Table 9. *Equations to planes*

Atoms in plane	Equations of planes
N(1), C(1), C(2), C(3), C(4), C(5)	$-5\cdot97x+9\cdot13y+7\cdot63z=1\cdot77$
N(2), C(6), C(7), C(8), C(9), C(10)	$6\cdot66x+9\cdot10y-0\cdot90z=1\cdot52$
Cu, O(1), O(2)	$2\cdot15x-5\cdot82y+6\cdot76z=0\cdot00$

x, y and z refer to fractional coordinates of the unit cell axes a, b and c.

Distances of atoms from planes

	Distance from first plane		Distance from second plane
N(1)	0·00 Å	N(2)	0·00 Å
C(1)	−0·01	C(6)	0·01
C(2)	0·01	C(7)	−0·01
C(3)	0·00	C(8)	0·00
C(4)	−0·01	C(9)	0·01
C(5)	0·01	C(10)	−0·01

Angles between planes and lines

Ring N(1)···C(5) to ring N(2)···C(10)	=82·8°
Ring N(1)···C(5) to square plane Cu, O(1), O(2)	=89·9
Ring N(2)···C(10) to square plane Cu, O(1), O(2)	=78·9
Line through C(1) and C(5) to line through C(6) and C(10)	=19·9

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Oxido Steroids. II. The Crystal and Molecular Structure of 11β,12β-Dibromo-3α,9-oxidocholanic Acid Methyl Ester

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The crystal structure of 11β,12β-dibromo-3α,9-oxidocholanic acid methyl ester has been analyzed and refined from three-dimensional intensity data to an R index of 0·14 for 2884 reflections. This steroid crystallizes from acetone in the orthorhombic space group $P2_12_12_1$ with unit-cell dimensions $a=11\cdot005$, $b=31\cdot383$, and $c=7\cdot133$ Å. The A ring is boat-shaped and the rings B and C are chair-shaped. The D ring is a distorted half-chair. The structural features of this molecule are discussed in comparison with those of its epimer 11β,12α-dibromo-3α,9-oxidocholanic acid methyl ester.

Introduction

11β,12β-Dibromo-3α,9-oxidocholanic acid methyl ester, $C_{25}H_{38}O_3Br_2$ (Fig. 1), is the second oxido steroid whose structure has been investigated in this laboratory. The other compound which was reported earlier is the 11β,12α-dibromo epimer of the above derivative (Gopalakrishna, Cooper & Norton, 1969). This derivative is a co-product of the 11β,12α-dibromo epimer formed in the process of bromination of 3α, 9-oxido-Δ^{11}-cholanic acid methyl ester (Mattox, Turner, Engel, McKenzie, McGuckin & Kendall, 1946). Both these epimers have the same stereochemical features, except that in one of them the bromine atom attached to C(12) is in the α-configuration and in the other it is

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in the β-configuration. Because of this difference, their chemical and physical properties are outstandingly different (Mattox *et al.*, 1946, 1948). In the above-mentioned process of bromination, the *cis* dibromo derivative has a yield of 35%, whereas the *trans* product has a 65% yield. When the latter is shaken with silver oxide or silver carbonate in aqueous acetone, the 11β-bromine atom is replaced by an hydroxyl group, pro-

Table 1. *Observed and calculated structure factors*

The values listed for FOBS and FCAL are ten times the absolute scale.

