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## The Crystal Structure of Diiodoacetylene; an Example of Pseudosymmetry

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Diiodoacetylene,  $C_2I_2$ , forms tetragonal crystals with  $a=15.68(3)$ ,  $c=4.30(1)$  Å, eight molecules in the unit cell, space group  $P4_2/n$ . The structure was determined from three-dimensional diffractometer data, and the refinement carried to a conventional  $R$  of 0.145. The problem was complicated by decomposition of the crystals, twinning and pseudosymmetry in the diffraction pattern. The linear molecules are in general positions, but each molecule points, at both ends, towards the middles of two adjacent molecules to give four  $C \cdots I$  distances of about 3.4 Å, which we interpret as donor( $C \equiv C$ )–acceptor( $I$ ) interactions. The intramolecular  $I \cdots I$  distance is 5.16 Å.

### Introduction

Several years ago Professor Jerry Donohue pointed out to one of us an apparently anomalous situation in the structure of crystalline diiodoacetylene,  $C_2I_2$ . Flannery & Nixon (Flannery, 1966) had made X-ray diffraction photographs that showed Laue symmetry  $4/mmm$  and systematic extinctions corresponding to an  $n$  glide plane perpendicular to the  $c$  axis. This evidence would require the space group to be  $P4/nmm$ , although there was also an indication of a  $4_2$  axis parallel to  $c$ . The cell dimensions,  $a=b=15.65$ ,  $c=4.29$  Å, and measured density suggested eight molecules in the unit cell. No hypothetical structure consistent with the  $P4/nmm$  space group with  $Z=8$  could be found, and an examination of the  $hk0$  reflexions (Patterson projection along the short  $c$  axis) did not provide a solution. The possibility of twinning was raised but not explored further. Additional complications are caused by gradual decomposition of the compound in the X-ray beam.

We have studied the problem further and report here our results.

### Experimental

A sample of diiodoacetylene was supplied to us by Dr E. Kloster-Jensen (Kloster-Jensen, 1969). Crystals

suitable for X-ray diffraction studies were prepared by sublimation at 50°C under reduced pressure; since the crystals are light-sensitive it was necessary to work in a darkened room. Precession photographs (Mo  $K\alpha$  radiation,  $\lambda=0.7107$  Å) showed the crystals to be tetragonal with  $a=15.68(3)$  and  $c=4.30(1)$  Å, in agreement with Flannery's values of 15.65 and 4.29 Å. Careful scrutiny of the photographs shows that the  $P4/mmm$  symmetry is only approximate; about 20% of the reflexion-pairs  $hkl$  and  $khl$  show small but significant intensity differences that cannot be explained away as absorption effects. The intensity differences vary from crystal to crystal but they affect the same reflexion pairs. The true Laue symmetry is only  $P4/m$ . Systematic extinctions:  $0k0$ ,  $k=2n+1$ ;  $hk0$ ,  $h+k=2n+1$  show the space group to be  $P4_2/n$ . (The following discussion is based on the second arrangement of  $P4_2/n$  given in *International Tables for X-ray Crystallography* (1959) with the origin at  $\bar{1}$ .) The density of 3.43(3) g.cm<sup>-3</sup> measured by flotation in thallos formate–thallous malonate solution agrees with the value of 3.49(1) g.cm<sup>-3</sup> calculated for  $Z=8$ .

Intensity data were collected using the Hilger and Watts linear diffractometer (Mo  $K\alpha$  radiation, balanced filters, crystal mounted with  $c$  as the rotation axis, two cycles per reflexion). At room temperature, at which all the measurements were made, the crystals decomposed in the X-ray beam at such a rate that it was necessary to use three different crystals to collect the data; one for  $hk0$ , one for  $hk1$  and  $hk2$ , and one for  $hk3$  and  $hk4$ . All the crystals were prisms elongated

