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The Crystal Structure of Ammonium Orotate Monohydrate

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The crystal structure of ammonium orotate monohydrate has been determined by X-ray crystallographic methods and refined to $R = 0.041$ ($R_w = 0.055$). The space group is *Pbca*. The intensities of 2285 reflections were measured on an automatic diffractometer using Mo$K\alpha$ radiation. The estimated standard deviations in bond lengths involving non-hydrogen atoms are 0.0011 – 0.0014 Å. The reflections have been divided into two parts, and the results of refinements of low and high order reflections are discussed.

Orotic acid (6-carboxy-uracil) is closely related to the biologically important pyrimidine bases. Horan and Snipes have carried out an ESR investigation of the ammonium salt of this acid, also predicting the orientation of the molecules in the crystals.[1] Using one of their crystals a complete crystal structure investigation was undertaken.

STRUCTURE DETERMINATION

The crystals are obtained from a solution of 50 % ethanol and 50 % 0.8 M aqueous NH_4OH saturated with orotic acid at 60°C and cooled slowly for a period of several days. The space group is *Pbca*. The unit cell dimensions were measured on a manual Picker diffractometer and found to be:

$$a = 18.664(1),\ b = 12.634(1),\ c = 6.6094(4)$$

Estimated standard deviations are given in parentheses. Flotation gave a density of 1.62 g/cm^3, corresponding to eight formula equiv. per unit cell ($\varrho_{calc} = 1.63$ g/cm^3). A crystal was cut to a somewhat irregular shape with the largest edge 0.62 and the smallest 0.30 mm. The intensities were measured at an automatic Picker diffractometer using Mo$K\alpha$ radiation. The 2θ-scan speed was 1 deg/min. The slowest varying index during data collection was l. No breakdown of the crystal could be observed. Out of a total of 2706 reflections with $2\theta < 65°$ 2288 had intensities greater than twice the standard deviation. At the end of the refinement three of these reflections were left out, being obviously in error when compared with the calculated values. The intensities were corrected for absorption effects.

Table 1. Observed and calculated structure factors on ten times absolute scale.

