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The Crystal Structures of Aflatoxin B_1. II. The Structure of an Orthorhombic and a Monoclinic Modification

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(*Received* 17 *November* 1969)

If aflatoxin B_1 is recrystallized from a chloroform–ethanol mixture, both an orthorhombic and a monoclinic modification are formed. The orthorhombic crystals have the unit-cell constants $a=7{\cdot}84$, $b=6{\cdot}36$ and $c=28{\cdot}35$ Å and the space group is $P2_12_12_1$, while the constants for the monoclinic crystals are $a=7{\cdot}93$, $b=6{\cdot}21$, $c=14{\cdot}04$ Å and $\alpha=95{\cdot}8°$. Their space group is $P2_1$. The crystal structures of the two modifications have been solved with the aid of the structure of aflatoxin $B_1.CHCl_3$ already known. The orientations of the aflatoxin B_1 molecule were assumed to be the same in all three structures and the positions of the molecules were determined by calculating the value of the residual while they were moved systematically through the unit cell. Both structures consist (just as the structure of aflatoxin $B_1.CHCl_3$) of strings of coplanar molecules in the directions [110] and [$\bar{1}$10]. The molecules within a string have again two short $CH_3\cdots O$ contacts: 2·97 and 3·18 Å for the orthorhombic form and 3·00 and 3·10 Å for the monoclinic form. These short contacts point to an interaction between the molecules and may be called hydrogen bonds.

Introduction

If aflatoxin B_1 is recrystallized by diffusion of ethanol (in which it is only slightly soluble) into a saturated solution of the toxin in chloroform, crystals containing chloroform (modification I) are formed (van Soest & Peerdeman, 1970*a*). However, if a solution of the toxin in a mixture of chloroform and ethanol is slowly evaporated, two new modifications (II and III) are formed. Their crystal structures were determined in order to compare them with the crystal structures already found for aflatoxin B_2 (van Soest & Peerdeman, 1970*b*) and for aflatoxin $B_1.CHCl_3$.

Experimental

For both modifications, the unit-cell dimensions were determined from Weissenberg and rotation photographs; their space groups followed from the systematically absent reflexions. The intensities were measured automatically with a PAILRED diffractometer, using nickel-filtered copper radiation. The monochromator was not applied in view of the small scattering power of the crystals. The intensities were corrected for Lorentz and polarization factors.

Most of the crystals obtained from the chloroform–ethanol solution are thin pale-yellow platelets. They

are monoclinic with the space group $P2_1$. The unit cell has the dimensions $a=7{\cdot}93$, $b=6{\cdot}21$, $c=14{\cdot}04$ Å and $\alpha=95{\cdot}8°$; it contains two molecules. For the intensity measurements, a crystal with dimensions 0·40

Table 1(*a*). *Observed and calculated structure factors* (×10) *and phase angles of the orthorhombic modification*

