Mg(2) and in addition by K(2). Atom O(3) appears therefore to be locked in, which is reflected in the fact that the amplitude of its thermal motion is the smallest of the three oxygen atoms and that its motion seems to be isotropic within the limits of error. The details of the orientation of the thermal ellipsoids thus are in qualitative agreement with the geometrical arrangements in this crystal structure.

Table 7. $K_2Mg_5Si_{12}O_{30}$, *root-mean-square thermal displacements along principal axes and their orientations relative to a, b and c*

	Axis	Displacement	Angle with axis [100]	[010]	[001]
K(1)	1	0·111 (4) Å	–	–	90°
	2	0·111	–	–	90
	3	0·154 (5)	90°	90°	0
K(2)	1	0·106 (5)	–	–	90
	2	0·106	–	–	90
	3	0·136 (6)	90	90	0
Mg(1)	1	0·077 (5)	–	–	90
	2	0·077	–	–	90
	3	0·119 (5)	90	90	0
Mg(2)	1	0·087 (6)	90	30	90
	2	0·112 (4)	90	90	0
	3	0·116 (5)	0	120	90
Si	1	0·088 (2)	68 (34)	87 (16)	28 (29)
	2	0·090 (2)	157 (32)	64 (5)	67 (33)
	3	0·109 (2)	98 (5)	26 (5)	104 (5)
O(1)	1	0·095 (6)	90	90	0
	2	0·155 (6)	32 (85)	152 (85)	90
	3	0·158 (5)	58 (85)	62 (85)	90
O(2)	1	0·105 (5)	27 (5)	145 (4)	81 (7)
	2	0·132 (4)	78 (8)	91 (8)	166 (8)
	3	0·157 (4)	67 (4)	55 (4)	79 (8)
O(3)	1	0·108 (5)	99 (32)	21 (29)	96 (21)
	2	0·113 (5)	158 (27)	73 (34)	109 (24)
	3	0·121 (4)	110 (24)	78 (17)	20 (23)

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References

BAUR, W. H. (1970). *Trans. Amer. Cryst. Assoc.* **6**, 129.

BAUR, W. H. (1971). *Amer. Miner.* **56**. 1573.

BAUR, W. H. & KHAN, A. A. (1970). *Acta Cryst.* B**26**, 1584.

BROWN, G. E. & GIBBS, G. V. (1969). *Amer. Miner.* **54**, 101.

DODD, R. R., VAN SCHMUS, W. R. & MARVIN, U. B. (1965). *Science*, **149**, 972.

FORBES, W. C. (1972). *Miner. Mag.* In the press.

ITO, T., MORIMOTO, N. & SADANAGA, R. (1952). *Acta Cryst.* **5**, 209.

MIYASHIRO, A. (1956). *Amer. Miner.* **41**, 104.

OLSEN, E. (1967). *Amer. Miner.* **52**, 1519.

OLSEN, E. & BUNCH, T. E. (1970). *Amer. Miner.* **55**, 875.

PASHEVA, Z. P. & TARKHOVA, T. N. (1953). *Dokl. Akad. Nauk SSSR*, **88**, 807.

PLUMIER, R. & TARDIEU, A. (1963). *C. R. Acad. Sci. Paris*, **257**, 3858.

ROEDDER, E. W. (1951). *Amer. J. Sci.* **249**, 81, 774.

SEIFERT, F. & SCHREYER, W. (1969). *Contr. Mineral. Petrol.* **22**, 190.

SMITH, J. V. (1953). *Amer. Miner.* **38**, 643.

ZOLTAI, T. (1960). *Amer. Miner.* **45**, 960.

ZORINA, N. G. & KVITKA, S. S. (1969). *Sov. Phys. Crystallogr.* **13**, 599

Acta Cryst. (1972). B**28**, 272

The Crystal Structures of Polymorphs I and III of Sulphathiazole

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The crystal structure of sulphathiazole II is known. The crystal structures of the other two known crystalline forms of sulphathiazole (*N*′-2-thiazolylsulphanilamide) have now been determined and are reported. The intensities were measured using Mo $K\alpha$ radiation and an automatic diffractometer. The structures were solved by the application of the Karle–Hauptman $\sum_2$ relationship and refinement was done by full-matrix least-squares methods. The main differences between the polymorphs of sulphathiazole lie in the hydrogen bonding and its effects on the arrangement of the molecules in the crystals.

Introduction

In the paper reporting the structure determination of sulphathiazole II (Kruger & Gafner, 1972) crystallographic data for the other two known polymorphs, modifications I and III, were listed. This information is repeated here in Table 1. In order to investigate the structural differences involved in the polymorphism of sulphathiazole, the crystal structures of sulphathiazole I and III have now been determined.

Experimental

The intensity data were collected from roughly cubical crystals with side lengths not exceeding 0·2 mm using a Hilger & Watts four-circle automatic diffractometer. In both cases the intensities were measured using the ω-scan method and Zr-filtered Mo radiation. Only the unique reflexions with $2\theta \leq 40°$ were measured for sulphathiazole I since the proportion of unobservable intensities became too high above this limit. All reflexions with $2\theta \leq 55°$ were measured for sulphathiazole III. Corrections for absorption were not applied as μR was less than 0·05 in both cases.

Determination of the structures

It was not found possible to use the heavy-atom method owing to the presence of two molecules in the asymmetric unit of each crystal. The structures were thus solved by the symbolic addition procedure using the phase determination programs included in the *X-ray* 67 (Stewart, 1967) computing system.

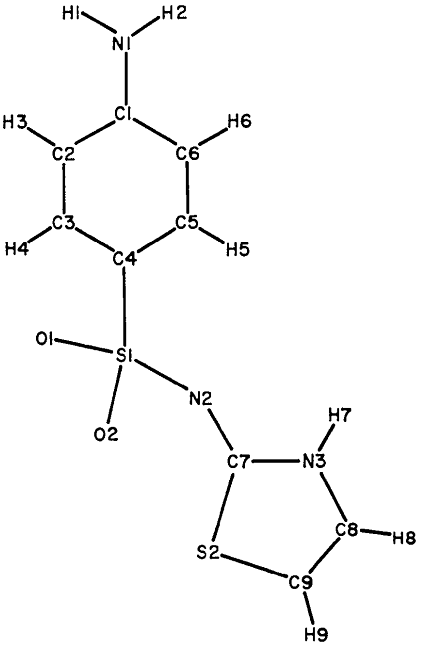

Fig. 1. The numbering of atoms in the sulphathiazole molecule.

In the case of sulphathiazole I, the phases of 173 reflexions with E values greater than 1·5 were determined and the E map calculated from them revealed the positions of the four sulphur atoms in the asymmetric unit. A Fourier synthesis phased on the contributions of the sulphur atoms gave the positions of the other 28 non-hydrogen atoms.

All reflexions with E values greater than 1·4 were used for the phase determination of sulphathiazole III. The phase determination process gave two possible sets of phases for the 362 reflexions. E maps were calculated with both sets. Only one of these could be interpreted and this gave the positions of the 32 non-hydrogen atoms.

The refinement of atomic parameters

Refinement was done by full-matrix least-squares procedures using the program *ORFLS* of Busing, Martin & Levy (1962). The atomic scattering factors used were those given by Hanson, Herman, Lea & Skillman (1964). Only the observed reflexions were used in the refinement of the structures (Dunning & Vand, 1969), that is, all the intensities higher than $2\sigma(I)$ where $\sigma(I)$ is the estimated standard deviation in intensity as determined from counting statistics.

(*a*) *Sulphathiazole* I

Of the 3328 reflexions recorded, 1843 were used in the refinement. After refinement of the positional and anisotropic thermal parameters, a three-dimensional difference Fourier synthesis was calculated. All hydrogen atoms could be found with the exception of the four bonded to amine nitrogen atoms. In subsequent refinement the 14 hydrogen atoms which could be located were included and given the anisotropic thermal parameters of the atoms to which they were bonded. Only their positional parameters were varied.

The most satisfactory method of weighting was found to be a modification of the weighting scheme proposed by Hughes (1941), where

Table 1. *Crystal data for the polymorphs of sulphathiazole*

Polymorph	I	II	III
Melting point (°C)	200–202	200–202	173–175 200–202 or
Transition point (°C)	–	173–175	– 173–175
Habit	elongated rods	hexagonal prisms	hexagonal plates
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	10·554 (5)	8·235 (4)	17·570 (9)
b (Å)	13·220 (7)	8·550 (4)	8·574 (4)
c (Å)	17·050 (8)	15·558 (8)	15·583 (8)
β (°)	108·06 (1)	93·67 (1)	112·93 (1)
Z	8	4	8
D_m (g.cm^{-3})	1·50	1·55	1·57
D_c (g.cm^{-3})	1·499	1·550	1·567

