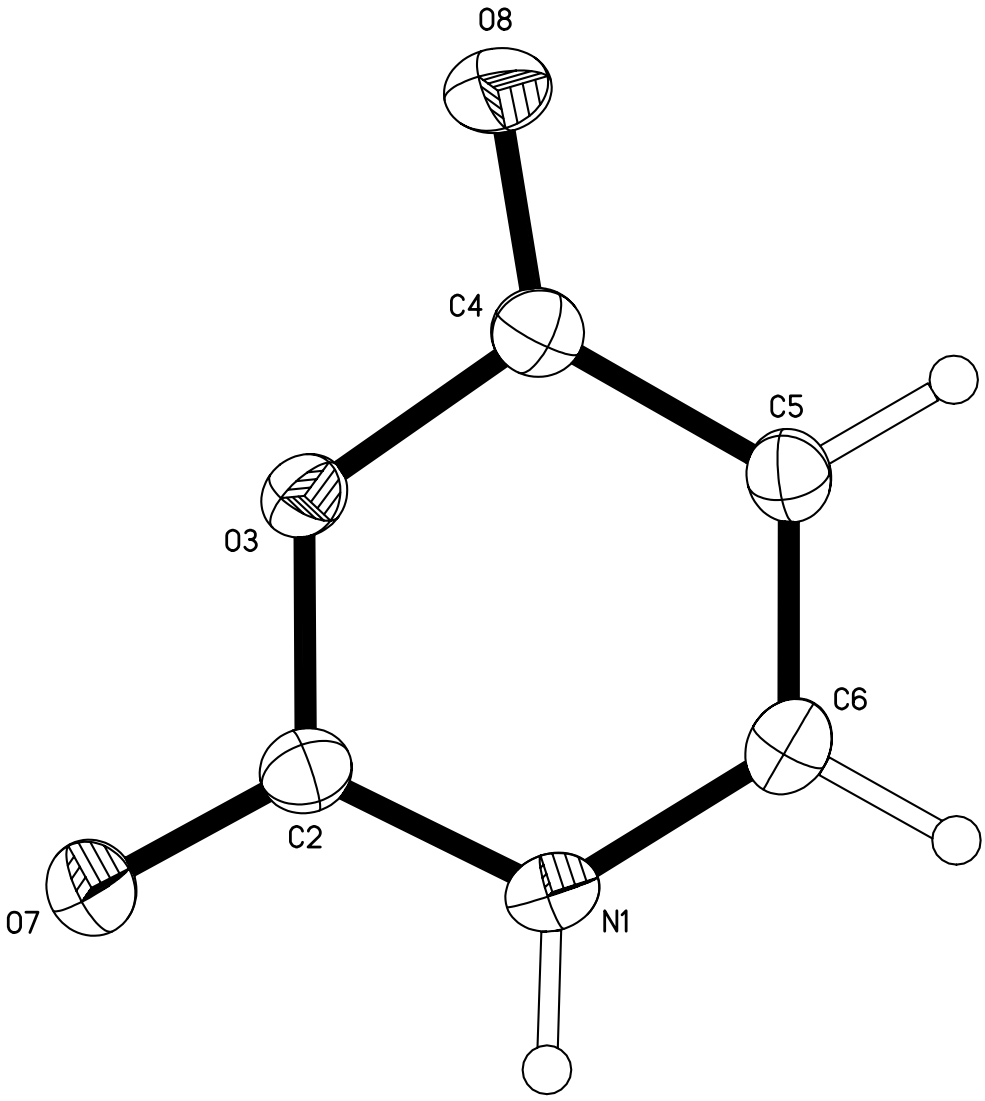
Supporting Information for the Crystal Structure of 3-Oxauracil (X4084AG2)



A view of a molecule of 3-oxauracil 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 3-oxauracil.

Identification code	X4084AG2	
Crystallization solvents	1,2-Dimethoxyethane and toluene	
Crystallization method	Slow evaporation	
Moiety formula	$C_4H_3NO_3$	
Empirical formula	$C_4H_3NO_3$	
Formula weight	113.07	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal size	0.22 x 0.16 x 0.04 mm	
Crystal habit	Colourless plate	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.7407(2) Å	α= 90°
	b = 5.54050(10) Å	β= 103.6430(10)°
	c = 10.4926(2) Å	γ = 90°
Volume	437.303(16) $Å^3$	
Z	4	
Density (calculated)	1.717 Mg/m^3	
Absorption coefficient	1.323 mm^{-1}	
F(000)	232	

Table 2. Data collection and structure refinement for X4084AG2.

