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The Structure of 2-*p*-Methoxyphenyl -3,4-dibenzyl-1,3,4-thiadiazolidine-5-thione, $C_{23}H_{22}N_2OS_2$

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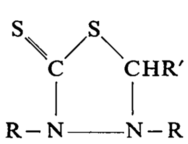
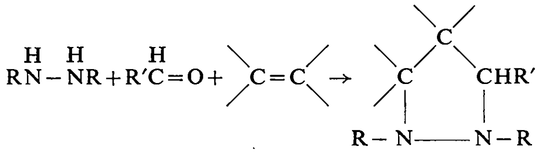
A new heterocyclic synthesis produced a product believed to be



The crystal structure of the derivative where R ≡ benzyl and R′ ≡ methoxyphenyl confirmed the chemical structure. The thiadiazolidine ring is not planar and is rather asymmetric since the lengths of the two C–N bonds are quite different from each other and the two C–S bonds are also different from each other. The bonds to the N atom adjacent to C=S lie in a plane, whereas the bonds to the N atom adjacent to CHR′ form approximately tetrahedral angles. The space group is $P\bar{1}$ with $Z=2$ and the cell dimensions $a=7{\cdot}74$, $b=12{\cdot}07$, $c=12{\cdot}32$ Å, $\alpha=111°\ 20'$, $\beta=88°\ 10'$, $\gamma=100°\ 43'$.

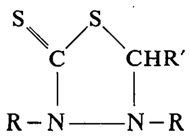
The structure was solved by obtaining phases directly from the structure factor magnitudes by the symbolic addition procedure. A well resolved *E*-map revealed the positions of all the atoms.

The reaction of *N,N′*-dialkylhydrazines with aromatic aldehydes and an unsaturated compound (a dipolarophile) represents a useful heterocyclic synthesis *via* 1,3-dipolar cycloaddition (Huisgen, 1963):



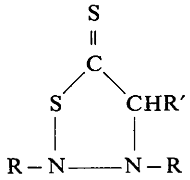
(1)

If CS_2 is used as the dipolarophile (Grashey, Huisgen, Sun & Moriarty, 1964), the resulting product of 1,3-dipolar cycloaddition was believed to be



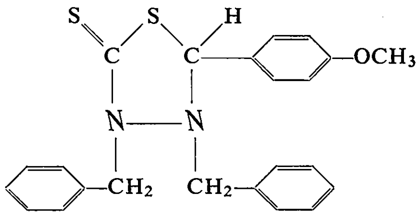
(*A*)

although the possibility existed of addition of the dipolarophile in the reverse sense, that is,



(*B*)

The present X-ray investigation made on the following derivative,



confirms configuration (*A*). A brief note describing the conformation of the molecule and its relationship to nuclear magnetic resonance studies has been published (Karle, Karle & Moriarty, 1964). Some very interesting structural features of the SCNNC ring will be described later in the paper.

Experimental

Crystals of $C_{23}H_{22}N_2OS_2$ were obtained from Prof. R. Moriarty of the Catholic University of America. They were colorless, transparent, elongated prisms of nearly square cross-section. Multiple-film, equi-inclination Weissenberg photographs were taken along the *a* axis from the zero through the sixth layer with copper radiation. Visual estimates of the intensities were made by comparison with a calibrated film strip. A total of 3780 data were collected.

Cell dimensions were determined from precession photographs with the crystal mounted on the a^* axis. The space group is triclinic (determined to be $P\bar{1}$ from statistical averages) and the unit-cell parameters are:

$a = 7{\cdot}74 \pm 0{\cdot}02$ Å $\quad \alpha = 111°20' \pm 20'$

$b = 12{\cdot}07 \pm 0{\cdot}03 \quad \beta = 88°10' \pm 20'$

$c = 12{\cdot}32 \pm 0{\cdot}03 \quad \gamma = 100°43' \pm 20'$

with $Z=2$. The computed density is $1{\cdot}282$ g.cm^{-3} while the density measured by flotation in mixed solvents was found to be $1{\cdot}264$ g.cm^{-3}. The measured density may be in some error since the crystals were dissolving in the solvents while measurements were being made.

The intensities were corrected for Lorentz and polarization factors and spot size; however, no correction was made for absorption. The data were adjusted to an absolute scale and structure factor magnitudes, $|F|$, and normalized structure factor magnitudes, $|E|$, were computed. For a triclinic space group,

$$E_{\mathbf{h}}^2 = F_{\mathbf{h}}^2 / \sum_{j=1}^{N} f_{j\mathbf{h}}^2 \qquad (2)$$

where F is on an absolute scale and corrected for vibrational motion, N is the number of atoms in the unit cell and f_j is the atomic scattering factor for the jth atom. Statistical averages for the normalized structure factors are listed in Table 1. The experimental values are compared with theoretical values computed for crystals with randomly distributed atoms. The statistical averages imply that the crystal is centrosymmetric and that its space group is therefore $P\bar{1}$.

Table 1. *Statistical averages*

	Experimental	Centrosymmetric	Non-centrosymmetric
$\langle \lvert E \rvert \rangle$	0·806	0·798	0·886
$\langle \lvert E^2-1 \rvert \rangle$	0·918	0·968	0·736
$\langle \lvert E \rvert^2 \rangle$	1·001	1·000	1·000

The distribution of normalized structure factors is near the expected values for centrosymmetric crystals. These are shown in Table 2.