h	k	l	F_o	F_c
6	0	0	708	665
8	0	0	23	- 27
10	0	0	1172	-1097
12	0	0	634	- 642
14	0	0	115	- 133
16	0	0	138	- 135
18	0	0	118	- 120
20	0	0	266	270
22	0	0	205	210
24	0	0	154	- 154
26	0	0	141	137
2	1	0	580	565
4	1	0	83	65
6	1	0	576	- 580
8	1	0	79	72
10	1	0	76	79
12	1	0	26	33
14	1	0	34	- 34
16	1	0	328	- 344
18	1	0	101	172
20	1	0	66	- 65
22	1	0	36	34
24	1	0	84	- 71
26	1	0	126	136
0	2	0	681	- 695
2	2	0	300	302
4	2	0	329	316
6	2	0	420	420
8	2	0	347	- 340
10	2	0	787	751
12	2	0	170	- 166
14	2	0	229	- 223
16	2	0	340	351
18	2	0	402	- 421
20	2	0	246	- 250
22	2	0	86	88
24	2	0	113	- 112
26	2	0	24	- 24
2	3	0	236	195
4	3	0	620	- 569
6	3	0	1616	-1588
8	3	0	52	44
10	3	0	15	15
24	3	0	103	102
26	3	0	172	- 165
0	4	0	320	280
2	4	0	674	- 646
4	4	0	257	295
6	4	0	667	693
8	4	0	291	- 285
10	4	0	53	45
12	4	0	317	324
14	4	0	141	- 157
16	4	0	125	- 134
18	4	0	56	- 42
20	4	0	87	- 97
22	4	0	128	- 129
24	4	0	50	51
26	4	0	40	38
2	5	0	312	- 301
4	5	0	118	- 134
6	5	0	144	135
8	5	0	377	- 372
10	5	0	102	- 108
12	5	0	381	- 390
14	5	0	83	- 81
16	5	0	62	- 66
18	5	0	48	45
20	5	0	76	76
22	5	0	38	- 35
24	5	0	38	32
26	5	0	333	325
0	6	0	534	- 476
2	6	0	970	925
4	6	0	91	- 90
6	6	0	222	- 246
8	6	0	465	- 461
10	6	0	286	281
12	6	0	333	- 342
14	6	0	177	- 196
16	6	0	27	21
18	6	0	169	174
20	6	0	157	163
22	6	0	51	- 51
24	6	0	58	58
26	6	0	51	- 53
2	7	0	248	- 224
4	7	0	585	557
6	7	0	243	- 245
8	7	0	236	- 251
10	7	0	146	156
12	7	0	184	- 176
14	7	0	158	- 210
16	7	0	143	- 145
18	7	0	99	- 105
22	7	0	177	172
24	7	0	39	- 36
0	8	0	615	- 637
2	8	0	108	- 96
4	8	0	117	- 128
6	8	0	93	- 90
8	8	0	140	140
10	8	0	268	- 287
12	8	0	512	540
14	8	0	52	55
16	8	0	63	- 71
18	8	0	167	166
20	8	0	64	- 65
22	8	0	22	- 16
24	8	0	55	- 54
2	9	0	234	- 217
4	9	0	547	- 536
6	9	0	253	- 263
8	9	0	425	- 435
10	9	0	102	96
12	9	0	295	- 296
14	9	0	465	502
16	9	0	87	76
20	9	0	167	195
24	9	0	154	- 157
0	10	0	370	- 390
2	10	0	24	- 31
4	10	0	185	211
6	10	0	325	- 356
8	10	0	175	181
10	10	0	64	- 82
12	10	0	55	- 65
14	10	0	215	226
16	10	0	97	- 98
18	10	0	100	104
22	10	0	72	67
2	11	0	542	- 565
4	11	0	515	528
6	11	0	143	164
8	11	0	23	15
10	11	0	98	- 103
14	11	0	22	- 21
16	11	0	140	- 143
20	11	0	36	- 39
22	11	0	36	- 40
0	12	0	136	- 144
2	12	0	107	- 109
4	12	0	159	- 177
6	12	0	243	- 244
8	12	0	368	375
10	12	0	34	- 36
12	12	0	152	144
14	12	0	18	- 14
16	12	0	25	25
18	12	0	191	186
20	12	0	98	- 97
2	13	0	133	130
4	13	0	173	187
6	13	0	54	- 65
8	13	0	179	191
10	13	0	72	- 62
12	13	0	62	58
16	13	0	151	- 143
18	13	0	134	- 135
20	13	0	191	187
0	14	0	23	27
4	14	0	202	- 213
8	14	0	208	201
10	14	0	242	- 235
12	14	0	120	- 118
14	14	0	329	324
18	14	0	160	- 155
2	15	0	49	- 40
4	15	0	19	- 14
6	15	0	119	- 115
8	15	0	27	- 24
10	15	0	95	93
12	15	0	64	61
14	15	0	22	- 23
16	15	0	142	143
0	16	0	36	- 45
2	16	0	91	98
6	16	0	61	58
8	16	0	183	- 180
10	16	0	45	44
12	16	0	141	- 137
14	16	0	60	56
2	17	0	231	221
4	17	0	89	- 78
6	17	0	39	- 38
8	17	0	340	327
10	17	0	20	- 18
12	17	0	102	- 96
0	18	0	166	- 160
2	18	0	22	- 15
4	18	0	19	- 18
6	18	0	75	- 66
8	18	0	69	70
1	1	1	166	137
2	1	1	21	- 36
