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The Crystal and Molecular Structure of 1,4-Dithiadiene

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A non-planar six-membered ring with the 'boat' configuration has been established for the molecular structure of 1,4-dithiadiene, $C_4H_4S_2$. Molecular parameters, which suggest a model of C_{2v} symmetry, are $C\text{–}S = 1{\cdot}78 \pm 0{\cdot}05$ Å, $C{=}C = 1{\cdot}29 \pm 0{\cdot}05$ Å, $C{=}C\text{–}S \cong 124°$ and $C\text{–}S\text{–}C \cong 100°$. The crystals are orthorhombic, the space group is $C_{2v}^{12}\text{–}Cmc2_1$, and the unit cell dimensions are $a = 11{\cdot}28$, $b = 6{\cdot}41$ and $c = 7{\cdot}36$ Å.

Introduction

In order to study the relative electronic effects of sulfur and oxygen, and to extend our knowledge of aromatic versus aliphatic character in the heterocyclic vinyl ethers, Parham, Wynberg & Ramp (1953) have prepared† 1,4-dithiadiene, and are continuing studies of its chemical properties.

Previous structural work on the oxygen analogue, 1,4-dioxadiene, is briefly reported by Beach (1941), who apparently tested only planar models in his electron-diffraction study. He interprets his results in terms of resonance which would give some aromatic character to the molecule. A tentative interpretation of the ultraviolet spectra has been made on the basis of the planar structure (Pickett & Sheffield, 1946). On the other hand, 1,4-dioxadiene does not undergo the usual aromatic reaction, such as nitration, acylation or reaction with metallic potassium (Lappin & Summerbell, 1948), but does undergo the reactions characteristic of an aliphatic vinyl ether, e.g. polymerization and reactions with halogens and hydrogen chloride. Clearly, reinvestigation of the molecular structure of 1,4-dioxadiene is desirable, in view of its chemical properties.

The molecular geometry of 1,4-dithiadiene is also of interest with respect to aromatic versus aliphatic character, and in the interpretation of its chemical properties. We have therefore carried out a study of its molecular structure by the X-ray diffraction method at −55° C., and have shown, as described below, that the molecule is non-planar and has the 'boat' configuration.

Experimental

A single crystal was grown at −25° C. by the usual techniques (Reed & Lipscomb, 1953), and zero-level photographs were taken at −55° C. about the axes [100], [010], [001] and [1$\bar{1}$0] at a precession angle of 30° with Mo $K\alpha$ radiation. Zero-, first- and second-level Weissenberg photographs were also taken about [001] with Mo $K\alpha$ radiation, but were not used in the refinement because they did not appreciably extend the precession data. In addition, zero-level precession photographs about [001] were taken down to −120° C., but there was no evidence of a transition.

Integrated intensities were estimated visually by means of intensity scales made with a single reflection of a 1,4-dithiadiene crystal exposed for varying lengths of time. Lorentz and polarization factors were applied (Waser, 1951), and the films were brought to a common scale by means of common reflections with the help of the intensity scale. In addition to the 123 observed reflections (Table 2), weak diffuse streamers parallel to c^* were observed on the $h0l$ precession photographs, and rough intensity measurements for those having indices $h01$ were obtained from the $hk1$ Weissenberg photographs.

Interpretation and molecular structure

The symmetry of reciprocal space is D_{2h}, and the orthorhombic unit cell has

$$a = 11{\cdot}28 \pm 0{\cdot}01,\; b = 6{\cdot}41 \pm 0{\cdot}01,\; c = 7{\cdot}36 \pm 0{\cdot}03 \text{ Å}.$$

Assumption of four molecules $C_4H_4S_2$ in this unit leads to a reasonable density of 1·45 g.cm.$^{-3}$ for the solid at −55° C., as compared with the experimental value† of 1·272 g.cm.$^{-3}$ for the liquid at 29° C. Reflections were observed for hkl only when $h+k = 2n$, and for $h0l$ only when $l = 2n$, except for the diffuse streamers. Thus the space group, aside from possible disorder, is $D_{2h}^{17}\text{–}Cmcm$ or one of the related subgroups $C_{2v}^{12}\text{–}Cmc2_1$ or $C_{2v}^{16}\text{–}C2cm$. A pyroelectric test was negative, and hence adds no information for decision among these space groups.