H	F-O	F-C	ARG
H	K= 0	L= 0	
2	407	473	180
4	891	891	180
6	878	873	180
8	106	97	180
10	86	87	180
12	420	418	180
14	260	264	0
16	256	245	180
18	89	96	0
20	12	8	0
22	109	94	0
24	118	112	0
26	40	29	180
28	34	28	180
30	214	209	180
32	38	48	180
34	241	253	0
H	K= 1	L= 0	
1	185	173	90
2	17	6	180
3	400	397	270
4	289	280	180
5	912	911	90
6	422	420	0
7	617	616	90
8	394	384	0
9	35	23	270
10	399	414	180
11	379	384	90
12	32	25	0
13	487	475	270
14	64	53	180
15	107	110	270
16	79	74	180
17	171	172	270
18	50	47	0
19	165	170	90
20	37	39	0
21	92	93	270
22	26	32	180
23	64	62	90
24	77	72	0
25	43	33	90
26	90	88	180
27	37	23	90
28	94	87	180
29	193	186	270
30	98	101	0
31	29	19	90
32	53	44	0
33	59	55	90
34	35	29	180
H	K= 2	L= 0	
0	75	75	0
1	250	246	90
2	26	19	180
3	60	61	270
4	218	209	0
5	606	597	270
6	189	185	180
7	239	230	270
8	422	399	0
9	434	438	90
10	46	45	0
11	329	320	90
12	182	177	180
13	107	107	270
14	23	26	180
15	51	55	270
16	19	5	180
17	141	132	90
18	81	77	180
19	108	108	270
20	25	23	180
21	167	167	270
22	41	38	180
23	212	210	90
24	145	142	180
25	7	3	90
26	174	174	0
27	20	6	90
28	49	47	180
29	126	132	270
30	85	80	0
31	35	28	90
32	37	31	0
33	14	5	90
H	K= 3	L= 0	
1	121	120	90
2	133	123	180
3	618	599	270
4	409	392	0
5	80	76	90
6	237	229	0
7	214	201	90
8	199	194	180
9	23	24	270
10	203	205	180
11	67	60	90
12	245	236	0
13	50	40	90
14	29	31	180
15	150	157	90
16	29	28	0
17	61	63	90
18	54	57	180
19	44	35	270
20	24	16	180
21	20	17	270
22	37	32	180
23	63	65	270
24	39	50	180
25	64	61	270
26	109	113	0
27	66	76	270
28	28	3	180
29	52	48	270
30	47	47	180
31	48	40	90
32	6	3	0
H	K= 4	L= 0	
0	156	148	0
2	8	9	180
3	35	32	270
4	103	108	0
5	23	15	270
6	78	75	0
7	64	57	90
8	199	199	180
9	43	39	270
10	123	127	0
11	31	10	90
12	105	108	180
13	136	131	90
14	150	151	0
15	16	14	270
16	111	115	180
17	70	76	270
18	77	81	180
19	22	23	270
20	42	43	0
21	19	13	270
22	10	18	180
23	64	62	90
24	24	22	180
25	26	29	270
26	43	36	180
27	31	24	90
28	32	34	0
29	20	1	270
30	23	30	0
H	K= 5	L= 0	
1	50	52	90
2	141	138	0
3	100	89	90
4	8	12	180
5	52	59	90
6	80	89	0
7	131	129	90
8	30	31	180
9	111	117	90
10	26	24	0
11	19	19	270
12	111	116	180
13	18	23	270
14	20	8	180
15	204	210	270
16	84	102	0
17	20	25	90
18	85	86	180
19	24	11	90
20	24	3	180
21	94	92	90
22	87	85	0
23	38	27	270
24	30	20	180
25	10	18	270
26	20	6	0
27	30	7	90
H	K= 6	L= 0	
0	45	58	0
1	118	111	270
2	127	133	0
3	71	65	90
4	37	28	180
5	12	33	270
6	93	91	0
7	90	87	90
8	138	136	180
9	27	19	270
10	86	88	180
11	33	26	270
12	64	63	0
13	63	69	90
14	84	88	180
15	23	15	270
17	20	17	270
18	29	27	180
19	33	32	270
20	47	60	0
21	41	44	90
H	K= 7	L= 0	
1	73	72	270
2	44	52	0
3	51	61	90
5	85	91	90
8	25	27	180
9	70	73	270
10	83	79	180
11	107	109	90
13	33	34	90
14	55	72	0
H	K= 0	L= 1	
1	843	858	90
2	382	382	270
3	410	415	270
4	179	187	270
5	228	239	90
6	354	372	270
7	247	242	90
8	47	39	270
9	580	578	270
10	175	181	90
11	126	134	270
12	271	267	270
13	193	197	270
14	118	120	270
15	54	56	90
16	33	34	90
17	54	49	90
18	46	50	90
19	133	131	90
20	88	89	90
21	73	76	90
22	0	0	0
23	34	31	270
24	66	61	90
25	50	47	270
26	40	41	270
27	25	29	270
28	36	43	90
29	21	1	90
30	60	53	270
31	46	58	270
32	69	69	90
33	50	46	90
34	59	65	90
H	K= 1	L= 1	
0	125	128	90
1	499	494	76
2	370	371	228
3	997	1007	257
4	999	1019	231
5	802	809	152
6	861	876	136
7	605	609	86
8	687	699	50
9	489	501	4
10	234	238	349
11	105	100	95
12	173	177	189
13	264	265	247
14	21	20	293
15	256	253	255
16	31	22	109
17	370	367	331
18	47	45	314
19	279	266	104
20	140	143	316
21	110	106	152
22	46	52	267
23	38	31	352
24	64	66	84
25	112	111	47
26	200	210	155
27	159	156	275
28	124	124	34
29	81	81	174
30	70	64	18
31	73	74	124
32	25	27	306
33	18	16	23
34	32	35	94
H	K= 2	L= 1	
0	581	584	0
1	238	243	181
2	173	169	308
3	154	150	350
4	89	95	223
5	274	280	67
6	230	223	223
7	328	323	30
8	308	296	97
9	39	31	50
10	251	244	242
11	383	378	232
12	322	321	230
13	176	173	224
14	257	244	31
15	208	209	74
16	102	101	180
17	127	127	225
18	118	126	22
19	109	109	131
20	110	104	271
21	79	79	32
22	63	63	54
23	219	231	304
24	189	186	117
25	39	36	174
26	83	85	349
27	55	51	57
28	35	35	191
29	51	50	67
30	16	20	159
32	28	13	125
33	21	23	196
H	K= 3	L= 1	
0	384	373	90
1	57	65	77
2	48	54	58
3	280	272	241
4	161	164	329
5	280	281	115
6	216	217	214
7	134	129	313
8	69	67	238
9	224	223	144
10	187	182	73
11	41	37	295
12	180	178	259
13	224	224	354
14	124	121	93
15	40	45	234
16	60	59	250
17	20	18	276
18	32	29	250
19	56	62	49
20	14	16	203
21	88	90	318
22	21	19	273
23	81	81	64
24	79	81	88
25	100	100	216
26	40	40	354
27	47	56	78
28	50	57	312
29	65	64	246
30	35	35	314
31	46	43	169
H	K= 4	L= 1	
0	399	392	0
1	89	91	85
2	369	360	236
3	30	31	291
4	35	33	326
5	153	159	150
6	130	128	147
7	158	165	216
8	119	110	297
9	104	104	129
10	136	131	355
11	119	118	258
12	115	111	187
13	173	169	351
14	77	84	318
15	100	101	27
16	117	114	247
17	39	47	69
18	107	112	50
19	29	39	9
20	137	139	132
21	86	91	199
23	51	60	246
24	28	13	151
25	20	12	148
26	26	28	45
27	24	16	136
28	24	20	264
29	30	29	8
H	K= 5	L= 1	
0	57	55	90
1	138	153	127
2	96	100	157
3	121	126	291
4	59	65	109
5	122	127	122
6	122	115	183
7	10	19	151
8	76	80	299
9	45	38	259
10	70	73	243
11	61	67	41
12	37	30	224
13	158	164	299
14	80	74	354
15	130	135	74
16	34	34	67
17	78	74	219
18	46	55	288
20	71	71	139
21	40	36	32
22	49	52	42
23	26	30	87
24	32	20	166
25	18	24	206
26	22	27	250
H	K= 6	L= 1	
0	199	190	0
1	137	131	141
2	55	54	85
3	95	89	252
4	21	34	40
5	144	139	30
6	173	170	225
7	69	71	125
8	69	65	209
9	63	65	246
10	24	13	305
11	83	91	223
12	53	58	355
13	52	25	341
14	36	35	132
15	31	31	222
16	25	10	4
17	29	22	48
18	27	11	100
19	6	2	28
20	16	5	247
H	K= 7	L= 1	
1	65	62	163
2	44	50	291
4	99	102	141
7	100	105	96
8	36	88	332
9	22	47	191
10	57	63	100
11	31	40	286
12	64	69	140
13	31	28	340
14	28	25	187
H	K= 0	L= 2	
0	565	569	180
1	330	336	180
2	547	549	0
3	105	117	0
4	491	494	180
5	209	194	180
6	470	472	0
7	197	211	0
8	531	537	0
9	400	408	180
10	158	155	180
11	410	403	0
12	453	439	180
13	298	293	0
14	302	314	180
15	140	131	180
16	332	333	0
17	51	51	0
18	46	39	180
19	93	93	0
20	51	58	0
21	127	118	180
22	221	218	180
23	124	119	180
24	53	45	0
25	17	13	180
26	102	100	0
27	21	16	0
28	29	28	0
29	79	83	180
30	17	7	180
31	61	63	0
32	17	15	180
33	27	20	180
H	K= 1	L= 2	
0	591	594	270
1	106	104	322
2	298	294	112
3	420	423	50
4	408	413	202
5	466	480	251
6	134	132	261
7	362	362	143
8	206	194	175
9	151	150	47
10	179	183	344
11	100	102	187
12	57	56	256
13	117	121	114
14	168	172	338
15	69	67	4
16	222	222	29
17	153	152	103
18	280	278	122
19	211	208	287
20	85	78	246
21	13	20	332
22	45	54	109
23	99	100	308
24	50	55	239
25	50	60	108
26	59	51	159
27	61	69	278
28	32	24	284
29	72	76	150
30	46	47	301
31	34	30	84
32	13	9	304
33	14	19	253
H	K= 2	L= 2	
0	285	285	180
1	275	272	15
2	92	93	45
3	186	175	146
4	8	12	330
5	162	161	274
6	68	66	18
7	274	270	27
8	237	227	104
9	217	212	11
10	308	312	17
11	504	499	324
12	315	310	266
13	492	488	211
14	186	187	162
15	196	192	119
16	60	57	357
17	242	239	99
18	78	70	234
19	94	97	82
20	130	130	223
21	195	199	352
22	187	195	131
23	159	163	231
24	165	169	6
25	91	92	140
26	46	39	226
27	59	60	213
28	38	40	7
29	31	30	310
30	33	37	16
31	25	14	255
32	21	19	355
H	K= 3	L= 2	
0	241	238	270
1	163	168	269
2	334	330	252
3	95	95	85
4	111	103	326
5	210	212	209
6	244	237	64
7	180	166	322
8	253	249	113
9	112	109	27
10	176	172	279
11	72	70	13
12	111	110	59
13	166	169	158
14	52	52	1
15	226	227	115
16	96	92	166
17	230	240	16
18	127	128	89
19	185	197	259
20	39	42	307
21	120	123	187
22	51	61	227
23	38	36	315
24	69	65	259
25	58	54	296
26	31	7	235
27	48	53	356
28	95	96	61
29	39	46	172
30	33	33	226
31	16	19	324
H	K= 4	L= 2	
0	67	74	180
1	131	121	28
2	131	127	268
3	131	129	282
4	134	137	302
5	82	79	270
6	74	76	289
7	151	152	51
8	68	69	130
9	121	120	345
10	46	38	356
11	98	102	128
12	129	128	349
13	91	92	24
14	99	101	123
15	31	45	198
16	104	102	223
17	65	63	40
18	128	132	124
19	136	146	218
20	58	60	207
21	19	11	10
22	71	69	324
23	29	24	185
24	57	60	66
25	33	36	189
26	18	22	236
27	26	29	341
28	29	29	297
29	31	26	101
H	K= 5	L= 2	
0	50	60	90
1	230	233	50
2	52	51	25
3	130	135	160
4	155	156	220
5	196	197	195
6	116	119	274
7	26	15	68
8	154	159	55
9	82	81	19
10	81	85	287
11	40	37	8
12	29	17	270
13	142	145	356
14	40	40	123
15	75	71	116
16	84	82	96
17	64	64	231
18	39	29	141
19	34	39	198
20	31	36	62
21	22	18	265
22	24	14	204
23	27	23	45
24	23	16	286
25	25	18	310
26	41	49	149
H	K= 6	L= 2	
0	112	107	180
1	53	52	51
2	197	202	269
3	88	89	168
4	188	184	10
5	28	10	15
6	64	61	142
7	89	84	302
8	48	52	131
9	7	28	279
10	25	29	245
11	60	60	313
12	70	74	225
14	33	20	294
15	39	40	45
16	10	12	163
17	14	16	52
18	50	54	17
19	42	35	103
20	20	14	129
H	K= 7	L= 2	
0	47	43	270
1	37	36	139
2	86	82	194
3	51	50	347
4	36	34	131
5	50	49	160
6	36	40	172
7	15	18	0
8	49	50	286
9	35	35	114
10	18	22	45
11	18	18	190
12	30	33	20
13	28	27	5
H	K= 0	L= 3	
1	131	132	90
2	108	104	270
3	131	148	270
4	245	243	270
5	443	441	90
6	172	174	270
7	225	235	270
8	295	294	270
9	283	272	90
10	156	142	270
11	48	44	270
12	358	359	90
13	151	143	270
14	80	77	90
15	25	25	270
16	133	130	90
17	204	208	270
18	91	100	90
19	106	112	90
20	85	85	270
21	175	177	270
22	110	102	270
23	58	61	90
24	73	78	270
25	78	77	90
26	97	98	90
27	49	47	90
28	92	89	270
29	24	15	90
30	29	27	90
31	12	11	90
32	6	15	90
H	K= 1	L= 3	
0	439	434	90
1	272	272	252
2	35	32	283
3	227	232	187
4	297	292	351
5	282	270	75
6	427	423	220
7	309	312	14
8	142	131	133
9	140	131	286
10	123	123	147
11	29	30	347
12	119	114	236
13	216	207	147
14	85	82	122
15	196	192	335
16	26	33	187
17	50	44	144
18	49	49	319
19	61	60	302
20	48	43	357
21	84	84	179
22	89	89	339
23	70	70	213
24	69	67	54
25	83	85	72
26	53	50	352
27	34	26	308
28	37	42	48
29	57	57	304
30	67	64	212
31	23	24	63
32	22	22	157
H	K= 2	L= 3	
0	448	427	0
1	192	183	317
2	409	382	71
3	181	181	127
4	488	471	160
5	206	197	47
6	207	204	14
7	179	171	147
8	98	95	186
9	136	136	152
10	72	65	357
11	76	81	32
12	72	73	285
13	168	161	301
14	146	146	234
15	99	90	230
16	105	99	92
17	47	55	250
18	94	96	245
19	58	61	306
20	38	32	336
21	22	26	348
22	63	69	111
23	67	66	226
24	72	79	8
25	47	52	14
26	33	42	109
27	42	44	80
28	28	20	349
29	46	38	80
30	29	28	178
31	59	64	112
H	K= 3	L= 3	
0	106	107	270
1	107	96	285
2	107	108	163
3	156	148	41
4	28	31	281
5	180	183	345
6	35	32	28
7	112	106	179
8	224	221	85
9	110	115	198
10	103	101	221
11	166	167	164
12	76	83	320
13	135	136	158
14	272	275	245
15	99	98	6
16	344	352	149
17	119	124	64
18	228	230	25
19	201	203	292
20	149	146	330
21	60	68	13
22	72	66	222
23	70	71	257