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slightly along *c* with prominent forms {110} and {001}. Their dimensions were 0.15 × 0.20 × 0.32 mm, 0.16 × 0.30 × 0.32 mm and 0.20 × 0.25 × 0.35 mm. The intensities of two test reflexions decreased by 0.5 to 1.5% per hour, depending on the crystal; the crystals were discarded after the intensities had decreased by about 20%. The measured intensities were rescaled by comparison with the test reflexions to eliminate the observed trend with time. Also, the data from the three crystals were put on a common scale by reference to the test reflexions. 845 symmetry-independent (on the basis of 4/*m* Laue symmetry) reflexions were measured. Eventually two of these were eliminated because of presumed extinction and 79 were discarded because the twin equivalents were not measured, so that 764 reflexions were finally used. The usual Lorentz and polarization corrections were made. Although the linear absorption coefficient is 118 cm<sup>-1</sup> for Mo *K*α radiation, absorption corrections were not made; the neglect of absorption corrections introduces systematic errors of up to 50% in the *F* values. These errors are partially compensated by adjustments of the temperature factors but certainly influence the results of the results of the eventual refinement. Unfortunately, at the time the data were collected, no absorption-correction program was available, and although the crystal dimensions were recorded, the orientations with respect to the X-ray beam were not.

### Solution of the structure

The Patterson map calculated from the diffraction data is shown schematically in Fig. 1(a); the deviations

from *P4/mmm* symmetry are very slight. A comparison of the symmetry of the special positions of *P4*<sub>2</sub>/*n* with the likely shape of the C<sub>2</sub>I<sub>2</sub> molecule makes it almost certain that there must be two sets of iodine atoms in general positions. Casual inspection of the Patterson map shows that all the peaks have *u* and *v* coordinates near *n*/4 and *w* coordinates near 0 or ½, strongly suggesting that the heavy iodine atoms all have *x* and *y* coordinates near *n*/8 and *z* coordinates near ±¼. This means that one set of iodine atoms, I(1), is grouped round the 4 axes with a second set, I(2), grouped round the 4<sub>2</sub> axes. A closer examination of the Patterson map shows that there are splittings and displacements of peaks from *u* and *v* coordinates of *n*/4, and also that the peaks fall into two classes with respect to their behaviour along *w*. There is a group of *sharp* peaks with half-widths along *w* approximately equal to the half-width of the origin peak, and a group of *diffuse* peaks with half-widths along *w* about ⅔ the half-width of the origin peak. The existence of *sharp* peaks near *u*=0, *v*=½, among others, requires that the two independent iodine atoms have nearly equal *z* parameters; from a detailed consideration of the half-width of the *diffuse* peaks, *z* must be approximately 0.20. There is, however, an ambiguity in assigning the *x* and *y* parameters, introduced by the apparent *P4/mmm* symmetry. The Patterson function shows [peak 1, Fig. 1(a)] that the atoms I(2) are rotated away from the diagonals more than the atoms I(1). The sense of this rotation may be chosen arbitrarily. The displacement of I(1) from *x*=½, *y*=½ can also be determined from the Patterson peak positions, but the rotation from the diagonals is too small to be estimated readily.