The nearly normal decline of the $00l$ reflections suggested that the molecular rings lay approximately parallel to the ab plane. Hence the Patterson projection along c was made, and easily interpreted in terms of

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† Although the preparation of 1,4-dithiadiene was first reported by Levi (1890), who named the compound 'biophene', the physical and chemical properties suggest that he was dealing with a different substance.

† Private communication from H. Wynberg.

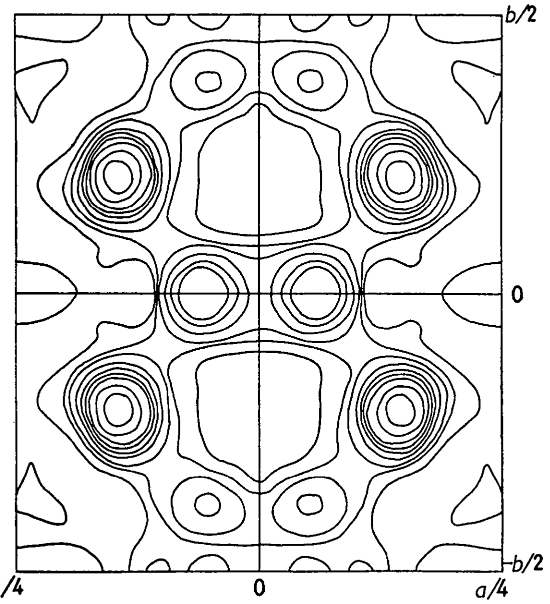

Fig. 1. Projection of electron density along the c axis. Contours are at 0, 2, 3, 4, 6, 8, 10, 12, 16 and 20 e.Å^{-2}.

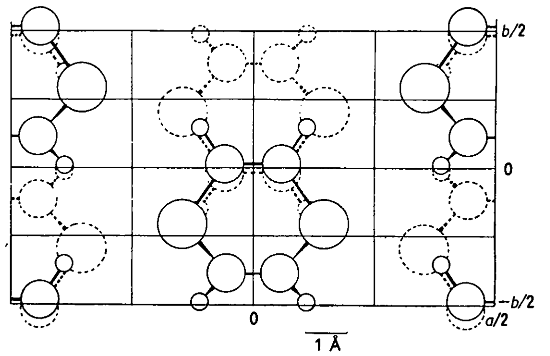

Fig. 2. Molecular interpretation of Fig. 1. Large, medium and small circles represent, respectively, sulfur, carbon and hydrogen atoms.

Table 1. *Final parameters found for* S *and* C *atoms and estimated parameters for* H *atoms*

	S	C_1	C_2	H_1	H_2
x	0·146	0·559	0·055	0·611	0·109
y	0·205	0·483	0·382	0·350	0·488
z	0·250	(*A*) 0·243 or (*B*) 0·257	0·117	(*A*) 0·239 or (*B*) 0·261	0·037

Table 2. *Comparison of structure factors* (*Model A*)