24	59	61	354
25	72	73	94
26	68	66	61
27	63	61	178
28	33	29	227
29	21	14	282
30	17	24	48
H	K= 4	L= 3	
0	98	95	180
1	91	92	111
2	199	192	54
3	69	80	175
4	172	169	152
5	44	49	183
6	8	19	175
7	183	187	285
8	203	202	333
9	194	190	60
10	133	139	329
11	205	209	78
12	193	189	153
13	173	173	249
14	46	53	137
15	97	106	226
16	91	87	25
17	33	25	96
18	106	106	220
19	56	59	280
20	39	48	307
21	163	153	311
22	127	131	190
23	71	72	103
24	54	55	14
25	118	115	130
26	96	97	27
27	75	69	262
28	38	41	76
H	K= 5	L= 3	
0	83	82	90
1	152	151	204
2	132	137	199
3	129	132	268
4	102	97	317
5	214	215	313
6	101	100	33
7	179	180	98
8	177	179	158
9	42	37	54
10	46	47	262
11	62	59	28
12	80	75	236
13	47	45	352
14	50	57	70
15	47	43	166
16	34	16	275
17	37	32	116
18	55	55	116
19	67	64	213
20	27	27	338
21	31	22	134
22	24	11	352
23	40	41	255
24	36	38	315
H	K= 6	L= 3	
0	24	29	180
1	21	13	67
2	48	45	220
3	61	58	109
4	119	119	296
5	58	56	213
6	33	32	345
7	86	83	48
8	42	55	196
9	21	19	186
10	83	83	26
11	66	72	325
12	44	30	58
13	65	66	242
14	71	67	172
16	18	21	59
17	40	36	139
18	14	20	176
19	24	30	304
H	K= 7	L= 3	
0	92	98	270
1	29	23	334
2	21	21	69
3	21	21	135
4	18	19	90
5	16	12	270
6	45	35	133
7	36	42	107
8	42	40	160
9	23	13	220
10	29	41	216
H	K= 0	L= 4	
0	150	154	180
1	143	136	0
2	7	10	180
3	10	13	0
4	29	28	0
5	261	266	0
6	50	44	0
7	35	42	0
8	24	18	0
9	88	95	180
10	165	169	180
11	90	90	0
12	68	76	180
13	49	47	0
14	77	81	0
15	9	15	180
16	23	18	0
17	67	67	180
18	169	171	0
19	24	19	0
20	63	69	180
21	45	50	180
22	158	163	0
23	42	50	180
24	144	149	180
25	67	64	0
26	39	36	180
27	27	20	180
28	27	20	180
29	50	46	180
30	20	0	0
31	5	5	0
H	K= 1	L= 4	
0	187	186	270
1	177	180	75
2	68	67	323
3	166	165	131
4	50	50	140
5	281	274	116
6	428	419	191
7	348	345	273
8	153	156	324
9	138	141	25
10	85	76	104
11	173	174	291
12	116	113	81
13	26	20	322
14	116	117	19
15	64	59	62
16	21	20	351
17	98	99	207
18	97	102	2
19	68	73	111
20	97	96	153
21	54	59	278
22	66	63	12
23	91	89	86
24	118	116	180
25	36	33	25
26	53	49	210
27	57	67	86
28	47	48	344
29	12	15	287
30	18	19	320
31	68	81	245
H	K= 2	L= 4	
0	101	103	0
1	310	301	74
2	68	62	220
3	323	309	307
4	60	54	176
5	35	35	104
6	155	159	242
7	119	110	169
8	117	115	49
9	77	84	329
10	153	153	198
11	80	84	289
12	23	18	18
13	73	70	349
14	98	95	356
15	98	97	309
16	112	106	110
17	55	60	63
18	124	121	342
19	64	70	149
20	66	67	213
21	81	71	154
22	84	81	15
23	38	40	90
24	45	50	159
25	48	53	167
26	33	20	197
27	37	29	322
28	17	14	236
29	17	22	238
30	22	35	187
H	K= 3	L= 4	
0	112	102	90
1	54	55	330
2	90	83	110
3	28	24	78
4	187	184	245
5	141	145	165
6	106	104	293
7	74	70	8
8	112	115	325
9	93	90	296
10	91	93	43
11	32	45	32
12	133	133	106
13	177	173	161
14	98	100	186
15	206	206	271
16	146	143	185
17	183	176	342
18	60	56	332
19	261	258	88
20	140	138	15
21	109	105	228
22	71	71	43
23	40	33	233
24	47	46	146
25	67	63	37
26	27	28	205
27	20	26	193
28	41	45	227
H	K= 4	L= 4	
0	51	43	180
1	105	106	298
2	86	80	112
3	108	107	285
4	71	63	105
5	87	92	8
6	102	100	354
7	110	103	65
8	111	113	6
9	312	318	102
10	309	310	198
11	100	99	277
12	30	7	23
13	124	121	279
14	87	88	340
15	88	88	52
16	28	44	50
17	50	53	217
18	27	25	178
19	21	10	48
20	112	113	358
21	96	97	253
22	21	23	275
23	69	73	257
24	110	112	157
25	60	62	82
26	45	42	69
H	K= 5	L= 4	
0	38	47	90
1	153	156	257
2	35	31	257
3	51	64	122
4	249	251	330
5	63	67	78
6	44	40	202
7	103	112	339
8	87	88	98
9	48	41	241
10	69	70	118
11	78	70	168
12	55	48	274
13	46	44	214
14	40	27	115
15	58	57	348
16	85	86	160
17	34	34	302
18	12	15	13
19	44	43	3
20	31	19	155
22	45	49	329
23	43	39	147
H	K= 6	L= 4	
0	38	19	0
1	32	24	257
2	56	58	277
3	13	31	18
5	34	34	88
6	36	25	187
7	31	30	312
8	62	62	191
9	36	37	354
10	37	45	274
11	52	63	87
12	73	73	354
13	87	82	281
14	43	40	59
15	25	13	0
16	47	45	118
H	K= 7	L= 4	
0	34	25	270
1	61	58	213
2	28	32	210
3	22	17	326
4	35	29	156
5	17	17	335
H	K= 0	L= 5	
1	32	31	270
2	11	3	90
3	174	167	90
4	27	34	90
5	115	119	270
6	131	130	90
7	13	11	270
8	188	187	270
9	193	183	270
10	79	79	270
11	206	210	90
12	124	118	90
13	159	157	90
14	149	150	90
15	146	149	270
16	14	16	270
17	19	20	270
18	107	112	90
19	141	147	270
20	90	87	270
21	104	112	90
22	91	102	270
23	10	16	90
24	29	31	270
25	28	19	270
26	24	32	90
27	32	38	270
28	31	30	270
29	28	32	90
H	K= 1	L= 5	
0	153	154	270
1	105	105	12
2	155	161	8
3	141	139	174
4	135	133	163
5	160	163	338
6	102	101	278
7	30	27	173
8	107	108	134
9	85	91	301
10	67	70	101
11	60	54	170
12	64	58	138
13	113	113	48
14	57	52	346
15	39	33	122
16	66	76	341
17	117	115	184
18	64	66	259
19	59	60	119
20	71	72	190
21	68	72	280
22	15	19	87
23	27	10	0
24	42	33	10
25	35	30	177
26	21	21	59
27	26	13	72
28	28	3	145
29	41	34	316
H	K= 2	L= 5	
0	31	28	180
1	210	203	85
2	148	143	142
3	28	28	135
4	158	156	310
5	77	77	311
6	117	118	122
7	72	70	245
8	224	221	359
9	125	126	265
10	280	283	100
11	129	135	316
12	156	158	196
13	159	159	78
14	142	141	267
15	208	206	174
16	91	89	350
17	145	146	263
18	91	89	339
19	124	115	15
20	100	98	115
21	98	97	68
22	70	64	177
23	56	54	175
24	79	79	233
25	60	57	285
26	48	49	323
27	20	14	334
28	17	12	44
H	K= 3	L= 5	
0	63	57	90
1	168	164	47
2	47	42	48
3	108	109	27
4	78	78	211
5	51	42	170
6	107	107	202
7	94	97	179
8	101	105	160
9	57	56	50
10	19	28	89
11	36	42	189
12	58	57	263
13	144	138	245
14	150	146	305
15	55	58	76
16	213	211	27
17	48	46	239
18	149	148	133
19	72	66	113
20	75	75	220
21	46	49	318
22	42	43	291
23	52	48	80
24	41	37	130
25	39	33	324
26	12	8	314
H	K= 4	L= 5	
0	224	230	0
1	49	47	43
2	72	82	108
3	41	41	128
4	37	28	145
5	75	65	286
6	12	12	270
7	125	124	117
8	112	112	86
9	44	45	216
10	86	86	173
11	118	114	299
12	34	33	162
13	48	46	274
14	42	41	234
15	78	81	0
16	19	31	306
17	58	55	90
18	77	77	9
19	64	56	153
20	39	36	194
21	24	31	328
22	40	40	22
23	44	42	222
24	41	43	243
H	K= 5	L= 5	
0	82	71	90
1	28	30	196
2	65	64	46
3	66	66	63
4	139	140	259
5	182	178	59
6	20	27	207
7	64	66	240
8	66	86	43
9	57	54	222
10	69	69	188
11	65	65	334
12	20	7	160
13	27	40	110
15	33	36	173
17	25	22	206
18	25	24	157
19	26	18	201
20	27	6	121
H	K= 6	L= 5	
0	40	36	180
1	114	116	42
2	36	32	296
3	102	101	301
4	42	42	332
5	41	30	275
6	34	27	60
7	24	28	63
9	44	43	117
10	35	37	186
11	28	17	340
12	31	28	90
13	17	20	72
H	K= 0	L= 6	
0	195	197	180
1	36	37	180
2	127	128	0
3	19	10	180
4	53	61	0
5	36	40	0
6	152	162	180
8	69	76	180
9	139	143	0
10	46	37	0
11	112	109	180
12	36	36	0
13	42	50	180
14	18	21	0
15	39	1	180
16	28	33	0
17	11	20	0
18	42	46	180
20	83	82	0
22	26	20	0
23	19	6	0
24	37	43	0
26	20	15	180
H	K= 1	L= 6	
0	35	34	90
1	55	57	239
2	155	165	321
3	139	145	199
4	140	140	55
5	216	222	273
6	104	107	164
7	264	268	20
8	168	165	221
9	111	117	101
10	92	90	332
11	120	123	204
12	131	133	91
13	78	81	270
14	87	90	87
15	49	43	261
16	105	109	325
17	105	102	20
18	115	121	243
19	38	33	225
20	60	61	90
21	80	75	75
22	40	30	102
23	91	95	162
24	33	42	205
25	26	25	244
26	28	29	280
27	52	55	329
H	K= 2	L= 6	
0	96	94	180
1	47	52	112
2	52	59	143
3	56	63	15
4	108	116	208
5	63	63	229
6	31	24	90
7	47	16	75
8	121	121	274
9	28	38	302
10	152	159	9
11	101	111	191
12	122	127	19
13	47	46	5
14	65	71	180
15	68	75	33
16	41	26	12
17	51	53	307
18	62	61	122
19	61	61	146
20	69	72	162
21	63	64	163
22	83	84	271
23	38	42	327
24	86	85	13
25	25	36	4
26	9	9	176
H	K= 3	L= 6	
0	12	19	270
1	54	62	0
2	36	58	2
3	94	97	183
4	73	83	92
5	160	141	286
6	67	73	197
7	181	190	237
8	39	46	229
9	151	153	0
10	58	57	112
11	82	81	136
12	113	112	286
13	28	27	63
14	62	66	19
15	26	34	67
16	24	24	90
17	41	47	109
18	21	24	134
20	16	17	194
21	34	37	167
22	21	26	210
23	39	44	291
24	6	23	21
H	K= 4	L= 6	
0	24	19	180
1	171	180	142
2	31	25	149
3	54	65	230
4	31	37	168
5	79	86	287
6	14	27	129
7	22	32	65
8	34	34	233
9	39	43	162
10	71	73	38
11	39	31	5
12	48	52	314
13	40	41	286
14	30	35	311
15	27	27	158
16	18	8	170
17	20	26	140
18	10	5	168
19	52	52	344
20	13	7	146
H	K= 5	L= 6	
0	64	54	90
1	30	32	102
3	18	21	317
4	61	56	228
5	20	27	11
6	31	38	75
7	35	19	128
9	9	28	163
10	25	27	132
11	47	48	243
12	37	43	281
13	48	43	270
14	26	13	314
16	19	27	129
H	K= 6	L= 6	
1	39	43	76
2	96	92	82
3	50	52	5
4	39	46	316
5	13	23	192
6	54	48	170
7	47	46	252
H	K= 0	L= 7	
1	362	372	270
2	97	101	270
3	272	277	90
4	90	88	270
5	164	164	90
6	55	56	90
7	82	79	270
8	140	140	90
9	21	17	270
10	44	35	90
11	18	13	270
12	32	6	90
13	32	8	270
14	54	60	270
16	38	29	90
17	52	51	90
18	61	63	270
19	28	8	90
20	68	60	90
23	22	24	270
H	K= 1	L= 7	
0	124	122	270
1	47	53	288
2	110	108	200
3	119	121	51
4	42	30	3
5	57	51	165
6	134	138	31
7	87	80	285
8	10	16	26
9	52	55	143
10	27	20	115
11	36	29	36
12	50	35	59
13	33	35	260
14	91	87	154
15	28	21	137
16	30	23	253
17	27	30	138
18	42	40	313
19	51	50	217
20	22	19	307
21	28	17	103
22	22	31	247
23	14	5	333
H	K= 2	L= 7	
21	22	13	270
H	K= 3	L= 7	
0	51	45	90
1	61	68	18
2	37	31	152
4	39	37	254
5	136	143	255
6	91	91	347
7	33	35	31
8	34	40	316
9	73	80	86
10	48	45	139
11	13	11	225
14	35	28	96
15	12	17	141
17	22	23	141
18	4	2	90
19	16	16	290
H	K= 4	L= 7	
0	64	59	180
1	48	46	197
2	29	22	67
3	24	13	170
4	42	39	211
5	45	41	229
6	43	39	30
7	25	19	90
8	30	34	342
9	11	17	174
10	55	60	99
11	27	13	119
12	47	31	339
13	52	53	330
15	44	42	351
16	15	14	201
H	K= 5	L= 7	
0	45	45	90
1	30	34	270
3	32	38	24
4	56	29	174
5	25	19	193
6	40	42	282
7	24	13	254
8	14	20	341
9	30	18	253
H	K= 0	L= 8	
0	233	236	0
1	48	37	180
2	67	71	180
3	43	49	180
4	9	14	180
5	29	38	180
7	36	30	180
8	64	60	180
9	26	7	0
10	62	64	180
11	12	17	0
12	19	8	0
13	27	28	180
14	51	42	0
15	27	23	0
17	13	15	0
18	22	16	0
H	K= 1	L= 8	
0	71	72	270
1	108	100	353
2	43	38	179
3	96	92	179
4	125	124	142
5	102	103	104
6	95	90	64
7	43	31	30
8	57	61	291
9	98	96	267
10	64	65	295
12	63	39	354
13	23	24	240
14	69	60	151
15	39	32	5
16	63	61	219
17	21	29	215
18	38	37	336
H	K= 2	L= 8	
0	19	7	0
1	42	42	273
2	26	24	144
3	55	52	133
4	45	36	124
5	49	46	119
6	31	26	300
7	64	60	324
8	54	50	7
9	37	27	328
10	41	35	185
11	75	72	162
12	55	54	148
13	31	29	193
14	45	50	335
15	37	17	273
16	41	39	339
H	K= 3	L= 8	
0	49	42	270
1	40	30	63
2	25	16	101
3	56	56	291
4	56	62	17
5	63	67	197
7	33	34	347
8	24	24	80
9	30	18	248
10	60	55	153
11	40	34	21
12	22	9	299
H	K= 4	L= 8	
0	16	19	0
1	25	30	199
2	42	39	255
3	61	63	178
4	25	25	223
5	30	34	338
6	25	17	160
7	19	13	122
8	18	17	108
H	K= 0	L= 9	
1	19	18	90
3	14	12	270
4	15	15	270
5	30	30	90
6	24	26	270
7	65	70	270
8	23	2	90
9	56	56	270
10	17	23	90
11	46	53	90
H	K= 1	L= 9	
1	34	30	123
2	8	23	335
3	24	23	292
4	33	39	203
5	29	27	90
6	48	45	116
7	25	24	129
8	43	44	350
9	36	34	354
10	27	28	319
H	K= 2	L= 9	
1	23	16	259
2	30	36	43
3	30	18	283
4	40	37	127
6	36	40	103
7	50	63	72

