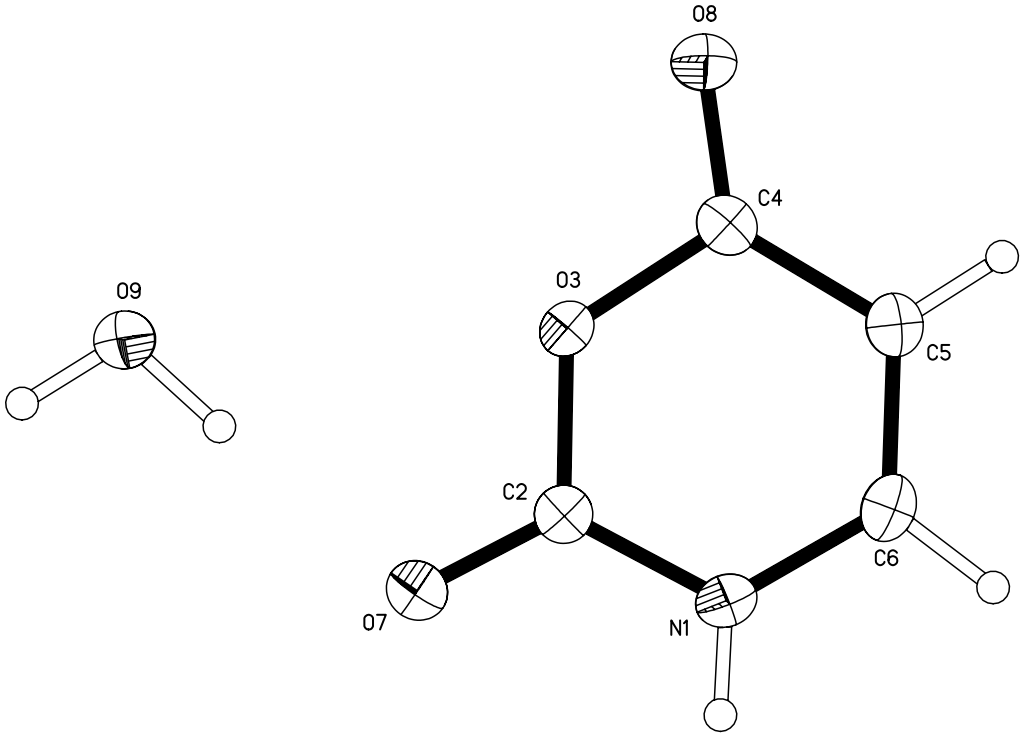
Supporting Information for the Crystal Structure of 3-Oxauracil Monohydrate (X4084AP4)



A view of a molecule of 3-oxauracil and a molecule of water 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 monohydrate X4084AP4.

Identification code	X4084AP4	
Crystallization solvents	Methanol and ethyl acetate	
Crystallization method	Slow evaporation	
Moiety formula	$C_4H_3NO_3 \cdot H_2O$	
Empirical formula	$C_4H_5NO_4$	
Formula weight	131.09	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal size	0.42 x 0.18 x 0.12 mm	
Crystal habit	Colourless block	
Crystal system	Orthorhombic	
Space group	Pnma	
Unit cell dimensions	a = 14.4737(3) Å	α= 90°
	b = 6.00300(10) Å	β= 90°
	c = 6.36260(10) Å	γ = 90°
Volume	552.818(17) $Å^3$	
Z	4	
Density (calculated)	1.575 Mg/m^3	
Absorption coefficient	1.268 mm^{-1}	
F(000)	272	

Table 2. Data collection and structure refinement for X4084AP4.

Diffractometer	Bruker AXS SMART 6000
Radiation source	Normal focus sealed tube, CuK_α
Data collection method	ω scans
Theta range for data collection	6.11 to 72.78°
Index ranges	$-17 \leq h \leq 17$, $-7 \leq k \leq 6$, $-7 \leq l \leq 6$
Reflections collected	4664
Independent reflections	596 [R(int) = 0.0150]
Coverage of independent reflections	98.7 %
Variation in check reflections	N/A
Absorption correction	Integration
Max. and min. transmission	0.8639 and 0.6821
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	596 / 0 / 70
Goodness-of-fit on F^2	1.083
Δ/σ_{max}	0.000
Final R indices	
593 data; $I>2\sigma(I)$	R1 = 0.0298, wR2 = 0.0818
all data	R1 = 0.0298, wR2 = 0.0819
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0620P)^2 + 0.0637P]$ where $P = [MAX(F_o^2, 0) + 2F_c^2]/3$
Largest diff. peak and hole	0.228 and -0.206 eÅ^{-3}