Index *hkl*	F_o	$\lvert F_c \rvert$
002	109	125
004	50·2	57·9
006	32·8	41·9
008	17·3	23·1
0,0,10	3·8	7·8
020	43·3	41·5
021	28·0	26·5*
022	42·2	45·5
023	41·6	40·5
024	23·1	29·4
025	20·2	22·6
026	10·2	17·1
027	< 3·9	5·3*
028	5·0	8·2
029	< 3·7	4·4*
040	20·7	19·6
041	43·8	47·2
042	30·8	28·0
043	32·3	35·6
044	30·3	26·7
045	20·2	23·9
046	14·9	12·1*
047	10·7	14·0
048	4·8	3·9*
049	4·2	6·6
060	5·7	6·5
061	18·2	23·8
062	7·9	7·1
063	7·2	12·5
064	7·7	6·4
065	6·5	9·8
066	5·0	3·3*
067	6·2	8·0
068	< 1·9	1·3*
080	4·6	2·5
081	6·8	8·7
082	5·5	5·0*
083	7·4	8·2
084	4·9	4·7
110	27·4	24·7
111	69·1	67·8
112	59·0	47·1*
113	26·7	27·0
114	33·4	29·8
115	13·3	19·8
116	13·3	12·0*
117	10·8	15·1
118	< 7·6	3·5*
119	< 6·9	6·2
1,1,10	< 6·1	3·1*
130	< 3·9	7·9
150	30·7	33·1
170	5·9	7·5
200	38·6	30·5
202	25·8	22·2*
204	11·3	13·6
206	< 4·3	3·9†
208	< 4·3	2·6*
2·0·10	< 3·2	2·0*
220	43·8	36·2
221	39·6	28·4*
222	30·8	26·9
223	8·4	6·8*
224	16·2	17·0
225	7·0	6·0*
226	9·2	10·5
227	7·7	6·8
228	< 7·6	5·4
229	< 6·9	2·8*
240	< 4·5	5·9
260	< 5·3	1·5
280	6·3	4·5
310	18·2	19·8
330	52·8	50·8
331	36·1	35·4
332	42·7	39·3
333	18·5	21·9
334	24·9	26·1
335	9·7	15·1
336	13·2	17·2
337	< 6·6	10·4
338	< 7·6	9·2
339	< 6·3	4·3
350	17·0	22·4
370	9·5	12·3
400	76·7	69·5
402	57·7	56·8
404	34·6	41·3
406	15·3	22·4
408	6·4	10·5
4,0,10	< 2·3	5·1
420	54·7	46·2
440	17·8	15·5
441	23·1	29·0
442	13·1	11·3
443	19·1	23·8
444	9·8	7·8
445	10·8	15·9
446	7·7	5·6
447	< 7·6	8·8
448	< 6·1	3·2
460	< 5·3	2·3
480	< 4·2	4·9

Table 2 (*cont.*)

Index *hkl*	F_o	$\|F_c\|$
510	< 3·9	4·0
530	< 4·6	2·2
550	< 6·9	5·2
551	< 6·9	0·5*
552	< 7·6	4·5
553	< 7·6	0·4*
554	< 7·6	2·6
555	< 7·6	0·2*
556	< 7·6	2·0
557	< 6·8	0·3*
570	< 5·2	1·0
600	22·2	22·4
602	26·2	29·6
604	21·1	24·0
606	10·9	11·3
608	5·6	5·0
620	32·5	36·9
640	5·6	8·8
660	< 7·6	0·2
661	9·6	11·3
662	< 7·6	0·6*
663	9·6	11·6
664	< 6·9	0·8*
665	8·2	7·7
666	< 4·3	0·5*
680	4·9	4·6
710	5·6	9·4
730	34·3	36·2
750	10·4	12·9
770	8·0	9·2
771	< 7·6	6·3
772	< 6·9	9·4
773	< 6·8	3·2
774	< 5·6	7·5
800	7·2	2·6
802	9·5	13·2*
804	8·0	13·0
806	< 4·5	4·0†
808	< 3·5	1·5*
820	26·6	22·8
840	7·8	5·0
860	6·2	1·0
910	11·1	5·4
930	5·8	2·6
950	12·1	11·9
970	< 4·3	2·0
10,0,0	33·4	37·4
10,0,2	30·4	28·3
10,0,4	21·5	16·7
10,0,6	12·4	14·0
10,0,8	5·6	8·2
10,2,0	13·5	14·2
10,4,0	8·7	5·8
10,6,0	< 4·1	2·0
11,1,0	6·5	4·6
11,3,0	5·9	5·1
11,5,0	8·1	10·5
12,0,0	< 4·6	3·3
12,0,2	< 4·5	2·3*
12,0,4	< 4·4	1·0
12,0,6	< 3·2	1·1*
12,2,0	< 5·2	1·3
12,4,0	< 4·7	0·8
12,6,0	< 2·8	0·1
13,1,0	5·2	3·6
13,3,0	7·6	6·0
13,5,0	7·0	4·6
14,0,0	12·7	11·1
14,0,2	11·1	9·7
14,0,4	8·7	7·1
14,2,0	7·3	6·0
14,4,0	4·3	2·9
15,1,0	< 3·9	1·5

* Reflection for which $B_{hkl} > \frac{1}{2}A_{hkl}$.