Table 2. *Distribution of normalized structure factors*

	$\lvert E \rvert > 3$	$\lvert E \rvert > 2$	$\lvert E \rvert > 1$
Expected	0·3 %	5·0 %	32·0 %
Observed	0·3	3·8	28·8

Phase determination

The phases were determined directly from the intensities by the symbolic addition procedure (Karle & Karle, 1963). In brief, the procedure consists of the use of the Σ_2 formula,

$$sE_{\mathbf{h}} \sim s\sum_{\mathbf{k}} E_{\mathbf{k}} E_{\mathbf{h}-\mathbf{k}}\,, \qquad (3)$$

where s means 'sign of'. The sign of $E_{\mathbf{h}}$ is determined as a function of the known signs of $E_{\mathbf{k}}$ and $E_{\mathbf{h}-\mathbf{k}}$. Previous experience has shown that a very small number of phases need be known in order to obtain the phases for a sufficient number of reflections to solve the crystal structure. The basic set of phases used to implement equation (3) consists of arbitrary phases (+ or −) assigned to three reflections (in space group $P\bar{1}$) in order to fix the origin, plus a small number of other reflections whose phases are specified by an unknown symbol, *a*, *b*, *c*, *etc.*, where each symbol has the value + or −. The initial set used in this determination is listed in Table 3.

Table 3. *Assignment of three origin specifying reflections and six other reflections as a starting set for the application of* Σ_2

Sign	*hkl*	*E*
+	$0,5,\bar{1}\bar{1}$	3·32
+	$1\bar{1}6$	2·84
+	$1\bar{7}\bar{7}$	3·22
a	$2,\overline{10},4$	3·00
b	$08\bar{4}$	3·17
c	625	2·41
d	$2,\bar{4},10$	2·87
g	190	2·94
h	075	3·66

It should be emphasized that the initial set was selected on the basis that each reflection had a large $|E|$ value and that the reflections entered into many combinations among themselves applicable to the Σ_2 formula. The unknown symbols were not assigned all at once, but as needed to continue the Σ_2 procedure. Initially, only phases for those reflections with large $|E|$ magnitudes, usually those with $|E| > 2{\cdot}0$, are determined in order to be assured that the indications from the Σ_2 formula are correct. The probability that the sign of $E_{\mathbf{h}}$ is plus is determined by the formula

$$P_+(E_{\mathbf{h}}) = \tfrac{1}{2} + \tfrac{1}{2} \tanh \frac{\sigma_3 |E_{\mathbf{h}}| \sum_{\mathbf{k}} E_{\mathbf{k}} E_{\mathbf{h}-\mathbf{k}}}{\sigma_2^{3/2}} \qquad (4)$$

where $\sigma_n = \sum_{j=1}^{N} Z_j^n$, Z_j being the atomic number of the jth atom in a cell containing N atoms. After the phases of many of the reflections with large $|E|$ magnitudes are determined, the process is continued with reflections having somewhat smaller $|E|$ magnitudes.

As many pairs of $E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}$ as possible are used in the formula in order to determine the phase of each $E_{\mathbf{h}}$.* Although, in general, most of the contributors to Σ_2 will agree in sign, there will be occasional disagreements. Phases of a few reflections may be indeterminate because the indications from Σ_2 will be nearly equally divided between + and −. Very often relationships will occur among the letters used as unknown symbols. In this determination, for example, the relationships $a \equiv cg$, $ab \equiv bcg$, and $ac \equiv g$ kept recurring in many of the phase determinations, hence it seemed likely that the symbol a had the same sign as cg. Other relationships occurred also, so that after 150 phases were de-

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* To facilitate the application of Σ_2, a computer program has been prepared to list the sets of interacting pairs of each *hkl* arranged in order of decreasing $|E|$ values.

termined as functions of *a*, *b*, *c*, *d*, *g* and *h*, it was obvious that the symbols had the following values:

$$a \equiv +$$
$$b \equiv b$$
$$c \equiv c$$
$$d \equiv bc$$
$$g \equiv c$$
$$h \equiv + \, .$$

Only two letters remained as unknowns. If both *b* and *c* were positive, then all phases would be positive; therefore this combination was eliminated. For the remaining three possibilities for *b* and *c*, (+ −), (− −) and (− +), the number of known phases was rapidly expanded to 468 (all $|E| > 1{\cdot}5$) by the use of a computer program and three three-dimensional *E*-maps were computed. *E*-maps are Fourier maps in which *E* values rather than *F* values are used as the coefficients (Karle, Hauptman, Karle & Wing, 1958). The advantage of using *E*-maps is that the atoms are represented as essentially point atoms. Since many of the reflections with large $|E|$ values have relatively high indices, the resolution of an *E*-map is very good. Upon examination of three *E*-maps computed, it was immediately obvious that the one with $b+$ and $c-$ was the correct one. It is illustrated on the left-hand side of Fig. 1.

The refinement

The coordinates of the twenty-eight atoms as read from the *E*-map in Fig. 1 were subjected to a least-squares refinement with the ORFLS program (Busing, Martin & Levy, 1962) which was adapted in our laboratory to the IBM 7030 (STRETCH). The quantity minimized was $\Sigma w(F_o - F_c)^2$ with the weighting function equal to unity for all reflections with $|F_o| > 0$. Individual scale factors were used for each level ($h = 0 \rightarrow 6$) since diffraction data were obtained only about the *a* axis. Several cycles of refinement with isotropic temperature factors brought the *R* index to 18·4%. Two cycles with anisotropic temperature factors reduced *R* to 10·7%. At this point the refinement was not continued any further. Hydrogen atoms were not included. The fractional coordinates and anisotropic temperature factors are listed in Table 4. Observed and calculated structure factors are listed in Table 5.