Refinement summary:

Ordered Non-H atoms, XYZ	Freely refining
Ordered Non-H atoms, U	Freely refining - anisotropic
H atoms (on carbon), XYZ	Freely refining
H atoms (on carbon), U	Freely refining - isotropic
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 X4084AP4.
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	0.29810(7)	0.2500	0.12634(17)	0.0220(3)
C2	0.26795(8)	0.2500	0.32735(19)	0.0215(3)
O3	0.33353(5)	0.2500	0.48092(13)	0.0220(3)
C4	0.42863(8)	0.2500	0.4419(2)	0.0224(3)
C5	0.45590(8)	0.2500	0.2256(2)	0.0247(3)
C6	0.39028(9)	0.2500	0.0766(2)	0.0237(3)
O7	0.18733(6)	0.2500	0.37884(15)	0.0295(3)
O8	0.47658(6)	0.2500	0.59703(15)	0.0286(3)
O9	0.16617(7)	0.2500	0.82028(15)	0.0272(3)

Table 4. Selected bond lengths (Å) for X4084AP4.

N1-C2	1.3513(16)	N1-C6	1.3713(16)
C2-O7	1.2121(15)	C2-O3	1.3622(14)
O3-C4	1.3986(14)	C4-O8	1.2065(16)
C4-C5	1.4321(19)	C5-C6	1.3418(19)

Table 5. Selected bond angles (°) for X4084AP4.

C2-N1-C6	122.18(11)	O7-C2-N1	124.52(12)
O7-C2-O3	118.49(11)	N1-C2-O3	117.00(10)
C2-O3-C4	123.95(9)	O8-C4-O3	114.90(11)
O8-C4-C5	128.88(11)	O3-C4-C5	116.22(11)
C6-C5-C4	118.94(11)	C5-C6-N1	121.71(12)

Table 6. Selected torsion angles (°) for X4084AP4.

C6-N1-C2-O7	180.0	C6-N1-C2-O3	0.0	O7-
C2-O3-C4	180.0	N1-C2-O3-C4	0.0	C2-
O3-C4-O8	180.0	C2-O3-C4-C5	0.0	O8-
C4-C5-C6	180.0	O3-C4-C5-C6	0.0	C4-
C5-C6-N1	0.0	C2-N1-C6-C5	0.0	

Table 7. Anisotropic atomic displacement parameters (Å^2) for X4084AP4.
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	0.0213(6)	0.0287(6)	0.0162(6)	0.000	-0.0025(4)	0.000
C2	0.0194(6)	0.0258(6)	0.0193(6)	0.000	0.0000(4)	0.000
O3	0.0192(5)	0.0320(5)	0.0149(5)	0.000	0.0004(3)	0.000
C4	0.0187(6)	0.0257(6)	0.0227(7)	0.000	-0.0003(5)	0.000
C5	0.0201(6)	0.0328(7)	0.0214(7)	0.000	0.0023(5)	0.000
C6	0.0251(7)	0.0280(6)	0.0182(6)	0.000	0.0044(5)	0.000
O7	0.0191(5)	0.0472(6)	0.0221(5)	0.000	-0.0007(3)	0.000
O8	0.0213(5)	0.0436(6)	0.0209(5)	0.000	-0.0033(3)	0.000
O9	0.0205(5)	0.0414(6)	0.0196(5)	0.000	-0.0010(3)	0.000

Table 8. Hydrogen atom coordinates and isotropic atomic displacement parameters (Å^2) for X4084AP4.

	x/a	y/b	z/c	U
H1	0.2563(14)	0.2500	0.035(3)	0.032(4)
H5	0.5195(13)	0.2500	0.198(3)	0.028(4)
H6	0.4014(13)	0.2500	-0.073(3)	0.033(5)
H9A	0.1712(14)	0.2500	0.673(4)	0.049(6)
H9B	0.1061(18)	0.2500	0.848(3)	0.048(6)

Table 9. Selected hydrogen bond information for X4084AP4 (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1...O9#1	0.84(2)	1.89(2)	2.7273(14)	178(2)
O9-H9A...O7	0.94(2)	1.88(2)	2.8253(14)	177.3(19)
O9-H9B...O8#2	0.89(3)	1.91(3)	2.7940(14)	179(2)
C5-H5...O7#3	0.936(18)	2.478(18)	3.4149(15)	179.4(16)
C6-H6...O8#1	0.97(2)	2.36(2)	3.2970(16)	162.2(16)

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