Diffractometer	Bruker AXS SMART 6000
Radiation source	Normal focus sealed tube, CuK_α
Data collection method	ω scans
Theta range for data collection	5.88 to 72.48°
Index ranges	$-9 \leq h \leq 9$, $-6 \leq k \leq 6$, $-12 \leq l \leq 12$
Reflections collected	3872
Independent reflections	852 [R(int) = 0.0200]
Coverage of independent reflections	97.8 %
Variation in check reflections	N/A
Absorption correction	Integration
Max. and min. transmission	0.9503 and 0.7771
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	852 / 0 / 77
Goodness-of-fit on F^2	1.067
Δ/σ_{max}	0.000
Final R indices	
783 data; $I>2\sigma(I)$	R1 = 0.0299, wR2 = 0.0822
all data	R1 = 0.0324, wR2 = 0.0849
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.1476P]$ where $P = [MAX(F_o^2, 0) + 2F_c^2]/3$
Largest diff. peak and hole	0.240 and -0.172 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	Freely refining
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 X4084AG2.
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	0.34147(14)	0.28064(19)	0.48351(10)	0.0220(3)
C2	0.34752(15)	0.2136(2)	0.36019(11)	0.0196(3)
O3	0.25732(10)	0.35568(15)	0.26087(8)	0.0206(3)
C4	0.15709(15)	0.5601(2)	0.27810(11)	0.0200(3)
C5	0.16533(16)	0.6255(2)	0.41136(12)	0.0205(3)
C6	0.25421(15)	0.4843(2)	0.50823(11)	0.0211(3)
O7	0.42643(12)	0.03986(17)	0.33256(8)	0.0271(3)
O8	0.07715(12)	0.65607(17)	0.17900(9)	0.0281(3)

Table 4. Selected bond lengths (Å) for X4084AG2.

N1-C2	1.3576(16)	N1-C6	1.3709(16)
C2-O7	1.2115(15)	C2-O3	1.3600(14)
O3-C4	1.4085(14)	C4-O8	1.2013(15)
C4-C5	1.4312(17)	C5-C6	1.3373(17)

Table 5. Selected bond angles (°) for X4084AG2.

C2-N1-C6	122.32(10)	O7-C2-N1	125.32(11)
O7-C2-O3	118.24(10)	N1-C2-O3	116.44(10)
C2-O3-C4	124.46(9)	O8-C4-O3	115.57(11)
O8-C4-C5	128.96(12)	O3-C4-C5	115.46(10)
C6-C5-C4	119.40(11)	C5-C6-N1	121.72(11)

Table 6. Selected torsion angles (°) for X4084AG2.

C6-N1-C2-O7	177.83(11)	C6-N1-C2-O3	-1.97(17)
O7-C2-O3-C4	178.68(10)	N1-C2-O3-C4	-1.50(16)
C2-O3-C4-O8	-175.64(10)	C2-O3-C4-C5	4.66(16)
O8-C4-C5-C6	175.82(12)	O3-C4-C5-C6	-4.52(16)
C4-C5-C6-N1	1.51(18)	C2-N1-C6-C5	1.96(18)

Table 7. Anisotropic atomic displacement parameters (Å^2) for X4084AG2.
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	0.0249(5)	0.0237(5)	0.0166(5)	0.0032(4)	0.0031(4)	0.0031(4)
C2	0.0182(5)	0.0213(6)	0.0190(6)	0.0013(5)	0.0037(4)	-0.0007(4)
O3	0.0225(4)	0.0241(5)	0.0159(4)	0.0017(3)	0.0060(3)	0.0031(3)
C4	0.0196(5)	0.0199(6)	0.0214(6)	0.0024(4)	0.0067(5)	-0.0010(5)
C5	0.0223(5)	0.0186(6)	0.0221(6)	-0.0001(4)	0.0082(5)	0.0000(4)
C6	0.0234(6)	0.0227(6)	0.0181(6)	-0.0018(5)	0.0064(5)	-0.0030(5)
O7	0.0303(5)	0.0270(5)	0.0238(5)	-0.0013(4)	0.0058(4)	0.0083(4)
O8	0.0328(5)	0.0300(5)	0.0209(5)	0.0074(4)	0.0053(4)	0.0068(4)

Table 8. Hydrogen atom coordinates and isotropic atomic displacement parameters (Å^2) for X4084AG2.

	x/a	y/b	z/c	U
H1	0.400(2)	0.186(3)	0.5452(19)	0.040(5)
H5	0.1082	0.7679	0.4308	0.025
H6	0.2569	0.5262	0.5965	0.025

Table 9. Selected hydrogen bond information for X4084AG2 (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1...O7#1	0.87(2)	2.05(2)	2.9103(14)	168.9(17)
C6-H6...O7#2	0.95	2.54	3.3520(14)	143.4
C6-H6...O8#3	0.95	2.52	3.1965(15)	128.2

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