H	K	L	FOBS	FCAL
0	0	2	388	409
0	0	4	276	306
0	0	6	774	812
0	0	8	281	284
0	1	1	321	310
0	1	2	1323	1306
0	1	3	359	419
0	1	4	231	253
0	1	5	448	401
0	1	6	188	171
0	1	7	214	205
0	1	8	112	88
0	2	0	1155	1238
0	2	1	1495	1371
0	2	2	425	438
0	2	3	1596	1552
0	2	4	184	112
0	2	5	415	430
0	2	6	413	358
0	2	7	93	55
0	2	8	123	129
0	3	1	576	474
0	3	2	1540	1413
0	3	3	72	56
0	3	4	587	521
0	3	5	203	157
0	3	6	348	325
0	3	7	93	14
0	3	8	133	114
0	4	0	1251	1420
0	4	1	1712	1700
0	4	2	964	955
0	4	3	1096	1044
0	4	4	314	367
0	4	5	94	10
0	4	6	222	87
0	4	7	107	81
0	4	8	112	86
0	5	1	913	885
0	5	2	294	237
0	5	3	1165	1164
0	5	4	728	723
0	5	5	663	635
0	5	6	149	34
0	5	7	222	238
0	5	8	71	26
0	6	0	946	1027
0	6	1	1285	1209
0	6	2	610	558
0	6	3	405	333
0	6	4	270	186
0	6	5	133	85
0	6	6	382	375
0	6	7	37	22
0	6	8	214	188
0	7	1	1050	1017
0	7	2	1355	1301
0	7	3	130	47
0	7	4	209	161
0	7	5	335	306
0	7	6	448	427
0	7	7	287	281
0	7	8	69	117
0	8	0	471	459
0	8	1	704	610
0	8	2	395	452
0	8	3	1581	1568
0	8	4	145	93
0	8	5	291	190
0	8	6	160	18
0	8	7	93	11
0	8	8	83	65
0	9	1	443	376
0	9	2	530	502
0	9	3	849	789
0	9	4	203	138
0	9	5	370	388
0	9	6	240	247
0	9	7	118	114
0	9	8	117	99
0	10	0	1962	2021
0	10	1	453	478
0	10	2	417	422
0	10	3	927	906
0	10	4	122	255
0	10	5	393	406
0	10	6	284	281
0	10	7	37	2
0	10	8	157	170
0	11	1	672	622
0	11	2	110	11
0	11	3	271	300
0	11	4	629	631
0	11	5	486	442
0	11	6	162	136
0	11	7	211	248
0	11	8	46	44
0	12	0	1152	1105
0	12	1	573	536
0	12	2	913	708
0	12	3	785	754
0	12	4	118	80
0	12	5	184	149
0	12	6	132	185
0	12	7	53	3
0	12	8	187	219
0	13	1	693	659
0	13	2	704	697
0	13	3	128	13
0	13	4	200	131
0	13	5	125	100
0	13	6	276	259
0	13	7	276	320
0	13	8	62	76
0	14	0	1181	1121
0	14	1	157	149
0	14	2	504	528
0	14	3	673	700
0	14	4	367	332
0	14	5	400	403
0	14	6	109	107
0	14	7	51	17
0	14	8	29	21
0	15	1	217	170
0	15	2	271	255
0	15	3	466	461
0	15	4	538	545
0	15	5	516	519
0	15	6	54	7
0	15	7	102	11
0	15	8	27	21
0	16	0	425	474
0	16	1	1222	1079
0	16	2	184	164
0	16	3	75	7
0	16	4	139	47
0	16	5	393	359
0	16	6	132	111
0	16	7	51	0
0	16	8	85	109
0	17	1	643	685
0	17	2	294	332
0	17	3	352	333
0	17	4	428	445
0	17	5	240	249
0	17	6	193	203
0	17	7	214	248
0	17	8	72	61
0	18	0	222	226
0	18	1	318	254
0	18	2	557	618
0	18	3	270	236
0	18	4	300	241
0	18	5	208	150
0	18	6	185	172
0	18	7	50	17
0	19	1	568	509
0	19	2	656	606
0	19	3	477	465
0	19	4	200	165
0	19	5	155	97
0	19	6	152	160
0	19	7	205	220
0	20	0	774	766
0	20	1	658	672
0	20	2	276	260
0	20	3	185	124
0	20	4	157	55
0	20	5	339	356
0	20	6	128	128
0	20	7	66	14
0	21	1	208	187
0	21	2	115	36
0	21	3	339	286
0	21	4	620	615
0	21	5	152	146
0	21	6	36	32
0	21	7	77	20
0	22	0	390	321
0	22	1	582	603
0	22	2	750	700
0	22	3	248	229
0	22	4	327	275
0	22	5	185	170
0	22	6	153	140
0	22	7	96	19
0	23	1	468	412
0	23	2	533	409
0	23	3	209	98
0	23	4	171	162
0	23	5	37	11
0	23	6	101	98
0	23	7	137	148
0	24	0	189	200
0	24	1	206	156
0	24	2	1027	910
0	24	3	130	132
0	24	4	281	328
0	24	5	140	181
0	24	6	171	182
0	24	7	51	31
0	25	1	211	118
0	25	2	355	361
0	25	3	235	161
0	25	4	418	436
0	25	5	91	121
0	25	6	67	70
0	26	0	201	186
0	26	1	759	819
0	26	2	118	87
0	26	3	54	50
0	26	4	53	51
0	26	5	206	276
0	26	6	32	43
0	27	1	238	271
0	27	2	132	109
0	27	3	54	10
0	27	4	265	301
0	27	5	36	88
0	27	6	61	22
0	28	0	299	330
0	28	1	265	299
0	28	2	477	545
0	28	3	93	40
0	28	4	165	178
0	28	5	71	66
0	28	6	112	88
0	29	1	359	442
0	29	2	37	87
0	29	3	37	34
0	29	4	88	16
0	29	5	48	34
0	30	0	276	281
0	30	1	412	408
0	30	2	240	356
0	30	3	53	35
0	30	4	114	110
0	30	5	118	152
0	31	1	75	107
0	31	2	37	44
0	31	3	104	39
0	31	4	238	279
0	31	5	40	35
0	32	0	140	93
0	32	1	361	393
0	32	2	53	117
0	32	3	36	6
0	32	4	106	89
0	32	5	93	146
0	33	1	180	205
0	33	2	86	9
0	33	3	71	76
0	33	4	113	144
0	34	0	51	1
0	34	1	72	28
0	34	2	219	298
0	34	3	94	116
0	34	4	27	98
0	35	1	101	167
0	35	2	34	17
0	35	3	45	42
0	36	0	34	116
0	36	1	144	267
0	36	2	32	83
0	36	3	80	13
0	37	1	31	13
0	37	2	59	6
0	38	0	29	99
0	38	1	58	147
0	38	2	26	174
1	0	1	82	142
1	0	2	486	478
1	0	3	956	931
1	0	4	779	766
1	0	5	305	282
1	0	6	91	117
1	0	7	37	9
1	0	8	50	69
1	1	0	1070	1049
1	1	1	926	836
1	1	2	782	841
1	1	3	443	431
1	1	4	287	294
1	1	5	316	337
1	1	6	287	276
1	1	7	54	39
1	1	8	142	148
1	2	0	640	966
1	2	1	767	709
1	2	2	1045	981
1	2	3	701	718
1	2	4	552	509
1	2	5	174	169
1	2	6	222	220
1	2	7	318	281
1	2	8	150	163
1	3	0	1337	1536
1	3	1	852	861
1	3	2	782	700
1	3	3	761	695
1	3	4	390	364
1	3	5	455	513
1	3	6	372	357
1	3	7	107	84
1	3	8	200	214
1	4	0	187	424
1	4	1	1848	1765
1	4	2	589	614
1	4	3	721	751
1	4	4	450	466
1	4	5	188	156
1	4	6	128	99
1	4	7	240	273
1	4	8	132	113
1	5	0	281	351
1	5	1	798	831
1	5	2	906	944
1	5	3	650	612
1	5	4	243	209
1	5	5	364	424
1	5	6	356	430
1	5	7	37	43
1	5	8	110	101
1	6	0	1120	1156
1	6	1	790	740
1	6	2	913	856
1	6	3	479	433
1	6	4	702	671
1	6	5	185	84
1	6	6	249	212
1	6	7	53	87
1	6	8	69	45
1	7	0	97	84
1	7	1	524	704
1	7	2	362	313
1	7	3	860	823
1	7	4	265	258
1	7	5	450	464
1	7	6	233	217
1	7	7	37	57
1	7	8	109	131
1	8	0	1879	1930
1	8	1	1103	1084
1	8	2	304	268
1	8	3	460	436
1	8	4	400	395
1	8	5	359	392
1	8	6	273	282
1	8	7	265	272
1	8	8	137	131
1	9	0	1075	981
1	9	1	659	661
1	9	2	572	521
1	9	3	110	187
1	9	4	171	102
1	9	5	246	202
1	9	6	314	371
1	9	7	93	81
1	9	8	150	191
1	10	0	132	91
1	10	1	653	647
1	10	2	364	310
1	10	3	974	1010
1	10	4	370	401
1	10	5	228	249
1	10	6	179	131
1	10	7	236	217
1	10	8	114	127
1	11	0	696	704
1	11	1	546	488
1	11	2	319	315
1	11	3	767	704
1	11	4	188	137
1	11	5	418	470
1	11	6	222	184
1	11	7	158	128
1	11	8	112	105
1	12	0	903	898
1	12	1	106	86
1	12	2	637	671
1	12	3	362	392
1	12	4	564	575