The structure

An electron density map including all the data and computed with *F* values for the Fourier coefficients is shown on the right-hand side of Fig. 1 for direct comparison with the original *E*-map computed from the

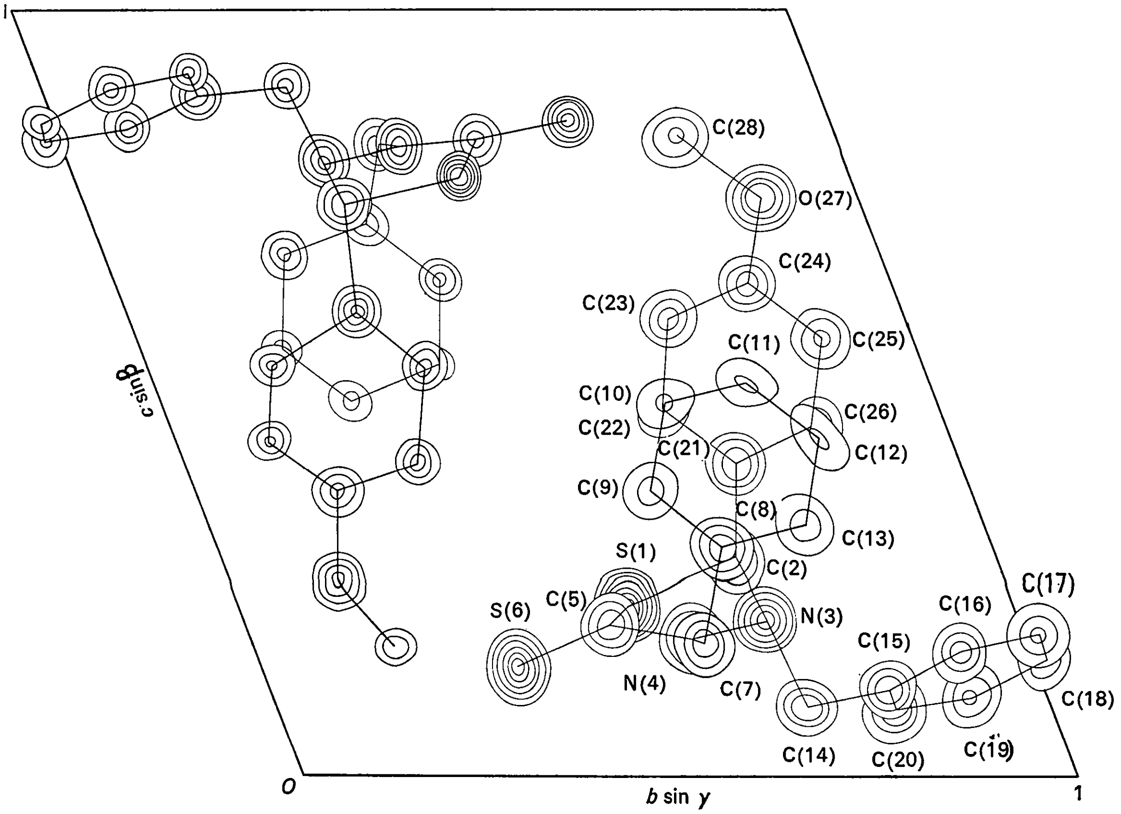

Fig. 1. On the left-hand side, sections through maximum densities of a three-dimensional *E*-map are projected on the (100) plane. The *E*-map was computed from 468 phases determined by the symbolic addition procedure. Contours are at equally spaced, arbitrary levels. Every other contour for the sulfur atoms has been omitted. On the right-hand side is the final electron density map. Contours are at intervals of 2 e.Å^{-3}, starting with the 2 e.Å^{-3}. Every other contour for the sulfur atoms has been omitted.

468 initially determined phases. Another view of the molecule is shown in Fig. 2. Rings I and III are approximately parallel to each other and approximately perpendicular to the SCNNC ring. The constituents attached to C(2) and N(3) are *trans* to each other. Bond distances and angles are listed in Table 6 and displayed in Fig. 3.

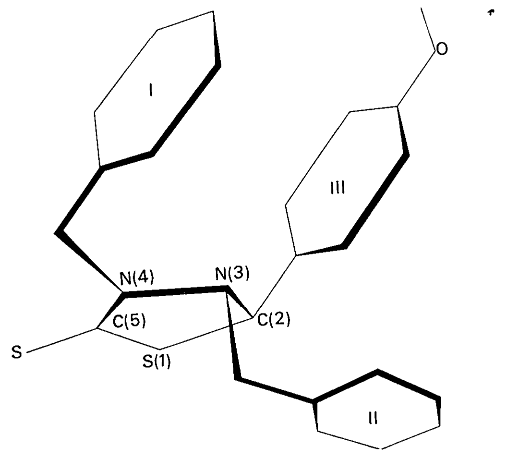

Fig. 2. Configuration of 2-*p*-methoxyphenyl-3,4-dibenzyl-1,3,4-thiadiazolidine-5-thione