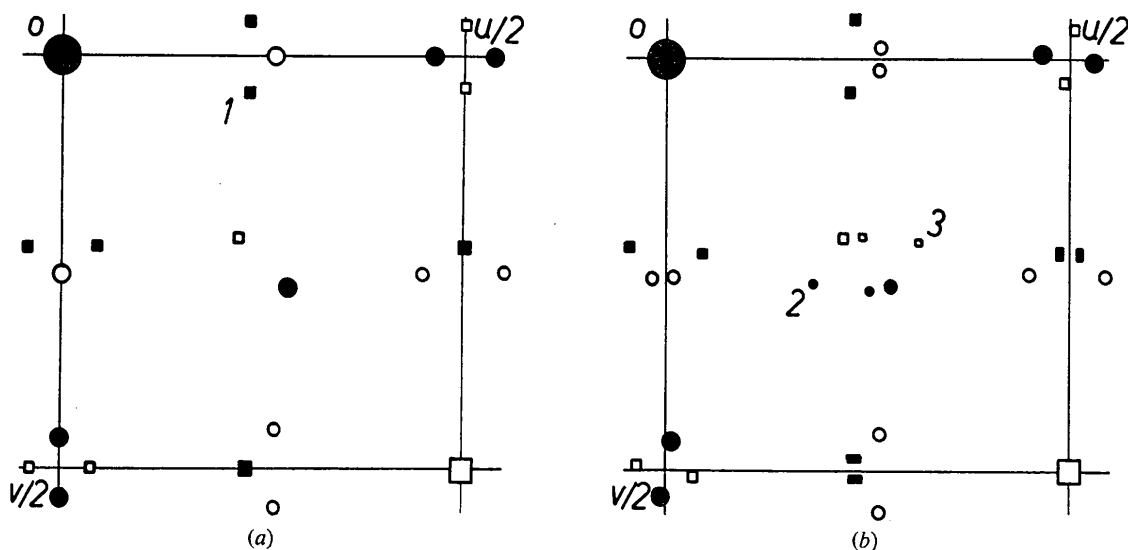


Fig. 1. (a) The observed Patterson map. Solid circles represent *sharp* (see text) peaks at *w*=0; open circles, *diffuse* peaks at *w*=0; solid squares, *sharp* peaks at *w*=½; open squares, *diffuse* peaks at *w*=½. The sizes of the peaks correspond approximately to the peak heights. (b) The calculated Patterson map. Solid circles, peaks at *w*=0; open circles, peaks at *w*=±0.11; solid squares, peaks at *w*=0.50; open squares, peaks at *w*=±0.39. The sizes of the peaks correspond to the number of overlapping peaks at the point. The numbered peaks in both figures are referred to in the text,

However, a small rotation in the same sense as for I(2) appeared to be indicated.

The trial set of iodine atom positions thus found differs only slightly from the final, refined positions. Fig. 1(b) shows the Patterson map based on these positions (the final parameters were used to draw the map). Several features merit comment: (i) most of the peaks on the experimental Patterson map represent the superposition of more than one peak from the calculated Patterson map; (ii) the deviation from  $P4/mmm$  symmetry in the calculated map is rather small; (iii) the two peaks [2 and 3, Fig. 1(b)] that would break the  $P4/mmm$  symmetry most clearly were not recorded on Fig. 1(a). A re-examination of the Patterson map after the trial structure was deduced showed very slight peaks (less than  $\frac{1}{3}$  the height of the next lowest peak) at the indicated positions and even slighter peaks (by about one-half) at the  $P4/mmm$  symmetry-related positions across the diagonal mirror plane. The former peaks confirmed our choice of the sense of the rotation of I(2). A Fourier synthesis based on the trial structure ( $R=0.49$  with  $B=3 \text{ \AA}^2$  assumed) gave rise to spherical peaks at approximately the same positions; the  $R$  value improved to 0.30,  $B=3.5 \text{ \AA}^2$ .

#### A digression on pseudosymmetry

As an exercise, the question was raised – what conditions on the coordinates *maximize* the pseudosymmetry of the Patterson map? Suppose the positional parameters of the two independent iodine atoms at  $x_1, y_1, z_1$  (near  $\frac{1}{8}, \frac{1}{8}, 0.2$ ) and  $x_2, y_2, z_2$  (near  $\frac{3}{8}, -\frac{1}{8}, -0.2$ ) to be related such that  $x_2 = x_1 + 2y_1$  and  $y_2 = -y_1$ . This is approximately the case in our structure and corresponds to pairs of molecules being related by the translation with components  $2(x_1 + y_1), 0, (z_1 + z_2)$ . Of the  $16^2 (=256)$  Patterson interactions, 224 comprise a set with exact  $P4/mmm$  symmetry, and only the remaining set of 32 interactions [8 for  $2x_i, 2y_i, 2z_i$ , etc., 4 double-weight for  $\frac{1}{2} - 2x_i, \frac{1}{2} - 2y_i, 0$ , etc. ( $i=1,2$ )] have the  $P4/m$  symmetry appropriate to the space group. If, as a further condition,  $x_1 = y_1$ ,

