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Redetermination of the crystal structure of uracil.

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The crystal structure of uracil, originally reported by Parry in 1954, has been redetermined. The unit-cell parameters are $a=11{\cdot}938\pm0{\cdot}001$, $b=12{\cdot}376\pm0{\cdot}0009$, $c=3{\cdot}6552\pm0{\cdot}0003$ Å; $\beta=120°54'\pm0{\cdot}4'$. The space group is $P2_1/a$. Three dimensional X-ray diffraction data were measured by diffractometry with Mo $K\alpha$ radiation. The final R was 0·045. The redetermined structure is essentially a confirmation of Parry's structure. The C(5)–C(6) bond length (1·340 Å, e.s.d. 0·002 Å) in this work, however, is 0·07 Å shorter than the value (1·41 Å, e.s.d. 0·011 Å) reported by Parry.

The crystal structure of uracil was first reported by Parry (1954). One interesting feature of the structure is the close approach of an oxygen atom to carbon atoms in different molecules. The reported distances are 3·19 and 3·28 Å. Another interesting result is the C(5)–C(6) bond length of $1{\cdot}41\pm0{\cdot}01$ Å, a value considerably greater (0·07 Å) than for a similar bond found in 1-methylthymine (Hoogsteen, 1963*a*, *b*), thymine monohydrate (Gerdil, 1961) and 1-methyluracil (Green, Mathews & Rich, 1962). The accuracy of the results, unfortunately, was limited by the quality of the uracil crystal. We report here the structural results of an X-ray diffraction investigation of a uracil crystal.

High quality single crystals of uracil were grown by heating the powder to its decomposition point in a Pyrex test tube with a sharp temperature gradient. Single crystals of stubby habit with prominent forms {001} and {110} grew on the walls of the tube at a temperature somewhat below the decomposition point. One precession and several Weissenberg photographs confirmed the space group $P2_1/a$ as reported by Parry (1954). Accurate cell parameters were determined on a Picker X-ray diffractometer with a General Electric quarter circle goniostat. The parameters for the monoclinic cell are:

$$
\begin{aligned}
a &= 11{\cdot}938\pm0{\cdot}001 \text{ Å}\\
b &= 12{\cdot}376\pm0{\cdot}0009\\
c &= 3{\cdot}6552\pm0{\cdot}0003\\
\beta &= 120°54'\pm0{\cdot}4'\\
\lambda(\text{Mo } K\alpha) &= 0{\cdot}71069 \text{ Å}.
\end{aligned}
$$

Table 1. *Final atomic parameters*

The temperature factors are of the form

$T_i=\exp\,[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$ and $T_H=\exp\,[-B(\sin\theta/\lambda)^2]$.

Estimated standard deviations, in parenthesis, are right adjusted:

e.g. For O(7), $\sigma(x)=11\cdot10^{-5}$ and for H(9), $\sigma(x)=16\cdot10^{-4}$.

	x	y	z	$10^4\beta_{11}$	$10_4\beta_{22}$	$10^4\beta_{33}$	$10^4\beta_{12}$	$10^4\beta_{13}$	$10^4\beta_{23}$
O(7)	0·08497 (11)	0·28677 (9)	−0·02173 (43)	80 (1)	41 (0·8)	1670 (22)	11 (0·8)	252 (4)	30 (3)
O(8)	0·12987 (10)	−0·07706 (8)	0·01962 (44)	66 (1)	35 (0·7)	1537 (19)	−6 (0·8)	228 (4)	−17 (3)
N(1)	0·27283 (12)	0·21750 (11)	0·05336 (50)	58 (1)	36 (0·9)	1157 (22)	−7 (0·9)	176 (4)	5 (4)
N(3)	0·11208 (12)	0·10468 (10)	0·00406 (48)	43 (1)	37 (0·8)	1040 (19)	−2 (0·8)	143 (4)	0 (3)
C(2)	0·15191 (14)	0·20933 (12)	0·00913 (56)	58 (1)	41 (1)	924 (22)	−3 (1)	143 (5)	10 (4)
C(4)	0·17988 (14)	0·01237 (12)	0·03494 (54)	52 (1)	40 (1)	829 (21)	−2 (1)	129 (5)	−10 (4)
C(5)	0·30519 (14)	0·02857 (13)	0·08193 (58)	51 (1)	44 (1)	1026 (25)	2 (1)	158 (5)	−9 (4)
C(6)	0·34620 (15)	0·12977 (12)	0·08905 (59)	49 (1)	51 (1)	940 (22)	−6 (1)	145 (5)	−14 (4)
H(9)	0·3536 (16)	−0·0322 (14)	0·0986 (56)	3·41 (39): B_H					
H(10)	0·4279 (16)	0·1464 (13)	0·1120 (50)	3·04 (35)					
H(11)	0·2964 (15)	0·2804 (14)	0·0416 (52)	3·15 (39)					
H(12)	0·0343 (16)	0·0947 (13)	−0·0320 (52)	3·33 (39)					

The parameters a and c are 1 % greater than those reported by Parry and the angle β is 0·9° larger. The discrepancy evidently lies in the determination of the angle β, since b, d_{100} and d_{001} for both sets of measurements agree well.