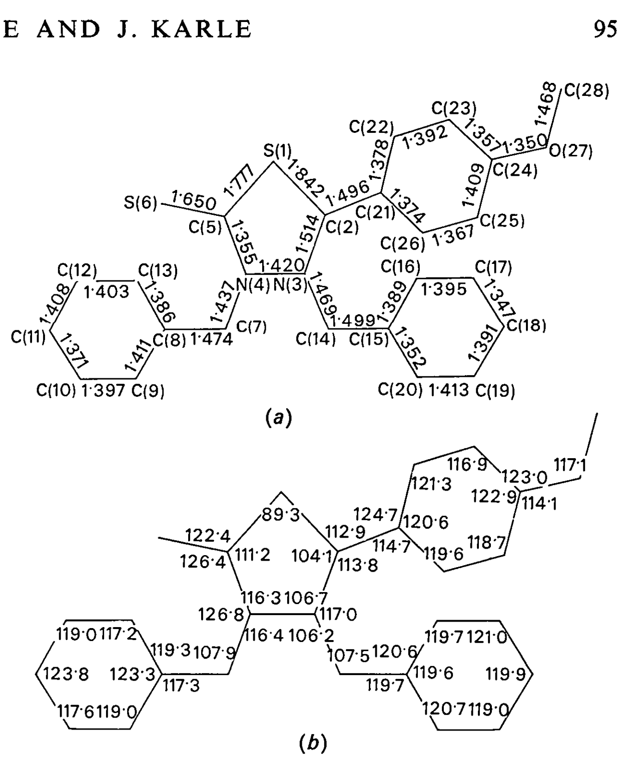

Fig. 3. Bond distances and angles.

Table 4. *Fractional coordinates* for 2-p-methoxyphenyl*-3,4-*dibenzyl*-1,3,4-*thiadiazolidine*-5-*thione*

The thermal parameters are of the form $T = \exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.
Each thermal parameter is multiplied by 10^4.

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
S(1)	0·0540	0·5000	0·2168	24	52	55	−8	−20	12
C(2)	0·1503	0·6627	0·2754	54	47	39	15	−5	14
N(3)	0·3078	0·6740	0·2015	43	42	33	34	−1	12
N(4)	0·3795	0·5678	0·1769	35	38	52	26	−5	12
C(5)	0·2656	0·4673	0·1755	43	47	58	3	−29	13
S(6)	0·3099	0·3304	0·1407	158	35	99	29	−38	10
C(7)	0·5676	0·5821	0·1709	53	67	65	29	1	4
C(8)	0·6439	0·6485	0·2902	49	74	64	30	−9	14
C(9)	0·6291	0·5847	0·3670	164	166	98	9	−51	58
C(10)	0·6961	0·6453	0·4816	260	270	118	42	−83	70
C(11)	0·7783	0·7639	0·5125	202	270	109	135	−57	−24
C(12)	0·7941	0·8284	0·4365	165	120	174	76	−99	−52
C(13)	0·7236	0·7691	0·3220	139	77	146	41	−63	−8
C(14)	0·2745	0·6824	0·0883	145	56	33	45	−12	14
C(15)	0·2120	0·7990	0·1118	85	59	31	28	0	19
C(16)	0·3262	0·9094	0·1602	112	55	62	14	−24	19
C(17)	0·2654	1·0168	0·1808	178	68	85	31	−19	30
C(18)	0·0979	1·0153	0·1532	193	79	95	40	−22	43
C(19)	−0·0180	0·9055	0·1047	186	106	95	51	−24	53
C(20)	0·0438	0·7967	0·0834	86	86	59	22	−20	35
C(21)	0·1948	0·7095	0·4034	47	46	35	11	−8	13
C(22)	0·1590	0·6420	0·4736	124	59	47	−3	−21	26
C(23)	0·1979	0·6936	0·5932	141	78	50	−3	−25	33
C(24)	0·2701	0·8132	0·6371	112	69	33	15	−14	18
C(25)	0·3131	0·8831	0·5667	228	55	39	−5	−22	14
C(26)	0·2729	0·8297	0·4497	205	57	43	6	−13	23
O(27)	0·3132	0·8747	0·7515	196	91	34	5	−32	19
C(28)	0·2729	0·8074	0·8302	213	132	53	14	−28	49
Standard error									
S	0·0003	0·0001	0·0001	1	1	1	2	2	1
C	0·0011	0·0006	0·0006	7	6	5	9	8	5
N	0·0007	0·0003	0·0004	4	3	3	5	5	2
O	0·0007	0·0004	0·0003	4	4	3	6	5	3

* Coordinates are so chosen that they may be substituted directly into the equations representing the least-squares planes.

Table 5. *Observed and calculated structure factors*

The three columns within each group contain the values of l, $10F_o$, $10F_c$. Reflections indicated by an asterisk were given zero weight in the least-squares calculation.