3	1	1	260	235
4	1	1	230	211
5	1	1	616	- 596
6	1	1	130	121
7	1	1	264	260
8	1	1	281	271
9	1	1	600	598
10	1	1	267	260
11	1	1	777	- 735
12	1	1	204	195
13	1	1	332	336
14	1	1	129	126
15	1	1	165	- 182
16	1	1	78	76
17	1	1	68	70
20	1	1	40	- 38
21	1	1	58	- 50
22	1	1	87	- 87
23	1	1	48	45
24	1	1	70	- 68
25	1	1	23	24
26	1	1	57	- 58
27	1	1	39	- 44
0	2	1	301	- 298
1	2	1	299	- 295
2	2	1	28	16
3	2	1	1250	1212
4	2	1	132	124
5	2	1	310	288
6	2	1	162	195
7	2	1	225	190
8	2	1	177	172
9	2	1	149	144
10	2	1	152	143
11	2	1	131	120
12	2	1	52	48
13	2	1	13	12
14	2	1	71	- 71
15	2	1	554	- 595
16	2	1	76	- 77
17	2	1	60	- 70
18	2	1	100	- 102
19	2	1	64	65
20	2	1	93	- 95
21	2	1	73	- 77
22	2	1	59	- 58
23	2	1	28	32
25	2	1	116	116
27	2	1	27	17
1	3	1	576	- 518
2	3	1	507	485
3	3	1	636	625
4	3	1	524	507
5	3	1	568	- 538
6	3	1	450	472
7	3	1	534	517
8	3	1	366	355
9	3	1	200	- 187
10	3	1	202	201
11	3	1	12	- 5
12	3	1	55	- 55
13	3	1	316	328
15	3	1	114	130
16	3	1	33	- 35
17	3	1	127	- 120
18	3	1	91	- 97
19	3	1	75	- 86
20	3	1	28	- 28
21	3	1	41	- 42
23	3	1	59	95
25	3	1	81	- 76
27	3	1	74	- 65
0	4	1	640	608
1	4	1	230	181
2	4	1	510	491
3	4	1	43	40
4	4	1	262	293
5	4	1	1628	-1577
6	4	1	140	133
7	4	1	216	206
8	4	1	64	- 95
9	4	1	28	24
10	4	1	119	- 115
11	4	1	153	- 150
12	4	1	147	- 148
13	4	1	218	- 218
14	4	1	74	- 76
15	4	1	470	476
16	4	1	133	- 140
17	4	1	255	270
18	4	1	50	- 50
19	4	1	41	- 44
21	4	1	79	- 80
22	4	1	38	- 38
23	4	1	32	27
25	4	1	82	79
27	4	1	286	- 270
1	5	1	625	578
2	5	1	76	- 67
3	5	1	115	102
4	5	1	222	215
5	5	1	11	15
6	5	1	137	142
7	5	1	266	- 251
8	5	1	21	27
9	5	1	175	- 135
10	5	1	19	22
11	5	1	250	- 292
12	5	1	61	62
13	5	1	141	- 151
16	5	1	88	- 56
17	5	1	188	- 204
18	5	1	26	31
19	5	1	329	345
21	5	1	54	48
23	5	1	18	- 13
24	5	1	18	- 12
25	5	1	44	42
26	5	1	21	23
0	6	1	404	387
1	6	1	215	188
2	6	1	530	514
4	6	1	369	382
5	6	1	219	214
6	6	1	61	- 58
7	6	1	80	- 67
8	6	1	112	- 110
9	6	1	205	206
10	6	1	154	- 155
11	6	1	124	- 127
12	6	1	172	- 177
13	6	1	184	191
14	6	1	190	- 195
15	6	1	292	- 310
16	6	1	51	- 50
17	6	1	77	85
18	6	1	17	- 10
19	6	1	27	25
20	6	1	35	- 31
21	6	1	285	- 293
23	6	1	214	212
24	6	1	25	19
25	6	1	58	- 60
1	7	1	707	- 686
2	7	1	85	- 82
3	7	1	422	407
4	7	1	289	- 288
5	7	1	18	17
6	7	1	184	- 182
7	7	1	256	- 248
8	7	1	125	- 138
9	7	1	62	54
10	7	1	30	- 30
11	7	1	864	891
13	7	1	390	- 404
14	7	1	100	104
15	7	1	33	- 22
16	7	1	75	76
17	7	1	110	107
18	7	1	30	28
19	7	1	84	81
20	7	1	27	25
21	7	1	319	- 313
23	7	1	50	- 46
24	7	1	44	43
25	7	1	93	88
0	8	1	177	180
1	8	1	438	424
2	8	1	69	72
3	8	1	67	- 60
4	8	1	79	40
5	8	1	100	- 112
6	8	1	151	151
7	8	1	153	154
8	8	1	121	124
9	8	1	186	- 188
10	8	1	77	- 40
11	8	1	15	12
12	8	1	29	- 21
13	8	1	178	192
15	8	1	108	- 102
16	8	1	122	- 122
17	8	1	164	- 158
18	8	1	109	- 107
19	8	1	112	- 108
20	8	1	45	- 44
21	8	1	76	72
22	8	1	52	- 53
24	8	1	32	- 31
25	8	1	91	- 88
1	9	1	22	- 33
2	9	1	109	- 105
3	9	1	308	- 311
4	9	1	48	- 51
5	9	1	475	484
6	9	1	69	- 72
7	9	1	189	- 205
8	9	1	146	- 150
9	9	1	24	- 17
10	9	1	124	- 136
11	9	1	96	- 83
13	9	1	188	188
14	9	1	69	- 65
15	9	1	27	18
17	9	1	35	- 36

