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1-Benzyluracil

Jin-Chang Ding, Miao-Chang Liu, Hua-Yue Wu, Mao-Lin Hu and Hong-Ping Xiao*

Department of Chemistry and Materials Science, Wenzhou Normal College, Wenzhou 325027, People's Republic of China

Correspondence e-mail: hp_xiao@wznc.zj.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean *σ*(C–C) = 0.007 Å
R factor = 0.054
wR factor = 0.126
Data-to-parameter ratio = 6.8

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

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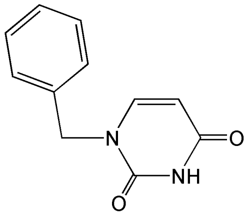
In the title compound, $C_{11}H_{10}N_2O_2$, the benzene ring is almost perpendicular to the heterocycle; the dihedral angle is 91.2 (2)°. A chain structure is formed *via* an intermolecular N—H···O hydrogen bond.

Comment

Uracil and thymine are important nucleobases in biology, being responsible for a wide range of biochemical processes, such as complementary base pairing in genetic information storage and transfer and some enzymatic reactions (Bazzicalupi *et al.*, 2001; Honda *et al.*, 2002; Leiros *et al.*, 2003). Therefore, considerable efforts have been made in the research field of uracil, thymine and their derivatives (Jolibois *et al.*, 1998; Koike *et al.*, 1998). In previous studies, we reported two thymine derivatives which were obtained by the benzylation of thymine (Ding *et al.*, 2002, 2003). We present here the structure of the title compound, (I), where thymine is replaced by uracil.



(I)

Compound (I) contains one benzene ring and one uracil heterocycle (Fig. 1). The benzene ring (C1–C6) is essentially planar, with an average deviation from planarity of 0.002 Å. The atoms of the uracil ring (C8/C9/C10/C11/N1/N2) are also coplanar, with an average deviation of 0.011 Å; the value in 1-benzylthymine is very similar, *viz*. 0.010 Å. The benzene ring is almost perpendicular to the heterocycle; the dihedral angle is 91.3 (2)°.

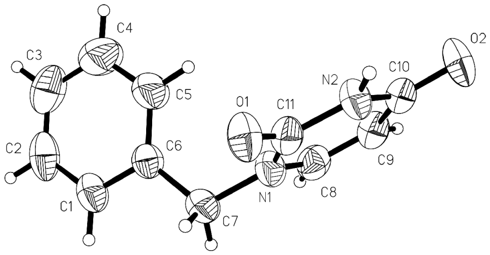


Figure 1
The molecule structure of (I), with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

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In 1-benzyluracil, there is an N—H···O hydrogen bond, leading to a one-dimensional linear chain structure. Moreover, the benzene rings of adjacent molecules are partially overlapped (Fig. 2), with a distance of about 3.40 Å between the centres of the rings, suggesting the existence of π–π stacking interactions.

Experimental

The title compound, (I), was synthesized by the benzylation of uracil (0.20 g) with benzyl bromide (0.45 ml), with neutralization by potassium carbonate (2.00 g) and catalysis by tetrabutylammonium bromide (0.20 g) in a mixture of solvents *N,N'*-dimethylacetamide and diethylene glycol (1:10 *v*/*v*); the reaction time was 40 s in a National NN-S568WFS 900 W microwave oven. Crystals were obtained by recrystallization from dichloremethane.

Crystal data

$C_{11}H_{10}N_2O_2$
$M_r = 202.21$
Monoclinic, $P2_1$
$a = 6.5304$ (4) Å
$b = 6.9483$ (3) Å
$c = 10.9214$ (6) Å
$\beta = 101.934$ (2)°
$V = 484.85$ (5) Å^3
$Z = 2$
$D_x = 1.385$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 578 reflections
$\theta = 2.5$–23.5°
$\mu = 0.10$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.37 × 0.32 × 0.10 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.965$, $T_{max} = 0.986$
2594 measured reflections
1683 independent reflections
921 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 25.2°$
$h = -6 \rightarrow 7$
$k = -8 \rightarrow 8$
$l = -13 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.126$
$S = 1.27$
1683 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.2061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1N···O2^{i}	0.85 (5)	1.97 (5)	2.813 (5)	174 (5)

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

The H atom bonded to N2 was located in a difference map and refined freely; all other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 Å [$U_{iso} = 1.2U_{eq}$(parent atom)] for Csp^2 atoms and 0.97 Å [$U_{iso} = 1.5U_{eq}$(parent atom)] for Csp^3 atoms. In the absence of significant anomalous scattering, Friedel pairs were merged.

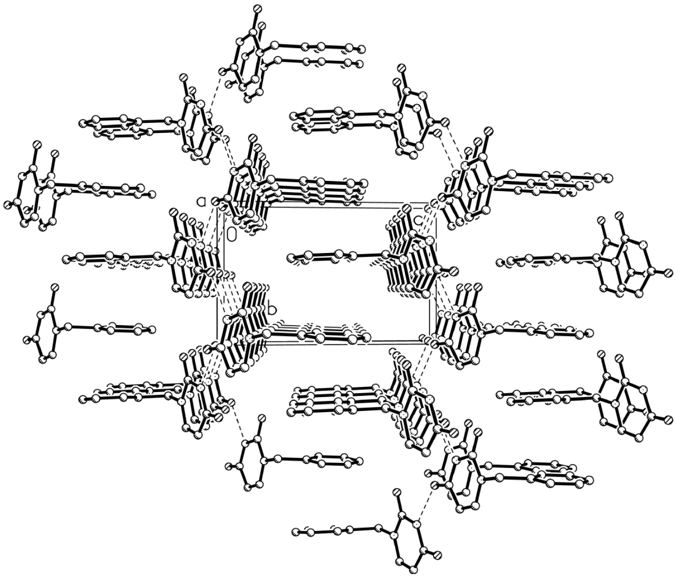

Figure 2
The crystal packing of (I), viewed down the *a* axis. H atoms have been omitted. Hydrogen bonds are shown as dashed lines.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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