0, 0, *l*		
1	0	-72
2	1202	-1366
3	1945*	-2805
4	991	-810
5	631	448
6	212	241
7	79	63
8	151	-93
9	94	-82
10	121	98
11	197	136
12	0	68
13	0	36
14	0	56
0, 1, *l*		
-14	113	-122
-13	128	-114
-12	107	84
-11	243	-204
-10	109	-124
-9	566	596
-8	651	558
-7	391	321
-6	78	-73
-5	1313	-1198
-4	1138	-969
-3	282	12
-2	1024	1117
-1	830	-917
0	848*	-1200
1	800	875
2	846	862
3	918	907
4	186	48
5	285	70
6	673	-536
7	596	600
8	335	-318
9	466	-466
10	517	-554
11	390	437
12	307	335
13	45	35
14	95	-146
0, 2, *l*		
-14	46	18
-13	201	176
-12	97	75
-11	70	-8
-10	593	-577
-9	111	62
-8	433	-373
-7	141	-139
-6	1136	1037
-5	1709	1808
-4	378	351
-3	1622	-2038
-2	1811*	-2355
-1	1610*	2229
0	928	-970
1	119	54
2	628	-463
3	368	377
4	642	612
5	412	451
6	128	-133
7	503	-467
8	176	-157
9	197	168
10	317	337
11	94	-58
12	225	-177
0, 3, *l*		
-15	241	247
-14	0	7
-13	0	-50
-12	0	39
-11	230	-250
-10	572	567
-9	909	-871
-8	0	69
-7	305	287
-6	418	398
-5	198	40
-4	148	-34
-3	407	-329
-2	134	-100
-1	23	-48
0	88	62
1	590	436
2	631	496
3	100	47
4	916	-788
5	1054	-998
6	433	373
7	886	878
8	326	295
9	378	-368
10	145	-142
11	0	-38
12	0	-4
0, 4, *l*		
-15	142	-123
-14	129	86
-13	0	-19
-12	130	-147
-11	454	-438
-10	738	730
-9	382	352
-8	196	-93
-7	692	-637
-6	224	-210
-5	429	381
-4	642	-547
-3	811	779
-2	319	-144
-1	729	714
0	580	-372
1	223	203
2	822	-735
3	709	-658
4	444	345
5	808	742
6	523	484
7	573	-567
8	243	-267
9	49	20
10	0	46
11	49	48
0, 5, *l*		
-15	87	-91
-14	295	-250
-13	85	-54
-12	98	142
-11	920	875
-10	593	-582
-9	584	-578
-8	454	-448
-7	391	373
-6	742	654
-5	298	272
-4	517	-457
-3	181	140
-2	349	228
-1	573	-464
0	819	-801
1	34	23
2	950	864
3	562	448
4	320	-259
5	1008	-963
6	570	556
7	172	-174
8	110	135
9	0	0
10	0	45
11	102	109
0, 6, *l*		
-15	189	186
-14	338	323
-13	0	51
-12	337	-314
-11	122	-127
-10	84	-79
-9	175	122
-8	285	192
-7	188	178
-6	431	329
-5	524	-459
-4	0	20
-3	888	-869
-2	399	-270
-1	121	-64
0	1623	1522
1	387	355
2	623	-555
3	649	-610
4	193	201
5	477	440
6	502	-469
7	49	-79
8	0	-10
9	238	247
10	138	137
0, 7, *l*		
-15	0	38
-14	225	-188
-13	0	20
-12	180	124
-11	86	-11
-10	283	-300
-9	126	-17
-8	380	333
-7	630	589
-6	0	-14
-5	712	-651
-4	576	-574
-3	558	438
-2	878	787
-1	68	56
0	587	-520
1	598	-508
2	166	-182
3	46	36
4	97	-94
5	1034	1082
6	70	-60
7	67	98
8	332	-364
9	371	-405
10	0	-75
0, 8, *l*		
-15	129	121
-14	0	33
-13	161	140
-12	47	-48
-11	98	-86
-10	210	-226
-9	155	147
-8	213	-223
-7	436	-352
-6	344	-268
-5	436	358
-4	1349	1425
-3	120	-168
-2	362	-252
-1	235	-200
0	319	-304
1	295	-258
2	227	-231
3	354	352
4	277	277
5	69	-55
6	124	-93
7	148	-145
8	168	134
9	208	263
0, 9, *l*		
-15	119	-125
-14	112	81
-13	0	24
-12	348	394
-11	0	28
-10	185	-158
-9	494	-543
-8	0	20
-7	498	448
-6	434	396
-5	573	-594
-4	725	-672
-3	296	-284
-2	440	410
-1	875	799
0	613	574
1	0	67
2	591	-574
3	381	-332
4	128	-128
5	225	-245
6	145	136
7	244	288
8	0	47
0, 10, *l*		
-14	0	28
-13	0	6
-12	160	-128
-11	226	-222
-10	490	514
-9	544	565
-8	225	201
-7	454	-442
-6	797	-759
-5	469	448
-4	538	-534
-3	169	161
-2	69	-81
-1	275	234
0	420	398
1	111	84
2	169	-175
3	360	-374
4	109	53
5	196	207
6	110	110
7	96	-112
0, 11, *l*		
-14	134	-149
-13	0	18
-12	264	258
-11	149	118
-10	369	-385
-9	330	-323
-8	69	56
-7	543	563
-6	333	309
-5	0	-28
-4	390	-396
-3	172	-119
-2	157	146
-1	0	-12
0	299	-320
1	337	-398
2	388	448
3	280	308
4	158	129
5	191	-251
0, 12, *l*		
-12	164	-181
-11	124	-138
-10	72	-62
-9	63	41
-8	103	-99
-7	0	28
-6	474	442
-5	48	78
-4	48	46
-3	460	-461
-2	423	-418
-1	183	151
0	448	448
1	242	262
2	221	-208
3	281	-317
4	71	-85
0, 13, *l*		
-8	112	105
-7	104	107
-6	43	-66
-5	310	-326
-4	218	-199
-3	272	290
-2	426	390
-1	152	100
0	286	-327
1	180	-183
0, 14, *l*		
-10	74	83
-9	132	-129
-8	0	-28
-7	239	-242
-6	0	29
-5	165	199
-4	301	336
-3	42	-66
-2	125	-165
-1	133	-162
0, 15, *l*		
-7	153	226
-6	134	182
-5	133	-183
-4	124	-169
1, -15, *l*		
4	85	-89
5	75	69
6	83	124
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3	187	-113
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3	292	-263
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7	368	335
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9	251	236
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1, -9, *l*		
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6	150	136
7	128	-105
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13	161	-117
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8	160	-138
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2	982	909
3	77	68
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8	147	152
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7	702	735
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-8	178	-111
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3	413	-439
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13	379	419
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7	551	462
8	379	-412
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8	697	-652
9	359	-348
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13	169	-164
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9	215	194
10	200	232
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14	116	131
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Table 5 (*cont.*)