1	12	5	223	211
1	12	6	241	214
1	12	7	53	52
1	12	8	31	59
1	13	0	144	153
1	13	1	173	125
1	13	2	471	473
1	13	3	455	449
1	13	4	401	375
1	13	5	365	341
1	13	6	109	80
1	13	7	74	23
1	13	8	106	125
1	14	0	817	808
1	14	1	1191	1112
1	14	2	273	309
1	14	3	305	312
1	14	4	150	73
1	14	5	383	373
1	14	6	180	200
1	14	7	252	273
1	14	8	110	119
1	15	0	382	390
1	15	1	681	597
1	15	2	555	515
1	15	3	166	131
1	15	4	166	143
1	15	5	222	240
1	15	6	222	241
1	15	7	153	174
1	15	8	106	126
1	16	0	168	133
1	16	1	359	331
1	16	2	858	856
1	16	3	450	486
1	16	4	316	323
1	16	5	130	66
1	16	6	142	116
1	16	7	114	127
1	16	8	54	71
1	17	0	200	20
1	17	1	284	251
1	17	2	482	508
1	17	3	539	489
1	17	4	297	287
1	17	5	355	328
1	17	6	118	73
1	17	7	87	93
1	18	0	680	649
1	18	1	587	583
1	18	2	482	525
1	18	3	230	203
1	18	4	372	353
1	18	5	259	272
1	18	6	160	170
1	18	7	69	95
1	19	0	436	426
1	19	1	228	159
1	19	2	438	470
1	19	3	443	401
1	19	4	473	456
1	19	5	162	154
1	19	6	259	244
1	19	7	117	92
1	20	0	96	53
1	20	1	564	601
1	20	2	401	370
1	20	3	400	351
1	20	4	117	84
1	20	5	180	199
1	20	6	74	65
1	20	7	114	149
1	21	0	590	618
1	21	1	347	392
1	21	2	350	333
1	21	3	133	49
1	21	4	160	96
1	21	5	94	111
1	21	6	187	200
1	21	7	117	141
1	22	0	463	470
1	22	1	294	262
1	22	2	568	559
1	22	3	426	360
1	22	4	434	444
1	22	5	160	181
1	22	6	72	77
1	22	7	72	46
1	23	0	173	33
1	23	1	174	110
1	23	2	174	100
1	23	3	246	240
1	23	4	230	217
1	23	5	118	186
1	23	6	71	39
1	23	7	39	34
1	24	0	110	82
1	24	1	459	504
1	24	2	225	245
1	24	3	118	19
1	24	4	188	239
1	24	5	166	214
1	24	6	69	119
1	24	7	36	54
1	25	0	413	380
1	25	1	281	252
1	25	2	216	166
1	25	3	132	92
1	25	4	201	192
1	25	5	53	26
1	25	6	142	152
1	26	0	188	23
1	26	1	240	240
1	26	2	342	405
1	26	3	75	119
1	26	4	37	82
1	26	5	72	107
1	26	6	91	47
1	27	0	259	247
1	27	1	287	271
1	27	2	107	96
1	27	3	236	256
1	27	4	93	103
1	27	5	114	98
1	27	6	112	145
1	28	0	132	110
1	28	1	259	287
1	28	2	188	241
1	28	3	152	142
1	28	4	128	130
1	28	5	85	143
1	28	6	123	80
1	29	0	109	35
1	29	1	188	164
1	29	2	54	68
1	29	3	219	250
1	29	4	231	234
1	29	5	67	118
1	30	0	132	116
1	30	1	222	253
1	30	2	278	305
1	30	3	106	132
1	30	4	123	135
1	30	5	109	117
1	31	0	37	171
1	31	1	130	121
1	31	2	106	78
1	31	3	88	21
1	31	4	149	111
1	31	5	71	86
1	32	0	75	112
1	32	1	192	250
1	32	2	222	234
1	32	3	102	72
1	32	4	94	131
1	32	5	36	139
1	33	0	104	170
1	33	1	104	67
1	33	2	88	97
1	33	3	110	142
1	33	4	145	134
1	34	0	51	79
1	34	1	145	266
1	34	2	51	135
1	34	3	80	65
1	34	4	39	86
1	35	0	112	124
1	35	1	101	78
1	35	2	107	40
1	35	3	115	177
1	36	0	67	97
1	36	1	32	99
1	36	2	110	192
1	36	3	39	62
1	37	0	64	141
1	37	1	77	76
1	37	2	101	35
1	38	0	71	9
1	38	1	99	167
1	38	2	36	111
1	39	0	24	35
2	0	0	551	551
2	0	1	1454	1481
2	0	2	648	568
2	0	3	102	84
2	0	4	426	462
2	0	5	115	13
2	0	6	150	104
2	0	7	431	509
2	0	8	130	131
2	1	0	79	50
2	1	1	828	849
2	1	2	522	500
2	1	3	499	509
2	1	4	352	309
2	1	5	481	503
2	1	6	192	105
2	1	7	170	160
2	1	8	157	174
2	2	0	82	40
2	2	1	1181	1160
2	2	2	570	665
2	2	3	420	475
2	2	4	600	615
2	2	5	297	325
2	2	6	158	111
2	2	7	214	248
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4	22	1	318	353
4	22	2	271	278
4	22	3	93	141
4	22	4	248	232
4	22	5	149	138
4	22	6	137	92
4	23	0	145	1
4	23	1	147	130
4	23	2	308	348
4	23	3	187	145
4	23	4	107	107
4	23	5	36	69
4	23	6	46	63
4	24	0	439	398
4	24	1	299	321
4	24	2	93	66
4	24	3	180	190
4	24	4	107	88
4	24	5	36	102
4	24	6	62	103
4	25	0	342	308
4	25	1	352	402
4	25	2	170	241
4	25	3	132	163
4	25	4	158	136
4	25	5	133	174
4	25	6	58	43
4	26	0	54	33
4	26	1	54	64
4	26	2	132	106
4	26	3	185	245
4	26	4	208	267
4	26	5	109	105
4	26	6	26	69
4	27	0	153	73
4	27	1	321	374
4	27	2	235	264
4	27	3	75	91
4	27	4	125	136
4	27	5	66	78
4	28	0	120	129
4	28	1	216	221
4	28	2	37	50
4	28	3	128	85
4	28	4	36	124
4	28	5	31	22
4	29	0	53	71
4	29	1	152	172
4	29	2	249	315
4	29	3	72	122
4	29	4	50	133
4	29	5	58	47
4	30	0	177	187
4	30	1	106	83
4	30	2	117	152
4	30	3	51	50
4	30	4	163	168
4	30	5	64	40
4	31	0	117	112
4	31	1	214	294
4	31	2	88	96
4	31	3	71	55
4	31	4	31	48
4	32	0	88	98
4	32	1	36	57
4	32	2	51	116
4	32	3	117	134
4	32	4	107	168
4	33	0	36	56
4	33	1	87	84
4	33	2	195	273
4	33	3	88	57
4	33	4	87	165
4	34	0	83	170
4	34	1	34	101
4	34	2	79	66
4	34	3	58	65
4	35	0	32	36
4	35	1	102	136
4	35	2	104	178
4	35	3	80	101
4	36	0	29	4
4	36	1	29	90
4	36	2	37	36
4	37	0	66	48
4	37	1	36	123
5	0	1	219	175
5	0	2	903	915
5	0	3	490	573
5	0	4	254	260
5	0	5	127	59
5	0	6	241	274
5	0	7	115	91
5	0	8	72	82
5	1	0	1101	1101
5	1	1	878	917
5	1	2	256	287
5	1	3	613	618
5	1	4	195	207
5	1	5	180	223
5	1	6	120	128
5	1	7	104	97
5	1	8	59	88
5	2	0	656	652
5	2	1	217	225
5	2	2	337	359
5	2	3	445	506
5	2	4	163	186
5	2	5	330	317
5	2	6	171	148
5	2	7	51	123
5	2	8	29	9
5	3	0	2091	1945
5	3	1	415	370
5	3	2	324	314
5	3	3	278	272
5	3	4	270	231
5	3	5	203	198
5	3	6	286	315
5	3	7	72	71
5	3	8	144	182
5	4	0	190	202
5	4	1	441	472
5	4	2	646	678
5	4	3	434	434
5	4	4	144	32
5	4	5	173	153
5	4	6	248	299
5	4	7	51	119
5	4	8	82	61
5	5	0	252	163
5	5	1	575	601
5	5	2	206	217
5	5	3	924	986
5	5	4	136	73
5	5	5	241	273
5	5	6	75	80
5	5	7	36	47
5	5	8	80	118
5	6	0	118	95
5	6	1	160	76
5	6	2	539	571
5	6	3	495	490
5	6	4	188	74
5	6	5	279	290
5	6	6	241	249
5	6	7	88	50
5	6	8	69	50
5	7	0	1070	1079
5	7	1	174	129
5	7	2	508	495
5	7	3	439	510
5	7	4	249	233
5	7	5	192	200
5	7	6	201	217
5	7	7	36	33
5	7	8	117	122
5	8	0	374	341
5	8	1	524	551
5	8	2	140	77
5	8	3	522	566
5	8	4	324	357
5	8	5	443	470
5	8	6	246	232
5	8	7	123	152
5	8	8	75	57
5	9	0	779	816
5	9	1	697	649
5	9	2	217	202
5	9	3	359	376
5	9	4	173	76
5	9	5	118	68
5	9	6	160	200
5	9	7	71	55
5	9	8	80	146