Table 1. Continued.

h	k	l	F_o	F_c
18	9	1	33	31
19	9	1	178	- 172
20	9	1	31	32
21	9	1	244	235
23	9	1	144	- 142
24	9	1	44	41
1	10	1	40	- 44
2	10	1	19	16
3	10	1	633	- 646
5	10	1	523	544
7	10	1	27	26
8	10	1	71	73
9	10	1	366	- 386
10	10	1	52	53
11	10	1	49	46
13	10	1	186	196
14	10	1	19	- 20
15	10	1	150	- 154
16	10	1	25	- 26
17	10	1	70	73
18	10	1	62	- 63
19	10	1	107	103
20	10	1	68	- 66
21	10	1	81	- 80
22	10	1	22	- 21
1	11	1	406	419
2	11	1	63	62
3	11	1	270	- 292
4	11	1	50	- 53
5	11	1	165	188
7	11	1	127	- 131
8	11	1	21	- 20
9	11	1	109	- 105
10	11	1	95	- 97
11	11	1	74	- 85
12	11	1	128	- 127
13	11	1	225	- 217
14	11	1	73	- 75
15	11	1	74	63
16	11	1	31	- 31
17	11	1	25	32
19	11	1	55	50
21	11	1	101	102
22	11	1	79	75
0	12	1	55	52
2	12	1	76	78
3	12	1	258	271
4	12	1	33	- 32
5	12	1	286	- 307
7	12	1	358	377
8	12	1	44	- 42
9	12	1	47	- 55
10	12	1	78	- 75
11	12	1	41	- 40
12	12	1	23	- 25
18	12	1	28	25
19	12	1	181	- 183
20	12	1	50	45
21	12	1	109	112
2	13	1	47	- 44
3	13	1	287	- 286
4	13	1	90	- 94
5	13	1	40	- 41
6	13	1	76	- 80
7	13	1	125	128
8	13	1	103	- 107
9	13	1	170	172
10	13	1	61	- 64
11	13	1	34	38
13	13	1	86	79
14	13	1	35	- 36
17	13	1	153	158
18	13	1	289	- 291
20	13	1	27	25
0	14	1	48	- 52
1	14	1	141	135
2	14	1	45	- 45
3	14	1	93	- 98
5	14	1	58	- 57
6	14	1	34	- 35
7	14	1	173	- 173
9	14	1	114	- 105
10	14	1	34	32
11	14	1	237	233
13	14	1	91	- 85
14	14	1	30	30
15	14	1	49	41
16	14	1	31	25
17	14	1	106	105
18	14	1	40	36
2	15	1	29	- 26
3	15	1	22	- 27
4	15	1	71	- 71
5	15	1	105	104
6	15	1	74	- 72
7	15	1	44	43
8	15	1	47	- 44
9	15	1	217	- 215
10	15	1	36	- 32
11	15	1	117	117
13	15	1	109	- 112
14	15	1	31	27
15	15	1	103	105
0	16	1	112	- 132
1	16	1	140	- 138
2	16	1	69	- 73
3	16	1	141	138
4	16	1	66	- 64
5	16	1	45	- 40
7	16	1	167	163
8	16	1	23	25
9	16	1	22	28
10	16	1	52	52
11	16	1	52	- 47
12	16	1	63	65
13	16	1	63	- 62
14	16	1	32	33
1	17	1	23	25
2	17	1	22	24
3	17	1	58	53
4	17	1	24	26
5	17	1	114	- 107
6	17	1	32	32
7	17	1	52	50
8	17	1	21	13
0	18	1	22	- 14
1	18	1	67	77
2	18	1	43	- 46
3	18	1	27	- 31
4	18	1	19	- 13
5	18	1	118	114
6	18	1	27	- 21
7	18	1	188	- 185
1	0	2	96	- 91
2	0	2	2069	-2172
3	0	2	581	574
4	0	2	736	- 693
5	0	2	373	395
6	0	2	262	247
7	0	2	357	351
8	0	2	230	211
9	0	2	12	- 11
10	0	2	463	- 435
11	0	2	100	92
12	0	2	132	- 137
13	0	2	31	- 37
14	0	2	188	189
15	0	2	214	- 215
16	0	2	91	96
17	0	2	13	16
20	0	2	241	241
21	0	2	29	- 33
22	0	2	168	168
23	0	2	45	47
24	0	2	131	- 134
25	0	2	68	68
26	0	2	120	118
1	1	2	182	192
2	1	2	902	877
3	1	2	645	627
4	1	2	611	598
5	1	2	36	38
6	1	2	69	57
7	1	2	320	- 297
8	1	2	445	419
9	1	2	119	- 116
10	1	2	185	186
11	1	2	27	- 15
12	1	2	19	- 15
13	1	2	185	- 182
14	1	2	70	- 68
15	1	2	66	- 62
16	1	2	363	- 377
17	1	2	168	176
20	1	2	79	- 75
21	1	2	39	39
22	1	2	62	56
23	1	2	57	57
24	1	2	61	- 51
25	1	2	29	24
26	1	2	135	125
27	1	2	58	- 52
0	2	2	1175	-1154
1	2	2	438	412
2	2	2	509	- 478
3	2	2	26	- 17
4	2	2	330	- 326
5	2	2	184	- 170
6	2	2	65	66
7	2	2	103	95
8	2	2	319	- 305
9	2	2	126	124
10	2	2	686	667
11	2	2	41	- 41
12	2	2	50	53
13	2	2	48	- 46
14	2	2	55	62
15	2	2	105	111
16	2	2	473	495
18	2	2	203	- 212
19	2	2	60	- 61
20	2	2	85	- 79
21	2	2	18	15
22	2	2	136	136
24	2	2	94	- 91
25	2	2	41	- 42
26	2	2	31	- 28
1	3	2	307	305
2	3	2	494	465
3	3	2	28	34
4	3	2	204	194
5	3	2	80	80
6	3	2	563	- 546
7	3	2	54	50
8	3	2	500	501
9	3	2	208	- 204
10	3	2	319	336
11	3	2	35	- 32
12	3	2	76	61
13	3	2	26	- 30
14	3	2	368	- 390
16	3	2	689	734
17	3	2	64	- 67
18	3	2	313	- 334
19	3	2	100	103
24	3	2	66	66
26	3	2	178	- 168
0	4	2	263	241
1	4	2	270	- 252
2	4	2	473	- 462
3	4	2	282	- 272
4	4	2	124	130
5	4	2	62	- 58
6	4	2	286	288
7	4	2	130	- 124
8	4	2	442	- 425
9	4	2	182	- 181
10	4	2	74	- 71
11	4	2	120	126
12	4	2	235	241
13	4	2	159	168
14	4	2	85	- 89
16	4	2	24	22
17	4	2	81	88
18	4	2	113	124
19	4	2	76	75
20	4	2	42	36
21	4	2	51	- 51
22	4	2	28	- 25
23	4	2	66	- 62
24	4	2	91	90
1	5	2	237	- 217
2	5	2	155	- 154
3	5	2	32	- 24
4	5	2	28	- 28
5	5	2	78	81
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6	7	7	97	96
7	7	7	27	22
8	7	7	58	- 54
10	7	7	51	51
11	7	7	178	177
13	7	7	61	- 65
14	7	7	35	32
16	7	7	26	- 25
0	8	7	22	21
1	8	7	22	25
2	8	7	51	- 55
3	8	7	47	46
4	8	7	66	- 62
5	8	7	60	54
6	8	7	22	20
7	8	7	30	20
8	8	7	31	29
9	8	7	34	- 35
10	8	7	32	- 29
11	8	7	60	61
13	8	7	57	57
14	8	7	99	96
15	8	7	69	- 71
1	9	7	36	- 35
2	9	7	32	29
3	9	7	28	28
4	9	7	40	35
5	9	7	132	133
6	9	7	49	47
7	9	7	109	- 109
8	9	7	36	37
9	9	7	24	19
10	9	7	26	- 29
14	9	7	41	- 39
0	10	7	34	34
1	10	7	28	28
2	10	7	57	- 57
3	10	7	125	- 127
5	10	7	120	122
6	10	7	47	- 45
7	10	7	27	25
8	10	7	64	57
10	10	7	19	- 11
11	10	7	26	19
1	11	7	166	166
2	11	7	72	69
3	11	7	85	- 92
4	11	7	23	- 22
5	11	7	47	45
6	11	7	24	- 22
8	11	7	75	74
9	11	7	66	- 61
10	11	7	26	22
11	11	7	64	- 58
0	12	7	69	- 71
1	12	7	19	- 8
2	12	7	98	98
3	12	7	48	48
4	12	7	49	- 52
5	12	7	86	- 91
6	12	7	26	26
7	12	7	88	90
2	13	7	35	34
0	0	8	379	390
1	0	8	56	- 57
2	0	8	69	- 72
3	0	8	117	117
4	0	8	24	33
5	0	8	105	- 104
7	0	8	43	37
9	0	8	25	- 22
10	0	8	56	- 52
11	0	8	29	- 31
12	0	8	55	- 52
13	0	8	26	- 14
14	0	8	91	- 88
15	0	8	62	- 61
1	1	8	24	- 22
2	1	8	164	165
3	1	8	90	95
4	1	8	64	- 68
5	1	8	24	- 33
6	1	8	67	- 65
7	1	8	38	- 35
8	1	8	60	61
9	1	8	48	- 47
12	1	8	36	- 36
14	1	8	45	45
15	1	8	52	- 49
16	1	8	57	- 58
0	2	8	48	- 52
1	2	8	89	92
2	2	8	27	25
3	2	8	72	- 70
4	2	8	23	24
6	2	8	31	32
7	2	8	30	- 20