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6	984	-903
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12	205	-206
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9	33	54
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12	126	-134
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2	102	-61
3	323	-306
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7	43	-55
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7	107	113
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-7	270	266
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8	0	-8
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-2	211	186
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7	219	-255
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6	133	-151
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-5	209	-235
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4	139	-168
5	142	154
	4, 10, *l*	
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-2	0	8

Table 5 (*cont.*)

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-3	75	57
-2	158	-154
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9	198	-237
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4	231	237
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10	93	-88
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8	71	-90
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11	86	-87
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12	52	76
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1	183	163
2	241	239
3	101	77
4	0	0
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10	143	129
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-3	269	-294
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3	294	326
4	267	248
5	126	-111
6	377	-358
7	265	-211
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9	118	92
10	0	57
11	0	-18
12	0	-15
13	97	-132
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-4	96	73
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2	175	-189
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9	542	-631
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7	89	-70
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9	320	395
10	62	-59
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7	296	-275
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9	205	209
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3	217	190
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5	260	273
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7	240	-253
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10	126	-139
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3	304	290
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7	75	-30
8	178	-149
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-2	315	313
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8	230	224
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-8	224	234
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-4	408	415
-3	129	139
-2	119	-81
-1	104	-116
0	48	41
1	280	270
2	0	25
3	392	-368
4	135	-123
5	86	8
6	228	241
7	76	54
8	94	-100
	5, 6, *l*	
-10	89	99
-9	163	-149
-8	78	-88
-7	111	99
-6	0	22
-5	120	102
-4	199	-212
-3	0	20
-2	183	169
-1	185	186
0	183	-141
1	419	-381
2	64	-81
3	392	369
4	240	249
5	112	-73
6	261	-272
	5, 7, *l*	
-10	84	-81
-9	87	-50
-8	235	219
-7	96	-65
-6	87	52
-5	247	-261
-4	222	-257
-3	215	223
-2	252	224
-1	245	261
0	143	-138
1	264	-264
5	83	-45
6	116	124
	5, 8, *l*	
-9	74	39
-8	0	-22
-7	54	-39
-6	154	143
-5	39	-63
-4	135	-114
-3	175	-175
-2	174	184
-1	219	241
0	0	-23
1	247	-239
2	165	-150
3	131	111
4	153	173
	5, 9, *l*	
-6	51	-61
-5	128	-120
-4	235	248
-3	234	259
-2	74	-78
-1	177	-174
0	252	-222
1	162	172
2	56	60
3	82	-91
4	32	-58
	5, 10, *l*	
-9	85	-86
-8	101	-127
-7	66	-48
-6	126	112
-5	99	118
-4	115	-136
-3	107	-101
-2	56	52
-1	107	111
0	0	9
1	0	-34
2	78	99
	5, 11, *l*	
-6	156	-173
-5	173	-182
-4	98	99
	6, -13, *l*	
1	37	49
2	101	86
3	93	96
4	90	-74
5	128	131
6	62	-63
7	157	-197
8	106	-150
9	28	42
	6, -12, *l*	
0	46	22
1	0	9
2	0	9
3	185	151
4	93	-70
5	120	-99
6	0	-34
7	81	82
8	136	129
	6, -11, *l*	
-3	107	87
-2	83	91
-1	52	53
0	0	-31
1	40	16
2	164	-137
3	232	-212
4	95	73
5	198	198
6	94	86
7	39	-33
8	133	-110
	6, -10, *l*	
-4	45	46
-3	0	3
-2	55	35
-1	0	1
0	198	-177
1	139	-114
2	171	104
3	266	260
4	110	90
5	139	-110
6	264	-234
7	68	-55
8	94	72
9	145	102
10	72	41
11	98	-90
	6, -9, *l*	
-6	137	-116
-5	0	3
-4	65	44
-3	0	-8
-2	129	-121
-1	35	-98
0	240	209
1	207	194
2	0	6
3	181	-193
4	0	-17
5	146	-89
6	0	18
7	0	-38
8	48	30
9	75	70
10	188	151
	6, -8, *l*	
-6	49	31
-5	0	-32
-4	107	-109
-3	49	44
-2	139	129
-1	34	61
0	89	-59
1	93	-97
2	170	158
3	91	69
4	0	-1
5	246	-234
6	108	-68
7	92	116
8	170	164
9	0	23
10	412	-431
11	102	100
	6, -7, *l*	
-7	69	-55
-6	87	-86
-5	34	39
-4	60	71
-3	69	72
-2	95	-108
-1	96	-111
0	175	-141
1	209	-181
2	91	72
3	431	390
4	249	247
5	231	203
6	173	-153
7	393	-358
8	402	-398
9	183	178
10	200	207
11	105	105
	6, -6, *l*	
-8	140	-119
-7	54	18
-6	180	186
-5	120	120
-4	91	70
-3	88	98
-2	131	115
-1	204	206
0	70	33
1	112	-72
2	64	77
3	173	-119
4	38	-44
5	142	-104
6	70	-33
7	345	351
8	279	283
9	339	-350
10	0	-11
11	100	-129
12	0	11
	6, -5, *l*	
-9	116	99
-8	119	132
-7	95	-100
-6	155	-157
-5	263	-269
-4	114	114
-3	297	310
-2	407	435
-1	42	53
0	389	-429
1	38	-51
2	145	-175
3	225	-211
4	80	46
5	252	191
6	199	150
7	185	-153
8	0	43
9	98	135
10	89	116
	6, -4, *l*	
-9	100	-69
-8	132	-132
-7	35	-46
-6	0	-6
-5	47	49
-4	69	-66
-3	77	-28
-2	23	23
-1	425	465
0	273	-323
1	78	-106
2	17	-3
3	273	298
4	114	68
5	244	-249
6	119	-135
7	103	-104
8	48	-8
9	156	158
10	75	87
11	37	-41
	6, -3, *l*	
-9	86	78
-8	136	115
-7	99	69
-6	209	-189
-5	32	-27
-4	89	85
-3	212	178
-2	260	-306
-1	368	-510
0	353	383
1	341	375
2	144	151
3	124	-111
4	238	-197
5	45	-28
6	95	56
7	73	-98
8	0	12
9	34	24
10	104	139
11	0	-39
	6, -2, *l*	
-10	71	-60
-9	0	-22
-8	0	17
-7	92	106
-6	182	154
-5	95	-116
-4	278	-306
-3	87	-93
-2	322	489
3	29	37
4	148	135
5	92	55
6	97	-80
7	142	120
8	92	79
9	0	28
10	311	-301
11	0	8
	6, -1, *l*	
-10	159	-110
-9	75	63
-8	0	-2
-7	167	-154
-6	120	-124
-5	64	80
-4	307	393
-3	26	41
0	86	37
1	72	22
2	98	60
3	182	-105
4	37	36
5	240	209
6	55	14
7	153	-127
8	171	-214
9	0	21
10	141	156
	6, 0, *l*	
-11	33	-27
-10	67	59
-9	48	-50
-8	49	-50
-7	127	99
-6	110	90
-5	69	-45
-4	68	-59
-3	49	-59
-2	54	-87
-1	5	21
0	83	31
1	218	-162
2	75	45
3	249	200
4	67	68
5	309	-264
6	336	-339
7	228	211
8	304	303
9	0	0
10	78	-104
	6, 1, *l*	
-10	78	46
-9	84	64
-8	60	60
-7	101	-80
-6	200	-192
-5	49	36
-4	70	39
-3	36	49
-2	48	-78
-1	74	66
0	69	76
1	370	322
2	36	-28
3	374	-329
4	405	-358
5	206	206
6	178	189
7	121	91
8	106	-113
	6, 2, *l*	
-11	155	137
-10	105	88
-9	0	11
-8	69	-66
-7	34	-55
-6	0	-5
-5	66	54
-4	120	-103
-3	0	17
-2	45	33
-1	138	119
0	337	-336
1	209	-175
2	240	184
3	627	635
4	236	212
5	549	-570
6	143	-133
7	120	-127
8	133	142
9	81	92
	6, 3, *l*	
-11	49	-48
-10	39	-18
-9	0	-25
-8	77	47
-7	0	0
-6	148	142
-5	140	130
-4	118	128
-3	96	-109
-2	339	-410
-1	364	-397
0	235	223
1	489	438
2	203	124
3	347	-337
4	59	33
5	41	51
6	192	215
7	81	-66
8	155	-153
9	58	-85
	6, 4, *l*	
-6	83	61
-5	80	59
-4	156	-141
-3	164	169
-2	247	283
-1	30	0
0	327	-303
1	360	-361
2	223	158
3	206	162
4	130	-104
5	87	76
6	98	-113
7	132	146
	6, 5, *l*	
-10	105	-73
-9	0	16
-8	0	-47
-7	49	-63
-6	170	-177
-5	91	-66
-4	294	337
-3	115	126
-2	74	-47
-1	82	-58
0	34	4
1	0	11
2	144	-111
3	57	-52
4	38	-11
5	173	148
6	65	76
	6, 6, *l*	
-9	0	6
-8	105	-91
-7	40	-51
-6	170	148
-5	170	-139
-4	49	28
-3	85	-80
-2	0	29
-1	0	8
0	0	-28
1	121	102
2	0	15
3	157	123
4	0	13
5	153	-201
	6, 7, *l*	
-9	101	92
-8	214	187
-7	0	-10
-6	233	-218
-5	34	24
-4	0	15
-3	109	87
-2	0	-8
-1	81	-89
0	45	34
1	204	140
2	42	-33
3	174	-143
4	88	-102
	6, 8, *l*	
-8	110	-106
-7	83	54
-6	0	37
-5	137	101
-4	106	-75
-3	106	-69
-2	97	62
-1	103	82
0	58	-38
1	245	-246
2	0	7
	6, 9, *l*	
-4	151	145
-3	35	34
-2	196	-188