† Reflection for which $B_{hkl} > \frac{1}{2}A_{hkl}$ and value calculated for model *B* is greater than observed limiting value.

a six-membered ring which appeared flat in this projection (see Figs. 1 and 2). Two refinements were made with the assumption of 8 S, 8 C_1 and 8 C_2 in three sets of the eightfold positions, x, y; $\bar{x}, y$; $x, \bar{y}$; $\bar{x}, \bar{y}$, plus 0, 0 and $\frac{1}{2}, \frac{1}{2}$. The second refinement resulted in no sign changes and a value of $R = \Sigma||F_o|-|F_c|| \div \Sigma|F_o| = 0{\cdot}186$.

In order to resolve the space-group ambiguity a sharpened Patterson projection along *a*, with the origin peak removed, was calculated. In addition to a striking ridge along $z = \frac{1}{2}$, there were peaks at y, z coordinates of (0·176, 0·133), (0·092, 0·37), and a fairly large peak at ($\frac{1}{4}$, 0). The ridge and peaks along $z = \frac{1}{2}$ indicated that the sulfur parameters of $y = 0{\cdot}205$ and $z = \frac{1}{4}$ are consistent with the projection along *c*. The peak at $y = 0{\cdot}176$, $z = 0{\cdot}133$, then, is a C–S vector within the ring, and was in fact similarly interpreted in the *c*-axis projection. Now if we assume a mirror plane at $z = \frac{1}{4}$, as required in the space groups *Cmcm* or *C2cm*, this C–S vector is mirrored about $z = \frac{1}{4}$ and the C–S–C bond angle would be about 65°, instead of its usual value of about 102° (Allen & Sutton, 1950). Hence we rejected *Cmcm* and *C2cm* as possible space groups, and chose $Cmc2_1$, which proved to be satisfactory.

Vector overlap methods (Beevers & Robertson, 1950) then led uniquely to a non-planar 'boat' configuration (Fig. 8), with S, C_1 and C_2 in separate sets of the eight-fold positions x, y, z; $\bar{x}, y, z$; $x, \bar{y}, \frac{1}{2}+z$; $\bar{x}, \bar{y}, \frac{1}{2}+z$ plus 0, 0, 0 and $\frac{1}{2}, \frac{1}{2}, 0$. Complete Fourier refinements were then made on the three principal zones, including hydrogen atom contributions in the later stages and backshift corrections with the use of the corresponding F_c syntheses. Final parameters represent a weighted average from resolved atoms in these three projections.

In the refinement of the *a*-axis projection a Patterson ambiguity arose associated with the *z* coördinate of C_1. Displacement of C_1 by 0·05 Å from its starting value of $z = \frac{1}{4}$ was indicated, but the Patterson projection is equally consistent with a positive or negative displacement, i.e. with a final value of $z(C_1) = 0{\cdot}243$ (Model *A*) or $z(C_1) = 0{\cdot}257$ (Model *B*). This ambiguity is illustrated in Fig. 7. Refinement of this projection was found to lead to either of these models, depending upon which was closest to the starting model. Hence coordinates for both Model *A* and Model *B* are included in Table 1, which lists expected values of parameters for hydrogen atoms as well.

For both Models *A* and *B* the structure factors of the forms 0*kl*, *h*0*l*, *hk*0 and *hhl* were calculated with the use of International Business Machines. For both models the usual logarithmic plot gave a temperature factor $\exp\left[-4{\cdot}0 \sin^2 \theta/\lambda^2\right]$. Values of *R* are 0·165 for Model *A* and 0·167 for Model *B* (observed reflections only), and 0·197 and 0·200, respectively, when unobserved reflections are included. Calculated structure factors for Model *A* are compared with observed values in Table 2, and some indication of their comparison with values for Model *B* are indicated.