$\times 0{\cdot}35 \times 0{\cdot}10$ mm was used. Seven levels around the *a* axis were recorded. 1200 reflexions were measured, 64 of which appeared to be too weak.

A few needle-shaped crystals were also formed. They were orthorhombic with the space group $P2_12_12_1$. The unit cell ($a=7{\cdot}84$, $b=6{\cdot}36$ and $c=28{\cdot}35$ Å) contains four molecules. A crystal with dimensions $0{\cdot}45 \times 0{\cdot}05 \times 0{\cdot}05$ mm was used to collect the intensity data. Seven levels around the *a* axis and six levels around the *b* axis were recorded. Using the mean value of the reflexions measured more than once, 1564 reflexions remained.

Determination and refinement of the structures

The *a* and *b* axes of the three aflatoxin B_1 modifications are of the same order of magnitude but the *c* axes differ appreciably. These differences can be explained

Table 1(*b*). *Observed and calculated structure factors* ($\times 10$) *and phase angles of the monoclinic modification*

	F-O	F-C	ARG
H	K= 0	L= 0	
17	73	80	180
16	86	95	180
15	119	122	0
14	16	11	0
13	15	7	180
12	59	56	0
11	36	33	180
10	21	3	0
9	42	43	180
8	128	124	180
7	113	113	180
6	223	220	180
4	43	38	180
3	408	420	0
2	357	371	180
1	165	168	0
H	K= 1	L= 0	
16	41	38	180
14	146	148	0
13	19	13	0
12	83	85	180
10	19	21	0
9	91	99	0
8	135	137	0
7	50	53	180
6	253	258	0
5	27	24	0
4	195	199	180
2	323	336	180
1	39	40	180
0	165	170	180
-2	464	467	180
-3	429	442	180
-4	387	397	0
-5	251	247	0
-6	289	288	0
-7	131	128	0
-8	57	57	180
-9	87	86	0
-10	95	101	0
-11	36	36	0
-12	66	63	0
-13	15	17	0
-14	19	22	0
-15	15	19	0
-16	8	2	180
-17	10	6	180
H	K= 2	L= 0	
14	102	104	180
13	53	48	180
12	70	69	180
11	99	100	180
10	89	92	180
9	26	19	0
8	113	115	0
7	28	23	0
6	46	45	180
5	300	289	180
4	296	285	0
3	343	326	0
2	207	206	180
1	94	95	0
0	136	139	0
-1	97	95	180
-2	79	82	0
-3	344	341	0
-4	38	32	0
-5	82	86	180
-6	63	57	0
-7	44	51	0
-8	53	51	180
-9	21	24	180
-10	45	41	180
-11	131	117	0
-12	46	41	0
-13	122	111	180
-14	15	15	0
-15	12	5	0
-16	6	16	0
-17	10	8	0
H	K= 3	L= 0	
14	21	23	0
13	8	13	180
12	48	48	0
11	25	28	0
10	45	48	180
9	35	32	0
8	84	87	180
7	47	45	0
6	24	15	0
5	113	108	180
4	47	43	180
3	176	163	0
2	81	85	0
1	456	440	180
0	161	163	180
-1	18	18	180
-2	127	125	180
-3	18	16	180
-4	25	26	180
-5	11	5	0
-6	166	165	0
-7	50	49	0
-8	77	81	0
-9	22	21	0
-10	23	22	180
-11	15	14	0
-12	14	19	180
-13	6	13	180
-14	65	61	180
-15	49	39	0
-16	22	26	0
H	K= 4	L= 0	
13	13	8	180
12	10	15	0
11	24	27	180
10	24	25	180
9	29	32	0
8	24	22	0
7	89	89	180
6	33	36	180
5	27	19	180
4	66	63	180
3	110	110	180
2	55	49	180
1	86	85	0
0	11	13	0
-1	82	79	0
-3	37	38	0
-4	22	17	180
-5	70	65	180
-6	24	29	180
-7	99	91	180
-8	102	90	180
-9	11	5	180
-10	45	46	0
-11	13	11	0
-12	35	24	0
-13	15	21	0
-14	21	23	0
H	K= 5	L= 0	
11	15	2	0
10	22	24	0
9	17	14	180
8	22	22	180
7	53	63	180
6	112	108	180
5	76	79	0
4	22	1	180
3	38	39	180
2	102	101	0
1	34	35	180
0	89	80	0
-1	20	23	180
-2	54	54	180
-3	16	5	180
-4	20	25	180
-5	21	18	0
-6	80	76	180
-7	25	23	180
-8	50	43	180
-9	36	33	180
-10	61	51	0
-11	14	18	180
-12	64	54	180
-13	10	1	0
-14	11	2	0
H	K= 6	L= 0	
9	17	8	0
8	49	46	0
5	64	60	0
4	18	21	0
2	114	100	180
1	26	22	180
0	67	65	180
-1	53	51	180
-2	55	45	0
-4	8	7	0
-5	28	27	180
-6	6	9	0
-7	27	24	0
-9	8	5	0
H	K= 7	L= 0	
5	10	10	0
3	21	22	0
2	15	17	0
1	15	5	0
-1	31	43	0
-2	4	3	0
-3	13	4	0
-4	25	27	180
-5	50	60	180
-6	27	31	0
-7	54	58	0
-8	24	27	180
H	K= 0	L= 1	
16	49	51	209
15	30	35	177
14	32	26	113
13	29	29	161
12	53	53	90
11	41	36	247
10	47	41	157
9	57	56	55
8	62	59	263
7	137	137	91
6	125	122	315
5	94	97	336
4	330	334	43
3	194	195	165
2	81	92	279
H	K= 1	L= 1	
16	22	26	97
15	49	50	192
14	69	65	315
13	177	176	46
12	141	149	104
11	49	51	297
10	71	71	28
9	144	147	203
8	154	157	170
7	148	147	61
6	219	224	254
5	143	144	201
4	43	52	97
3	144	145	13
-1	274	287	334
-2	818	845	69
-3	787	817	156
-4	664	681	267
-5	278	276	359
-6	84	78	180
-7	27	21	154
-8	141	129	357
-9	234	216	275
-10	123	111	186
-11	16	13	76
-12	15	15	148
-13	9	17	193
-14	16	18	208
-15	20	18	109
-16	27	24	254
H	K= 2	L= 1	
14	35	32	255
13	22	25	74
12	62	62	80
11	127	128	161
10	66	64	293
9	107	113	344
8	111	107	58
7	139	137	58
6	211	199	39
5	173	166	287
4	173	156	175
3	280	269	119
2	194	193	235
1	123	124	75
0	253	258	171
-1	151	145	222
-2	177	170	76
-3	79	70	346
-4	95	96	223
-5	184	181	323
-6	152	147	21
-7	207	189	120
-8	53	52	198
-9	57	51	108
-10	29	19	275
-11	54	51	102
-12	139	134	49
-13	23	22	0
-14	27	24	83
-15	17	15	4
-16	17	9	253
H	K= 3	L= 1	
14	36	29	242
13	21	8	180
12	54	54	258
11	89	87	302
10	46	40	175
9	41	33	201
8	30	16	270
7	44	30	151
6	137	128	133
4	56	45	3
3	64	60	6
0	39	36	30
-3	34	28	74
-7	36	25	338
-8	34	15	129
-13	7	9	213
-15	47	32	223
-16	49	37	354
H	K= 4	L= 1	
13	34	25	312
12	33	16	0
10	33	21	234
8	54	53	3
7	62	50	322
5	104	100	338
4	58	53	139
3	76	66	283
2	127	121	249
1	78	70	161
0	177	162	194
-1	167	151	227
-2	159	148	299
-3	73	64	146
-4	40	36	106
-6	134	127	68
-7	110	103	3
-8	21	7	333
-9	92	82	111
-10	45	46	59
-12	25	14	50
-13	23	18	42
-14	14	8	122
H	K= 5	L= 1	
11	19	22	291
10	33	31	214
9	9	17	186
8	45	47	285
7	44	39	287
6	82	76	234
5	107	97	206
4	48	46	342
3	3	12	137
2	78	75	66
1	96	90	9
0	67	74	25
-1	96	91	35
-2	54	51	148
-3	67	61	61
-4	10	15	221
-5	48	48	212
-6	6	14	180
-7	32	36	245
-8	19	32	254
-9	45	40	211
-10	9	7	241
-11	48	36	23
-13	19	14	166
H	K= 6	L= 1	
7	9	0	0
6	24	25	279
5	25	24	291
4	52	48	256
3	40	32	45
2	25	15	90
1	104	86	237
0	25	19	295
-1	95	81	208
-2	59	48	163
-3	65	59	55
-4	111	96	304
-5	34	29	257
-6	17	13	101
-7	27	25	321
-8	17	15	212
-9	12	10	310
-10	5	11	90
H	K= 7	L= 1	
4	23	20	255
3	20	27	68
1	12	14	223
-1	24	31	321
-2	13	16	86
-3	19	21	0
-4	32	36	0
-5	40	38	224
-6	43	47	187
-7	28	28	75
H	K= 0	L= 2	
15	40	39	4
14	36	34	51
13	41	41	297
12	20	21	219
11	134	128	124
10	114	113	31
9	13	7	59
8	139	133	104
7	226	222	135
6	193	183	271
5	287	284	11
4	304	312	83
3	262	266	314
2	241	249	285
1	219	258	303
H	K= 1	L= 2	
16	15	19	125
15	10	13	123
14	38	50	197
13	53	62	311
12	15	20	261
11	33	33	272
10	8	12	338
9	119	118	311
8	186	192	284
7	132	135	181
6	39	32	26
5	20	25	90
4	125	121	66
3	135	138	62
-2	270	278	8
-3	213	216	116
-4	155	152	199
-5	151	142	263
-6	43	42	205
-7	152	147	297
-8	119	120	142
-9	152	142	358
-10	82	79	323
-11	22	24	0
-12	83	81	329
-13	6	7	237
-14	60	55	325
-15	11	11	0
-16	12	15	125
H	K= 2	L= 2	
15	17	15	154
14	17	23	244
13	33	36	145
12	68	73	62
11	152	158	112
10	180	197	183
9	99	100	281
8	156	159	77
7	41	44	182
6	134	132	335
5	87	78	38
4	95	94	242
3	183	181	352
2	110	108	255
1	90	90	213
-1	155	163	242
-2	88	93	147
-3	65	62	76
-4	59	61	50
-5	223	212	235
-6	451	434	340
-7	337	327	54
-8	87	83	140
-9	72	69	302
-10	36	33	102
-11	13	16	168
-12	46	43	99
-13	8	5	280
-14	27	26	172
-15	8	2	90
H	K= 3	L= 2	
14	9	17	212
13	58	79	208
11	37	52	3
10	60	71	213
9	40	42	270
8	143	158	336
7	128	128	76
6	51	51	152
5	140	137	208
4	63	60	154
3	101	90	192
2	75	72	77
1	49	50	193
0	91	86	156
-1	144	143	58
-2	200	193	160
-3	196	185	28
-4	149	137	337
-5	190	184	214
-6	48	34	162
-7	61	54	0
-8	54	46	142
-9	92	88	211
-10	92	85	295
-11	53	47	26
-12	14	13	46
-13	16	16	35
-14	18	13	80
-15	25	20	157
H	K= 4	L= 2	
13	15	17	134
12	18	20	30
11	20	26	34
10	12	15	302
9	20	23	227
8	131	146	153
7	41	45	210
6	67	64	165
5	69	68	126
4	55	50	252
3	49	52	267
2	111	110	320
1	69	73	161
0	81	72	56
-1	86	84	216
-2	81	78	224
-3	66	66	32
-4	55	54	100
-5	35	33	201
-6	44	47	153
-7	68	60	113
-8	21	23	344
-9	28	32	315
-10	12	18	254
-11	37	35	270
-12	30	33	213
-13	16	14	134
-14	13	13	39
H	K= 5	L= 2	
11	11	12	328
10	9	7	90
9	15	14	206
8	25	26	323
7	31	33	162
6	16	26	90
5	65	74	6
4	51	52	178
3	24	22	253
2	83	90	198
1	84	87	130
0	115	117	27
-1	89	98	286
-2	101	104	220
-3	43	40	355
-4	31	24	9
-5	85	88	170
-6	40	47	199
-7	16	17	165
-8	31	38	154
-9	36	41	134
-11	15	21	180
-13	13	8	17
H	K= 6	L= 2	
8	23	24	302
7	16	24	230
6	21	18	9
5	20	14	263
4	13	14	149
3	25	26	349
2	22	24	62
1	54	60	118
0	27	31	65
-1	29	28	341
-2	61	70	224
-3	77	96	156
-4	33	39	77
-5	36	47	303
-6	5	23	162
-7	31	42	327
-8	10	11	270
-9	10	3	90
-10	13	15	281
H	K= 7	L= 2	
3	11	10	343
2	11	15	282
1	15	15	216
0	21	33	195
-1	22	34	263
-2	15	19	45
-3	16	13	104
-4	16	22	325
-5	15	17	70
-6	13	20	333
H	K= 0	L= 3	
16	9	3	20
15	9	5	335
14	48	43	61
13	44	44	80
12	71	71	31
11	79	74	187
10	74	73	136
9	105	107	106
8	95	98	192
7	51	53	60
6	188	180	216