Table 6. *Bond lengths and angles*

Bond		Angle	
S(1)–C(2)	1·842 Å	C(5)–S(1)–C(2)	89·3°
C(2)–N(3)	1·514	S(1)–C(2)–N(3)	104·1
N(3)–N(4)	1·420	C(2)–N(3)–N(4)	106·7
N(4)–C(5)	1·355	N(3)–N(4)–C(5)	116·3
C(5)–S(1)	1·777	N(4)–C(5)–S(1)	111·2
C(5)–S(6)	1·650	N(4)–C(5)–S(6)	126·4
		S(6)–C(5)–S(1)	122·4
N(4)–C(7)	1·437	C(5)–N(4)–C(7)	126·8
C(7)–C(8)	1·474	N(3)–N(4)–C(7)	116·4
C(8)–C(9)	1·411	N(4)–C(7)–C(8)	107·9
C(9)–C(10)	1·397	C(7)–C(8)–C(9)	117·3
C(10)–C(11)	1·371	C(7)–C(8)–C(13)	119·3
C(11)–C(12)	1·408	C(8)–C(9)–C(10)	119·0
C(12)–C(13)	1·403	C(9)–C(10)–C(11)	117·6
C(13)–C(8)	1·386	C(10)–C(11)–C(12)	123·8
		C(11)–C(12)–C(13)	119·0
		C(12)–C(13)–C(8)	117·2
		C(13)–C(8)–C(9)	123·3
N(3)–C(14)	1·469	N(4)–N(3)–C(14)	106·2
C(14)–C(15)	1·499	C(2)–N(3)–C(14)	117·0
C(15)–C(16)	1·389	N(3)–C(14)–C(15)	107·5
C(16)–C(17)	1·395	C(14)–C(15)–C(16)	120·6
C(17)–C(18)	1·347	C(14)–C(15)–C(20)	119·7