240 peaks would comprise the set with  $P4/mmm$  symmetry and only 16 peaks (8 for  $2x_2, 2y_2, 2z_2$ , etc., 4 double-weight for  $\frac{1}{2} - 2x_2, \frac{1}{2} - 2y_2, 0$ , etc.) would have  $P4/m$  symmetry. Furthermore, if the positions were exactly  $\frac{1}{8}, \frac{1}{8}, z_1$  and  $\frac{3}{8}, -\frac{1}{8}, z_2$ , then the Patterson map would have *exact*  $P4/mmm$  symmetry even though the symmetry of the structure would only be  $P4_2/n!$  In this case the diffraction pattern would also have  $P4/mmm$  symmetry although it would show an unusual pattern of extinctions. If  $z_2 = -z_1$ , further extinctions result and finally if  $z_1 = \frac{1}{4}, z_2 = -\frac{1}{4}$ , the space group becomes  $I4/m$ . Fig. 2 shows the effect of these successive requirements on the diffraction pattern ( $hkl$  is chosen to illustrate the changes in the entire pattern).

By coincidence, the low-temperature form of dimethylacetylene (Miksic, Segerman & Post, 1959), which is also tetragonal, shows an unusual pattern of extinctions due to an accidental relationship between the coordinates of the atoms. (Also see the discussion of the packing.)

#### Refinement of the structure

In the course of the intensity measurements the positive direction of the  $c$  axis had been chosen arbitrarily for each crystal. This arbitrary choice introduces an ambiguity in the sense of the 4-fold rotation axis with respect to the  $+c$  direction, *i.e.* an ambiguity in the indexing of reflexions as  $hkl$  or  $khl$ , from crystal to crystal. The  $hk0$  reflexions, measured from a single crystal, were known at least to be self-consistent in this respect, so it was decided first of all to refine these data separately. Of the three possible orientations for a particular molecule, parallel to (100), (010), or (110), only the last gave a reasonable intramolecular  $I \cdots I$  distance of about  $5.2 \text{ \AA}$ ; the carbon atoms were included so as to correspond to this orientation. Three cycles of least-squares analysis with isotropic vibration parameters gave  $R=0.175$  (0.164 if the two most intense reflexions, which appeared to suffer from secondary extinction, were omitted).

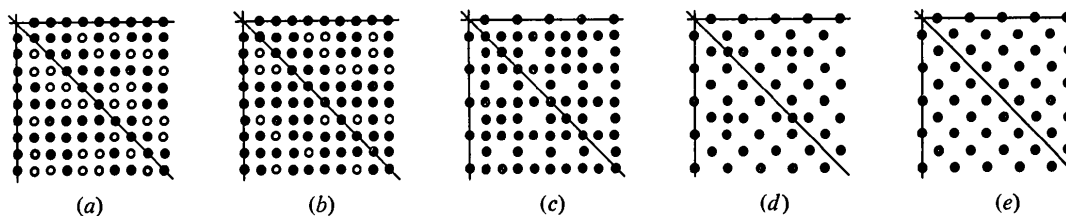


Fig. 2. The pseudosymmetry of the diffraction pattern. The positive quadrant of the layer  $l=1$  is shown as an example. Intensity differences are not shown, except for  $hkl-khl$  pairs or systematic extinctions. (a) No conditions on the positional parameters for the two atoms:  $x_1=0.121, y_1=0.109, z_1=0.200, x_2=0.320, y_2=-0.115, z_2=-0.190$ . The open circles represent reflexions that have intensities less than 50% of the intensities of the related reflexion. (b)  $x_1, y_1, z_1, z_2$ , as in (a);  $x_2 = x_1 + 2y_1, y_2 = -y_1$ . Adding the conditions  $x_1 = y_1$  and/or  $z_2 = -z_1$  has little effect on this pattern. (c)  $x_1 = y_1 = \frac{1}{8}; z_1, x_2, y_2, z_2$ , as in (b). (d)  $x_1, y_1, z_1, x_2, y_2$  as in (c);  $z_2 = -z_1$  (e)  $x_1, y_1, x_2, y_2$  as in (c);  $z_1 = -z_2 = \frac{1}{4}$ . The space group changes here to  $I4/m$ . The space group in (a)-(d) is  $P4_2/n$ . It should be emphasized that for none of these arrangements does the diagonal mirror plane or its equivalent occur in the atomic arrangement.