Table 2. *Observed and calculated structure factors on a* × 10 *absolute scale*

(*a*) Sulphathiazole I

-11, K, L			
3	9	116	-121
2	10	117	104
2	8	129	135
2	7	150	-155
1	10	168	151
1	5	110	119
0	8	160	-177
0	2	117	-122
-10, K, L			
7	6	124	123
7	4	128	138
6	10	166	-146
6	6	193	170
6	4	141	149
3	10	109	125
3	8	253	248
3	4	112	-160
1	13	151	-161
1	4	349	-351
1	3	134	-135
0	12	118	138
0	10	302	299
0	6	483	-476
0	4	150	-183
-9, K, L			
7	10	144	-130
7	7	134	-147
7	3	250	246
7	2	119	131
6	11	116	-148
6	5	136	165
5	12	174	161
5	8	219	-234
5	3	125	127
4	11	123	-143
4	10	138	147
4	9	282	-270
4	8	161	170
4	6	176	189
4	5	252	244
4	3	167	155
3	14	142	128
3	12	163	169
3	10	172	-163
3	8	160	-146
3	7	99	-133
3	6	215	-201
3	3	128	-135
3	2	154	170
2	9	160	-159
2	8	104	-89
2	6	145	-117
2	5	176	168
2	3	116	138
2	2	152	-156
1	14	113	110
1	12	150	150
1	11	114	121
1	9	363	352
1	7	298	302
1	6	97	112
1	3	275	-291
1	2	286	-299
1	1	185	-218
0	14	243	216
0	10	116	-128
0	4	129	-117
-8, K, L			
9	10	126	-102
9	8	180	161
9	6	184	190
9	4	126	-113
9	2	175	-171
8	10	125	121
8	8	115	95
8	6	132	-116
8	4	181	-157
7	11	157	-173
7	7	109	137
6	10	164	176
6	7	156	-183
6	4	128	-112
5	14	111	-92
5	12	112	98
5	11	113	-119
5	9	166	-188
5	8	267	-277
5	7	143	163
5	5	112	120
5	4	289	277
5	3	148	143
5	2	512	504
5	1	162	114
4	15	121	-71
4	10	234	-221
4	8	96	-103
4	6	159	-147
4	4	94	-59
3	10	118	-141
3	8	445	-450
3	7	165	-172
3	6	462	-472
3	2	254	263
2	15	134	-121
2	12	134	148
2	11	203	210
2	10	219	-226
2	8	252	-258
2	6	260	253
2	5	101	106
2	4	263	269
2	3	232	254
2	1	106	118
1	13	248	271
1	11	179	151
1	10	106	-107
1	9	279	-283
1	8	197	-208
1	7	251	-244
1	6	110	-110
1	5	111	-106
1	4	182	190
1	2	388	377
1	1	237	247
0	12	100	-129
0	10	422	-435
0	8	545	-527
0	6	280	284
0	4	457	474
-7, K, L			
10	1	176	-183
9	12	168	143
9	10	147	151
9	8	139	-159
9	7	162	154
9	6	134	-160
9	3	220	-230
9	1	221	-241
8	8	137	131
8	6	111	105
8	3	105	83
8	2	147	-173
7	11	253	-246
7	10	250	238
7	9	226	228
7	8	373	375
7	7	286	285
7	5	125	115
7	3	285	-287
7	1	378	-387
6	9	220	232
6	8	161	-184
6	7	172	147
6	6	189	206
6	1	105	73
6	1	145	167
5	16	122	75
5	14	113	-98
5	13	130	-134
5	12	151	-149
5	10	119	-100
5	8	186	183
5	7	352	358
5	5	135	143
5	4	111	-94
5	3	186	-185
5	1	270	-279
4	14	158	172
4	10	102	-103
4	9	257	255
4	8	114	127
4	6	91	-91
4	4	118	-129
4	2	179	-195
3	13	108	84
3	12	329	-321
3	9	120	-145
3	8	429	430
3	7	95	-129
3	6	318	328
3	5	184	191
3	4	345	356
3	3	168	196
3	2	383	380
3	1	112	94
2	15	116	-121
2	14	170	-163
2	12	187	-185
2	9	310	318
2	7	272	256
2	5	461	-467
2	3	214	-223
2	2	90	87
1	13	157	144
1	12	242	-233
1	11	135	119
1	10	195	-191
1	9	216	-246
1	8	221	-219
1	7	543	-549
1	6	122	132
1	5	147	-129
1	3	290	279
1	2	155	159
1	1	523	516
0	16	118	80
0	14	101	-80
0	10	201	196
0	2	197	209
-6, K, L			
11	8	116	-113
11	7	136	-90
11	6	174	-166
11	2	259	254
10	4	202	-207
10	3	110	-80
10	2	142	-136
9	12	120	91
9	11	159	141
9	10	248	256
9	7	125	-132
9	6	352	-361
9	4	109	-105
9	3	117	-130
9	2	272	287
8	12	132	125
8	4	438	445
8	3	130	-172
8	2	189	204
7	15	126	-108
7	9	171	179
7	7	137	-166
7	5	135	-134
7	4	109	-118
7	1	164	-177
6	16	118	-12
6	12	140	154
6	9	124	-137
6	8	282	-282
6	7	172	174
6	3	110	-100
6	2	119	-107
6	1	112	-107
5	17	164	-118
5	15	131	-111
5	11	281	281
5	9	221	215
5	8	318	336
5	6	271	281
5	5	128	-153
5	2	338	-324
4	17	131	-125
4	8	265	282
4	5	82	120
4	4	151	147
4	2	459	450
4	1	173	-162
3	15	113	-125
3	14	111	-141
3	12	311	-293
3	10	325	-323
3	6	485	481
3	5	139	119
3	4	105	66
3	3	575	595
3	2	500	-479
3	1	105	-94
2	18	120	82
2	13	160	184
2	9	156	-171
2	8	340	363
2	7	149	171
2	6	112	-101
2	5	190	191
2	4	674	-688
2	1	119	140
1	17	122	120
1	15	126	129
1	14	109	105
1	11	193	-186
1	10	105	77
1	8	107	108
1	7	137	127
1	6	393	401
1	5	99	99
1	4	108	-109
1	3	429	437
1	2	249	-240
1	1	337	336
0	18	163	-152
0	16	116	-59
0	14	178	-166
0	12	206	-213
0	10	96	99
0	8	685	681
0	6	111	99
0	2	600	612
-5, K, L			
13	4	134	38
13	1	133	-87
12	8	190	-195
12	3	197	-177
11	9	116	72
11	8	126	-85
10	9	105	82
10	6	126	103
10	4	234	265
10	3	227	-227
9	14	131	81
9	10	289	-284
9	6	161	151
9	3	96	91
9	2	110	-160
9	1	202	206
8	15	118	38
8	9	186	187
8	6	349	-347
8	5	192	-204
8	4	186	-186
8	3	125	-152
8	1	108	-100
7	16	120	90
7	14	151	167
7	11	166	136
7	9	209	227
7	8	275	-280
7	7	233	-234
7	5	373	-365
7	4	117	-113
7	2	462	-458
7	1	339	326
6	16	186	154
6	11	151	174
6	10	247	248
6	8	111	128
6	3	156	-143
6	1	197	-211
5	17	128	-70
5	16	237	-222
5	14	122	-137
5	12	118	-119
5	11	203	196
5	10	181	194
5	8	191	199
5	7	147	-136
5	6	111	-153
5	5	100	-101
4	13	205	222
4	12	321	-335
4	10	109	-138
4	8	317	-321
4	7	236	-236
4	6	340	-344
4	5	118	131
4	4	261	-206
4	1	603	-599
3	18	117	58
3	17	151	117
3	16	111	-76
3	14	256	-266
3	13	189	200
3	12	104	74
3	10	301	287
3	9	102	82
3	7	104	96
3	6	237	-244
3	5	237	-227
3	3	121	-143
3	2	542	-555
3	1	440	438
2	15	109	100
2	14	106	-115
2	13	99	149
2	12	193	179
2	10	265	254
2	9	110	127
2	8	214	-193
2	7	213	-193
2	6	402	404
2	4	343	353
2	2	82	-46
2	1	371	-359
1	16	217	-209
1	15	226	241
1	14	327	-340
1	13	232	-251
1	11	502	-497
1	10	156	161
1	9	500	-484
1	8	97	-104
1	7	179	188
1	6	312	303
1	5	603	608
1	4	151	137
1	3	174	-186
1	2	114	119
1	1	714	-736
0	18	127	-102
0	16	168	-179
0	14	196	182
0	12	433	453
0	10	147	-135
0	8	330	-348
0	6	480	-473
0	4	244	227
0	2	256	243
-4, K, L			
12	10	135	80
12	2	107	35
11	10	130	-72
11	6	255	260
11	4	321	334
10	10	117	-116
10	9	162	-190
10	4	100	99
10	3	102	84
10	2	179	157
10	1	224	257
9	13	111	42
9	12	123	101
9	10	264	-261
9	9	106	-107
9	8	122	-97
9	4	373	376
9	2	112	-120
9	1	114	98
8	15	138	-34
8	8	169	150
8	7	102	90
8	6	250	256
8	4	236	-235
8	3	111	134
8	2	428	-444
8	1	104	111
7	16	116	-60
7	15	253	251
7	13	263	257
7	9	298	-312
7	8	155	-167
7	6	351	366
7	5	149	147
7	4	249	259
7	3	159	-169
7	2	185	203
6	17	133	41
6	16	141	-115
6	12	244	-245
6	10	257	-271
6	9	135	155
6	7	223	235
6	6	91	74
6	4	78	-100
6	3	81	101
6	1	289	271
5	17	114	35
5	15	170	148
5	13	137	88
5	10	126	133
5	6	530	-534
5	4	554	-569
5	3	338	-343
5	1	276	-286
4	17	158	142
4	12	135	113
4	11	244	-246
4	10	173	200
4	9	87	-65
4	8	282	292
4	7	382	380
4	6	75	20
4	4	80	-65
4	2	500	-487
4	1	296	-283
3	18	212	-187
3	16	145	-141
3	15	166	-170
3	14	211	-190
3	12	314	349
3	11	192	-190
3	10	510	507
3	9	149	155
3	8	744	753
3	7	214	221
3	6	292	300
3	5	230	219
3	3	627	-628
3	2	168	185
3	1	345	-337
2	18	120	-65
2	17	159	144
2	15	100	76
2	13	319	-318
2	12	144	-137
2	11	165	-149
2	10	90	-89
2	9	106	-88
2	7	196	-173
2	5	513	-507
2	4	221	212
2	3	414	-416
2	2	158	171
2	1	183	169
1	18	136	-78
1	15	230	-245
1	13	294	-290
1	11	124	-119
1	10	213	207
1	9	256	265
1	8	401	389
1	7	720	712
1	6	230	-233
1	5	210	185
1	4	99	-127
1	3	352	-341
1	2	247	-261
1	1	967	-954
0	18	148	94
0	14	99	-35
0	12	148	155
0	10	647	668
0	8	339	325
0	6	1005	-981
0	4	490	495
0	2	114	-81
-3, K, L			
14	8	141	60
14	7	185	-44
14	6	150	-23
14	4	168	-163
14	2	174	-113
14	1	138	29
13	7	163	-34
13	6	130	97
13	5	121	-52
13	4	183	103
13	1	115	21
12	10	132	-36
12	2	192	116
11	12	177	-191
11	5	208	-229
11	3	123	-97
10	13	151	63
10	11	218	223
10	10	115	-108
10	7	150	-135
10	6	111	-87
10	4	273	-266
10	3	209	193
10	2	234	-243
10	1	203	168
9	11	123	-87
9	13	126	57
9	9	113	-110
9	8	164	173
9	7	189	-174
9	5	112	93
9	3	173	384
9	2	141	136
9	1	119	116
8	13	151	81
8	12	112	73
8	11	133	116
8	10	168	149
8	8	167	-124
8	7	344	-353
8	3	316	325
8	2	192	221
8	1	231	226
7	16	137	50
7	12	134	-103
7	9	136	-124
7	8	127	-138
7	7	290	-279
7	6	221	-227
7	5	289	279
7	4	102	-97
7	3	249	269
7	2	273	255
6	17	166	07
6	16	198	-189
6	13	129	98
6	13	108	98
6	12	112	104
6	10	191	197
6	9	219	-223
6	8	134	113
6	7	170	173
6	[illegible]	301	-499
6	[illegible]	308	301
6	[illegible]	229	-216
6	[illegible]	351	-346
6	2	183	195
6	1	134	-150
5	16	132	95
5	15	136	112
5	14	366	381
5	12	227	225
5	11	125	-124
5	10	111	105
5	9	245	-231
5	6	87	102
5	4	120	132
5	3	355	358
5	2	130	-152
4	18	192	-154
4	16	190	-163
4	15	115	-82
4	14	179	-185
4	12	111	102
4	10	175	-184
4	8	93	96
4	7	119	-151
4	6	523	503
4	4	601	598
4	3	234	-257
4	2	526	530
4	1	178	141
3	18	188	-153
3	16	122	74
3	14	281	291
3	13	99	-81
3	12	378	373
3	11	114	140
3	10	246	-247
3	9	433	430
3	8	1010	-1016
3	7	88	82
3	6	479	-465
3	5	464	-453
3	4	233	-220
3	3	388	-399
3	2	539	-535
3	1	386	378
2	17	133	-65
2	15	105	114
2	14	127	99
2	13	257	-288
2	10	146	-149
2	9	196	227
2	8	278	-278
2	7	371	363
2	6	395	375
2	5	237	203
2	4	410	-439
2	3	340	-318
2	2	281	-286
2	1	746	-760
1	18	131	-90
1	17	115	-103
1	15	256	-267
1	14	457	489
1	13	220	-233
1	12	269	276
1	11	271	289
1	10	186	-197
1	9	556	574
1	7	600	590
1	6	157	203
1	5	225	-247
1	3	109	-151
1	2	146	-135
1	1	427	447
0	16	163	168
0	12	574	-548
0	10	512	-539
0	8	1045	1046
0	6	843	821
0	4	506	-491
0	2	269	258
-2, K, L			
14	4	130	120
14	3	132	-38
13	8	125	55
13	7	119	-58
13	1	116	-74
12	2	141	-102
12	9	117	73
12	4	167	-40
12	3	111	146
12	2	226	-197
12	1	155	-125
11	12	138	25
11	11	148	-25
11	10	136	70
11	9	149	-13
11	8	213	197
11	7	108	120
11	6	123	140
11	5	155	123
11	4	166	-166
11	3	171	169
11	2	379	-388
11	1	132	107
10	13	167	-92
10	12	110	108
10	11	164	-151
10	10	118	-48
10	8	152	151
10	5	102	76
10	2	223	240
10	1	104	-78
9	13	167	-156
9	12	138	-111
9	11	138	-77
9	10	109	91
9	9	193	178
9	8	250	241
9	4	161	-196
9	3	111	122
9	1	115	109
8	13	136	82
8	12	143	-140
8	11	155	-189
8	8	417	-437
8	6	254	-253
8	2	238	261
8	1	304	-291
7	13	144	-134
7	12	119	140
7	9	219	-233
7	8	124	91
7	7	204	203
7	4	313	-305
7	3	101	128
7	2	337	-324
7	1	293	292
6	16	121	70
6	15	138	-66
6	11	359	357
6	10	141	129
6	9	181	198
6	7	411	-421
6	6	350	-318
6	5	226	-248
6	4	389	386
6	3	521	490
6	2	951	978
6	1	136	-128
5	13	161	-144
5	11	204	-183
5	10	414	-415
5	9	92	-105
5	8	543	-561
5	7	122	111
5	6	422	-442
5	5	104	98
5	4	356	358
5	3	315	319
5	2	421	439
5	1	137	-125
4	17	149	-80
4	16	140	129
4	15	137	-125
4	14	155	153
4	13	262	277
4	12	166	193
4	11	381	385
4	10	100	-88
4	9	179	164
4	8	180	-175
4	7	591	-589
4	6	357	-375
4	5	460	-450
4	2	616	-586
4	1	92	119
3	18	177	110
3	17	112	-27
3	16	178	110
3	15	201	205
3	14	166	141
3	12	271	275
3	11	88	93
3	10	153	140
3	8	347	-341
3	7	795	-787
3	5	100	-68
3	3	545	537
3	1	179	141
2	18	113	-49
2	17	113	-118
2	15	214	-215
2	14	285	288
2	11	308	298
2	10	135	132
2	9	191	-190
2	8	154	154
2	7	339	-363
2	6	491	497
2	5	939	-912
2	4	985	961
2	3	345	-335
2	2	924	-838
2	1	94	-51
1	17	193	-175
1	16	125	-118
1	15	234	218
1	14	158	161
1	13	549	561
1	11	171	[illegible]
1	10	81	75
1	9	83	77
1	8	581	-573
1	7	699	-695
1	6	800	-791
1	5	651	-622
1	4	1650	1604
1	3	134	-112
1	2	1998	1993
1	1	275	-274
0	16	111	62
0	12	97	117
0	10	310	-309
0	8	1063	-1027
0	6	309	334
0	4	962	908
0	2	2268	-2267
-1, K, L			
14	3	140	-123
13	8	114	-58
13	6	158	-84
13	5	145	99
13	3	136	111
13	2	128	-77
12	10	249	258
12	7	146	118
11	12	156	73
11	6	120	103
11	2	133	130
10	12	144	-95
10	11	131	-95
10	10	121	-112
10	7	192	235
10	5	425	434
10	1	286	-271
9	12	130	107
9	11	114	-84
9	9	202	196
9	8	327	-370
9	7	222	213
9	6	271	-299
9	5	95	101
9	4	215	-213
9	3	227	-236
9	1	316	-306
8	15	128	-69
8	14	182	118
8	12	122	-168
8	10	[illegible]	-137
8	8	196	188
8	7	143	143
8	6	322	318
8	5	352	348
8	4	263	268
8	3	146	-136
8	2	142	-138
8	1	128	143
7	16	135	-67
7	14	[illegible]	[illegible]
7	13	187	-17
7	7	422	442
7	6	300	299
7	5	285	288
7	4	437	418
7	3	148	-162
7	2	677	-693
7	1	268	-261
6	13	193	-198
6	12	309	-302
6	10	466	-458
6	9	230	-236
6	6	283	283
6	5	618	-597
6	4	136	119
6	3	224	-208
6	2	125	-117
6	1	750	714
5	16	236	202
5	15	113	-102
5	14	132	-121
5	13	105	-82
5	12	231	-214
5	8	350	-359
5	7	174	146
5	6	309	328
5	5	254	-220
5	4	455	-471
5	3	118	-131
5	1	576	-573
4	17	139	-28
4	15	107	-88
4	14	106	111
4	9	142	-153
4	8	185	193
4	7	549	-553
4	6	794	767
4	5	232	-256
4	4	399	391
4	3	120	163
4	2	150	-155
4	1	1962	1941
3	16	180	185
3	14	189	-202
3	12	403	-407
3	11	129	114
3	9	142	-127
3	7	331	-335
3	6	435	443
3	5	181	-267
3	2	815	812
3	1	545	-542
2	18	139	97
2	16	147	-139
2	14	158	-149
2	10	262	266
2	9	101	-116
2	8	174	148
2	7	111	93
2	6	[illegible]	-811
2	5	236	211
2	4	1098	-1075
2	3	581	-612
2	2	[illegible]	-113
2	1	1681	1623
1	18	155	125
1	16	127	103
1	14	116	-147
1	13	242	248
1	12	209	-216
1	11	354	365
1	9	314	-317
1	8	236	261
1	7	450	-451
1	6	738	-729
1	5	565	520
1	4	2105	-2110
1	3	755	734
1	2	199	136
1	1	320	325
0	16	104	76
0	14	418	-433
0	12	463	453
0	10	780	801
0	8	133	123
0	6	1390	-1355
0	4	700	-656
0	2	558	-615
0, K, L			
0	2	1201	1140
0	4	1881	-1824
0	6	377	-387
0	8	161	-164
0	11	410	-417
1	1	75	91
1	2	502	-495
1	3	284	-346
1	4	557	549
1	5	77	45
1	6	472	475
1	7	333	-304
1	8	127	138
1	10	132	132
1	13	173	-171
1	14	143	-131
1	15	149	161
1	17	164	159
2	0	907	854
2	1	514	552
2	2	537	537
2	3	244	294
2	4	757	-748
2	5	569	560
2	6	498	-499
2	7	523	519
2	9	448	-452
2	11	447	-433
2	13	316	-319
2	14	151	177
2	15	265	231
3	1	1320	1464
3	2	1065	-1031
3	3	592	-596
3	[illegible]	198	195
3	[illegible]	81	-71
3	7	262	-219
3	8	143	138
3	9	114	[illegible]
3	10	475	-508
3	11	190	167
3	12	329	-318
3	13	118	-136
4	0	1019	999
4	3	506	508
4	4	451	-425
4	5	838	834
4	6	213	[illegible]
4	8	197	-206
4	9	138	-133
4	11	145	-143
4	13	113	161
4	14	148	-138
4	15	183	194
5	1	748	723
5	2	333	-331
5	3	293	288
5	4	88	-51
5	5	208	201
5	6	137	460
5	7	296	-306
5	8	375	[illegible]
5	9	110	-125
5	11	138	137
5	13	121	-164
6	0	740	[illegible]
6	1	660	-611
6	2	624	[illegible]
6	[illegible]	107	92
6	5	339	[illegible]
6	6	351	[illegible]
6	7	306	[illegible]
6	8	120	141
6	9	166	-183
6	11	157	-155
6	13	145	137
7	1	403	-399
7	2	317	298
7	3	208	198
7	4	212	-236
7	6	286	-290
7	7	299	-332
7	9	122	-107
7	11	224	228
7	13	112	113
7	15	137	-132
8	0	84	12
8	1	109	-113
8	2	108	[illegible]
8	3	306	-410
8	4	383	383
8	5	167	-182
8	6	369	[illegible]
8	8	162	-81
8	10	157	[illegible]
9	1	126	-103
9	2	275	286
9	3	92	71
9	4	371	369
9	6	100	-99
9	8	217	203
9	10	348	312
9	11	164	111
9	13	133	[illegible]
10	0	418	-410
10	1	104	-106
10	2	211	-244
10	3	128	-131
10	5	107	-90
10	6	125	-141
10	7	122	-136
10	8	110	83
10	9	219	206
10	11	140	135
11	2	323	325
11	3	126	-109
11	4	118	-93
11	5	101	72
11	6	262	[illegible]
11	8	116	-101
12	0	166	109
12	2	129	100

$$w = F_{\mathrm{obs}}/16{\cdot}0 \text{ for } F_{\mathrm{obs}} \leq 16{\cdot}0$$
$$w = 16{\cdot}0/F_{\mathrm{obs}} \text{ for } F_{\mathrm{obs}} > 16{\cdot}0.$$

When refinement was terminated the final unweighted R was 0·080 and the weighted R was 0·069.

The observed and calculated structure factors of the observed reflexions are listed in Table 2(*a*) and the final atomic parameters and estimated standard deviations are given in Table 3. The numbering of the atoms is as in Fig. 1.

(*b*) *Sulphathiazole* III

2729 of the 6137 reflexions recorded were regarded as observable and the refinement was based on them.