Table 1 (*cont.*)

H	K	L	FOBS	FCAL
5	10	0	230	198
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5	10	2	586	654
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5	10	5	208	201
5	10	6	256	286
5	10	7	150	175
5	11	0	276	228
5	11	1	289	276
5	11	2	533	570
5	11	3	595	655
5	11	4	319	283
5	11	5	270	275
5	11	6	53	63
5	11	7	85	106
5	12	0	182	223
5	12	1	123	71
5	12	2	233	261
5	12	3	337	374
5	12	4	273	250
5	12	5	286	272
5	12	6	177	159
5	12	7	83	107
5	13	0	1113	1030
5	13	1	587	587
5	13	2	238	216
5	13	3	166	131
5	13	4	238	182
5	13	5	281	325
5	13	6	106	101
5	13	7	67	49
5	14	0	337	282
5	14	1	356	397
5	14	2	230	182
5	14	3	214	159
5	14	4	340	342
5	14	5	230	220
5	14	6	128	154
5	14	7	174	173
5	15	0	182	151
5	15	1	385	404
5	15	2	367	359
5	15	3	629	660
5	15	4	177	123
5	15	5	132	147
5	15	6	180	145
5	15	7	31	74
5	16	0	91	35
5	16	1	415	440
5	16	2	364	400
5	16	3	168	132
5	16	4	256	159
5	16	5	120	54
5	16	6	155	136
5	16	7	145	170
5	17	0	720	688
5	17	1	231	230
5	17	2	365	365
5	17	3	231	265
5	17	4	179	138
5	17	5	246	237
5	17	6	51	63
5	17	7	29	64
5	18	0	107	47
5	18	1	216	171
5	18	2	251	185
5	18	3	314	308
5	18	4	415	441
5	18	5	206	227
5	18	6	101	107
5	18	7	39	20
5	19	0	289	267
5	19	1	616	625
5	19	2	153	97
5	19	3	118	67
5	19	4	144	154
5	19	5	254	264
5	19	6	122	132
5	19	7	82	53
5	20	0	166	2
5	20	1	369	382
5	20	2	312	321
5	20	3	152	152
5	20	4	236	224
5	20	5	36	61
5	20	6	153	126
5	21	0	145	63
5	21	1	187	150
5	21	2	605	681
5	21	3	75	66
5	21	4	170	182
5	21	5	72	74
5	21	6	115	117
5	22	0	127	11
5	22	1	203	204
5	22	2	244	260
5	22	3	259	280
5	22	4	75	256
5	22	5	51	95
5	22	6	77	50
5	23	0	347	259
5	23	1	410	475
5	23	2	208	219
5	23	3	54	47
5	23	4	37	81
5	23	5	168	226
5	23	6	43	19
5	24	0	152	117
5	24	1	187	220
5	24	2	109	112
5	24	3	37	57
5	24	4	292	340
5	24	5	34	88
5	24	6	27	14
5	25	0	120	25
5	25	1	339	383
5	25	2	334	385
5	25	3	160	152
5	25	4	51	109
5	25	5	82	83
5	25	6	80	55
5	26	0	94	122
5	26	1	259	284
5	26	2	132	117
5	26	3	93	37
5	26	4	72	128
5	26	5	79	29
5	27	0	310	330
5	27	1	152	168
5	27	2	240	338
5	27	3	36	64
5	27	4	101	143
5	27	5	122	137
5	28	0	292	55
5	28	1	168	205
5	28	2	91	33
5	28	3	36	62
5	28	4	195	210
5	28	5	80	63
5	29	0	74	7
5	29	1	274	374
5	29	2	91	137
5	29	3	36	40
5	29	4	46	30
5	29	5	62	124
5	30	0	74	60
5	30	1	165	191
5	30	2	125	129
5	30	3	34	21
5	30	4	145	160
5	31	0	115	120
5	31	1	115	116
5	31	2	195	284
5	31	3	80	52
5	31	4	56	85
5	32	0	36	78
5	32	1	142	202
5	32	2	83	95
5	32	3	109	99
5	33	0	50	4
5	33	1	117	217
5	33	2	137	154
5	33	3	40	28
5	34	0	32	20
5	34	1	64	65
5	34	2	112	31
5	34	3	61	77
5	35	0	43	87
5	35	1	82	150
5	35	2	66	136
5	36	0	54	48
5	36	1	51	104
6	0	0	1040	1095
6	0	1	136	140
6	0	2	283	354
6	0	3	490	546
6	0	4	122	66
6	0	5	233	266
6	0	6	256	302
6	0	7	112	122
6	0	8	118	172
6	1	0	425	468
6	1	1	335	320
6	1	2	343	381
6	1	3	354	434
6	1	4	378	368
6	1	5	93	85
6	1	6	93	103
6	1	7	166	174
6	1	8	36	57
6	2	0	560	467
6	2	1	152	143
6	2	2	267	317
6	2	3	299	288
6	2	4	217	192
6	2	5	267	283
6	2	6	273	324
6	2	7	36	35
6	3	0	139	1
6	3	1	519	543
6	3	2	488	516
6	3	3	347	374
6	3	4	481	528
6	3	5	107	73
6	3	6	75	110
6	3	7	122	110
6	4	0	259	177
6	4	1	217	192
6	4	2	407	405
6	4	3	356	364
6	4	4	152	149
6	4	5	179	134
6	4	6	193	185
6	4	7	34	82
6	5	0	1136	1086
6	5	1	517	558
6	5	2	350	380
6	5	3	153	80
6	5	4	410	452
6	5	5	179	195
6	5	6	75	80
6	5	7	171	227
6	6	0	249	154
6	6	1	147	103
6	6	2	259	159
6	6	3	297	242
6	6	4	184	152
6	6	5	142	116
6	6	6	185	204
6	6	7	65	17
6	7	0	458	435
6	7	1	701	805
6	7	2	174	119
6	7	3	448	506
6	7	4	211	197
6	7	5	120	165
6	7	6	130	122
6	7	7	155	168
6	8	0	205	217
6	8	1	281	275
6	8	2	235	257
6	8	3	302	325
6	8	4	225	179
6	8	5	236	252
6	8	6	205	210
6	8	7	97	23
6	9	0	630	593
6	9	1	365	358
6	9	2	455	533
6	9	3	274	268
6	9	4	356	344
6	9	5	75	50
6	9	6	117	94
6	9	7	82	105
6	10	0	377	378
6	10	1	162	37
6	10	2	184	207
6	10	3	488	516
6	10	4	128	90
6	10	5	254	245
6	10	6	157	167
6	10	7	115	32
6	11	0	300	212
6	11	1	629	691
6	11	2	294	308
6	11	3	211	151
6	11	4	150	166
6	11	5	230	227
6	11	6	53	71
6	11	7	185	210
6	12	0	565	527
6	12	1	259	335
6	12	2	337	330
6	12	3	155	169
6	12	4	249	245
6	12	5	170	154
6	12	6	171	220
6	12	7	77	53
6	13	0	385	380
6	13	1	351	429
6	13	2	324	315
6	13	3	244	260
6	13	4	240	222
6	13	5	179	141
6	13	6	36	83
6	13	7	87	132
6	14	0	217	214
6	14	1	274	300
6	14	2	120	36
6	14	3	503	539
6	14	4	201	128
6	14	5	233	274
6	14	6	88	128
6	14	7	59	113
6	15	0	530	497
6	15	1	284	252
6	15	2	495	510
6	15	3	139	114
6	15	4	271	330
6	15	5	130	105
6	15	6	114	96
6	15	7	40	67
6	16	0	274	177
6	16	1	163	154
6	16	2	184	183
6	16	3	236	228
6	16	4	243	231
6	16	5	118	139
6	16	6	87	89
6	16	7	122	59
6	17	0	209	166
6	17	1	544	549
6	17	2	225	197
6	17	3	292	288
6	17	4	120	51
6	17	5	184	213
6	17	6	130	34
6	17	7	114	138
6	18	0	267	218
6	18	1	240	157
6	18	2	214	148
6	18	3	120	14
6	18	4	37	28
6	18	5	51	114
6	18	6	136	159
6	19	0	477	480
6	19	1	200	179
6	19	2	461	475
6	19	3	120	128
6	19	4	240	262
6	19	5	137	107
6	19	6	123	71
6	20	0	157	5
6	20	1	166	115
6	20	2	152	60
6	20	3	153	177
6	20	4	227	141
6	20	5	136	152
6	20	6	62	29
6	21	0	158	123
6	21	1	337	339
6	21	2	235	262
6	21	3	222	240
6	21	4	184	176
6	21	5	87	160
6	21	6	43	67
6	22	0	383	365
6	22	1	132	114
6	22	2	236	232
6	22	3	162	134
6	22	4	117	189
6	22	5	85	81
6	22	6	144	175
6	23	0	252	188
6	23	1	305	299
6	23	2	248	271
6	23	3	152	155
6	23	4	88	84
6	23	5	118	86
6	23	6	82	44
6	24	0	248	269
6	24	1	94	91
6	24	2	152	175
6	24	3	130	152
6	24	4	51	46
6	24	5	147	135
6	25	0	187	196
6	25	1	107	117
6	25	2	233	249
6	25	3	36	80
6	25	4	144	146
6	25	5	59	118
6	26	0	53	41
6	26	1	130	100
6	26	2	106	49
6	26	3	88	137
6	26	4	149	151
6	26	5	40	102
6	27	0	118	26
6	27	1	53	215
6	27	2	165	206
6	27	3	51	135
6	27	4	106	119
6	27	5	59	124
6	28	0	128	124
6	28	1	117	55
6	28	2	72	101
6	28	3	71	60
6	28	4	118	127
6	29	0	36	135
6	29	1	127	197
6	29	2	198	246
6	29	3	83	69
6	29	4	94	91
6	30	0	72	31
6	30	1	87	97
6	30	2	85	65
6	30	3	102	133
6	30	4	66	101
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6	32	1	82	69
6	32	2	125	77
6	32	3	102	101
6	33	0	77	204
6	33	1	140	142
6	33	2	82	108
6	34	0	82	113
6	34	1	91	94
6	34	2	51	20
6	35	0	53	98
7	0	1	484	579
7	0	2	112	141
7	0	3	265	334
7	0	4	453	558
7	0	5	259	323
7	0	6	165	195
7	0	7	32	58
7	1	0	114	15
7	1	1	466	478
7	1	2	413	422
7	1	3	139	46
7	1	4	196	263
7	1	5	180	141
7	1	6	117	131
7	1	7	66	62
7	2	0	257	211
7	2	1	273	251
7	2	2	319	325
7	2	3	335	375
7	2	4	196	141
7	2	5	153	185
7	2	6	117	133
7	2	7	66	179
7	3	0	329	254
7	3	1	418	460
7	3	2	512	536
7	3	3	185	166
7	3	4	289	272
7	3	5	109	192
7	3	6	157	150
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7	4	0	130	75
7	4	1	300	316
7	4	2	308	349
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7	4	6	127	157
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7	5	1	680	746
7	5	2	149	254
7	5	3	200	154
7	5	4	347	392
7	5	5	216	184
7	5	6	137	137
7	5	7	102	99
7	6	0	243	191
7	6	1	174	189
7	6	2	133	128
7	6	3	173	109
7	6	4	469	530
7	6	5	170	162
7	6	6	88	50
7	6	7	64	97
7	7	0	393	352
7	7	1	182	189
7	7	2	598	640
7	7	3	312	312
7	7	4	278	292
7	7	5	37	39
7	7	6	104	88
7	7	7	77	102
7	8	0	217	172
7	8	1	499	521
7	8	2	259	211
7	8	3	279	279
7	8	4	75	17
7	8	5	162	99
7	8	6	51	68
7	8	7	158	205
7	9	0	102	35
7	9	1	755	785
7	9	2	206	143
7	9	3	364	372
7	9	4	208	109
7	9	5	179	131
7	9	6	136	115
7	9	7	96	99
7	10	0	287	199
7	10	1	307	358
7	10	2	287	319
7	10	3	187	156
7	10	4	228	210
7	10	5	222	218
7	10	6	125	127
7	10	7	72	85
7	11	0	911	898
7	11	1	460	467
7	11	2	539	543
7	11	3	256	186
7	11	4	236	214
7	11	5	213	238
7	11	6	123	129
7	11	7	27	40
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7	12	1	289	263
7	12	2	190	135
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7	12	4	144	138
7	12	5	160	187
7	12	6	36	43
7	12	7	67	73
7	13	0	645	559
7	13	1	415	389
7	13	2	458	498
7	13	3	343	355
7	13	4	203	259
7	13	5	74	32
7	13	6	71	98
7	13	7	53	100
7	14	0	180	144
7	14	1	271	215
7	14	2	259	250
7	14	3	185	137
7	14	4	162	161
7	14	5	91	78
7	14	6	83	93
7	15	0	340	295
7	15	1	570	613
7	15	2	182	125
7	15	3	270	246
7	15	4	162	145
7	15	5	117	136
7	15	6	96	85
7	16	0	236	233
7	16	1	155	65
7	16	2	130	136
7	16	3	170	188
7	16	4	187	160
7	16	5	187	202
7	16	6	32	61
7	17	0	638	564
7	17	1	166	114
7	17	2	350	419
7	17	3	180	100
7	17	4	213	269
7	17	5	88	80
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7	18	2	377	389
7	18	3	144	111
7	18	4	53	19
7	18	5	114	67
7	18	6	61	84
7	19	0	233	150
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12	6	2	130	136
12	6	3	64	68
12	6	4	36	42
12	7	0	36	13
12	7	1	71	62
12	7	2	97	78
12	7	3	117	92
12	7	4	107	130
12	8	0	112	124
12	8	1	200	221
12	8	2	107	120
12	8	3	45	58
12	9	0	50	9
12	9	1	110	77
12	9	2	67	80
12	9	3	106	75
12	10	0	233	192
12	10	1	50	101
12	10	2	162	180
12	10	3	110	122
12	11	0	69	51
12	11	1	127	127
12	11	2	64	44
12	11	3	40	30
12	12	0	96	18
12	12	1	195	229
12	12	2	77	17
12	12	3	110	124
12	13	0	48	59
12	13	1	46	27
12	13	2	115	59
12	13	3	26	55
12	14	0	240	230
12	14	1	118	128
12	14	2	132	158
12	15	0	88	121
12	15	1	97	77
12	15	2	56	59
12	16	0	106	72
12	16	1	125	122
12	16	2	142	145
12	17	0	40	60
12	17	1	56	51
12	18	0	102	118
12	18	1	139	140
12	19	0	24	47
13	0	1	166	213
13	0	2	40	17
13	1	0	79	81
13	1	1	62	69
13	1	2	58	20
13	2	0	128	144
13	2	1	31	38
13	2	2	170	199
13	3	0	91	107
13	3	1	45	34
13	3	2	58	35
13	4	0	62	52
13	4	1	145	152
13	4	2	114	124
13	5	0	45	7
13	5	1	61	61
13	5	2	39	23
13	6	0	31	92
13	6	1	149	107
13	6	2	77	113
13	7	0	61	38
13	7	1	59	67
13	7	2	54	85
13	8	0	94	90
13	8	1	71	53
13	8	2	97	95
13	9	0	40	26
13	9	1	56	24
13	9	2	36	44
13	10	0	79	63
13	10	1	115	133
13	11	0	26	63
13	11	1	26	43
13	12	0	36	70