Comparison of the observed and calculated structure factors showed that the observed values of  $|F(hkl)|$  and  $|F(khl)|$  were generally more nearly equal than the corresponding pairs of calculated values. That is, even though we expected an intensity pattern close to  $P4/mmm$  symmetry, the observed pattern is too close. This confirmed what we already suspected: that twinning was present. The distribution of the ratio  $F^2(hkl)/[F^2(hkl)+F^2(khl)]$  for all twin-related pairs (Britton, 1972) suggested that the larger twin was about 70% of the total for the crystal used for the  $hk0$  reflexions. After correction for the twinning, further least-squares analysis (isotropic vibrational parameters) gave  $R=0.152$ . The estimated standard deviations in the positions were about 0.007 Å for the iodine atoms and 0.09 Å for the carbon atoms; the molecule was still linear within the error limits.

Similar treatments of the data for  $l=1$  and 2 (crystal 2) and  $l=3$  and 4 (crystal 3) were not successful. The fractional volume of the larger twin in each case appeared to be nearer 0.60; the errors in the data, due in part to crystal decomposition and in part to the neglect of absorption corrections, are such that the twinning correction gave only insignificant improvement of the  $R$  value. In order to avoid the problem of the twinning correction, the  $h0l$  and  $hhl$  data, which are unaffected by the twinning, were used to refine the  $z$  parameters. This refinement (isotropic vibration parameters) gave  $R=0.165$  with standard deviations of about 0.013 Å for the iodine atoms and 0.16 Å for the carbon atoms. We believe that the inherent quality of the data corresponds to an  $R$  value near 0.15; further refinement with the present data therefore seems pointless since, except for the  $I\cdots I$  distances, we could guess the molecular parameters better than we could measure them. As a final test of the structure

and the data, we refined only the iodine atom positions with the  $h0l$  and  $hhl$  data, averaged the results with those from the corrected  $hk0$  data, put in carbon atoms so as to correspond to a linear  $C_2I_2$  molecule with normal bond lengths, and calculated  $R$  values for the original data and for a data set that allowed for the twinning in the following way:  $\langle F(hkl) \rangle = \{[F^2(hkl) + F^2(khl)]/2\}^{1/2}$ . The corresponding  $R$  values, layer by layer, are given in Table 1 (the data for  $l=4$  were also rescaled). The parameters are given in Table 2. Since our data are for three different crystals with three different degrees of twinning, it does not seem worthwhile to publish them; a set of observed and calculated structure factors is available from the authors on request.

### Discussion

The structure is shown in Fig. 3. The intramolecular  $I\cdots I$  distance of 5.16 Å is comparable with the distances found in donor-acceptor complexes such as 1,4-dioxane-diiodoacetylene, 4.97 Å (Gagnaux & Susz, 1960), 1,4-cyclohexadione-diiodoacetylene, 5.13 Å (Groth & Hassel, 1965), and 1,4-dithiane- and 1,4-diselenane-diiodoacetylene, 5.243(4) and 5.167(6) Å respectively (Holmesland & Rømming, 1966). It also agrees within experimental error with an unpublished electron-diffraction study of diiodoacetylene vapour mentioned by Groth & Hassel (1965).