Table 6 (*cont.*)

Bond		Angle	
C(18)–C(19)	1·391	C(15)–C(16)–C(17)	119·7
C(19)–C(20)	1·413	C(16)–C(17)–C(18)	121·0
C(20)–C(15)	1·352	C(17)–C(18)–C(19)	119·9
		C(18)–C(19)–C(20)	119·0
		C(19)–C(20)–C(15)	120·7
		C(20)–C(15)–C(16)	119·6
C(2)–C(21)	1·496	S(1)–C(2)–C(21)	112·9
C(21)–C(22)	1·378	N(3)–C(2)–C(21)	113·8
C(22)–C(23)	1·392	C(2)–C(21)–C(22)	124·7
C(23)–C(24)	1·357	C(2)–C(21)–C(26)	114·7
C(24)–C(25)	1·409	C(21)–C(22)–C(23)	121·3
C(25)–C(26)	1·367	C(22)–C(23)–C(24)	116·9
C(26)–C(21)	1·374	C(23)–C(24)–C(25)	122·9
C(24)–O(27)	1·350	C(24)–C(25)–C(26)	118·7
O(27)–C(28)	1·468	C(25)–C(26)–C(21)	119·6
		C(26)–C(21)–C(22)	120·6
		C(23)–C(24)–O(27)	123·0
		C(25)–C(24)–O(27)	114·1
		C(24)–O(27)–C(28)	117·1

The standard deviations for the bond lengths range from 0·007 to 0·010 Å and the standard deviations for the angles range from 0·4° to 0·9°.

The SCNNC ring is of particular interest in this investigation. The atoms S(1), N(3), N(4) and C(5) lie within 0·02 Å of a plane whose equation is

$$1{\cdot}8422x-1{\cdot}8020y+11{\cdot}641z=1{\cdot}7113\,, \qquad (5)$$

referred to the triclinic axes and where the quantity on the right hand side of the equation is the origin-to-plane distance in Å. Atom C(2), however, is 0·58 Å out of the plane. The puckering of the ring is similar to that found in saturated five-membered rings composed of all carbon atoms. The two adjacent nitrogen atoms in the ring are quite different from each other. The bonds to N(3) form tetrahedral angles whereas the bonds to N(4) lie in a plane. Furthermore, the bond distance C(2)–N(3) is 1·51 Å, a value near that found in saturated compounds while the C(5)–N(4) distance is much shorter, 1·35 Å. The latter value for C–N is characteristically found in compounds where C–N is adjacent to C=S as in thiourea (Kuncher & Truter, 1958) and its derivatives (Dias & Truter, 1964). Apparently the presence of the C=S has a profound effect not only on the neighboring nitrogen atom, N(4), but also on the neighboring sulfur atom, S(1). The two C–S distances in the ring are also considerably different from each other, 1·78 and 1·84 Å, with the lower value adjacent to the C=S. The C=S distance, 1·65 Å, is somewhat shorter than that found in thiourea derivatives, 1·72 Å (Dias & Truter, 1964).

The usual values have been obtained for the bond distances and angles in the benzyl and methoxyphenyl substituents. The equations for the least-squares planes through rings I, II, and III are, respectively,

$$7{\cdot}2663x-4{\cdot}3274y-\ 2{\cdot}1285z=\ 1{\cdot}2524 \qquad (6)$$

$$-1{\cdot}8937x-3{\cdot}3007y+11{\cdot}835z=\ 0{\cdot}1323 \qquad (7)$$

and

$$7{\cdot}4924x-4{\cdot}6072y-\ 0{\cdot}3992z=-1{\cdot}9598\,, \qquad (8)$$

where the x, y and z values refer to coordinates in the triclinic system.

The thermal motion of the atoms in ring I is considerably greater than that of atoms in the other rings. The thermal parameters increase for atoms C(9), C(10), C(11), C(12) and C(13) as their distance from C(8) increases. The electron density map (Fig. 1) shows the effect of the thermal motion on these atoms.

The nearest intermolecular approaches are O(27)–C(17′) at 3·30 Å, O(27)–C(18′) at 3·66 Å, C(28)–C(20″) at 3·59 Å, and S(6)–C(20‴) at 3·62 Å.

We wish to express our appreciation to Mr Stephen Brenner, who performed all the high-speed machine calculations.

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Calculation of Exact Transmission Factors for Crystals with Constant Cross-Section

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Formulae for the calculation of exact transmission factors are derived by the block-mosaic method. The solutions of the integral for a cross-section are presented in a form which relates the area a_{qr} of a block to the paths of the X-rays diffracted at the corners of the a_{qr}. The use of the formulae is simplified if the a_{qr}'s are divided into triangles and parallelograms. The formulae are suitable for application to automatic computers.

Introduction

The intensities of the reflexions in X-ray diffraction patterns are affected by absorption. An exact evaluation of the absorption factor (or of the transmission factor) is needed to obtain good accuracy in structure determinations (Jeffery & Rose, 1964).

The transmission factor is usually defined as

$$A=\frac{1}{\tau}\int_{\tau}\exp\,(-\mu l)d\tau \qquad (1)$$

in which l represents the length in cm of X-ray path in the crystal, μ is the absorption coefficient in cm^{-1} and τ can be either an area or a volume. The integral,