The Bragg scattered intensities were measured for the upper hemisphere (the crystal was mounted along c^* with Mo $K\alpha$ radiation on a Picker diffractometer. The 2θ scan technique was employed (Alexander & Smith, 1964). All reflections out to $2\theta=50°$ ($\sin\theta/\lambda=0{\cdot}595$ Å^{-1}) were measured; in the shell from 2θ of 50 to 80°, only reflections with expected net intensities greater than 200 counts were measured. The overall agreement, $R_{\rm exp}$, for the equivalent reflections hkl and $h\bar{k}l$ was 0·0168. We define $R_{\rm exp}=\Sigma\,|I_{hkl}-I_{h\bar{k}l}|/\,\Sigma\,I_{\rm mean}$. The most intense reflections were measured by powder diffractometry. These intensities, from the planes (001), (200), and (120), were judged free from

Table 2. *List of structure factors for uracil*

The three columns of each row contain the values for k, $10F_o$, $10F_c$. The F_c values were calculated from the parameters in Table 1.

0,K,0		
2	55	-51
4	201	210
6	191	-187
8	32	28
10	210	212
12	101	-105
14	100	101
16	69	+66
1,K,0		
1	218	231
2	340	-355
3	145	144
4	121	125
5	289	-282
6	57	-53
7	54	-52
8	38	-38
9	16	-11
10	228	-233
11	120	123
12	70	-72
13	25	23
14	17	-13
16	<15	-3
2,K,0		
0	471	-485
1	190	-195
2	95	-83
3	368	369
4	251	-252
5	<7	-14
6	84	-78
7	19	16
8	42	-46
9	55	58
10	16	-21
11	155	-158
12	29	32
13	13	-6
14	29	-25
17	59	54
21	49	-39
3,K,0		
1	142	-143
2	74	65
3	43	-47
4	109	-109
5	20	18
6	393	381
7	142	140
8	90	-92
9	45	-45
10	52	48
11	108	-114
12	68	-70
13	60	-59
14	36	30
16	50	52
4,K,0		
0	532	-542
1	307	-304
2	111	-109
3	<7	-6
4	230	219
5	71	-69
6	142	141
7	56	52
8	31	20
9	<10-	-2
10	80	-88
11	52	-53
12	12	-0
13	33	40
17	27	29
5,K,0		
1	190	-182
2	73	72
3	19	-17
4	131	-131
5	211	204
6	29	-24
7	43	43
8	27	26
9	23	14
10	115	120
11	<10	-2
12	40	44
13	21	21
14	32	-30
15	46	41
6,K,0		
0	41	44
1	126	120
2	221	219
3	130	-131
4	13	-12
5	22	21
6	101	106
7	18	17
8	42	49
9	<13	16
10	19	-20
11	107	114
12	15	17
16	33	29
17	59	-55
18	34	-32
7,K,0		
1	135	134
2	47	-46
3	53	-52
4	26	-24
5	127	127
6	117	-117
7	208	-211
8	68	-72
9	64	71
10	22	-22
11	14	-10
12	<10	-1
13	28	31
16	69	-62
17	45	-41
8,K,0		
0	33	39
1	18	18
2	43	-43
3	108	108
4	146	-148
5	75	-77
6	144	-147
7	79	-80
8	43	-45
9	<10	0
10	15	22
11	14	-15
9,K,0		
1	45	45
2	13	-14
3	24	-25
4	153	156
5	177	-182
6	<10	1
7	36	36
8	85	88
9	32	-27
10	43	-46
12	43	38
14	45	37
10,K,0		
0	<10	12
1	70	71
2	62	65
3	54	-55
4	37	40
5	76	77
6	18	16
7	14	23
8	<11	4
9	34	-34
13	27	-28
14	36	-34
15	53	50
11,K,0		
1	15	-8
2	<10	5
3	<10	10
4	36	-38
5	15	19
6	<12	0
7	58	57
9	37	34
12	42	-39
12,K,0		
0	<11	0
1	46	-48
2	43	-50
3	38	-39
4	29	29
6	38	40
7	58	52
13,K,0		
1	38	-42
3	44	42
4	44	-42
5	37	37
9	44	-46
14,K,0		
2	53	-48
5	35	-36
7	33	-35
16,K,0		
2	53	49
3	50	48
17,K,0		
1	36	32
0,K,1		
0	1565	1449
1	112	-115
2	45	-48
3	24	-23
4	145	145
5	<8	8
6	143	-140
7	18	-18
8	22	18
9	58	-58
10	176	176
11	41	-43
12	82	-83
13	<10	6
14	86	83
16	57	-56
1,K,1		
1	<7	-2
2	133	-134
3	85	84
4	103	101
5	235	-231
6	79	-73
7	40	-39
8	<9	-6
9	42	-42
10	172	-173
11	114	117
12	55	-57
13	15	16
-1,K,1		
1	399	409
2	295	308
3	102	100
4	75	-74
5	169	-164
6	14	11
7	35	-36
8	38	40
9	42	43
10	195	197
11	73	74
12	64	64