The crystal packing shows several noteworthy features. The molecules are not located on crystallographic centres of symmetry, in contradiction to the general rule (Kitaigorodskii, 1961) that molecules retain their inversion centres and lose their other symmetry elements in the crystal structure. The two ends of the molecule have distinctly different environments:  $I(1)$ , near the  $\bar{4}$  axis, has seven iodine neighbours at distances less than 4.4 Å;  $I(2)$ , near the  $4_2$  axis, has nine neighbours of this sort. However, there is considerable near symmetry in the environment of each molecule. If we consider, for a given molecule, only the near neighbours in the  $z$  direction, the local symmetry is  $2/m$ . If we consider only the near neighbours in the  $xy$  directions located at the sides of the molecule, the local symmetry is close to  $m$ . If we consider only the near neighbours in the  $xy$  directions located at the ends of the molecule the local symmetry is close to 2. The conditions to make the latter two local symmetries exact are:  $x_2 = x_1 + 2y_1$ ,  $y_2 = -y_1$ ,  $z_2 = -z_1$ . The first two of these are just the conditions required to maximize the  $P4/mmm$  pseudosymmetry of the diffraction pattern and they are approximately fulfilled in the actual structure.

The presence of a number of similar short intermolecular  $I\cdots I$  distances might suggest that  $I\cdots I$  interactions alone are sufficient to determine the packing. This is wrong since, if we choose the intramolecular  $I\cdots I$  distance to be 5.16 Å, and set all intermolecular  $I\cdots I$  distances less than 4.4 Å equal to 4.30 Å, we find there is still one degree of freedom

Table 1. Summary of  $R$  values for different groups of reflexions

$l$	$F(h0l)$ and $F(hhl)$		$F(hkl)$		$\langle F(hkl) \rangle$	
	No.	$R$	No.	$R$	No.	$R$
0	15	0.074	141	0.179	78	0.116
1	27	0.106	229	0.221	128	0.133
2	23	0.172	185	0.259	104	0.176
3	20	0.141	170	0.242	95	0.158
4	11	0.317	39	0.300	25	0.226
Total	96	0.131	764	0.224	430	0.145

Table 2. Atomic positions and isotropic thermal parameters

The origin is taken at  $\bar{1}$ , corresponding to the second arrangement of  $P4_2/n$  given in *International Tables for X-ray Crystallography*.

	$x$	$y$	$z$	$B(\text{Å}^2)$
I(1)	0.1242	0.1083	0.1963	4.2
I(2)	0.3447	-0.1116	-0.1955	3.9
C(1)	0.2090	0.0237	0.0456	2.5
C(2)	0.2599	-0.0271	-0.0448	2.5

left undetermined. For there are eight parameters to be fixed ( $a=b$ ,  $c$ ,  $x_1$ ,  $y_1$ ,  $z_1$ ,  $x_2$ ,  $y_2$ ,  $z_2$ ) whereas the geometrical constraints in this hypothetical structure can be defined in terms of seven equations. However, if we choose  $z_1=0.200$  to eliminate this degree of freedom and calculate the other parameters, we find  $a=15.81$ ,  $c=4.30$  Å,  $x_1=0.1208$ ,  $y_1=0.1088$ ,  $x_2=0.3384$ ,  $y_2=-0.1088$ ,  $z_2=-0.200$ , in very good agreement with the observed parameters. Now we must ask why  $z_1$  should be near 0.200. If we consider values of  $z_1$  between 0 (where the molecules are not tilted at all out of a plane perpendicular to the  $c$  direction) and 0.36 (where any further tilt would lead to  $I \cdots I$  distances less than 4.30 Å), we find  $z_1=0.200$  corresponds approximately to the maximum molecular volume in this range, that is, to the least efficient packing subject to the other constraints. (The calculated molecular volumes are:  $z_1=0$ ,  $V=119$  Å<sup>3</sup>;  $z_1=0.20$ ,  $V=134$  Å<sup>3</sup>;  $z_1=0.36$ ,  $V=126$  Å<sup>3</sup>.) Clearly

there must be some factor other than overall packing efficiency involved.

