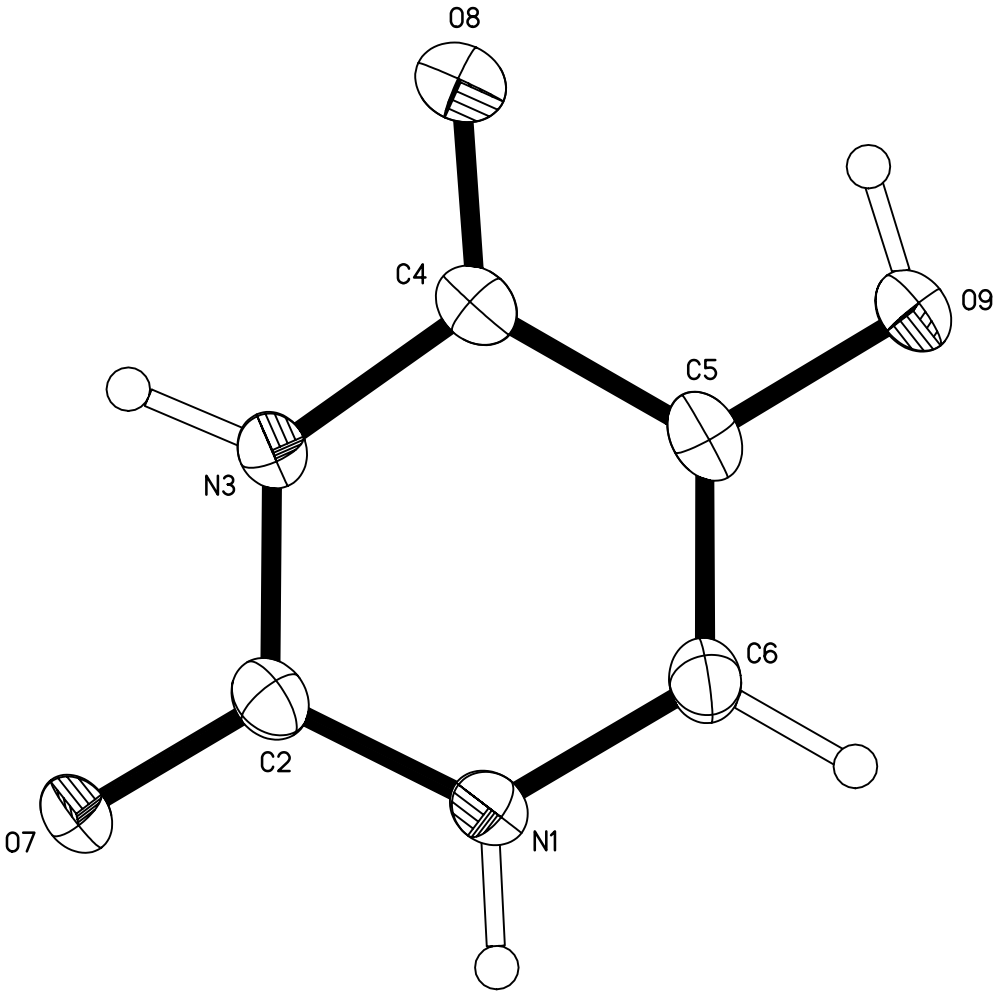
Supporting Information for the Crystal Structure of 5-Hydroxyuracil (X4183O2)



A view of a molecule of 5-hydroxyuracil from the crystal structure showing the numbering scheme employed. Anisotropic atomic displacement ellipsoids for the non-hydrogen atoms are shown at the 50% probability level. Hydrogen atoms are displayed with an arbitrarily small radius.

Table 1. Sample and crystal data for 5-hydroxyuracil **X4183O2.**

Identification code	X4183O2	
Crystallization solvents	DMF and water	
Crystallization method	Slow evaporation	
Moiety formula	$C_4H_4N_2O_3$	
Empirical formula	$C_4H_4N_2O_3$	
Formula weight	128.09	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal size	0.11 x 0.07 x 0.04 mm	
Crystal habit	Colourless blade	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 4.61950(10) Å	α= 88.1690(10)°
	b = 7.04930(10) Å	β= 81.5040(10)°
	c = 7.3452(2) Å	γ = 86.2450(10)°
Volume	235.998(9) $Å^3$	
Z	2	
Density (calculated)	1.803 Mg/m^3	
Absorption coefficient	1.373 mm^{-1}	
F(000)	132	

Table 2. Data collection and structure refinement for X4183O2.

Diffractometer	Bruker AXS SMART 6000
Radiation source	Normal focus sealed tube, CuK_α
Data collection method	ω scans
Theta range for data collection	6.09 to 72.56°
Index ranges	$-5 \leq h \leq 5$, $-8 \leq k \leq 8$, $-9 \leq l \leq 8$
Reflections collected	3677
Independent reflections	902 [R(int) = 0.0157]
Coverage of independent reflections	96.6 %
Variation in check reflections	N/A
Absorption correction	Integration
Max. and min. transmission	0.9556 and 0.8538
Structure solution technique	Direct methods
Structure solution program	SHELXTL V6.10 UNIX (Bruker, 2001)
Refinement technique	Full-matrix least-squares on F^2
Refinement program	SHELXTL V6.10 UNIX (Bruker, 2001)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	902 / 3 / 94
Goodness-of-fit on F^2	1.069
Δ/σ_{max}	0.000
Final R indices	
788 data; $I>2\sigma(I)$	R1 = 0.0409, wR2 = 0.1193
all data	R1 = 0.0463, wR2 = 0.1236
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0920P)^2 + 0.0243P]$ where $P = [MAX(F_o^2, 0) + 2F_c^2]/3$
Largest diff. peak and hole	0.597 and -0.228 eÅ^{-3}

