Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Bromopyrimidin-2(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.007 Å
R factor = 0.036
wR factor = 0.092
Data-to-parameter ratio = 12.6

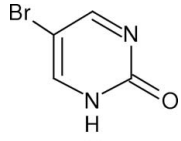
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 18 January 2007
Accepted 19 January 2007

The geometric parameters of the title compound, $C_4H_3BrN_2O$, are in the usual ranges. The crystal packing is characterized by N—H···N and C—H···O hydrogen bonds and short O···Br contacts.

Comment

Pyrimidine and its derivatives are biologically important components of nucleic acids (DNA, RNA) and coenzymes. They can be the parent compound of many drugs, including the barbiturates. Over the years, the pyrimidine system has proved to be an important pharmacophore, interacting with the synthesis and functions of nucleic acids or the HIV drug zidovudine (Logoja, 2005). 5-Bromopyrimidine is used as an intermediate for the synthesis of pharmaceuticals, especially for sulfa drugs and disinfectants. Because the purines, pyrimidines and pteridines are widely distributed in natural materials and living organisms, it is not surprising that so many derivatives of these compounds have biological activity, but the range of activity reaches beyond analogues and antimetabolite action and it seems that, in some cases, the heterocyclic ring acts as a useful carrier for biologically active substituents (Hurst, 1980).



(I)

A perspective view of the title compound, (I), is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.28, November 2006; Allen, 2002; *Mogul* Version 1.1; Bruno et al., 2004).

The crystal packing shows zigzag chains of hydrogen-bonded molecules (Fig. 2) running along the vector [101]. The molecules in a chain are held together by N—H···N and C—H···O hydrogen bonds. Two parallel chains are further connected by O···Br contacts [O1···Br1^{ii} = 2.895 (3)°, C1—O1···Br1^{ii} = 162.9 (3)° and O1···Br1^{ii}—C4^{ii} = 177.68 (16)°; symmetry code: (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$].

It is remarkable that compound (I) is not isostructural with either 5-chloro-pyrimidin-2-one (Furberg & Solbakk, 1974) or 5-fluoro-pyrimidin-2-one (Furberg & Petersen, 1972).

Experimental

The title compound was prepared according to the literature procedure of Langerman (1951) and X-ray quality crystals were obtained

by slow evaporation of a solution in acetone (m.p. 523 K). Analysis (%) for $C_4H_3BrN_2O$: found (calculated): C 27.32 (27.46), H 1.61 (1.73), N 15.92 (16.01).

Crystal data

$C_4H_3BrN_2O$
M_r = 174.99
Monoclinic, $P2_1/n$
a = 3.9481 (6) Å
b = 17.383 (2) Å
c = 7.7968 (11) Å
β = 102.461 (12)°
V = 522.49 (12) Å^3
Z = 4
D_x = 2.225 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 7.75 mm^{-1}
T = 173 (2) K
Block, colourless
0.32 × 0.30 × 0.27 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.111, T_{max} = 0.129
3791 measured reflections
982 independent reflections
868 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 25.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.092
S = 1.12
982 reflections
78 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.2707P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.030 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N6^{i}	0.84 (6)	2.00 (6)	2.829 (6)	167 (5)
C3—H3···O1^{i}	0.95	2.52	3.229 (6)	132

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

H atoms were found in a difference map, but those bonded to C atoms were refined using a riding model, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atom bonded to N was refined freely.

Data collection: *X-AREA* (Stoe & Cie, 2001); 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: *PLATON* (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

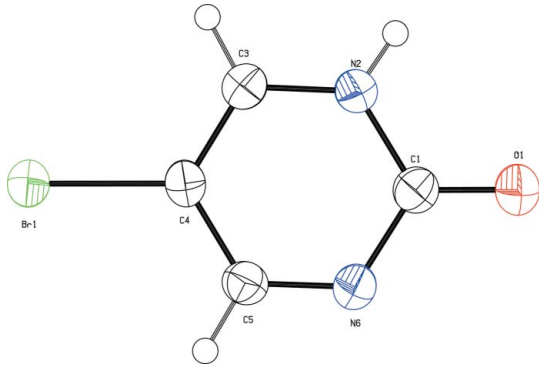


Figure 1
The molecular structure of compound (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

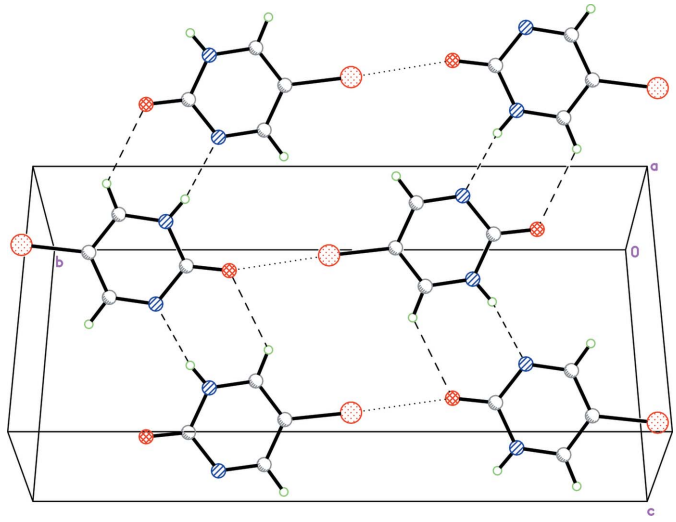


Figure 2
A packing diagram for (I). Hydrogen bonds are shown as dashed lines and O···Br contacts as dotted lines.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruno, I. J., Cole, J. C., Kessler, M., Luo Jie, Motherwell, W. D. S., Purkis, L. H., Smith, B. R., Taylor, R., Cooper, R. I., Harris, S. E. & Orpen, A. G. (2004). *J. Chem. Inf. Comput. Sci.* **44**, 2133–2144.
Furberg, S. & Petersen, C. S. (1972). *Acta Chem. Scand.* **26**, 760–768.
Furberg, S. & Solbakk, J. (1974). *Acta Chem. Scand. A*, **28**, 435–438.
Hurst, D.T. (1980). *An Introduction to the Chemistry and Biochemistry of Pyrimidines, Purines and Pteridines.* Chichester, New York, Brisbane and Toronto: John Wiley.
Langerman, M. J. (1951). *J. Am. Chem. Soc.* **73**, 3011–3012.
Logoja, I. M. (2005). *Chem. Biodivers.* **2**, 1–50.
Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.