5	165	160	286
4	192	185	30
3	206	209	302
2	170	177	3
H	K= 1	L= 3	
15	21	26	68
14	6	11	159
13	22	15	56
12	37	40	142
10	65	64	33
9	41	39	132
8	47	45	10
7	99	100	101
6	45	39	90
5	50	49	216
4	107	101	346
3	293	287	78
2	333	332	159
1	102	103	267
0	248	256	31
-1	110	115	352
-2	71	72	31
-3	129	127	9
-4	59	62	270
-5	94	89	339
-6	118	112	205
-7	144	133	226
-8	66	61	203
-9	54	44	144
-10	32	32	270
-11	42	42	149
-12	62	64	75
-13	55	55	154
-14	32	29	347
-15	57	55	1
-16	20	17	163
H	K= 2	L= 3	
15	49	50	110
14	27	34	335
13	12	4	315
12	24	24	60
11	67	70	350
10	46	47	77
9	58	62	281
8	59	58	224
7	37	37	294
6	14	13	106
5	61	56	118
4	80	80	243
3	158	149	103
2	79	80	117
1	256	247	134
0	279	273	50
-1	242	232	298
-2	133	135	133
-3	265	256	122
-4	29	33	53
-5	98	92	169
-6	85	79	268
-7	126	117	10
-8	68	64	73
-9	47	43	8
-10	9	12	82
-11	40	40	281
-12	35	31	65
-13	24	23	341
-14	16	17	279
-15	16	16	21
-16	20	25	285
H	K= 3	L= 3	
14	13	18	281
13	28	26	270
12	51	56	239
11	78	77	137
10	30	32	146
9	106	101	163
8	49	49	311
7	168	169	7
6	213	207	88
5	93	89	230
4	55	52	67
3	108	104	68
2	163	155	250
1	50	47	38
0	32	27	207
-1	93	89	302
-2	83	83	301
-3	31	34	14
-4	119	112	66
-5	67	61	15
-6	71	66	10
-7	35	30	314
-8	74	75	65
-9	224	218	136
-10	126	119	196
-11	49	42	11
-12	29	30	82
-13	33	31	197
-14	21	22	102
-15	11	9	286
H	K= 4	L= 3	
12	9	7	75
11	41	40	287
10	14	10	0
9	54	52	73
8	68	66	296
7	52	47	302
6	47	43	25
5	202	189	177
4	85	82	150
3	195	187	355
2	93	87	294
1	105	103	159
0	88	88	74
-1	47	44	180
-2	93	93	173
-3	64	65	108
-4	41	44	195
-5	18	16	169
-6	72	78	96
-7	49	55	320
-8	17	11	337
-9	40	53	45
-10	13	13	309
-11	37	39	356
-12	84	105	348
-13	30	38	203
-14	44	62	162
H	K= 5	L= 3	
10	14	25	180
9	12	16	77
8	48	52	207
7	12	15	148
6	28	35	239
5	55	55	282
4	28	35	54
3	33	41	349
2	126	131	320
1	94	95	249
0	97	99	130
-1	69	78	41
-2	60	61	287
-3	18	20	84
-4	68	73	340
-5	38	45	118
-6	19	30	103
-7	37	37	240
-8	16	18	110
-10	16	17	161
-11	8	10	57
-12	6	13	180
H	K= 6	L= 3	
7	24	19	287
6	12	12	324
5	15	10	225
4	16	27	213
3	19	23	128
2	36	45	180
1	12	14	126
0	31	33	46
-1	11	15	270
-2	18	18	97
-3	32	39	309
-4	33	43	248
-6	22	36	197
-7	18	29	191
-8	20	39	330
-9	8	8	0
-10	6	5	180
H	K= 7	L= 3	
2	14	26	326
1	11	15	244
-2	8	18	256
-3	3	10	46
-4	9	12	341
-5	7	15	336
H	K= 0	L= 4	
15	10	9	62
14	16	25	77
13	17	21	270
12	42	52	333
11	79	86	16
10	27	32	42
9	79	75	25
8	32	26	117
7	54	51	310
6	52	47	57
5	86	87	174
4	56	59	118
3	63	59	313
2	102	92	285
1	18	29	141
H	K= 1	L= 4	
15	22	25	50
12	22	22	177
11	104	101	189
10	49	44	202
9	97	95	195
8	45	37	274
7	60	65	179
6	34	35	250
5	118	116	359
4	132	129	100
3	430	405	9
2	132	125	346
1	118	127	203
0	154	150	59
-1	58	50	347
-2	61	71	298
-3	51	57	100
-4	31	33	285
-5	49	47	47
-6	48	47	354
-7	33	30	12
-8	52	46	146
-9	19	22	95
-10	50	52	336
-11	28	25	159
-12	47	45	1
-13	25	33	230
-14	42	55	192
-15	18	36	355
H	K= 2	L= 4	
14	4	16	150
13	20	13	53
12	33	38	149
11	62	66	22
10	9	13	0
9	49	47	352
8	40	39	25
7	72	79	136
6	78	76	341
5	95	90	180
4	42	40	183
3	22	19	171
2	59	58	123
1	149	145	163
0	179	167	202
-1	120	111	349
-2	162	149	58
-3	40	41	275
-4	141	136	268
-5	76	71	224
-6	30	23	227
-7	61	60	347
-8	44	45	30
-9	96	94	331
-10	28	32	34
-11	53	49	60
-12	22	24	0
-13	24	18	102
-14	7	7	90
-15	10	13	174
H	K= 3	L= 4	
13	19	23	160
12	31	29	59
11	2	1	0
10	40	40	174
9	57	54	261
8	143	146	178
7	65	67	92
6	157	156	347
5	110	114	265
4	91	94	154
3	33	25	36
2	104	100	283
1	75	73	132
0	50	42	114
-1	65	59	288
-2	68	65	116
-3	109	103	80
-4	27	21	16
-5	93	92	172
-6	56	56	13
-7	21	20	135
-8	76	73	31
-9	86	95	340
-10	137	151	208
-11	54	64	168
-12	44	43	35
-13	35	45	307
-14	14	5	116
H	K= 4	L= 4	
11	12	9	147
10	14	21	64
9	11	13	149
8	20	19	175
7	24	34	90
6	67	66	41
5	41	45	29
4	245	244	189
3	131	131	180
2	119	113	19
1	52	59	198
0	4	19	285
-1	47	51	328
-2	64	62	162
-3	86	91	347
-4	33	28	225
-5	17	24	90
-6	24	27	270
-7	30	32	193
-8	3	8	310
-9	33	36	175
-11	69	82	194
-12	27	26	350
-13	53	81	11
H	K= 5	L= 4	
9	20	25	247
8	11	9	251
7	46	39	196
6	24	27	279
5	7	7	160
4	56	55	106
3	40	38	299
2	69	76	310
1	92	96	64
-1	69	85	215
-2	30	38	192
-3	64	76	185
-4	25	36	128
-5	11	18	25
-7	7	10	142
-8	20	36	120
-9	18	30	8
-11	11	14	90
H	K= 6	L= 4	
6	5	17	96
5	18	35	336
4	14	15	160
3	22	25	21
1	13	23	184
0	16	21	68
-1	9	16	99
-5	18	8	0
-6	9	17	310
-7	24	43	208
-8	21	33	188
H	K= 0	L= 5	
14	27	26	94
13	19	19	118
12	21	23	195
11	48	50	346
10	82	79	78
9	78	76	126
8	4	7	334
7	133	132	106
6	48	55	348
5	140	136	274
4	108	101	181
3	91	91	158
2	76	77	271
1	34	51	242
H	K= 1	L= 5	
14	29	29	36
12	13	18	152
11	23	17	225
9	34	36	72
8	71	78	184
7	40	43	0
6	18	17	262
5	63	66	348
4	57	49	72
3	30	27	125
2	107	103	29
1	85	85	38
0	102	102	350
-1	82	85	220
-2	99	101	183
-3	105	104	139
-4	60	55	196
-5	53	52	81
-6	48	48	203
-7	73	71	208
-8	65	62	26
-9	17	12	0
-10	19	13	126
-11	21	14	24
-12	17	13	61
-13	27	23	345
-14	14	14	157
H	K= 2	L= 5	
13	15	20	19
12	49	46	251
11	67	69	176
10	80	82	73
9	98	101	313
8	85	87	270
7	88	97	143
6	61	57	36
5	43	40	165
4	83	82	148
3	132	129	71
2	87	83	161
1	79	75	101
0	125	116	92
-1	106	103	276
-2	83	84	56
-3	73	69	18
-4	37	31	64
-5	154	143	41
-6	187	176	302
-7	139	132	207
-8	137	130	127
-9	71	61	39
-10	44	38	259
-11	50	45	177
-12	19	21	45
-13	16	12	205
H	K= 3	L= 5	
12	9	11	3
11	43	34	94
10	21	14	90
9	69	65	26
8	52	48	305
7	93	89	210
6	131	129	102
5	45	37	12
4	43	40	321
3	42	42	55
2	60	55	255
1	75	73	111
0	50	47	320
-1	103	96	216
-2	43	30	336
-3	44	38	340
-4	79	84	135
-5	69	58	229
-6	15	16	47
-7	41	34	36
-8	60	64	140
-9	116	118	63
-10	52	47	13
-11	18	17	211
-12	26	30	107
-13	12	15	180
H	K= 4	L= 5	
10	26	31	170
9	20	19	234
8	46	50	199
7	32	31	60
6	35	38	339
5	29	25	272
4	75	72	60
3	50	47	293
2	52	54	226
1	22	19	241
0	39	42	140
-1	100	104	81
-2	16	20	353
-3	22	21	64
-4	52	50	106
-5	55	59	118
-6	47	46	345
-7	18	30	229
-8	32	35	50
-9	16	25	296
-10	30	32	227
-11	15	16	135
-12	25	31	233
H	K= 5	L= 5	
8	19	22	283
7	10	12	192
6	13	16	315
5	16	17	217
4	24	27	195
3	33	31	185
2	54	52	254
1	76	81	313
0	46	51	60
-1	27	30	169
-2	11	18	320
-3	33	34	329
-4	48	60	219
-5	23	33	121
-6	27	35	66
-7	25	28	302
-8	15	8	155
-10	5	11	15
H	K= 6	L= 5	
4	21	21	0
2	16	15	270
1	16	17	189
0	30	43	49
-1	22	25	134
-2	38	45	214
-3	13	20	290
-4	16	18	44
H	K= 0	L= 6	
13	10	10	90
12	36	35	303
11	26	25	154
10	39	36	308
9	23	25	309
8	4	13	307
7	21	27	200
6	11	12	259
5	83	77	31
4	42	39	87
3	74	82	308
2	32	38	315
1	38	58	119
H	K= 1	L= 6	
13	48	54	60
12	24	31	316
11	67	67	229
10	44	39	131
9	61	61	52
8	64	66	151
7	67	74	186
6	54	58	350
5	12	17	154
4	29	23	291
3	99	95	355
2	31	29	274
1	10	5	270
0	85	96	325
-1	58	60	106
-2	124	120	22
-3	171	178	288
-4	172	169	199
-5	121	117	99
-6	117	114	32
-7	65	60	240
-8	19	19	221
-9	101	98	11
-10	39	35	66
-11	16	16	52
-12	17	21	21
-13	10	11	226
H	K= 2	L= 6	
12	8	20	11
11	41	52	268
10	67	81	203
9	45	46	90
8	45	46	20
7	26	30	188
6	56	64	305
5	36	41	348
4	94	97	92
3	64	62	347
2	74	71	139
1	9	8	49
-1	51	52	148
-2	41	40	234
-3	56	50	158
-4	69	59	262
-5	70	66	148
-6	75	76	35
-7	78	72	318
-8	48	40	251
-9	40	40	313
-10	15	13	65
-11	29	26	105
-12	29	28	321
-13	10	14	341
H	K= 3	L= 6	
11	14	20	118
10	42	40	83
9	24	25	326
8	29	28	140
7	23	23	34
6	33	31	280
5	84	85	186
4	74	70	231
3	103	101	165
1	40	39	309
0	43	48	216
-1	22	15	321
-2	51	68	71
-3	101	112	332
-4	30	35	86
-5	53	63	68
-6	51	58	303
-7	35	33	180
-8	17	9	104
-12	8	5	90
H	K= 4	L= 6	
9	7	13	195
8	13	21	238
7	6	5	46
6	17	22	134
5	9	12	0
3	13	16	148
2	13	16	51
1	37	40	105
0	45	54	284
-1	59	67	207
-2	44	52	141
-3	23	24	26
-4	16	26	294
-5	25	36	170
-6	33	35	173
-7	20	29	273
-8	17	19	31
-9	13	11	147
-10	20	18	196
-11	2	3	213
H	K= 5	L= 6	
5	18	23	265
4	26	35	158
2	5	15	226
1	20	28	235
-1	24	31	74
-3	17	23	170
-4	10	10	144
-6	9	20	167
-7	9	5	235
-8	11	13	300
H	K= 6	L= 6	
0	4	2	90
-2	12	36	168
-3	19	44	215

with the aid of Fig. 5 of the preceding paper (van Soest & Peerdeman, 1970*a*). This figure shows a projection of the structure of aflatoxin $B_1.CHCl_3$ along the *a* axis. Within a period of 36·25 Å, there are two aflatoxin B_1 layers separated by a chloroform layer. The shortening of the *c* axis of the orthorhombic form to a value of 28·35 Å can be explained from the absence of the chloroform layers and a further shortening to a value of 14·04 Å in the case of the monoclinic form can be accounted for by 'removing' one of the two aflatoxin B_1 layers.

In view of this it seems likely that the orientations of the aflatoxin B_1 molecule will be the same in all three structures. This assumption was easily verified by making use of a simple technique. Coordinates of the molecules (calculated from those of the known structure I) were used to calculate the minimum residual functions $R(0YZ)$ and $R(X0Z)$. In other words, the *R* value defined as $\sum||F_o|-|F_c||/\sum|F_o|$ was repeatedly calculated for a number of reflexions when the molecule was systematically moved through the unit cell (*e.g.* van Soest & Peerdeman, 1970*a*). For the orthorhombic modification, 18 strong low-order $0kl$ reflexions and 20 strong low-order $h0l$ reflexions were used. The minimum value of *R* was 0·10 for both functions. In this way, the approximate position of the molecule was determined and further refined by calculating $R(XYZ)$ for a small area with 47 strong low-order *hkl* reflexions. $R(XYZ)$ was 0·10 for the final position. The same procedure was followed for the monoclinic modification. For the space group $P2_1$, only the function $R(0YZ)$ needed to be calculated.

The structures were refined with the aid of an IBM 1800 computer, using a block-diagonal least-squares program. The *R* for the orthorhombic form decreased without complications to a value of 0·053. The number of reflexions used was 1564. Thirty-five atomic positions, the anisotropic temperature factors of the 23 heavy atoms and one scaling factor were varied. During the refinement of the monoclinic form it appeared that the reflexions from $43l$ to $46l$ were systematically calculated too high. As they were measured separately from the others, a second scaling factor was introduced for these reflexions. The final *R* was 0·076 for the 1144 reflexions observed and 0·084 if the 64 zeros were included. The hydrogen atoms were given isotropic temperature factors equal to those of the carbon atoms to which they are bound; these factors were obtained from the refinement. The atomic scattering factors used in these refinements were taken from *International Tables for X-ray Crystallography* (1962). The final structure factors are detailed in Table 1 and the structural parameters in Tables 2 to 4. The arbitrary numbering of the atoms of the molecule is given in Fig. 1.

Table 3. *Final parameters and e.s.d.'s* ($\times 10^4$) *and the isotropic temperature factors* (Å) *for the hydrogen atoms*

Orthorhombic modification

	x/a	*y/b*	*z/c*	*B*
H(1)	6093 (56)	5088 (73)	4987 (14)	2·9
H(2)	5182 (58)	6499 (73)	5368 (14)	2·9
H(3)	4639 (57)	2279 (77)	5281 (14)	2·7
H(4)	3835 (56)	3485 (71)	5700 (14)	2·7
H(5)	2110 (62)	6854 (79)	5715 (15)	4·1
H(6)	917 (63)	9179 (80)	5647 (15)	4·1
H(7)	1379 (63)	8441 (78)	6170 (15)	4·1
H(8)	3620 (57)	6354 (73)	6454 (14)	3·0
H(9)	9869 (60)	7368 (76)	6998 (14)	3·0
H(10)	8450 (59)	−5828 (74)	7203 (15)	3·4
H(11)	9113 (59)	403 (77)	7585 (15)	3·5
H(12)	7666 (61)	8057 (77)	8256 (15)	3·6

Table 2. *Final positional parameters and e.s.d.'s* ($\times 10^5$) *for the non-hydrogen atoms*

	Orthorhombic modification			Monoclinic modification		
	x/a	*y/b*	*z/c*	*x/a*	*y/b*	*z/c*
C(1)	75043 (58)	53704 (69)	55708 (13)	39165 (118)	63859 (117)	−60682 (45)
C(2)	58313 (58)	51418 (66)	53148 (13)	22927 (120)	62432 (119)	−55162 (50)
C(3)	49526 (55)	31993 (64)	55241 (12)	13910 (118)	41548 (119)	−59590 (48)
C(4)	76630 (53)	35499 (62)	58866 (13)	40810 (105)	44003 (110)	−67042 (44)
C(5)	62301 (49)	23397 (59)	58663 (12)	26747 (111)	31506 (107)	−66724 (41)
C(6)	90976 (58)	30920 (68)	61891 (14)	54811 (121)	37870 (125)	−73150 (51)
C(7)	60883 (50)	4999 (58)	61510 (12)	24975 (111)	11687 (102)	−72587 (43)
C(8)	46765 (51)	−8973 (64)	61602 (13)	10794 (110)	−2503 (116)	−72820 (47)
C(9)	74793 (47)	767 (60)	64570 (12)	38432 (110)	5746 (113)	−78751 (44)
C(10)	46459 (52)	−26617 (66)	64451 (13)	10715 (120)	−21867 (114)	−78671 (48)
C(11)	74637 (52)	−16816 (61)	67484 (12)	38441 (111)	−13016 (115)	−84782 (45)
C(12)	60720 (56)	−29825 (62)	67279 (13)	24454 (122)	−26361 (107)	−84383 (46)
C(13)	86793 (55)	−24198 (66)	71231 (13)	50393 (111)	−22523 (118)	−92471 (47)
C(14)	77945 (61)	−44821 (70)	72860 (14)	41316 (131)	−44311 (119)	−95696 (49)
C(15)	18581 (58)	−16057 (83)	58583 (18)	−16650 (120)	−8691 (142)	−66502 (67)
C(16)	86302 (62)	−11502 (68)	75705 (14)	49798 (123)	−11385 (117)	−1522 (41)
C(17)	78521 (61)	−22276 (83)	78990 (14)	42197 (135)	−23665 (131)	−8225 (54)
O(1)	85136 (47)	68025 (57)	55236 (12)	48846 (86)	79474 (81)	−59881 (35)
O(2)	4251 (42)	40052 (57)	62233 (12)	68384 (91)	46433 (99)	−73661 (44)
O(3)	88869 (35)	13244 (44)	64787 (9)	52632 (71)	18494 (76)	−79108 (31)
O(4)	62288 (40)	−46731 (44)	70200 (9)	25719 (89)	−44878 (75)	−90423 (34)
O(5)	33874 (37)	−3649 (37)	58685 (10)	−1792 (80)	4554 (83)	−66853 (37)
O(6)	73564 (44)	−42350 (52)	77662 (9)	36926 (96)	−43860 (87)	−5471 (34)

Table 3 (*cont.*)

Monoclinic modification

	x/a	*y/b*	*z/c*	*B*
H(1)	2880 (117)	6008 (112)	−4821 (53)	3·7
H(2)	1659 (123)	7543 (126)	−5491 (54)	3·7
H(3)	903 (126)	3154 (125)	−5400 (54)	3·7
H(4)	253 (121)	4444 (122)	−6289 (54)	3·7
H(5)	−1169 (137)	7317 (132)	−6305 (56)	4·4
H(6)	−2345 (133)	9946 (125)	−6169 (55)	4·4
H(7)	−2151 (134)	8698 (129)	−7217 (56)	4·4
H(8)	85 (123)	6819 (121)	−7901 (53)	3·7
H(9)	6358 (123)	7742 (123)	−9002 (50)	3·6
H(10)	4946 (123)	−6090 (124)	−9428 (55)	3·8
H(11)	5915 (121)	488 (128)	−115 (59)	3·8
H(12)	3784 (133)	7913 (127)	−1610 (57)	4·2

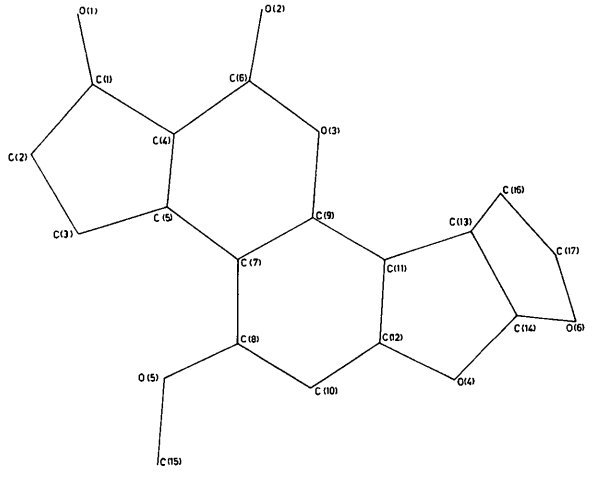

Fig. 1. Arbitrary numbering of the atoms of the aflatoxin B_1 molecule.

Discussion

The bond lengths and the bond angles (not corrected for thermal motion) of the aflatoxin B_1 molecules together with their standard deviations, are listed in Tables 5 and 6. Except for the outer dihydrofuran ring, the structure of the molecule is very similar to that of the aflatoxin B_2 molecule (*cf.* van Soest & Peerdeman, 1970*b*). Twenty of the 23 heavy atoms are approximately lying in one plane, just as the five atoms of the protruding dihydrofuran ring. The least-squares equations of these planes and the distances from the atoms to the planes are given in Table 7. Projections of the structures on the (100) plane are shown in Fig. 2(*a*) and (*b*). Comparison of the projection of the orthorhombic modification [Fig. 2(*a*)] with that of aflatoxin $B_1.CHCl_3$ shows that the first structure can be derived from the second by 'removing' the chloroform layers and by 'moving' the aflatoxin B_1 layers towards one another. The resulting packing of the cyclopentenone rings is rather close: the distances C(2)···O(1) and C(3)···O(1) are 3·24 and 3·32 Å respectively. If we also 'remove' one of the two aflatoxin B_1 layers, the monoclinic structure results [Fig. 2(*b*)] showing a different packing of the cyclopentenone rings. Except for the 3·35 Å of the C(3)···O(1) contact, none of its intermolecular distances is shorter than 3·40 Å.

The mode of packing of the aflatoxin B_1 layer has already been described (van Soest & Peerdeman, 1970*a*). It is now clear that this layer occurs in all three structures. It is characterized by strings of coplanar molecules in the directions [110] and [$\bar{1}$10]. The molecules within a string are coupled by an interac-

Table 4(*a*). *Final thermal parameters and e.s.d.'s* ($\times 10^5$) *for the non-hydrogen atoms*

Orthorhombic modification

The anisotropic temperature factor is defined as

$$\exp\left[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)\right].$$

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	1809 (80)	2171 (112)	104 (5)	−243 (94)	24 (18)	78 (21)
C(2)	1915 (82)	1816 (103)	98 (4)	−269 (91)	−44 (17)	73 (19)
C(3)	1655 (76)	1913 (106)	88 (4)	−170 (86)	−55 (17)	13 (19)
C(4)	1508 (72)	1864 (98)	90 (4)	−171 (78)	−3 (17)	12 (19)
C(5)	1210 (63)	1706 (93)	91 (4)	−47 (73)	32 (15)	−18 (18)
C(6)	1630 (78)	2103 (111)	129 (5)	−327 (90)	−11 (19)	84 (22)
C(7)	1355 (66)	1533 (89)	89 (4)	−190 (73)	31 (15)	31 (17)
C(8)	1342 (69)	2028 (126)	97 (4)	−302 (80)	−23 (16)	−21 (20)
C(9)	1080 (56)	1728 (93)	88 (4)	−30 (71)	17 (14)	−20 (18)
C(10)	1469 (72)	1971 (105)	105 (4)	−613 (83)	16 (16)	−0 (20)
C(11)	1335 (67)	1748 (96)	91 (4)	−46 (78)	−23 (16)	19 (18)
C(12)	1685 (77)	1684 (97)	93 (4)	−289 (84)	−6 (17)	69 (18)
C(13)	1501 (72)	2126 (110)	108 (4)	−136 (86)	1 (17)	122 (21)
C(14)	1932 (89)	2151 (116)	115 (5)	79 (100)	−29 (19)	68 (22)
C(15)	1438 (81)	3181 (150)	186 (7)	−763 (101)	−98 (22)	78 (30)
C(16)	1954 (92)	2262 (117)	116 (5)	−164 (98)	−111 (20)	82 (22)
C(17)	1889 (89)	3325 (150)	114 (5)	−33 (112)	−79 (19)	4 (26)
O(1)	2364 (74)	3468 (112)	205 (5)	−1382 (87)	−169 (18)	422 (21)
O(2)	1830 (64)	3600 (114)	227 (5)	−1493 (78)	−223 (17)	407 (23)
O(3)	1249 (47)	2114 (73)	128 (4)	−372 (55)	−56 (12)	118 (14)
O(4)	2132 (61)	1932 (75)	125 (4)	−466 (67)	−85 (14)	144 (15)
O(5)	1534 (53)	2494 (84)	160 (4)	−750 (63)	−149 (14)	154 (18)
O(6)	2343 (68)	3076 (96)	100 (3)	−617 (80)	11 (14)	114 (16)

tion between the methyl group and the carbonyl oxygen atoms O(1) and O(2), as is indicated by the short intermolecular distances of 2·97 and 3·18 Å of the orthorhombic modification and 3·00 and 3·10 Å of the monoclinic modification (see Fig. 2). Sutor (1963) has reported a number of crystal structures containing

Table 4(*b*). *Final thermal parameters and e.s.d.'s* ($\times 10^4$) *for the non-hydrogen atoms*

Monoclinic modification

The anisotropic temperature factor is defined as

$$\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)].$$

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	182 (18)	292 (21)	39 (3)	−13 (17)	−15 (6)	−6 (6)
C(2)	163 (18)	299 (22)	51 (3)	−36 (17)	13 (7)	−15 (7)
C(3)	159 (18)	291 (21)	47 (3)	−39 (16)	26 (7)	−19 (7)
C(4)	124 (16)	262 (19)	38 (3)	−30 (14)	−3 (6)	−10 (6)
C(5)	164 (17)	275 (19)	29 (3)	−14 (13)	−6 (6)	3 (6)
C(6)	174 (19)	329 (23)	49 (4)	−39 (18)	−0 (7)	−18 (8)
C(7)	143 (16)	225 (17)	35 (3)	−21 (14)	−5 (6)	−1 (6)
C(8)	137 (17)	279 (20)	44 (3)	−48 (15)	−8 (6)	10 (7)
C(9)	123 (16)	287 (19)	39 (3)	−27 (15)	−6 (6)	16 (6)
C(10)	178 (19)	247 (19)	48 (3)	−44 (15)	−1 (7)	−9 (7)
C(11)	132 (16)	286 (19)	40 (3)	−23 (15)	−5 (6)	−6 (7)
C(12)	200 (19)	232 (18)	43 (3)	−26 (16)	−3 (7)	−9 (6)
C(13)	147 (18)	306 (21)	45 (3)	−1 (17)	2 (7)	−13 (7)
C(14)	256 (23)	262 (21)	46 (3)	−1 (18)	3 (8)	−2 (7)
C(15)	101 (19)	395 (28)	94 (6)	−97 (19)	17 (9)	−14 (11)
C(16)	201 (20)	297 (21)	46 (4)	16 (19)	19 (7)	−3 (7)
C(17)	258 (25)	322 (24)	53 (4)	21 (20)	15 (8)	9 (8)
O(1)	213 (14)	304 (15)	53 (3)	−65 (13)	−1 (5)	−22 (5)
O(2)	185 (14)	411 (20)	88 (4)	−102 (14)	36 (6)	−64 (7)
O(3)	135 (12)	302 (14)	43 (2)	−37 (10)	4 (4)	−17 (5)
O(4)	252 (14)	245 (14)	57 (3)	−49 (12)	22 (6)	−22 (5)
O(5)	147 (12)	311 (15)	70 (3)	−70 (12)	33 (5)	−28 (5)
O(6)	273 (15)	351 (17)	45 (3)	−47 (14)	−3 (6)	−13 (5)

Table 5. *Bond lengths and e.s.d.'s* (Å) *of the aflatoxin* B_1 *molecules*

	Orthorhombic	Monoclinic
C–C bonds		
sp^3–sp^3		
C(2)—C(3)	1·534 (6)	1·554 (11)
C(13)–C(14)	1·554 (6)	1·559 (11)
sp^2–sp^3		
C(1)—C(2)	1·505 (6)	1·510 (12)
C(3)—C(5)	1·497 (5)	1·517 (11)
C(11)–C(13)	1·502 (5)	1·511 (11)
C(13)–C(16)	1·504 (6)	1·508 (9)
sp^2–sp^2		
C(1)—C(4)	1·469 (6)	1·453 (9)
C(4)—C(6)	1·444 (6)	1·431 (11)
C(5)—C(7)	1·426 (5)	1·417 (9)
C=C bonds		
C(4)—C(5)	1·363 (6)	1·362 (11)
C(16)–C(17)	1·307 (6)	1·298 (12)
C···C bonds		
C(7)—C(8)	1·419 (6)	1·427 (11)
C(7)—C(9)	1·419 (5)	1·400 (11)
C(8)—C(10)	1·383 (6)	1·386 (10)
C(9)—C(11)	1·391 (5)	1·369 (9)
C(10)–C(12)	1·390 (6)	1·365 (12)
C(11)–C(12)	1·370 (6)	1·389 (12)
C=O bonds		
C(1)—O(1)	1·214 (6)	1·233 (10)
C(6)—O(2)	1·195 (6)	1·206 (11)
–C–O bonds		
C(14)–O(4)	1·445 (5)	1·436 (12)
C(14)–O(6)	1·413 (5)	1·419 (8)
C(15)–O(5)	1·435 (6)	1·441 (11)
=C–O bonds		
C(6)—O(3)	1·402 (5)	1·405 (9)
C(9)—O(3)	1·360 (5)	1·385 (9)
C(8)—O(5)	1·349 (5)	1·347 (10)
C(12)–O(4)	1·363 (5)	1·362 (8)
C(17)–O(6)	1·387 (6)	1·412 (10)
C–H bonds		
C(2)—H(1)	0·95 (4)	1·1 (1)
C(2)—H(2)	1·01 (5)	1·0 (1)
C(3)—H(3)	0·94 (4)	1·1 (1)
C(3)—H(4)	1·02 (4)	1·0 (1)
C(10)–H(8)	1·02 (5)	1·0 (1)
C(13)–H(9)	1·01 (5)	1·1 (1)
C(14)–H(10)	1·03 (5)	1·3 (1)
C(15)–H(5)	1·07 (5)	1·3 (1)
C(15)–H(6)	1·08 (5)	1·0 (1)
C(15)–H(7)	0·96 (5)	0·9 (1)
C(16)–H(11)	1·06 (5)	1·3 (1)
C(17)–H(12)	1·04 (4)	1·1 (1)

short CH···O contacts; these interactions would be due to hydrogen bonding.

Table 6. *Bond angles and e.s.d.'s of the aflatoxin* B_1 *molecules*

	Orthorhombic	Monoclinic
C(2)—C(1)—O(1)	125·9 (4)°	124·8 (7)°
C(4)—C(1)—O(1)	127·2 (4)	127·6 (7)
C(2)—C(1)—C(4)	106·9 (4)	107·6 (7)
C(1)—C(2)—C(3)	106·4 (3)	106·1 (7)
C(2)—C(3)—C(5)	104·2 (3)	103·1 (7)
C(1)—C(4)—C(5)	110·5 (3)	110·9 (7)
C(1)—C(4)—C(6)	125·9 (4)	126·6 (7)
C(5)—C(4)—C(6)	123·5 (3)	122·5 (7)
C(3)—C(5)—C(4)	111·8 (3)	111·9 (7)
C(3)—C(5)—C(7)	127·9 (3)	126·3 (7)
C(4)—C(6)—O(2)	128·9 (4)	129·5 (7)
C(4)—C(6)—O(3)	114·7 (4)	114·9 (7)
O(2)—C(6)—O(3)	116·4 (4)	115·5 (7)
C(5)—C(7)—C(8)	125·8 (3)	126·1 (7)
C(5)—C(7)—C(9)	116·2 (3)	116·3 (7)
C(8)—C(7)—C(9)	117·9 (3)	117·6 (7)
C(7)—C(8)—O(5)	114·5 (3)	114·1 (7)
C(7)—C(8)—C(10)	122·2 (3)	120·9 (7)
C(10)—C(8)—O(5)	123·3 (4)	125·0 (7)
C(8)—O(5)—C(15)	120·0 (3)	118·4 (7)
C(6)—O(3)—C(9)	122·5 (3)	122·6 (7)
C(7)—C(9)—O(3)	122·7 (3)	121·9 (7)
C(7)—C(9)—C(11)	120·6 (3)	122·5 (8)
O(3)—C(9)—C(11)	116·7 (3)	115·6 (7)
C(8)—C(10)—C(12)	116·2 (4)	117·3 (7)
C(9)—C(11)—C(12)	117·9 (3)	116·6 (8)
C(9)—C(11)—C(13)	131·8 (3)	133·5 (7)
C(12)—C(11)—C(13)	110·2 (3)	109·8 (6)
C(10)—C(12)—C(11)	125·1 (3)	125·0 (7)
C(10)—C(12)—O(4)	122·6 (3)	122·3 (8)
C(11)—C(12)—O(4)	112·3 (3)	112·7 (8)
C(11)—C(13)—C(14)	101·0 (3)	100·4 (7)
C(11)—C(13)—C(16)	114·3 (2)	113·8 (7)
C(14)—C(13)—C(16)	101·0 (3)	101·5 (6)
C(13)—C(14)—O(4)	107·1 (3)	108·2 (6)
C(13)—C(14)—O(6)	107·5 (3)	107·0 (6)
O(4)—C(14)—O(6)	107·8 (3)	106·8 (8)
C(13)—C(16)—C(17)	109·3 (4)	109·9 (7)
C(16)—C(17)—O(6)	114·8 (4)	114·3 (7)
C(14)—O(6)—C(17)	107·2 (3)	107·3 (6)
C(12)—O(4)—C(14)	109·1 (3)	108·6 (7)
C(1)—C(2)—H(1)	107 (3)	96 (7)
C(1)—C(2)—H(2)	106 (3)	112 (7)
C(3)—C(2)—H(1)	116 (3)	112 (7)
C(3)—C(2)—H(2)	114 (3)	116 (7)
H(1)—C(2)—H(2)	106 (4)	112 (7)
C(2)—C(3)—H(3)	110 (3)	112 (7)
C(2)—C(3)—H(4)	115 (3)	114 (7)
C(5)—C(3)—H(3)	115 (3)	118 (7)
C(5)—C(3)—H(4)	109 (3)	111 (7)
H(3)—C(3)—H(4)	104 (4)	98 (7)
O(5)—C(15)—H(5)	111 (3)	106 (7)
O(5)—C(15)—H(6)	109 (3)	103 (7)
O(5)—C(15)—H(7)	107 (3)	116 (7)
H(5)—C(15)—H(6)	110 (4)	108 (7)
H(5)—C(15)—H(7)	116 (4)	105 (7)
H(6)—C(15)—H(7)	103 (4)	118 (7)
C(8)—C(10)—H(8)	116 (3)	122 (7)
C(12)—C(10)—H(8)	122 (3)	121 (7)
C(13)—C(14)—H(10)	114 (3)	115 (7)
O(4)—C(14)—H(10)	104 (3)	107 (7)
O(6)—C(14)—H(10)	116 (3)	112 (7)
C(11)—C(13)—H(9)	112 (3)	113 (7)
C(14)—C(13)—H(9)	114 (3)	120 (7)
C(16)—C(13)—H(9)	113 (3)	108 (7)
C(13)—C(16)—H(11)	122 (3)	113 (7)
C(17)—C(16)—H(11)	129 (3)	136 (7)
C(16)—C(17)—H(12)	132 (3)	133 (7)
O(6)—C(17)—H(12)	113 (3)	113 (7)

Table 6 (*cont.*)

Thermal motion

The atomic vibration ellipsoids of the two molecules have been analysed in terms of rigid-body tensors of translation (**T**), libration (**L**) and screw motion (**S**) (Schomaker & Trueblood, 1968). All 23 heavy atoms were considered and the results of the analysis are given in Tables 8(*a*) and 8(*b*).