13	19	20
14	<13	7
16	<14	6
2,K,1		
0	147	-149
1	53	-51
2	60	-58
3	189	185
4	162	-158
5	36	34
6	39	-37
7	29	25
8	<9	-7
9	63	62
10	33	-32
11	91	-93
12	<11	-7
13	<10	-11
17	41	39
21	41	-34
-2,K,1		
0	502	-527
1	304	308
2	50	-35
3	326	-322
4	195	-193
5	60	59
6	93	-89
7	<8	-2
8	70	-70
9	24	-22
10	<10	-2
11	183	184
12	61	64
13	<10	-1
14	26	-22
15	33	27
17	55	-52
21	40	33
3,K,1		
1	96	-95
2	27	-27
3	12	-1
4	74	-73
5	36	35
6	236	231
7	84	82
8	55	-56
9	35	-36
10	<10	7
11	82	-83
12	50	-48
13	40	-42
14	25	26
-3,K,1		
1	179	-178
2	177	-169
3	88	-90
4	87	89
5	40	-36
6	356	-343
7	136	133
8	77	78
9	57	-56
10	75	-73
11	96	-100
12	71	72
13	49	-51
14	27	-22
16	57	-55
22	34	31
4,K,1		
0	323	-320
1	154	-155
2	66	-67
3	14	18
4	128	122
5	70	-70
6	75	77
7	23	25
8	<10	1
9	20	14
10	49	-52
11	29	-27
12	22	21
-4,K,1.		
0	479	-487
1	288	285
2	80	-80
3	49	48
4	223	211
5	10	-6
6	163	159
7	79	-71
8	39	38
9	15	18
10	101	-106
11	47	50
12	28	-29
13	38	-42
14	36	-34
5,K,1		
1	48	-47
2	63	61
3	<9	6
4	72	-71
5	93	92
6	21	19
7	58	60
8	11	15
9	15	7
10	99	101
11	<10	1
12	32	32
15	44	37
-5,K,1		
1	293	-288
2	36	-38
3	33	-26
4	148	145
5	300	291
6	75	68
7	<9	0
8	21	-24
9	27	18
10	81	-87
11	14	-10
12	41	-45
13	27	28
14	36	33
15	33	30
6,K,1		
0	68	67
1	51	52
2	103	106
3	80	-81
4	34	31
5	21	19
6	59	58
7	<11	-0
8	19	17
9	18	-18
10	<10	-5
11	57	59
17	46	-44
-6,K,1		
0	44	-42
1	185	-176
2	265	262
3	127	131
4	63	-60
5	<8	-1
6	134	135
7	17	-17
8	64	67
9	51	-53
10	28	-29
11	136	-147
12	29	30
13	<10	7
16	52	50
17	50	51
18	34	-31
7,K,1		
1	37	40
2	<10	-5
3	48	-46
4	<10	-9
5	67	64
6	102	-101
7	142	-145
8	50	-54
9	42	42
10	15	-20
16	43	-40
-7,K,1		
1	233	230
2	78	83
3	42	-38
4	30	29
5	154	158
6	89	88
7	202	-205
8	55	62
9	75	84
10	<12	10
11	14	-15
12	<10	-10
13	27	25
16	80	70
17	50	-47
8,K,1		
0	13	10
1	<10	-1
2	24	-27
3	84	83
4	117	-118
5	36	-35
6	79	-82
7	30	-31
8	12	-14
-8,K,1		
0	95	92
1	29	-33
2	59	-58
3	83	-85
4	111	-115
5	103	106
6	184	-190
7	123	124
8	76	-78
9	21	23
10	32	41
11	22	24
12	23	24
15	42	36
9,K,1		
1	26	28
2	19	-17
3	<11	5
4	78	77
5	84	-86
6	21	23
7	22	24
8	41	42
14	32	28
-9,K,1		
1	48	46
2	<9	-0
3	64	-67
4	214	-217
5	264	-274
6	56	58
7	33	32
8	121	-125
9	34	-32
10	66	66
11	21	18
12	50	-44
14	38	-30
10,K,1		
0	<10	6
1	43	42
2	37	38
3	29	-32
4	27	27
13	20	-24
-10,K,1		
0	21	25
1	82	-87
2	74	83
3	61	62
4	19	21
5	139	-142
6	17	14
7	54	-59
8	11	5
9	44	46
10	13	12
14	51	-46
15	73	-70
11,K,1		
7	34	34
-11,K,1		
1	26	-20
2	20	-22
3	55	55
4	55	58
5	37	41
6	<10	-9
7	76	75
8	21	21
9	35	28
12	60	57
16	41	-34
12,K,1		
3	29	-27
4	31	23
7	33	32
-12,K,1		
0	14	17
1	58	62
2	92	-99
3	39	40
4	37	37
5	<13	-7
6	57	57
7	62	-55
8	47	44
11	24	29
12	44	-42
14	40	34
13,K,1		
4	25	-26
-13,K,1		
1	58	-64
2	41	43
3	60	59
4	54	51
5	53	51
6	49	-47
9	61	-62
14,K,1		
2	39	-34
-14,K,1		
2	53	-46
5	65	62
7	57	52
8	42	-37
-15,K,1		
3	61	-57
7	44	-41
-16,K,1		
2	68	63
3	78	-74
12	45	40
13	50	-46
-17,K,1		
1	59	55
2	50	-49
8	38	37
-18,K,1		
4	29	-31
9	38	34
0,K,2		
0	493	506
1	89	-86
2	23	-24
3	20	-18
4	66	65
5	<10	0
6	64	-65
7	20	-20
8	<11	4
9	66	-65
10	109	108
11	51	-53
12	41	-41
14	49	49
16	36	-33
1,K,2		
1	39	-40
2	27	-25
3	18	21
4	54	52
5	117	-115
6	58	-57
7	22	-22
8	20	15
9	32	-33
10	82	-83
11	71	72