Table 2 (*cont.*)

12	4	123	-130
12	5	108	-58
12	8	160	-45
13	2	125	109
13	7	112	64
14	0	142	114
14	4	186	-166
1, K, L			
0	0	634	-630
0	2	1083	-1051
0	4	582	578
0	6	162	145
0	8	310	-323
0	10	453	-462
0	12	231	232
0	14	358	353
1	0	306	206
1	1	565	-541
1	2	55	-26
1	3	215	-239
1	4	293	283
1	6	81	72
1	7	474	471
1	8	306	-312
1	9	420	-421
1	10	205	-212
1	11	446	-456
1	13	185	200
1	14	274	-275
1	15	249	265
2	0	59	13
2	1	1086	-1024
2	2	1547	1560
2	3	519	544
2	4	547	530
2	5	671	696
2	6	383	373
2	7	417	396
2	8	104	72
2	9	181	-180
2	10	228	-241
2	12	144	191
2	14	202	242
3	0	969	-980
3	1	203	148
3	2	602	585
3	3	423	-404
3	4	510	504
3	5	284	-255
3	6	360	-337
3	7	584	590
3	9	93	74
3	10	208	205
3	11	256	-280
3	12	272	285
3	14	106	-118
3	16	204	-206
4	0	506	-492
4	1	775	-787
4	2	378	-356
4	3	315	320
4	4	249	-259
4	5	677	663
4	6	385	-394
4	7	341	356
4	8	171	-168
4	9	134	-135
4	11	214	-219
4	16	115	101
5	0	792	-787
5	1	131	-119
5	2	351	363
5	3	131	146
5	4	336	352
5	5	192	187
5	6	246	242
5	8	140	-151
5	9	145	130
5	13	129	157
5	16	210	-187
6	0	79	86
6	1	437	-442
6	2	98	103
6	3	207	215
6	4	187	-205
6	7	154	138
6	8	482	495
6	9	91	-85
6	10	206	210
6	12	187	-175
6	14	184	-161
7	0	607	-623
7	1	437	443
7	3	529	521
7	4	80	65
7	6	289	297
7	7	133	-140
7	10	111	99
7	11	198	244
7	12	187	187
8	0	334	-343
8	2	238	-237
8	3	172	-205
8	4	463	-478
8	5	104	-119
8	6	217	-228
8	7	145	143
8	10	221	206
8	12	124	-110
8	14	185	-157
9	1	121	135
9	2	145	-136
9	3	103	119
9	4	136	-134
9	5	210	-236
9	6	124	120
9	8	124	121
9	10	253	-249
9	12	136	-130
10	0	101	96
10	1	133	137
10	2	177	176
10	3	109	-83
10	4	440	466
10	5	258	-265
10	6	125	110
10	9	174	181
10	12	129	48
11	0	203	-208
11	2	259	-274
11	3	113	-106
11	6	108	118
11	8	129	126
11	11	128	-32
12	8	211	-189
14	1	115	-33
14	4	181	179
2, K, L			
0	0	1194	-1206
0	2	1119	1096
0	4	778	804
0	6	636	637
0	8	214	206
0	12	141	-163
0	16	160	121
1	0	1150	1073
1	1	286	-260
1	2	292	-321
1	3	95	108
1	5	297	275
1	6	178	-201
1	8	321	-311
1	10	193	193
1	12	103	62
1	13	107	-147
1	14	141	-154
1	15	224	-237
1	16	126	89
2	0	1506	-1456
2	1	1045	-999
2	2	932	897
2	3	107	-96
2	4	471	478
2	5	385	-374
2	6	234	-234
2	7	310	318
2	8	542	-551
2	9	442	432
2	10	140	-152
2	12	138	-181
2	13	325	-332
3	0	234	256
3	2	1034	1024
3	3	670	-641
3	4	478	457
3	5	313	331
3	6	167	-159
3	7	774	766
3	8	244	232
3	9	100	-124
3	11	150	-170
3	12	215	-229
3	16	135	-126
4	0	184	-189
4	1	195	174
4	2	290	-288
4	3	286	-299
4	8	343	343
4	9	286	271
4	10	163	163
4	13	362	-351
4	14	161	-141
4	15	197	-203
5	0	472	-463
5	1	177	-185
5	2	251	-229
5	3	171	-170
5	5	157	150
5	6	259	-262
5	7	121	137
5	8	139	-131
5	10	276	269
5	14	115	48
6	0	302	308
6	1	296	284
6	2	322	-321
6	3	181	153
6	4	555	-573
6	6	240	-238
6	7	145	141
6	8	233	232
6	9	114	121
6	11	177	-194
6	13	245	-251
7	0	152	152
7	1	650	-646
7	3	422	-420
7	4	296	295
7	6	94	-126
7	7	137	137
7	8	95	-54
7	13	130	-91
7	14	148	-99
8	0	228	219
8	1	273	275
8	3	89	86
8	4	377	-372
8	6	326	346
8	7	172	-162
8	8	333	340
8	10	103	119
9	0	340	-342
9	2	406	-407
9	3	175	-160
9	4	234	233
9	5	141	-163
9	6	113	145
9	7	121	129
9	8	356	-366
9	10	130	-104
9	12	114	44
10	2	95	-105
10	3	107	91
10	5	177	-168
10	6	324	-334
10	7	155	-131
10	10	137	105
10	11	129	70
11	0	136	100
11	4	252	265
11	10	147	-106
12	0	125	-144
12	5	114	106
12	7	130	-63
12	8	138	92
13	0	127	-127
13	2	161	-151
14	2	126	60
3, K, L			
0	0	524	-522
0	2	409	405
0	4	887	893
0	6	158	200
0	8	433	429
0	10	286	-292
0	12	633	-624
0	14	130	-75
1	0	482	447
1	1	693	707
1	2	164	146
1	3	235	236
1	4	329	335
1	5	433	-440
1	6	450	432
1	7	517	-510
1	8	209	231
1	9	233	219
1	13	111	-95
1	14	161	176
1	15	147	-70
2	1	1317	-1269
2	2	334	-352
2	3	619	-610
2	5	109	-118
2	6	273	285
2	7	280	277
2	8	123	129
2	9	195	210
2	12	157	-146
2	13	150	-133
2	14	108	-77
3	0	727	-711
3	1	357	-336
3	2	330	-326
3	3	474	486
3	4	386	-385
3	5	121	-105
3	6	161	156
3	7	239	-239
3	9	127	148
3	10	198	-193
3	13	104	-114
3	14	197	206
4	0	795	779
4	1	114	81
4	2	306	310
4	3	427	-435
4	4	359	362
4	5	382	-386
4	6	426	-421
4	7	281	278
4	8	449	-460
4	9	386	385
4	10	161	-156
4	11	214	234
4	15	180	-146
5	0	193	-160
5	1	190	-194
5	2	333	-333
5	4	277	282
5	5	116	116
5	6	378	380
5	10	170	-181
6	0	90	-75
6	2	101	-103
6	5	116	-128
6	6	388	-399
6	7	283	292
6	8	246	-244
6	9	309	323
6	10	145	178
6	12	325	312
6	13	125	99
6	14	200	164
7	0	201	-213
7	1	87	-75
7	2	223	-210
7	4	203	-209
7	5	145	123
7	6	279	-279
7	7	156	-182
8	2	118	118
8	3	243	255
8	4	170	184
8	5	127	163
8	6	102	-71
8	7	268	-255
8	8	373	-384
8	9	156	-151
8	10	121	75
8	11	124	89
8	12	226	221
9	0	119	106
9	2	535	562
9	4	116	-105
9	8	173	192
9	10	231	259
10	1	102	117
10	2	131	-127
10	3	326	336
10	4	213	-204
10	7	108	-89
10	8	121	95
10	9	151	-154
10	10	131	89
11	6	108	-89
12	0	161	151
12	1	128	128
12	3	106	127
12	4	121	-93
12	7	155	-130
13	0	119	79
13	2	170	116
13	3	111	-18
13	4	144	78
4, K, L			
0	0	1618	-1586
0	2	1415	-1386
0	4	428	-405
0	6	417	409
0	8	375	388
0	10	109	-110
0	12	238	244
1	0	468	460
1	1	430	419
1	2	109	-121
1	3	265	270
1	4	129	-134
1	5	462	464
1	6	125	-91
1	7	314	322
1	8	107	-99
1	11	137	-140
1	14	193	-170
2	0	437	-423
2	1	262	-262
2	2	436	-454
2	4	457	458
2	5	157	-170
2	6	735	719
2	7	490	-512
2	8	118	117
2	10	179	169
2	11	343	335
2	13	290	305
2	14	164	-149
3	0	857	-841
3	1	103	-107
3	3	205	217
3	4	331	319
3	5	174	-162
3	6	398	412
3	7	99	75
3	8	141	146
3	10	176	176
4	0	366	-358
4	1	160	166
4	2	245	241
4	3	611	-592
4	4	87	66
4	5	300	-306
4	7	280	-297
4	9	99	93
4	11	389	392
4	13	150	122
4	14	134	79
5	0	192	173
5	1	306	309
5	2	394	-413
5	3	207	-217
5	5	287	-293
5	6	154	146
5	8	176	-180
5	11	192	183
5	12	136	105
5	13	137	77
6	0	329	338
6	2	588	604
6	3	178	199
6	4	361	366
6	7	123	-132
6	8	268	-279
6	11	176	165
6	13	121	46
7	0	85	67
7	1	230	231
7	2	169	175
7	5	138	-102
7	8	189	206
7	9	213	203
7	11	128	88
8	2	254	252
8	5	257	239
8	6	431	-442
8	7	101	101
8	8	266	-274
8	9	140	105
8	10	126	-93
9	0	490	506
9	1	133	132
9	3	130	-117
9	4	459	-481
10	0	135	116
10	4	158	164
10	6	137	99
10	7	148	140
10	9	116	53
12	0	134	-110
12	2	178	-156
12	4	123	-81
12	6	152	32
13	0	142	75
13	1	144	-82
13	3	126	-28
5, K, L			
0	0	273	194
0	2	152	-169
0	6	430	-422
0	8	174	176
0	10	620	624
0	12	219	193
1	0	289	-296
1	1	295	-294
1	2	381	-387
1	3	125	108
1	4	387	-395
1	5	270	285
1	6	291	-299
1	8	462	475
1	10	249	243
1	12	122	44
1	13	117	-44
2	1	849	865
2	2	321	-325
2	3	139	130
2	4	416	-434
2	5	279	-269
2	6	293	-288
2	7	462	-473
2	9	280	-270
2	10	112	115
2	13	136	88
3	0	475	482
3	1	352	-342
3	4	539	-537
3	5	107	84
3	6	265	-261
3	8	234	224
3	9	185	183
3	10	229	211
3	13	127	-75
4	0	115	-132
4	1	322	357
4	2	245	252
4	3	213	212
4	5	291	-301
4	6	165	154
4	7	476	-472
4	8	199	185
4	12	157	-110
5	0	236	220
5	1	274	308
5	2	294	-297
5	3	142	-158
5	4	497	-491
5	6	286	-277
5	10	156	151
5	11	109	53
5	12	140	-16
6	2	238	-253
6	5	311	-331
6	6	340	356
6	10	241	-246
7	0	336	361
7	1	259	255
7	2	192	200
7	3	183	-167
7	5	445	-459
7	6	268	-258
7	11	159	-95
8	1	157	-167
8	3	135	-141
8	4	215	210
8	5	103	69
8	6	241	237
8	8	242	223
8	10	148	-109
9	0	329	-336
9	2	193	-181
9	3	139	-131
9	4	115	111
9	7	124	54
9	8	124	-66
9	9	117	-17
10	1	187	-177
10	3	162	-169
10	4	194	-182
10	7	143	67
11	3	114	-23
11	4	213	154
11	5	115	35
12	1	149	-146
12	2	120	48
6, K, L			
0	0	836	799
0	4	900	-933
0	6	575	-597
1	0	554	557
1	1	148	-154
1	2	86	-77
1	3	231	-236
1	5	432	-448
1	6	169	169
1	9	307	312
1	10	200	-228
1	11	210	194
1	12	120	47
2	0	430	437
2	1	194	201
2	4	293	-295
2	5	157	161
2	6	280	-273
2	7	175	191
2	9	118	-131
2	10	139	151
2	12	176	153
3	0	371	386
3	1	352	-345
3	2	264	-256
3	3	124	-138
3	4	378	-390
3	5	279	-284
3	6	227	-237
3	7	130	-124
3	8	177	-169
4	1	142	-159
4	2	189	208
4	5	292	294
4	6	103	-142
4	7	134	136
4	8	140	149
4	9	156	-176
4	11	178	-174
5	0	398	386
5	1	173	165
5	2	181	189
5	4	150	-168
5	6	98	121
5	7	282	-273
6	0	288	-281
6	2	317	-317
6	3	131	-127
6	4	98	109
6	5	176	190
6	6	211	231
6	9	183	-212
7	3	599	613
7	4	134	-140
7	5	130	142
7	9	179	-164
8	0	228	-231
8	1	98	-112
8	2	132	-116
8	3	115	-96
8	8	131	33
9	0	106	-68
9	2	195	212
9	3	184	181
9	4	216	217
9	5	162	128
9	6	150	101
9	7	132	-59
10	4	146	98
10	5	121	-16
10	6	133	52
11	0	202	-167
11	2	119	-23
11	4	158	80
12	0	191	129
7, K, L			
0	0	224	-208
0	2	388	-401
0	4	243	268
0	6	506	535
0	8	316	-304
0	10	167	-173
1	0	117	-107
1	3	385	-395
1	4	266	276
1	6	235	-256
1	8	278	-280
2	0	259	255
2	3	142	156
2	4	160	148
2	5	236	202
2	7	133	136
2	8	166	-161
2	9	211	-173
2	10	121	-36
3	2	319	348
3	4	379	378
3	5	199	241
3	7	177	162
3	8	204	-225
3	9	120	-104
3	10	128	-70
4	0	225	-244
4	1	168	-184
4	2	263	-273
4	3	201	202
4	5	162	166
4	9	143	-88
5	2	418	423
5	3	158	158
5	4	276	288
5	5	330	365
5	6	117	-118
5	8	219	-204
5	9	123	-75
6	0	185	173
6	1	108	-78
6	2	138	132
6	5	206	202
6	7	112	-76
7	0	142	152
7	3	217	216
7	6	179	181
8	1	185	162
8	5	113	-85
9	2	168	-162
9	3	117	106
10	1	127	98
8, K, L			
0	0	386	-373
0	2	511	522
0	4	279	282
0	6	141	-122
0	8	196	-160
1	1	148	157
1	2	226	233
1	4	127	-87
1	6	125	-55
1	7	186	-178
1	8	116	21
2	2	153	-163
2	3	101	125
2	8	149	-107
3	2	300	301
3	6	128	-34
3	8	197	-176
4	0	144	138
4	1	179	180
4	5	140	-142
5	0	318	-128
5	1	193	-201
5	2	231	237
5	3	134	-133
5	6	177	-147
5	7	158	111
6	1	314	323
6	2	143	-155
6	3	111	-55
6	4	246	-233
6	5	153	-142
6	6	121	-15
7	1	156	-162
7	3	244	-216
7	5	147	99
8	0	135	100
8	3	119	55
8	4	120	-67
9	1	135	-62
9	2	129	-17
9, K, L			
0	0	343	316
0	2	307	279
0	4	198	-205
0	6	125	-75
1	0	100	-33
1	1	264	281
1	2	147	-127
1	3	166	128
1	4	132	49
1	5	193	-145
1	6	192	162
2	0	105	37
2	2	115	124
2	5	126	39
2	6	125	-60
3	0	209	-204
3	1	185	166
3	2	178	-175
3	4	131	32
3	5	155	-91
3	6	286	272
4	4	183	-135
4	5	138	71
5	3	116	-81
5	4	211	185
6	0	206	-196
6	2	115	50
6	3	131	-12
6	4	129	72
7	1	204	-151
7	2	162	-24
8	0	143	81
8	1	162	48
10, K, L			
0	4	121	97
1	0	262	-256
1	1	108	30
1	2	111	-26
1	3	205	168
2	0	127	74
2	2	150	65
2	3	113	10
3	0	137	-95
3	1	116	26
3	2	161	-183
3	3	195	121
4	0	126	-43
4	2	130	55
5	0	199	-157
5	1	115	33
6	0	145	-53

After anisotropic refinement a difference Fourier synthesis was calculated and this revealed the positions of the 18 hydrogen atoms. During further refinement they were included with the same temperature factors as the atoms to which they were bonded and these parameters were kept constant. The weighting scheme of Hughes was again used. The final residuals were $R = 0{\cdot}063$ and $R_w = 0{\cdot}048$.