Molecular parameters, calculated from the data in Table 1, are not greatly different for the two models. Values of bond lengths and angles are given in Table 3, where the probable errors are estimates based on comparisons with other studies, but are comparable with the backshift corrections.

Table 3. *Bond lengths and angles*

	Length (Å)	Angle	Angle (all ±2°)
$C_2=C_2'$	1·24±0·04	$C_2=C_2$–S	124·4
$C_1=C_1'$	1·33±0·02	$C_1=C_1$–S	124·6
$C=C_{av.}$	1·29±0·05	$C=C-S_{av}$	124·5
C_2–S	1·82±0·04	C_1–S–C_2	100·2 (Model *A*)
C_1–S	1·73±0·04	φ	137·1 (Model *A*)
$C-S_{av.}$	1·78±0·05		
		C_1–S–C_2	102·1 (Model *B*)
C–H	1·06 (assumed)	φ	141·3 (Model *B*)
		C=C–H	124 (assumed)

Models *A* and *B* have so nearly the same parameters that one cannot decide between them on chemical grounds. They differ only in the 0·1 Å difference in the *z* parameter of C_1, and in no sense represent an ambiguity relative to the gross molecular structure. Thus it is certain that the molecule is non-planar, and has the 'boat' configuration. One cannot hope to distinguish between these models on the basis of the overall *R* values. However, one can arrive at a very slight preference for Model *A* from a detailed comparison of those 12 reflections which are most sensitive to the carbon parameters, i.e. those for which $B_{hkl} > \frac{1}{2}A_{hkl}$ (the S atoms contribute nothing to B_{hkl}). For Model *B* there are two reflections for which $|F_c|$ is greater than the lower limit of observation, whereas there are no such cases for Model *A*. Turning to the 12 observed reflections we find that 7 favor Model *A*, 4 favor Model *B*, and one is the same for both models. The two most sensitive of these reflections favor Model *A*. Values of *R* are 0·189 for Model *A* and 0·204 for Model *B*. The reflections which are used in this argument are indicated in Table 2.

Thus, while we may express a very slight preference for Model *A*, actually we felt it wise to increase our probable errors so that both models are included. For results of chemical interest it seems to us that the gross molecular configuration was the chief point of interest, and hence have not investigated the ambiguity further.

Discussion

The boat configuration (Fig. 8) is consistent with the assumptions of a nearly normal S–C single bond, and a nearly normal ethylenic double bond between the carbon atoms. Ethylenic hybridization is certainly consistent with a planar S–C=C–S configuration. The dihedral angle, φ, between the planes is 137° (Model *A*). Within the limit of the accuracy of our results the symmetry of the isolated molecule is C_{2v}, with average parameters C–S = 1·78±0·05 Å, C=C = 1·29±0·05 Å, C–C–S = 124° and C–S–C = 100°.

Although the C–S bond distance is insignificantly shorter than that of 1·81 Å given in the table of covalent radii (Pauling, 1942, p. 164), our value is the same as that found in the electron-diffraction studies of dimethyl disulfide (Stevenson & Beach, 1938) and dimethyl trisulfide (Donohue & Schomaker, 1948), and is greater than that found in thiophene (Schomaker & Pauling, 1939). We cannot be sure that the observed C=C distance is really significantly shorter than the 'normal' C=C distance because of our relatively large probable errors.

Bond angles are certainly reasonable when compared

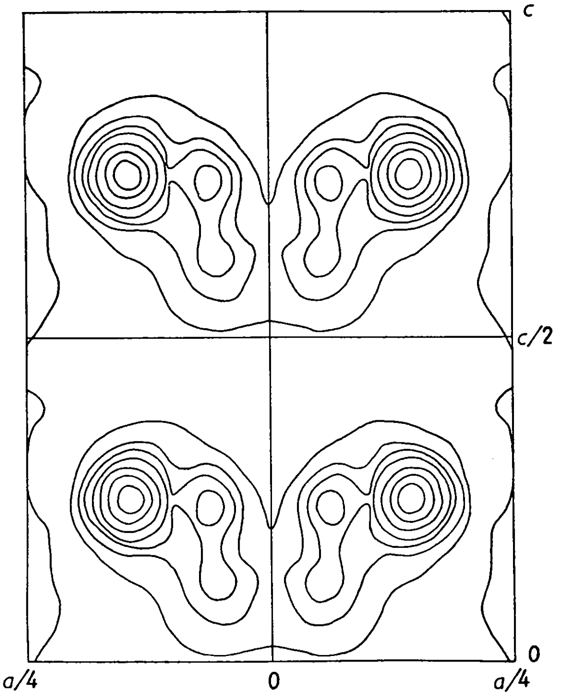

Fig. 3. Projection of electron density along the *b* axis. Contours are at 0, 2, 4, 6, 8, 12, 16 and 20 e.Å^{-2}.

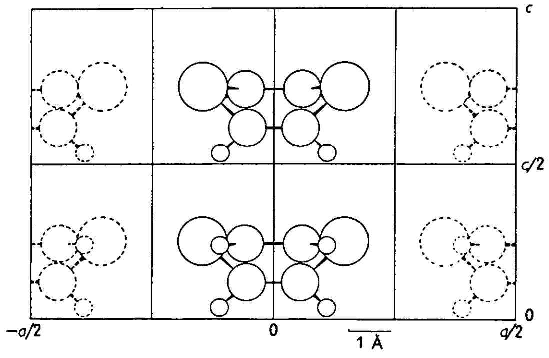

Fig. 4. Molecular interpretation of Fig. 3.

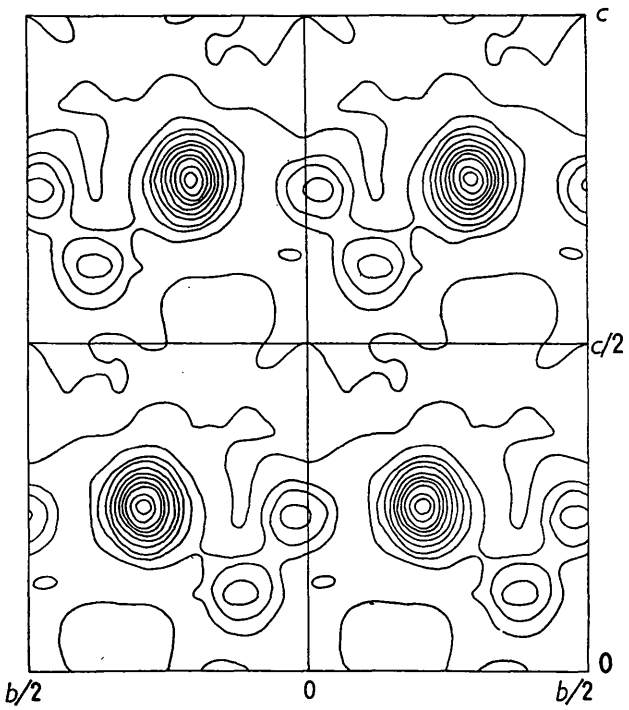

Fig. 5. Projection of electron density along the *a* axis. Contours are at intervals of 4 e.Å^{-2}, starting with the lowest contour at 2 e.Å^{-2}.

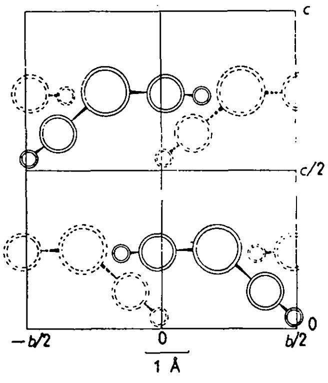

Fig. 6. Molecular interpretation of Fig. 5.

with similar angles in other molecules. The C=C–C angle in 1,3-butadiene is 122° (Allen & Sutton, 1950), and the C=C–Cl angle is 123° in tetrachloroethylene (Karle & Karle, 1952; Lipscomb, 1946). The C–S–C bond angle varies between extremes of 91° in thiophene to 107° in dimethyldisulfide, but when constraints are small our value of 100° seems very reasonable.

The packing in the crystal is best grasped by reference to the three projections on (001), (100), and (010), along with the atomic interpretation shown in Figs. 2, 4 and 6. The molecules lie in layers with their sulfur–sulfur axes parallel to the crystallographic *a* axis. The $S–C_1–C_1–S$ plane lies essentially parallel to the *ab* crystal face with the $S–C_2–C_2–S$ plane inclined at about 43°. The molecules are stacked in the *c* direction with the $S–C_1–C_1–S$ planes overlapped and the $S–C_2–C_2–S$ planes sticking out in alternative plus and minus *b* directions, as may best be seen in Fig. 6. It is interesting to note that the crystal seems to employ both common modes of organic crystal packing, one with rings parallel to each other, and the other with rings inclined at nearly right angles to each other.

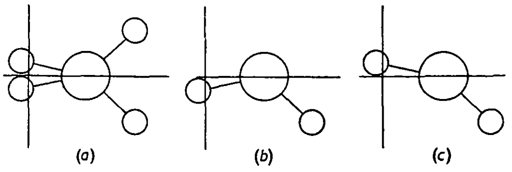

Fig. 7. Illustration of the ambiguity in the *a*-axis projection; the effect has been exaggerated for clarity. The composite molecule obtained by vector overlap methods is represented by (*a*). Model *A* is represented by (*b*), and Model *B* by (*c*).

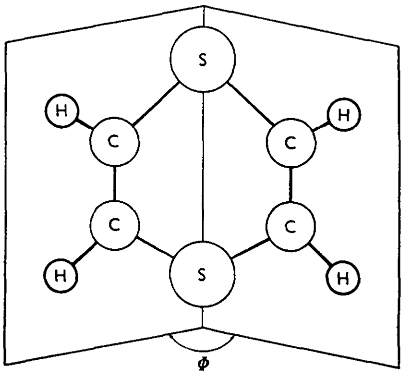

Fig. 8. The molecular structure of 1,4-dithiadiene.

The packing of the molecules into the unit cell is reasonable, all molecules being in van der Waals contact. Within a given layer (assuming C_1 at $z = \frac{1}{4}$), the shortest contacts are $S \cdots C_1 = 3{\cdot}8$ Å and $C_2 \cdots C_1 = 4{\cdot}0$ Å. Between layers the shortest contacts are $S \cdots C_1 = 4{\cdot}0$ Å and $S \cdots C_2 = 3{\cdot}9$ Å. These distances are quite consistent with the normal van der Waals radii; R_S 1·85 Å, R_{CH_2} 2·0 Å (Robertson, 1953, p. 227).

The diffuse reflections

The weak diffuse streamers parallel to c^*, described in the experimental section, had indices $h0l$ with h even. Hence, we sought an explanation associated with violation of the *c* glide. A possible, but not necessarily unique, explanation is to have those pairs of molecules related by this *c* glide slightly displaced in opposite directions about axes parallel to *b*. Rough structure-factor calculations showed that displacement of the coordinate of the sulfur atoms by only 0·2 Å gave fair agreement with the $h01$ reflections. Observed structure factors are 2·7, 6·7, 6·4, 5·9, 14·5, 4·9 and 6·9 for h = 2, 4, 6, 8, 10, 12 and 14 respectively, on the same scale as those listed in Table 2. Because the quality and quantity of these diffuse reflections is low, and because they are sufficiently faint that they do not represent a major disorder in the structure, we have not investigated them further. It does seem likely that they represent such a limited disorder that no doubt remains about the correctness of the ordered structure.

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References

ALLEN, P. W. & SUTTON, L. E. (1950). *Acta Cryst.* **3**, 46.