Table 1. Continued.

h	k	l	F_o	F_c
8	2	8	17	- 20
9	2	8	17	- 21
10	2	8	53	54
12	2	8	56	- 58
13	2	8	47	- 51
14	2	8	42	41
15	2	8	24	23
16	2	8	25	22
1	3	8	18	- 19
2	3	8	57	- 59
6	3	8	63	- 60
8	3	8	66	- 65
9	3	8	42	- 38
11	3	8	47	44
12	3	8	60	60
13	3	8	35	- 33
14	3	8	133	- 132
15	3	8	47	43
1	4	8	62	- 62
2	4	8	37	- 40
3	4	8	42	- 36
4	4	8	58	60
5	4	8	27	- 24
6	4	8	39	40
7	4	8	18	- 19
8	4	8	54	- 54
9	4	8	68	- 69
12	4	8	69	71
13	4	8	45	44
14	4	8	53	- 51
1	5	8	49	- 45
2	5	8	17	16
3	5	8	58	- 56
4	5	8	106	- 110
6	5	8	52	57
8	5	8	18	- 8
9	5	8	53	53
10	5	8	68	- 70
11	5	8	22	19
12	5	8	55	- 55
13	5	8	50	45
14	5	8	24	26
0	6	8	42	- 38
1	6	8	25	25
2	6	8	111	112
4	6	8	66	- 66
5	6	8	44	38
6	6	8	23	- 35
7	6	8	29	- 36
9	6	8	43	42
10	6	8	37	42
11	6	8	40	- 36
12	6	8	84	- 81
13	6	8	19	22
1	7	8	30	- 28
2	7	8	18	- 16
4	7	8	61	63
5	7	8	36	- 36
6	7	8	22	- 21
7	7	8	28	33
8	7	8	88	- 92
9	7	8	40	- 44
10	7	8	41	39
12	7	8	31	31
0	8	8	34	- 38
1	8	8	28	26
2	8	8	38	- 37
3	8	8	24	18
4	8	8	25	- 27
5	8	8	28	26
6	8	8	29	32
7	8	8	51	47
8	8	8	25	24
10	8	8	80	- 84
11	8	8	19	16
2	9	8	33	33
3	9	8	43	- 42
7	9	8	102	- 101
5	9	8	46	47
6	9	8	44	- 38
7	9	8	78	- 76
9	9	8	34	37
0	10	8	124	- 127
1	10	8	79	- 84
4	10	8	57	57
6	10	8	77	- 80
1	1	9	36	33
2	1	9	23	- 22
3	1	9	51	51
4	1	9	39	37
5	1	9	25	- 32
6	1	9	35	- 33
8	1	9	29	30
9	1	9	27	26
11	1	9	46	- 42
0	2	9	36	- 36
1	2	9	24	- 21
2	2	9	19	20
3	2	9	40	42
6	2	9	30	26
7	2	9	51	- 50
11	2	9	20	22
1	3	9	18	- 27
2	3	9	48	50
5	3	9	22	17
10	3	9	51	46
0	4	9	34	35
1	4	9	61	- 64
2	4	9	21	14
4	4	9	19	20
5	4	9	56	- 53
8	4	9	39	- 37
1	5	9	23	21
2	5	9	18	- 23
4	5	9	30	35
6	5	9	28	- 25
0	6	9	21	12
1	6	9	27	24
2	6	9	44	47
4	6	9	54	44
6	6	9	26	- 28
7	6	9	31	- 33
2	7	9	23	- 19
3	7	9	25	- 25
4	7	9	52	- 52

Attempts to solve the structure by direct methods were unsuccessful. By inspection of the sharpened Patterson map the orientation of the pyrimidine ring was found, and, in accordance with Horan and Snipes's conclusion, it seemed likely that the ring plane lay in the *ab*-plane. The *R* factor was calculated for each position as the postulated orotate anion was moved stepwise in this plane, and the nitrogen of NH_4^+ and oxygen of H_2O were then derived

Table 2. Positional parameters for the atoms (estimated standard deviations in parentheses).

Atom	*x*	*y*	*z*
O	.03038(5)	.45630(7)	.26256(15)
N	.04980(5)	.14067(8)	.35358(18)
O2	.14806(3)	.21871(6)	.04876(15)
O4	.31568(4)	−.03808(6)	−.01425(15)
O8	.45395(3)	.30861(6)	.00616(13)
O9	.36391(4)	.42446(6)	−.01556(14)
N1	.26461(4)	.26934(6)	.01446(13)
C2	.21106(5)	.19546(7)	.02677(15)
N3	.23324(4)	.09227(7)	.01266(14)
C4	.30281(5)	.05754(8)	−.00526(16)
C5	.35609(5)	.14025(7)	−.01219(16)
C6	.33560(4)	.24228(7)	−.00134(14)
C7	.38932(4)	.33310(7)	−.00385(15)
H N1	.2495(7)	.3330(13)	.0168(18)
H N3	.1995(11)	.0477(17)	.0161(23)
H C5	.4083(8)	.1264(12)	−.0239(22)
H1 W	.0615(11)	.4773(15)	.3250(30)
H2 W	.0046(9)	.4172(16)	.3380(30)
H1 N	.0823(9)	.1664(14)	.2601(28)
H2 N	.0236(9)	.0837(15)	.3070(26)
H3 N	.0155(9)	.1963(14)	.3910(31)
H4 N	.0787(10)	.1217(16)	.4623(30)