ducing 12α-bromo-11β-hydroxy-3α,9-oxidocholanic acid methyl ester, whereas the other epimer resists similar attempts to eliminate one of the bromine atoms.

Experimental

Transparent, well-formed prismatic crystals were grown from an acetone solution, from a sample prepared by Squibb Products and supplied by the Cancer Chemotherapy Division of the National Institutes of Health. All the X-ray measurements were made on a General Electric single crystal diffractometer with Cu $K\alpha$ radiation.

The observed systematic extinctions ($h00$ for $h=2n+1$; $0k0$ for $k=2n+1$; $00l$ for $l=2n+1$) determined the space group as $P2_12_12_1$. The unit-cell dimensions are $a=11{\cdot}005\pm0{\cdot}007$, $b=31{\cdot}383\pm0{\cdot}013$, and $c=7{\cdot}133\pm0{\cdot}004$ Å (measured at 20°C, Cu $K\alpha_1=1{\cdot}54051$ Å).

There are four molecules per unit cell. The density, measured by flotation, was 1·45 g.cm^{-3}, as compared with the calculated value of 1·47 g.cm^{-3}.

The intensities of 2884 independent reflections in the θ-range 0°–74° were measured by the stationary crystal-stationary counter method with balanced nickel and cobalt filters. With each filter, the intensity was measured for ten seconds for each reflection. Appropriate corrections were made for Lorentz and polarization factors, but no corrections were made for extinction or absorption. Of the 2884 observed reflections, 696 were found to have intensities less than twice their standard deviations. Wilson's (1942) method was used to put the observed structure amplitudes on an absolute scale.