BEACH, J. Y. (1941). *J. Chem. Phys.* **9**, 54.

BEEVERS, C. A. & ROBERTSON, J. H. (1950). *Acta Cryst.* **3**, 164.

DONOHUE, J. & SCHOMAKER, V. (1948). *J. Chem. Phys.* **16**, 92.

KARLE, I. L. & KARLE, J. (1952). *J. Chem. Phys.* **20**, 63.

LAPPIN, G. R. & SUMMERBELL, R. K. (1948). *J. Organ. Chem.* **13**, 671.

LEVI, L. E. (1890). *Chem. News*, **62**, 216.

LIPSCOMB, W. N. (1946). Ph.D. Thesis, California Institute of Technology.

PARHAM, W. E., WYNBERG, H. & RAMP, F. L. (1953). *J. Amer. Chem. Soc.* **75**, 2065.

PAULING, L. (1942). *The Nature of the Chemical Bond.* Ithaca: Cornell University Press.

PICKETT, L. W. & SHEFFIELD, E. (1946). *J. Amer. Chem. Soc.* **68**, 216.

REED, T. B. & LIPSCOMB, W. N. (1953). *Acta Cryst.* **6**, 45.

ROBERTSON, J. M. (1953). *Organic Crystals and Molecules.* Ithaca: Cornell University Press.

SCHOMAKER, V. & PAULING, L. (1939). *J. Amer. Chem. Soc.* **61**, 1769.

STEVENSON, D. P. & BEACH, J. Y. (1938). *J. Amer. Chem. Soc.* **60**, 2872.

WASER, J. (1951). *Rev. Sci. Instrum.* **22**, 567.

Acta Cryst. (1954). **7**, 503

The Effect of Anisotropic Thermal Vibration on the Atomic Scattering Factor

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A discussion of the effect of anisotropic thermal vibration of the atoms in a crystal on the intensity of the Bragg reflexions leads to a method by which these anisotropic temperature factors can easily be evaluated numerically.

It is well known that the effect of isotropic thermal vibration of atoms in a crystal is to reduce the atomic scattering factor for Bragg reflexions by a factor

$$\exp\left[-2\pi^2u^2S^2\right], \quad (1)$$

where u^2 is the mean square displacement of an atom from its average position and $S = 2\sin\theta/\lambda$. It has generally been assumed that when the thermal vibration is anisotropic, the surfaces of constant temperature factor in reciprocal space are ellipsoids. As far as I am aware, no proof of this has been offered. The following derivation shows the circumstances in which the result is true, and has the merit of suggesting a way in which the calculation of structure factors, with allowance for anisotropic temperature effects, can be simplified.

Let r, having rectangular components (x, y, z), be a distance in space, and S, with rectangular components (ξ, η, ζ), a distance in reciprocal space. The directions (x, y, z) and (ξ, η, ζ) coincide; they are not however the directions of the crystallographic axes (which need not be rectangular), but are the 'principal directions of vibration' of an atom. Let $\varrho_0(r)$ be the electron distribution in the atom at rest, and $f_0(S)$ its atomic scattering factor. $f_0(S)$ is the Fourier transform of $\varrho_0(r)$; the latter is assumed to have spherical symmetry and therefore $f_0(S)$ also has this symmetry. Now suppose the atom to be displaced from its mean position so that the probability that its centre lies within a volume element $dx\,dy\,dz$ is

$$p(x, y, z)dxdydz = ((2\pi)^{3/2}u_xu_yu_z)^{-1} \times \exp\left[-(x^2/2u_x^2+y^2/2u_y^2+z^2/2u_z^2)\right]dxdydz\,, \quad (2)$$

u_x^2, u_y^2 and u_z^2 being the mean square displacements in the three directions at right angles. The resulting average electron distribution $\varrho(r)$ may be described as the convolute of $\varrho_0(r)$ with $p(x, y, z)$. It follows that the resulting atomic scattering factor, $f(S)$, is the product of $f_0(S)$ with the Fourier transform of $p(x, y, z)$. This transform may be shown to be