Each  $C_2I_2$  molecule points almost to the centre of the adjacent molecule at either end (at each end the extended line of the molecule misses the next molecule by only about 0.3 Å. This suggests that the other factor is provided by donor-acceptor interactions, with the  $C \equiv C$  triple bond donating  $\pi$  electrons to low-lying unoccupied orbitals on the iodine atoms. For maximum participation of the  $\pi$  electrons in the  $C \equiv C$  triple bond in two donor-acceptor interactions of this type, the directions to the acceptor molecules should be roughly orthogonal. However, in this structure, linearity of the  $\left(\begin{smallmatrix} C \\ C \end{smallmatrix}\right) \cdots I-C$  arrangement and orthogonality of the  $I \cdots \left(\begin{smallmatrix} C \\ C \end{smallmatrix}\right) \cdots I$  arrangement cannot both be satisfied simultaneously. The actual structure

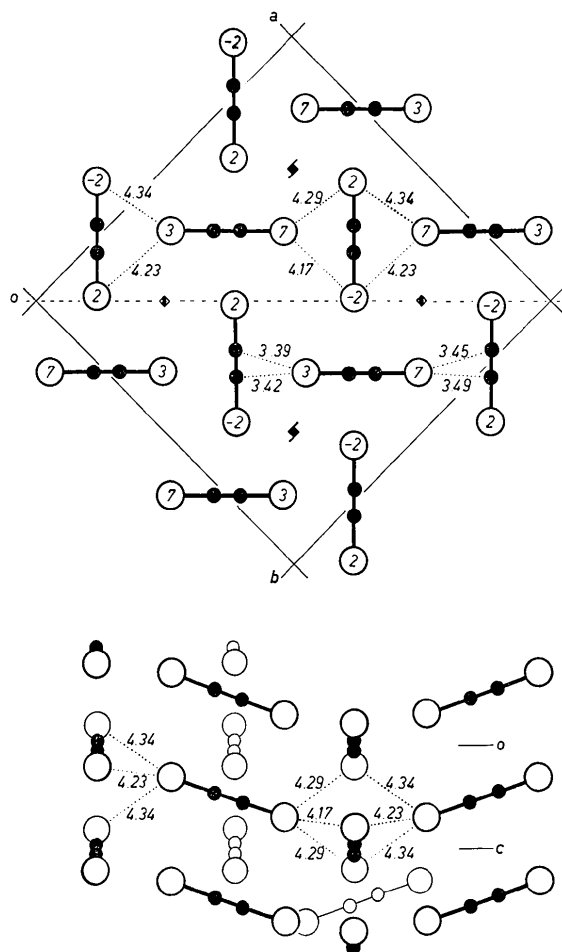


Fig. 3. The crystal structure of  $C_2I_2$ . Above: view along  $c$ . Intermolecular distances are shown in Å. The heights of the I atoms are indicated in the atom in units of  $c/10$ . The dotted line shows the starting point for the lower view. Below: view perpendicular to the  $(110)$  plane.

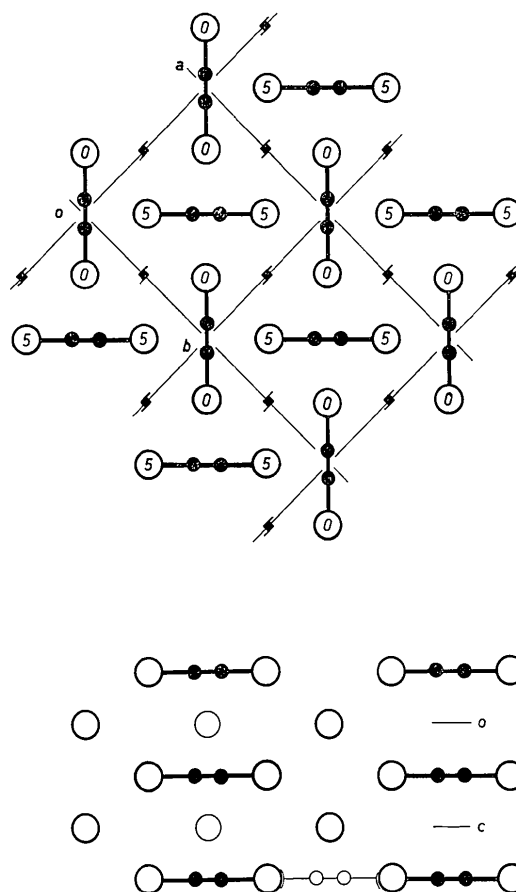


Fig. 4. Hypothetical structure for  $C_2I_2$ , 10% more dense than the actual structure. Views as in Fig. 3. Note, most clearly in the lower view, the poorer geometry for a  $(C \equiv C) \cdots I$  donor-acceptor interaction. This is the structure of the high-temperature form of dimethylacetylene, where no donor-acceptor interaction is expected.