from a difference electron density map based on the set of parameters giving the best value of R. The structure was refined by full matrix least squares. The weighting scheme was based on standard deviation from counter statistics and 2 % fluctuation in diffractometer stability. The hydrogen atoms were refined isotropically. At the end of the refinement the data were corrected for secondary extinction. The final R-value was 0.041 ($R_w = 0.055$). In Table 1 the observed and calculated structure factors for this refinement are listed. The positional parameters are given in Table 2 and the thermal parameters in Table 3.

Table 3. Temperature parameters of the atoms (estimated standard deviations in parentheses).

Atom	B_{11}(B)	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
O	.00190(2)	.00373(5)	.01800(21)	−.00081(6)	−.00058(12)	.00153(17)
N	.00131(2)	.00321(6)	.01880(25)	−.00026(6)	−.00063(12)	.00065(19)
O2	.00101(2)	.00311(5)	.02563(25)	.00029(5)	.00221(11)	.00302(17)
O4	.00142(2)	.00175(4)	.03342(31)	.00008(5)	.00043(12)	−.00108(18)
O8	.00102(2)	.00252(5)	.02403(24)	−.00013(5)	−.00044(10)	.00052(16)
O9	.00133(2)	.00184(4)	.02732(26)	.00020(5)	.00126(11)	.00121(16)
N1	.00094(2)	.00171(4)	.01404(20)	−.00002(4)	.00052(10)	.00013(15)
C2	.00099(2)	.00195(5)	.01282(22)	−.00012(5)	.00044(11)	.00114(17)
N3	.00091(2)	.00169(4)	.01984(25)	−.00032(5)	.00048(11)	.00056(17)
C4	.00107(2)	.00185(5)	.01556(25)	−.00008(6)	−.00012(12)	.00001(18)
C5	.00098(2)	.00179(5)	.01596(25)	−.00012(5)	−.00009(12)	−.00021(18)
C6	.00095(2)	.00188(5)	.01012(20)	−.00024(5)	−.00003(11)	.00022(16)
C7	.00105(2)	.00182(5)	.01239(22)	−.00030(6)	.00032(12)	−.00010(17)
H N1	2.35(29)					
H N3	3.64(38)					
H C5	2.79(33)					
H1 W	4.11(44)					
H2 W	4.38(42)					
H1 N	4.04(37)					
H2 N	3.40(34)					
H3 N	4.39(39)					
H4 N	4.64(46)					

Omitting the strong reflections from the least squares refinement did not make R_w any better, and secondary extinction or attenuator constants were excluded as explanations for the relative high R_w-value. The reflections were then divided into two sets. Set II consists of 1325 reflections with $2\theta > 45°$, set III comprises the remaining 960 reflections, while set I denotes the whole collected data set. Least squares refinements were then done on data sets II and III, not refining the hydrogen atom parameters. The results which are given in Table 4 suggest that the weighting scheme used in the least squares refinement does not properly weight the low order reflections. This is probably mainly caused by the assumption of spherical atomic structure factors. Data set III was not good enough, however, to show the bonding electrons when the parameters from II were used as input for a difference Fourier map calculation on III. Random errors obscured the map, although there were no peaks higher than ± 0.4 e$^-$/Å^3.

Table 4. Reliability constants and scale factors for the three data sets. R_{total} is the R-factor calculated for all the reflections (data set I).

	R	R_w	R_{total}	Scale factor
III	0.031	0.053	0.060	0.9522
I	0.041	0.055	0.041	1.0000
II	0.034	0.031	0.048	1.0549

Table 5. For each data set are given the r.m.s. difference between "observed" U_{ij} and U_{ij} calculated from the rigid body model (in Å²), the r.m.s. translational amplitudes (in Å) and last the r.m.s. librational amplitudes (in deg).

	$(\sum \Delta U_{ij}^2)^{\frac{1}{2}}$	T_1	T_2	T_3	L_1	L_2	L_3
III	0.0027	0.147	0.143	0.139	4.42	3.56	1.57
I	0.0022	0.145	0.128	0.118	4.33	3.37	1.65
II	0.0019	0.145	0.119	0.107	4.28	3.23	1.75

A rigid body analysis was performed on the thermal parameters of the orotate anion.[3] Some of the resulting TLS-parameters are given in Table 5. The corresponding corrections in bond lengths amount to between two and three times the estimated standard deviation in the bond lengths.

The atomic scattering factors of Hanson *et al.*[4] were used for the non-hydrogen atoms, those of Stewart *et al.*[5] for the hydrogen atoms. All programs used are included in Ref. 2.