12	32	-34
-1,K,2		
1	274	274
2	133	133
3	30	31
4	25	-24
5	36	-38
6	<10	1
7	14	-10
8	18	15
9	68	68
10	108	108
11	21	21
12	40	40
2,K,2		
0	22	-21
1	<10	-11
2	27	-26
3	49	52
4	77	-76
5	33	33
6	15	-14
7	20	23
8	<13	8
9	43	40
10	26	-29
11	44	-43
12	23	-24
-2,K,2		
0	241	-242
1	224	222
2	<15	12
3	136	-135
4	75	-76
5	46	48
6	56	-55
7	<10	3
8	53	-51
9	<10	11
10	<13	7
11	151	151
12	58	60
14	17	-15
15	30	31
17	37	-34
3,K,2		
1	52	-55
2	46	-44
3	11	10
4	34	-34
5	22	20
6	94	94
7	30	28
8	24	-21
9	28	-27
10	14	-13
11	44	-41
12	26	-24
-3,K,2		
1	152	-146
2	132	-128
3	64	-63
4	40	40
5	66	-61
6	168	-166
7	69	69
8	30	29
9	56	-57
10	56	-58
11	51	-53
12	54	54
13	29	-25
16	44	-41
4,K,2		
0	139	-143
1	44	-45
2	24	-23
3	13	16
4	52	49
5	36	-37
6	31	33
7	13	11
8	<11	-1
9	21	20
10	24	-24
-4,K,2		
0	224	-225
1	112	112
2	14	-27
3	49	48
4	95	92
5	63	-58
6	104	105
7	62	-60
8	36	36
9	16	16
10	91	-93
11	20	19
12	37	-40
13	29	-29
14	31	-30
5,K,2		
1	<10	8
2	33	36
3	13	15
4	30	-29
5	34	37
6	29	30
7	50	48
8	<12	3
10	56	56
-5,K,2		
1	209	-208
2	9	7
3	<9	-2
4	91	90
5	243	239
6	53	53
7	28	-26
8	11	-8
9	19	12
10	31	-30
11	17	-14
12	32	-35
14	23	21
6,K,2		
0	42	43
1	19	19
2	33	35
3	39	-39
4	40	39
5	<11	7
6	23	24
9	24	-27
17	30	-26
-6,K,2		
0	95	-97
1	146	-143
2	158	157
3	60	64
4	53	-52
5	26	25
6	110	110
7	<10	1
8	52	53
9	56	-56
10	17	-20
11	120	-126
12	29	33
16	51	50
17	34	33
7,K,2		
1	<11	0
2	<11	11
3	34	-35
5	<21	19
6	64	-64
7	74	-74
9	18	20
-7,K,2		
1	219	215
2	63	66
3	12	-14
4	13	15
5	117	117
6	36	34
7	115	-116
8	32	34
9	66	71
10	13	-8
11	13	-14
12	25	-21
16	68	59
17	42	-37
8,K,2		
3	43	44
4	65	-67
6	32	-35
-8,K,2		
0	122	122
1	23	-24
2	52	-53
3	25	-25
4	33	-31
5	87	88
6	158	-161
7	119	120
8	78	-81
9	36	38
10	38	48
11	26	28
15	39	34
16	32	-31
9,K,2		
4	27	28
5	29	-30
-9,K,2		
1	19	18
2	12	-12
3	85	-87
4	191	-193
5	267	-275
6	110	113
7	10	8
8	113	-117
9	28	-28
10	64	66
11	16	20
12	33	-32
10,K,2		
1	23	19
-10,K,2		
0	26	30
1	64	-65
2	73	75
3	40	38
4	31	-31
5	154	-158
6	<11	-0
7	83	-86
8	<11	12
9	35	36
10	<13	0
14	47	-45
15	75	-69
-11,K,2		
1	26	-18
2	24	-28
3	96	98
4	60	64
5	48	53
6	37	-40
7	75	74
8	41	41
9	15	10
12	60	57
16	45	-40
-12,K,2		
0	35	34
1	46	50
2	115	-120
3	29	29
4	49	47
5	17	19
6	60	61
7	39	-33
8	59	56
11	34	37
12	52	-49
14	46	42
-13,K,2		
1	67	-73
2	60	62
3	49	45
4	46	44
5	53	51
6	70	-70
7	36	37
9	53	-56
-14,K,2		
0	28	-35
1	11	7
2	32	-26
4	44	46
5	70	68
7	52	51
8	57	-52
9	36	-31
-15,K,2		
3	85	-79
7	55	-53
-16,K,2		
1	37	35
2	59	56
3	86	-84
6	23	-28
12	51	48
13	66	-63
-17,K,2		
1	71	67
2	67	-65
3	56	51
8	31	31
-18,K,2		
0	25	30
1	39	-38
4	40	-43
9	55	48
-19,K,2		
3	36	-33
0,K,3		
0	144	145
1	47	-47
2	<11	-11
3	<13	-10
4	27	27
5	<11	-6
6	25	-24
7	17	-14
8	<11	-3
9	44	-41
10	54	-54
11	38	-36
14	21	21
1,K,3		
1	23	-25
2	<11	-0
3	<11	-3
4	25	23
5	52	-49
6	33	-31
7	<12	-10
8	19	18
9	15	-16
10	25	-25
11	31	30
-1,K,3		
1	134	139
2	46	45
3	<10	6
4	<11	-8
5	<10	9
6	<11	4
7	<11	1
8	<11	-3
9	57	55
10	41	38
2,K,3		
0	<11	1
1	<11	-9
2	<10	-9
3	<11	5
4	34	-35
5	20	19
6	<11	-6
12	21	-19
-2,K,3		
0	72	-76
1	118	119
2	18	17
3	30	-31
4	18	-18
5	23	27
6	16	-21
7	<11	4
8	21	-20
9	19	21
10	15	8
11	97	94
12	34	34
15	22	24
3,K,3		
1	33	-32
2	28	-28
3	<11	8
4	14	-12
6	30	29