Structure analysis

The positions of the two bromine atoms of the molecule were located from a three-dimensional sharpened Patterson synthesis, computed by the use of coefficisten which had been modified so as to approximate those to be expected for point atoms without thermal motion. Other atoms in the molecule were then located from two successive Fourier syntheses calculated with the phases of the structure factors determined by the atoms which had already been located. The positional and thermal parameters (anisotropic for bromine atoms and isotropic for the lighter atoms) were refined by least squares with a block-diagonal approximation to the least-squares normal equations. Weights which were inversely proportional to the variances in the observed

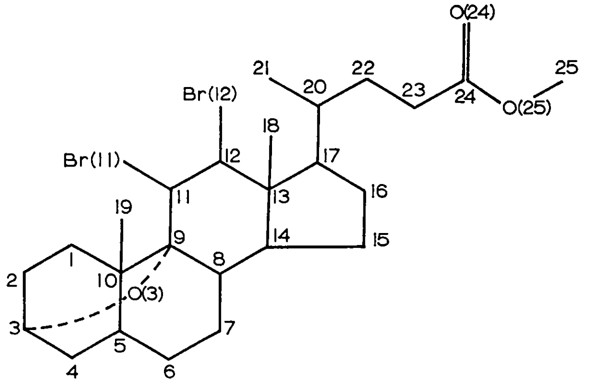

Fig. 1. Schematic representation of the molecule with the atoms numbered for reference in text.

Table 2. *Final positional and thermal parameters*

Standard deviations are given in parentheses.

	x/a	y/b	z/c	B_{iso}
C(1)	0·6583 (14)	0·2600 (4)	0·9205 (23)	3·91 (40)
C(2)	0·6899 (14)	0·2786 (4)	0·7201 (24)	3·80 (42)
C(3)	0·6382 (13)	0·2510 (4)	0·5708 (22)	3·13 (37)
C(4)	0·4943 (13)	0·2476 (4)	0·5989 (21)	3·50 (41)
C(5)	0·4633 (15)	0·2242 (4)	0·7915 (25)	4·08 (43)
C(6)	0·3970 (13)	0·1805 (4)	0·7695 (27)	4·44 (45)
C(7)	0·4692 (14)	0·1474 (4)	0·6460 (21)	3·94 (42)
C(8)	0·5982 (12)	0·1414 (4)	0·7199 (23)	3·32 (38)
C(9)	0·6649 (13)	0·1853 (3)	0·7599 (24)	3·20 (36)
C(10)	0·5913 (14)	0·2176 (4)	0·8917 (24)	3·69 (43)
C(11)	0·8101 (13)	0·1792 (4)	0·8029 (22)	3·19 (39)
C(12)	0·8639 (14)	0·1501 (4)	0·6673 (21)	3·45 (42)
C(13)	0·8046 (14)	0·1028 (4)	0·6395 (21)	3·03 (39)
C(14)	0·6727 (15)	0·1162 (4)	0·5826 (24)	3·74 (40)
C(15)	0·6193 (13)	0·0707 (4)	0·5140 (22)	3·43 (42)
C(16)	0·7294 (15)	0·0525 (4)	0·4123 (25)	4·34 (47)
C(17)	0·8432 (14)	0·0782 (4)	0·4551 (23)	3·67 (40)
C(18)	0·8101 (14)	0·0746 (4)	0·8241 (22)	3·60 (42)
C(19)	0·5598 (16)	0·1963 (4)	1·0875 (27)	5·26 (51)
C(20)	0·9720 (14)	0·0544 (4)	0·4590 (22)	3·46 (40)
C(21)	0·9963 (16)	0·0468 (4)	0·2510 (31)	6·49 (55)
C(22)	0·9633 (15)	0·0089 (4)	0·5431 (25)	4·77 (47)
C(23)	1·1013 (16)	−0·0012 (5)	0·5994 (28)	6·36 (60)
C(24)	1·1178 (18)	−0·0487 (5)	0·5994 (31)	8·32 (70)
C(25)	1·2284 (17)	−0·1091 (5)	0·7483 (34)	7·92 (64)
O(3)	0·6765 (9)	0·2067 (2)	0·5791 (15)	3·31 (25)
O(24)	1·0399 (13)	−0·0770 (3)	0·5519 (22)	9·91 (49)
O(25)	1·1970 (11)	−0·0636 (3)	0·7107 (21)	9·29 (46)
Br(11)	0·8395 (11)	0·1627 (3)	1·0695 (21)	4·69 *
Br(12)	1·0431 (11)	0·1459 (3)	0·7204 (21)	4·50 *

* These are the equivalent isotropic temperature factors for atoms Br(11) and Br(12). The anisotropic temperature factors are:

$$\exp -10^{-4}(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{12}hk+b_{13}hl+b_{23}kl)\,.$$

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Br(11)	144	10	144	4	−96	−1
Br(12)	71	9	329	0	−58	−11

structure factors (obtained from counting statistics alone) were used, and the quantity minimized was $\Sigma w(F_o|-F_c|)^2$. The scattering factor values given in *International Tables for X-ray Crystallography* (1962) were used throughout, with the scattering factors for bromine atoms corrected for the real part of the anomalous dispersion factor only. The refinement of the structure was terminated when the calculated positional parameter shifts were less than one fifth of their estimated standard derivations and the final R value ($\Sigma\,||F_o|-|F_c||/\Sigma\,|F_o|$) was 14% for the 2884 reflections. No attempt was made to locate the hydrogen atoms. The absolute configuration of the molecule was not determined but it was chosen to correspond with that normally observed in naturally occuring steroids; it is for this configuration that the observed and calculated structure amplitudes are listed in Table 1 and the positional (and thermal) parameters are listed in Table 2. The standard deviations listed in Table 2 were calculated from the inverses of the least-squares normal-equation blocks for each atom.

Bond lengths and bond angles

The bond lengths and bond angles are shown in Fig. 2(*a*) and (*b*), respectively. The estimated standard deviations in bond lengths are in the range 0·02–0·03 Å, and in bond angles in the range 1·0–2·0°. Four of the twenty six carbon–carbon single bonds of the type sp^3–sp^3 deviate from the expected value of 1·533 Å (Bonham & Bartell, 1959) by more than twice the standard deviation. Of these four, C(9)–C(11) with 1·64 Å, C(12)–C(13) with 1·63 Å, and C(14)–C(15) with 1·62 Å are longer than expected, and C(11)–C(12) with 1·46 Å is shorter.

Among the bond angles, C(10)–C(9)–C(11), with a value of 117°, is larger and C(12)–C(13)–C(14), with a value of 99°, is smaller than the normally expected value of about 109°. Also, as a result of the high thermal motions of the atoms at the end of the side chain, the geometry about atom O(25) is somewhat distorted.

Torsional angles

Table 3 lists the torsional angles calculated for this molecule. The two torsional angles $\theta(1,2)$ and $\theta(4,5)$ in the *A* ring, having values of 4° and 6° respectively, show a nearly eclipsed configuration. The other four torsional angles $\theta(2,3)$, $\theta(3,4)$, $\theta(5,10)$, and $\theta(10,1)$ with values 58°, −64°, 58°, and −65°, respectively, are of staggered configuration within experimental error. With the exception of $\theta(7,8)$, all torsional angles in the *B* ring are nearly of staggered configuration; $\theta(7,8)$ with a value of −48°, however, deviates by 12° from

Table 3. *Torsional angles in the rings*

θ_{A-B} is the torsional angle about the *A*–*B* bond, in which the other two atoms required to define the angle are those attached to either end of the bond and are in the ring in question.

A ring		*B* ring		*C* ring		*D* ring	
Bond	θ_{A-B}*	Bond	θ_{A-B}	Bond	θ_{A-B}	Bond	θ_{A-B}
C(1)—C(2)	3·7	C(5)—C(6)	−60·9	C(8)—C(9)	−47·1	C(13)–C(14)	50·9
C(2)—C(3)	58·0	C(6)—C(7)	54·0	C(9)—C(11)	45·4	C(14)–C(15)	−39·3
C(3)—C(4)	−64·4	C(7)—C(8)	−48·0	C(11)–C(12)	−54·6	C(15)–C(16)	12·7
C(4)—C(5)	5·8	C(8)—C(9)	52·7	C(12)–C(13)	58·5	C(16)–C(17)	18·5
C(5)—C(10)	57·5	C(9)—C(10)	−56·0	C(13)–C(14)	−61·4	C(13)–C(17)	−42·9
C(10)–C(1)	−65·1	C(10)–C(5)	58·7	C(8)—C(14)	61·5		

* The sign convention for the direction of the torsional angle is that of Klyne & Prelog (1960).