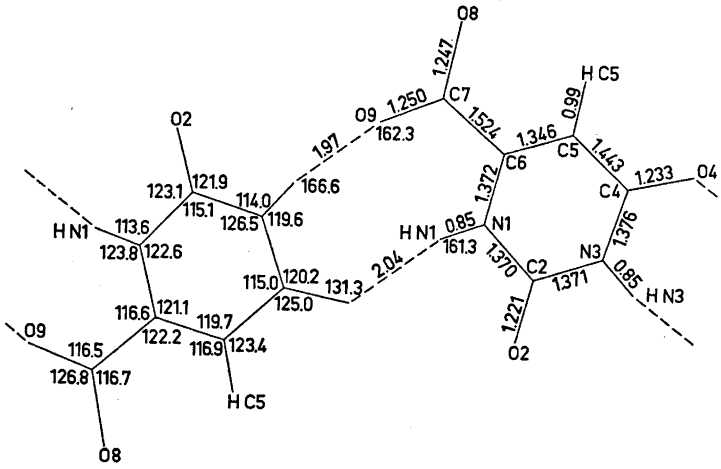

Fig. 1. The (001) projection of the orotate anion showing uncorrected bond distances (in Å) and angles (in deg).

Table 6. Bond distances (in Å) as calculated from the parameters from the refinements of data sets III, I, and II. σ_I is the estimated standard deviations calculated for I, for II the corresponding values are about 0.0004 Å smaller and for III 0.0010 Å larger. The rigid body motion corrections are equal for the three sets. The angles given (in deg) are calculated from data set I. For comparsion the bond lengths and angles of uracil are given.

	III	I	II	σ_I	R.b.m. corr.	Uracil
N1–C2	1.3693	1.3699	1.3715	.0012	.0028	1.371
C2–N3	1.3675	1.3710	1.3738	.0013	.0040	1.376
N3–C4	1.3701	1.3756	1.3788	.0013	.0032	1.371
C4–C5	1.4434	1.4432	1.4415	.0014	.0028	1.430
C5–C6	1.3373	1.3464	1.3546	.0014	.0041	1.340
C6–N1	1.3727	1.3724	1.3748	.0012	.0034	1.358
C2–O2	1.2202	1.2205	1.2265	.0011	.0018	1.215
C4–O4	1.2339	1.2332	1.2350	.0013	.0017	1.245
C6–C7	1.5265	1.5237	1.5208	.0013	.0028	
C7–O8	1.2442	1.2471	1.2507	.0011	.0024	
C7–O9	1.2480	1.2503	1.2520	.0012	.0026	

	I	σ_I	Uracil		I	σ_I	Uracil
N1–H N1	0.852	0.016	0.836	C6–N1–H N1	123.8	1.0	122.1
N3–H N3	0.846	0.021	0.877	C2–N1–H N1	113.6	1.0	115.1
C5–H C5	0.993	0.015	0.931	C2–N3–H N3	114.0	1.4	117.8
N1–C2–N3	115.05	0.08	114.0	C4–N3–H N3	119.6	1.4	115.5
C2–N3–C4	126.46	0.09	126.7	C4–C5–H C5	123.4	0.9	118.1
N3–C4–C5	114.97	0.09	115.5	C6–C5–H C5	116.9	0.9	123.0
C4–C5–C6	119.72	0.09	118.9	N–H1 N	0.926	0.019	
C5–C6–N1	121.12	0.09	122.3	N–H2 N	0.923	0.019	
C6–N1–C2	122.63	0.08	122.7	N–H3 N	0.983	0.018	
N1–C2–O2	123.09	0.09	123.7	N–H4 N	0.930	0.021	
N3–C2–O2	121.86	0.09	122.3	O–H1 W	0.760	0.021	
N3–C4–O4	120.23	0.09	119.2	O–H2 W	0.851	0.020	
C5–C4–O4	125.01	0.09	125.3	H1 N–N–H2 N	113.5	1.5	
C5–C6–C7	122.24	0.08	123.2[a]	H1 N–N–H3 N	110.1	1.6	
N1–C6–C7	116.64	0.08	114.5[a]	H1 N–N–H4 N	103.0	1.4	
C6–C7–O8	116.68	0.09		H2 N–N–H3 N	107.2	1.3	
C6–C7–O9	116.51	0.08		H2 N–N–H4 N	111.4	1.6	
O8–C7–O9	126.81	0.09		H3 N–N–H4 N	111.6	1.6	
				H1 W–O–H2 W	108.4	1.9	

[a] The angles are to the hydrogen atom which is substituted by the carboxyl group in orotic acid.

RESULTS AND DISCUSSION

Bond distances and rigid body motion corrected bond distances as calculated from the parameters from the refinements of data sets III, I, and II are given in Table 6. The differences between the bond angles from the three refinements are negligible, and only the result of data set I is listed. Fig. 1 shows the bond distances and angles for this set. The uncertainties given are

those of set I. They range from 0.0011 to 0.0014 Å, the corresponding values for II being about 0.0004 Å smaller, for III about 0.0010 Å greater. The bond lengths derived from refinements of the three sets of data agree within the experimental error, except for C5 – C6 which is significantly shorter in the low order structure than in the high order structure. There is a tendency, although not significant for each bond, towards a lengthening of the double bonds when high order reflections are included in the refinement, and a corresponding slight shortening of the two almost single bonds, C4 – C5 and C6 – C7.

The pyrimidine ring is planar, the largest deviations from the least squares plane defined by the six ring atoms being 0.012 Å and – 0.014 Å for N1 and C2, respectively. O2 and C7 are displaced significantly from this plane, the deviations being 0.052 and 0.037 Å. The carboxyl group is both twisted and bended in relation to the pyrimidine ring, the displacements of O8 and O9 being 0.213 and – 0.114 Å, respectively. However, the angle between the two planes is not greater than 8.5°. The angle between the ring plane and the z-axis is 84.9°, and the orotate anion could somewhat unprecisely be described as lying in (001).