-3,K,3		
1	93	-94
2	54	-55
3	26	-26
4	19	12
5	51	-51
6	49	-49
7	21	21
8	<11	-0
9	46	-46
10	25	-26
12	35	32
16	27	-21
4,K,3		
0	53	-54
1	<12	-4
3	17	11
5	14	-13
6	16	14
9	<13	16
-4,K,3		
0	74	-76
1	<10	13
2	<11	-7
3	30	27
4	<13	9
5	51	-50
6	44	44
7	38	-38
8	22	21
9	<11	3
10	63	-63
12	27	-31
5,K,3		
4	<13	-11
5	17	17
6	23	21
7	27	26
10	20	21
-5,K,3		
1	88	-90
2	18	17
3	21	15
4	36	38
5	129	131
6	12	13
7	24	-23
8	<11	5
9	<11	2
10	<11	1
6,K,3		
3	13	-14
4	29	25
-6,K,3		
0	69	-70
1	80	-80
2	50	52
3	11	9
4	<10	-12
5	32	30
6	59	62
7	12	14
8	24	24
9	36	-34
10	<11	-5
11	73	-75
12	25	27
16	38	33
7,K,3		
3	19	-21
6	30	-30
7	25	-28
-7,K,3		
1	125	128
2	21	23
3	<9	-5
4	<10	-0
5	57	57
6	<10	3
7	30	-31
8	<11	13
9	43	46
10	13	-19
12	20	-20
16	44	37
8,K,3		
4	29	-28
-8,K,3		
0	99	99
1	<10	-2
2	26	-28
3	<11	8
4	19	21
5	44	44
6	89	-90
7	75	77
8	52	-54
9	34	35
10	36	38
16	37	-33
-9,K,3		
1	<11	-10
2	11	-11
3	68	-69
4	110	-110
5	183	-184
6	115	115
7	18	-15
8	71	-72
9	20	-18
10	45	48
-10,K,3		
0	10	14
1	23	-25
2	45	45
3	<11	5
4	74	-72
5	111	-111
6	15	-16
7	78	-79
8	16	17
14	35	-33
15	52	-47
-11,K,3		
1	<10	-3
2	16	-16
3	98	101
4	46	48
5	40	42
6	65	-68
7	56	54
8	40	38
12	40	39
16	38	-35
-12,K,3		
0	36	37
1	17	19
2	88	-89
3	21	19
4	55	54
5	35	36
6	50	51
8	48	44
11	26	32
12	42	-38
14	39	37
-13,K,3		
1	54	-57
2	56	57
3	16	9
4	28	27
5	43	39
6	62	-60
7	35	37
9	28	-30
-14,K,3		
0	48	-54
4	55	54
5	45	45
7	30	29
8	59	-53
-15,K,3		
3	76	-69
6	43	42
7	52	-51
8	24	28
-16,K,3		
1	46	40
2	31	30
3	70	-69
4	32	-32
6	34	-36
12	45	39
13	68	-60
-17,K,3		
1	64	58
2	61	-58
3	68	60
11	38	32
-18,K,3		
0	40	41
1	57	-53
2	37	33
4	38	-40
8	37	34
9	55	47
-19,K,3		
3	47	-44
-21,K,3		
2	36	33
0,K,4		
6	<13	-9
9	20	-16
10	27	22
1,K,4		
5	27	-20
9	<12	-5
-1,K,4		
1	58	61
9	31	30
-2,K,4		
0	<12	-10
1	57	57
2	<16	13
3	<12	-0
11	46	46
3,K,4		
1	17	-16
-3,K,4		
1	50	-52
2	15	-14
3	<11	-6
5	29	-28
9	27	-27
12	21	17
4,K,4		
0	21	-14
-4,K,4		
0	29	-30
1	12	-11
2	15	-5
3	<11	9
4	18	-14
5	24	-25
6	15	12
7	<20	-19
10	35	-34
-5,K,4		
1	26	-28
2	14	13
3	18	13
4	<13	13
5	56	55
-6,K,4		
0	34	-35
1	37	-36
2	<12	11
3	<11	-0
4	17	11
5	22	21
6	26	28
11	31	-32
-7,K,4		
1	57	60
2	<11	-3
3	<11	-5
4	<13	-5
5	19	21
9	25	25
-8,K,4		
0	64	62
1	<11	8
2	<11	-8
3	<11	12
4	26	26
5	16	12
6	34	-35
7	36	35
8	22	-23
9	22	22
10	21	22
-9,K,4		
1	14	-18
2	<11	-5
3	35	-37
4	45	-43
5	89	-88
6	79	79
8	32	-30
10	27	28
-10,K,4		
0	<12	-4
1	<11	-2
2	19	16
3	<13	-9
4	73	-73
5	49	-51
6	23	-20
7	46	-48
-11,K,4		
1	14	6
2	<11	-1
3	65	67
4	23	25
6	66	-67
7	29	32
-12,K,4		
0	27	28
2	40	-39
4	48	50
5	26	30
6	34	35
-13,K,4		
1	30	-30
2	35	34
6	34	-30
-14,K,4		
0	46	-50
4	43	40
8	42	-39
-15,K,4		
3	42	-38
6	40	42
7	37	-37
-16,K,4		
1	32	29
3	45	-42
4	37	-39
6	29	-31
13	45	-41
-17,K,4		
1	38	35
2	36	-34
3	52	48
4	30	-32
-18,K,4		
0	40	39
1	56	-51
2	51	45
9	36	32
-19,K,4		
3	43	-42
-1,K,5		
1	18	21
-2,K,5		
1	23	22
11	22	17
-3,K,5		
1	18	-22
-4,K,5		
0	<16	-16
-5,K,5		
5	20	17
-6,K,5		
0	16	-13
-7,K,5		
1	23	22
-8,K,5		
0	38	33
-9,K,5		
5	31	-30
6	39	39
-10,K,5		
4	47	-47
-11,K,5		
3	28	30
6	45	-45
-12,K,5		
0	22	15
4	34	36
-14,K,5		
0	29	-30
-18,K,5		
1	39	-34
2	42	38
-9,K,6		
0	21	14
-10,K,6		
4	26	-21
-11,K,6		
6	19	-21
-12,K,6		
4	19	19