Table 4(*a*). *Least-squares planes through the atoms**

Plane	Atoms	*l*	*m*	*n*	*p*
*A*1	C(2), C(3), C(4)	−0·1279	0·8018	−0·5838	3·040
*A*2	C(1), C(2), C(4), C(5)	−0·5088	0·8204	0·2608	4·685
*A*3*B*1	C(1), C(5), C(6), C(10)	−0·4360	0·1174	0·8923	3·649
*B*2	C(6), C(7), C(9), C(10)	0·0505	−0·6405	0·7663	0·814
*B*3*C*1	C(7), C(8), C(9), C(11)	−0·2697	−0·0591	0·9612	2·830
*C*2	C(8), C(11), C(12), C(14)	0·1559	−0·6846	0·7120	1·631
*C*3*D*1	C(12), C(13), C(14), C(15)	−0·2965	−0·0959	0·9501	1·325
*D*2	C(13), C(15), C(16), C(17)	0·1654	−0·7610	0·6274	1·808
*D*3	C(14), C(15), C(16), C(17)	0·1830	−0·4555	0·8711	3·359
A	C(1), C(2), C(3), C(4), C(5), C(10)	−0·5009	0·8251	0·2612	4·531
B	C(5), C(6), C(7), C(8), C(9), C(10)	−0·1200	−0·4286	0·8955	1·714
C	C(8), C(9), C(11), C(12), C(13), C(14)	−0·0032	−0·4602	0·8878	2·271
D	C(13), C(14), C(15), C(16), C(17)	0·0429	−0·6240	0·7801	1·598
C(1)–C(17)		−0·0008	−0·3245	0·9459	2·816
C(5)–C(17)		−0·0418	−0·5124	0·8577	1·486

* The planes are in the form $lX+mY+nZ+p=0$, where X, Y, Z and p are in Å units, and X, Y and Z are referred to the crystal axes.

this configuration. The two angles θ(8,9) and θ(9,11) in the *C* ring, with values −47° and 45°, respectively, are considerably smaller than those for a staggered configuration; this deformation could be either the result of the interaction of Br(11) with the methyl group attached to C(10) or the oxido bridge between C(3) and C(9). In the *D* ring, θ(15,16) is 13° and θ(16,17) is 18°, as compared with values of approximately 16° in a regular half-chair.

Least-square planes

A perspective view of the molecule is shown in Fig. 3. Ring *A* has a boat conformation in which atoms C(1), C(2), C(4), and C(5) are coplanar within 0·04 Å, and atoms C(3) and C(10) both lie at a distance of 0·73 Å from this plane. Atom C(9), at the *B*/*C* ring junction, appears to have been drawn closer to the mean plane of the *B* and *C* rings than is normally observed in steroids having a *trans A*/*B* ring junction. Ring *D* is a distorted half-chair and is quite similar to the *D* ring in 11β,12α-dibromo-3α,9-oxidocholanic acid methyl ester. The equations of the usual least-squares planes and the atoms included in the calculation of these planes are given in Table 4(*a*).

Table 4(*b*). *Interplanar angles*

Plane 1	Plane 2	Angle
*A*1	*A*2	125°
*A*3*B*1	*A*2	123
*A*3*B*1	*B*2	126
*B*3*C*1	*B*2	140
*B*3*C*1	*C*2	133
*C*3*D*1	*C*2	134
*C*3*D*1	*D*2	128
*C*3*D*1	*D*3	35
A	*B*	87
B	*C*	7
C	*D*	12
C(1)–C(17)	(100)	90
C(1)–C(17)	(010)	71
C(1)–C(17)	(001)	161

Important interplanar angles calculated for this molecule are listed in Table 4(*b*). The mean plane of the *A* ring is practically perpendicular (87°) to the mean plane of the *B* ring, while the mean planes of rings *B* and *C* are inclined to each other at 7° and those of *C* and *D* at 12°.

Packing of the molecules

The molecules pack in the unit cell solely by weak van der Waals forces. There are only twenty-one intermolecular contacts shorter than 4·0 Å and nine shorter than 3·8 Å (see Table 5). The side chain and the methyl groups seem to play a major part in the packing of the molecules in the crystal, with four contacts involving the C(18) and C(19) methyl groups and twelve contacts involving the side chain. Of the latter, six are with the carboxyl oxygen atom O(24). The *A* ring also carries seven intermolecular contacts. The two bromine atoms together carry only three intermolecular contacts, in the range 3·82–3·98 Å. Fig. 4 shows the main features of this packing arrangement.

Comparative study of the two epimers

The two epimers are alike stereochemically, except for the configurations of the 12-bromine atom. In the 11β,12β-dibromo epimer (I), the bromine atoms are

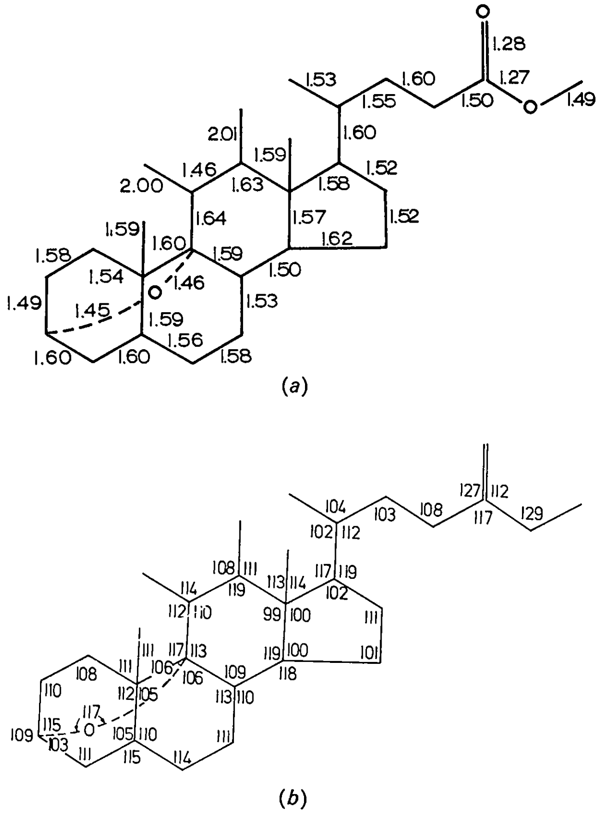

Fig. 2. (*a*) Interatomic distances. Standard deviations are in the range 0·02–0·03 Å. (*b*) Bond angles. Standard deviations are in the range 1·5–2·0°.

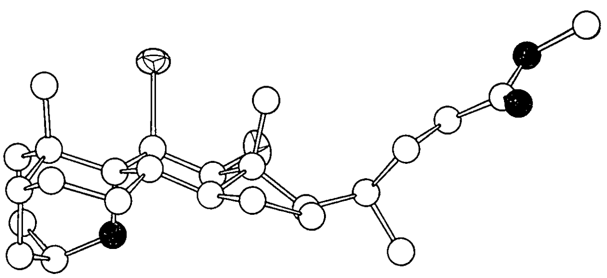

Fig. 3. Perspective view of the molecule as seen from the side. Shaded circles are oxygen atoms; the bromine atoms are drawn as ellipsoids which indicate their thermal motions.

in a *cis* configuration, and in the 11β,12α-dibromo epimer (II), they have a *trans* configuration. This difference leaves the gross features of the two molecules the same, but when finer details are considered, there are various structural differences arising out of the configuration of Br(12). The most outstanding difference is in the distortion of the *C* ring conformation. In the *cis* dibromo derivative, θ(Br(11)–11–12–13), with a value of 72°, has a distortion of only 12° from the normal staggered configuration, whereas in the *trans* dibromo epimer the same torsional angle, with a value of 92°, has a distortion of 32°, *i.e.* more than three times the distortion in the former; it is nearly midway between a staggered and an eclipsed configuration.

