Tetrahedron Lett.* **39**, 6267–6270.
Bazgir, A., Amani, V. & Khavasi, H. R. (2006). *Acta Cryst.* **E62**, o3533–o3534.
Domling, A. & Ugi, I. (2000). *Angew. Chem. Int. Ed.* **39**, 3169–3210.
Heck, S. & Domling, A. (2000). *Synlett*, pp. 424–426.
Majer, P. & Randa, R. S. (1994). *J. Org. Chem.* **59**, 1937–1938.
Nowick, J. S., Powell, N. A., Nguyen, T. M. & Noronha, G. (1992). *J. Org. Chem.* **57**, 7364–7366.
Ozaki, S. (1972). *Chem. Rev.* **72**, 457–496.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2000). *X-STEP32*. Version 1.07e. Stoe & Cie, Darmstadt, Germany.
Stoe & Cie (2005). *X-AREA* (Version 1.31), *X-RED32* (Version 1.28b) and *X-SHAPE* (Version 2.05). Stoe & Cie, Darmstadt, Germany.
Ugi, I., Domling, A. & Horl, W. (1994). *Endeavour*, **18**, 115–122.