The observed and calculated structure factors of the observed reflexions are listed in Table 2(*b*) and the final atomic parameters and estimated standard deviations are given in Table 3.

Discussion

Two molecules are contained in each asymmetric unit and this situation allowed the determination of two independent molecular structures in each case. In the discussion following and in the Tables and Figures the two molecules belonging to each structure are distinguished by labelling them *A* and *B*.

Intramolecular bond lengths and angles were calculated with the function and error program *ORFFE* of Busing, Martin & Levy (1964) and are listed in Table 4. The estimated errors given for individual bond lengths and angles take into account both the least-squares estimated standard deviations and the estimated cell constant errors. Neither the bond lengths nor their errors have been corrected for thermal motion. The standard deviations of bond lengths and angles involving hydrogen atoms have average values of approximately ±0·05 Å and ±3°, respectively, and are not listed separately. Since the hydrogen atoms which could be found could not be accurately located, no further discussion of their positions is made.

Comparison of the values found here with the bond lengths and angles obtained for sulphathiazole II indicates that the molecular structure of sulphathiazole is the same in all three crystalline modifications. The differences between the bond lengths and angles determined in the five independent molecules and their mean

Table 2 (*cont.*)

(*b*) Sulphathiazole III

0, K, L			
12	0	129	-98
11	1	154	130
11	4	133	-158
10	5	133	109
10	7	108	-92
10	8	143	-149
9	1	100	113
9	5	205	-219
9	6	235	230
9	10	134	-118
9	11	163	-157
8	3	131	147
8	6	191	186
8	8	245	-246
8	9	117	137
8	13	151	-160
7	1	311	-323
7	2	199	218
7	3	319	324
7	4	519	511
7	5	391	-386
7	7	187	-178
7	8	104	-102
7	14	128	-129
6	0	133	165
6	1	140	-150
6	3	85	-92
6	4	459	-441
6	5	76	99
6	6	478	476
6	7	849	857
6	8	152	160
6	9	378	-381
6	11	142	-154
6	12	163	-154
6	13	98	107
5	1	268	-269
5	2	159	-148
5	3	291	-285
5	4	835	813
5	5	379	377
5	6	169	-165
5	7	150	166
5	8	289	276
5	9	207	-236
5	10	161	147
5	11	215	227
5	12	91	-74
5	17	117	-113
5	18	181	-191
4	0	623	-620
4	1	304	-284
4	2	334	326
4	3	488	486
4	4	303	-264
4	5	204	-213
4	6	216	-210
4	7	182	192
4	8	621	616
4	10	180	183
4	11	566	547
4	15	169	-165
4	16	308	-300
3	1	575	563
3	3	1328	-1324
3	5	426	418
3	6	81	67
3	7	380	397
3	8	158	169
3	9	231	246
3	12	631	632
3	13	115	-142
3	15	150	138
3	16	116	131
3	19	244	-257
2	0	230	213
2	1	1862	-1877
2	3	157	-169
2	4	1394	1356
2	5	377	-366
2	6	79	-70
2	7	297	-298
2	8	324	287
2	9	473	481
2	11	88	-104
2	12	329	336
2	15	726	701
2	16	209	-206
1	1	106	-114
1	2	295	267
1	3	1486	1474
1	4	1547	-1517
1	5	426	399
1	6	185	-181
1	7	592	-580
1	8	179	-152
1	9	154	-157
1	10	100	-92
1	11	676	-701
1	13	272	289
1	14	93	66
1	15	195	-180
1	16	174	-164
1	18	175	163
0	2	145	119
0	4	633	-605
0	6	267	268
0	8	221	237
0	10	370	-375
0	12	161	-148
0	14	162	-167
0	16	586	590
0	18	120	61
1, K, L			
12	0	181	-132
12	2	214	206
11	-2	211	-201
11	2	186	192
11	3	134	-150
11	4	112	-103
10	-9	147	-111
10	-3	154	155
10	0	151	-131
10	1	252	-289
10	2	166	-171
10	3	149	178
10	5	108	117
10	6	143	128
9	-11	113	-101
9	-10	114	77
9	-9	117	89
9	-7	127	151
9	-6	129	150
9	-1	121	-140
9	0	100	106
9	2	109	102
9	3	126	96
9	4	152	-151
9	5	323	-334
9	6	100	90
9	13	133	106
8	-14	201	-189
8	-10	138	154
8	-7	97	-86
8	-6	168	186
8	-4	139	-161
8	-2	128	-115
8	2	478	-484
8	4	99	-105
8	5	478	-496
8	13	142	-174
7	-10	129	-134
7	-9	297	317
7	-7	219	-221
7	-6	360	380
7	-3	310	332
7	-2	501	498
7	1	244	-263
7	2	227	-204
7	3	140	155
7	5	162	-175
7	6	431	-409
7	7	156	137
7	8	179	-173
7	9	124	-145
7	14	208	235
6	-14	280	286
6	-13	167	-178
6	-12	96	94
6	-10	354	-356
6	-9	139	-150
6	-8	230	-239
6	-7	500	-516
6	-5	603	583
6	-4	121	-119
6	-2	178	-188
6	0	76	-75
6	2	510	492
6	3	435	-437
6	4	100	91
6	5	394	-392
6	6	633	-629
6	8	163	-164
6	9	566	-556
6	10	144	-152
6	11	94	104
6	12	140	-139
6	13	143	164
6	14	105	-98
6	17	137	123
5	-18	156	165
5	-17	265	288
5	-16	124	-94
5	-11	127	126
5	-9	199	-202
5	-7	304	-303
5	-5	254	-266
5	-3	516	-519
5	-2	388	-380
5	-1	743	720
5	0	208	-217
5	1	213	203
5	2	574	541
5	4	314	315
5	5	566	565
5	6	830	-802
5	7	174	-191
5	8	233	247
5	9	521	-520
5	13	229	-229
5	16	123	107
5	17	140	133
4	-18	160	166
4	-16	145	148
4	-12	136	-122
4	-10	414	421
4	-8	156	-158
4	-7	318	-329
4	-6	1390	-1363
4	-5	686	692
4	-4	135	151
4	-3	570	-567
4	-2	485	463
4	-1	329	328
4	0	305	-309
4	1	892	-861
4	3	251	-269
4	5	509	499
4	6	125	154
4	7	170	191
4	8	100	97
4	10	448	-436
4	11	253	-258
4	13	94	-105
4	16	125	-118
4	18	149	154
3	-18	265	-231
3	-17	123	-127
3	-16	178	168
3	-13	472	454
3	-10	139	151
3	-9	586	-610
3	-8	104	114
3	-7	122	135
3	-6	281	-286
3	-4	305	-313
3	-3	767	-765
3	-2	1780	-1730
3	-1	830	-799
3	0	189	182
3	1	339	-317
3	2	377	-358
3	3	602	593
3	4	93	92
3	5	632	589
3	7	191	-194
3	8	173	194
3	9	434	463
3	10	196	-200
3	12	192	222
3	13	120	-117
3	14	206	-220
3	15	107	84
2	-20	128	-126
2	-16	157	132
2	-15	197	-202
2	-14	169	-176
2	-13	335	312
2	-12	141	-161
2	-11	98	76
2	-10	216	221
2	-9	92	102
2	-7	270	287
2	-6	848	-776
2	-4	222	-215
2	-2	1370	-1306
2	-1	1505	1525
2	0	115	-101
2	1	1079	-1074
2	2	300	278
2	3	346	367
2	5	377	-366
2	6	447	-432
2	7	91	-106
2	8	82	99
2	9	1063	1064
2	10	425	452
2	11	118	-118
2	12	147	161
2	13	125	-95
2	14	91	-74
2	15	119	-117
2	17	107	76
1	-18	222	-218
1	-14	238	-239
1	-13	394	-387
1	-12	270	283
1	-11	247	-265
1	-10	616	615
1	-9	576	578
1	-7	257	-263
1	-6	215	-204
1	-5	69	61
1	-4	106	-120
1	-3	1600	1617
1	-2	1361	-1292
1	-1	154	-141
1	0	59	-26
1	1	241	-237
1	2	1383	-1353
1	3	381	-370
1	5	867	822
1	6	720	712
1	7	212	224
1	8	181	-190
1	9	207	215
1	10	412	-407
1	11	200	188
1	12	340	345
1	13	702	695
1	16	145	-141
1	17	157	111
0	-18	105	-65
0	-16	493	-497
0	-14	540	-548
0	-12	218	195
0	-10	712	-696
0	-8	115	-168
0	-6	556	569
0	-4	178	177
0	-2	465	-431
0	0	195	188
0	2	2013	-1961
0	4	82	-80
0	6	475	-463
0	10	768	763
0	12	125	-64
0	14	106	88
0	16	154	149
0	18	143	-123
2, K, L			
12	-2	132	-29
12	-1	183	171
11	-8	165	-164
11	0	164	192
11	3	175	186
10	-11	182	-193
10	-7	105	44
10	-4	204	-183
10	-1	118	98
10	0	137	69
10	1	127	109
10	3	203	218
10	4	186	198
10	6	149	133
9	-11	120	149
9	-9	147	111
9	-7	253	-264
9	-6	110	102
9	-4	104	-92
9	-1	158	-168
9	1	146	154
9	3	111	86
9	4	178	188
9	6	103	87
9	7	272	278
8	-12	241	248
8	-11	190	192
8	-9	181	146
8	-8	143	151
8	-6	137	134
8	-5	167	191
8	-4	212	-200
8	-3	92	120
8	1	326	-328
8	4	305	306
8	5	274	282
8	6	114	-107
8	7	164	184
8	10	136	121
8	11	154	148
8	12	121	-137
7	-16	149	-163
7	-15	198	192
7	-12	104	-132
7	-10	144	149
7	-9	190	188
7	-8	517	531
7	-4	324	-306
7	0	229	-224
7	3	111	-117
7	4	253	-271
7	8	442	443
6	-14	185	-171
6	-11	112	144
6	-8	150	171
6	-7	596	596
6	-6	202	184
6	-5	652	641
6	-4	619	597
6	-3	478	-467
6	-2	111	107
6	0	181	190
6	1	73	56
6	2	75	-88
6	3	364	-354
6	4	432	-418
6	5	152	150
6	6	86	-105
6	7	280	296
6	8	94	99
6	11	225	235
5	-19	163	138
5	-16	133	-120
5	-15	158	-146
5	-11	134	-156
5	-9	363	-366
5	-8	379	-399
5	-7	837	820
5	-6	117	-135
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5	-4	300	299
5	-3	371	370
5	-2	105	91
5	-1	377	380
5	0	603	-574
5	3	442	-439
5	4	284	274
5	5	358	-362
5	6	375	-379
5	7	707	-701
5	8	510	-510
5	9	263	261
5	12	153	123
5	16	130	-133
4	-19	113	145
4	-18	163	-164
4	-17	133	75
4	-16	101	88
4	-15	253	260
4	-12	235	-229
4	-11	322	-330
4	-8	151	148
4	-5	778	-773
4	-4	427	425
4	-3	467	460
4	-2	157	160
4	-1	1020	1026
4	0	143	132
4	1	440	443
4	3	351	-345
4	4	265	-205
4	5	271	-276
4	7	272	285
4	8	288	-298
4	10	243	-222
4	11	624	-609
4	12	303	293
4	14	147	129
4	15	154	179
4	16	161	-127
3	-20	127	80
3	-19	200	202
3	-18	111	86
3	-16	226	229
3	-15	203	-177
3	-13	167	196
3	-11	284	293
3	-10	117	-104
3	-9	275	-277
3	-8	200	-208
3	-7	124	-148
3	-5	478	473
3	-4	493	-458
3	-2	103	-89
3	-1	665	-637
3	0	474	474
3	1	201	169
3	2	58	99
3	3	295	-279
3	4	227	194
3	5	217	-200
3	6	82	78
3	8	516	-521
3	10	207	-206
3	11	349	-361
3	12	115	-137
3	15	256	252
2	-20	159	-134
2	-19	156	158
2	-16	148	137
2	-15	119	89
2	-14	128	129
2	-13	101	153
2	-12	190	-187
2	-9	441	-438
2	-8	383	386
2	-7	495	-490
2	-5	93	-83
2	-4	1073	-1024
2	-3	425	460
2	-2	204	-207
2	-1	520	-508
2	0	488	462
2	1	173	-202
2	2	131	132
2	3	485	498
2	4	434	-427
2	6	291	-294
2	7	995	-988
2	8	525	520
2	9	285	-281
2	10	270	306
2	12	144	-165
2	13	90	88
2	14	122	-142
2	15	164	-162
2	19	164	180
1	-16	199	208
1	-15	143	137
1	-14	86	93
1	-11	128	-115
1	-10	171	-177
1	-9	265	280
1	-7	86	-85
1	-6	241	227
1	-4	166	-166
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1	-2	46	-85
1	-1	514	-522
1	0	1111	1048
1	1	135	-147
1	3	213	232
1	4	1293	-1265
1	5	193	-191
1	6	123	123
1	7	251	263
1	8	222	235
1	9	364	-366
1	10	247	-261
1	11	256	-261
1	14	121	143
1	15	96	-86
1	16	193	187
0	-18	157	116
0	-16	470	-462
0	-14	190	191
0	-12	771	738
0	-8	838	-851
0	-6	86	69
0	-4	121	98
0	-2	49	29
0	0	101	-80
0	2	118	-136
0	4	746	756
0	6	192	203
0	8	264	-280
0	12	189	-177
0	16	207	191
3, K, L			
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11	-3	207	186
11	2	210	-223
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10	-3	106	64
10	-2	177	158
10	-1	137	-129
10	0	167	162
10	1	145	158
10	5	106	-121
10	6	120	-100
9	-10	114	-152
9	-7	123	-124
9	-5	148	161
9	-4	144	-120
9	-1	106	82
9	0	127	125
9	1	179	183
9	2	166	174
9	3	99	-16
9	4	103	68
9	6	102	-75
8	-12	115	51
8	-11	115	106
8	-9	100	-114
8	-7	265	-282
8	-6	128	-115
8	-5	247	-253
8	-3	203	212
8	-2	221	230
8	0	89	-104
8	2	149	150
8	3	147	160
8	4	192	227
8	5	314	326
8	7	117	-95
7	-15	128	140
7	-14	228	216
7	-13	185	-142
7	-8	98	-105
7	-6	84	-107
7	-2	130	-116
7	1	115	126
7	2	507	499
7	3	93	-120
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7	7	204	203
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6	-11	143	160
6	-10	255	258
6	-9	357	-369
6	-8	150	161
6	-6	126	120
6	-5	226	-218
6	-4	151	-135
6	-3	456	-448
6	-1	109	87
6	1	148	161
6	2	195	192
6	3	203	-200
6	6	143	163
6	8	122	141
6	10	184	198
6	11	101	-44
6	12	173	-176
6	13	248	-248
5	-17	295	-257
5	-15	106	-127
5	-13	158	173
5	-12	127	-122
5	-11	194	202
5	-10	495	498
5	-9	118	121
5	-8	301	304
5	-7	172	165
5	-6	408	-398
5	-5	352	-362
5	-4	165	145
5	-3	288	263
5	-2	522	509
5	-1	78	-91
5	0	212	-213
5	1	343	-332
5	2	70	83
5	3	388	394
5	4	129	131
5	5	595	601
5	6	254	242
5	16	130	-121
4	-18	201	-221
4	-16	120	120
4	-13	178	173
4	-11	201	-205
4	-10	156	143
4	-9	289	-289
4	-7	196	208
4	-6	353	322
4	-5	820	814
4	-3	124	-117
4	-2	248	-225
4	-1	818	-794
4	0	177	163
4	1	293	-271
4	2	240	-208
4	3	367	384
4	4	158	-183
4	5	181	-186
4	6	652	621
4	7	175	-178
4	11	90	90
4	12	177	170
4	13	159	-154
4	14	157	-138
4	16	245	-241
3	-17	162	142
3	-16	122	-87
3	-14	168	-166
3	-13	123	-135
3	-12	161	170
3	-10	132	131
3	-9	114	123
3	-7	91	127
3	-5	611	-597
3	-4	140	85
3	-3	73	-94
3	-2	528	485
3	-1	277	-274
3	0	213	198
3	2	515	-494
3	3	823	797
3	4	150	-161
3	6	367	-359
3	7	109	-147
3	9	520	519
3	10	197	213
3	13	221	-217
3	18	162	-173
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2	-17	118	115
2	-13	276	-292
2	-12	88	113
2	-10	233	228
2	-9	1194	1190
2	-8	357	-358
2	-6	684	-666
2	-4	54	58
2	-3	735	773
2	-2	431	427
2	-1	201	-183
2	1	874	-881
2	2	557	-551
2	3	392	-388
2	4	66	105
2	5	230	-233
2	6	588	579
2	7	514	504
2	10	449	-449
2	13	241	234
2	14	123	128
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1	-18	146	-133
1	-17	103	60
1	-16	126	-134
1	-13	415	-423
1	-12	297	285
1	-11	352	-371
1	-10	466	-469
1	-7	470	-469
1	-6	1676	1625
1	-5	93	109
1	-4	156	-178
1	-3	76	95
1	-2	1467	-1445
1	-1	712	700
1	1	405	-394
1	2	635	-629
1	3	341	-365
1	4	331	-343
1	5	151	151
1	6	296	-271
1	9	628	-627
1	10	397	393
1	11	109	158
1	13	238	248
1	14	161	-153
1	18	134	-129
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0	-16	101	-67
0	-12	207	-201
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0	-8	180	175
0	-6	434	436
0	-4	45	-24
0	-2	977	942
0	0	414	359
0	2	345	331
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0	10	536	528
0	14	121	-148
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4, K, L			
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10	-4	120	-140
10	-3	139	132
10	2	117	-89
10	3	125	-106
10	4	113	-38
10	7	134	143
9	-10	103	-79
9	-7	130	-110
9	-6	175	160
9	-5	207	232
9	-1	126	-138
9	4	156	-193
9	6	156	-164
9	11	191	172
8	-13	154	-160
8	-12	149	-135
8	-11	141	-159
8	-8	128	125
8	-7	261	276
8	-6	149	-159
8	-4	125	-156
8	0	190	-176
8	3	98	-96
8	8	151	153
8	11	152	145
8	12	116	-104
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7	-5	196	199
7	-4	306	294
7	-3	307	-307
7	-2	113	140
7	-1	196	193
7	0	222	-231
7	1	227	241
7	3	116	-141
7	4	456	-433
7	7	157	173
7	14	123	150
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6	-9	268	-242
6	-8	434	-446
6	-7	613	617
6	-6	212	-198
6	-5	188	220
6	-4	498	491
6	-3	123	116
6	-1	138	120
6	0	152	-183
6	1	114	-126
6	2	113	134
6	3	131	-141
6	4	149	145
6	5	213	225
6	6	276	-289
6	7	95	-107
6	8	247	-262
6	9	121	125
6	11	111	81
6	12	202	224
6	13	109	-76
6	15	119	146
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5	-17	124	89
5	-16	176	193
5	-12	246	-235
5	-11	399	-406
5	-8	343	327
5	-7	152	172
5	-6	209	-225
5	-5	216	-227
5	-4	121	-127
5	-3	213	210
5	-1	460	457
5	0	622	614
5	2	127	106
5	3	90	88
5	4	608	-597
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5	10	135	-150
5	11	204	-194
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4	-13	203	223
4	-9	96	-100
4	-8	441	-408
4	-6	131	137
4	-4	381	-358
4	-3	621	608
4	-2	273	-269
4	-1	261	-249
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4	1	330	338
4	3	550	545
4	4	272	-263
4	5	132	157
4	11	243	-243
4	12	157	-156
4	16	282	294
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3	-13	94	138
3	-12	559	566
3	-11	101	148
3	-10	105	-89
3	-8	264	230
3	-7	324	-310
3	-3	268	284
3	-2	175	-201
3	-1	1111	-1088
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3	2	75	56
3	3	873	874
3	4	526	518
3	5	217	-184
3	7	296	-274
3	9	138	-141
3	12	315	-308
3	14	135	-159
3	15	233	-233
3	16	120	42
2	-19	275	-273
2	-15	455	454
2	-12	142	148
2	-11	191	-224
2	-9	504	501
2	-8	645	-611
2	-7	106	118
2	-6	81	85
2	-4	163	-174
2	-3	329	-330
2	-2	48	-93
2	-1	312	-328
2	0	793	-767
2	1	570	594
2	2	215	-213
2	3	438	-424
2	4	462	-461
2	5	270	-258
2	12	160	-153
2	15	318	-295
1	-18	203	205
1	-16	171	-171
1	-15	207	189
1	-12	823	813
1	-11	446	455
1	-10	92	96
1	-9	112	137
1	-8	83	67
1	-7	1023	1049
1	-6	176	-184
1	-5	116	165
1	-4	536	-521
1	-3	1265	-1193
1	-2	76	51
1	-1	337	352
1	0	74	58
1	1	366	363
1	2	77	-110
1	3	563	-574
1	4	621	647
1	5	271	-261
1	7	248	263
1	8	77	55
1	11	91	133
1	12	182	-188
1	13	133	-98
1	15	119	115
0	-16	408	-407
0	-12	136	140
0	-10	325	319
0	-8	115	39
0	-6	97	-118
0	-4	354	316
0	-2	125	-79
0	0	3279	-3432
0	4	332	-298
0	6	506	-502
0	8	171	67
0	10	301	310
0	14	179	-180
0	16	156	-170
5, K, L			
11	-3	114	82
11	-2	128	142
10	0	111	74
10	2	151	131
10	6	148	-161
10	7	160	77
9	-10	121	103
9	-7	157	-164
9	-6	184	-218
9	-1	179	189
9	0	152	-165
9	3	164	-172
9	4	186	185
9	5	211	222
9	7	112	-53
9	9	142	-155
8	-15	111	65
8	-14	168	170
8	-8	158	172
8	-7	129	114
8	-6	128	-120
8	-5	189	-209
8	-1	98	-117
8	1	92	-103
8	2	257	248
8	5	251	-261
8	6	118	108
7	-10	198	204
7	-9	209	-196
7	-6	295	-316
7	-5	128	155
7	-4	128	-167
7	-3	266	-286
7	-2	355	-343
7	-1	105	-133
7	2	350	348
7	3	249	-237
7	6	203	199
7	9	121	141
7	14	160	-167
6	-15	116	-137
6	-14	231	-241
6	-13	111	122
6	-11	113	133
6	-10	325	325
6	-9	342	-346
6	-8	310	319
6	-7	240	263
6	-6	81	-64
6	-5	257	-257
6	-4	109	119
6	-3	197	182
6	-2	149	164
6	-1	336	-331
6	1	328	-328
6	2	623	-590
6	3	187	208
6	4	124	165
6	5	471	486
6	6	378	377
6	7	246	-254
6	12	127	153
5	-18	144	-162
5	-17	183	-199
5	-14	170	-150
5	-11	286	-291
5	-9	337	331
5	-7	261	268
5	-6	215	-241
5	-4	89	101
5	-3	260	248
5	-2	361	348
5	-1	372	-375
5	0	157	80
5	1	173	-163
5	2	96	-77
5	3	143	112
5	4	272	-261
5	5	231	-246
5	6	379	376
5	9	265	272
5	13	191	177
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4	-15	103	41
4	-13	414	-411
4	-11	161	-161
4	-10	129	-128
4	-7	162	162
4	-6	593	619
4	-5	97	97
4	-4	101	[illegible]
4	-3	458	446
4	-2	100	41
4	-1	274	-277
4	0	367	375
4	1	514	508
4	2	392	-408
4	3	96	-99
4	4	131	-128
4	5	232	-227
4	6	118	136
4	10	129	146
3	-17	141	121
3	-14	188	-211
3	-13	341	-360
3	-11	78	113
3	-10	345	-343
3	-9	367	371
3	-8	95	-104
3	-7	144	-123
3	-6	244	-220
3	-5	454	-454
3	-4	139	139
3	-3	457	464
3	-2	909	900
3	-1	655	662
3	1	70	-91
3	2	422	371

values are small and do not justify a discussion of the effects of external influences on the molecular structures.

The equations of the equally weighted least-squares planes through the benzene and thiazole rings (excluding the S(2) sulphur atoms), as well as the deviations of the individual atoms from these planes, are listed in Table 5. As in the case of sulphathiazole II the deviations of the benzene ring atoms from the best planes are very small while the substituent sulphur and nitrogen atoms are markedly displaced. The five membered ring is non-planar as shown by the displacement of the sulphur atom and the substituent nitrogen atoms also deviate considerably from the best planes. The dihedral

Table 2 (*cont.*)

3	4	96	98
3	6	323	-307
3	7	199	195
3	8	138	-176
3	9	282	-289
3	10	287	302
3	14	151	154
2	-21	192	187
2	-18	132	-100
2	-17	98	-128
2	-15	154	172
2	-14	317	345
2	-11	154	-164
2	-9	223	-209
2	-8	83	-103
2	-6	787	759
2	-5	128	119
2	-3	350	349
2	-2	496	472
2	-1	205	-204
2	0	61	68
2	1	264	285
2	2	664	662
2	3	132	-151
2	5	274	261
2	6	341	350
2	7	135	138
2	9	568	-566
2	10	92	-106
2	13	311	289
2	14	119	-120
1	-18	242	247
1	-17	100	-90
1	-15	138	149
1	-14	292	-295
1	-10	164	-169
1	-9	366	-382
1	-7	471	459
1	-6	256	285
1	-5	144	175
1	-4	99	-127
1	-3	1147	-1199
1	-2	488	497
1	0	124	94
1	1	415	422
1	2	350	-310
1	3	467	467
1	4	172	-146
1	5	342	-352
1	6	194	-214
1	7	122	-136
1	8	91	102
1	9	384	-391
1	10	476	485
1	12	114	-80
1	13	315	-313
1	14	130	112
0	-18	183	166
0	-16	167	168
0	-14	346	340
0	-12	171	-169
0	-10	837	804
0	-8	115	124
0	-6	591	-605
0	-4	66	-72
0	-2	3767	4016
0	0	240	-154
0	2	155	-163
0	6	684	673
0	8	136	-167
0	10	447	-439
0	14	232	237
	6, K, L		
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0	-2	122	-130
0	0	336	328
0	2	107	89
0	4	516	525
0	10	183	159
0	12	105	-32
	11, K, L		
10	-7	131	114
9	-13	145	-161
9	-8	145	-142
9	-7	105	-81
9	-5	157	137
9	-3	131	119
9	-1	113	89
9	1	121	134
9	5	162	-176
8	-10	139	-118
8	-8	118	-90
8	-7	133	-131
8	-6	103	103
8	-5	149	-162
8	-3	111	-117
8	-2	218	230
8	-1	186	190
8	1	111	142
8	4	131	141
8	6	117	-115
7	-17	143	-164
7	-15	116	100
7	-14	254	247
7	-10	201	-198
7	-6	156	-164
7	-5	135	146
7	-3	149	150
7	1	123	109
7	2	181	182
7	3	155	168
7	6	122	-108
7	7	128	122
6	-17	150	152
6	-15	104	57
6	-10	204	204
6	-9	107	-126
6	-8	94	-101
6	-7	405	-405
6	-5	103	135
6	-3	341	-338
6	1	180	187
6	2	119	122
6	6	106	124
6	9	162	-170
5	-18	176	165
5	-14	115	99
5	-13	126	121
5	-11	327	322
5	-7	206	220
5	-6	300	-306
5	-5	178	-171
5	-3	266	-253
5	-2	358	357
5	2	288	-297
5	3	183	201
5	4	204	224
5	5	208	190
5	9	148	171
5	10	200	-214
4	-18	156	-184
4	-17	127	-55
4	-14	253	255
4	-13	134	142
4	-11	190	-216
4	-9	180	201
4	-7	167	169
4	-6	141	-152
4	-5	271	275
4	-3	465	-461
4	-2	355	-352
4	0	157	-177
4	1	123	135
4	2	446	440
4	5	350	-352
4	6	352	358
4	8	248	233
4	10	158	-151
3	-21	114	-85
3	-15	226	-210
3	-11	290	314
3	-10	123	137
3	-9	154	-159
3	-7	219	-224
3	-6	528	519
3	-5	187	-207
3	-4	199	196
3	-2	537	-549
3	-1	111	113
3	2	496	-500
3	4	189	-224
3	5	399	398
3	9	119	160
3	10	113	85
3	12	153	120
3	13	218	-220
2	-15	156	-180
2	-13	110	134
2	-10	701	-721
2	-9	512	525
2	-8	95	-57
2	-7	293	302
2	-6	143	-124
2	-5	173	-154
2	-4	124	132
2	-3	105	105
2	-2	268	-274
2	-1	97	-101
2	1	824	-837
2	2	110	129
2	4	149	148
2	6	265	-263
2	7	123	99
2	8	131	-123
2	9	249	244
2	13	124	150
1	-21	193	189
1	-18	137	-81
1	-11	377	-383
1	-10	378	385
1	-8	77	-88
1	-7	97	-106
1	-6	181	-154
1	-5	308	314
1	-3	538	540
1	-2	601	-582
1	-1	144	-127
1	1	426	422
1	3	215	-231
1	4	272	-301
1	5	407	-402
1	6	104	106
1	8	134	141
1	9	187	176
1	13	228	225
1	14	139	-103
0	-14	801	-801
0	-10	330	-344
0	-6	72	-105
0	-4	128	112
0	-2	539	-513
0	0	234	236
0	2	806	-807
0	6	219	-212
0	8	108	-120
0	14	116	113
	12, K, L		
9	-9	136	139
9	-7	119	-79
9	-6	125	159
8	-9	170	162
8	-8	116	93
8	-2	189	183
8	1	112	-128
7	-16	116	-112
7	-11	109	-118
7	-9	101	-80
7	-5	209	212
7	-4	122	125
7	-3	133	-130
7	0	211	-204
6	-17	114	106
6	-11	161	153
6	-9	91	96
6	-7	118	126
6	-5	252	275
6	-2	136	108
6	2	98	86
6	7	181	-165
5	-15	103	-120
5	-14	102	93
5	-13	98	82
5	-12	262	-255
5	-8	223	245
5	-6	114	-114
5	-5	155	-169
5	-4	312	328
5	-3	98	112
5	-1	366	369
5	1	119	-166
5	2	112	-98
5	3	216	-221
5	4	118	-110

angles in the four molecules are listed in Table 5. The big differences between them are the only significant quantitative differences between the molecular geometry in the polymorphs of sulphathiazole.

The crystal structures of sulphathiazole I and III are illustrated by the stereo pairs (Johnson, 1965) of their unit-cell contents in Figs. 2 and 3. Hydrogen bond distances and other close intermolecular approaches are listed in Table 6.

In sulphathiazole I, centrosymmetric dimers are formed by pairs of molecules through symmetrical hydrogen bonds between nitrogen atoms N(2) and N(3). Separate dimers are bonded together through hydrogen bonds between atoms N(1) and O(1) and O(2). Only

Table 2 (*cont.*)

5	10	188	-201
4	-16	163	136
4	-15	121	-100
4	-13	256	261
4	-12	106	-84
4	-11	211	191
4	-8	428	-422
4	-5	224	237
4	-4	235	227
4	-3	240	231
4	-1	200	214
4	0	356	357
4	2	147	189
4	4	162	-186
4	5	134	124
4	6	141	104
4	7	253	-248
4	8	181	-196
4	10	164	-164
3	-16	237	229
3	-15	130	142
3	-13	126	134
3	-12	294	291
3	-11	392	-413
3	-9	236	-235
3	-8	257	252
3	-7	145	148
3	-5	412	-421
3	-4	105	-141
3	-3	265	264
3	-2	211	-220
3	-1	80	105
3	0	557	558
3	1	171	-162
3	3	165	179
3	4	328	323
3	7	397	-403
3	12	119	-121
2	-15	418	403
2	-13	177	198
2	-11	190	-204
2	-9	437	447
2	-8	228	221
2	-7	302	-329
2	-5	569	-570
2	-4	155	-147
2	-2	118	-127
2	-1	181	-184
2	0	84	49
2	1	449	448
2	3	254	248
2	6	99	86
2	7	130	95
2	11	316	-333
2	12	130	-119
1	-19	114	-93
1	-15	97	79
1	-12	659	655
1	-11	340	358
1	-9	226	214
1	-8	511	-499
1	-7	87	-74
1	-5	282	-296
1	-4	304	298
1	-3	385	-373
1	-2	151	167
1	-1	495	-497
1	0	93	-57
1	2	93	-80
1	3	660	-692
1	4	630	625
1	6	150	117
1	7	173	181
1	8	111	-137
1	9	99	-41
0	-20	125	-137
0	-13	139	150
0	-12	452	451
0	-8	638	631
0	-6	98	30
0	-4	215	-227
0	-2	191	-235
0	0	749	-769
0	2	363	-355
0	4	288	301
0	10	131	136
9	-7	223	-251
9	-4	136	-90
8	-13	113	88
8	-10	206	-183
8	-6	123	-132
8	-3	261	-298
8	5	122	125
7	-13	134	-105
7	-10	202	189
7	-7	111	75
7	-6	226	-209
7	-3	162	-171
7	2	217	231
7	4	107	53
7	6	118	151
6	-14	120	-81
6	-11	112	89
6	-10	133	138
6	-9	215	-221
6	-6	136	-148
6	-5	148	-156
6	-4	118	150
6	-3	155	-140
6	-2	199	-184
6	0	99	-124
6	2	136	-145
6	6	144	153
6	9	132	115
5	-18	147	-187
5	-17	156	-167
5	-15	128	-126
5	-14	130	127
5	-13	180	178
5	-12	96	-56
5	-7	229	229
5	-6	374	363
5	-4	129	128
5	-3	104	96
5	-2	224	-229
5	-1	194	-229
5	1	132	-133
5	2	283	264
5	5	109	98
5	6	142	124
5	9	244	245
4	-17	136	-114
4	-15	130	-139
4	-14	301	-299
4	-13	173	-171
4	-7	172	174
1	-6	391	393
1	-4	133	115
1	-3	340	352
4	-2	344	-318
1	2	111	-113
1	4	101	-80
4	10	161	175
3	-18	155	148
3	-14	334	-301
3	-13	150	-130
3	-11	106	-110
3	-10	197	-204
3	-9	271	284
3	-6	215	223
3	-4	175	201
3	-3	521	535
3	-2	530	522
3	0	156	158
3	2	291	-282
3	5	106	-83
2	-21	203	193
2	-17	157	-130
2	-15	196	195
2	-14	117	107
2	-13	110	130
2	-11	101	-123
2	-9	133	-162
2	-5	297	317
2	-3	212	211
2	-2	310	307
2	1	579	591
2	2	209	213
2	5	102	-87
2	6	256	-245
2	8	117	-129
2	12	155	-119
1	-18	125	111
1	-17	132	140
1	-15	101	98
1	-14	111	-105
1	-13	153	151
1	-11	190	204
1	-10	267	-280
1	-9	205	-214
1	-7	116	-107
1	-5	447	117
1	-3	84	-136
1	-2	98	94
1	-1	239	229
1	1	162	181
1	2	194	218
1	3	158	142
1	4	153	152
1	6	138	-161
1	9	148	-137
0	-18	213	218
0	-14	303	311
0	-10	359	361
0	-6	236	-255
0	-2	263	249
0	0	225	-209
0	2	348	363
0	4	134	151
0	8	176	-143
14, K, L			
9	-7	119	151
9	2	130	-119
8	-9	113	-155
8	-5	107	-41
8	-4	105	[illegible]
8	-2	110	132
8	-1	123	132
8	0	182	-167
7	-13	131	-190
7	-11	111	98
7	-8	226	-230
7	-7	121	-129
7	[illegible]	113	-131
7	-4	115	88
6	-10	122	-75
6	-9	127	-111
6	[illegible]	123	-129
6	[illegible]	228	-221
6	-4	371	-369
6	-3	111	115
6	-1	228	206
6	0	120	120
6	6	133	142
5	-17	111	-76
5	-15	137	152
5	-13	173	158
5	-12	191	-159
5	-11	116	-109
5	-9	164	-128
5	-5	228	-231
5	-4	158	-163
5	-1	302	-305
5	0	112	-104
5	3	152	164
5	4	119	-156
4	-17	109	-90
4	-15	101	51
4	-12	167	163
4	-11	112	105
4	-9	92	104
4	-8	294	-293
4	-4	192	-196
4	-3	118	-127
4	0	238	239
4	2	94	100
3	-16	214	-207
3	-12	141	137
3	-11	167	-175
3	-9	139	161
3	-8	101	117
3	-5	287	-281
3	-4	306	-283
3	-1	229	214
3	0	376	-379
3	2	150	-153
3	4	356	351
3	6	157	137
3	11	162	-158
2	-17	130	-146
2	-16	149	-157
2	-12	196	-200
2	-9	120	129
2	-7	249	-265
2	-6	100	96
2	-4	148	163
2	-3	91	-106
2	-1	142	-152
2	7	383	384
1	-20	133	-116
1	-16	165	153
1	-5	517	537
1	-4	164	[illegible]
1	[illegible]	88	[illegible]
1	-1	148	171
1	0	137	160
1	1	98	-110
1	2	113	83
1	7	107	113
1	11	161	150
0	-16	131	-147
0	-12	231	-271
0	-8	419	[illegible]
0	-4	190	[illegible]
0	0	198	181
0	2	85	-78
0	4	109	-85
0	8	313	331
15, K, L			
9	-8	118	96
9	-5	135	133
9	-3	150	-153
8	-7	157	112
7	-10	137	100
7	-7	116	-116
7	-4	111	104
7	1	177	-177
6	-14	112	17
6	-9	101	-103
6	-7	108	103
6	-6	102	53
6	-5	106	-99
6	1	123	-105
5	-10	98	89
5	-9	121	128
5	-2	164	-119
5	3	103	-63
5	4	110	-117
5	5	162	-168
4	-11	189	-186
4	-7	105	-122
4	-6	112	119
4	-5	172	-159
4	1	130	-128
4	2	342	-323
4	6	145	-86
3	-17	152	-119
3	-16	103	70
3	-14	107	96
3	-11	160	-182
3	-10	389	-382
3	-5	195	233
3	-3	260	263
3	-1	155	-166
3	1	129	-114
3	2	122	106
3	3	97	68
3	4	183	174
3	5	191	-172
3	6	248	-260
2	-14	107	-38
2	-13	121	-109
2	-10	317	325
2	-9	187	-187
2	-7	388	-401
2	-5	160	140
2	1	398	399
2	4	124	82
2	5	123	-140
2	9	184	-196
1	-21	158	-142
1	-18	111	117
1	-14	172	-163
1	-11	187	197
1	-10	98	-91
1	[illegible]	163	-158
1	[illegible]	178	-195
1	-5	83	-122
1	-3	278	-287
1	-2	118	[illegible]
1	1	164	-170
1	2	128	-140
1	4	122	170
1	5	306	286
1	10	134	-136
0	-14	419	425
0	-10	160	121
0	-6	104	-38
0	0	98	-113
0	2	418	414
0	4	105	73
0	8	198	202
16, K, L			
7	-7	119	131
7	0	118	173
6	-12	152	148
6	-9	116	-128
6	-5	172	-193
5	-13	137	121
5	-12	117	112
5	-9	170	141
5	-8	162	-157
5	-5	97	-51
5	-1	135	-122
5	0	101	-117
5	7	141	127
4	-15	153	122
4	-13	127	-139
4	-8	168	153
4	-7	91	86
4	-5	131	-147
4	-1	242	-230
4	0	103	84
4	1	101	-70
4	2	110	-132
4	3	225	-198
4	4	159	178
3	-17	120	-102
3	-12	133	-131
3	-8	232	220
3	-5	200	221
3	-4	173	-190
3	-3	90	-81
3	-1	126	-114
3	0	310	-302
3	1	159	-115
3	7	123	119
2	-16	129	-95
2	-15	119	-111
2	-13	138	-137
2	-12	237	-213
2	-11	161	150
2	-8	90	-110
2	-7	90	111
2	-5	280	274
2	1	121	-92
2	3	149	-146
2	4	166	-158
2	6	107	-121
1	-11	111	-138
1	-9	126	-150
1	-5	209	215
1	-4	311	333
0	-16	186	-186
0	-12	315	-311
0	-8	311	-317
0	-4	113	-190
0	0	117	78
0	2	172	174
0	4	175	-167
17, K, L			
8	-10	128	109
8	-3	153	189
7	-6	171	176
7	-4	119	-75
6	-10	110	-90
6	-7	112	84
6	-3	114	156
6	-2	138	115
6	2	133	119
5	-9	111	-96
5	-7	190	-213
5	0	127	-93
5	1	104	23
1	-18	112	103
1	-15	171	115
1	-14	106	[illegible]
1	-13	155	102
1	-11	117	100
1	-10	116	-120
1	-2	217	213
1	0	122	86
1	[illegible]	129	-116
3	-14	179	192
3	-10	250	231
3	-7	130	-121
3	-6	172	-168
3	-4	151	-161
3	0	121	-118
3	2	221	212
3	5	110	-130
2	-11	162	189
2	-10	151	171
2	-9	103	-71
2	-7	189	-162
2	-3	193	-186
2	-2	100	-96
2	-1	122	136
2	2	109	-92
1	-14	197	182
1	-6	136	165
1	-5	168	-159
1	-3	155	-141
1	-1	126	-95
1	1	359	-361
1	2	188	196
1	-10	178	172
0	-2	175	-162
18, K, L			
7	-4	141	-115
6	-7	108	-76
6	-6	108	102
5	-9	114	90
5	-8	112	53
5	-5	191	197
5	-3	103	-71
5	[illegible]	142	[illegible]
4	-1	133	[illegible]
4	-8	226	230
4	0	197	-203
3	-12	189	-186
3	-11	181	178
3	-5	317	297
3	-4	254	[illegible]
3	4	156	-156
2	-17	115	111
2	-16	115	83
2	-9	164	-143
2	-7	230	225
2	-5	129	99
2	-4	116	17
2	-1	331	[illegible]
2	1	110	-75
2	4	115	-91
2	7	134	[illegible]
1	-15	129	89
1	-13	161	109
1	-12	137	-123
1	-5	150	-148
1	-4	122	129
1	3	139	[illegible]
1	4	151	-180
0	-12	157	118
0	-8	334	-326
0	0	225	198
0	2	121	118
19, K, L			
7	-10	147	-170
6	-7	156	-171
6	1	126	132
5	-10	131	-119
5	-3	199	-187
4	-14	203	221
4	-10	114	-75
4	-6	245	-214
4	-1	113	-77
4	2	223	232
3	-18	121	-100
3	-13	117	-81
3	-11	129	123
3	-10	257	266
3	-3	143	-137
3	-2	245	-251
3	0	176	-121
3	5	153	149
2	-15	111	-124
2	-14	132	-87
2	-11	122	76
2	-7	229	245
2	-5	155	-133
1	-11	165	-174
1	-10	123	156
1	-7	187	183
1	-3	232	237
1	-2	151	-127
0	-14	303	-290
0	-2	124	109
0	0	104	113
0	2	277	-273
20, K, L			
7	-8	141	123
6	-5	177	170
5	-8	172	178
5	-1	136	138
1	-12	[illegible]	[illegible]
4	-4	[illegible]	[illegible]
4	-1	158	[illegible]
3	-8	111	[illegible]
3	-7	[illegible]	101
3	[illegible]	[illegible]	[illegible]
3	0	179	[illegible]
2	-15	180	[illegible]
2	-12	[illegible]	[illegible]
2	-11	121	-211
2	-9	128	[illegible]
2	-5	[illegible]	-258
2	3	152	[illegible]
1	-8	[illegible]	-111
1	[illegible]	[illegible]	[illegible]
1	-1	[illegible]	[illegible]
1	0	188	[illegible]
1	2	111	86
0	1	133	120
0	-12	302	287
0	-4	177	-172
21, K, L			
4	-10	142	143
4	-5	117	106
3	-14	133	-123
3	-7	[illegible]	[illegible]
3	-6	141	[illegible]
3	-4	115	98
2	-11	[illegible]	-158
2	-7	173	[illegible]
2	-3	[illegible]	[illegible]
1	-11	138	-138
1	-10	101	[illegible]
1	-5	104	88
1	-2	140	[illegible]
1	-1	[illegible]	[illegible]
1	0	131	87
1	1	[illegible]	[illegible]
1	2	[illegible]	-124
0	-16	250	-232
0	-6	139	-128
0	-4	109	[illegible]
0	-2	187	183
22, K, L			
3	-3	161	-186
1	-13	128	71
1	-8	161	-137
3	-12	133	128
0	-8	198	[illegible]
23, K, L			
3	-10	115	-114
3	-7	135	129
1	-11	123	118
1	-10	144	-171
0	-14	118	107
0	-6	170	-152
24, K, L			
2	-5	118	106
1	-8	145	124
0	-12	167	-160
0	-8	128	-129
0	-4	152	156

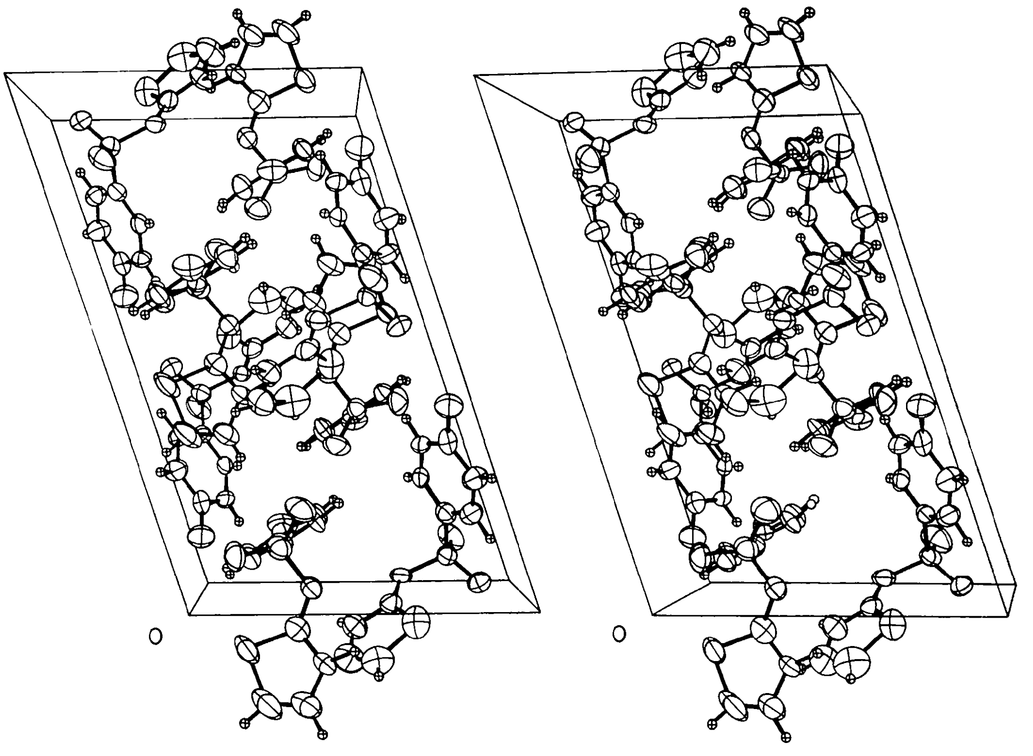

Fig. 2. A stereopair showing the unit cell and its contents of sulphathiazole I viewed along the *b* axis with the *a* axis horizontal.

Table 3. *Positional and thermal parameters*

(*a*) Atomic parameters (× 10^4) with e.s.d.'s for the non-hydrogen atoms of sulphathiazole I and III.
Positional parameters are given as fractional coordinates and thermal parameters are given according to the expression

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

The e.s.d.'s are given in brackets and refer to the least significant figures in the parameter values. The values given for each parameter are from top to bottom, for sulphathiazole I, molecules *A* and *B*, and sulphathiazole III, molecules *A* and *B* respectively.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
S(1)	3221 (3)	709 (2)	1220 (2)	109 (3)	71 (2)	40 (1)	−1 (2)	11 (2)	9 (1)
	8063 (2)	4260 (2)	884 (2)	84 (3)	84 (2)	32 (1)	−2 (2)	10 (1)	11 (1)
	3829 (1)	3982 (2)	5584 (1)	22 (1)	87 (2)	29 (1)	3 (1)	5 (1)	1 (1)
	8916 (1)	3802 (2)	8178 (1)	23 (1)	77 (2)	27 (1)	4 (1)	3 (1)	0 (1)
S(2)	1301 (3)	4338 (3)	4303 (2)	90 (3)	149 (3)	57 (2)	−14 (3)	−9 (2)	25 (2)
	6434 (3)	2537 (2)	4660 (2)	157 (4)	61 (2)	72 (2)	−3 (3)	36 (2)	6 (2)
	3558 (1)	1741 (2)	3781 (1)	64 (1)	139 (3)	29 (1)	16 (1)	13 (1)	1 (1)
	8635 (1)	1513 (2)	6404 (1)	71 (1)	128 (3)	26 (1)	13 (1)	12 (1)	1 (1)
O(1)	1868 (6)	402 (5)	1801 (4)	106 (8)	96 (6)	68 (4)	−23 (5)	29 (4)	10 (4)
	8375 (6)	5270 (5)	1193 (4)	146 (9)	79 (6)	60 (4)	−32 (6)	2 (4)	13 (4)
	4314 (2)	4781 (4)	6445 (2)	28 (2)	100 (6)	41 (2)	3 (3)	−1 (2)	−10 (3)
	9397 (2)	4611 (4)	9027 (3)	33 (2)	102 (6)	42 (2)	−3 (3)	−1 (2)	−20 (3)
O(2)	4206 (7)	345 (6)	1951 (4)	167 (10)	90 (6)	48 (4)	12 (7)	7 (5)	20 (4)
	8726 (6)	3875 (6)	342 (4)	120 (9)	162 (8)	36 (3)	12 (7)	29 (4)	18 (4)
	3761 (2)	4755 (5)	4733 (3)	31 (2)	141 (6)	44 (2)	6 (3)	14 (2)	27 (3)
	8870 (2)	4502 (5)	7323 (3)	33 (2)	136 (7)	40 (2)	3 (3)	13 (2)	20 (3)
N(1)	3359 (8)	5164 (7)	1483 (5)	197 (13)	53 (7)	45 (4)	−1 (8)	26 (6)	7 (4)
	9410 (8)	1607 (7)	3827 (5)	169 (12)	93 (8)	49 (4)	22 (8)	26 (6)	38 (5)
	449 (3)	3047 (7)	5498 (3)	26 (3)	95 (7)	37 (3)	−4 (7)	7 (3)	1 (3)
	5538 (3)	3230 (6)	8172 (3)	31 (2)	104 (8)	43 (3)	7 (4)	10 (2)	13 (4)
N(2)	3758 (7)	345 (6)	476 (5)	87 (8)	77 (6)	41 (4)	6 (6)	8 (5)	−1 (4)
	6470 (7)	4295 (6)	462 (4)	106 (9)	66 (6)	27 (3)	6 (7)	10 (4)	−4 (4)
	4202 (3)	2246 (5)	5693 (3)	30 (2)	108 (8)	29 (2)	19 (3)	7 (2)	2 (4)
	9258 (3)	2050 (5)	8318 (3)	29 (2)	82 (6)	29 (2)	11 (3)	4 (2)	−1 (3)
N(3)	3433 (6)	4937 (6)	4086 (5)	88 (9)	66 (6)	36 (4)	−10 (6)	−7 (5)	1 (4)
	4550 (8)	1308 (6)	4508 (5)	109 (10)	58 (6)	47 (4)	12 (7)	4 (5)	7 (4)
	4107 (3)	−219 (5)	5081 (3)	33 (2)	102 (7)	40 (3)	0 (3)	15 (2)	−2 (4)
	9202 (3)	−439 (5)	7706 (3)	29 (2)	83 (7)	33 (2)	4 (3)	14 (2)	−4 (3)
C(1)	3324 (9)	4137 (8)	1383 (5)	104 (13)	83 (9)	22 (4)	−4 (9)	14 (5)	5 (5)
	9085 (9)	2234 (8)	3144 (6)	78 (11)	69 (9)	50 (5)	−2 (8)	16 (6)	−1 (5)
	1233 (3)	3298 (6)	5491 (3)	23 (2)	79 (8)	32 (3)	−3 (3)	9 (2)	−10 (4)
	6334 (3)	3374 (6)	8142 (3)	28 (2)	75 (7)	28 (3)	2 (3)	5 (2)	1 (4)
C(2)	4467 (9)	3558 (8)	1703 (6)	103 (12)	66 (8)	49 (5)	−8 (9)	11 (6)	−8 (5)
	9512 (9)	1992 (7)	2456 (6)	151 (14)	66 (7)	44 (5)	38 (9)	30 (7)	9 (5)
	1357 (3)	4184 (6)	4813 (3)	25 (2)	81 (8)	24 (3)	4 (3)	2 (2)	−4 (4)
	6452 (3)	4135 (6)	7420 (3)	20 (2)	99 (9)	28 (3)	8 (4)	1 (2)	2 (4)
C(3)	4466 (8)	2528 (10)	1644 (5)	56 (9)	102 (10)	38 (5)	8 (9)	−10 (5)	1 (6)
	9145 (9)	2582 (9)	1766 (6)	130 (12)	93 (9)	35 (5)	20 (10)	28 (6)	−1 (6)
	2152 (3)	4391 (6)	4831 (3)	27 (2)	100 (8)	25 (2)	1 (3)	7 (2)	−2 (4)
	7225 (3)	4267 (6)	7408 (3)	33 (3)	83 (8)	23 (2)	6 (4)	6 (2)	6 (3)
C(4)	3281 (8)	2031 (7)	1254 (5)	83 (10)	66 (7)	27 (4)	12 (7)	9 (5)	15 (4)
	8400 (8)	3456 (7)	1738 (5)	73 (11)	63 (7)	33 (4)	3 (8)	5 (5)	−7 (4)
	2830 (3)	3743 (6)	5548 (3)	23 (2)	76 (7)	23 (2)	2 (3)	4 (2)	−4 (4)
	7900 (3)	3630 (6)	8141 (3)	25 (2)	76 (7)	28 (2)	−2 (3)	7 (2)	−2 (3)
C(5)	2136 (9)	2591 (9)	908 (6)	90 (11)	83 (8)	44 (5)	−12 (9)	6 (6)	−9 (6)
	8023 (8)	3711 (7)	2416 (5)	73 (10)	66 (7)	36 (4)	5 (7)	16 (5)	−8 (5)
	2710 (4)	2866 (7)	6237 (4)	25 (3)	109 (8)	25 (3)	−2 (4)	2 (2)	3 (4)
	7778 (4)	2888 (7)	8867 (4)	33 (3)	107 (8)	27 (3)	19 (4)	4 (2)	11 (4)
C(6)	2152 (8)	3628 (9)	974 (5)	68 (11)	91 (9)	44 (4)	8 (9)	−7 (5)	−7 (5)
	8335 (9)	3114 (7)	3095 (5)	96 (11)	78 (8)	28 (4)	17 (8)	19 (5)	14 (4)
	1943 (4)	2670 (6)	6225 (4)	32 (3)	80 (9)	33 (3)	−3 (4)	12 (2)	9 (4)
	6991 (4)	2770 (6)	8880 (4)	30 (3)	103 (8)	26 (3)	8 (4)	9 (2)	13 (4)
C(7)	2970 (9)	4654 (7)	4707 (6)	110 (11)	44 (7)	48 (5)	13 (7)	11 (6)	1 (5)
	5873 (9)	1402 (8)	4944 (6)	116 (13)	63 (7)	38 (4)	−9 (8)	30 (6)	−17 (5)
	3982 (3)	1324 (7)	4958 (4)	28 (2)	112 (9)	37 (3)	7 (4)	14 (2)	12 (4)
	9062 (3)	1101 (7)	7600 (3)	18 (2)	103 (8)	30 (3)	2 (4)	2 (2)	1 (4)
C(8)	2544 (11)	4866 (8)	3319 (6)	138 (15)	91 (9)	45 (5)	−26 (10)	−9 (7)	1 (5)
	4053 (12)	2068 (10)	3951 (7)	159 (18)	74 (8)	68 (7)	38 (11)	12 (9)	7 (6)
	3875 (4)	−1084 (7)	4268 (4)	46 (3)	126 (9)	49 (3)	1 (5)	16 (3)	23 (5)
	8972 (4)	−1309 (7)	6907 (4)	35 (3)	139 (10)	47 (4)	5 (5)	16 (3)	−20 (5)
C(9)	1388 (11)	4521 (11)	3310 (7)	129 (14)	148 (13)	60 (6)	−51 (12)	−23 (7)	24 (7)
	4924 (14)	2791 (9)	3957 (7)	262 (22)	47 (9)	76 (7)	10 (11)	44 (10)	13 (6)
	3562 (5)	−217 (8)	3504 (4)	58 (4)	156 (11)	39 (3)	9 (6)	10 (3)	−13 (5)
	8648 (5)	−452 (7)	6141 (4)	75 (5)	123 (10)	47 (4)	15 (6)	26 (4)	−21 (5)

Table 3 (*cont.*)

(*b*) Fractional coordinates (× 10^3) with e.s.d.'s for the hydrogen atoms of sulphathiazole I and III

	x	*y*	*z*
H(1)	—	—	—
	—	—	—
	22 (5)	327 (10)	494 (6)
	508 (4)	356 (9)	770 (5)
H(2)	—	—	—
	—	—	—
	50 (4)	199 (8)	574 (5)
	537 (4)	223 (9)	831 (5)
H(3)	519 (12)	402 (10)	203 (7)
	−3 (13)	129 (10)	248 (7)
	95 (5)	464 (10)	432 (5)
	603 (5)	459 (10)	686 (6)
H(4)	531 (11)	212 (10)	200 (7)
	942 (12)	243 (10)	128 (7)
	229 (5)	479 (10)	439 (6)
	744 (6)	477 (10)	676 (5)
H(5)	145 (12)	216 (10)	65 (7)
	766 (11)	432 (10)	244 (7)
	317 (5)	246 (10)	667 (6)
	819 (5)	255 (10)	921 (6)
H(6)	128 (11)	401 (9)	67 (7)
	814 (11)	329 (9)	358 (7)
	189 (5)	199 (10)	673 (6)
	696 (5)	221 (10)	946 (6)
H(7)	441 (12)	523 (9)	435 (7)
	422 (12)	66 (10)	454 (8)
	439 (5)	− 58 (10)	565 (6)
	941 (5)	− 86 (10)	838 (6)
H(8)	727 (13)	16 (10)	217 (8)
	318 (15)	209 (10)	376 (9)
	389 (6)	−225 (11)	424 (6)
	902 (6)	−246 (11)	698 (6)
H(9)	57 (14)	445 (12)	296 (8)
	483 (15)	330 (10)	371 (9)
	311 (6)	− 60 (12)	273 (6)
	880 (6)	− 74 (11)	534 (6)

symmetry-related molecules are bonded, *i.e.* no hydrogen bonds exist between the independent molecules I*A* and I*B*. This means that two intermeshed but independent systems of hydrogen bonded molecules exist in the crystal. These systems are the same except that N(1*A*) is bonded only to O(1*A*) while N(1*B*) is bonded to both O(1*B*) and O(2*B*). All the hydrogen bond distances have normal values. The hydrogen bonding network is shown in Fig. 4.

The crystal structure of, and the hydrogen bonding in, sulphathiazole III is very similar to that of sulphathiazole II. The nitrogen atom N(2) does not participate in any hydrogen bonding and its only close approach that can be regarded as a van der Waals interaction is the N(1*A*)···N(2*B*) distance of 3·223 Å. The independent molecules III*A* and III*B* are bonded into integrated, irregular sheets of molecules that are parallel to the (001) plane. The hydrogen bonding in sulphathiazole III is illustrated by the schematic diagram in Fig. 5. Neighbouring molecules are hydrogen bonded through N(1)···O(1) and N(1)···N(3) bonds. The absence of one N(1*A*)···O(1*B*) bond implies that the oxygen atom of molecule III*A* that participates in hydrogen bonding, is bonded to the amine nitrogen atoms of two separate III*B* molecules, while the oxygen atom of molecule III*B* is bonded to the amine nitrogen atom of only one III*A* molecule.

Table 4. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s of sulphathiazole* I *and* III

(*a*) Bond lengths

	I*A*	I*B*	III*A*	III*B*	Mean
N(1)–C(1)	1·368 (11)	1·382 (11)	1·399 (8)	1·422 (8)	1·394 (18)
C(1)–C(2)	1·390 (12)	1·419 (13)	1·386 (7)	1·385 (7)	1·395 (13)
C(2)–C(3)	1·365 (14)	1·363 (12)	1·398 (8)	1·370 (8)	1·375 (13)
C(3)–C(4)	1·386 (12)	1·389 (13)	1·393 (6)	1·399 (7)	1·392 (5)
C(4)–C(5)	1·384 (12)	1·377 (11)	1·393 (7)	1·386 (8)	1·385 (9)
C(5)–C(6)	1·375 (14)	1·355 (11)	1·350 (9)	1·395 (9)	1·369 (16)
C(6)–C(1)	1·390 (12)	1·395 (12)	1·430 (7)	1·375 (7)	1·397 (18)
C(4)–S(1)	1·749 (9)	1·748 (10)	1·745 (5)	1·769 (6)	1·754 (9)
S(1) —O(1)	1·432 (6)	1·436 (7)	1·450 (4)	1·440 (4)	1·440 (6)
S(1) —O(2)	1·437 (6)	1·415 (7)	1·446 (4)	1·435 (4)	1·434 (10)
S(1) -N(2)	1·615 (8)	1·612 (7)	1·610 (5)	1·602 (5)	1·606 (9)
N(2)–C(7)	1·316 (10)	1·296 (10)	1·321 (7)	1·316 (7)	1·312 (10)
S(2) -C(7)	1·733 (9)	1·736 (10)	1·727 (6)	1·752 (5)	1·738 (9)
C(7)–N(3)	1·349 (11)	1·369 (10)	1·344 (7)	1·343 (7)	1·347 (12)
N(3)–C(8)	1·357 (10)	1·371 (12)	1·385 (7)	1·371 (7)	1·372 (9)
C(8)–C(9)	1·297 (13)	1·324 (14)	1·327 (9)	1·327 (8)	1·318 (11)
C(9)–S(2)	1·742 (12)	1·705 (12)	1·735 (7)	1·737 (7)	1·728 (14)
N(1)–H(1)	—	—	0·82	0·90	0·87
N(1)–H(2)	—	—	0·98	0·96	0·93
C(2)–H(3)	1·00	1·04	0·91	0·98	0·97
C(3)–H(4)	1·06	0·98	0·88	1·28	1·03
C(5)–H(5)	0·91	0·90	0·90	0·78	0·88
C(6)–H(6)	1·03	0·94	1·02	1·04	0·99
N(3)–H(7)	1·06	0·93	0·89	1·03	0·96
C(8)–H(8)	1·00	0·87	1·00	1·00	0·96
C(9)–H(9)	0·89	0·79	1·20	1·40	1·03

Table 4 (*cont.*)

(*b*) Bond angles	I*A*	I*B*	III*A*	III*B*	Mean
N(1)–C(1)–C(2)	120·7 (9)	120·1 (9)	122·5 (5)	121·9 (5)	121·5 (9)
N(1)–C(1)–C(6)	121·9 (9)	122·6 (9)	119·4 (5)	117·2 (5)	120·1 (19)
C(1)–C(2)–C(3)	122·6 (9)	120·4 (9)	120·5 (5)	120·9 (5)	121·0 (8)
C(2)–C(3)–C(4)	119·3 (8)	120·8 (9)	120·1 (5)	119·1 (5)	119·9 (6)
C(3)–C(4)–C(5)	119·3 (9)	118·9 (9)	119·6 (5)	119·6 (5)	119·4 (4)
C(4)–C(5)–C(6)	120·8 (8)	121·2 (9)	120·5 (5)	121·0 (5)	120·7 (4)
C(5)–C(6)–C(1)	120·7 (9)	121·4 (9)	121·2 (6)	118·4 (5)	120·5 (11)
C(6)–C(1)–C(2)	117·4 (9)	117·3 (9)	118·0 (5)	120·9 (5)	118·4 (13)
C(3)–C(4)–S(1)	120·5 (7)	120·1 (7)	120·9 (4)	121·2 (4)	120·7 (4)
C(5)–C(4)–S(1)	120·2 (7)	120·8 (8)	119·5 (4)	119·1 (4)	119·9 (7)
C(4)–S(1) –O(1)	108·2 (4)	107·1 (4)	107·9 (2)	107·1 (3)	107·5 (5)
C(4)–S(1) –O(2)	107·3 (4)	108·1 (4)	107·6 (2)	108·3 (2)	107·8 (4)
O(1)–S(1) –O(2)	117·7 (4)	118·1 (5)	116·1 (2)	116·8 (3)	117·1 (8)
N(2)–S(1) –O(1)	104·2 (4)	103·1·(4)	105·7 (2)	105·8 (2)	104·8 (9)
N(2)–S(1) –O(2)	111·2 (4)	112·2 (4)	113·9 (3)	113·6 (3)	113·0 (11)
N(2)–S(1) –C(4)	107·8 (4)	107·7 (4)	105·0 (3)	104·3 (3)	105·9 (17)
S(1) –N(2)–C(7)	120·9 (5)	120·2 (5)	119·6 (4)	120·4 (4)	120·2 (5)
N(2)–C(7)–S(2)	130·3 (8)	132·0 (8)	131·1 (5)	129·8 (4)	130·8 (8)
N(2)–C(7)–N(3)	120·7 (10)	120·2 (9)	119·4 (5)	122·0 (5)	120·6 (8)
C(7)–N(3)–C(8)	115·3 (8)	114·6 (9)	115·1 (5)	116·7 (5)	115·6 (8)
N(3)–C(8)–C(9)	113·8 (10)	114·1 (10)	113·0 (6)	112·8 (6)	113·5 (5)
C(8)–C(9)–S(2)	111·7 (8)	111·0 (8)	111·1 (5)	111·4 (5)	111·3 (4)
C(9)–S(2) –C(7)	90·0 (5)	92·4 (6)	91·2 (3)	90·9 (3)	91·1 (8)
S(2) –C(7)–N(3)	109·0 (7)	107·8 (8)	109·5 (4)	108·1 (4)	108·6 (6)
H(1)–N(1)–C(1)	—	—	92	122	110
H(2)–N(1)–C(1)	—	—	101	118	112
H(3)–C(2)–C(1)	107	111	125	128	118
H(4)–C(3)–C(4)	120	117	112	111	116
H(5)–C(5)–C(4)	109	120	115	109	114
H(6)–C(6)–C(1)	122	115	122	126	121
H(7)–N(3)–C(7)	123	102	119	116	116
H(8)–C(8)–N(3)	138	134	124	117	127
H(9)–C(9)–C(8)	91	95	129	123	114

Comparison of these two crystal structures with that of sulphathiazole II shows that the main difference lies in the types of hydrogen bonds present and their effects on the arrangement of molecules in the crystal. Although sulphathiazole I has the additional N(2)···N(3) bond and uses O(2) in a N(1)···O(2) bond, the number of bonds per molecule is the same as in form III. The strengths of the hydrogen bonds as shown by their bond distances are very similar and no definite conclusion as to changes in stability due to differing hydrogen bonding can be made. A similar situation has been encountered with the crystal structures of barbital I and II (Craven, Vizzini & Rodrigues, 1969) and amobarbital I and II (Craven & Vizzini, 1969). These structures are also characterized by the small differences between polymorphs.

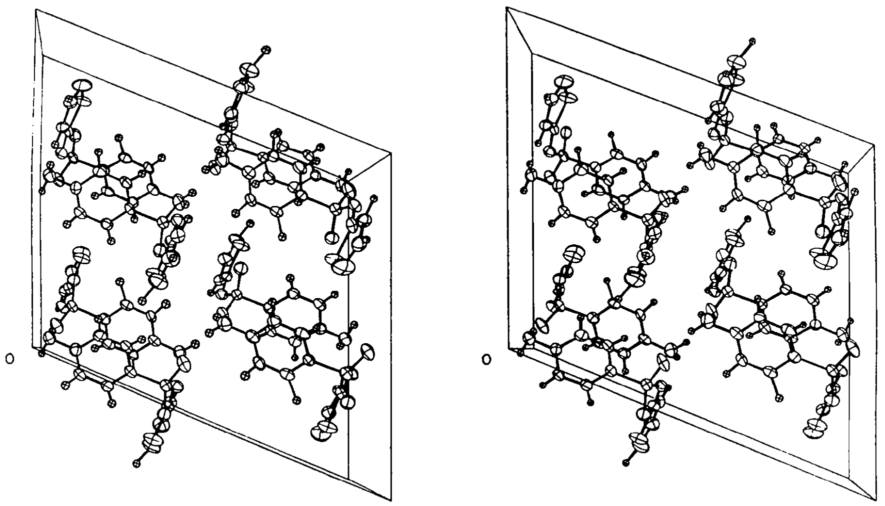

Fig. 3. A stereo pair showing the unit cell and its contents of sulphathiazole III viewed along the *b* axis with the *c* axis vertical.

Modification I is the most suitable form of sulphathiazole for pharmaceutical use owing to its higher rate of dissolution. It is clear from these structure analyses that this is not a result of striking differences in the numbers of hydrogen bonds in the different polymorphs but rather a consequence of more subtle bonding effects. Evidence of the weaker bonding in modification I lies in its density which is significantly (4%) lower than that of the other two polymorphs.

Table 5. *The least-squares planes through the benzene and thiazole rings for sulphathiazole* I *and* III

The equations of the planes are of the form $AX+BY+CZ+D=0$ and were calculated with reference to the orthogonal coordinate system a,b,c^*. The deviations from the planes are in Å.

(*a*) Planes through the six benzene ring atoms

Coefficients	Molecules			
	I*A*	I*B*	III*A*	III*B*
A	−0·499	0·760	−0·125	−0·066
B	−0·070	0·528	0·830	0·869
C	0·863	0·379	0·544	0·491
D	0·151	9·525	6·793	7·849
C(1)	0·011	−0·009	−0·014	−0·012
C(2)	−0·006	0·018	0·010	0·005
C(3)	−0·007	−0·011	−0·003	0·003
C(4)	0·014	−0·005	0·001	−0·004
C(5)	−0·009	0·014	−0·006	−0·003
C(6)	−0·004	−0·007	0·013	0·011
N(1)	0·063	−0·041	−0·014	−0·003
S(1)	0·112	0·104	−0·017	0·033
H(3)	0·11	−0·10	0·00	−0·02
H(4)	0·17	0·01	−0·12	−0·13
H(5)	−0·04	0·16	−0·03	−0·05
H(6)	−0·08	0·06	−0·02	0·03

(*b*) Planes through the atoms C(7), N(3), C(8) and C(9)

Coefficients	Molecules			
	I*A*	I*B*	III*A*	III*B*
A	−0·347	−0·501	0·994	0·991
B	0·935	0·496	0·111	0·131
C	0·072	0·709	−0·001	−0·010
D	6·076	4·814	4·082	11·229
C(7)	0·002	−0·007	0·001	−0·002
N(3)	−0·004	0·013	−0·002	0·003
C(8)	0·004	−0·013	0·002	−0·003
C(9)	−0·002	0·007	−0·001	0·002
S(2)	0·102	0·037	0·013	0·037
N(2)	−0·054	−0·048	0·030	0·003
H(7)	0·08	−0·18	0·11	−0·10
H(8)	0·14	0·19	−0·06	−0·10
H(9)	0·11	0·05	−0·36	0·72

(*c*) Dihedral angles

I*A*	I*B*	III*A*	III*B*
101·26	98·62	91·87	100·04

Polymorphs II and III change into polymorph I on slow heating to 173–175°C. Rapid heating causes III to melt at this temperature with no apparent phase change before melting. The presence of the most active form (I) can thus be ensured by slow heating to temperatures between 175and 200°C. Reversion from the metastable polymorph I to one of the other two forms takes

Table 6. *Intermolecular distances*

(*a*) Hydrogen bonding

I*A*		I*B*	
N(1*A*)···O(2*A*)	3·088 Å	N(1*B*)···O(1*B*)	2·940 Å
N(2*A*)···N(3*A*)	2·874	N(1*B*)···O(2*B*)	2·959
N(2*A*)···H(7*A*)	1·87	N(2*B*)···N(3*B*)	2·877
		N(2*B*)···H(7*B*)	1·95

III*A*		III*B*	
N(1*A*)···O(1*B*)	3·026 Å	N(1*B*)···O(1*A*)	3·010 Å
N(1*A*)···N(3*B*)	2·925	N(1*B*)···O(1*A*)	3·022
N(1*A*)···H(7*B*)	1·91	N(1*B*)···N(3*A*)	2·871
O(1*A*)···N(1*B*)	3·010	N(1*B*)···H(7*A*)	2·06
O(1*A*)···H(1*B*)	2·16	O(1*B*)···N(1*A*)	3·026
O(1*A*)···N(1*B*)	3·022	O(1*B*)···H(2*A*)	2·07
O(1*A*)···H(2*B*)	2·17	N(3*B*)···N(1*A*)	2·925
N(3*A*)...N(1*B*)	2·871		

(*b*) Other close approaches

Form I

N(1*A*)···C(7*B*)	3·238 Å		
N(1*A*)···N(1*B*)	3·392	O(1*B*)···N(3*B*)	3·249
N(1*A*)···O(2*B*)	3·449		
N(1*A*)···N(2*B*)	3·451	C(4*B*)···C(7*B*)	3·383
O(1*A*)···C(6*B*)	3·369	C(5*B*)···N(2*B*)	3·316
O(1*A*)···C(5*B*)	3·375		
O(2*A*)···C(2*A*)	3·288		
C(4*A*)···C(7*A*)	3·389		
N(2*A*)···C(3*A*)	3·455		
N(3*A*)···C(9*B*)	3·285		

Form III

N(1*A*)···N(2*B*)	3·223 Å	O(1*B*)···C(6*A*)	3·445
N(1*A*)···O(1*B*)	3·252	O(2*B*)···C(3*A*)	3·271
O(1*A*)···C(6*B*)	3·344	O(2*B*)···C(2*A*)	3·388
O(1*A*)···C(1*B*)	3·432	O(2*B*)···N(3*B*)	3·406
O(2*A*)···C(3*B*)	3·215	N(3*B*)···C(1*A*)	3·366
O(2*A*)···C(2*B*)	3·366	N(3*B*)···C(6*A*)	3·473
C(7*A*)···C(8*A*)	3·484		
N(3*A*)···N(3*A*)	3·266		
N(3*A*)···C(1*B*)	3·375		
N(3*A*)···C(6*B*)	3·429		
N(3*A*)···C(8*A*)	3·471		

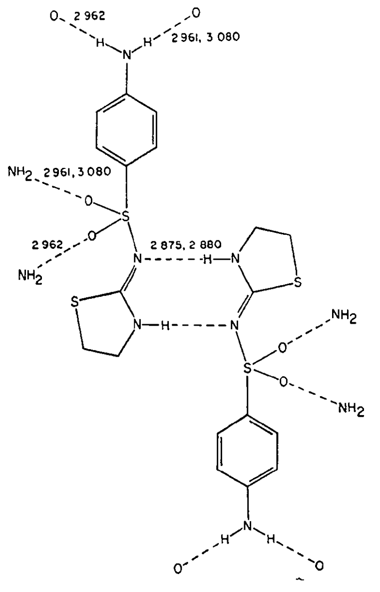

Fig. 4. The hydrogen bonding in sulphathiazole I.

place slowly at room temperature but the kinetics of the process has not been studied as extremely long times are involved.

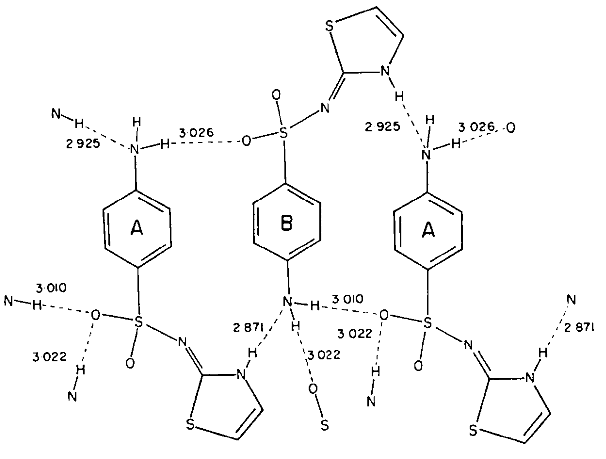

Fig. 5. The hydrogen bonding in sulphathiazole III.

References

Busing, W. R., Martin, K. O. & Levy, H. A. (1962). *ORFLS*. ORNL-TM-305, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Busing, W. R., Martin, K. O. & Levy, H. A. (1964). *ORFFE*. ORNL-TM-306, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Craven, B. M. & Vizzini, E. A. (1969). *Acta Cryst*. B**25**, 1993.

Craven, B. M., Vizzini, E. A. & Rodrogues, M. M. (1969). *Acta Cryst*. B**25**, 1978.

Dunning, A. J. & Vand, V. (1969). *Acta Cryst*. **15**, 1092.

Hanson, H. P., Herman, F., Lea, J. D. & Skillman, S. (1964). *Acta Cryst*. **17**, 1040.

Hughes, E. W. (1941). *J. Amer. Chem. Soc*. **63**, 1737.

Johnson, C. K. (1965). *ORTEP, A Fortran Thermal Ellipsoid Plot Program for Crystal Structure Illustrations*. ORNL-3794, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Kruger, G. J. & Gafner, G. (1972). *Acta Cryst*. To be published.

Stewart, J. M. (1967). Technical Report 67–58. Computer Science Center, Univ. of Maryland.

Acta Cryst. (1972). B**28**, 283

The Crystal and Molecular Structure of 2-Thioamidopyridine

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Crystals of 2-thiamidopyridine, $C_6H_6N_2S$, are monoclinic, space group $P2_1/c$ with four molecules in a unit cell of dimensions $a=5\cdot79$, $b=7\cdot42$ and $c=16\cdot26$ Å, $\beta=106\cdot9°$. The crystal structure was solved by three-dimensional Patterson and Fourier syntheses using the heavy-atom technique. The atomic parameters were refined by block-matrix least-squares calculations. Hydrogen atoms were located but their parameters were not refined. The final R index was 0·069 from 1004 observed reflexions, collected using Cu $K\alpha$ radiation. The mean bond lengths are C–C = 1·383, C–N = 1·336 Å in the pyridine ring and C–C = 1·505, C–N = 1·325, C–S = 1·657 Å in the thioamido group with a mean e.s.d. of 0·006 Å. Bond lengths and angles in the thioamido group suggest that the electron configuration contains contributions from the ionic canonical form as well as the amide form. The angle between the plane of the pyridine ring and that of the thioamido group is 10·5°. Non-bonded contact radii of some atoms are proposed to interpret the twisting between the thioamido group and the pyridine ring. Pairs of hydrogen bonds of the type N–H···S and 3·43 Å in length join molecules together across centres of symmetry.

Introduction

The corrosion inhibitive properties of aliphatic and aromatic amines, as well as nitrogen heterocyclic compounds, have been known for some time. (Rhodes & Khun, 1929; Mann, Lauer & Hultin, 1936). Sulphur-containing compounds such as thiourea derivatives and mercapto-imidazole derivatives have also been extensively used as inhibitors. (Aronson & Belen'kii, 1964). In view of the chelating ability of 2-thioamidopyridine (2-thiopic) to group IIB metals (Sutton, 1963) and certain transition metals (Sutton, 1966) the corrosion inhibitive properties of 2-thiopic were investigated, the compound was found to reduce the corrosion rate of carbon steels in 0·2N sulphuric acid by 40%. (Osborne, 1968).

In its chelation with metals, 2-thiopic always uses its pyridine nitrogen atom as well as either the nitrogen atom or the sulphur atom of the side chain. Spectro-

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