In (I), θ(Br(12)–12–11–9) with a value of 178° is within experimental error of the undistorted angle 180°, whereas in (II), θ(Br(12)–12–11–9) is 89° and has a distortion of 29° from the expected staggered configuration. The angle θ(9–11–12–13) in (II), with a value of −29°, is midway between the staggered and eclipsed configurations, whereas in (I) the angle is −55°, and close to the staggered configuration. The bond between C(11) and C(12) in the *cis* dibromo epimer is shortened (1·46 Å), whereas in the *trans* epimer it is lengthened (1·64 Å). The distortion in the *C* ring, though of different degree in each, is in the same direction, whereas the distortions in the *B* rings of the two epimers are of opposite sense to each other. In the *cis* dibromo derivative, θ(8,9), with a value of 53°, is 7° smaller in magnitude than in the staggered configuration, whereas in the *trans* dibromo epimer, the angle is 65° and is larger in magnitude by 5°. Angles θ(9,10) and θ(10,5) are also larger in magnitude than in a staggered configuration in (II), and smaller in (I). In both molecules, the distortion is transmitted as far as the *A* ring. For example, θ(5,10) is +58° in I, and +48° in II; these angles would have been +60° if distortion-free. The *D* ring in neither of these epimers, however, seems to have been affected by the *C* ring distortion or by the 3,9-oxido bond. The *D* rings in both these steroids have practically the same

Table 5. *Intermolecular distances less than* 4·0 Å

C(1)–C(5)	(3/000)	3·97 Å	C(7)—O(24)	(2/100)	3·64 Å
C(1)–C(6)	(3/000)	3·91	C(8)—O(24)	(2/100)	3·46
C(2)–C(25)	(4/201)	3·64	C(15)–O(24)	(2/10$\bar{1}$)	3·74
C(3)–C(19)	(1/00$\bar{1}$)	3·95	C(16)–C(22)	(2/10$\bar{1}$)	3·89
C(3)–Br(12)	(3/$\bar{1}$0$\bar{1}$)	3·99	C(16)–O(24)	(2/10$\bar{1}$)	4·00
C(4)–C(12)	(3/$\bar{1}$0$\bar{1}$)	4·00	C(17)–Br(11)	(1/00$\bar{1}$)	3·82
C(4)–O(3)	(3/$\bar{1}$0$\bar{1}$)	3·99	C(18)–C(21)	(1/001)	3·77
C(5)–Br(11)	(3/$\bar{1}$00)	3·93	C(19)–O(3)	(1/001)	3·75
C(6)–O(24)	(2/100)	3·89	C(19)–O(24)	(2/100)	3·91
C(7)–C(25)	(2/10$\bar{1}$)	3·77	C(21)–C(25)	(2/20$\bar{1}$)	3·61
			C(21)–O(25)	(2/20$\bar{1}$)	3·43

The equivalent positions are:

1	x	y	z
2	$\frac{1}{2}-x$	$-y$	$\frac{1}{2}+z$
3	$\frac{1}{2}+x$	$\frac{1}{2}-y$	$-z$
4	$-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$

C(7)–C(25) (2/10$\bar{1}$) means C(7) at equivalent position 1 to C(25) at equivalent position 2, translated one unit cell in the x direction and one unit cell in the $-z$ direction.

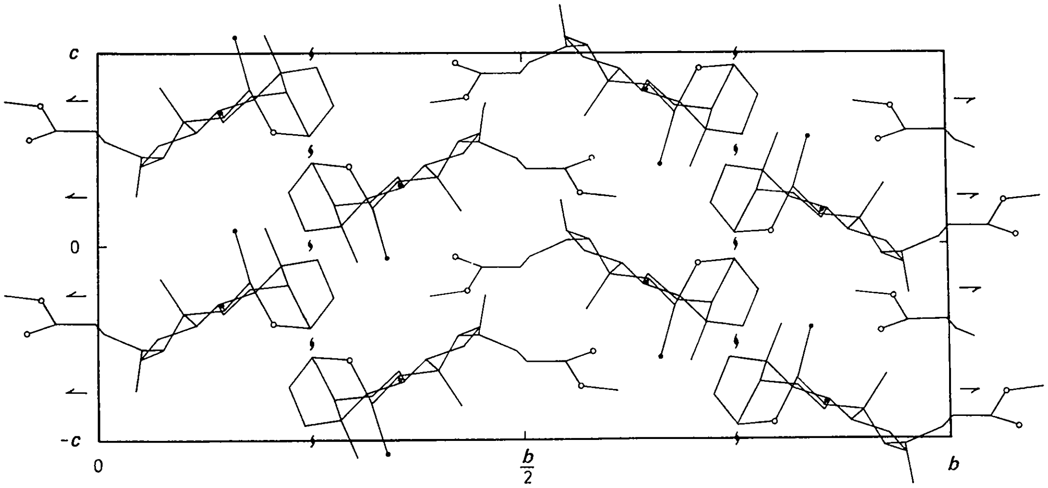

Fig. 4. Projection of the structure along the *a* axis of the unit cell. Shaded circles are bromine atoms; open circles are oxygen atoms.

conformation as that of the *D* ring in 2β,3α-dichloro-5α-cholestane, in which the *A* ring is normal, and in which there is no bromine atom attached to the *C* ring (Geise, Romers & Rutten, 1966). The packing of the molecules in the two cases is quite different. In the case of the 12α-bromo derivative, the bulky bromine group on the α-surface causes a fairly large intermolecular separation. This loosened packing arrangement allows a comparatively free rotation of the side chain about the C(17)–C(20) bond, resulting in the unusual side chain orientation observed in this molecule. The more compact packing arrangement achieved in the 12β-bromo derivative causes the side chain to take up the more frequently observed 'extended' conformation.

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The Crystal and Molecular Structure of Hypoxanthine Hydrochloride Monohydrate

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The structure of hypoxanthine hydrochloride monohydrate, $[C_5N_4H_5O]Cl.H_2O$, has been solved by X-ray crystallographic methods. The crystals are monoclinic, space group $P2_1/c$, with $a=4\cdot8295$ Å, $b=17\cdot7285$ Å, $c=9\cdot0077$ Å and $\beta=94\cdot59°$ ($t=20°\pm2°C$). 1769 reflections were measured on a manually operated diffractometer with Mo *Kα* radiation. The structure was refined to $R=0\cdot030$. Standard deviations in bond lengths and angles involving nonhydrogen atoms are in the range 0·0014–0·0018 Å and 0·03–0·07° respectively. The hypoxanthine cation is present in the lactam form and the nitrogen atoms N(1), N(7) and N(9) carry hydrogen atoms. The molecules are linked together through extensive hydrogen bonding. The spacing between layers of molecules is 3·18 Å, and there is virtually no overlap between molecules in adjacent layers.

Introduction

The hypoxanthine nucleotide inosinic acid is the first purine compound formed in the biosynthesis of purine nucleotides, and it is the precursor of both adenylic and guanylic acid. Any structure which is an antagonist for hypoxanthine will block nucleic acid synthesis. The structure of one such antagonist, 6-mercaptopurine, has already been determined (Sletten, Sletten & Jensen, 1969), and it is important to establish dimensional similarities and differences between this structure and hypoxanthine. The present paper is a report of the structure of the monohydrate of hypoxanthine hydrochloride.

Experimental

Hypoxanthine was obtained from Sigma Chemical Company, St. Louis, Missouri, and crystals of hypoxanthine hydrochloride were grown from a 1*N* HCl solution by slow evaporation.

Cell parameters were determined by least-squares treatment of the 2θ settings for 14 reflections as measured on the diffractometer. The mean deviation between the observed and computed 2θ values, $1/14\ (\Sigma\ |2\theta_{\rm obs}-2\theta_c|)$, was 0·007°.

The density of the crystals was determined by flotation in a mixture of chloroform and tetrabromoethane, and the value obtained agreed satisfactorily with that calculated for hypoxanthine hydrochloride crystallized with one molecule of water.

Crystal data

$[C_5N_4H_5O]$ Cl. H_2O. *M.W.* = 190·6 .

Crystal system: