Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: HA1063). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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6-Amino-5-hydroxyiminomethyl-1,3-dimethyluracil

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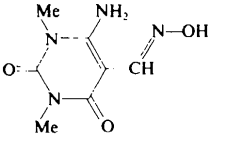
Abstract

The structure of the title compound [6-amino-5-hydroxyiminomethyl-1,3-dimethyl-2,4(1*H*,3*H*)-pyrimidinedione, $C_7H_{10}N_4O_3$] shows that there is extensive electronic delocalization in the uracil ring, as found in analogous uracil derivatives.

Comment

The bonds and angles of the title compound, (I), are very similar to those found for 6-amino-1,3-dimethyluracil (Ferguson, Gallagher, Low, Howie, Hueso-Ureña & Moreno Carretero, 1993). The bonds are longer than those found in 5-formyl and 5-nitroso derivatives (Low, Howie, Hueso-Ureña & Moreno-Carretero, 1992). Only the exocyclic C=O bonds show true double-bond character, and the C6—N6 distance is intermediate between that of a single and a double bond. The C4—C5 and C5—C6 distances in the present compound do show some difference due to the different substituents. The structure is fully hydrogen bonded.



(I)

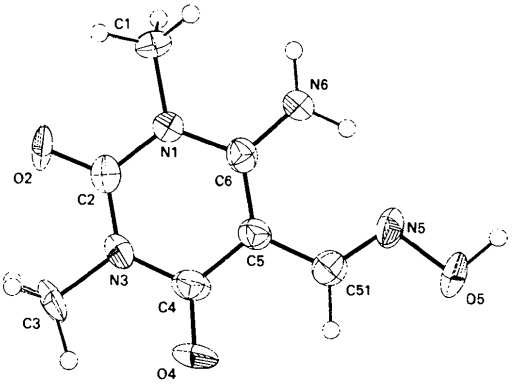


Fig. 1. Perspective view of the molecule. Displacement ellipsoids are shown at the 50% probability level.

Experimental

Crystal data

$C_7H_{10}N_4O_3$
M_r = 198.18
Tetragonal
$I4_1/a$
a = 23.0740 (19) Å
c = 6.9535 (9) Å
V = 3702.1 (6) Å^3
Z = 16
D_x = 1.422 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 12.00–31.00°
μ = 0.11 mm^{-1}
T = 293 K
Prism
0.440 × 0.243 × 0.243 mm
Yellow

Data collection

Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
4107 measured reflections
2010 independent reflections
1059 observed reflections [$I > 3.0\sigma(I)$]
R_{int} = 0.009
θ_{max} = 26.87°
$h = 0 \rightarrow 29$
$k = 0 \rightarrow 29$
$l = 0 \rightarrow 8$
3 standard reflections
frequency: 120 min
intensity variation: 2.5%

Refinement

Refinement on F
R = 0.042
wR = 0.056
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

$S = 1.56$
1059 reflections
127 parameters
H atoms treated using a riding model
$w = 1/[\sigma^2(F) + 0.0008F^2]$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
N1	0.72058 (9)	0.83028 (9)	0.9271 (4)	0.0379 (14)
C1	0.75047 (13)	0.88604 (12)	0.9092 (6)	0.0559 (20)
C2	0.66158 (12)	0.83080 (12)	0.8929 (5)	0.0411 (17)
O2	0.63641 (8)	0.87533 (9)	0.8498 (4)	0.0589 (14)
N3	0.63326 (9)	0.77892 (10)	0.9079 (4)	0.0443 (15)
C3	0.57093 (13)	0.77953 (15)	0.8660 (7)	0.074 (3)
C4	0.65969 (12)	0.72629 (12)	0.9550 (4)	0.0424 (16)
O4	0.62912 (9)	0.68245 (9)	0.9629 (4)	0.0637 (16)
C5	0.72019 (11)	0.72830 (11)	0.9949 (4)	0.0350 (14)
C51	0.74753 (12)	0.67496 (11)	1.0559 (4)	0.0397 (16)
N5	0.80196 (10)	0.67109 (9)	1.0894 (4)	0.0438 (14)
O5	0.81672 (9)	0.61491 (9)	1.1516 (4)	0.0618 (15)
C6	0.74957 (11)	0.78094 (11)	0.9800 (4)	0.0341 (14)
N6	0.80628 (9)	0.78507 (9)	1.0154 (4)	0.0415 (15)

Table 2. *Selected geometric parameters* (Å, °)

N1—C1	1.465 (4)	C4—O4	1.234 (3)
N1—C2	1.382 (3)	C4—C5	1.424 (4)
N1—C6	1.371 (3)	C5—C51	1.447 (4)
C2—O2	1.218 (3)	C5—C6	1.395 (4)
C2—N3	1.368 (4)	C51—N5	1.280 (4)
N3—C3	1.468 (4)	N5—O5	1.408 (3)
N3—C4	1.398 (4)	C6—N6	1.335 (3)
C1—N1—C2	116.20 (22)	N3—C4—C5	116.44 (23)
C1—N1—C6	121.50 (22)	O4—C4—C5	125.3 (3)
C2—N1—C6	122.27 (22)	C4—C5—C51	117.20 (23)
N1—C2—O2	121.3 (3)	C4—C5—C6	119.35 (23)
N1—C2—N3	116.75 (23)	C51—C5—C6	123.41 (24)
O2—C2—N3	121.96 (25)	C5—C51—N5	122.72 (24)
C2—N3—C3	116.40 (23)	C51—N5—O5	110.93 (22)
C2—N3—C4	124.72 (22)	N1—C6—C5	120.40 (23)
C3—N3—C4	118.86 (24)	N1—C6—N6	117.94 (22)
N3—C4—O4	118.2 (3)	C5—C6—N6	121.66 (23)

Data reduction: *NRCVAX DATRD2* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *NRCVAX SOLVER*. Program(s) used to refine structure: *NRCVAX LSTSQ*. Molecular graphics: *NRCVAX* and *PLUTON92* (Spek, 1992). Software used to prepare material for publication: *NRCVAX TABLES*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, torsion angles and complete geometry have been deposited with the IUCr (Reference: HA1109). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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4-Amino-2-methylthio-6-oxo-1,6-dihydropyrimidine and its 1-Methyl Derivative and 4-Amino-2-methoxy-1-methyl-6-oxo-1,6-dihydropyrimidine and its 5-Nitroso Derivative

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Abstract

The molecular structures of 4-amino-2-methylthio-6-oxo-1,6-dihydropyrimidine trihydrate (AMT, $C_5H_7N_3OS.3H_2O$), 4-amino-1-methyl-2-methylthio-6-oxo-1,6-dihydropyrimidine (AMEMT, $C_6H_9N_3OS$), 4-amino-2-methoxy-1-methyl-6-oxo-1,6-dihydropyrimidine (AMH, $C_6H_9N_3O_2$) and 4-amino-2-methoxy-1-methyl-5-nitroso-6-oxo-1,6-dihydropyrimidine monohydrate (AMEMONO, $C_6H_8N_4O_3.H_2O$) show that, as has been reported for analogous compounds, there is extensive electron delocalization in the pyrimidine rings of all four compounds.

Comment

Knowledge of the molecular structure of free pyrimidine ligands is of interest because it permits an understanding