Refinement summary:

Ordered Non-H atoms, XYZ	Freely refining
Ordered Non-H atoms, U	Freely refining - anisotropic
H atoms (on carbon), XYZ	Idealized positions riding on attached atoms
H atoms (on carbon), U	Appropriate multiple of U(eq) for bonded atom
H atoms (on heteroatoms), XYZ	Refined with distance restraints [N-H 0.88(1) Å, O-H 0.84(1) Å]
H atoms (on heteroatoms), U	Freely refining - isotropic
Disordered atoms, OCC	No disorder
Disordered atoms, XYZ	
Disordered atoms, U	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for X4183O2.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
N1	0.3091(3)	0.07643(19)	0.33662(18)	0.0210(4)
C2	0.1840(3)	0.2428(2)	0.4025(2)	0.0199(4)
N3	0.3209(3)	0.40227(17)	0.33474(17)	0.0201(4)
C4	0.5706(3)	0.4055(2)	0.2063(2)	0.0203(4)
C5	0.6837(3)	0.2213(2)	0.1356(2)	0.0225(4)
C6	0.5548(3)	0.0636(2)	0.2043(2)	0.0212(4)
O7	-0.0434(2)	0.25430(15)	0.51771(15)	0.0239(3)
O8	0.6848(3)	0.55421(17)	0.15938(17)	0.0283(4)
O9	0.9196(3)	0.21100(17)	0.00291(19)	0.0325(4)

Table 4. Selected bond lengths (Å) for X4183O2.

N1-C2	1.345(2)	N1-C6	1.381(2)
C2-O7	1.2477(19)	C2-N3	1.3696(19)
N3-C4	1.3788(19)	C4-O8	1.221(2)
C4-C5	1.450(2)	C5-C6	1.345(2)
C5-O9	1.3501(19)		

Table 5. Selected bond angles (°) for X4183O2.

C2-N1-C6	123.15(13)	O7-C2-N1	122.99(14)
O7-C2-N3	121.13(13)	N1-C2-N3	115.88(13)
C2-N3-C4	125.75(13)	O8-C4-N3	121.22(14)
O8-C4-C5	123.82(15)	N3-C4-C5	114.96(14)
C6-C5-O9	121.04(14)	C6-C5-C4	119.66(15)
O9-C5-C4	119.29(15)	C5-C6-N1	120.48(14)

Table 6. Selected torsion angles (°) for X4183O2.

C6-N1-C2-O7	177.62(13)	C6-N1-C2-N3	-2.1(2)
O7-C2-N3-C4	-179.36(13)	N1-C2-N3-C4	0.4(2)
C2-N3-C4-O8	-176.93(14)	C2-N3-C4-C5	2.5(2)
O8-C4-C5-C6	175.57(15)	N3-C4-C5-C6	-3.8(2)
O8-C4-C5-O9	-3.7(2)	N3-C4-C5-O9	176.92(12)
O9-C5-C6-N1	-178.34(13)	C4-C5-C6-N1	2.4(2)
C2-N1-C6-C5	0.7(2)		

Table 7. Anisotropic atomic displacement parameters (Å^2) for X4183O2.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + ... + 2hka^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.0208(7)	0.0210(6)	0.0201(7)	-0.0003(5)	0.0020(5)	-0.0038(5)
C2	0.0188(7)	0.0242(8)	0.0164(8)	-0.0011(6)	-0.0015(6)	-0.0026(6)
N3	0.0186(7)	0.0201(7)	0.0203(7)	-0.0031(5)	0.0024(5)	-0.0022(5)
C4	0.0176(8)	0.0248(8)	0.0184(8)	0.0005(6)	-0.0014(6)	-0.0033(6)
C5	0.0176(7)	0.0285(8)	0.0199(8)	-0.0007(6)	0.0015(6)	-0.0002(6)
C6	0.0200(8)	0.0220(8)	0.0204(8)	-0.0023(6)	0.0000(6)	0.0010(6)
O7	0.0227(6)	0.0235(6)	0.0228(6)	-0.0026(4)	0.0075(4)	-0.0045(4)
O8	0.0255(6)	0.0256(6)	0.0320(7)	0.0004(5)	0.0036(5)	-0.0059(4)
O9	0.0274(7)	0.0251(7)	0.0390(8)	-0.0004(5)	0.0158(5)	-0.0024(5)

Table 8. Hydrogen atom coordinates and isotropic atomic displacement parameters (Å^2) for X4183O2.

	x/a	y/b	z/c	U
H1	0.225(4)	-0.030(2)	0.373(3)	0.027(5)
H3	0.234(4)	0.505(2)	0.382(3)	0.030(5)
H6	0.6332	-0.0576	0.1615	0.025
H9	0.965(4)	0.3233(16)	-0.011(3)	0.024(5)

Table 9. Selected hydrogen bond information for X4183O2 (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1...O7#1	0.884(10)	1.934(10)	2.8132(18)	173.3(18)
N3-H3...O7#2	0.863(10)	1.971(10)	2.8336(17)	178(2)
O9-H9...O8#3	0.832(10)	2.037(16)	2.6696(17)	132.3(17)
O9-H9...O8	0.832(10)	2.294(18)	2.7959(16)	119.2(16)
C6-H6...O9#4	0.95	2.44	3.231(2)	140.7

#1 -x,-y,-z+1 #2 -x,-y+1,-z+1 #3 -x+2,-y+1,-z #4 -x+2,-y,-z