For comparison the dimensions of uracil[6] are given in Table 6. The two molecules are almost equal, showing that the introduction of a carboxyl group

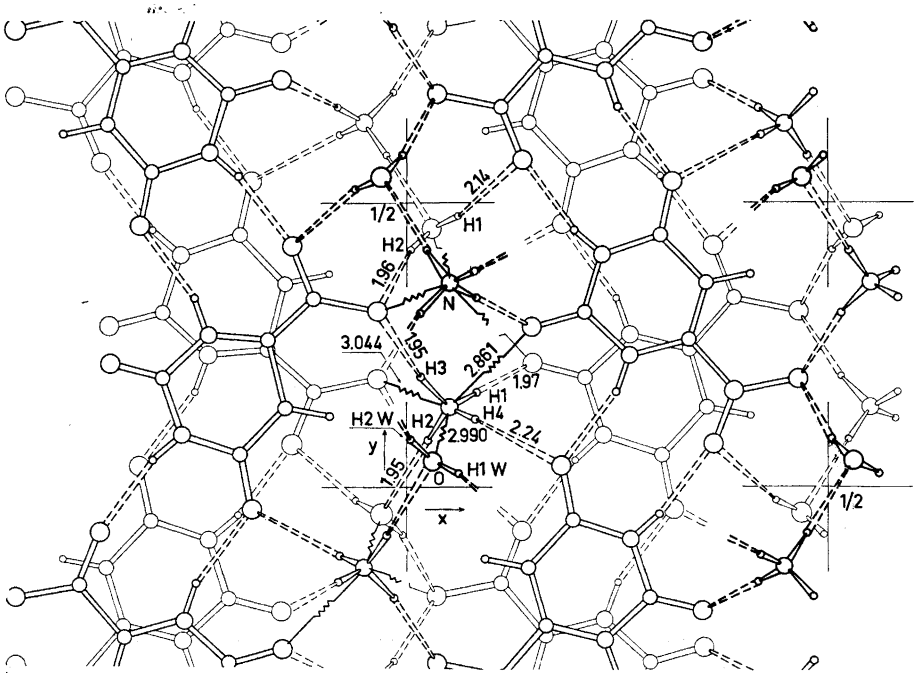

Fig. 2. Orthographic projection of the compound onto (001). Light print, molecules near $z = 0$. Heavy print, molecules near $z = 1/2$. Zig-zag lines denote short contacts between atoms.

in the 6-position has very little influence on the uracil nucleus. However, the two bonds C5–C6 and C6–N1 are significantly longer in orotic acid than in uracil.

The hydrogen bond distances and angles are given in Table 7, and the molecular packing is shown in Fig. 2. The orotate anions are held together by two hydrogen bonds in the y-direction, forming roughly planar ribbons, as shown in Fig. 1. These ribbons are cross-linked by five hydrogen bonds in the x-direction to H_2O and the NH_4^+-ion whereas there are only van der Waals contacts in the z-direction. All oxygen atoms in the anion, except O2,

Table 7. Hydrogen bond lengths (in Å) and angles (in deg). Three short contacts to the ammonium ion are included in the list.

	I	σ_I		I	σ_I
H N1···O4	2.044	.016	N1–H N1···O4	161.3	1.3
N1···O4	2.864	.001	C4–O4···H N1	131.3	0.4
H N3···O9	1.966	.021	N3–H N3···O9	166.6	1.8
N3···O9	2.796	.001	C7–O9···H N3	162.3	0.6
H1 N···O2	1.973	.019	N–H1 N···O2	176.8	1.6
N···O2	2.897	.001	C2–O2···H1 N	127.1	0.5
H3 N···O8	1.947	.019	N–H3 N···O8	173.3	1.6
N···O8	2.926	.001	C7–O8···H3 N	140.3	0.5
H4 N···O4	2.242	.020	N–H4 N···O4	133.2	1.5
N···O4	2.957	.001	C4–O4···H4 N	129.5	0.5
H1 W···O9	2.142	.021	O–H1 W···O9	165.0	1.9
O···O9	2.883	.001	C7–O9···H1 W	108 6	0.5
H2 W···O8	1.959	.021	O–H2 W···O8	171.0	1.8
O···O8	2.803	.001	C7–O8···H2 W	108.7	0.5
H2 N···O	1.953	.019	N–H2 N···O	173.6	1.6
N···O	2.873	.001			
			H N1···O4···H4 N	98.9	0.7
N···O2	2.861	.001	H3 N···O8···H2 W	92.4	0.8
N···O8	3.044	.001	H N3···O9···H1 W	89.1	0.8
N···O	2.990	.002	N···O2···H1 N	97.4	0.5
			H2 N···O–H1 W	103.5	0.8
			H2 N···O–H2 W	109.0	0.8
			H2 N···O···N	100.8	0.5
			N···O–H1 W	122.8	1.5
			N···O–H2 W	111.1	1.3
			O8···N–H4 N	177.3	1.2
			O2···N–H2 N	167.0	1.0
			O···N–H1 N	145.8	1.0

take part in two hydrogen bonds. The orotate ion has accordingly a very restricted motion in the ring plane. The r.b.m. analysis confirms this. The librational axis which has the smallest amplitude is normal to the ring plane, and so is the translational axis having the greatest amplitude.

The ammonium ion has seven closest neighbouring atoms, four of which are connected to the nitrogen atom by hydrogen bonds through the ammonium hydrogens. The ammonium hydrogen atoms are nearly situated in the corners of a tetrahedron having the nitrogen in the center, and then there are short

contacts to oxygen atoms normal to three of the sides of this assumed tetrahedron. One of these contacts, to O2, is as short as 2.861 Å, and may perhaps not be repulsive as seen from the angles given in Table 7.

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