Table 7. *Equations of the least-squares planes and the distances from the atoms to these planes*

Orthorhombic modification

$-0{\cdot}4219X+0{\cdot}5451Y+0{\cdot}7245Z-10{\cdot}8087=0$

C(1)	+0·016 Å	C(11)	+0·002 Å
C(2)	−0·036	C(12)	−0·031
C(3)	+0·011	C(13)	+0·114
C(4)	−0·019	C(14)	+0·026
C(5)	−0·007	C(15)	+0·053
C(6)	−0·031	O(1)	+0·082
C(7)	−0·014	O(2)	−0·083
C(8)	−0·013	O(3)	+0·020
C(9)	+0·008	O(4)	−0·069
C(10)	−0·029	O(5)	−0·001

$-0{\cdot}8862X+0{\cdot}3716Y-0{\cdot}2768Z+12{\cdot}1932=0$

C(13)	+0·005	C(17)	+0·015
C(14)	+0·003	O(6)	−0·011
C(16)	−0·012		

Angle between the two planes: 112·1°

Monoclinic modification

$+0{\cdot}4208X-0{\cdot}5550Y+0{\cdot}7176Z+7{\cdot}4222=0$

C(1)	−0·032 Å	C(11)	−0·012 Å
C(2)	+0·072	C(12)	+0·024
C(3)	+0·012	C(13)	−0·117
C(4)	+0·020	C(14)	−0·018
C(5)	+0·015	C(15)	−0·023
C(6)	+0·038	O(1)	−0·161
C(7)	+0·006	O(2)	+0·140
C(8)	−0·004	O(3)	−0·011
C(9)	−0·007	O(4)	+0·051
C(10)	+0·028	O(5)	−0·022

$+0{\cdot}8803X-0{\cdot}3815Y-0{\cdot}2820Z-7{\cdot}1915=0$

C(13)	+0·002	C(17)	−0·008
C(14)	−0·006	O(6)	+0·009
C(16)	+0·004		

112·3°

Table 8(*a*). *Rigid-body thermal parameters*

Orthorhombic modification

$$\mathbf{T} = \begin{pmatrix} 360 & -39 & 26 \\ & 337 & -17 \\ & & 331 \end{pmatrix} \times 10^{-4}\ \text{Å}^2$$

$$\sigma(\mathbf{T}) = \begin{pmatrix} 16 & 14 & 14 \\ & 15 & 14 \\ & & 15 \end{pmatrix} \times 10^{-4}\ \text{Å}^2$$

$$\mathbf{L} = \begin{pmatrix} 52 & -29 & 48 \\ & 92 & -62 \\ & & 120 \end{pmatrix} \times 10^{-1}\ (^\circ)^2$$

$$\sigma(\mathbf{L}) = \begin{pmatrix} 6 & 5 & 6 \\ & 8 & 6 \\ & & 8 \end{pmatrix} \times 10^{-1}\ (^\circ)^2$$

Unique origin (Å)*	4·884	0·429	17·699

Principal axes of **I**†

Eigenvalue	Direction cosines (×10⁴)		
1265 Å²	−775	7187	−6910
2738	−8458	−4143	−3360
3671	−5278	5584	6400

Principal axes of **T**‡

Eigenvalue	Direction cosines (×10⁴)		
0·0402 Å²	−7421	5122	−4321
0·0310	6621	4608	−5908
0·0296	−1035	−7246	−6812

Table 8(*a*) (*cont.*)

Principal axes of **L**

Eigenvalue	Direction cosines (×10⁴)		
19·2 (°)²	−3710	5657	−7363
4·5	−3604	−8185	−4472
2·7	−8558	994	5075

R.m.s. difference between 'observed' and calculated U_{ij}: 50×10^{-4} Å².

* This origin symmetrizes **S**.

† Calculated for the unique origin, using atomic weights instead of mass weights.

‡ Calculated after **S** had been symmetrized.

Table 8(*b*). *Rigid-body thermal parameters*

Monoclinic modification

$$\mathbf{T} = \begin{pmatrix} 406 & -52 & -16 \\ & 498 & -38 \\ & & 386 \end{pmatrix} \times 10^{-4}\ \text{Å}^2$$

$$\sigma(\mathbf{T}) = \begin{pmatrix} 19 & 16 & 17 \\ & 17 & 16 \\ & & 17 \end{pmatrix} \times 10^{-4}\ \text{Å}^2$$

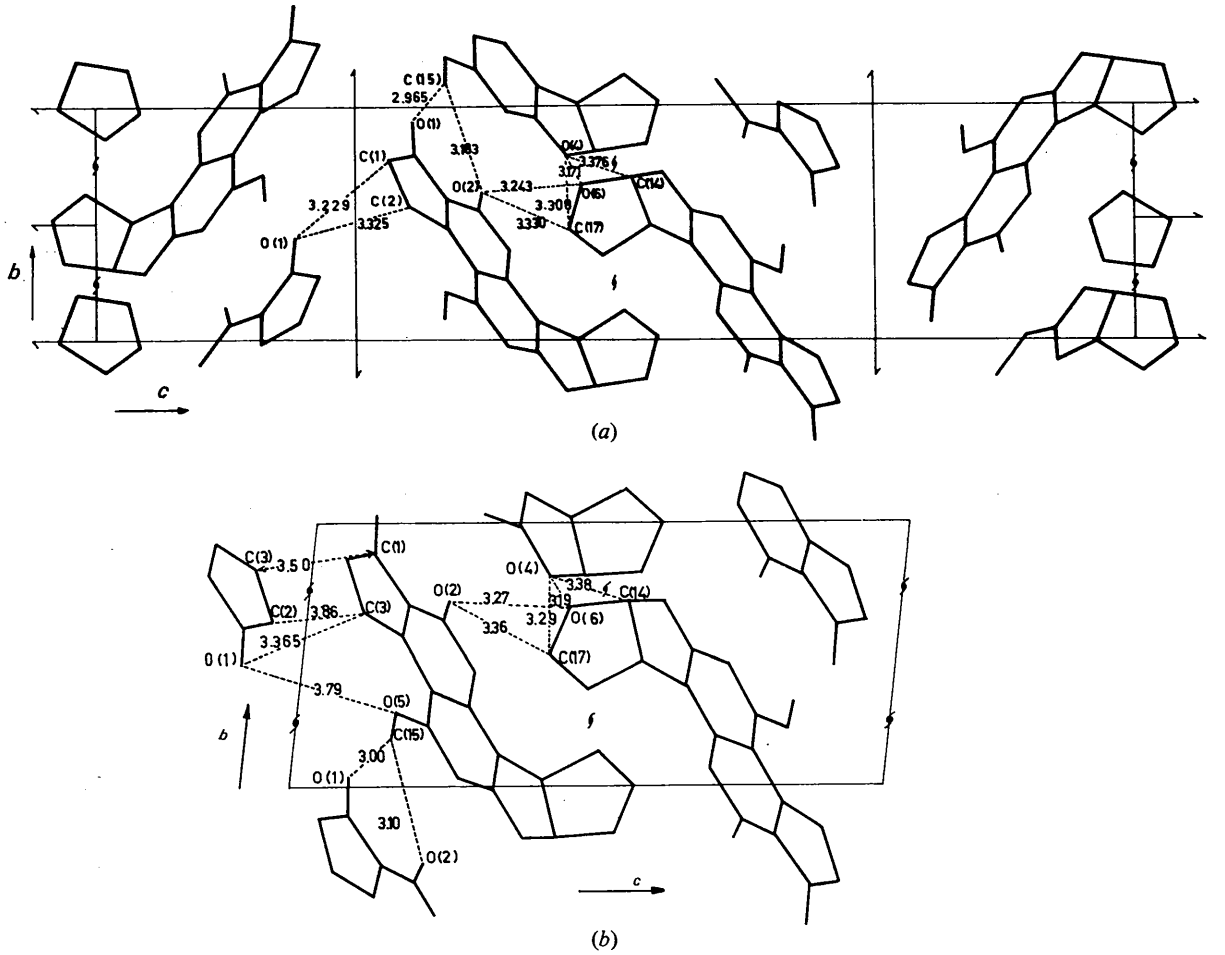

Fig. 2. Projection of the structure of aflatoxin B_1 on the (100) plane: (*a*) orthorhombic modification; (*b*) monoclinic modification.

Table 8(*b*) (*cont.*)

$$\mathbf{L} = \begin{pmatrix} 26 & -17 & -20 \\ & 92 & 49 \\ & & 103 \end{pmatrix} \times 10^{-1}\ (^\circ)^2$$

$$\sigma(\mathbf{L}) = \begin{pmatrix} 6 & 6 & 7 \\ & 9 & 8 \\ & & 10 \end{pmatrix} \times 10^{-1}\ (^\circ)^2$$

Unique origin (Å)*	2·292	2·134	−10·356
Principal axes of **I**†			
Eigenvalue	Direction cosines ($\times 10^4$)		
1217 Å^2	−755	7130	6970
2832	−8591	−4014	3176
3721	5063	5748	6428
Principal axes of **T**‡			
Eigenvalue	Direction cosines ($\times 10^4$)		
0·0524 Å^2	−3560	9137	−1930
0·0405	−6827	−1141	7228
0·0346	6381	3907	6630
Principal axes of **L**			
Eigenvalue	Direction cosines ($\times 10^4$)		
15·2 (°)^2	2037	−6531	−7292
4·8	197	7475	−6638
2·0	9788	1228	1635

R.m.s. difference between 'observed' and calculated U_{ij}: 59×10^{-4} Å^2.

* This origin symmetrizes **S**.

† Calculated for the unique origin, using atomic weights instead of mass weights.

‡ Calculated after **S** had been symmetrized.

The r.m.s. deviation between the thermal parameters obtained by the least-squares refinement and those calculated from the rigid-body tensors is 0·0050 Å^2 for the orthorhombic and 0·0059 Å^2 for the monoclinic modification.

The translation tensors are slightly anisotropic; however, an explanation for the directions of their principal axes could not be found. The libration tensors are clearly anisotropic in both cases: one of the principal axes is always appreciably longer than the other two.

The inertia tensors **I** (the principal axes and their directions with respect to an orthogonal axial system) for the two aflatoxin B_1 molecules were calculated using the unique origins obtained by symmetrizing the screw tensors **S**. The tensors **I** have one principal axis being appreciably shorter than the other two. The angle between the largest principal axis of the libration tensor and the smallest principal axis of the inertia tensor is 19° for the orthorhombic form and 8° for the monoclinic form.

The same anisotropy of the libration tensors has also been observed for the aflatoxin B_2 molecule and for the aflatoxin B_1 molecule of modification I. For both molecules, the axes showing the highest degree of libration are also approximately parallel to the axes, the moment of inertia of which is smallest; the angles between the corresponding axes are 3° and 11° respectively.

The conclusion seems justified that in all four structures, the libration of the aflatoxin molecule is influenced by its moment of inertia.

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