secondary extinction. Adsorption differences were found to be small (~1·5 %) and no corrections were made.

The averaged intensities were converted to structure factors within the ideal mosaic approximation and with appropriate account of Lorentz and polarization effects. Weights were based on the counting statistics and on other fluctuations in the diffractometer – the latter amounting to a 1 % relative standard error. A total of 1163 unique reflections, of which 132 were unobserved, were used in the least-squares analysis.

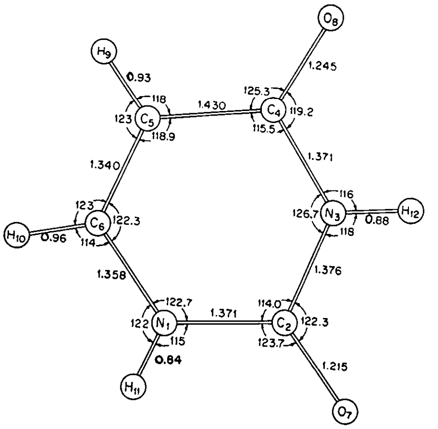

Fig. 1. Dimensions of the uracil molecule.

The structure factor calculation with Parry's (1954) atomic and thermal parameters for all atoms yielded an R of 0·18. The scattering factors for O, N, and C were from Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) and for H were from Stewart, Davidson & Simpson (1965). Refinement proceeded by full-matrix least-squares whereby an overall scale factor, atomic positions, and anisotropic thermal parameters (isotropic for H atoms) were varied. For these 89 parameters the sum of the weighted, squared residuals, $w(|F_o|-|F_c|)^2$ was minimized. After three cycles the refinement terminated, with marginal shifts in the parameters, the largest being $0{\cdot}25\sigma$. The final R was 0·045, omitting the unobserved reflections. The final weighted R was 0·037. The goodness of fit was 2·34. The average estimated standard deviation for positions of the heavy atoms was 0·0016 Å; for the hydrogen 0·018 Å. The final atomic parameters are listed in Table 1. All calculations were carried out on an IBM 7094 computer with programs from X-RAY 63 (Stewart *et al.*, 1964).

The observed and calculated structure factors are listed in Table 2.

The distances and angles among the least-squares adjusted precalculated scattering centers are listed in Table 3 and shown in Fig. 1. For comparison the values reported by Parry (1954), corrected to our unit cell parameters are also shown in Table 3. The C(5)–C(6) bond is 0·07 Å shorter than Parry's value, but is in agreement with the C(5)–C(6) bond in thymine (Gerdil, 1961) and 1-methylthymine (Hoog-

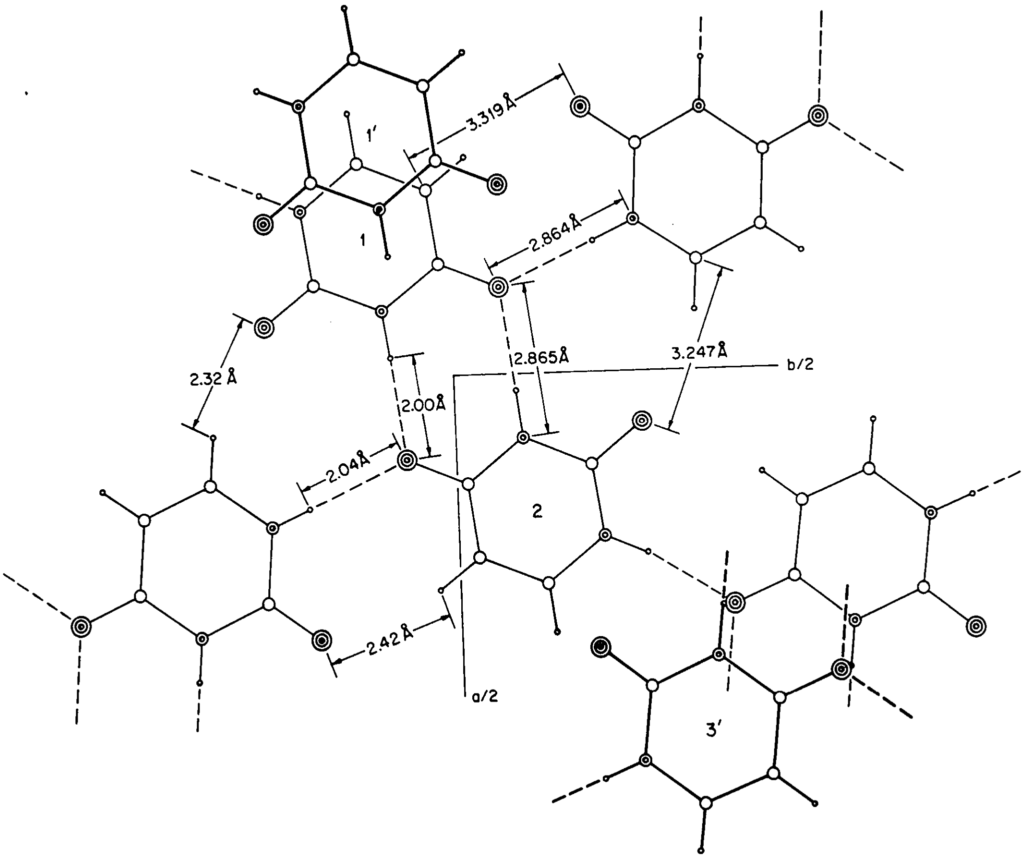

Fig. 2. Orthographic projection of uracil molecules onto (001). Heavy print, molecules near $z=1$. Light print, molecules near $z=0$. Single large circles, carbon atoms. Single small circles, hydrogen atoms. Double circles, nitrogen atoms. Triple circles, oxygen atoms.

steen, 1963*a*, *b*). The corresponding bond lengths and angles for 1-methylthymine, also listed in Table 3, are in remarkable agreement with the refined uracil structure. The C(2)–O(7) bond length has not been corrected for the bending motion implied by the thermal parameters. A significantly different bond length is the C(6)–N(1) distance where the bond for uracil (1·358 Å) is 0·025 Å shorter than for 1-methylthymine (1·383 Å). In thymine (Gerdil, 1961), moreover, the C(6)–N(1) bond length is also the same as for 1-methylthymine.

Table 3. *Bond distances and angles of uracil*

U (1966): this investigation.
U (1954): uracil (Parry, 1954); (corrected to unit-cell parameters in this work).
1-MT: 1-methylthymine (Hoogsteen, 1963*a*).

Estimated standard deviations in parenthesis

	U (1966)	U (1954)	1-MT
N(1)–C(2)	1·371 ($0{\cdot}002_5$)	1·354 (0·012)	1·379 (0·004)
C(2)–N(3)	1·376 ($0{\cdot}002_0$)	1·389 (0·008)	1·379 (0·004)
N(3)–C(4)	1·371 ($0{\cdot}002_1$)	1·379 (0·010)	1·375 (0·004)
C(4)–C(5)	1·430 ($0{\cdot}002_6$)	1·421 (0·014)	1·432 (0·004)
C(5)–C(6)	1·340 ($0{\cdot}002_3$)	1·413 (0·011)	1·346 (0·004)
C(6)–N(1)	1·358 ($0{\cdot}002_2$)	1·347 (0·012)	1·383 (0·004)
C(2)–O(7)	1·215 ($0{\cdot}002_1$)	1·236 (0·010)	1·214 (0·004)
C(4)–O(8)	1·245 ($0{\cdot}001_9$)	1·245 (0·010)	1·237 (0·004)
C(5)–H(9)	0·931 (0·020)		
C(6)–H(10)	0·957 (0·020)		
N(1)–H(11)	0·836 (0·018)		
N(3)–H(12)	0·877 (0·021)		
N(1)–C(2)–N(3)	114·0 (0·1)	115·7	115·4° (0·2)
C(2)–N(3)–C(4)	126·7 (0·2)	124·2	126·3 (0·2)
N(3)–C(4)–C(5)	115·5 (0·1)	118·3	116·1 (0·2)
C(4)–C(5)–C(6)	118·9 (0·2)	116·6	118·3 (0·2)
C(5)–C(6)–N(1)	122·3 (0·2)	121·4	123·3 (0·2)
C(6)–N(1)–C(2)	122·7 (0·1)	123·7	120·6 (0·2)
N(1)–C(2)–O(7)	123·7 (0·2)	124·7	123·3 (0·2)
N(3)–C(2)–O(7)	122·3 (0·2)	119·5	121·3 (0·2)
N(3)–C(4)–O(8)	119·2 (0·2)	118·0	120·0 (0·2)
C(5)–C(4)–O(8)	125·3 (0·2)	123·7	123·9 (0·2)
C(4)–C(5)–H(9)	118·1 (1·2)		
C(6)–C(5)–H(9)	123·0 (1·2)		
C(5)–C(6)–H(10)	123·2 (1·0)		
N(1)–C(6)–H(10)	114·5 (1·0)		
C(6)–N(1)–H(11)	122·12 (1·4)		
C(2)–N(1)–H(11)	115·1 (1·3)		
C(2)–N(3)–H(12)	117·8 (1·0)		
C(4)–N(3)–H(12)	115·5 (1·0)		

The least-squares plane through the eight non-hydrogen atoms of the uracil molecule is

$$-1{\cdot}2601x+0{\cdot}2390y+3{\cdot}3162z=-0{\cdot}1100$$

(x, y, and z in fractions of unit-cell axes) and leads to an average standard deviation of 0·0046 Å. The root mean square average for the estimated standard deviations of these atoms along the direction normal to the plane is 0·0017 Å. On the average the deviation of the atoms from the plane is $2{\cdot}7\sigma$; one may conclude that they depart significantly from a plane. The largest departures are for N(3) (−0·0073 Å) and for O(8) (+0·0070 Å). The other distances in Å are 0·0006, 0·0048, 0·0011, −0·0022, −0·0040, and −0·0001 for atoms O(7), N(1), C(2), C(4), C(5), and C(6), respectively. The least-squares plane for the pyrimidine ring alone [O(7) and O(8) omitted] is given by the equation

$$-1{\cdot}2404x+0{\cdot}2728y+3{\cdot}3135z=-0{\cdot}1004.$$

The standard deviation of the six atoms from this plane is 0·0025 Å. Atoms N(3) and C(4) are appreciably out of this plane; $-0{\cdot}003_4$ and $+0{\cdot}003_5$ Å, respectively. The atom O(8) is $0{\cdot}016_7$ Å above the plane. The uracil least-squares plane forms a dihedral angle with (001) of 6°9′; the pyrimidine ring least-squares plane is at a similar angle of 6°6′.

Fig. 2 is an orthographic projection of the atoms in the uracil molecules onto (001). The heavy line molecules are at $z=1$; the light line at $z=0$. The N(3)–O(8) hydrogen bond length to the centric related molecule is 2·865 ± 0·002 Å and the N(1)–O(8) length to the screw axis related molecule is 2·864 ± 0·002 Å. These distances are in agreement with Parry's structure (corrected to the *a* axis reported here.) The corresponding distances from O(8) to H(12) and to H(11) are 2·00 ± 0·02 and 2·04 ± 0·02 Å, respectively. The distance from C(5) to O(7) of a screw related molecule is 3·319 Å; the corresponding H(9)–O(7) length is 2·42 Å. The distance from C(6) to O(7) of a glide related molecule is 3·246 Å and the corresponding H(10)–O(7) distance is 2·32 Å. These approach distances are also in agreement with Parry (again corrected to the present *a*-axis value). Although the H(10)–O(7) approach, 2·32 Å, is close, it is not as close as the distance reported for the 1-methythymine crystal structure (Hoogsteen, 1963). For the latter case the O(7)–C(6) distance was 3·11 Å and for O(7)–H(9) the length was 2·14 Å.

Aside from the N(1)–O(8) and N(3)–O(8) hydrogen bonds, the closest heavy atom interatomic distance is 3·20 Å between C(6) of molecule 2 and O′(7) of molecule 3′ as depicted in Fig. 2. The other close approaches are C(2′)–N(1) 3·317 Å, and C(4′)–C(5) 3·323 Å between molecules 1′ and 1 in Fig. 2. The spacing between the (001) planes is 3·136 Å.

The details of data gathering and refinement in this investigation will be submitted elsewhere.

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