

Intermolecular N—H···O==C Hydrogen-Bonding in the Crystal Structure of 6-Amino-1,3-dimethyluracil

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Abstract

The 6-amino-1,3-dimethyluracil molecule [6-amino-1,3-dimethyl-2,4(1H,3H)-pyrimidinedione], C6H9N3O2 (I), lies on a crystalographic mirror plane and participates in an extensive two-dimensional hydrogen-bonding network in the solid state. Each molecule is involved in N—H···O==C hydrogen bonding involving the amino and carbonyl groups, with O···N separations of 2.894 (3) and 2.904 (3) Å.

Comment

Hydrogen bonds often provide the strongest intermolecular forces between molecules in organic molecular crystals and hence often dictate the preferred packing arrangement. The general principles underlying hydrogen-bond formation are reasonably well understood and the structures of hydrogen-bonded crystals can often be rationalized in terms of the preferred combinations of hydrogen-bond donors and acceptors (Etter, 1990; Etter, McDonald & Bernstein, 1990; Etter & Reutzel, 1991). In general, the strongest hydrogen-bond donors pair off with the strongest hydrogen-bond acceptors. Similar pairing processes are repeated until all the hydrogen-bond donors and acceptors have been utilized. Herein we report the formation of a two-dimensional network of intermolecular N—H···O==C hydrogen bonds in the structure of 6-amino-1,3-dimethyluracil (I).

Fig. 1. A view of the two-dimensional hydrogen-bonding environment in the crystal structure of 6-amino-1,3-dimethyluracil (I). The non-H atoms are depicted with thermal ellipsoids drawn at the 50% probability level. For clarity the H atoms are drawn as small spheres of an arbitrary size.
C(4)—C(5). As the molecule lies on a mirror plane, all the torsion angles involving non-H atoms are either 0 or 180°.

There have been many structural determinations of uracil derivatives reported, both as organic structures and metal-complex derivatives. A search of the January 1992 release of the Cambridge Structural Database (Allen, Kennard & Taylor, 1983) reveals that the most closely related structural determinations to the present study include: (i) 6-amino-5-cinnamoyl-1,3-dimethyluracil (Warin, Foulon, Baert, Bernier & Henichart, 1980); (ii) 5-cinnamoyl-1,3-dimethyl-6-[2-(morfolinoethyl)amino]-uracil hydrochloride (Warin, Baert, Bernier & Henichart, 1984); (iii) 6-[cinnamoyl(2-morpholinoethyl)amino]-1,3-dimethyluracil (Warin, Lobry, Bernier & Henichart, 1984); and (iv) 5-(acridin-9-yl)-6-amino-1,3-dimethyluracil hydrochloride dihydrate (Kimura, 1987); their dimensions generally agree with those reported here.

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

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<th>x</th>
<th>y</th>
<th>z</th>
<th>Ueq</th>
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<td>0.25000</td>
<td>0.03879 (24)</td>
<td>0.23018 (13)</td>
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<td>-0.0589 (3)</td>
<td>0.07871 (13)</td>
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<td>0.3552 (3)</td>
<td>0.26783 (14)</td>
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<td>0.04668 (16)</td>
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<td>0.2230 (3)</td>
<td>0.20369 (15)</td>
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</table>

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References


Structure of N\(^1\)-(3-Phenoxypropyl)-4,7-diaza-1-azoniatricyclo[5.2.1.0\^4\^10]decane Bromide Hydrate
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Abstract
The structure of the title compound shows a distortion towards the amidinium form with the bond between the capping C atom and the quaternary N atom [1.668 (9) Å] being significantly longer than the distances between this C atom and the other two N atoms [1.419 (9) and 1.398 (9) Å].

Comment
The structure of the title compound was determined as it is an intermediate in the general preparative route to mono-N-substituted cyclic triazanonanes. It was prepared in near quantitative yield by allowing equimolar amounts of 1-bromo-3-phenoxypropane and 1,4,7-triazatricyclo[5.2.1.0\^4\^10]decane to react in tetrahydrofuran at room temperature in the dark (Atkins, 1980). The preparation of a related N-CH\(_2\)Ph derivative has been reported (Weisman, Vachon, Johnson & Gronbeck, 1987). The most interesting feature of the structure concerns the bonding of the 'capping' C atom, C(1). Formally, the N(1) atom is a quaternary nitrogen as in (I), bearing a positive charge, and has C—N—C angles in the range 102.3 (6)–116.1 (6)°. However, the structure shows considerable distortion towards the amidinium form, (II); the C(1)—N(1) distance [1.668 (9) Å] is long for a C—N single bond and is significantly longer than C(1)—N(4) [1.419 (9) Å] and C(1)—N(7) [1.398 (9) Å]. These in turn are significantly shorter than the other C—N bond distances. The structure also contains water of solvation [O(2)] at less than full occupancy; least-squares refinement afforded a site occupancy factor of 0.72 (2).

Experimental
Crystal data
C\(_{16}\)H\(_{24}\)N\(_3\)O\(_2\), Br\(^-\).0.72H\(_2\)O
Mr = 367.25
Monoclinic
P\(_2_1\)/a
\(a = 8.431\) (1) Å
\(b = 20.452\) (3) Å
\(c = 10.615\) (3) Å
\(\beta = 111.42\) (1)°

\(D_x = 1.38\) Mg m\(^{-3}\)
Mo K\(_\alpha\) radiation
\(\lambda = 0.71069\) Å
Cell parameters from 25 reflections
\(\theta = 17–20°\)
\(\mu = 2.389\) mm\(^{-1}\)
\(T = 298\) K
Cleaved from large prism

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