seems to be a compromise between these two requirements, but the exact equilibrium point cannot be assessed at this simple level of discussion. The limiting case for  $z_1=0$  is shown in Fig. 4. It can be seen that the donor-acceptor interactions would be less favourable in this case in spite of more efficient packing. This limit corresponds to space group  $P4_2/mnm$  with a unit cell halved along the **a** and **b** directions; it turns out to be just the structure found by Pignataro & Post (1955) for the high-temperature form of dimethylacetylene. It seems likely to us that methyliodoacetylene (1-iodopropyne) should crystallize in the same space group as diiodoacetylene since the difference between the two ends of the molecule should have no effect crystallographically and the donor-acceptor interaction could still occur at the iodine end.

The occurrence of twinning can be understood by assuming the two twin fragments join along a plane parallel to (110) or (1 $\bar{1}$ 0). This leaves all of the atoms in the twin plane with an approximately correct set of nearest neighbours and with half the second nearest neighbours across the plane also correct.

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### Structure Cristalline de l'Ekanite de St-Hilaire, P. Q.

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The crystal structure of ekanite ( $\text{Th}_{1.76}, \text{Ce}_{0.05}, \text{Pb}_{0.01}, \square_{0.18}$ ) ( $\text{K}_{1.21}, \square_{0.79}$ ) ( $\text{Na}_{1.80}, \text{Ca}_{1.46}, \text{Mn}_{0.38}, \text{Mg}_{0.07}, \square_{0.29}$ )  $\text{Si}_{16}(\text{O}_{38.08}, \text{OH}_{1.92})$  was determined by the symbolic addition method with data collected on a single-crystal diffractometer using Mo  $K\alpha$  radiation. The crystals are tetragonal, space group  $P4/mcc$ , with  $a=7.58$ ,  $c=14.77$  Å. The structure was refined by least-squares methods to an  $R$  value of 0.058 for 1602 reflexions of measurable intensity. Eight  $\text{SiO}_4$  tetrahedra are grouped together in a tetragonal double-ring (with mirror symmetry in the plane of the ring), the rings being linked together by cations of K, Th and Na, distributed on the vertices, the edges and the faces of the tetragonal cell. The structure is very porous.

#### Introduction

A l'occasion de travaux d'identification minérale sur des matériaux de St-Hilaire (Québec, Canada), Chao, Harris, Hounslow, Mandarino & Perrault (1967) assignèrent l'indicatif UK-4 à un silicate de thorium, sodium, calcium et potassium qui ne s'accordait, quant à ses propriétés physiques et chimiques, avec aucune espèce minérale connue. Nous en entreprîmes la définition minéralogique et l'étude structurale.

Nous avons tout juste complété l'une et l'autre quand les travaux d'Anderson, Claringbull, Davis & Hill (1961), Ginzburg & Semenov (1965), et Mokeyeva & Golovastikov (1966) sur l'ékanite furent portés à notre attention. Un examen attentif de ces travaux nous amena à la conclusion que le matériel UK-4 de St-Hilaire, l'ékanite du Ceylan (Anderson *et al.*, 1961) et l'ékanite alcaline d'Asie Centrale (Ginzburg *et al.*, 1965) ne constituaient effectivement que des variétés d'une même espèce minérale. De plus, la structure de l'ékanite d'Asie Centrale définie par Mokeyeva & Golovastikov (1966) est essentiellement la même que celle que nous avons déterminée pour UK-4 de St-Hilaire. Nous avons donc adopté le nom d'ékanite pour désigner UK-4.

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